

Supporting Information for

Theoretical Investigations of the Chiral Transition of α -Amino Acid Confined in Various Sized Armchair Boron-Nitride Nanotubes

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Contents

Figure S0. Potential energy surface of isolated α -Ala chiral transition.

Figure S1. Optimized structures of transition states (STS*@A) and intermediates (S α -Ala@A and R*_S α -Ala@A).

Table S0. The details of S- α -Ala@A and R*_S α -Ala@A geometries parameters.

Figure S2. Optimized structures of transition states and intermediates, and the vibration mode of the transition state along pathway, where α -Ala confined in SWBNNT(5,5).

Figure S3. Intrinsic reaction coordinate for proton transfer reaction of R*_S α -Ala@A $\rightarrow$ INT1@A.

Table S1. Energy (E), Thermal Correction to the Gibbs Free Energy (G_{tc}), Total Energies (G_{total} , Including the ZPE Correction) and Relative Total Energies (ΔG_{total}), and the Transition State Imaginary Frequency (I_{ma}) at 298.15 K of all Stationary Points in the Pathway a of α -Ala Chiral Transition Confined in SWBNNT(6,6), (7,7) and (8,8).

Figure S4. Optimized structures of transition states and intermediates, and the vibration mode of the transition state along pathway a, where α -Ala confined in SWBNNT(6,6).

Figure S5. Potential energy surface of α -Ala chiral transformation confined in SWBNNT(7,7) in pathway a.

Figure S6. Potential energy surface of α -Ala chiral transformation confined in SWBNNT(8,8) in pathway a.

Figure S7. Optimized structures of transition states and intermediates, and the vibration mode of the transition state along pathway b, where α -Ala confined in SWBNNT(6,6).

Table S2. Energy (E), Thermal Correction to the Gibbs Free Energy (G_{tc}), Total Energies (G_{total} , Including the ZPE Correction) and Relative Total Energies (ΔG_{total}), and the Transition State Imaginary Frequency (I_{ma}) at 298.15 K of all Stationary Points in the Pathway b of α -Ala Chiral Transition Confined in SWBNNT(6,6), (7,7) and (8,8).

Figure S8. Potential energy surface of the first three steps of α -Ala chiral transformation confined in the SWBNNT(7,7) in pathway b.

Figure S9. Potential energy surface of the first three steps of α -Ala chiral transformation confined in the SWBNNT(8,8) in pathway b.

Simulation models

Figure S10. Optimized reactant-included complexes structures of model S α -Ala@A, S α -Ala@A_k, S α -Ala@A_n, S α -Ala@A_p and S α -Ala@A_q for α -Ala chiral transition confined in SWBNNT(5,5).

Table S3. Energy (E), Thermal Correction to the Gibbs Free Energy (G_{tc}), Total Energies (G_{total} , Including the ZPE Correction) and Relative Total Energies (ΔG_{total}), the location of the chiral carbon of α -Ala Molecule (x) at 298.15 K of all Reactant-Included Complexes in the Pathway of α -Ala Chiral Transition Confined in SWBNNT(5,5).

Figure S11. Optimized reactant-included complexes structures of model S α -Ala@B, S α -Ala@B_u, S α -Ala@C, S α -Ala@C_u, S α -Ala@D, S α -Ala@D_u and S α -Ala@D_v for α -Ala chiral transition confined in SWBNNT(6,6), SWBNNT(7,7) and SWBNNT(8,8).

Table S4. Energy (E), Thermal Correction to the Gibbs Free Energy (G_{tc}), Total Energies (G_{total} , Including the ZPE Correction) and Relative Total Energies (ΔG_{total}) at 298.15 K of all Reactant-Included Complexes in the Pathway of α -Ala Chiral Transition Confined in SWBNNT(6,6), SWBNNT(7,7) and SWBNNT(8,8).

Coordinates of all stationary points in the pathway of α -Ala chiral transformation confined in SWBNNT(5,5)

Coordinates of all stationary points in the pathway a of α -Ala chiral transformation confined in SWBNNT(6,6)

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Coordinates of all stationary points in the pathway a of α -Ala chiral transformation confined in SWBNNT(8,8)

Coordinates of all stationary points in the pathway b of α -Ala chiral transformation confined in SWBNNT(6,6)

Coordinates of all stationary points in the pathway b of α -Ala chiral transformation confined in SWBNNT(7,7)

Coordinates of all stationary points in the pathway b of α -Ala chiral transformation confined in SWBNNT(8,8)

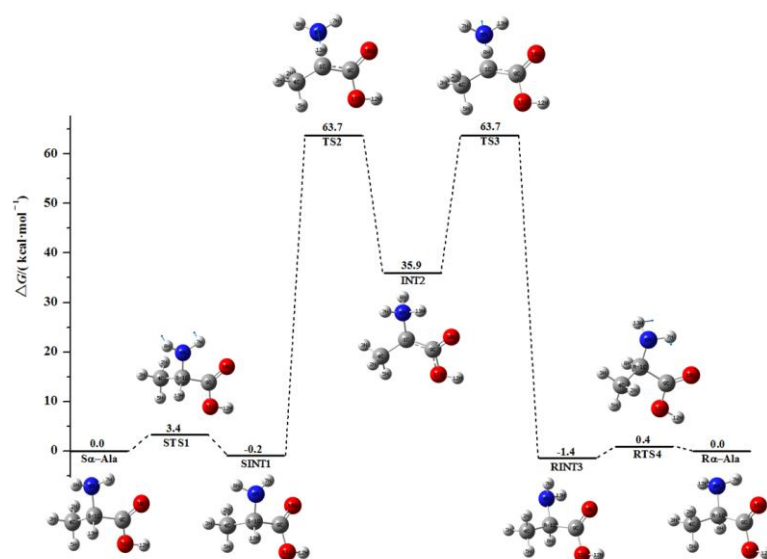


Figure S0. Potential energy surface of isolated α -Ala chiral transition.

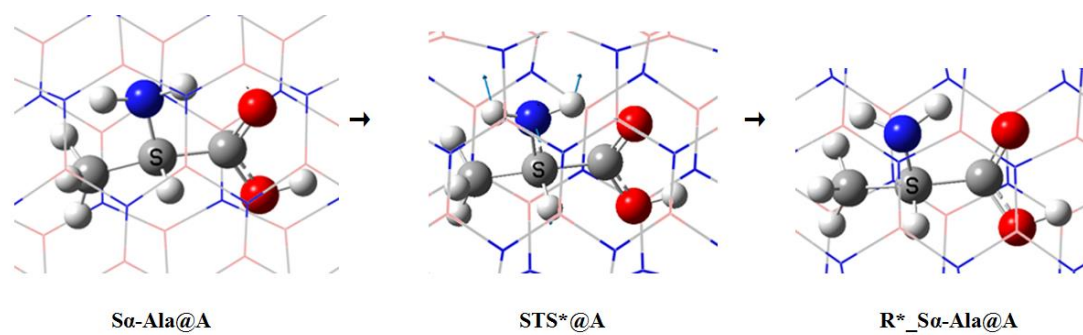


Figure S1. Optimized structures of transition states ($STS^*\text{@A}$) and intermediates ($S\alpha\text{-Ala@A}$ and $R^*_S\alpha\text{-Ala@A}$).

Table S0. The details of S- α -Ala@A and R*_ α -Ala@A geometries parameters.

Structures	C9-C1-C4	O10-C9-C1-N6	C9-C1-N6-C4	H13-C1-N6-H7	N6-H13	O10-H7
S- α -Ala@A	154.0	19.0	160.0	59.3	1.38	1.83
R*_ α -Ala@A	151.4	-18.4	154.5	120.0	1.40	1.73

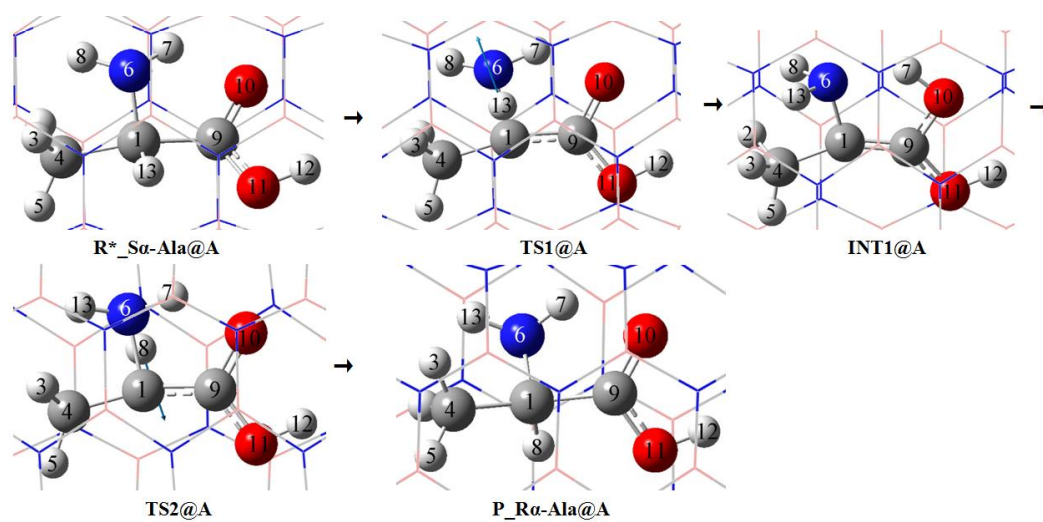


Figure S2. Optimized structures of transition states and intermediates, and the vibration mode of the transition states along pathway, where α -Ala confined in SWBNNT(5,5).

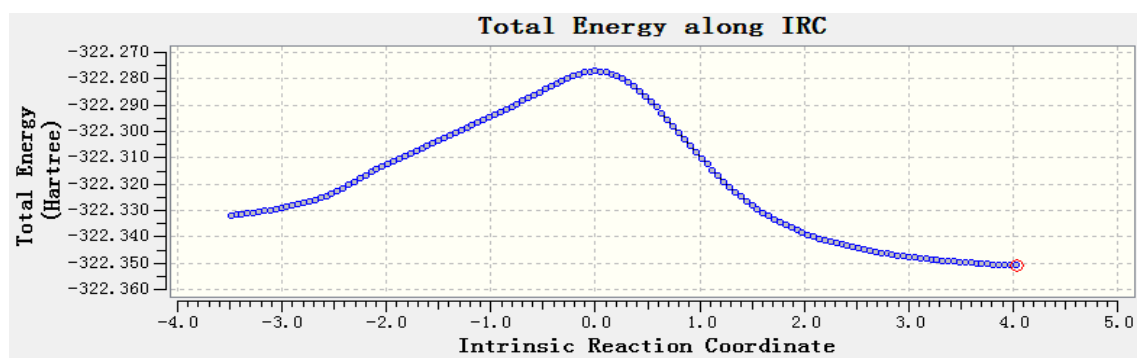


Figure S3. Intrinsic reaction coordinate for proton transfer reaction of $R^*_{S\alpha}\text{-Ala}@A \rightarrow \text{INT1}@A$.

Table S1. Energy (E), Thermal Correction to the Gibbs Free Energy (G_{tc}), Total Energies (G_{total} , Including the ZPE Correction) and Relative Total Energies (ΔG_{total}), and the Transition State Imaginary Frequency (I_{ma}) at 298.15 K of all Stationary Points in the Pathway a of α -Ala Chiral Transition Confined in SWBNNT(6,6), (7,7) and (8,8).

Structures	E (Hartree)	G_{tc} (Hartree)	G_{total} (Hartree)	ΔG_{total} (Kcalmol ⁻¹)	I_{ma} (cm ⁻¹)
S α -Ala@B	-321.84977	1.85596	-319.99381	0.0	
aSTS1@B	-321.84465	1.85581	-319.98884	3.1	599.90
aSINT1@B	-321.85041	1.85650	-319.99391	-0.1	
aTS2@B	-321.75037	1.85068	-319.89969	59.1	1639.35
aINT2@B	-321.81006	1.85430	-319.95576	23.9	
aTS3@B	-321.75046	1.85066	-319.8998	59.0	1636.12
aRINT3@B	-321.85049	1.85653	-319.99396	-0.1	
aRTS4@B	-321.84450	1.85580	-319.9887	3.2	600.23
aR α -Ala@B	-321.84983	1.85604	-319.99379	0.0	
S α -Ala @C	-321.65953	2.14435	-319.51518	0.0	
aSTS1@C	-321.65320	2.14255	-319.51065	3.1	605.25
aSINT1@C	-321.65968	2.14362	-319.51606	-0.5	
aTS2@C	-321.55483	2.14196	-319.41287	63.1	1669.59
aINT2@C	-321.62104	2.14377	-319.47727	23.8	
S α -Ala @D	-321.40554	2.43869	-318.96685	0.0	
aSTS1@D	-321.39886	2.43692	-318.96194	2.8	601.34
aSINT1@D	-321.40562	2.43799	-318.96763	-0.5	
aTS2@D	-321.29966	2.43343	-318.86623	64.2	1657.48
aINT2@D	-321.36772	2.42750	-318.94022	16.7	

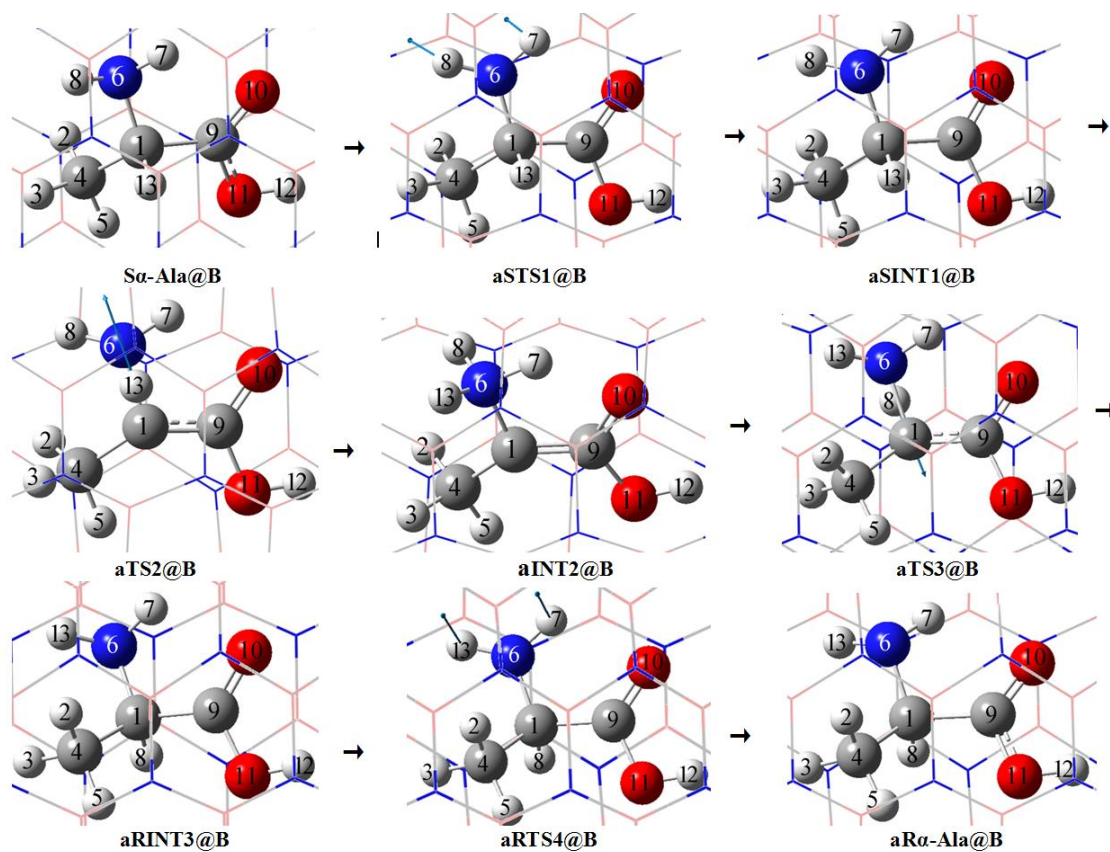


Figure S4. Optimized structures of transition states and intermediates, and the vibration mode of the transition states along pathway a, where α -Ala confined in SWBNNT(6,6).

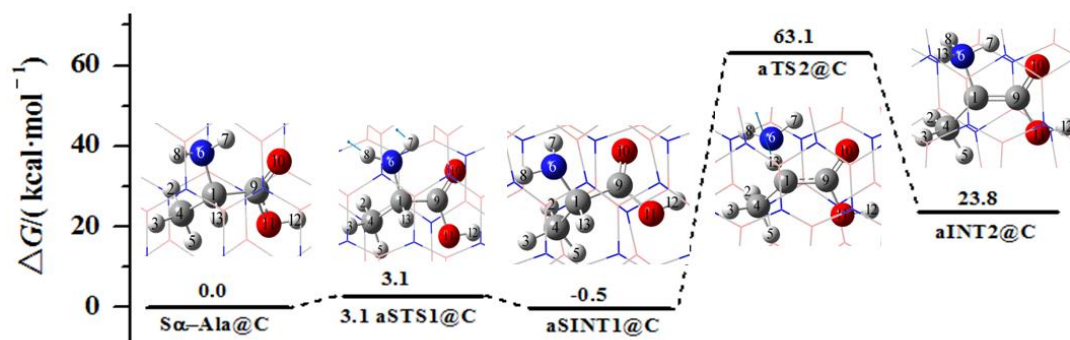


Figure S5. Potential energy surface of α -Ala chiral transformation confined in SWBNNT(7,7) in pathway a.

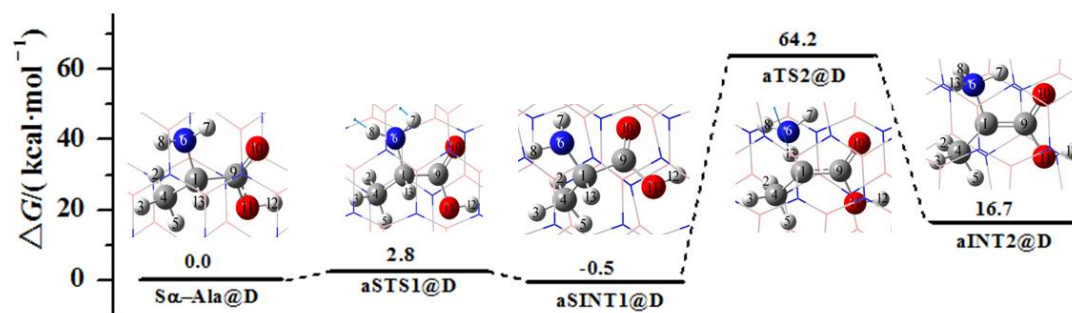


Figure S6. Potential energy surface of α -Ala chiral transformation confined in SWBNNT(8,8) in pathway a.

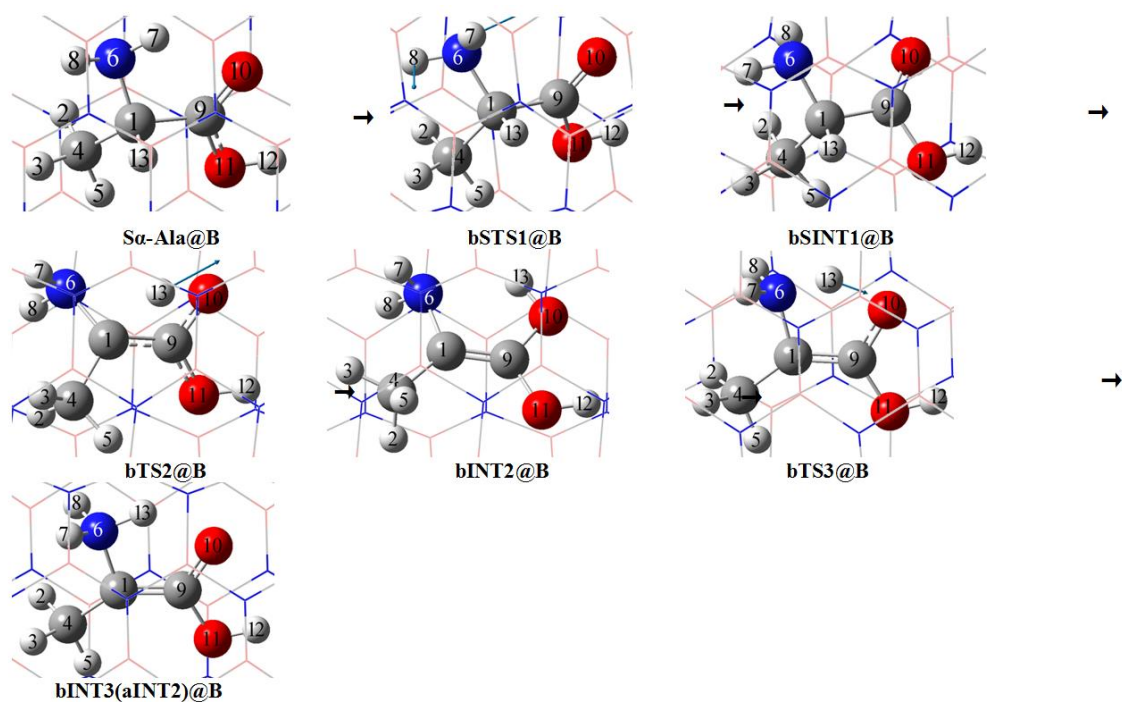


Figure S7. Optimized structures of transition states and intermediates, and the vibration mode of the transition state along pathway b, where α -Ala confined in SWBNNT(6,6).

Table S2. Energy (E), Thermal Correction to the Gibbs Free Energy (G_{tc}), Total Energies (G_{total} , Including the ZPE Correction) and Relative Total Energies (ΔG_{total}), and the Transition State Imaginary Frequency (I_{ma}) at 298.15 K of all Stationary Points in the Pathway b of α -Ala Chiral Transition Confined in SWBNNT(6,6), (7,7) and (8,8).

Structures	E (Hartree)	G_{tc} (Hartree)	G_{total} (Hartree)	ΔG_{total} (Kcalmol ⁻¹)	I_{ma} (cm-1)
S α -Ala@B	-321.84977	1.85596	-319.99381	0.0	
bSTS1@B	-321.84591	1.85640	-319.98951	2.7	159.94
bSINT1@B	-321.85096	1.85685	-319.99411	-0.2	
bTS2@B	-321.73471	1.85030	-319.88441	68.6	2129.95
bINT2@B	-321.81268	1.85677	-319.95591	23.8	
bTS3@B	-321.79801	1.85082	-319.94719	29.3	794.82
bINT3@B	-321.80998	1.85421	-319.95577	23.9	
S α -Ala@C	-321.65953	2.14398	-319.51555	0.0	
bSTS1@C	-321.65467	2.14364	-319.51103	2.8	200.63
bSINT1@C	-321.65849	2.14466	-319.51383	1.1	
bTS2@C	-321.53313	2.13903	-319.3941	76.2	2169.80
bINT2@C	-321.62659	2.14669	-319.4799	22.4	
bTS3@C	-321.60591	2.14110	-319.46481	31.8	874.31
bINT3@C	-321.62092	2.14353	-319.47739	23.9	
S α -Ala@D	-321.40554	2.43869	-318.96685	0.0	
bSTS1@D	-321.39929	2.43811	-318.96118	3.6	238.29
bSINT1@D	-321.40459	2.44041	-318.96418	1.7	
bTS2@D	-321.27823	2.43301	-318.84522	76.3	2071.94
bINT2@D	-321.37340	2.43916	-318.93424	20.5	
bTS3@D	-321.35187	2.43486	-318.91701	31.3	865.61
bINT3@D	-321.36769	2.43692	-318.93077	22.6	

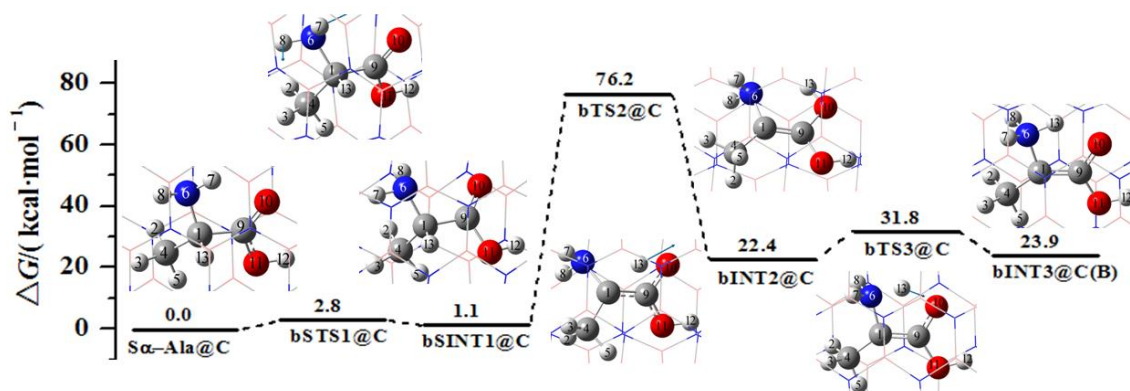


Figure S8. Potential energy surface of the first three steps of α -Ala chiral transformation confined in the SWBNNT(7,7) in pathway b.

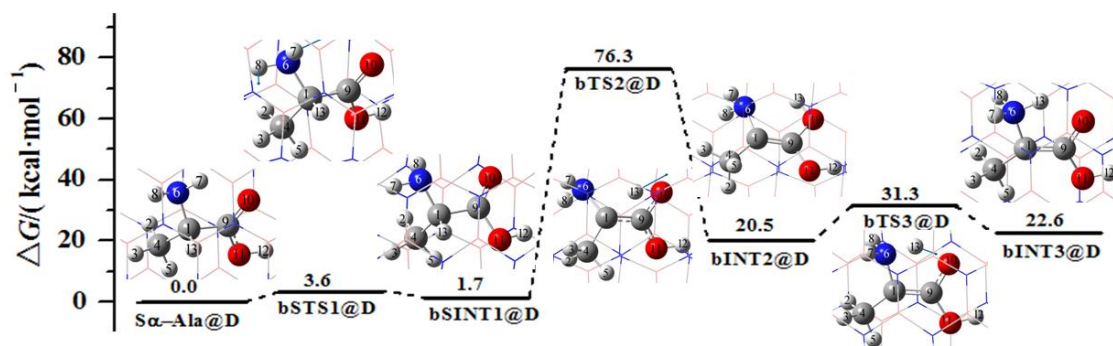


Figure S9. Potential energy surface of the first three steps of α -Ala chiral transformation confined in the SWBNNT(8,8) in pathway b.

Simulation models

It formed the reactant-included complexes after the α -Ala entering SWBNNTs. The α -Ala molecule can be oriented in different ways, thereby results in many different conformations of the reactant-included complexes. From the available computational cost, it does not seem possible to exclude any of those conformations. Therefore, an investigation was performed by comparing the relative energies of different conformations of several reactant-included complexes in the reaction studied. Several reactant-included complexes were taken as the initial guesses to perform the ground state geometry optimization.

The diameters of SWBNNT(5,5) nanotube is 0.6732 nm, and the size of α -Ala molecule is ~ 0.4488 nm $\times 0.3811$ nm. Thus, α -Ala molecule under confinement in the SWBNNT(5,5) nanotube, only when the direction of C-C-C backbone of the α -Ala molecule is the parallel to the axial direction of the nanotube, does the confinement effect behave physical absorption and α -Ala achieve chiral transition. Finally, we obtained several minimum-energy geometries with quite different conformations for reactant-included complexes in SWBNNT(5,5) ($S\alpha$ -Ala@A, $S\alpha$ -Ala@A_k, $S\alpha$ -Ala@A_n, $S\alpha$ -Ala@A_p and $S\alpha$ -Ala@A_q) (Figure S10), since α -Ala molecule has different position in nanotube.

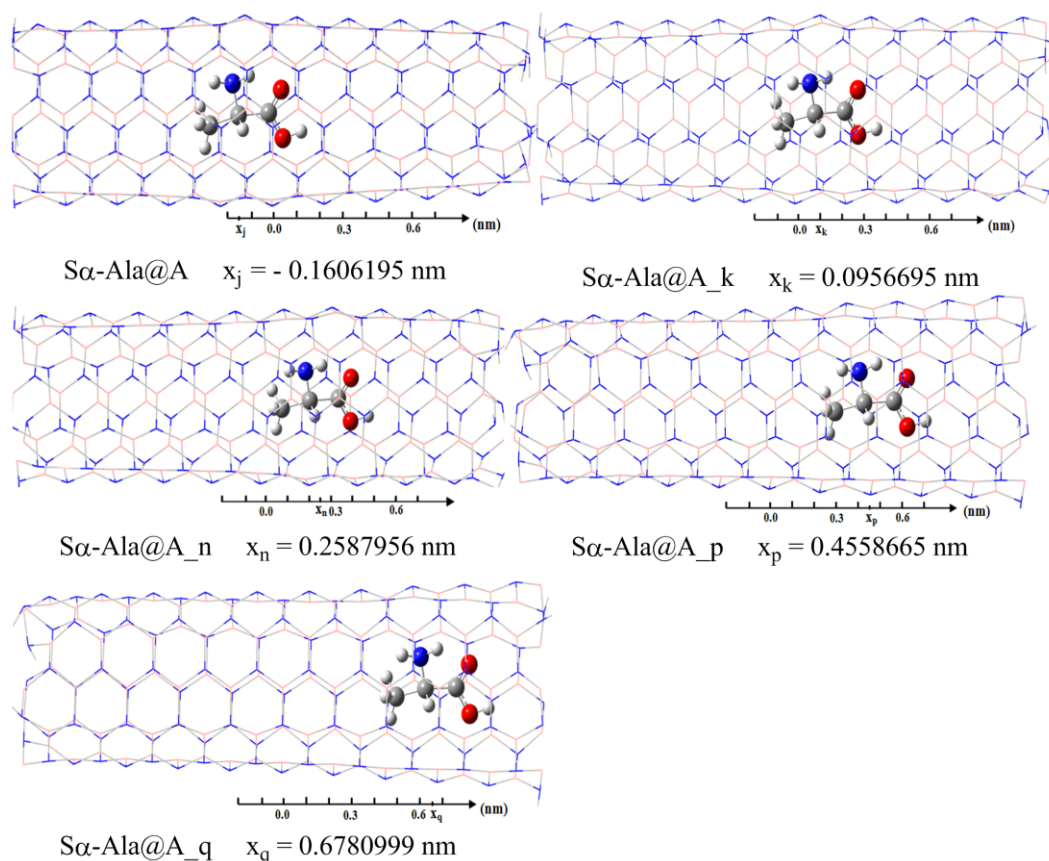


Figure S10. Optimized reactant-included complexes structures of model $S\alpha$ -Ala@A, $S\alpha$ -Ala@A_k, $S\alpha$ -Ala@A_n, $S\alpha$ -Ala@A_p and $S\alpha$ -Ala@A_q for α -Ala chiral transition confined in SWBNNT(5,5).

The details of these different conformations of reactant-included complexes in SWBNNT(5,5) are as follows: First we define a one-dimensional coordinate axis. In this coordinate axis, the tube axis is taken as the x-axis, and the center of the tube taken as the coordinate origin 0. In $S\alpha$ -Ala@A, α -Ala@A_k, $S\alpha$ -Ala@A_n, $S\alpha$ -Ala@A_p and $S\alpha$ -Ala@A_q, the abscissas of the chiral carbon of α -Ala molecule locate at $x = -0.1606195$,

+0.0956695, +0.2587956, +0.4558665 and +0.6780999 nm on the x-axis, respectively. As it turned out, the relative energy of the S α -Ala@A conformation is the lowest, the computational details is shown in Table S3. Thus, it is reasonable for the simulation model of S α -Ala@A in the text.

Table S3. Energy (E), Thermal Correction to the Gibbs Free Energy (G_{tc}), Total Energies (G_{total} , Including the ZPE Correction) and Relative Total Energies (ΔG_{total}), the location of the chiral carbon of α -Ala Molecule (x) at 298.15 K of all Reactant-Included Complexes in the Pathway of α -Ala Chiral Transition Confined in SWBNNT(5,5).

Models	E (Hartree)	Gtc(Hartree)	G_{total} (Hartree)	ΔG_{total} (Kcal/mol)	x (nm)
S α -Ala @A	-321.76791	1.57317	-320.19474	0.0	-0.161
S α -Ala @A_k	-321.74241	1.57213	-320.17028	15.4	0.096
S α -Ala @A_n	-321.74430	1.57246	-320.17184	14.4	0.259
S α -Ala @A_p	-321.74704	1.57380	-320.17324	13.5	0.456
S α -Ala @A_q	-321.74890	1.57454	-320.17436	12.8	0.678

Reactant-included complexes in SWBNNT(6,6), SWBNNT(7,7), and SWBNNT(8,8) models are similar to that in SWBNNT(5,5). In other word, when the α -Ala molecules locate the center of the SWBNNTs, the relative energies of different conformations are lowest. However, due to sizes of SWBNNT(6,6), SWBNNT(7,7), and SWBNNT(8,8) are bigger than that of the SWBNNT(5,5), the direction of C-C-C backbone of the α -Ala molecule have other different ways after the α -Ala entering to SWBNNT(6,6), SWBNNT(7,7), and SWBNNT(8,8). Finally, we obtained several minimum-energy geometries with quite different conformations of reactant-included complexes in SWBNNT(6,6), SWBNNT(7,7) and SWBNNT(8,8). There are S α -Ala@B, S α -Ala@B_u, S α -Ala@C, S α -Ala@C_u, S α -Ala@D, S α -Ala@D_u and S α -Ala@D_v, respectively. (Figure S11)

The S α -Ala@B, S α -Ala@C and S α -Ala@D are similar to the S α -Ala@A, in their geometries, the direction of C-C-C backbone of the α -Ala molecule is the parallel to the axial direction of the nanotube, the abscissas of the chiral carbon of α -Ala molecule locate at x = - 0.0088381, +0.0367987 and +0.0292628 nm on the x-axis, respectively. However, in S α -Ala@B_n, S α -Ala@C_u and S α -Ala@D_u, the abscissas of the chiral carbon of α -Ala molecule locates at x = +0.0065261, +0.0532896 and +0.0074601 nm on the x-axis, respectively. In addition, the α -Ala molecules in these complexes are clockwise rotation 90 degree relative to their orientation in the S α -Ala@B, S α -Ala@C and S α -Ala@D. Especially, in S α -Ala@D_v, the direction of C-C-C backbone of the α -Ala molecule is perpendicular to the axial direction of the nanotube. As it turned out, the relative energy of the S α -Ala@B, S α -Ala@C and S α -Ala@D conformations are the lowest, the computational details is shown in Table S4. Thus, it is reasonable for the simulation models of S α -Ala@B, S α -Ala@C and S α -Ala@D in the text.

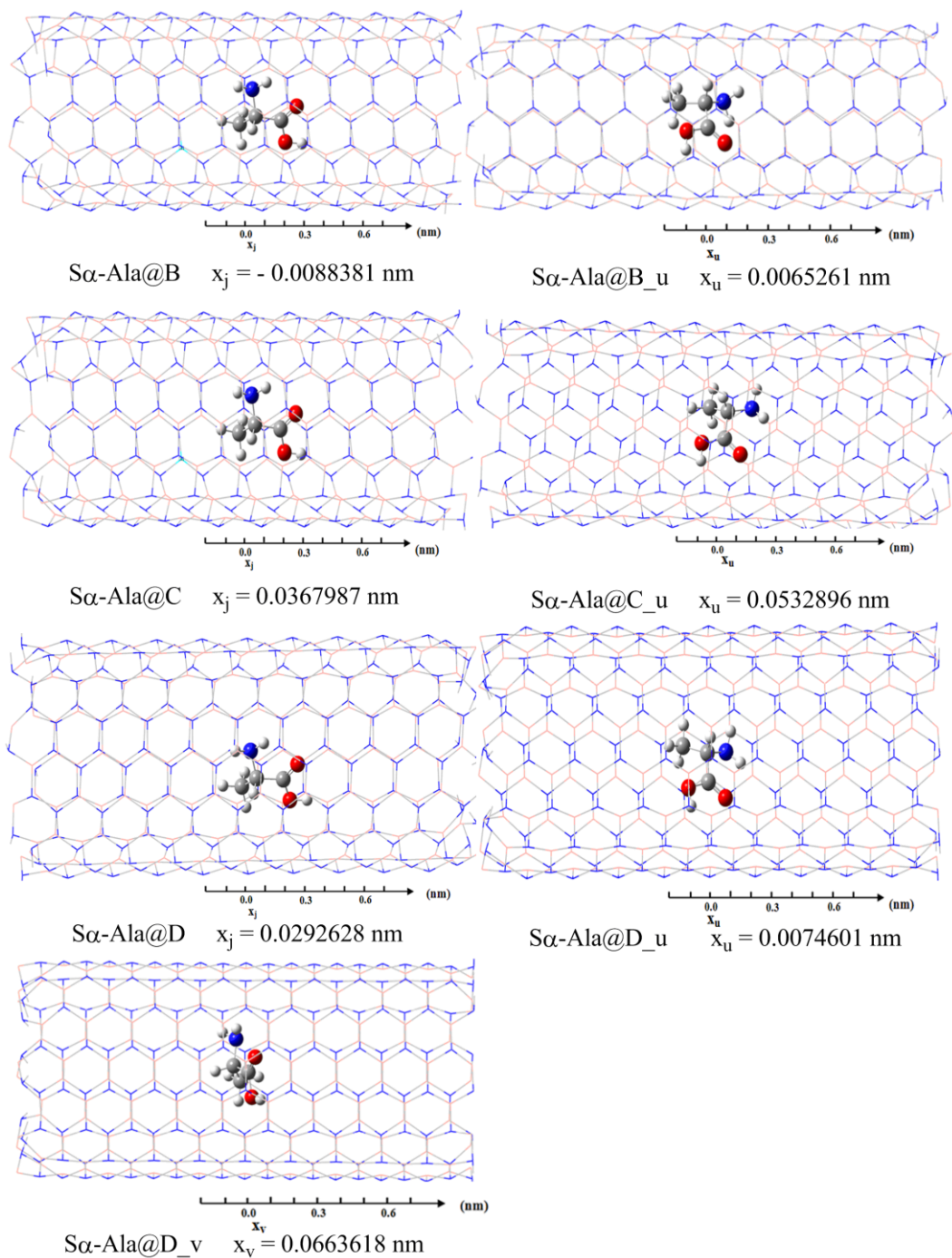


Figure S11. Optimized reactant-included complexes structures of model $S\alpha\text{-Ala@B}$, $S\alpha\text{-Ala@B}_u$, $S\alpha\text{-Ala@C}$, $S\alpha\text{-Ala@C}_u$, $S\alpha\text{-Ala@D}$, $S\alpha\text{-Ala@D}_u$ and $S\alpha\text{-Ala@D}_v$ for α -Ala chiral transition confined in SWBNNT(6,6), SWBNNT(7,7) and SWBNNT(8,8).

Table S4. Energy (E), Thermal Correction to the Gibbs Free Energy (G_{tc}), Total Energies (G_{total} , Including the ZPE Correction) and Relative Total Energies (ΔG_{total}) at 298.15 K of all Reactant-Included Complexes in the Pathway of α -Ala Chiral Transition Confined in SWBNNT(6,6), SWBNNT(7,7) and SWBNNT(8,8).

Structures	E (Hartree)	G _{tc} (Hartree)	G _{total} (Hartree)	ΔG_{total} (Kcal/mol)
S α -Ala@B_u	-321.79227	1.85865	-319.93362	37.80
S α -Ala@B	-321.84977	1.85596	-319.99381	0.0
S α -Ala@C_u	-321.62965	2.14837	-319.48128	21.3
S α -Ala@C	-321.65953	2.14435	-319.51518	0.0
S α -Ala@D_u	-321.37846	2.44034	-318.93812	18.0
S α -Ala@D_v	-321.37709	2.44086	-318.93623	19.2
S α -Ala @D	-321.40554	2.43869	-318.96685	0.0

In addition, nothing optimization was done for α -Ala adsorption on SWBNNTs surface. Because when the α -Ala molecule under confinement in nanotubes adsorption on SWBNNTs surface, the confinement effect behaved chemical absorption, which made α -Ala molecule could not achieve chiral transition. Although this work studies the situation in α -Ala under confinement in different diameters of SWBNNTs, the real purpose is not focusing on α -Ala adsorption on SWBNNTs or the interaction of α -Ala and SWBNNTs. Instead this work tries to study the chiral transition process of the α -Ala molecule under confined different sizes armchair SWBNNTs for exploring the confinement effect, which is an important issue in realizing the role of the confinement environment in the chiral transition process and providing fundamental references for chiral drug molecule transport and enantiomer curing.

Coordinates of all stationary points in the pathway of α -Ala chiral transformation confined in SWBNNT(5,5)

S α -Ala@A

B-B_2	0	10.30436900	-0.21287700	3.65580200 L
N-N_3	0	11.57393100	-1.01757000	3.80970800 L
B-	0	12.82965900	-0.16438500	4.11026300 L
B-B_2	0	5.17566700	-0.25397600	3.27175300 L
N-N_3	0	6.45460800	-1.03373900	3.55895700 L
B-B_2	0	7.74270100	-0.22903100	3.40025700 L
B-B_2	0	9.07712300	-2.10788100	2.57729000 L
N-N_3	0	9.00952800	-1.02378500	3.66862300 L
N-N_3	0	10.41461300	-2.79675100	2.25004700 L
B-B_2	0	11.62318800	-1.88510800	2.55782700 L
B-	0	12.95844000	-3.02958800	0.83123100 L
N-N_3	0	12.71884200	-1.67712200	1.51961800 L
B-B_2	0	0.04000500	-0.28275900	3.26674400 L
N-N_3	0	1.33328500	-1.07265200	3.49161400 L
B-B_2	0	2.60584800	-0.28049600	3.20020300 L
B-B_2	0	3.91918200	-2.27069100	2.55663100 L
N-N_3	0	3.89119400	-1.05277600	3.48875000 L
N-N_3	0	5.23169200	-3.01811300	2.29870600 L
B-B_2	0	6.49901900	-2.20007200	2.56350400 L
B-B_2	0	7.82042000	-3.27611200	0.78394900 L
N-N_3	0	7.81862300	-2.93090400	2.27674800 L
N-N_3	0	9.12267900	-3.68725700	0.08941600 L
B-B_2	0	10.39706500	-3.16293300	0.75765300 L
B-B_2	0	11.64295700	-2.90993700	-1.35729500 L
N-N_3	0	11.70715600	-3.51124200	0.05057600 L
N-N_3	0	12.96435700	-2.65379400	-2.09512400 L
B-B_2	0	-5.11080100	-0.28073300	3.22445600 L
N-N_3	0	-3.83854500	-1.07705100	3.52310700 L
B-B_2	0	-2.54136800	-0.27600900	3.35403300 L
B-B_2	0	-1.24686000	-2.34332200	2.59643600 L
N-N_3	0	-1.24251000	-1.08477100	3.52283200 L
N-N_3	0	0.04656000	-3.14243900	2.36131000 L
B-B_2	0	1.33906600	-2.34776600	2.61441600 L
B-B_2	0	2.64885400	-3.53575600	0.85288500 L
N-N_3	0	2.64797900	-3.09697600	2.32837000 L
N-N_3	0	3.95689600	-3.90984200	0.14394300 L
B-B_2	0	5.23689500	-3.40325400	0.81712600 L
B-B_2	0	6.50658600	-3.20843700	-1.29049400 L
N-N_3	0	6.54351500	-3.80199400	0.12068300 L
N-N_3	0	7.77844900	-3.15287600	-2.14001300 L
B-B_2	0	9.08667600	-3.12752500	-1.34275100 L

B-B_2	0	10.28533500	-1.98016300	-3.21592000 L
N-N_3	0	10.36851300	-3.12275300	-2.19161000 L
N-N_3	0	11.53256300	-1.41548900	-3.85955900 L
B-	0	12.79687100	-2.26589900	-3.58193200 L
B-B_2	0	-10.26948900	-0.25288900	3.26043700 L
N-N_3	0	-8.98415100	-1.05264300	3.51462000 L
B-B_2	0	-7.69192900	-0.27029000	3.24116800 L
B-B_2	0	-6.40919100	-2.27309900	2.54317700 L
N-N_3	0	-6.40240300	-1.05940800	3.48074700 L
N-N_3	0	-5.13363800	-3.09215100	2.32212900 L
B-B_2	0	-3.83156500	-2.33816800	2.61495000 L
B-B_2	0	-2.54198400	-3.79310100	0.93854700 L
N-N_3	0	-2.54004600	-3.13775300	2.36180300 L
N-N_3	0	-1.24221100	-4.07799100	0.16981500 L
B-B_2	0	0.05489900	-3.74461700	0.92325400 L
B-B_2	0	1.34008000	-3.41925400	-1.25549300 L
N-N_3	0	1.37006200	-4.03820200	0.16885200 L
N-N_3	0	2.62633800	-3.20262800	-2.05945600 L
B-B_2	0	3.92348900	-3.27850100	-1.25271400 L
B-B_2	0	5.17173600	-1.80692100	-2.78927400 L
N-N_3	0	5.20094600	-3.16673400	-2.08522000 L
N-N_3	0	6.42360300	-1.29518600	-3.49132900 L
B-B_2	0	7.73401100	-1.84812200	-2.94107200 L
B-B_2	0	9.03345900	0.17630900	-3.40418000 L
N-N_3	0	8.97199200	-1.34044300	-3.65755300 L
N-N_3	0	10.35242100	0.94098500	-3.61384700 L
B-B_2	0	11.58839000	0.03757200	-3.39311100 L
B-	0	12.92150800	2.05140400	-2.79064100 L
N-N_3	0	12.78386600	0.53428600	-2.58947700 L
B-	0	-12.82159800	-0.20606400	2.97678800 L
B-B_2	0	-11.55774500	-2.31943000	2.68016700 L
N-N_3	0	-11.59226100	-1.01154600	3.48578400 L
N-N_3	0	-10.26396700	-3.04343200	2.31978900 L
B-B_2	0	-8.98568000	-2.25673400	2.56895700 L
B-B_2	0	-7.71774900	-3.45797400	0.82745100 L
N-N_3	0	-7.70429200	-3.04555500	2.30422000 L
N-N_3	0	-6.43626500	-3.93607800	0.14251800 L
B-B_2	0	-5.13291500	-3.55662600	0.85128700 L
B-B_2	0	-3.83531300	-3.45161200	-1.27234500 L
N-N_3	0	-3.85759600	-4.06217100	0.16536700 L
N-N_3	0	-2.52636900	-3.22204900	-2.03529600 L
B-B_2	0	-1.24976200	-3.33154600	-1.19308900 L
B-B_2	0	0.03123500	-1.82438400	-2.72042000 L
N-N_3	0	0.02906400	-3.21323300	-2.02576500 L

N-N_3	0	1.31496100	-1.25575900	-3.31453800 L
B-B_2	0	2.60144900	-1.80073700	-2.69839100 L
B-B_2	0	3.88447900	0.26212600	-3.21346100 L
N-N_3	0	3.86659600	-1.26510900	-3.36551600 L
N-N_3	0	5.17070900	1.03643100	-3.50837600 L
B-B_2	0	6.45637200	0.22863700	-3.31534300 L
B-B_2	0	7.78753200	2.15516200	-2.56098200 L
N-N_3	0	7.75377700	1.00614800	-3.57320500 L
N-N_3	0	9.09424000	2.89800200	-2.28481100 L
B-B_2	0	10.36623700	2.11224500	-2.61834600 L
B-B_2	0	11.65367000	2.98216900	-0.75874500 L
N-N_3	0	11.67448500	2.81417600	-2.27743800 L
N-N_3	0	12.92012000	2.69661900	0.05298700 L
B-	0	-12.84633800	-3.00147200	0.75721200 L
N-N_3	0	-12.84501200	-3.02004700	2.29235600 L
N-N_3	0	-11.62768300	-3.75229400	0.14754900 L
B-B_2	0	-10.29614600	-3.35779400	0.81653700 L
B-B_2	0	-8.99313000	-3.26527800	-1.26698300 L
N-N_3	0	-9.02291900	-3.87507800	0.13628200 L
N-N_3	0	-7.69658600	-3.17197900	-2.06697900 L
B-B_2	0	-6.41476100	-3.28469800	-1.24555900 L
B-B_2	0	-5.10881200	-1.80429400	-2.71635200 L
N-N_3	0	-5.12743300	-3.20658900	-2.06527500 L
N-N_3	0	-3.82414000	-1.26599400	-3.35362700 L
B-B_2	0	-2.53626100	-1.83707500	-2.74977500 L
B-B_2	0	-1.25545400	0.29820800	-3.19689500 L
N-N_3	0	-1.25000100	-1.25203800	-3.33443400 L
N-N_3	0	0.03437500	1.08567400	-3.43939100 L
B-B_2	0	1.31549200	0.28417200	-3.17240800 L
B-B_2	0	2.62447900	2.29480200	-2.53218500 L
N-N_3	0	2.60089300	1.06108500	-3.44754500 L
N-N_3	0	3.93682400	3.05002200	-2.30288200 L
B-B_2	0	5.20665100	2.22564300	-2.54433300 L
B-B_2	0	6.53090700	3.36383100	-0.81063800 L
N-N_3	0	6.52000500	2.97161400	-2.29142500 L
N-N_3	0	7.83689900	3.76412600	-0.11439500 L
B-B_2	0	9.11203200	3.23928200	-0.78315000 L
B-B_2	0	10.36585200	3.20262100	1.37225100 L
N-N_3	0	10.42954700	3.64585200	-0.09790300 L
N-N_3	0	11.62770300	3.13781900	2.21656000 L
B-	0	12.90247700	3.44712600	1.39511900 L
N-N_3	0	-12.83833000	-3.16665600	-2.14136700 L
B-B_2	0	-11.56592800	-3.37402400	-1.34338800 L
B-B_2	0	-10.27252600	-1.80449400	-2.76924800 L

N-N_3	0	-10.25654300	-3.19215500	-2.10880700 L
N-N_3	0	-8.97881300	-1.27210800	-3.40578600 L
B-B_2	0	-7.69222900	-1.79897700	-2.75264500 L
B-B_2	0	-6.39722300	0.26989700	-3.20790800 L
N-N_3	0	-6.39114300	-1.25843700	-3.35530100 L
N-N_3	0	-5.11893200	1.07126400	-3.47720500 L
B-B_2	0	-3.82306700	0.28925100	-3.26538300 L
B-B_2	0	-2.54631200	2.42324800	-2.66965000 L
N-N_3	0	-2.53288700	1.09370500	-3.49211400 L
N-N_3	0	-1.24626900	3.21402400	-2.38006400 L
B-B_2	0	0.04054000	2.39328200	-2.59857400 L
B-B_2	0	1.35632400	3.65054300	-0.87163900 L
N-N_3	0	1.35460200	3.13550100	-2.32671600 L
N-N_3	0	2.66840600	3.97414800	-0.14549100 L
B-B_2	0	3.94697100	3.49078100	-0.83661500 L
B-B_2	0	5.22052400	3.21502600	1.25117300 L
N-N_3	0	5.25430100	3.86702700	-0.13336600 L
N-N_3	0	6.49278300	3.13814700	2.09468700 L
B-B_2	0	7.79564100	3.17016400	1.29751600 L
B-B_2	0	9.05023200	1.81018500	2.93594300 L
N-N_3	0	9.05657900	3.13516700	2.15335800 L
N-N_3	0	10.33772100	1.31949800	3.62468600 L
B-B_2	0	11.61317500	1.75485700	2.87518000 L
N-N_3	0	12.95210500	1.08910800	3.21760300 L
B-	0	-12.82480000	-1.67628200	-2.51520200 L
B-B_2	0	-11.54511700	0.25004000	-3.39694900 L
N-N_3	0	-11.58915000	-1.28438400	-3.37638700 L
N-N_3	0	-10.24658700	1.04218200	-3.53548200 L
B-B_2	0	-8.97539700	0.25164600	-3.25464900 L
B-B_2	0	-7.70850200	2.25636100	-2.53994000 L
N-N_3	0	-7.68676100	1.04391500	-3.47910200 L
N-N_3	0	-6.42801900	3.06361900	-2.30644000 L
B-B_2	0	-5.12487700	2.29796300	-2.54441800 L
B-B_2	0	-3.84834600	3.65135600	-0.87727900 L
N-N_3	0	-3.85799800	3.14260000	-2.34260100 L
N-N_3	0	-2.56304600	4.12170900	-0.16780800 L
B-B_2	0	-1.24675400	3.90061400	-0.95915200 L
B-B_2	0	0.05231700	3.44586100	1.25149700 L
N-N_3	0	0.07034500	4.11156000	-0.16295500 L
N-N_3	0	1.34889700	3.19544700	2.03390200 L
B-B_2	0	2.63900900	3.27642500	1.22007100 L
B-B_2	0	3.89870100	1.78526100	2.74115300 L
N-N_3	0	3.91927300	3.15234600	2.04943100 L
N-N_3	0	5.16179000	1.26941900	3.43022100 L

B-B_2	0	6.47202300	1.80260700	2.84732900 L
N-N_3	0	7.73902800	1.29526500	3.54296000 L
B-	0	-12.83673800	1.96367500	-2.29736100 L
N-N_3	0	-12.82817600	1.04630500	-3.52647700 L
N-N_3	0	-11.61976200	2.93140500	-2.26784100 L
B-B_2	0	-10.28572600	2.20259700	-2.52814500 L
B-B_2	0	-9.00601400	3.47330000	-0.84051300 L
N-N_3	0	-9.01340900	3.03016900	-2.30532900 L
N-N_3	0	-7.72342500	3.91357300	-0.14334700 L
B-B_2	0	-6.42963700	3.50831400	-0.84117800 L
B-B_2	0	-5.13140300	3.29680700	1.22819500 L
N-N_3	0	-5.15243900	3.98061900	-0.14790200 L
N-N_3	0	-3.84741200	3.22394700	2.05579700 L
B-B_2	0	-2.54404800	3.52787200	1.28919800 L
B-B_2	0	-1.25094500	1.86280500	2.74540700 L
N-N_3	0	-1.24007100	3.27544400	2.06511100 L
N-N_3	0	0.03954400	1.27272700	3.33173100 L
B-B_2	0	1.32173500	1.79480700	2.68446100 L
N-N_3	0	2.59621100	1.24999200	3.33275000 L
N-N_3	0	-12.86267000	3.85823200	-0.11017400 L
B-B_2	0	-11.58071500	3.56991100	-0.86790500 L
B-B_2	0	-10.29727700	3.17768600	1.21961800 L
N-N_3	0	-10.28329100	3.89927200	-0.13633400 L
N-N_3	0	-9.01002500	3.13904100	2.05573300 L
B-B_2	0	-7.71748500	3.23910700	1.23347000 L
B-B_2	0	-6.40444600	1.78102200	2.71708900 L
N-N_3	0	-6.42196600	3.15743700	2.04346300 L
N-N_3	0	-5.10753200	1.25579200	3.33638400 L
B-B_2	0	-3.82160400	1.81836900	2.71375900 L
N-N_3	0	-2.53897900	1.29070800	3.36167600 L
B-	0	-12.84681600	2.87800100	1.07406800 L
B-B_2	0	-11.55234700	1.84422700	2.91867800 L
N-N_3	0	-11.61724500	3.07973700	2.00680800 L
N-N_3	0	-10.24185100	1.27136800	3.45865800 L
B-B_2	0	-8.98191100	1.78975000	2.77902200 L
N-N_3	0	-7.67950300	1.25756000	3.38006600 L
N-N_3	0	-12.82489700	1.24317300	3.48098500 L
H-H_	0	12.36131500	-0.99839700	0.80933600 L
H-H_	0	13.46360500	-1.86831700	-1.62367600 L
H-H_	0	12.57341100	0.34642700	-1.58495200 L
H-H_	0	12.93334400	1.67465000	0.25945200 L
H-H_	0	-12.77430100	-4.01586600	2.60186300 L
H-H_	0	-12.75488500	-3.71860300	-3.02498800 L
H-H_	0	13.40990100	0.78641500	2.33117700 L

H-H_	0	-12.74940900	1.64682900	-4.37832200 L
H-H_	0	-12.79432500	4.82675600	0.27672500 L
H-H_	0	-12.73720800	1.22285100	4.52230100 L
C-C_3	0	-1.60618100	-0.10344100	0.12608000 H
H-H_	0	-3.52448000	-0.30639000	-0.85434200 H
H-H_	0	-3.55784600	-0.08792200	0.81268000 H
C-C_3	0	-3.03253000	-0.63224600	0.03629900 H
H-H_	0	-3.26517600	-1.62173400	0.22362100 H
N-N_3	0	-1.89610200	1.17672600	-0.31033100 H
H-H_	0	-1.09151900	1.69479900	-0.07391900 H
H-H_	0	-2.80830200	1.43511200	-0.00876600 H
C-C_R	0	-0.08931500	-0.15886600	-0.14035600 H
O-O_R	0	0.52976400	0.87506700	-0.27959500 H
O-O_R	0	0.61548500	-1.21397800	0.15954600 H
H-H_	0	1.53599300	-0.90042200	0.14932700 H
H-H_	0	-1.40959000	-0.15832400	1.17213100 H

STS*@A

B-B_2	0	10.34741200	-0.43636500	3.29869800 L
N-N_3	0	11.64767000	-1.22191500	3.40166600 L
B-	0	12.90199000	-0.31334300	3.45969800 L
B-B_2	0	5.18905800	-0.53210400	3.21401800 L
N-N_3	0	6.49224900	-1.31114300	3.41432800 L
B-B_2	0	7.76967800	-0.48352200	3.23363500 L
B-B_2	0	9.09300600	-2.36119700	2.32421000 L
N-N_3	0	9.06721100	-1.27110800	3.41200000 L
N-N_3	0	10.41379100	-3.07455600	1.97660300 L
B-B_2	0	11.63800100	-2.16458900	2.20002600 L
B-	0	12.90147600	-3.68094800	0.61375800 L
N-N_3	0	12.90786200	-2.33885700	1.36307600 L
B-B_2	0	0.03920500	-0.57709800	3.31748400 L
N-N_3	0	1.33767500	-1.38511800	3.48210800 L
B-B_2	0	2.60900900	-0.57512200	3.20965900 L
B-B_2	0	3.92290700	-2.52012800	2.42992800 L
N-N_3	0	3.91079000	-1.35245600	3.42383200 L
N-N_3	0	5.23319800	-3.23484200	2.08505300 L
B-B_2	0	6.50956700	-2.43889000	2.37711700 L
B-B_2	0	7.79126000	-3.44606900	0.53052500 L
N-N_3	0	7.81819100	-3.16290200	2.03557000 L
N-N_3	0	9.06182800	-3.85024900	-0.20840200 L
B-B_2	0	10.36341700	-3.48403900	0.49657100 L
B-B_2	0	11.61337000	-3.01277800	-1.53475700 L
N-N_3	0	11.63241700	-3.85348100	-0.25390300 L
N-N_3	0	12.94859300	-2.60405000	-2.16977600 L
B-B_2	0	-5.12159300	-0.54671200	3.21317900 L
N-N_3	0	-3.84846400	-1.36194000	3.45018000 L
B-B_2	0	-2.54807200	-0.55887500	3.32183600 L
B-B_2	0	-1.25879400	-2.56630400	2.46202400 L
N-N_3	0	-1.25744000	-1.38346000	3.47819700 L
N-N_3	0	0.02789800	-3.35148300	2.16629500 L
B-B_2	0	1.33521700	-2.63170100	2.55535100 L
B-B_2	0	2.63048400	-3.59308200	0.62398000 L
N-N_3	0	2.64657700	-3.32388900	2.14328200 L
N-N_3	0	3.92400700	-3.90234700	-0.13427500 L
B-B_2	0	5.21413800	-3.49664200	0.57699800 L
B-B_2	0	6.47444800	-3.12146500	-1.50814500 L
N-N_3	0	6.49832700	-3.86168600	-0.16651500 L
N-N_3	0	7.74434600	-3.00812900	-2.35525100 L
B-B_2	0	9.05245800	-3.12672600	-1.56615000 L

B-B_2	0	10.29336600	-1.73811400	-3.21318300 L
N-N_3	0	10.34087000	-3.04010400	-2.40433100 L
N-N_3	0	11.55596500	-1.12313600	-3.77087900 L
B-	0	12.81890700	-1.99945200	-3.58488600 L
B-B_2	0	-10.27990600	-0.51298800	3.25479200 L
N-N_3	0	-8.99672500	-1.33347900	3.44531800 L
B-B_2	0	-7.70227000	-0.53457400	3.23760200 L
B-B_2	0	-6.42194700	-2.47798700	2.38876900 L
N-N_3	0	-6.41353600	-1.34113100	3.41690400 L
N-N_3	0	-5.14719800	-3.27512000	2.09972000 L
B-B_2	0	-3.84556000	-2.55119600	2.45649200 L
B-B_2	0	-2.55299200	-3.84470300	0.66712400 L
N-N_3	0	-2.55562500	-3.32893200	2.14518100 L
N-N_3	0	-1.25065700	-4.02875500	-0.12514900 L
B-B_2	0	0.03901100	-3.75424600	0.66066800 L
B-B_2	0	1.32228700	-3.20965600	-1.45683200 L
N-N_3	0	1.34668900	-3.98888500	-0.11282800 L
N-N_3	0	2.60514800	-2.96633500	-2.25207300 L
B-B_2	0	3.89760100	-3.11903600	-1.45391900 L
B-B_2	0	5.16554200	-1.55427500	-2.87497100 L
N-N_3	0	5.16937800	-2.96893300	-2.28663100 L
N-N_3	0	6.43523600	-1.00347100	-3.51670800 L
B-B_2	0	7.73235700	-1.61412100	-2.98887400 L
B-B_2	0	9.05152700	0.43503900	-3.25083100 L
N-N_3	0	8.99058300	-1.05595800	-3.63198300 L
N-N_3	0	10.38270300	1.20127000	-3.35744400 L
B-B_2	0	11.59927100	0.27022900	-3.15495100 L
B-	0	12.93875500	2.16158800	-2.31872000 L
N-N_3	0	12.71096200	0.64849600	-2.18434000 L
B-	0	-12.83593300	-0.43687100	2.98582900 L
B-B_2	0	-11.57171300	-2.51414100	2.49402600 L
N-N_3	0	-11.60440900	-1.28493600	3.41548900 L
N-N_3	0	-10.27874100	-3.21149600	2.08004300 L
B-B_2	0	-8.99853300	-2.45496400	2.40322100 L
B-B_2	0	-7.72598900	-3.49635300	0.56768500 L
N-N_3	0	-7.71837300	-3.22146800	2.07607600 L
N-N_3	0	-6.44109100	-3.90638500	-0.15365400 L
B-B_2	0	-5.14135500	-3.59274000	0.59251100 L
B-B_2	0	-3.83689600	-3.22984300	-1.48037700 L
N-N_3	0	-3.86330000	-4.01810400	-0.13741400 L
N-N_3	0	-2.53158800	-2.99548500	-2.24710300 L
B-B_2	0	-1.25840600	-3.15038900	-1.40834800 L
B-B_2	0	0.02731000	-1.54994600	-2.85195800 L
N-N_3	0	0.02118000	-2.97230100	-2.22796800 L

N-N_3	0	1.31526000	-0.95673300	-3.42096900 L
B-B_2	0	2.59472100	-1.53032500	-2.81317800 L
B-B_2	0	3.89225000	0.55140200	-3.20500400 L
N-N_3	0	3.87136400	-0.96628300	-3.43578600 L
N-N_3	0	5.19451700	1.33209000	-3.41240900 L
B-B_2	0	6.47210400	0.50418100	-3.23406200 L
B-B_2	0	7.79806500	2.37674900	-2.32717600 L
N-N_3	0	7.78324900	1.28610300	-3.40354700 L
N-N_3	0	9.10486900	3.10023500	-1.98436900 L
B-B_2	0	10.37643000	2.30172800	-2.28551500 L
B-B_2	0	11.64291500	3.19380400	-0.37109600 L
N-N_3	0	11.69014500	2.97390000	-1.88597600 L
N-N_3	0	12.97198900	3.33851000	0.38291300 L
B-	0	-12.84884400	-3.02398500	0.51095500 L
N-N_3	0	-12.86031700	-3.17104400	2.03906300 L
N-N_3	0	-11.63287000	-3.73522900	-0.14853100 L
B-B_2	0	-10.30391900	-3.39625100	0.55480900 L
B-B_2	0	-8.99411500	-3.12939000	-1.50969200 L
N-N_3	0	-9.02764900	-3.85410100	-0.16190600 L
N-N_3	0	-7.69389200	-2.97393500	-2.29575100 L
B-B_2	0	-6.41625500	-3.12654800	-1.47343600 L
B-B_2	0	-5.11379400	-1.55343600	-2.85554700 L
N-N_3	0	-5.12349300	-2.98437600	-2.27802300 L
N-N_3	0	-3.83157100	-0.97327800	-3.45965700 L
B-B_2	0	-2.53821500	-1.58515500	-2.91072400 L
B-B_2	0	-1.25920400	0.58485300	-3.22330600 L
N-N_3	0	-1.24985500	-0.95570600	-3.44821500 L
N-N_3	0	0.02659900	1.39647800	-3.43423900 L
B-B_2	0	1.31648600	0.58130900	-3.23518000 L
B-B_2	0	2.62372800	2.53807900	-2.41705600 L
N-N_3	0	2.61412400	1.37162800	-3.42029500 L
N-N_3	0	3.93627400	3.26180400	-2.09347900 L
B-B_2	0	5.21286300	2.45870400	-2.37584900 L
B-B_2	0	6.50749100	3.48395000	-0.54503500 L
N-N_3	0	6.52450500	3.18217800	-2.04601800 L
N-N_3	0	7.79235300	3.86682300	0.19305300 L
B-B_2	0	9.08756300	3.40001500	-0.47616100 L
B-B_2	0	10.30190400	3.39447600	1.71219400 L
N-N_3	0	10.38104000	3.82578900	0.23862000 L
N-N_3	0	11.55380900	3.21379100	2.54297800 L
B-	0	12.82073500	3.78044000	1.85604100 L
N-N_3	0	-12.83533300	-2.99619400	-2.39585600 L
B-B_2	0	-11.56551100	-3.24844800	-1.60717400 L
B-B_2	0	-10.27616200	-1.57769100	-2.91594900 L

N-N_3	0	-10.25382000	-3.00676000	-2.35164300 L
N-N_3	0	-8.98459900	-0.99773900	-3.51279500 L
B-B_2	0	-7.69644600	-1.56132100	-2.89472900 L
B-B_2	0	-6.40950400	0.53522600	-3.20805700 L
N-N_3	0	-6.39832400	-0.97797500	-3.46098000 L
N-N_3	0	-5.13138300	1.35514500	-3.41310000 L
B-B_2	0	-3.83391800	0.56478900	-3.24133300 L
B-B_2	0	-2.56352600	2.64992400	-2.51688600 L
N-N_3	0	-2.54974300	1.38734800	-3.43402100 L
N-N_3	0	-1.26887400	3.42546000	-2.17575200 L
B-B_2	0	0.03264700	2.65892200	-2.51895000 L
B-B_2	0	1.33431900	3.70429200	-0.63208100 L
N-N_3	0	1.34764400	3.35329300	-2.13847300 L
N-N_3	0	2.63632400	3.95364600	0.13416600 L
B-B_2	0	3.92443300	3.56691000	-0.59320700 L
B-B_2	0	5.18177100	3.11552500	1.47068100 L
N-N_3	0	5.21466600	3.89887400	0.15605200 L
N-N_3	0	6.43867200	2.99535400	2.32243700 L
B-B_2	0	7.74597400	3.18333900	1.56294200 L
B-B_2	0	9.03412000	1.64157300	2.96658000 L
N-N_3	0	8.98967200	3.08222300	2.42623500 L
N-N_3	0	10.34466000	1.08067900	3.54401700 L
B-B_2	0	11.58706700	1.72541300	2.88650700 L
N-N_3	0	12.79098500	0.87750700	2.49390500 L
B-	0	-12.83206300	-1.48349300	-2.66503000 L
B-B_2	0	-11.55722400	0.51047300	-3.39484600 L
N-N_3	0	-11.59415500	-1.02177800	-3.48775800 L
N-N_3	0	-10.26215800	1.31679400	-3.46766800 L
B-B_2	0	-8.98678000	0.51177400	-3.25602100 L
B-B_2	0	-7.72581000	2.45410000	-2.38359800 L
N-N_3	0	-7.70140100	1.32383800	-3.41974300 L
N-N_3	0	-6.44839100	3.24151800	-2.08097200 L
B-B_2	0	-5.14278300	2.50820600	-2.39461000 L
B-B_2	0	-3.86511800	3.68054000	-0.61183100 L
N-N_3	0	-3.87747800	3.33089500	-2.11995100 L
N-N_3	0	-2.58064800	4.07924000	0.13381400 L
B-B_2	0	-1.26960300	3.95685200	-0.68663800 L
B-B_2	0	0.02844100	3.23968300	1.45000800 L
N-N_3	0	0.04631300	4.07253500	0.12537100 L
N-N_3	0	1.32324200	2.95767100	2.22059600 L
B-B_2	0	2.60892800	3.11035700	1.41585400 L
B-B_2	0	3.88514800	1.52737000	2.82790700 L
N-N_3	0	3.88035300	2.94590000	2.24565500 L
N-N_3	0	5.16311400	0.97869300	3.46715700 L

B-B_2	0	6.45657400	1.57795600	2.90984900 L
N-N_3	0	7.74629500	1.02043200	3.52570000 L
B-	0	-12.85183100	2.11535400	-2.14490400 L
N-N_3	0	-12.84401700	1.30953000	-3.45014100 L
N-N_3	0	-11.63870000	3.08207000	-2.03420600 L
B-B_2	0	-10.30296500	2.38559000	-2.36382400 L
B-B_2	0	-9.02108200	3.49586100	-0.57049100 L
N-N_3	0	-9.03337800	3.19493300	-2.07108600 L
N-N_3	0	-7.73655400	3.88112400	0.15604800 L
B-B_2	0	-6.44548100	3.53608900	-0.57864100 L
B-B_2	0	-5.13978900	3.13560200	1.45675000 L
N-N_3	0	-5.16595000	3.94295400	0.14977000 L
N-N_3	0	-3.84996600	3.00244700	2.26959800 L
B-B_2	0	-2.55424800	3.29559100	1.49348400 L
B-B_2	0	-1.25739600	1.60540700	2.89698400 L
N-N_3	0	-1.25326500	3.03953200	2.26671000 L
N-N_3	0	0.03863500	0.97797600	3.44233300 L
B-B_2	0	1.31016200	1.52386500	2.79752300 L
N-N_3	0	2.59442100	0.95012300	3.40459500 L
N-N_3	0	-12.87634200	3.81808900	0.19757700 L
B-B_2	0	-11.59559100	3.58845900	-0.58161600 L
B-B_2	0	-10.30567200	3.04878300	1.46872900 L
N-N_3	0	-10.29612300	3.86710000	0.16831100 L
N-N_3	0	-9.01518000	2.94949700	2.29570600 L
B-B_2	0	-7.72563500	3.10016600	1.47580500 L
B-B_2	0	-6.41208800	1.54330700	2.86036800 L
N-N_3	0	-6.42554700	2.95784300	2.27230000 L
N-N_3	0	-5.11714800	0.97473600	3.44344300 L
B-B_2	0	-3.83023300	1.57022100	2.85979200 L
N-N_3	0	-2.54609800	0.99650900	3.46845300 L
B-	0	-12.85374100	2.75575100	1.30812800 L
B-B_2	0	-11.55846700	1.60690900	3.08254700 L
N-N_3	0	-11.62386900	2.89785700	2.25109600 L
N-N_3	0	-10.24786500	0.99100200	3.57000700 L
B-B_2	0	-8.98886300	1.55481000	2.92667200 L
N-N_3	0	-7.68747100	0.97915700	3.48667900 L
N-N_3	0	-12.82983600	0.96786100	3.60377400 L
H-H_	0	12.91790100	-1.57663700	0.65193700 L
H-H_	0	13.39465900	-1.87762400	-1.56973700 L
H-H_	0	12.37247900	0.44488100	-1.21639800 L
H-H_	0	13.45661900	2.41460200	0.38487500 L
H-H_	0	-12.79836000	-4.18968600	2.26485200 L
H-H_	0	-12.74298400	-3.48471400	-3.31521200 L
H-H_	0	12.60476600	0.51364200	1.53414400 L

H-H_	0	-12.77024100	1.98316900	-4.24590400 L
H-H_	0	-12.80992400	4.75681300	0.65231500 L
H-H_	0	-12.73536700	0.86395600	4.63949400 L
C-C_3	0	-1.37644800	-0.11786000	0.13749600 H
H-H_	0	-3.29587500	-0.26057200	-0.88104200 H
H-H_	0	-3.33517200	-0.00193300	0.77920200 H
C-C_3	0	-2.83187700	-0.59315700	0.02360900 H
H-H_	0	-3.12847100	-1.56561700	0.23321500 H
N-N_2	0	-1.61033000	1.16039600	-0.30000400 H
H-H_	0	-0.75367000	1.64734000	-0.30738500 H
H-H_	0	-2.54252900	1.46947200	-0.19611200 H
C-C_R	0	0.15250100	-0.19367600	-0.14467100 H
O-O_R	0	0.76987700	0.80829200	-0.44177500 H
O-O_R	0	0.86843300	-1.17495100	0.32956000 H
H-H_	0	1.78522100	-0.85661700	0.27598900 H
H-H_	0	-1.20565200	-0.22409100	1.18517400 H

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B-B_2	0	-10.35924800	-0.92279500	-3.25622100 L
N-N_3	0	-11.66398800	-1.70749300	-3.22300000 L
B-	0	-12.91387100	-0.81070500	-3.40631500 L
B-B_2	0	-5.19580200	-1.03508500	-3.21622800 L
N-N_3	0	-6.50608200	-1.82645800	-3.28301500 L
B-B_2	0	-7.77899000	-0.97517400	-3.21429500 L
B-B_2	0	-9.10111900	-2.67414000	-2.00807700 L
N-N_3	0	-9.08319900	-1.77122200	-3.25526600 L
N-N_3	0	-10.41821900	-3.31900300	-1.53711900 L
B-B_2	0	-11.64489000	-2.45511100	-1.89052700 L
B-	0	-12.89331800	-3.71909000	-0.08639700 L
N-N_3	0	-12.90999300	-2.50456500	-1.02918500 L
B-B_2	0	-0.03038100	-1.09852800	-3.31819300 L
N-N_3	0	-1.33349000	-1.92351900	-3.36539500 L
B-B_2	0	-2.61189600	-1.08601100	-3.22170900 L
B-B_2	0	-3.92969000	-2.87628500	-2.14670400 L
N-N_3	0	-3.91903500	-1.88119900	-3.31280700 L
N-N_3	0	-5.23987800	-3.49592700	-1.64789800 L
B-B_2	0	-6.51782800	-2.77121700	-2.07735300 L
B-B_2	0	-7.78675000	-3.41734000	-0.06347900 L
N-N_3	0	-7.82435400	-3.41427200	-1.59517200 L
N-N_3	0	-9.04820400	-3.72398600	0.73584800 L
B-B_2	0	-10.35663400	-3.48067500	-0.01018000 L
B-B_2	0	-11.60581300	-2.74234100	1.94046200 L
N-N_3	0	-11.61876500	-3.75485700	0.79085700 L
N-N_3	0	-12.94499800	-2.25953600	2.51164800 L
B-B_2	0	5.13077700	-1.02279700	-3.14526400 L
N-N_3	0	3.86487200	-1.87056900	-3.28312900 L
B-B_2	0	2.56010500	-1.06585200	-3.29242900 L
B-B_2	0	1.26366500	-2.93564800	-2.17110200 L
N-N_3	0	1.27208900	-1.91202600	-3.34781400 L
N-N_3	0	-0.02886000	-3.63155700	-1.71789200 L
B-B_2	0	-1.33645700	-3.02443600	-2.26733600 L
B-B_2	0	-2.63010200	-3.50278000	-0.16162200 L
N-N_3	0	-2.65018000	-3.59469700	-1.70005700 L
N-N_3	0	-3.91613100	-3.70432100	0.64354400 L
B-B_2	0	-5.21166600	-3.43816900	-0.11841500 L
B-B_2	0	-6.46835400	-2.77331800	1.90405500 L
N-N_3	0	-6.48588200	-3.70127200	0.68371300 L
N-N_3	0	-7.73539100	-2.58521100	2.74230400 L
B-B_2	0	-9.04443900	-2.81496100	1.97779500 L

B-B_2	0	-10.29956700	-1.24565500	3.44243400 L
N-N_3	0	-10.33229600	-2.63912000	2.80367000 L
N-N_3	0	-11.56941500	-0.57077100	3.90588500 L
B-	0	-12.82479500	-1.47343000	3.83485200 L
B-B_2	0	10.28906300	-0.97492700	-3.12892300 L
N-N_3	0	9.00994200	-1.81888500	-3.21194100 L
B-B_2	0	7.71176900	-1.00303700	-3.13847400 L
B-B_2	0	6.42650500	-2.80232600	-2.02617700 L
N-N_3	0	6.42759500	-1.83208500	-3.21270100 L
N-N_3	0	5.15007200	-3.54436800	-1.62481400 L
B-B_2	0	3.85119500	-2.90542500	-2.12913600 L
B-B_2	0	2.53778600	-3.76165000	-0.13058800 L
N-N_3	0	2.55771600	-3.60490000	-1.68466000 L
N-N_3	0	1.23147500	-3.84839400	0.66478200 L
B-B_2	0	-0.04576300	-3.65833900	-0.16138300 L
B-B_2	0	-1.32829000	-2.77009500	1.81698800 L
N-N_3	0	-1.35152400	-3.76707200	0.63178400 L
N-N_3	0	-2.60489300	-2.49062000	2.60552300 L
B-B_2	0	-3.89686600	-2.73118800	1.83011000 L
B-B_2	0	-5.17042900	-1.06139400	3.12028200 L
N-N_3	0	-5.16257900	-2.52213000	2.65749300 L
N-N_3	0	-6.44887400	-0.45742100	3.69111700 L
B-B_2	0	-7.73753200	-1.13110600	3.22219100 L
B-B_2	0	-9.07027700	0.92080500	3.21455000 L
N-N_3	0	-9.00486500	-0.50865100	3.78263800 L
N-N_3	0	-10.40730600	1.68417700	3.18792300 L
B-B_2	0	-11.61786000	0.72687200	3.10815700 L
B-	0	-12.95065000	2.47925500	1.99621400 L
N-N_3	0	-12.72569400	0.96233600	2.08862300 L
B-	0	12.83746500	-0.85056000	-2.83419100 L
B-B_2	0	11.57521000	-2.84654700	-2.07709400 L
N-N_3	0	11.61676100	-1.75733000	-3.16014800 L
N-N_3	0	10.27842600	-3.47781300	-1.57793400 L
B-B_2	0	9.00229500	-2.77521900	-2.01626500 L
B-B_2	0	7.71425700	-3.52649100	-0.05541400 L
N-N_3	0	7.71938400	-3.48510100	-1.58853400 L
N-N_3	0	6.42009600	-3.81452500	0.71049300 L
B-B_2	0	5.12853500	-3.59663200	-0.08370400 L
B-B_2	0	3.81748200	-2.92243400	1.91863700 L
N-N_3	0	3.83743900	-3.88401000	0.69363400 L
N-N_3	0	2.51253300	-2.58133900	2.65006000 L
B-B_2	0	1.24283100	-2.81487400	1.82742500 L
B-B_2	0	-0.03602900	-1.05966300	3.12874600 L
N-N_3	0	-0.04324000	-2.52316000	2.60607400 L

N-N_3	0	-1.32282400	-0.40698100	3.64691700 L
B-B_2	0	-2.60072700	-1.02297700	3.07311500 L
B-B_2	0	-3.90616100	1.07149800	3.26076000 L
N-N_3	0	-3.88329800	-0.41627600	3.63718300 L
N-N_3	0	-5.21930600	1.86153500	3.31010300 L
B-B_2	0	-6.49010200	1.00769400	3.23939600 L
B-B_2	0	-7.81157400	2.69415600	2.02159200 L
N-N_3	0	-7.80955800	1.79371500	3.26112500 L
N-N_3	0	-9.11325200	3.34901000	1.54718500 L
B-B_2	0	-10.38986800	2.61262000	1.96345300 L
B-B_2	0	-11.63927100	3.19931900	-0.07746700 L
N-N_3	0	-11.69832000	3.21610500	1.45330500 L
N-N_3	0	-12.96285700	3.22767600	-0.85403200 L
B-	0	12.83949700	-3.08050800	-0.03448800 L
N-N_3	0	12.85960700	-3.43600400	-1.52790400 L
N-N_3	0	11.61709700	-3.69106300	0.70899600 L
B-B_2	0	10.29334700	-3.44505600	-0.04158700 L
B-B_2	0	8.97678800	-2.88151900	1.95755300 L
N-N_3	0	9.00943000	-3.78854900	0.72538100 L
N-N_3	0	7.67518500	-2.60252900	2.70579900 L
B-B_2	0	6.39852500	-2.85510900	1.90679800 L
B-B_2	0	5.10761300	-1.10203200	3.07112300 L
N-N_3	0	5.10557000	-2.59489600	2.68221300 L
N-N_3	0	3.83159600	-0.44012300	3.59892500 L
B-B_2	0	2.53086300	-1.10200000	3.13670200 L
B-B_2	0	1.26144700	1.08994700	3.21270200 L
N-N_3	0	1.25383300	-0.40973000	3.62552500 L
N-N_3	0	-0.01536600	1.93783300	3.34485500 L
B-B_2	0	-1.32312500	1.11687400	3.34549800 L
B-B_2	0	-2.63192600	2.87007800	2.14305000 L
N-N_3	0	-2.62954400	1.92093500	3.35544500 L
N-N_3	0	-3.94304000	3.50586300	1.65980200 L
B-B_2	0	-5.22561900	2.78470100	2.08952500 L
B-B_2	0	-6.50347500	3.43816700	0.07996800 L
N-N_3	0	-6.53256300	3.43112900	1.61105600 L
N-N_3	0	-7.77791300	3.72610500	-0.71760700 L
B-B_2	0	-9.08362100	3.39122900	0.00977100 L
B-B_2	0	-10.29020700	3.05843600	-2.15532200 L
N-N_3	0	-10.36816400	3.71868000	-0.77024200 L
N-N_3	0	-11.53774700	2.80137300	-2.97086900 L
B-	0	-12.80332300	3.46409500	-2.37282300 L
N-N_3	0	12.81397500	-2.65858200	2.84157700 L
B-B_2	0	11.54652800	-3.01537800	2.09048600 L
B-B_2	0	10.26856000	-1.15001400	3.11839800 L

N-N_3	0	10.23415800	-2.64753000	2.77878300 L
N-N_3	0	8.98274800	-0.47841800	3.62294300 L
B-B_2	0	7.68895800	-1.11977500	3.09999900 L
B-B_2	0	6.41291700	1.00541700	3.12287800 L
N-N_3	0	6.39783400	-0.45674700	3.58649400 L
N-N_3	0	5.13981800	1.85154700	3.21882300 L
B-B_2	0	3.83810900	1.05184300	3.17598000 L
B-B_2	0	2.56218500	2.99706600	2.16379000 L
N-N_3	0	2.56127500	1.90030500	3.26908800 L
N-N_3	0	1.26502000	3.70097400	1.70881500 L
B-B_2	0	-0.03666800	3.03325200	2.23060900 L
B-B_2	0	-1.33715300	3.57981400	0.15141600 L
N-N_3	0	-1.35563800	3.60368200	1.69575900 L
N-N_3	0	-2.63337400	3.74360300	-0.64203300 L
B-B_2	0	-3.92293100	3.47601300	0.12965700 L
B-B_2	0	-5.17685300	2.76658600	-1.86637400 L
N-N_3	0	-5.20234300	3.72127000	-0.66942900 L
N-N_3	0	-6.43222000	2.56702500	-2.70434700 L
B-B_2	0	-7.73811100	2.84455600	-1.96958900 L
B-B_2	0	-9.03378200	1.17017100	-3.20354400 L
N-N_3	0	-8.97828400	2.66094900	-2.82415500 L
N-N_3	0	-10.35120400	0.54890200	-3.70010000 L
B-B_2	0	-11.58995700	1.28389500	-3.13491400 L
N-N_3	0	-12.79309100	0.50384900	-2.61946500 L
B-	0	12.83004500	-1.12217500	2.87127100 L
B-B_2	0	11.56179700	0.97399100	3.23881900 L
N-N_3	0	11.59042900	-0.51914200	3.59482000 L
N-N_3	0	10.27272500	1.79498300	3.21902800 L
B-B_2	0	8.99013300	0.97580900	3.14307100 L
B-B_2	0	7.72578300	2.77559700	2.01054100 L
N-N_3	0	7.70998800	1.81039100	3.20206400 L
N-N_3	0	6.44506400	3.50556600	1.59719200 L
B-B_2	0	5.14285500	2.83501100	2.03741900 L
B-B_2	0	3.84895900	3.65605800	0.08935900 L
N-N_3	0	3.87260600	3.59390900	1.63484600 L
N-N_3	0	2.56038700	3.94201000	-0.69654000 L
B-B_2	0	1.25143500	3.90170500	0.14284000 L
B-B_2	0	-0.03432400	2.84805700	-1.83767500 L
N-N_3	0	-0.06521400	3.86752900	-0.65859100 L
N-N_3	0	-1.32416500	2.51040200	-2.58951900 L
B-B_2	0	-2.60975400	2.74543000	-1.80584300 L
B-B_2	0	-3.88590600	1.04417300	-3.06841400 L
N-N_3	0	-3.87733200	2.51060700	-2.62144100 L
N-N_3	0	-5.16759100	0.43618100	-3.64134600 L

B-B_2	0	-6.45697200	1.09809000	-3.14730200 L
N-N_3	0	-7.75168200	0.48045200	-3.69020600 L
B-	0	12.83809400	2.37724300	1.74960800 L
N-N_3	0	12.85532100	1.76041200	3.15348800 L
N-N_3	0	11.63593300	3.34005800	1.54204500 L
B-B_2	0	10.30198900	2.69912600	1.97531200 L
B-B_2	0	9.00702800	3.54571200	0.05486300 L
N-N_3	0	9.03013300	3.46192600	1.58317500 L
N-N_3	0	7.71529100	3.80346600	-0.71504600 L
B-B_2	0	6.43142500	3.54850200	0.06704100 L
B-B_2	0	5.12688300	2.85536900	-1.89516700 L
N-N_3	0	5.14440300	3.83096000	-0.70745600 L
N-N_3	0	3.83963600	2.61156800	-2.68656100 L
B-B_2	0	2.54425400	2.98966600	-1.94679800 L
B-B_2	0	1.25632900	1.12140300	-3.14752400 L
N-N_3	0	1.23705200	2.61148300	-2.66244900 L
N-N_3	0	-0.03565000	0.42973100	-3.62184300 L
B-B_2	0	-1.31137800	1.03521700	-3.03914200 L
N-N_3	0	-2.59648900	0.40692500	-3.58593600 L
N-N_3	0	12.85258500	3.82031400	-0.76964600 L
B-B_2	0	11.57918000	3.68050900	0.04168800 L
B-B_2	0	10.29396700	2.82022400	-1.89889800 L
N-N_3	0	10.27441200	3.82187400	-0.73538300 L
N-N_3	0	9.00468400	2.58625900	-2.69987100 L
B-B_2	0	7.71286900	2.84199700	-1.90971300 L
B-B_2	0	6.41263100	1.10031700	-3.07270200 L
N-N_3	0	6.41526800	2.58102800	-2.67949200 L
N-N_3	0	5.12494000	0.45233200	-3.58426100 L
B-B_2	0	3.83024300	1.11619000	-3.09940800 L
N-N_3	0	2.55250700	0.45915300	-3.63452400 L
B-	0	12.85379500	2.60618700	-1.71325300 L
B-B_2	0	11.56171400	1.15287200	-3.25223200 L
N-N_3	0	11.61277500	2.56700600	-2.65296700 L
N-N_3	0	10.25819400	0.46717500	-3.66102500 L
B-B_2	0	8.99042600	1.11414400	-3.11946500 L
N-N_3	0	7.69587600	0.45899600	-3.60236100 L
N-N_3	0	12.84124700	0.44650200	-3.65371900 L
H-H_	0	-12.91778900	-1.64574200	-0.43812700 L
H-H_	0	-13.39209200	-1.62227100	1.81816900 L
H-H_	0	-12.38496100	0.61745700	1.16237600 L
H-H_	0	-13.44162700	2.30912000	-0.72976900 L
H-H_	0	12.79696000	-4.47593600	-1.61193600 L
H-H_	0	12.70827400	-2.99568300	3.82523500 L
H-H_	0	-12.60136000	0.27968200	-1.61901200 L

H-H_	0	12.80568100	2.53779200	3.85041200 L
H-H_	0	12.76413400	4.67997000	-1.35748000 L
H-H_	0	12.76322900	0.19061300	-4.66410900 L
C-C_3	0	1.47519300	-0.19670400	-0.21499800 H
H-H_	0	3.34857500	-0.12876900	0.93788600 H
H-H_	0	3.43520000	0.04896800	-0.73723700 H
C-C_3	0	2.95748700	-0.54552100	0.03231600 H
H-H_	0	3.39052000	-1.48726800	-0.11413600 H
N-N_3	0	1.62303600	1.18733700	-0.09241300 H
H-H_	0	0.89053900	1.46973400	0.51798400 H
H-H_	0	2.53945500	1.37628400	0.24577200 H
C-C_R	0	-0.03531500	-0.26064300	0.18553500 H
O-O_R	0	-0.59984900	0.62824100	0.77477400 H
O-O_R	0	-0.80678400	-1.03833500	-0.53480700 H
H-H_	0	-1.71087100	-0.72972000	-0.36009800 H
H-H_	0	1.30225300	-0.51520800	-1.20706800 H

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B-B_2	0	-10.37875500	-0.82279000	-3.23114100 L
N-N_3	0	-11.67857200	-1.61544300	-3.23431900 L
B-	0	-12.93358100	-0.72327900	-3.40895600 L
B-B_2	0	-5.21980600	-0.90602800	-3.13963300 L
N-N_3	0	-6.52313000	-1.70481400	-3.23804600 L
B-B_2	0	-7.80060500	-0.86124900	-3.16251500 L
B-B_2	0	-9.12289200	-2.60890900	-2.02216000 L
N-N_3	0	-9.09825700	-1.66482600	-3.23893300 L
N-N_3	0	-10.44311900	-3.27409600	-1.58834900 L
B-B_2	0	-11.66718400	-2.39861300	-1.92325400 L
B-	0	-12.93092700	-3.69371300	-0.16180600 L
N-N_3	0	-12.92357600	-2.43955000	-1.05013900 L
B-B_2	0	-0.06337100	-0.95631100	-3.14919000 L
N-N_3	0	-1.36083100	-1.77504600	-3.24893600 L
B-B_2	0	-2.64046500	-0.94306000	-3.11270500 L
B-B_2	0	-3.95489800	-2.76860500	-2.09813300 L
N-N_3	0	-3.93966900	-1.74483200	-3.23802100 L
N-N_3	0	-5.26368500	-3.44688600	-1.68192800 L
B-B_2	0	-6.53988200	-2.69079100	-2.06504300 L
B-B_2	0	-7.82113900	-3.47137700	-0.11047100 L
N-N_3	0	-7.84810700	-3.36956100	-1.63863100 L
N-N_3	0	-9.09097400	-3.78748500	0.67103000 L
B-B_2	0	-10.39232100	-3.49857800	-0.06906400 L
B-B_2	0	-11.64096500	-2.81198300	1.90308400 L
N-N_3	0	-11.66143800	-3.78376200	0.71821000 L

N-N_3	0	-12.97659300	-2.35116900	2.50066300 L
B-B_2	0	5.08776400	-0.96644500	-3.14038600 L
N-N_3	0	3.80163700	-1.78908800	-3.28905100 L
B-B_2	0	2.51358000	-0.95886200	-3.16140200 L
B-B_2	0	1.22086500	-2.89364700	-2.17315000 L
N-N_3	0	1.22315500	-1.78208200	-3.25823300 L
N-N_3	0	-0.08145000	-3.60395500	-1.76116500 L
B-B_2	0	-1.37091400	-2.86247300	-2.15344900 L
B-B_2	0	-2.66442100	-3.65016000	-0.19031800 L
N-N_3	0	-2.67930300	-3.53312600	-1.72206600 L
N-N_3	0	-3.95736500	-3.85712500	0.60004400 L
B-B_2	0	-5.24612300	-3.53956100	-0.15439100 L
B-B_2	0	-6.50043300	-2.91461200	1.87463300 L
N-N_3	0	-6.52947700	-3.80758900	0.62896300 L
N-N_3	0	-7.76812200	-2.70823600	2.70775400 L
B-B_2	0	-9.07859100	-2.91769700	1.94015100 L
B-B_2	0	-10.31900700	-1.35654500	3.42654300 L
N-N_3	0	-10.36549300	-2.74008500	2.76601600 L
N-N_3	0	-11.58359000	-0.67621800	3.89760000 L
B-	0	-12.84430300	-1.57201300	3.82748300 L
B-B_2	0	10.24795300	-0.94191500	-3.16264500 L
N-N_3	0	8.96489200	-1.77540800	-3.28857300 L
B-B_2	0	7.66959200	-0.96196500	-3.15259300 L
B-B_2	0	6.38791800	-2.82954600	-2.14076600 L
N-N_3	0	6.37866800	-1.78213000	-3.26327100 L
N-N_3	0	5.12157400	-3.60029800	-1.76412000 L
B-B_2	0	3.80775100	-2.98648100	-2.28867200 L
B-B_2	0	2.52000400	-3.76639000	-0.22221400 L
N-N_3	0	2.50638500	-3.62475100	-1.77209300 L
N-N_3	0	1.23251900	-3.96948500	0.58185200 L
B-B_2	0	-0.07542700	-3.87647300	-0.22618700 L
B-B_2	0	-1.34857500	-2.92873000	1.75156100 L
N-N_3	0	-1.37923300	-3.94433300	0.58731700 L
N-N_3	0	-2.62154300	-2.64026400	2.54861800 L
B-B_2	0	-3.92529900	-2.90174800	1.79787600 L
B-B_2	0	-5.19075900	-1.19551600	3.04735200 L
N-N_3	0	-5.19023000	-2.66752100	2.62310400 L
N-N_3	0	-6.46113800	-0.57825500	3.62513300 L
B-B_2	0	-7.75799500	-1.25128500	3.17842900 L
B-B_2	0	-9.08326700	0.80862200	3.18409800 L
N-N_3	0	-9.01732100	-0.62204500	3.75023300 L
N-N_3	0	-10.41700700	1.57764700	3.18923400 L
B-B_2	0	-11.62947700	0.62442000	3.10471900 L
B-	0	-12.97424700	2.37889600	2.01938300 L

N-N_3	0	-12.73094700	0.86338900	2.07973800 L
B-	0	12.79940500	-0.84360900	-2.87700300 L
B-B_2	0	11.53900100	-2.89488800	-2.25548400 L
N-N_3	0	11.57398900	-1.72418100	-3.25243400 L
N-N_3	0	10.24455400	-3.50925700	-1.73452000 L
B-B_2	0	8.96601300	-2.80226100	-2.15398300 L
B-B_2	0	7.69661200	-3.57764300	-0.19274500 L
N-N_3	0	7.68676000	-3.51408700	-1.72588200 L
N-N_3	0	6.41526000	-3.87475800	0.58700500 L
B-B_2	0	5.11568000	-3.73444100	-0.21576800 L
B-B_2	0	3.81110800	-3.00646400	1.81550300 L
N-N_3	0	3.82042900	-3.95601700	0.57766200 L
N-N_3	0	2.50815500	-2.65946000	2.54612100 L
B-B_2	0	1.23087100	-2.94356000	1.74669500 L
B-B_2	0	-0.05375700	-1.15143300	2.94355800 L
N-N_3	0	-0.05536000	-2.63928600	2.51258800 L
N-N_3	0	-1.33617600	-0.51488500	3.47229000 L
B-B_2	0	-2.62162500	-1.15779300	2.95362700 L
B-B_2	0	-3.92554800	0.93723000	3.12660100 L
N-N_3	0	-3.89595000	-0.54218400	3.52991300 L
N-N_3	0	-5.23022700	1.73304500	3.24442900 L
B-B_2	0	-6.50402100	0.88492600	3.16479000 L
B-B_2	0	-7.83487000	2.62341800	2.02730600 L
N-N_3	0	-7.81882100	1.67661300	3.23216100 L
N-N_3	0	-9.14255500	3.29478500	1.59447400 L
B-B_2	0	-10.41152000	2.53208100	1.98542200 L
B-B_2	0	-11.67614100	3.19599600	-0.02552000 L
N-N_3	0	-11.72728700	3.14517600	1.50453700 L
N-N_3	0	-13.00407500	3.26800800	-0.79201400 L
B-	0	12.83013100	-3.12672500	-0.22482500 L
N-N_3	0	12.82383800	-3.49413600	-1.71709800 L
N-N_3	0	11.60456500	-3.70127000	0.54371800 L
B-B_2	0	10.27617600	-3.46839800	-0.20017900 L
B-B_2	0	8.96894700	-2.87455100	1.79660600 L
N-N_3	0	9.00109400	-3.80570400	0.58201400 L
N-N_3	0	7.66830300	-2.63270100	2.56355300 L
B-B_2	0	6.38749200	-2.88554800	1.76629100 L
B-B_2	0	5.09050700	-1.18710200	3.03816600 L
N-N_3	0	5.10344700	-2.66600700	2.56996400 L
N-N_3	0	3.79259100	-0.52669200	3.53130600 L
B-B_2	0	2.51386000	-1.16570600	2.98185200 L
B-B_2	0	1.22773100	1.01354100	3.16350300 L
N-N_3	0	1.22558700	-0.50783400	3.48413300 L
N-N_3	0	-0.07166000	1.82182900	3.26468600 L

B-B_2	0	-1.34813100	0.98142200	3.10408800 L
B-B_2	0	-2.66655900	2.82600800	2.12323700 L
N-N_3	0	-2.64797600	1.77702200	3.24082100 L
N-N_3	0	-3.98005800	3.49085700	1.69889800 L
B-B_2	0	-5.25204000	2.72546200	2.07907000 L
B-B_2	0	-6.54132000	3.50047800	0.12454300 L
N-N_3	0	-6.56446900	3.39293000	1.65214200 L
N-N_3	0	-7.82367400	3.80102400	-0.65478000 L
B-B_2	0	-9.12076300	3.41293700	0.06120500 L
B-B_2	0	-10.33175100	3.16798300	-2.11684400 L
N-N_3	0	-10.41258100	3.75639800	-0.69869500 L
N-N_3	0	-11.58334700	2.89139200	-2.92145000 L
B-	0	-12.84955400	3.53667700	-2.30619900 L
N-N_3	0	12.81550600	-2.62019400	2.63788200 L
B-B_2	0	11.54141000	-2.96222300	1.89127600 L
B-B_2	0	10.24943300	-1.17803700	3.03786000 L
N-N_3	0	10.23103300	-2.65721600	2.61906800 L
N-N_3	0	8.95930700	-0.54738800	3.58258900 L
B-B_2	0	7.66922800	-1.16896200	3.02918700 L
B-B_2	0	6.37839900	0.94598300	3.13904000 L
N-N_3	0	6.37585200	-0.53546200	3.55358500 L
N-N_3	0	5.10267500	1.78883400	3.26861600 L
B-B_2	0	3.80096600	0.99310600	3.19135900 L
B-B_2	0	2.52476400	3.06849300	2.33265500 L
N-N_3	0	2.51564500	1.83877800	3.31152600 L
N-N_3	0	1.21317600	3.69881000	1.79357100 L
B-B_2	0	-0.07773300	2.96401100	2.21525700 L
B-B_2	0	-1.37217400	3.66218800	0.20283000 L
N-N_3	0	-1.39306000	3.59211500	1.73860500 L
N-N_3	0	-2.66578500	3.86701300	-0.58885100 L
B-B_2	0	-3.96008400	3.57448800	0.17105600 L
B-B_2	0	-5.21098900	2.91018800	-1.83920700 L
N-N_3	0	-5.24497200	3.83079200	-0.61646800 L
N-N_3	0	-6.46771200	2.69771400	-2.67338500 L
B-B_2	0	-7.77590800	2.97156100	-1.94144600 L
B-B_2	0	-9.06499400	1.27896100	-3.15617800 L
N-N_3	0	-9.01938900	2.77259700	-2.78801100 L
N-N_3	0	-10.37631500	0.65269600	-3.66042900 L
B-B_2	0	-11.61869200	1.37279000	-3.08643400 L
N-N_3	0	-12.82634900	0.57987900	-2.60056300 L
B-	0	12.79685000	-1.08948900	2.75130400 L
B-B_2	0	11.52653900	0.95363300	3.33682500 L
N-N_3	0	11.56834200	-0.56663800	3.54892700 L
N-N_3	0	10.22919300	1.75701500	3.31461600 L

B-B_2	0	8.95676000	0.93142800	3.18539400 L
B-B_2	0	7.69387400	2.77316500	2.11951100 L
N-N_3	0	7.66974300	1.75334100	3.26487900 L
N-N_3	0	6.41888800	3.52173300	1.72511700 L
B-B_2	0	5.11071300	2.85609300	2.15312600 L
B-B_2	0	3.82484100	3.78171600	0.21825500 L
N-N_3	0	3.84339700	3.64042800	1.77229500 L
N-N_3	0	2.52929300	4.01832200	-0.58154900 L
B-B_2	0	1.22097900	3.88441600	0.23155300 L
B-B_2	0	-0.05729600	2.95088100	-1.76724100 L
N-N_3	0	-0.08506900	3.94733000	-0.57995000 L
N-N_3	0	-1.34520800	2.64541900	-2.53832200 L
B-B_2	0	-2.63984100	2.89318000	-1.77101200 L
B-B_2	0	-3.91494000	1.18251400	-3.01419500 L
N-N_3	0	-3.90738100	2.65515300	-2.58886100 L
N-N_3	0	-5.19433700	0.56131400	-3.57995700 L
B-B_2	0	-6.48674500	1.22300700	-3.09642600 L
N-N_3	0	-7.77775300	0.59518600	-3.63767500 L
B-	0	12.82722200	2.41374900	1.92491400 L
N-N_3	0	12.81016900	1.75903400	3.31263100 L
N-N_3	0	11.60679300	3.34933900	1.68883400 L
B-B_2	0	10.27165800	2.69656000	2.10009400 L
B-B_2	0	8.98679000	3.57266300	0.18763100 L
N-N_3	0	9.00234700	3.46481800	1.71397500 L
N-N_3	0	7.69883900	3.83826200	-0.58532000 L
B-B_2	0	6.40855500	3.60637400	0.19513800 L
B-B_2	0	5.10160900	2.91181900	-1.76681000 L
N-N_3	0	5.12645800	3.90013700	-0.58404300 L
N-N_3	0	3.82383900	2.70215600	-2.58259400 L
B-B_2	0	2.52123300	3.10732100	-1.86496000 L
B-B_2	0	1.22409400	1.22933700	-3.06186300 L
N-N_3	0	1.21589800	2.71899400	-2.58327500 L
N-N_3	0	-0.06661800	0.54566200	-3.52880600 L
B-B_2	0	-1.34151700	1.16854400	-2.96877900 L
N-N_3	0	-2.62416200	0.53788900	-3.51421700 L
N-N_3	0	12.84153400	3.78709900	-0.62310400 L
B-B_2	0	11.56224900	3.67096700	0.18359200 L
B-B_2	0	10.27093000	2.83196100	-1.76462500 L
N-N_3	0	10.26106700	3.83222000	-0.59847300 L
N-N_3	0	8.97931800	2.61571200	-2.56769500 L
B-B_2	0	7.69021400	2.86712100	-1.77170100 L
B-B_2	0	6.38085800	1.15203200	-2.97477500 L
N-N_3	0	6.39235900	2.62446600	-2.54554800 L
N-N_3	0	5.09383200	0.53238800	-3.51915400 L

B-B_2	0	3.80275100	1.21368600	-3.04042600 L
N-N_3	0	2.51446900	0.55504700	-3.54540500 L
B-	0	12.81865700	2.57628200	-1.57019500 L
B-B_2	0	11.52690800	1.18522100	-3.15912900 L
N-N_3	0	11.58774000	2.58134600	-2.52244000 L
N-N_3	0	10.21961000	0.53047200	-3.60486600 L
B-B_2	0	8.95798500	1.15337000	-3.02219900 L
N-N_3	0	7.65944700	0.52564200	-3.53172900 L
N-N_3	0	12.80177200	0.50238900	-3.61199500 L
H-H_	0	-12.89348400	-1.60605800	-0.42427500 L
H-H_	0	-13.44421400	-1.71367300	1.82087500 L
H-H_	0	-12.37699800	0.54349600	1.14949900 L
H-H_	0	-13.49992200	2.35595200	-0.68845900 L
H-H_	0	12.74728600	-4.53398800	-1.78969500 L
H-H_	0	12.73753100	-3.01555900	3.60226200 L
H-H_	0	-12.64819400	0.33932900	-1.60142900 L
H-H_	0	12.72683200	2.51804800	4.02636100 L
H-H_	0	12.77299100	4.65060600	-1.20795400 L
H-H_	0	12.71819400	0.31241200	-4.63639000 L
C-C_R	0	2.15246500	-0.19240700	-0.14160600 H
H-H_	0	4.01893300	-0.39677800	0.86786100 H
H-H_	0	4.16280100	0.01143200	-0.74884800 H
C-C_3	0	3.58300500	-0.62983700	-0.09273300 H
H-H_	0	3.88344000	-1.59160400	-0.33068200 H
N-N_R	0	2.45556300	1.23170300	0.20413600 H
H-H_	0	1.54996200	1.48948400	0.59654200 H
H-H_	0	3.35285800	1.26376800	0.64146300 H
C-C_R	0	0.73053600	-0.20690700	0.01571000 H
O-O_R	0	0.13223600	0.84731500	0.31294800 H
O-O_R	0	-0.07214400	-1.20787800	-0.25252500 H
H-H_	0	-0.95733600	-0.82288800	-0.15579200 H
H-H_	0	2.29207000	0.80005500	-0.86056200 H

INT1@A

B-B_2	0	10.37695600	3.35649900	-0.42584000 L
N-N_3	0	11.67436600	3.65263100	0.32128700 L
B-	0	12.93131500	3.33138000	-0.52505400 L
B-B_2	0	5.21593700	3.55810200	-0.47372500 L
N-N_3	0	6.51880900	3.86900800	0.27038100 L
B-B_2	0	7.79948000	3.43538800	-0.44616000 L
B-B_2	0	9.06418600	3.03325500	1.64230900 L
N-N_3	0	9.09425800	3.77381400	0.29417500 L
N-N_3	0	10.34662400	2.91710800	2.48412200 L

B-B_2	0	11.62170600	2.84795900	1.62438400 L
B-	0	12.78841600	1.86771900	3.71260700 L
N-N_3	0	12.94556900	2.44880000	2.29001400 L
B-B_2	0	0.01810100	3.86469700	-0.54729200 L
N-N_3	0	1.33134600	4.07216900	0.24165100 L
B-B_2	0	2.62286600	3.68125700	-0.50002100 L
B-B_2	0	3.90148400	3.14098900	1.54591500 L
N-N_3	0	3.92968600	3.96394800	0.25457500 L
N-N_3	0	5.17665200	2.92951500	2.36298000 L
B-B_2	0	6.48363000	3.09134500	1.58906300 L
B-B_2	0	7.71943800	1.52090300	3.03148400 L
N-N_3	0	7.75335800	2.92851100	2.42859700 L
N-N_3	0	8.96040200	0.94025500	3.68602800 L
B-B_2	0	10.27299200	1.62322700	3.30778600 L
B-B_2	0	11.57404000	-0.39556800	3.25867100 L
N-N_3	0	11.52130100	0.99457200	3.88506300 L
N-N_3	0	12.73332400	-0.78060300	2.34844100 L
B-B_2	0	-5.16756100	3.53563300	-0.48630000 L
N-N_3	0	-3.88950000	3.94214900	0.25128400 L
B-B_2	0	-2.58262600	3.70552700	-0.51805200 L
B-B_2	0	-1.27932800	3.42790100	1.66653700 L
N-N_3	0	-1.29604500	4.09378900	0.23709900 L
N-N_3	0	0.02799100	3.02407900	2.36743100 L
B-B_2	0	1.31417800	3.27601200	1.57581000 L
B-B_2	0	2.58750000	1.49144000	2.80195800 L
N-N_3	0	2.60853100	2.95891200	2.33389600 L
N-N_3	0	3.85544900	0.88493500	3.40370800 L
B-B_2	0	5.15665700	1.48848200	2.88322400 L
B-B_2	0	6.44584200	-0.59364500	3.19386000 L
N-N_3	0	6.41218000	0.90531800	3.52171400 L
N-N_3	0	7.74525200	-1.38843000	3.37896600 L
B-B_2	0	9.02194200	-0.54304700	3.27689000 L
B-B_2	0	10.35385800	-2.39618900	2.30495800 L
N-N_3	0	10.34383800	-1.32119500	3.40352700 L
N-N_3	0	11.66634000	-3.05495300	1.89185300 L
B-	0	12.91210600	-2.30401700	2.42672000 L
B-B_2	0	-10.32760800	3.34163000	-0.48051500 L
N-N_3	0	-9.05604200	3.78070000	0.25674800 L
B-B_2	0	-7.75030300	3.45313700	-0.48038100 L
B-B_2	0	-6.44612900	3.04150300	1.55443600 L
N-N_3	0	-6.46919300	3.85028100	0.25561600 L
N-N_3	0	-5.15270100	2.89995400	2.35431300 L
B-B_2	0	-3.86250500	3.13204400	1.56093800 L
B-B_2	0	-2.55466100	1.54923400	2.94265400 L

N-N_3	0	-2.58505900	3.01138400	2.39294800 L
N-N_3	0	-1.25109400	0.91013600	3.42349100 L
B-B_2	0	0.01524500	1.53244300	2.82911600 L
B-B_2	0	1.30576200	-0.63356600	3.11367300 L
N-N_3	0	1.30182200	0.89473400	3.36370200 L
N-N_3	0	2.59532700	-1.43875300	3.30847200 L
B-B_2	0	3.87322300	-0.62315800	3.11029500 L
B-B_2	0	5.19197700	-2.53921300	2.28588200 L
N-N_3	0	5.16251300	-1.41770600	3.33024300 L
N-N_3	0	6.50739000	-3.25211400	1.95714400 L
B-B_2	0	7.77499100	-2.45357900	2.27822100 L
B-B_2	0	9.08794000	-3.39108700	0.40793600 L
N-N_3	0	9.08350400	-3.16586800	1.93080400 L
N-N_3	0	10.39869000	-3.74321600	-0.31958900 L
B-B_2	0	11.63191600	-3.12432300	0.36497100 L
B-	0	12.84972800	-3.49851800	-1.85263300 L
N-N_3	0	12.93833600	-2.94493500	-0.41788000 L
B-	0	-12.86752800	2.94920200	-0.45911600 L
B-B_2	0	-11.59376400	3.09160700	1.66526800 L
N-N_3	0	-11.66013400	3.64463800	0.23183500 L
N-N_3	0	-10.28333000	2.87840800	2.42146600 L
B-B_2	0	-9.02149200	3.01699300	1.58340100 L
B-B_2	0	-7.71179300	1.46369300	2.97573300 L
N-N_3	0	-7.72297500	2.87610700	2.37605600 L
N-N_3	0	-6.40601000	0.88087000	3.52642200 L
B-B_2	0	-5.13095500	1.47207900	2.91860100 L
B-B_2	0	-3.83203300	-0.62983900	3.19724300 L
N-N_3	0	-3.83413200	0.89172600	3.48496600 L
N-N_3	0	-2.54557000	-1.44574100	3.37971000 L
B-B_2	0	-1.26233300	-0.63015600	3.16550600 L
B-B_2	0	0.02207300	-2.64446300	2.31743800 L
N-N_3	0	0.02591800	-1.44685900	3.30602100 L
N-N_3	0	1.32072300	-3.41457300	2.01982600 L
B-B_2	0	2.61128900	-2.63411600	2.33065700 L
B-B_2	0	3.91807800	-3.65806000	0.48588500 L
N-N_3	0	3.92292700	-3.35083000	1.99154400 L
N-N_3	0	5.22060300	-3.93251800	-0.27193100 L
B-B_2	0	6.50558600	-3.51955800	0.44915000 L
B-B_2	0	7.75511500	-3.09990000	-1.63253300 L
N-N_3	0	7.80480300	-3.84559400	-0.29569400 L
N-N_3	0	9.00485900	-2.96120000	-2.48879200 L
B-B_2	0	10.32260000	-3.20245100	-1.75657100 L
B-B_2	0	11.57257600	-1.54722200	-2.99275100 L
N-N_3	0	11.57631700	-3.02254600	-2.59133600 L

N-N_3	0	12.83808400	-0.70453400	-2.82362800 L
B-	0	-12.83873900	1.31483700	2.72558100 L
N-N_3	0	-12.86606400	2.82436300	2.44512500 L
N-N_3	0	-11.60404700	0.88661200	3.56942100 L
B-B_2	0	-10.29011700	1.45220700	2.99595600 L
B-B_2	0	-8.98369000	-0.62106200	3.32537500 L
N-N_3	0	-8.99319700	0.88612400	3.59390900 L
N-N_3	0	-7.69028000	-1.42813700	3.43615900 L
B-B_2	0	-6.40897400	-0.62279900	3.23052800 L
B-B_2	0	-5.14189900	-2.56489700	2.34028600 L
N-N_3	0	-5.11984500	-1.43541800	3.38356300 L
N-N_3	0	-3.87840000	-3.37532600	2.03233700 L
B-B_2	0	-2.56311600	-2.70361900	2.45469300 L
B-B_2	0	-1.27963100	-3.89412900	0.54549000 L
N-N_3	0	-1.26448500	-3.43196600	2.04196100 L
N-N_3	0	0.01766400	-4.10140600	-0.25500700 L
B-B_2	0	1.32400800	-3.89947200	0.53947500 L
B-B_2	0	2.60111800	-3.18484600	-1.53738100 L
N-N_3	0	2.63544500	-4.05123700	-0.25701000 L
N-N_3	0	3.87840900	-2.93092400	-2.34182300 L
B-B_2	0	5.18056400	-3.11094700	-1.56440200 L
B-B_2	0	6.44075600	-1.49846200	-2.94864200 L
N-N_3	0	6.44653800	-2.93005000	-2.39845300 L
N-N_3	0	7.71215700	-0.91910300	-3.57904200 L
B-B_2	0	9.01703100	-1.52665300	-3.04784600 L
B-B_2	0	10.29627600	0.56638400	-3.45952300 L
N-N_3	0	10.30927700	-0.95649600	-3.65907000 L
N-N_3	0	11.57614100	1.37294500	-3.57847300 L
B-	0	12.81881400	0.47935100	-3.80264100 L
N-N_3	0	-12.82777000	-1.46497000	3.57164400 L
B-B_2	0	-11.55153100	-0.64911200	3.52800700 L
B-B_2	0	-10.30262500	-2.44569200	2.36089500 L
N-N_3	0	-10.24855900	-1.44279500	3.52216800 L
N-N_3	0	-9.03472100	-3.23077600	2.00345200 L
B-B_2	0	-7.72414900	-2.51090300	2.35079500 L
B-B_2	0	-6.45626500	-3.50544500	0.48744400 L
N-N_3	0	-6.45044000	-3.28296600	2.00243400 L
N-N_3	0	-5.18257600	-3.91240600	-0.25171600 L
B-B_2	0	-3.87690200	-3.66822100	0.51018200 L
B-B_2	0	-2.57359100	-3.27090000	-1.59477600 L
N-N_3	0	-2.59882800	-4.06667200	-0.24686400 L
N-N_3	0	-1.26345400	-2.95469400	-2.32568700 L
B-B_2	0	0.01236800	-3.17789100	-1.50520900 L
B-B_2	0	1.29820500	-1.47916400	-2.82934900 L

N-N_3	0	1.29806400	-2.93640900	-2.30076900 L
N-N_3	0	2.57832400	-0.86978900	-3.39088400 L
B-B_2	0	3.86802400	-1.47751600	-2.84422000 L
B-B_2	0	5.15753600	0.61052600	-3.15812400 L
N-N_3	0	5.13617000	-0.89111700	-3.46579100 L
N-N_3	0	6.44506900	1.40299300	-3.37402000 L
B-B_2	0	7.72877300	0.57938400	-3.26154300 L
B-B_2	0	9.06464500	2.40904600	-2.31161400 L
N-N_3	0	9.00538400	1.38561600	-3.46037100 L
N-N_3	0	10.39949000	3.08048000	-1.93833000 L
B-B_2	0	11.61311800	2.19148300	-2.29107900 L
N-N_3	0	12.76701500	2.01967300	-1.30705600 L
B-	0	-12.86697500	-2.19330300	2.22040400 L
B-B_2	0	-11.60762300	-3.46943800	0.50169600 L
N-N_3	0	-11.63853300	-3.12370200	1.99927100 L
N-N_3	0	-10.31628000	-3.78058800	-0.25429500 L
B-B_2	0	-9.03249800	-3.43415700	0.48643200 L
B-B_2	0	-7.73865400	-3.03314000	-1.56398600 L
N-N_3	0	-7.75426400	-3.82561600	-0.25096200 L
N-N_3	0	-6.43839400	-2.89056700	-2.36008800 L
B-B_2	0	-5.15408800	-3.08983100	-1.54969400 L
B-B_2	0	-3.83994900	-1.48788100	-2.89625000 L
N-N_3	0	-3.86514300	-2.94179600	-2.36073300 L
N-N_3	0	-2.54538200	-0.88390600	-3.45485800 L
B-B_2	0	-1.26986000	-1.49215800	-2.86571500 L
B-B_2	0	0.01786300	0.67571700	-3.14726700 L

TS2@A

B-B_2	0	10.33191800	1.55374000	2.89871400 L
N-N_3	0	11.61791300	0.94088400	3.43448400 L
B-	0	12.88717800	1.71340400	2.98945400 L
B-B_2	0	5.17622300	1.52286700	2.82296200 L
N-N_3	0	6.46173300	0.91932100	3.39752000 L
B-B_2	0	7.75607500	1.51995800	2.83937500 L
B-B_2	0	9.04758100	-0.57930900	3.10136300 L
N-N_3	0	9.03545200	0.92688800	3.42644100 L

N-N_3	0	10.35508700	-1.37673100	3.26615400 L
B-B_2	0	11.59420600	-0.51002200	2.95938100 L
B-	0	12.85971900	-2.64944100	2.55237500 L
N-N_3	0	12.85182800	-1.12727300	2.34580400 L
B-B_2	0	0.01228400	1.59090400	2.88513100 L
N-N_3	0	1.30968300	0.94175900	3.39364800 L
B-B_2	0	2.59355200	1.54469300	2.82319900 L
B-B_2	0	3.88265600	-0.58093000	3.05858500 L
N-N_3	0	3.88219900	0.92108600	3.37649000 L
N-N_3	0	5.17050000	-1.38572500	3.25816400 L
B-B_2	0	6.46464600	-0.58179500	3.08436900 L
B-B_2	0	7.75129800	-2.51500900	2.23970800 L
N-N_3	0	7.75505000	-1.38943000	3.27926000 L
N-N_3	0	9.02972500	-3.29476500	1.94721200 L
B-B_2	0	10.32344700	-2.56622800	2.29571400 L
B-B_2	0	11.61098200	-3.42127600	0.42236300 L
N-N_3	0	11.60072700	-3.31666300	1.94988900 L
N-N_3	0	12.95946300	-3.49573600	-0.30543000 L
B-B_2	0	-5.14206800	1.50099400	2.91928500 L
N-N_3	0	-3.84344100	0.92664000	3.48928000 L
B-B_2	0	-2.56322100	1.57766200	2.93621000 L
B-B_2	0	-1.26533500	-0.58185500	3.16043000 L
N-N_3	0	-1.26258800	0.95134200	3.44367300 L
N-N_3	0	0.02637000	-1.39446700	3.29117500 L
B-B_2	0	1.30737500	-0.57874700	3.10054900 L
B-B_2	0	2.59691800	-2.56876700	2.26774500 L
N-N_3	0	2.59889800	-1.38958700	3.26292900 L
N-N_3	0	3.89255500	-3.32150600	1.96387100 L
B-B_2	0	5.17354100	-2.52527500	2.23339100 L
B-B_2	0	6.46906900	-3.63295100	0.45552700 L
N-N_3	0	6.46579700	-3.28985100	1.94891500 L
N-N_3	0	7.76131100	-4.00087500	-0.27598600 L
B-B_2	0	9.04810500	-3.58173800	0.43683000 L
B-B_2	0	10.30978500	-3.42320800	-1.70540000 L
N-N_3	0	10.35534100	-3.97738100	-0.27343000 L
N-N_3	0	11.58281300	-3.12622000	-2.46714800 L
B-	0	12.84833500	-3.74547000	-1.82587300 L
B-B_2	0	-10.30307100	1.46284600	2.98290600 L
N-N_3	0	-9.00561900	0.90107800	3.58416400 L
B-B_2	0	-7.72410300	1.48445900	2.97126900 L
B-B_2	0	-6.41616600	-0.59838900	3.22475700 L
N-N_3	0	-6.41718000	0.90466200	3.52360500 L
N-N_3	0	-5.12722700	-1.40963700	3.37654000 L
B-B_2	0	-3.83918600	-0.59744800	3.21903900 L

B-B_2	0	-2.56399700	-2.62058300	2.39201300 L
N-N_3	0	-2.54523200	-1.40755000	3.36936000 L
N-N_3	0	-1.27277700	-3.35904400	2.00524400 L
B-B_2	0	0.01541400	-2.58057000	2.29018000 L
B-B_2	0	1.30145500	-3.87242700	0.52166600 L
N-N_3	0	1.30715500	-3.35696300	1.99168400 L
N-N_3	0	2.60461800	-4.07362000	-0.26842300 L
B-B_2	0	3.88801500	-3.69502900	0.47333900 L
B-B_2	0	5.16761800	-3.19432400	-1.56563000 L
N-N_3	0	5.18210200	-4.01438800	-0.27201200 L
N-N_3	0	6.44539700	-2.99956800	-2.37482500 L
B-B_2	0	7.74078600	-3.24624000	-1.60779600 L
B-B_2	0	9.04365200	-1.56740900	-2.82588400 L
N-N_3	0	9.00836300	-3.05333200	-2.42154500 L
N-N_3	0	10.36123600	-0.95329100	-3.32502900 L
B-B_2	0	11.58156000	-1.61138600	-2.64823100 L
B-	0	12.91061000	0.43399300	-2.99068800 L
N-N_3	0	12.68519800	-0.75400500	-2.04166900 L
B-	0	-12.84784500	1.31028900	2.69788200 L
B-B_2	0	-11.55779500	-0.64331600	3.51745500 L
N-N_3	0	-11.61687900	0.89223900	3.55175400 L
N-N_3	0	-10.25180000	-1.43170300	3.51446500 L
B-B_2	0	-8.99099300	-0.60546100	3.31263400 L
B-B_2	0	-7.72491600	-2.49071500	2.33718100 L
N-N_3	0	-7.69541400	-1.40808200	3.42341700 L
N-N_3	0	-6.44617800	-3.25873000	1.99340100 L
B-B_2	0	-5.14306100	-2.52005200	2.31092400 L
B-B_2	0	-3.88321600	-3.69736100	0.50458700 L
N-N_3	0	-3.87569800	-3.32757900	2.01315000 L
N-N_3	0	-2.59397000	-4.05499900	-0.25732300 L
B-B_2	0	-1.28877300	-3.75635700	0.50072200 L
B-B_2	0	0.00578200	-3.22555000	-1.56598800 L
N-N_3	0	-0.00347700	-4.07589600	-0.26742200 L
N-N_3	0	1.29886900	-2.98721700	-2.34934400 L
B-B_2	0	2.59017600	-3.22974400	-1.56448700 L
B-B_2	0	3.88123000	-1.52339100	-2.83503600 L
N-N_3	0	3.87715700	-2.98407100	-2.35359700 L
N-N_3	0	5.17583500	-0.91780200	-3.39297800 L
B-B_2	0	6.46306600	-1.53792500	-2.84097700 L
B-B_2	0	7.76664200	0.56463300	-3.03711900 L
N-N_3	0	7.76406400	-0.92898200	-3.38567800 L
N-N_3	0	9.06081400	1.36821200	-3.20857800 L
B-B_2	0	10.34230200	0.55020500	-3.01522800 L
B-B_2	0	11.62051800	2.42646000	-2.03683800 L

N-N_3	0	11.65102600	1.33535800	-3.10987700 L
N-N_3	0	12.95991400	3.02788600	-1.58756800 L
B-	0	-12.87013800	-2.20442100	2.22676900 L
N-N_3	0	-12.83038000	-1.46399200	3.57138300 L
N-N_3	0	-11.63757100	-3.13045700	2.00913800 L
B-B_2	0	-10.30362100	-2.44255300	2.35982300 L
B-B_2	0	-9.03520900	-3.44945400	0.49193600 L
N-N_3	0	-9.03220700	-3.22470200	2.00571000 L
N-N_3	0	-7.75962400	-3.84637900	-0.24595600 L
B-B_2	0	-6.45844900	-3.52205700	0.48405200 L
B-B_2	0	-5.16196100	-3.12874800	-1.56138900 L
N-N_3	0	-5.18847800	-3.94174600	-0.25536500 L
N-N_3	0	-3.87714200	-2.97952200	-2.38136600 L
B-B_2	0	-2.57954400	-3.32063200	-1.63861600 L
B-B_2	0	-1.27017300	-1.53626100	-2.90840000 L
N-N_3	0	-1.27145700	-3.00172600	-2.38118500 L
N-N_3	0	0.02241500	-0.91613500	-3.46492300 L
B-B_2	0	1.30284300	-1.53052600	-2.88428900 L
B-B_2	0	2.60057500	0.59689700	-3.09412400 L
N-N_3	0	2.60015600	-0.91097100	-3.40838800 L
N-N_3	0	3.89936700	1.39101600	-3.25512800 L
B-B_2	0	5.18318500	0.57710300	-3.05660200 L
B-B_2	0	6.47503800	2.51917000	-2.21467800 L
N-N_3	0	6.47973400	1.37586300	-3.23449600 L
N-N_3	0	7.76410400	3.30336000	-1.94926700 L
B-B_2	0	9.05683100	2.51156700	-2.18007700 L
B-B_2	0	10.30842400	3.91583900	-0.51247000 L
N-N_3	0	10.35609300	3.29445200	-1.91913700 L
N-N_3	0	11.57827000	4.17272200	0.27215400 L
B-	0	12.83072300	4.23545800	-0.63321600 L
N-N_3	0	-12.90289600	-3.68162600	-0.25603000 L
B-B_2	0	-11.61062500	-3.49027000	0.51486400 L
B-B_2	0	-10.32462100	-2.98080100	-1.54529000 L
N-N_3	0	-10.32083700	-3.79994800	-0.24339600 L
N-N_3	0	-9.03742200	-2.89731000	-2.37845800 L
B-B_2	0	-7.74708900	-3.06187300	-1.56359500 L
B-B_2	0	-6.42587500	-1.49742300	-2.92628700 L
N-N_3	0	-6.44969300	-2.92268200	-2.36426800 L
N-N_3	0	-5.12447400	-0.91176400	-3.48068000 L
B-B_2	0	-3.84669200	-1.52125200	-2.89918800 L
B-B_2	0	-2.55046700	0.62244900	-3.23420200 L
N-N_3	0	-2.55372900	-0.91645400	-3.46453600 L
N-N_3	0	-1.26536800	1.45278300	-3.41781200 L
B-B_2	0	0.02677200	0.62786000	-3.25183800 L

B-B_2	0	1.30883300	2.58365000	-2.29250000 L
N-N_3	0	1.33009800	1.42750300	-3.32300300 L
N-N_3	0	2.60704200	3.32439700	-1.96555100 L
B-B_2	0	3.89320000	2.53088000	-2.23092300 L
B-B_2	0	5.17388300	3.68892100	-0.47458900 L
N-N_3	0	5.18379200	3.30373900	-1.95618500 L
N-N_3	0	6.45407200	4.03636100	0.26956400 L
B-B_2	0	7.74459300	3.74496300	-0.48188100 L
B-B_2	0	9.04681400	3.15803500	1.50842800 L
N-N_3	0	9.01479000	4.07887500	0.27709600 L
N-N_3	0	10.35738800	2.96260100	2.28598700 L
B-B_2	0	11.59441100	3.11100700	1.37282400 L
N-N_3	0	12.79323800	2.18068600	1.52658400 L
B-	0	-12.85424500	-2.61744600	-1.36162600 L
B-B_2	0	-11.56820000	-1.55266600	-3.19625700 L
N-N_3	0	-11.64604900	-2.81386000	-2.32001000 L
N-N_3	0	-10.25278900	-0.92376500	-3.64889400 L
B-B_2	0	-9.00073700	-1.50182700	-3.00803700 L
B-B_2	0	-7.71037700	0.58921000	-3.25563200 L
N-N_3	0	-7.69500000	-0.91676500	-3.54706200 L
N-N_3	0	-6.41799000	1.39932900	-3.38990900 L
B-B_2	0	-5.13006600	0.59691500	-3.19145700 L
B-B_2	0	-3.85737200	2.54037900	-2.30534800 L
N-N_3	0	-3.84837800	1.41876800	-3.36193300 L
N-N_3	0	-2.59363400	3.36608100	-2.02375100 L
B-B_2	0	-1.27652900	2.68859700	-2.45002200 L
B-B_2	0	0.00872000	3.88623200	-0.53562300 L
N-N_3	0	0.02774300	3.39714700	-2.02815500 L
N-N_3	0	1.31066900	4.09886100	0.25804100 L
B-B_2	0	2.59491500	3.70378200	-0.47608900 L
B-B_2	0	3.88749300	3.20224400	1.55215800 L
N-N_3	0	3.88611700	4.03418300	0.26513700 L
N-N_3	0	5.18225700	2.97615600	2.33881600 L
B-B_2	0	6.46715000	3.17118900	1.53477800 L
N-N_3	0	7.76426400	2.96311300	2.32487100 L
B-	0	-12.85306800	0.48778700	-3.07018300 L
N-N_3	0	-12.83267200	-0.90312000	-3.72096100 L
N-N_3	0	-11.61102900	1.34772900	-3.44590000 L
B-B_2	0	-10.28864800	0.57056500	-3.29516100 L
B-B_2	0	-9.01417600	2.47796400	-2.36443400 L
N-N_3	0	-9.00311200	1.39577500	-3.44684000 L
N-N_3	0	-7.73620300	3.23141300	-1.99976500 L
B-B_2	0	-6.43858800	2.49012400	-2.31598600 L
B-B_2	0	-5.17639100	3.55709600	-0.48112300 L

N-N_3	0	-5.16382500	3.26973000	-1.98662500 L
N-N_3	0	-3.90411000	3.97702500	0.25607200 L
B-B_2	0	-2.59466200	3.75278700	-0.51343100 L
B-B_2	0	-1.29479900	3.44591500	1.67588100 L
N-N_3	0	-1.30584500	4.11952500	0.24831100 L
N-N_3	0	0.01502000	3.07702000	2.40089300 L
B-B_2	0	1.30147900	3.32120500	1.60323500 L
N-N_3	0	2.60470300	3.01270600	2.35763500 L
N-N_3	0	-12.87994800	3.17680500	-2.00480500 L
B-B_2	0	-11.58731900	2.53990200	-2.47617100 L
B-B_2	0	-10.33488900	3.34798700	-0.49371700 L
N-N_3	0	-10.29805800	3.22152800	-2.02455500 L
N-N_3	0	-9.06691300	3.79123600	0.24583000 L
B-B_2	0	-7.75800100	3.46207000	-0.48428900 L
B-B_2	0	-6.46000800	3.06829200	1.55620200 L
N-N_3	0	-6.48219500	3.86993800	0.25273300 L
N-N_3	0	-5.16802800	2.93066100	2.35925400 L
B-B_2	0	-3.87716800	3.16957800	1.56891200 L
N-N_3	0	-2.59877700	3.04035000	2.39913100 L
B-	0	-12.87912300	2.96800800	-0.48392800 L
B-B_2	0	-11.60837500	3.09475500	1.64433300 L
N-N_3	0	-11.66959000	3.65420600	0.21304400 L
N-N_3	0	-10.30055400	2.88904200	2.40792400 L
B-B_2	0	-9.03526200	3.03292500	1.57570200 L
N-N_3	0	-7.73904900	2.89753200	2.37338400 L
N-N_3	0	-12.88361800	2.81943900	2.41678800 L
H-H_	0	12.81991700	-0.93927300	1.32049100 L
H-H_	0	13.45309600	-2.58442200	-0.19026800 L
H-H_	0	12.33694700	-0.38622700	-1.12737000 L
H-H_	0	13.50323600	2.29633000	-1.07932500 L
H-H_	0	-12.72018800	-2.17746300	4.32718800 L
H-H_	0	-12.86790300	-4.62159100	-0.71175100 L
H-H_	0	12.61166700	1.34767200	0.92504000 L
H-H_	0	-12.72161600	-0.77281900	-4.75202500 L
H-H_	0	-12.81743700	4.20379600	-2.18874800 L
H-H_	0	-12.81722000	3.31869200	3.33262300 L
C-C_R	0	-0.87866200	-0.21767400	-0.08439300 H
H-H_	0	-2.75155800	-0.15753200	0.93795200 H
H-H_	0	-2.88658500	-0.16498900	-0.73375100 H
C-C_3	0	-2.31272700	-0.62270900	0.06603400 H
H-H_	0	-2.61838800	-1.61087800	0.08264700 H
N-N_R	0	-1.17459300	1.24895200	-0.08059000 H
H-H_	0	-0.26737500	1.59270900	0.23537900 H
H-H_	0	-2.06845800	1.37892100	0.34555100 H

C-C_R	0	0.54413900	-0.20212800	0.06432400 H
O-O_R	0	1.14883400	0.88878700	0.11093700 H
O-O_R	0	1.33967000	-1.24361600	0.02322600 H
H-H_	0	2.22740700	-0.85221700	0.02454600 H
H-H_	0	-1.02063100	0.57788900	-1.01460300 H

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B-B_2	0	-10.32169800	1.82512400	-2.84247900 L
N-N_3	0	-11.61167300	1.23260500	-3.39207900 L
B-	0	-12.87631000	1.97959100	-2.89785200 L
B-B_2	0	-5.15324200	1.81915000	-2.85923600 L
N-N_3	0	-6.45257800	1.23728500	-3.42803400 L
B-B_2	0	-7.74054100	1.80274400	-2.82264700 L
B-B_2	0	-9.03083200	-0.28452700	-3.15172300 L
N-N_3	0	-9.02841900	1.23342400	-3.41562800 L
N-N_3	0	-10.33371700	-1.08240000	-3.34322400 L
B-B_2	0	-11.57563700	-0.24004700	-2.98684000 L
B-	0	-12.82823700	-2.40104500	-2.69620900 L
N-N_3	0	-12.81971500	-0.89646200	-2.38469800 L
B-B_2	0	0.02000400	1.81338000	-2.84332100 L
N-N_3	0	-1.26417500	1.25727100	-3.47500200 L
B-B_2	0	-2.56502700	1.87976700	-2.94830700 L
B-B_2	0	-3.86219000	-0.26128800	-3.17408000 L
N-N_3	0	-3.86844000	1.25135900	-3.47062200 L
N-N_3	0	-5.15420700	-1.06618400	-3.35558700 L
B-B_2	0	-6.44792800	-0.27161700	-3.15710500 L
B-B_2	0	-7.72368500	-2.23760400	-2.35832100 L
N-N_3	0	-7.73583000	-1.08036000	-3.36314300 L
N-N_3	0	-8.99189800	-3.05310900	-2.12727000 L
B-B_2	0	-10.29204300	-2.31384700	-2.42702800 L
B-B_2	0	-11.57645300	-3.35218000	-0.64255500 L
N-N_3	0	-11.56148600	-3.10680800	-2.15386700 L
N-N_3	0	-12.92909900	-3.51930300	0.06114500 L
B-B_2	0	5.17341300	1.69979900	-2.81984700 L
N-N_3	0	3.87713900	1.17913500	-3.44250100 L
B-B_2	0	2.59632600	1.77350500	-2.84737200 L
B-B_2	0	1.28702000	-0.32715100	-3.31518000 L
N-N_3	0	1.29978700	1.22296800	-3.44569900 L
N-N_3	0	-0.01132800	-1.12081100	-3.46551400 L
B-B_2	0	-1.28562900	-0.28655900	-3.27969600 L
B-B_2	0	-2.57869000	-2.26870200	-2.41765700 L
N-N_3	0	-2.58962400	-1.07863300	-3.40841100 L
N-N_3	0	-3.87018100	-3.03157600	-2.12349700 L

B-B_2	0	-5.14912400	-2.22394100	-2.34908100 L
B-B_2	0	-6.43451900	-3.46252500	-0.64180300 L
N-N_3	0	-6.43251400	-3.01551000	-2.10791900 L
N-N_3	0	-7.72265200	-3.96407100	0.01364000 L
B-B_2	0	-9.01178800	-3.46513400	-0.64560700 L
B-B_2	0	-10.29032400	-3.60142900	1.49521000 L
N-N_3	0	-10.31731300	-3.96283100	0.00157300 L
N-N_3	0	-11.57191400	-3.33934900	2.25647600 L
B-	0	-12.82883200	-3.90430400	1.55337200 L
B-B_2	0	10.33024000	1.64024400	-2.84667800 L
N-N_3	0	9.03563000	1.15435500	-3.51505600 L
B-B_2	0	7.75351700	1.67790200	-2.85292800 L
B-B_2	0	6.43854900	-0.36108700	-3.30791500 L
N-N_3	0	6.44950600	1.16190100	-3.46985500 L
N-N_3	0	5.14197500	-1.14798200	-3.51792800 L
B-B_2	0	3.86101700	-0.35150600	-3.26511600 L
B-B_2	0	2.57402100	-2.39864200	-2.60561200 L
N-N_3	0	2.57315600	-1.14229400	-3.51958600 L
N-N_3	0	1.26949900	-3.13726800	-2.24847000 L
B-B_2	0	-0.00419400	-2.30799600	-2.46244400 L
B-B_2	0	-1.27996100	-3.61737600	-0.71774700 L
N-N_3	0	-1.29665900	-3.07603100	-2.17530400 L
N-N_3	0	-2.57597300	-4.00496000	0.00867600 L
B-B_2	0	-3.85863100	-3.49091900	-0.65361200 L
B-B_2	0	-5.13974100	-3.41594800	1.45470600 L
N-N_3	0	-5.14693800	-3.95670500	0.01928100 L
N-N_3	0	-6.42981700	-3.25538200	2.25061600 L
B-B_2	0	-7.71743600	-3.45100700	1.45678400 L
B-B_2	0	-9.02717800	-1.82594500	2.74285100 L
N-N_3	0	-8.99927300	-3.28568000	2.25335000 L
N-N_3	0	-10.34567000	-1.23471900	3.26690000 L
B-B_2	0	-11.56268000	-1.83892400	2.53668700 L
B-	0	-12.88495900	0.18665000	3.01504400 L
N-N_3	0	-12.66310000	-0.93733700	1.99019700 L
B-	0	12.85995900	1.41882200	-2.53527500 L
B-B_2	0	11.57627000	-0.40505800	-3.62759200 L
N-N_3	0	11.64645500	1.12194600	-3.45913000 L
N-N_3	0	10.26708500	-1.18452600	-3.67472500 L
B-B_2	0	9.01087700	-0.37286900	-3.40493800 L
B-B_2	0	7.73881200	-2.32152700	-2.58254000 L
N-N_3	0	7.71134400	-1.15726700	-3.58047600 L
N-N_3	0	6.45729400	-3.09927300	-2.27468100 L
B-B_2	0	5.15595800	-2.34272500	-2.55445800 L
B-B_2	0	3.88893100	-3.49449400	-0.77174400 L

N-N_3	0	3.87668600	-3.13876400	-2.27343900 L
N-N_3	0	2.62025700	-3.95946500	-0.04564300 L
B-B_2	0	1.29903800	-3.67254000	-0.78034900 L
B-B_2	0	0.03337000	-3.37170100	1.40357000 L
N-N_3	0	0.01683800	-4.02087900	-0.01112400 L
N-N_3	0	-1.24456700	-3.25163600	2.24664700 L
B-B_2	0	-2.55546000	-3.49991300	1.47976100 L
B-B_2	0	-3.85451000	-1.82749800	2.82477900 L
N-N_3	0	-3.85103400	-3.26326600	2.26358400 L
N-N_3	0	-5.15747100	-1.23348700	3.38272300 L
B-B_2	0	-6.44378500	-1.81994500	2.79090000 L
B-B_2	0	-7.74152700	0.27944900	3.08258400 L
N-N_3	0	-7.74863000	-1.23041200	3.35091000 L
N-N_3	0	-9.03070100	1.08102800	3.29896200 L
B-B_2	0	-10.31662000	0.28514300	3.05388100 L
B-B_2	0	-11.58204700	2.23092800	2.19810900 L
N-N_3	0	-11.62086000	1.07092100	3.19648000 L
N-N_3	0	-12.91703400	2.86911800	1.78906500 L
B-	0	12.89198300	-2.06991300	-2.46972500 L
N-N_3	0	12.84330700	-1.22671700	-3.75347100 L
N-N_3	0	11.64972700	-2.99415500	-2.29980600 L
B-B_2	0	10.31878000	-2.27803600	-2.59961000 L
B-B_2	0	9.04907200	-3.37731500	-0.79148400 L
N-N_3	0	9.04479600	-3.07459200	-2.29154400 L
N-N_3	0	7.77032500	-3.80448700	-0.07433600 L
B-B_2	0	6.47149900	-3.40830600	-0.77567500 L
B-B_2	0	5.19226800	-3.16044200	1.30608800 L
N-N_3	0	5.19673200	-3.85506000	-0.06186000 L
N-N_3	0	3.91340000	-3.09424700	2.14037500 L
B-B_2	0	2.61440200	-3.28646800	1.35498700 L
B-B_2	0	1.31968700	-1.81222000	2.93793300 L
N-N_3	0	1.33614000	-3.18126600	2.19110400 L
N-N_3	0	0.01760100	-1.22806400	3.51746900 L
B-B_2	0	-1.26805600	-1.85321400	2.93664300 L
B-B_2	0	-2.57222300	0.28649500	3.15933200 L
N-N_3	0	-2.57843700	-1.23509000	3.43355100 L
N-N_3	0	-3.87191200	1.07581200	3.34190000 L
B-B_2	0	-5.15726800	0.27466900	3.10708000 L
B-B_2	0	-6.44276400	2.26325400	2.36010400 L
N-N_3	0	-6.45062700	1.07088100	3.32176600 L
N-N_3	0	-7.72305700	3.07434700	2.14616200 L
B-B_2	0	-9.02098100	2.28379400	2.34029200 L
B-B_2	0	-10.26376400	3.79911800	0.77220700 L
N-N_3	0	-10.31203700	3.09578600	2.13848600 L

N-N_3	0	-11.53203000	4.17256300	0.03658000 L
B-	0	-12.78084400	4.15935600	0.95022400 L
N-N_3	0	12.91785600	-3.69180700	-0.07694100 L
B-B_2	0	11.62466400	-3.44161800	-0.82883900 L
B-B_2	0	10.35059700	-3.05031600	1.26595900 L
N-N_3	0	10.33428400	-3.78571000	-0.08480600 L
N-N_3	0	9.06978500	-3.02241000	2.11199100 L
B-B_2	0	7.77318200	-3.11514800	1.29577200 L
B-B_2	0	6.46845700	-1.68501100	2.81728400 L
N-N_3	0	6.48474500	-3.04777500	2.11810900 L
N-N_3	0	5.17383300	-1.16309800	3.44356100 L
B-B_2	0	3.89158600	-1.71171000	2.81786000 L
B-B_2	0	2.58435400	0.35461200	3.29239200 L
N-N_3	0	2.61068000	-1.18496700	3.46973200 L
N-N_3	0	1.29003700	1.15130000	3.52706400 L
B-B_2	0	0.00690100	0.32389900	3.31680900 L
B-B_2	0	-1.28880300	2.34793800	2.48106600 L
N-N_3	0	-1.30377100	1.11329100	3.42615000 L
N-N_3	0	-2.58893700	3.08537600	2.16648600 L
B-B_2	0	-3.86451800	2.26451100	2.37278600 L
B-B_2	0	-5.14141600	3.50580400	0.67621500 L
N-N_3	0	-5.15090800	3.05192600	2.13763400 L
N-N_3	0	-6.41656400	3.97563000	-0.00458100 L
B-B_2	0	-7.70608500	3.57825800	0.69996600 L
B-B_2	0	-9.02007500	3.30263900	-1.33812000 L
N-N_3	0	-8.96976400	4.04724500	0.00631900 L
N-N_3	0	-10.34393800	3.17665500	-2.11101200 L
B-B_2	0	-11.57419200	3.24444300	-1.17657500 L
N-N_3	0	-12.78177400	2.34136200	-1.40619500 L
B-	0	12.88239200	-2.69795900	1.09259400 L
B-B_2	0	11.61165200	-1.73328500	2.98662800 L
N-N_3	0	11.67676400	-2.94396100	2.04281200 L
N-N_3	0	10.30301900	-1.16726200	3.53359500 L
B-B_2	0	9.04209500	-1.68405300	2.85702300 L
B-B_2	0	7.74777400	0.36536900	3.34043600 L
N-N_3	0	7.74391900	-1.16306300	3.47527900 L
N-N_3	0	6.45045600	1.15443400	3.55226800 L
B-B_2	0	5.16639000	0.36310700	3.29177200 L
B-B_2	0	3.87833700	2.34709100	2.54300800 L
N-N_3	0	3.87066800	1.15458300	3.51274200 L
N-N_3	0	2.60608100	3.16530400	2.28806200 L
B-B_2	0	1.29625100	2.45042200	2.65209300 L
B-B_2	0	0.01509200	3.82142200	0.83508700 L
N-N_3	0	-0.01268500	3.19354200	2.28540300 L

N-N_3	0	-1.28840300	4.06173000	0.02881700 L
B-B_2	0	-2.56731700	3.55411900	0.69919800 L
B-B_2	0	-3.85334200	3.33318100	-1.40875500 L
N-N_3	0	-3.85733200	3.96207100	-0.00747100 L
N-N_3	0	-5.15211800	3.20925600	-2.21468000 L
B-B_2	0	-6.43733500	3.31685200	-1.38895400 L
N-N_3	0	-7.74421900	3.19364200	-2.18338800 L
B-	0	12.88320800	0.31635700	3.05355600 L
N-N_3	0	12.88445000	-1.13544900	3.55142000 L
N-N_3	0	11.64942200	1.12078200	3.55515900 L
B-B_2	0	10.32663200	0.35752500	3.34199500 L
B-B_2	0	9.03658400	2.33361600	2.61489000 L
N-N_3	0	9.03966800	1.15638700	3.59262000 L
N-N_3	0	7.75132700	3.08756400	2.28446700 L
B-B_2	0	6.46089400	2.32124100	2.56252600 L
B-B_2	0	5.19405800	3.44349400	0.77471300 L
N-N_3	0	5.17974300	3.10212400	2.26788900 L
N-N_3	0	3.91946800	3.89580100	0.06443700 L
B-B_2	0	2.60981300	3.57241700	0.79206300 L
B-B_2	0	1.32526500	3.38200000	-1.35696700 L
N-N_3	0	1.33728100	4.03806900	0.06484000 L
N-N_3	0	0.03989800	3.22542700	-2.18130100 L
B-B_2	0	-1.26704300	3.46734900	-1.41927200 L
N-N_3	0	-2.56599900	3.25939900	-2.23340900 L
N-N_3	0	12.89039700	3.11846400	2.32145400 L
B-B_2	0	11.60856800	2.43223700	2.75128200 L
B-B_2	0	10.35266800	3.29961700	0.79446600 L
N-N_3	0	10.31123400	3.10666700	2.31694200 L
N-N_3	0	9.08161100	3.76298300	0.07178700 L
B-B_2	0	7.77411600	3.38201400	0.77977100 L
B-B_2	0	6.48388800	3.11879600	-1.29289500 L
N-N_3	0	6.49669700	3.82384200	0.06605700 L
N-N_3	0	5.19470700	3.05942700	-2.11199400 L
B-B_2	0	3.90332100	3.18768400	-1.29875100 L
N-N_3	0	2.62777900	3.14885300	-2.13886000 L
B-	0	12.91096400	2.98171100	0.79090400 L
B-B_2	0	11.63344700	3.11307300	-1.33084900 L
N-N_3	0	11.68443900	3.65354700	0.10671200 L
N-N_3	0	10.33379000	3.00263300	-2.13088600 L
B-B_2	0	9.05999200	3.07998700	-1.29885600 L
N-N_3	0	7.76884100	3.02391100	-2.11649900 L
N-N_3	0	12.91742800	2.89072700	-2.10671500 L
H-H_	0	-12.75933700	-0.78628200	-1.34916500 L
H-H_	0	-13.43990900	-2.61065300	0.02127000 L

H-H_	0	-12.31267600	-0.50977900	1.10320700 L
H-H_	0	-13.45568400	2.18403500	1.21548300 L
H-H_	0	12.72238400	-1.88037600	-4.56001200 L
H-H_	0	12.87604400	-4.65792300	0.31968600 L
H-H_	0	-12.61309900	1.46606300	-0.86467600 L
H-H_	0	12.79648800	-1.11886200	4.59277400 L
H-H_	0	12.80185000	4.13450100	2.55002100 L
H-H_	0	12.87793300	3.48105200	-2.96834900 L
C-C_3	0	0.24442500	-0.25504500	0.14939900 H
H-H_	0	2.10652600	0.16987600	-0.93581800 H
H-H_	0	2.20590600	-0.16847100	0.71850000 H
C-C_3	0	1.72812900	-0.50436100	-0.19538500 H
H-H_	0	2.17128000	-1.44157300	-0.34316600 H
N-N_3	0	0.38176400	1.10488100	0.44098000 H
H-H_	0	-0.33520000	1.55369600	-0.08288200 H
H-H_	0	1.30557700	1.38428400	0.20024800 H
C-C_R	0	-1.26785100	-0.20281300	-0.24571400 H
O-O_R	0	-1.83559200	0.81439200	-0.55933800 H
O-O_R	0	-2.03358400	-1.15553700	0.23038200 H
H-H_	0	-2.93967800	-0.81502300	0.15172700 H
H-H_	0	0.07918300	-0.85113000	1.00417700 H

Coordinates of all stationary points in the pathway a of α -Ala chiral transformation confined in SWBNNT(6,6)

S α -Ala@B

B-B_2	0	-10.30299100	2.14019300	-3.55760400 L
N-N_3	0	-11.57441400	1.60368300	-4.20192300 L
B-	0	-12.85892400	2.30371000	-3.68986900 L
B-B_2	0	-5.16315800	2.10801600	-3.39053700 L
N-N_3	0	-6.43469300	1.57828400	-4.05476300 L
B-B_2	0	-7.73551000	2.10483300	-3.44718000 L
B-B_2	0	-9.01163600	0.05221100	-4.02761800 L
N-N_3	0	-8.99666700	1.59015100	-4.13544300 L
N-N_3	0	-10.30736100	-0.70748500	-4.35934000 L
B-B_2	0	-11.55096600	0.09973300	-3.94014900 L
B-	0	-12.85166700	-2.03829900	-3.84240800 L
N-N_3	0	-12.76441300	-0.59390900	-3.32184900 L
B-B_2	0	-0.02134900	2.13799000	-3.34551100 L
N-N_3	0	-1.30264100	1.58679000	-3.97095200 L
B-B_2	0	-2.59116300	2.12203200	-3.35179300 L
B-B_2	0	-3.86703200	0.05067200	-3.88518800 L
N-N_3	0	-3.86624400	1.57899100	-4.00092300 L
N-N_3	0	-5.14275800	-0.71272300	-4.24135600 L
B-B_2	0	-6.43810200	0.04848500	-3.95142100 L
B-B_2	0	-7.72728400	-2.01929100	-3.49889500 L
N-N_3	0	-7.71578600	-0.71735600	-4.30842200 L
N-N_3	0	-9.00496600	-2.85236900	-3.44416400 L
B-B_2	0	-10.29502200	-2.04710100	-3.61091900 L
B-B_2	0	-11.57738100	-3.40766100	-2.07439900 L
N-N_3	0	-11.58085000	-2.85509600	-3.49703700 L
N-N_3	0	-12.77977700	-3.18308100	-1.15769300 L
B-B_2	0	5.12332800	2.11769600	-3.39290200 L
N-N_3	0	3.82742500	1.58470500	-4.00283000 L
B-B_2	0	2.54971000	2.13171900	-3.36129600 L
B-B_2	0	1.26187600	0.05948400	-3.83581100 L
N-N_3	0	1.26028100	1.58817600	-3.97163200 L
N-N_3	0	-0.01731600	-0.70633400	-4.16449300 L
B-B_2	0	-1.30168900	0.05643100	-3.84911700 L
B-B_2	0	-2.58534900	-2.03369600	-3.41834000 L
N-N_3	0	-2.57794400	-0.70973800	-4.19387900 L
N-N_3	0	-3.87255300	-2.85492200	-3.36751400 L
B-B_2	0	-5.15487100	-2.02215200	-3.44666300 L
B-B_2	0	-6.46065900	-3.60060500	-2.06085300 L
N-N_3	0	-6.44256500	-2.84312800	-3.39239700 L
N-N_3	0	-7.75981000	-4.25321100	-1.57751800 L

B-B_2	0	-9.03751400	-3.57556700	-2.08383800 L
B-B_2	0	-10.33117100	-4.22743500	-0.05573900 L
N-N_3	0	-10.35171600	-4.20656700	-1.59083700 L
N-N_3	0	-11.62041400	-4.47720700	0.71669200 L
B-	0	-12.89023600	-4.34818500	-0.16101300 L
B-B_2	0	10.27136100	2.09917000	-3.44432400 L
N-N_3	0	8.98013700	1.57989800	-4.09108300 L
B-B_2	0	7.69884300	2.10751900	-3.43237200 L
B-B_2	0	6.39816000	0.05425700	-3.92326400 L
N-N_3	0	6.39969200	1.58100700	-4.04664000 L
N-N_3	0	5.10503400	-0.70734800	-4.21842500 L
B-B_2	0	3.82872800	0.05813400	-3.86855200 L
B-B_2	0	2.54693200	-2.02289600	-3.38986700 L
N-N_3	0	2.54054800	-0.70480300	-4.17247600 L
N-N_3	0	1.26586700	-2.85737800	-3.33583600 L
B-B_2	0	-0.01895900	-2.03224300	-3.39088400 L
B-B_2	0	-1.30646900	-3.68696500	-2.05424100 L
N-N_3	0	-1.30092600	-2.86494400	-3.35228700 L
N-N_3	0	-2.60585400	-4.33702800	-1.57395900 L
B-B_2	0	-3.88301000	-3.63457600	-2.04873600 L
B-B_2	0	-5.18342500	-4.23637300	-0.04322600 L
N-N_3	0	-5.18222000	-4.28670300	-1.57218900 L
N-N_3	0	-6.47799100	-4.51369700	0.72221400 L
B-B_2	0	-7.75931400	-4.19262500	-0.04688800 L
B-B_2	0	-9.04525600	-3.62403200	1.99340100 L
N-N_3	0	-9.04203900	-4.49573600	0.72265300 L
N-N_3	0	-10.34520100	-3.47497900	2.80211500 L
B-B_2	0	-11.58276700	-3.49322400	1.88450700 L
B-	0	-12.86019200	-2.30258300	3.68471300 L
N-N_3	0	-12.78695900	-2.59673400	2.17667800 L
B-	0	12.79677700	1.91579000	-3.13528700 L
B-B_2	0	11.53223000	0.04033200	-4.10894900 L
N-N_3	0	11.58716100	1.57020100	-4.04508800 L
N-N_3	0	10.23169300	-0.72177500	-4.35796800 L
B-B_2	0	8.96932000	0.04995000	-3.99190400 L
B-B_2	0	7.68939300	-2.02173100	-3.47762300 L
N-N_3	0	7.67317700	-0.71153400	-4.27561200 L
N-N_3	0	6.40182800	-2.84469900	-3.37961600 L
B-B_2	0	5.11609500	-2.01864700	-3.42629900 L
B-B_2	0	3.84129200	-3.64162900	-2.03833600 L
N-N_3	0	3.83168800	-2.84763900	-3.34828200 L
N-N_3	0	2.56244800	-4.34711900	-1.57274300 L
B-B_2	0	1.26649600	-3.67828500	-2.03878500 L
B-B_2	0	-0.02041200	-4.41577000	-0.04289000 L

N-N_3	0	-0.01924000	-4.37707100	-1.58224300 L
N-N_3	0	-1.32435100	-4.64590500	0.73530400 L
B-B_2	0	-2.60422900	-4.31323700	-0.04036100 L
B-B_2	0	-3.89062900	-3.68467000	1.97753800 L
N-N_3	0	-3.90439100	-4.56847400	0.72711300 L
N-N_3	0	-5.17611400	-3.51039700	2.79108800 L
B-B_2	0	-6.46847500	-3.64708800	1.98525400 L
B-B_2	0	-7.73620800	-2.10423700	3.45352200 L
N-N_3	0	-7.75310900	-3.49386100	2.80657500 L
N-N_3	0	-8.99886600	-1.58944400	4.13908500 L
B-B_2	0	-10.30395100	-2.13991400	3.55919100 L
B-B_2	0	-11.55307000	-0.09911500	3.93977100 L
N-N_3	0	-11.57688700	-1.60331000	4.20084500 L
N-N_3	0	-12.76920800	0.59591400	3.32811700 L
B-	0	12.79469600	-1.82679200	-3.24523700 L
N-N_3	0	12.81380700	-0.74088200	-4.32597300 L
N-N_3	0	11.58562100	-2.78734000	-3.40374000 L
B-B_2	0	10.26085700	-2.00832000	-3.51431500 L
B-B_2	0	8.98772600	-3.59068000	-2.07660900 L
N-N_3	0	8.98055800	-2.84724000	-3.41609400 L
N-N_3	0	7.70952400	-4.26225100	-1.57593000 L
B-B_2	0	6.41503500	-3.60529500	-2.05144800 L
B-B_2	0	5.14212000	-4.26816100	-0.04039900 L
N-N_3	0	5.13915900	-4.30029000	-1.57034800 L
N-N_3	0	3.86316200	-4.59491600	0.73232100 L
B-B_2	0	2.56260000	-4.35403400	-0.03883600 L
B-B_2	0	1.26791300	-3.73076400	1.96802200 L
N-N_3	0	1.27671100	-4.65478400	0.73908100 L
N-N_3	0	-0.01870000	-3.55145700	2.77804200 L
B-B_2	0	-1.31267100	-3.74714100	1.98452200 L
B-B_2	0	-2.59073400	-2.12058700	3.37201900 L
N-N_3	0	-2.60161800	-3.53890000	2.78677500 L
N-N_3	0	-3.86799000	-1.57815100	4.01744000 L
B-B_2	0	-5.16333400	-2.10728800	3.40343300 L
B-B_2	0	-6.44088300	-0.04807100	3.95588700 L
N-N_3	0	-6.43695600	-1.57737000	4.06360100 L
N-N_3	0	-7.71861200	0.71860500	4.31027200 L
B-B_2	0	-9.01408900	-0.05158900	4.02984000 L
B-B_2	0	-10.29735300	2.04781600	3.61270600 L
N-N_3	0	-10.30998000	0.70796700	4.36067800 L
N-N_3	0	-11.58284400	2.85619600	3.50013000 L
B-	0	-12.85373500	2.04071100	3.84826300 L
N-N_3	0	12.84719600	-4.18769800	-1.55896700 L
B-B_2	0	11.55358000	-3.64195700	-2.13224100 L

B-B_2	0	10.29223000	-4.15269700	-0.06061600 L
N-N_3	0	10.26724000	-4.26251600	-1.59445100 L
N-N_3	0	9.01833100	-4.49267500	0.72181900 L
B-B_2	0	7.71943700	-4.21315800	-0.04412900 L
B-B_2	0	6.42444100	-3.65092800	1.97499400 L
N-N_3	0	6.43877400	-4.53627200	0.72676000 L
N-N_3	0	5.13321400	-3.51061900	2.78181600 L
B-B_2	0	3.84851100	-3.68807900	1.96686400 L
B-B_2	0	2.54969000	-2.11562900	3.36276600 L
N-N_3	0	2.55767800	-3.53072700	2.77133100 L
N-N_3	0	1.26243300	-1.58356000	3.98972500 L
B-B_2	0	-0.02030000	-2.12830300	3.36006400 L
B-B_2	0	-1.30331100	-0.05332500	3.87581000 L
N-N_3	0	-1.30217700	-1.58445300	3.99221900 L
N-N_3	0	-2.58306200	0.71333100	4.20090800 L
B-B_2	0	-3.86979800	-0.05074800	3.89491800 L
B-B_2	0	-5.15794100	2.01927600	3.44179300 L
N-N_3	0	-5.14636400	0.71429000	4.24373100 L
N-N_3	0	-6.44425000	2.84272700	3.39109900 L
B-B_2	0	-7.72972300	2.01954200	3.49883100 L
B-B_2	0	-9.04038900	3.57730100	2.08574400 L
N-N_3	0	-9.00714600	2.85303400	3.44544800 L
N-N_3	0	-10.35530700	4.20723400	1.59288300 L
B-B_2	0	-11.58045000	3.40802300	2.07734000 L
B-	0	-12.89430400	4.34024400	0.16226700 L
N-N_3	0	-12.77941700	3.17518500	1.15836600 L
B-	0	12.82280000	-3.77082300	-0.08390700 L
B-B_2	0	11.56518000	-3.66808300	2.03462600 L
N-N_3	0	11.62126700	-4.38881200	0.68216300 L
N-N_3	0	10.26654300	-3.49840800	2.82225900 L
B-B_2	0	8.99831100	-3.63088100	1.98836700 L
B-B_2	0	7.69842600	-2.09989700	3.43591800 L
N-N_3	0	7.70602800	-3.49277000	2.79371700 L
N-N_3	0	6.39932500	-1.57463300	4.05124300 L
B-B_2	0	5.12289400	-2.10681800	3.39408100 L
B-B_2	0	3.82856000	-0.04998700	3.89023200 L
N-N_3	0	3.82778100	-1.57745800	4.00916700 L
N-N_3	0	2.54199600	0.71341700	4.20147200 L
B-B_2	0	1.26194700	-0.05269500	3.87728100 L
B-B_2	0	-0.02276100	2.03103000	3.40369000 L
N-N_3	0	-0.02137800	0.71380500	4.19488900 L
N-N_3	0	-1.30655300	2.85978900	3.34629300 L
B-B_2	0	-2.58815300	2.02495600	3.40542000 L
B-B_2	0	-3.88514900	3.63713300	2.04541100 L

N-N_3	0	-3.87389700	2.84911400	3.35878100 L
N-N_3	0	-5.18496500	4.29305400	1.57526500 L
B-B_2	0	-6.46316900	3.60409700	2.06171700 L
B-B_2	0	-7.76303200	4.19847200	0.04969100 L
N-N_3	0	-7.76325300	4.25673400	1.58030200 L
N-N_3	0	-9.04627900	4.49831700	-0.72031500 L
B-B_2	0	-10.33493200	4.22765900	0.05775000 L
B-B_2	0	-11.58460800	3.49097400	-1.88357000 L
N-N_3	0	-11.62475000	4.47427300	-0.71509400 L
N-N_3	0	-12.79041700	2.59845200	-2.18163700 L
B-	0	12.79786800	-1.91308000	3.14497600 L
N-N_3	0	12.84879400	-3.40593400	2.79918800 L
N-N_3	0	11.58670900	-1.56428900	4.05162500 L
B-B_2	0	10.27113200	-2.09335100	3.45024900 L
B-B_2	0	8.96934600	-0.04362700	3.99845600 L
N-N_3	0	8.97967000	-1.57364100	4.09610000 L
N-N_3	0	7.67400900	0.71757700	4.28531700 L
B-B_2	0	6.39822400	-0.04747100	3.93484800 L
B-B_2	0	5.11529800	2.02252300	3.43951100 L
N-N_3	0	5.10653200	0.71390000	4.23549300 L
N-N_3	0	3.82882400	2.84815400	3.35456400 L
B-B_2	0	2.54500600	2.02197100	3.40272000 L
B-B_2	0	1.26240800	3.66084400	2.03056200 L
N-N_3	0	1.26231200	2.85453100	3.33705300 L
N-N_3	0	-0.02049000	4.37623600	1.58577500 L
B-B_2	0	-1.30885000	3.68230100	2.04802700 L
B-B_2	0	-2.60728100	4.33906800	0.04245500 L
N-N_3	0	-2.60694400	4.34277500	1.57627500 L
N-N_3	0	-3.90965100	4.58547200	-0.72431900 L
B-B_2	0	-5.18718800	4.25033300	0.04637300 L
B-B_2	0	-6.47093900	3.65209100	-1.97984800 L
N-N_3	0	-6.48273100	4.52224700	-0.71924000 L
N-N_3	0	-7.75437900	3.49548500	-2.80220000 L
B-B_2	0	-9.04740000	3.62555700	-1.99039200 L
N-N_3	0	-10.34633400	3.47501000	-2.80023700 L
N-N_3	0	12.81437700	0.74699500	4.32564100 L
B-B_2	0	11.53228300	-0.03426600	4.11119400 L
B-B_2	0	10.26003500	2.01519100	3.52040300 L
N-N_3	0	10.23231300	0.72787000	4.36309100 L
N-N_3	0	8.97932300	2.85366400	3.42341000 L
B-B_2	0	7.68864600	2.02771300	3.48723200 L
B-B_2	0	6.41238900	3.60360100	2.05630900 L
N-N_3	0	6.40033400	2.84953800	3.38810000 L
N-N_3	0	5.13452900	4.29286800	1.57216900 L

B-B_2	0	3.83827400	3.62849200	2.03732800 L
B-B_2	0	2.55958500	4.33390900	0.03614100 L
N-N_3	0	2.55841900	4.32909500	1.56788600 L
N-N_3	0	1.28110600	4.67190100	-0.73785000 L
B-B_2	0	-0.02405100	4.46346500	0.04608500 L
B-B_2	0	-1.31430900	3.76006800	-1.97393000 L
N-N_3	0	-1.32906500	4.67371800	-0.73497200 L
N-N_3	0	-2.60334500	3.54342900	-2.77455900 L
B-B_2	0	-3.89349100	3.69378100	-1.96889100 L
N-N_3	0	-5.17762600	3.51360700	-2.78350600 L
B-	0	12.79267200	1.83404100	3.24610900 L
B-B_2	0	11.55092700	3.65298200	2.14024000 L
N-N_3	0	11.58440000	2.79467300	3.40928100 L
N-N_3	0	10.26338700	4.26994800	1.60121100 L
B-B_2	0	8.98510400	3.59567600	2.08308900 L
B-B_2	0	7.71659400	4.21470700	0.04902700 L
N-N_3	0	7.70547400	4.26376500	1.58091100 L
N-N_3	0	6.43601200	4.53835500	-0.72188900 L
B-B_2	0	5.13970600	4.26148900	0.04266300 L
B-B_2	0	3.84808800	3.70204300	-1.97381300 L
N-N_3	0	3.86084000	4.59147600	-0.72812000 L
N-N_3	0	2.55796600	3.55105100	-2.78014700 L
B-B_2	0	1.26866600	3.75766900	-1.97503600 L
N-N_3	0	-0.02261300	3.56621600	-2.77358000 L
B-	0	12.82175300	3.78337300	0.09331100 L
N-N_3	0	12.84352900	4.20191100	1.56795800 L
N-N_3	0	11.61878700	4.39631600	-0.67473600 L
B-B_2	0	10.28960200	4.15900100	0.06755000 L
B-B_2	0	8.99762800	3.63681300	-1.98313400 L
N-N_3	0	9.01570900	4.49724400	-0.71567400 L
N-N_3	0	7.70689000	3.50070600	-2.79083700 L
B-B_2	0	6.42387600	3.65986800	-1.97487600 L
N-N_3	0	5.13463900	3.52318900	-2.78508300 L
N-N_3	0	12.84913900	3.40813800	-2.78755400 L
B-B_2	0	11.56444700	3.67159800	-2.02507900 L
N-N_3	0	10.26706700	3.50381000	-2.81515600 L
H-H_	0	-12.61357700	-0.62340000	-2.28974200 L
H-H_	0	-12.60190100	-2.30654800	-0.62020100 L
H-H_	0	-12.63282000	-1.69434100	1.67553700 L
H-H_	0	-12.62437100	0.62464000	2.29517200 L
H-H_	0	12.75247200	-1.20725400	-5.25939200 L
H-H_	0	12.80424300	-5.23109700	-1.60361800 L
H-H_	0	-12.59412900	2.30024700	0.62068700 L
H-H_	0	-12.64206100	1.69581600	-1.67926800 L

H-H_	0	12.80793300	-3.94883300	3.69142700 L
H-H_	0	12.75549600	1.21230400	5.25974900 L
H-H_	0	12.79735800	5.24522600	1.61133200 L
H-H_	0	12.81098300	3.95227900	-3.67915600 L
C-C_3	0	-0.08990500	0.06760100	0.29842700 H
H-H_	0	-1.39318700	-0.84285500	-1.11695900 H
H-H_	0	-2.00529500	-0.85616500	0.53747800 H
C-C_3	0	-1.10932600	-0.97398400	-0.07715100 H
H-H_	0	-0.70283500	-1.95305000	0.08216900 H
N-N_3	0	-0.50862200	1.32507700	-0.23578500 H
H-H_	0	0.26667600	1.95724600	-0.14162000 H
H-H_	0	-1.34913100	1.66132500	0.21016700 H
C-C_R	0	1.35058600	-0.12820800	-0.12563200 H
O-O_R	0	2.08859700	0.78066100	-0.43202800 H
O-O_R	0	1.79141400	-1.38335600	-0.00614400 H
H-H_	0	2.74213900	-1.36513400	-0.20254700 H
H-H_	0	0.00715300	0.05908000	1.39116800 H

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B-B_2	0	-10.30208500	2.48357400	-3.33427200 L
N-N_3	0	-11.57479400	2.00844700	-4.02302900 L
B-	0	-12.85867400	2.65258800	-3.44092500 L
B-B_2	0	-5.16155800	2.44731200	-3.18607300 L
N-N_3	0	-6.43422800	1.97935800	-3.89324100 L
B-B_2	0	-7.73414600	2.44320200	-3.23508200 L
B-B_2	0	-9.00867900	0.45259300	-4.00375400 L
N-N_3	0	-8.99650600	1.99386800	-3.96561700 L
N-N_3	0	-10.30348300	-0.27419700	-4.40503000 L
B-B_2	0	-11.54760200	0.48620100	-3.90730000 L
B-	0	-12.84461500	-1.65371700	-4.02213500 L
N-N_3	0	-12.76077900	-0.26705000	-3.36235500 L
B-B_2	0	-0.01693800	2.48654500	-3.15821500 L
N-N_3	0	-1.30113500	1.99053300	-3.82362400 L
B-B_2	0	-2.58887900	2.46531200	-3.15505300 L
B-B_2	0	-3.86386100	0.44780300	-3.86848900 L
N-N_3	0	-3.86552100	1.98035500	-3.84646800 L
N-N_3	0	-5.13883600	-0.28267300	-4.29081800 L
B-B_2	0	-6.43504400	0.44658700	-3.93154600 L
B-B_2	0	-7.72100000	-1.65706200	-3.67258800 L
N-N_3	0	-7.71190000	-0.28502600	-4.35677300 L
N-N_3	0	-8.99650600	-2.49466700	-3.70025300 L
B-B_2	0	-10.28834700	-1.67990400	-3.78964600 L
B-B_2	0	-11.56917800	-3.18842200	-2.39640300 L
N-N_3	0	-11.57232600	-2.49810300	-3.75752500 L
N-N_3	0	-12.77488700	-3.06108400	-1.46553600 L
B-B_2	0	5.13106700	2.46400500	-3.20522400 L
N-N_3	0	3.83538700	1.99378800	-3.86627500 L
B-B_2	0	2.55626300	2.48309200	-3.18104300 L
B-B_2	0	1.26631200	0.46178600	-3.83411700 L
N-N_3	0	1.26424700	1.99705400	-3.83552100 L
N-N_3	0	-0.01455900	-0.27522700	-4.21903300 L
B-B_2	0	-1.29844300	0.45531600	-3.83498900 L
B-B_2	0	-2.57984100	-1.66858400	-3.59372900 L
N-N_3	0	-2.57427900	-0.27935500	-4.24567300 L
N-N_3	0	-3.86530000	-2.49369300	-3.61694500 L
B-B_2	0	-5.14872600	-1.65929700	-3.61892000 L
B-B_2	0	-6.45216700	-3.36667300	-2.39047600 L
N-N_3	0	-6.43453100	-2.48445100	-3.64304200 L

N-N_3	0	-7.74989700	-4.06887700	-1.97825900 L
B-B_2	0	-9.02891600	-3.34769300	-2.41725400 L
B-B_2	0	-10.32398700	-4.20210500	-0.46704700 L
N-N_3	0	-10.34209800	-4.02834000	-1.99230200 L
N-N_3	0	-11.61381300	-4.52990300	0.27430000 L
B-	0	-12.88286000	-4.31887700	-0.58840800 L
B-B_2	0	10.28013200	2.43863400	-3.23970200 L
N-N_3	0	8.99017100	1.98634400	-3.93709800 L
B-B_2	0	7.70727000	2.45105600	-3.23561100 L
B-B_2	0	6.40514400	0.45700200	-3.91647800 L
N-N_3	0	6.40925900	1.98847300	-3.90158100 L
N-N_3	0	5.11111000	-0.27394200	-4.27738700 L
B-B_2	0	3.83454100	0.46115500	-3.86614100 L
B-B_2	0	2.55164900	-1.64985100	-3.55941400 L
N-N_3	0	2.54536000	-0.27238900	-4.23246300 L
N-N_3	0	1.27090800	-2.48556700	-3.57691800 L
B-B_2	0	-0.01454400	-1.66094000	-3.55879300 L
B-B_2	0	-1.29940000	-3.43706600	-2.38325600 L
N-N_3	0	-1.29347600	-2.49838500	-3.59973300 L
N-N_3	0	-2.59670800	-4.13733700	-1.97255600 L
B-B_2	0	-3.87481800	-3.39353900	-2.37641000 L
B-B_2	0	-5.17588200	-4.20416300	-0.44425300 L
N-N_3	0	-5.17230800	-4.09476500	-1.97038700 L
N-N_3	0	-6.47165900	-4.56215600	0.28486500 L
B-B_2	0	-7.75210800	-4.16439100	-0.44941900 L
B-B_2	0	-9.04217700	-3.80748400	1.63508600 L
N-N_3	0	-9.03583900	-4.54596000	0.28266600 L
N-N_3	0	-10.34429800	-3.73759700	2.45124100 L
B-B_2	0	-11.57982200	-3.66599800	1.53346200 L
B-	0	-12.86076200	-2.64915200	3.43326000 L
N-N_3	0	-12.78093700	-2.79492000	1.90420500 L
B-	0	12.80624600	2.22464800	-2.94600100 L
B-B_2	0	11.54027800	0.45143700	-4.09456000 L
N-N_3	0	11.59695000	1.96846800	-3.88561000 L
N-N_3	0	10.23884500	-0.28315100	-4.41286900 L
B-B_2	0	8.97688100	0.45397400	-3.98032000 L
B-B_2	0	7.69396400	-1.65186900	-3.65163000 L
N-N_3	0	7.67998100	-0.27702100	-4.33232300 L
N-N_3	0	6.40469400	-2.47731100	-3.62620400 L
B-B_2	0	5.12073700	-1.64723000	-3.59826700 L
B-B_2	0	3.84503600	-3.38575600	-2.35796200 L
N-N_3	0	3.83513300	-2.47707700	-3.59108300 L
N-N_3	0	2.56656300	-4.13294300	-1.96438200 L
B-B_2	0	1.27220700	-3.41868600	-2.35884800 L

B-B_2	0	-0.01391600	-4.35062100	-0.44857900 L
N-N_3	0	-0.01101100	-4.16325700	-1.97606200 L
N-N_3	0	-1.31570300	-4.68759000	0.29269500 L
B-B_2	0	-2.59709500	-4.27698800	-0.44411600 L
B-B_2	0	-3.88681400	-3.87451100	1.62891800 L
N-N_3	0	-3.89768700	-4.61633500	0.28899800 L
N-N_3	0	-5.17523500	-3.78181300	2.45110200 L
B-B_2	0	-6.46522000	-3.83281900	1.63171700 L
B-B_2	0	-7.73533800	-2.44292600	3.24199300 L
N-N_3	0	-7.75225100	-3.76147200	2.46055900 L
N-N_3	0	-8.99964100	-1.99330200	3.96927800 L
B-B_2	0	-10.30372600	-2.48270800	3.33506900 L
B-B_2	0	-11.55030300	-0.48442100	3.90587800 L
N-N_3	0	-11.57828200	-2.00689800	4.02049500 L
N-N_3	0	-12.76668700	0.27017600	3.36962300 L
B-	0	12.79894200	-1.48882100	-3.40346300 L
N-N_3	0	12.82120200	-0.30849600	-4.38032800 L
N-N_3	0	11.58872700	-2.42894600	-3.65097900 L
B-B_2	0	10.26545700	-1.64068200	-3.68873400 L
B-B_2	0	8.99008900	-3.34814800	-2.40219900 L
N-N_3	0	8.98334600	-2.48251100	-3.66643700 L
N-N_3	0	7.71055800	-4.06333000	-1.96916000 L
B-B_2	0	6.41773500	-3.35720400	-2.37359900 L
B-B_2	0	5.14530500	-4.22369500	-0.43737700 L
N-N_3	0	5.14071900	-4.09347500	-1.96221900 L
N-N_3	0	3.86668500	-4.63418700	0.29591000 L
B-B_2	0	2.56689900	-4.30005300	-0.43999200 L
B-B_2	0	1.27314700	-3.92830300	1.63178300 L
N-N_3	0	1.28121200	-4.69136600	0.29744100 L
N-N_3	0	-0.01488500	-3.83496200	2.45462500 L
B-B_2	0	-1.30814300	-3.94758500	1.64264200 L
B-B_2	0	-2.58848100	-2.46475300	3.17934300 L
N-N_3	0	-2.60090100	-3.81767500	2.45473300 L
N-N_3	0	-3.86777700	-1.98234000	3.86757500 L
B-B_2	0	-5.16193700	-2.44738000	3.20120700 L
B-B_2	0	-6.43856600	-0.44736100	3.93828800 L
N-N_3	0	-6.43732700	-1.97988200	3.90392800 L
N-N_3	0	-7.71558600	0.28604000	4.35913400 L
B-B_2	0	-9.01184400	-0.45201200	4.00607700 L
B-B_2	0	-10.29061100	1.68103100	3.79077600 L
N-N_3	0	-10.30669600	0.27518200	4.40585400 L
N-N_3	0	-11.57376800	2.50012000	3.76033600 L
B-	0	-12.84648000	1.65756100	4.02872400 L
N-N_3	0	12.84858800	-4.00093900	-1.95058900 L

B-B_2	0	11.55544800	-3.39783200	-2.46446200 L
B-B_2	0	10.29488600	-4.11787600	-0.45456900 L
N-N_3	0	10.26845600	-4.06842300	-1.99162000 L
N-N_3	0	9.02147100	-4.53714300	0.28916200 L
B-B_2	0	7.72229000	-4.17464000	-0.44049400 L
B-B_2	0	6.43020000	-3.83661100	1.63146000 L
N-N_3	0	6.44213600	-4.57816300	0.29295200 L
N-N_3	0	5.14113400	-3.78528200	2.45223300 L
B-B_2	0	3.85407900	-3.87747500	1.62748400 L
B-B_2	0	2.55552200	-2.46281900	3.17868700 L
N-N_3	0	2.56498900	-3.81129600	2.44804700 L
N-N_3	0	1.26673400	-1.99072500	3.85052200 L
B-B_2	0	-0.01698000	-2.47590100	3.17411700 L
B-B_2	0	-1.30015500	-0.45654500	3.87849000 L
N-N_3	0	-1.30053900	-1.99245500	3.85207300 L
N-N_3	0	-2.58059800	0.28205200	4.26156000 L
B-B_2	0	-3.86693000	-0.45019300	3.88553900 L
B-B_2	0	-5.15230700	1.65370100	3.61187700 L
N-N_3	0	-5.14371600	0.28334400	4.29616900 L
N-N_3	0	-6.43577300	2.48247300	3.63930100 L
B-B_2	0	-7.72355800	1.65652600	3.67138400 L
B-B_2	0	-9.03113200	3.34907700	2.41793300 L
N-N_3	0	-8.99822700	2.49519100	3.70034500 L
N-N_3	0	-10.34491500	4.02924300	1.99344900 L
B-B_2	0	-11.57173900	3.18944500	2.39887300 L
B-	0	-12.88657200	4.31006300	0.58799000 L
N-N_3	0	-12.77319100	3.05222700	1.46414700 L
B-	0	12.82513000	-3.73806900	-0.44064400 L
B-B_2	0	11.57085900	-3.85843300	1.67887700 L
N-N_3	0	11.62434200	-4.43235500	0.25785500 L
N-N_3	0	10.27360600	-3.76884900	2.48113000 L
B-B_2	0	9.00392900	-3.81580200	1.64056800 L
B-B_2	0	7.70604100	-2.44315300	3.23875400 L
N-N_3	0	7.71362900	-3.76360500	2.45873100 L
N-N_3	0	6.40794900	-1.98127400	3.90490700 L
B-B_2	0	5.12993000	-2.45154800	3.20467400 L
B-B_2	0	3.83437500	-0.45270800	3.88556600 L
N-N_3	0	3.83496500	-1.98457900	3.86930300 L
N-N_3	0	2.54697800	0.27975000	4.26041700 L
B-B_2	0	1.26613800	-0.45591700	3.87243100 L
B-B_2	0	-0.01757800	1.65877200	3.57890000 L
N-N_3	0	-0.01644900	0.28024500	4.25813000 L
N-N_3	0	-1.30071800	2.48976100	3.58917200 L
B-B_2	0	-2.58292300	1.65521200	3.57710700 L

B-B_2	0	-3.87657300	3.38995300	2.36722300 L
N-N_3	0	-3.86641800	2.48386700	3.60252200 L
N-N_3	0	-5.17369400	4.09794700	1.97143200 L
B-B_2	0	-6.45397600	3.36792700	2.38885300 L
B-B_2	0	-7.75526900	4.17118300	0.45149000 L
N-N_3	0	-7.75231900	4.07152500	1.97993600 L
N-N_3	0	-9.03982000	4.54947800	-0.28100200 L
B-B_2	0	-10.32729600	4.20276900	0.46813900 L
B-B_2	0	-11.58127800	3.66419800	-1.53383500 L
N-N_3	0	-11.61794300	4.52707100	-0.27384200 L
N-N_3	0	-12.78486000	2.79930100	-1.91152300 L
B-	0	12.80669000	-2.22368900	2.95613900 L
N-N_3	0	12.85546500	-3.67514800	2.46430600 L
N-N_3	0	11.59567800	-1.96343600	3.89256500 L
B-B_2	0	10.27910400	-2.43348000	3.24587900 L
B-B_2	0	8.97644800	-0.44779600	3.98661300 L
N-N_3	0	8.98880600	-1.98011400	3.94193200 L
N-N_3	0	7.68051100	0.28286400	4.34183800 L
B-B_2	0	6.40482800	-0.44998900	3.92719800 L
B-B_2	0	5.12006200	1.65220900	3.61276000 L
N-N_3	0	5.11241600	0.28029600	4.29398100 L
N-N_3	0	3.83277900	2.47989600	3.59957600 L
B-B_2	0	2.55002700	1.65092800	3.57518500 L
B-B_2	0	1.26749400	3.39875000	2.34713300 L
N-N_3	0	1.26734400	2.48477200	3.58034900 L
N-N_3	0	-0.01357500	4.15593300	1.97656100 L
B-B_2	0	-1.30204800	3.42028000	2.36599900 L
B-B_2	0	-2.59925600	4.30414200	0.44540100 L
N-N_3	0	-2.59652400	4.13518200	1.97033200 L
N-N_3	0	-3.90251800	4.63675500	-0.28622700 L
B-B_2	0	-5.17897600	4.21960800	0.44660600 L
B-B_2	0	-6.46749400	3.84016300	-1.62726100 L
N-N_3	0	-6.47615600	4.57273600	-0.28223200 L
N-N_3	0	-7.75339700	3.76393700	-2.45708100 L
B-B_2	0	-9.04404500	3.81004200	-1.63293300 L
N-N_3	0	-10.34506400	3.73834400	-2.45037200 L
N-N_3	0	12.82145500	0.31410200	4.38013400 L
B-B_2	0	11.53984900	-0.44577400	4.09674100 L
B-B_2	0	10.26469100	1.64728500	3.69543600 L
N-N_3	0	10.23914900	0.28881900	4.41805900 L
N-N_3	0	8.98244100	2.48894800	3.67467700 L
B-B_2	0	7.69330000	1.65811200	3.66195000 L
B-B_2	0	6.41548700	3.35689500	2.37919400 L
N-N_3	0	6.40362500	2.48305900	3.63595400 L

N-N_3	0	5.13641700	4.08747500	1.96349200 L
B-B_2	0	3.84227100	3.37494800	2.35731100 L
B-B_2	0	2.56442300	4.28071700	0.43424200 L
N-N_3	0	2.56153800	4.11470900	1.95680800 L
N-N_3	0	1.28759800	4.71033400	-0.29524100 L
B-B_2	0	-0.01618800	4.40000900	0.45526900 L
B-B_2	0	-1.30935700	3.96555900	-1.63382500 L
N-N_3	0	-1.31939500	4.71946300	-0.29116800 L
N-N_3	0	-2.60245600	3.82514000	-2.44448400 L
B-B_2	0	-3.88943700	3.88804700	-1.62186300 L
N-N_3	0	-5.17686900	3.78685800	-2.44485900 L
B-	0	12.79688900	1.49568200	3.40487500 L
B-B_2	0	11.55330300	3.40845100	2.47397500 L
N-N_3	0	11.58776900	2.43571600	3.65738300 L
N-N_3	0	10.26523800	4.07566700	1.99934400 L
B-B_2	0	8.98795200	3.35343600	2.40962200 L
B-B_2	0	7.72011800	4.17537800	0.44563100 L
N-N_3	0	7.70713800	4.06539500	1.97446100 L
N-N_3	0	6.44000700	4.57889200	-0.28796100 L
B-B_2	0	5.14352600	4.21603100	0.43891000 L
B-B_2	0	3.85480600	3.89259900	-1.63407000 L
N-N_3	0	3.86538400	4.62944600	-0.29246500 L
N-N_3	0	2.56709800	3.83554000	-2.45685400 L
B-B_2	0	1.27590900	3.96008700	-1.63810300 L
N-N_3	0	-0.01749700	3.85313300	-2.45085400 L
B-	0	12.82480100	3.74954800	0.45177600 L
N-N_3	0	12.84553000	4.01440400	1.96144000 L
N-N_3	0	11.62258900	4.43880100	-0.24948900 L
B-B_2	0	10.29293900	4.12339300	0.46233700 L
B-B_2	0	9.00405700	3.82072200	-1.63467500 L
N-N_3	0	9.01951400	4.54071300	-0.28255300 L
N-N_3	0	7.71543300	3.77126700	-2.45518500 L
B-B_2	0	6.43051100	3.84504700	-1.63070200 L
N-N_3	0	5.14376100	3.79880900	-2.45495200 L
N-N_3	0	12.85668900	3.67527400	-2.45193600 L
B-B_2	0	11.57092700	3.86016200	-1.66859200 L
N-N_3	0	10.27503900	3.77318000	-2.47331300 L
H-H_	0	-12.61169900	-0.39744100	-2.33781100 L
H-H_	0	-12.60302700	-2.24055600	-0.84430700 L
H-H_	0	-12.61828100	-1.84879200	1.49473400 L
H-H_	0	-12.62534200	0.39956300	2.34390900 L
H-H_	0	12.76055300	-0.68750900	-5.35254200 L
H-H_	0	12.80482700	-5.03413000	-2.10266100 L
H-H_	0	-12.59203400	2.23374800	0.84276000 L

H-H_	0	-12.62995100	1.85265500	-1.50037200 L
H-H_	0	12.81444400	-4.30346000	3.29859500 L
H-H_	0	12.76335700	0.69175300	5.35303500 L
H-H_	0	12.79862000	5.04767800	2.11200700 L
H-H_	0	12.81864900	4.30498800	-3.28531100 L
C-C_3	0	-0.24193000	0.03613500	0.34531200 H
H-H_	0	-1.55694400	-0.72502200	-1.16433100 H
H-H_	0	-2.19165800	-0.85008300	0.48195700 H
C-C_3	0	-1.29193600	-0.94769800	-0.13339000 H
H-H_	0	-0.92196900	-1.95148300	-0.04794700 H
N-N_3	0	-0.64440500	1.34645200	0.00990900 H
H-H_	0	0.09567900	1.94954400	-0.27459800 H
H-H_	0	-1.59332200	1.64311700	0.12075600 H
C-C_R	0	1.18405600	-0.13189000	-0.16195600 H
O-O_R	0	1.87005800	0.77255600	-0.59384100 H
O-O_R	0	1.67985000	-1.36609800	0.03299600 H
H-H_	0	2.61551800	-1.33411600	-0.22954600 H
H-H_	0	-0.10710700	-0.13469200	1.42295100 H

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B-B_2	0	-10.30234700	2.54671200	-3.28585600 L
N-N_3	0	-11.57715200	2.08627000	-3.98096600 L
B-	0	-12.85947800	2.71659700	-3.38059000 L
B-B_2	0	-5.16153300	2.50682700	-3.15373500 L
N-N_3	0	-6.43641100	2.05628100	-3.86786300 L
B-B_2	0	-7.73418700	2.50371800	-3.19459200 L
B-B_2	0	-9.01072900	0.53123800	-4.00346000 L
N-N_3	0	-8.99867700	2.07127800	-3.93163400 L
N-N_3	0	-10.30658300	-0.18755500	-4.41551100 L
B-B_2	0	-11.54949200	0.56182600	-3.89841600 L
B-	0	-12.84552500	-1.57668300	-4.05778500 L
N-N_3	0	-12.76297400	-0.20326000	-3.37066600 L
B-B_2	0	-0.01632300	2.54867100	-3.14358100 L
N-N_3	0	-1.30247700	2.07046500	-3.81822100 L
B-B_2	0	-2.58859300	2.52568700	-3.13231400 L
B-B_2	0	-3.86510600	0.52659100	-3.88675000 L
N-N_3	0	-3.86766200	2.05803300	-3.83084000 L
N-N_3	0	-5.14142400	-0.19684400	-4.31730500 L
B-B_2	0	-6.43679200	0.52489100	-3.94032600 L
B-B_2	0	-7.72160600	-1.58278000	-3.71573500 L
N-N_3	0	-7.71487200	-0.19874900	-4.37520900 L
N-N_3	0	-8.99662300	-2.42059600	-3.75548200 L
B-B_2	0	-10.28928500	-1.60543400	-3.82862800 L

B-B_2	0	-11.56729100	-3.13997200	-2.46139500 L
N-N_3	0	-11.57257900	-2.42504800	-3.80982100 L
N-N_3	0	-12.77361400	-3.03372900	-1.52860000 L
B-B_2	0	5.13226700	2.52745200	-3.18117200 L
N-N_3	0	3.83855400	2.07601700	-3.85959800 L
B-B_2	0	2.55719900	2.54673600	-3.16600500 L
B-B_2	0	1.26733400	0.54443800	-3.87132700 L
N-N_3	0	1.26512500	2.07956700	-3.83580900 L
N-N_3	0	-0.01490700	-0.18790800	-4.26257200 L
B-B_2	0	-1.29858500	0.53596300	-3.86415800 L
B-B_2	0	-2.57947500	-1.59021000	-3.64572700 L
N-N_3	0	-2.57622600	-0.19306100	-4.28036900 L
N-N_3	0	-3.86450900	-2.41640100	-3.67766100 L
B-B_2	0	-5.14898500	-1.58365900	-3.66690600 L
B-B_2	0	-6.44992600	-3.30992600	-2.46168100 L
N-N_3	0	-6.43432400	-2.40941800	-3.70118800 L
N-N_3	0	-7.74631500	-4.02111600	-2.06048000 L
B-B_2	0	-9.02685000	-3.29507100	-2.48696600 L
B-B_2	0	-10.31985900	-4.18694600	-0.55184300 L
N-N_3	0	-10.33869600	-3.98538300	-2.07361400 L
N-N_3	0	-11.60873400	-4.53299200	0.18274900 L
B-	0	-12.87856000	-4.30819000	-0.67540200 L
B-B_2	0	10.28177100	2.50548100	-3.20428000 L
N-N_3	0	8.99340000	2.06852200	-3.91387600 L
B-B_2	0	7.70876500	2.51615300	-3.20463900 L
B-B_2	0	6.40852500	0.53964400	-3.93375800 L
N-N_3	0	6.41266400	2.07022700	-3.88530000 L
N-N_3	0	5.11566800	-0.18496400	-4.31102600 L
B-B_2	0	3.83700600	0.54378400	-3.89411100 L
B-B_2	0	2.55379900	-1.56742000	-3.61412400 L
N-N_3	0	2.54841000	-0.18407600	-4.27523400 L
N-N_3	0	1.27286200	-2.40263400	-3.63789200 L
B-B_2	0	-0.01367700	-1.57972800	-3.61489600 L
B-B_2	0	-1.29724000	-3.37004400	-2.45680300 L
N-N_3	0	-1.29223800	-2.41827100	-3.66306000 L
N-N_3	0	-2.59300700	-4.07943200	-2.05600300 L
B-B_2	0	-3.87237500	-3.33229600	-2.44890200 L
B-B_2	0	-5.17210200	-4.17604600	-0.52882100 L
N-N_3	0	-5.16862100	-4.04191500	-2.05306400 L
N-N_3	0	-6.46690100	-4.55178800	0.19300400 L
B-B_2	0	-7.74822700	-4.14283000	-0.53345800 L
B-B_2	0	-9.03896000	-3.83237300	1.55855200 L
N-N_3	0	-9.03083600	-4.54242100	0.19093800 L
N-N_3	0	-10.34140300	-3.78285200	2.37567000 L

B-B_2	0	-11.57674600	-3.69473100	1.45909600 L
B-	0	-12.86063000	-2.71672700	3.37648100 L
N-N_3	0	-12.77781800	-2.83033500	1.84490800 L
B-	0	12.80941900	2.29004200	-2.91504500 L
B-B_2	0	11.54447700	0.53774200	-4.09719800 L
N-N_3	0	11.59981600	2.05060600	-3.85881600 L
N-N_3	0	10.24395000	-0.19192700	-4.43001600 L
B-B_2	0	8.98061800	0.53753900	-3.98885800 L
B-B_2	0	7.69729100	-1.57132100	-3.69522300 L
N-N_3	0	7.68496200	-0.18733800	-4.35696600 L
N-N_3	0	6.40766400	-2.39628400	-3.68191500 L
B-B_2	0	5.12366100	-1.56597300	-3.64800900 L
B-B_2	0	3.84635300	-3.31298800	-2.42436100 L
N-N_3	0	3.83760300	-2.39472100	-3.65025500 L
N-N_3	0	2.56741900	-4.06319700	-2.04069000 L
B-B_2	0	1.27402100	-3.34277900	-2.42557400 L
B-B_2	0	-0.01140800	-4.30228400	-0.53086400 L
N-N_3	0	-0.00732000	-4.09598400	-2.05542800 L
N-N_3	0	-1.31162200	-4.66268400	0.20015500 L
B-B_2	0	-2.59387500	-4.24290700	-0.52966900 L
B-B_2	0	-3.88426500	-3.88703600	1.55214100 L
N-N_3	0	-3.89340200	-4.59999700	0.19649400 L
N-N_3	0	-5.17269100	-3.81863100	2.37635500 L
B-B_2	0	-6.46221100	-3.85152800	1.55529300 L
B-B_2	0	-7.73478800	-2.50348800	3.19859100 L
N-N_3	0	-7.74941400	-3.80272000	2.38539200 L
N-N_3	0	-9.00069500	-2.07162200	3.93380600 L
B-B_2	0	-10.30330600	-2.54718400	3.28623800 L
B-B_2	0	-11.55185200	-0.56229800	3.89741500 L
N-N_3	0	-11.57933900	-2.08684400	3.97946000 L
N-N_3	0	-12.76672600	0.20295500	3.37292300 L
B-	0	12.80192900	-1.41278500	-3.43327100 L
N-N_3	0	12.82627300	-0.21739200	-4.39176500 L
N-N_3	0	11.59214300	-2.34899200	-3.69761500 L
B-B_2	0	10.26903600	-1.56016900	-3.72629800 L
B-B_2	0	8.99118000	-3.28487100	-2.46572900 L
N-N_3	0	8.98664700	-2.40195000	-3.71808800 L
N-N_3	0	7.71010000	-4.00493500	-2.04503400 L
B-B_2	0	6.41878500	-3.28981000	-2.43891300 L
B-B_2	0	5.14445700	-4.18548700	-0.51595200 L
N-N_3	0	5.14035200	-4.02926800	-2.03844400 L
N-N_3	0	3.86520900	-4.61161600	0.20714900 L
B-B_2	0	2.56716300	-4.25309900	-0.51937900 L
B-B_2	0	1.27365000	-3.94265300	1.56303700 L

N-N_3	0	1.28211500	-4.66516000	0.20660400 L
N-N_3	0	-0.01559100	-3.87149800	2.38583300 L
B-B_2	0	-1.30610600	-3.95333400	1.56595600 L
B-B_2	0	-2.58813900	-2.52045200	3.14540100 L
N-N_3	0	-2.59920200	-3.85057800	2.38029900 L
N-N_3	0	-3.86882300	-2.05772700	3.84387100 L
B-B_2	0	-5.16143900	-2.50495700	3.16227400 L
B-B_2	0	-6.43971400	-0.52526800	3.94614500 L
N-N_3	0	-6.43827200	-2.05641200	3.87438000 L
N-N_3	0	-7.71838600	0.19891900	4.37779800 L
B-B_2	0	-9.01341600	-0.53160600	4.00524300 L
B-B_2	0	-10.29200000	1.60498300	3.82903900 L
N-N_3	0	-10.30964600	0.18707900	4.41596000 L
N-N_3	0	-11.57509300	2.42468800	3.81043800 L
B-	0	-12.84812400	1.57676100	4.05959400 L
N-N_3	0	12.84869600	-3.94953300	-2.02249100 L
B-B_2	0	11.55645500	-3.33557900	-2.52583600 L
B-B_2	0	10.29354500	-4.09496600	-0.53125700 L
N-N_3	0	10.26830000	-4.01429600	-2.06714800 L
N-N_3	0	9.01896400	-4.52823600	0.20251200 L
B-B_2	0	7.72107500	-4.14464700	-0.51855700 L
B-B_2	0	6.42946600	-3.85701100	1.56336600 L
N-N_3	0	6.43984600	-4.56225200	0.20532300 L
N-N_3	0	5.14105700	-3.82764500	2.38649300 L
B-B_2	0	3.85371800	-3.89437500	1.56035400 L
B-B_2	0	2.55615800	-2.52567800	3.15359900 L
N-N_3	0	2.56487600	-3.85201900	2.38339900 L
N-N_3	0	1.26719100	-2.06958700	3.83703700 L
B-B_2	0	-0.01682000	-2.53612200	3.14802500 L
B-B_2	0	-1.30025900	-0.53436000	3.90158100 L
N-N_3	0	-1.30169700	-2.06913000	3.83558900 L
N-N_3	0	-2.58166300	0.19693600	4.29689600 L
B-B_2	0	-3.86758800	-0.52668800	3.90170200 L
B-B_2	0	-5.15260700	1.58015900	3.66476000 L
N-N_3	0	-5.14591900	0.19766100	4.32376800 L
N-N_3	0	-6.43660300	2.40802800	3.70014300 L
B-B_2	0	-7.72449600	1.58200600	3.71605500 L
B-B_2	0	-9.02937200	3.29469600	2.48716800 L
N-N_3	0	-8.99922000	2.42015400	3.75566200 L
N-N_3	0	-10.34144400	3.98475200	2.07384300 L
B-B_2	0	-11.56992300	3.13914200	2.46182700 L
B-	0	-12.88149600	4.30305200	0.67433000 L
N-N_3	0	-12.77416800	3.02851100	1.52698300 L
B-	0	12.82314700	-3.71839000	-0.50747400 L

B-B_2	0	11.56963700	-3.88956200	1.60867600 L
N-N_3	0	11.62209000	-4.42848200	0.17411100 L
N-N_3	0	10.27275900	-3.81739000	2.41287200 L
B-B_2	0	9.00297100	-3.84096200	1.57162200 L
B-B_2	0	7.70733400	-2.50924900	3.20631200 L
N-N_3	0	7.71319600	-3.80849700	2.39158100 L
N-N_3	0	6.41038500	-2.06307300	3.88545700 L
B-B_2	0	5.13100300	-2.51576000	3.17628700 L
B-B_2	0	3.83643500	-0.53405700	3.90461800 L
N-N_3	0	3.83675800	-2.06514900	3.85416500 L
N-N_3	0	2.54934800	0.19165500	4.29466200 L
B-B_2	0	1.26717200	-0.53553200	3.89406100 L
B-B_2	0	-0.01638600	1.58420800	3.64047900 L
N-N_3	0	-0.01539600	0.19368800	4.29500000 L
N-N_3	0	-1.29945400	2.41653200	3.66452600 L
B-B_2	0	-2.58218700	1.58255000	3.63776600 L
B-B_2	0	-3.87488800	3.32925100	2.44485000 L
N-N_3	0	-3.86658800	2.41023500	3.67045000 L
N-N_3	0	-5.17075400	4.04193900	2.05378400 L
B-B_2	0	-6.45232300	3.30930900	2.46114900 L
B-B_2	0	-7.75065100	4.14570000	0.53462300 L
N-N_3	0	-7.74881200	4.02136400	2.06141600 L
N-N_3	0	-9.03367600	4.54380800	-0.19004200 L
B-B_2	0	-10.32250500	4.18657700	0.55210600 L
B-B_2	0	-11.57803200	3.69285800	-1.45973400 L
N-N_3	0	-11.61170400	4.53071400	-0.18308600 L
N-N_3	0	-12.77979500	2.83077600	-1.84881200 L
B-	0	12.80929400	-2.28870500	2.92410000 L
N-N_3	0	12.85443800	-3.72834400	2.39845900 L
N-N_3	0	11.59820200	-2.04646000	3.86539800 L
B-B_2	0	10.28053200	-2.50111500	3.20981800 L
B-B_2	0	8.97963600	-0.53219300	3.99422800 L
N-N_3	0	8.99147400	-2.06309000	3.91775700 L
N-N_3	0	7.68468300	0.19235500	4.36480500 L
B-B_2	0	6.40758100	-0.53277100	3.94081300 L
B-B_2	0	5.12301800	1.57288900	3.66293100 L
N-N_3	0	5.11598200	0.19097700	4.32333100 L
N-N_3	0	3.83631200	2.40108000	3.66284700 L
B-B_2	0	2.55221600	1.57384500	3.63217100 L
B-B_2	0	1.26989600	3.33400300	2.42624400 L
N-N_3	0	1.27004700	2.40846500	3.65051400 L
N-N_3	0	-0.01000800	4.09414100	2.06045900 L
B-B_2	0	-1.30055900	3.36395500	2.45388300 L
B-B_2	0	-2.59484100	4.24697300	0.52994700 L

N-N_3	0	-2.59476400	4.07672500	2.05500100 L
N-N_3	0	-3.89542000	4.60729000	-0.19355100 L
B-B_2	0	-5.17441100	4.18121800	0.53029200 L
B-B_2	0	-6.46394200	3.85676000	-1.55327000 L
N-N_3	0	-6.46959300	4.55689700	-0.19105500 L
N-N_3	0	-7.75070400	3.80444900	-2.38360900 L
B-B_2	0	-9.04050200	3.83350500	-1.55749800 L
N-N_3	0	-10.34225700	3.78248500	-2.37544800 L
N-N_3	0	12.82584000	0.22184200	4.39373600 L
B-B_2	0	11.54353900	-0.53313100	4.10051800 L
B-B_2	0	10.26826800	1.56560600	3.73300900 L
N-N_3	0	10.24353300	0.19654900	4.43526400 L
N-N_3	0	8.98612900	2.40758700	3.72625400 L
B-B_2	0	7.69664700	1.57737000	3.70530600 L
B-B_2	0	6.41735800	3.29095400	2.44610400 L
N-N_3	0	6.40732700	2.40270800	3.69276600 L
N-N_3	0	5.13747900	4.02557200	2.04139700 L
B-B_2	0	3.84449500	3.30777000	2.42921000 L
B-B_2	0	2.56470200	4.22799700	0.51626700 L
N-N_3	0	2.56386500	4.05081800	2.03762600 L
N-N_3	0	1.28653600	4.66921100	-0.20294100 L
B-B_2	0	-0.01357500	4.32834000	0.53796900 L
B-B_2	0	-1.30728000	3.97277600	-1.56473000 L
N-N_3	0	-1.31480200	4.67879500	-0.19654000 L
N-N_3	0	-2.60098900	3.86158200	-2.37790900 L
B-B_2	0	-3.88599700	3.89811300	-1.55051300 L
N-N_3	0	-5.17462500	3.82414400	-2.37395700 L
B-	0	12.80026300	1.41806500	3.43633600 L
B-B_2	0	11.55487400	3.34346400	2.53429300 L
N-N_3	0	11.59136900	2.35432300	3.70399400 L
N-N_3	0	10.26597900	4.01987600	2.07425300 L
B-B_2	0	8.98968900	3.28934100	2.47304400 L
B-B_2	0	7.71920900	4.14386400	0.52363400 L
N-N_3	0	7.70774300	4.00694900	2.05047500 L
N-N_3	0	6.43735600	4.55992100	-0.20048000 L
B-B_2	0	5.14287200	4.17522500	0.51853800 L
B-B_2	0	3.85396300	3.90086300	-1.56477500 L
N-N_3	0	3.86293000	4.60036000	-0.20321100 L
N-N_3	0	2.56671900	3.87015400	-2.39010600 L
B-B_2	0	1.27598100	3.95950300	-1.56676800 L
N-N_3	0	-0.01582600	3.88770000	-2.38569900 L
B-	0	12.82272700	3.72696100	0.51703500 L
N-N_3	0	12.84645100	3.95937800	2.03190700 L
N-N_3	0	11.62055600	4.43348600	-0.16653300 L

B-B_2	0	10.29192600	4.09895700	0.53831800 L
B-B_2	0	9.00292500	3.84432200	-1.56618600 L
N-N_3	0	9.01703900	4.53026000	-0.19641100 L
N-N_3	0	7.71446000	3.81416700	-2.38803000 L
B-B_2	0	6.42938800	3.86140900	-1.56203600 L
N-N_3	0	5.14285900	3.83725600	-2.38812100 L
N-N_3	0	12.85543300	3.72911600	-2.38799000 L
B-B_2	0	11.56965200	3.89133200	-1.59984700 L
N-N_3	0	10.27385100	3.82093300	-2.40588800 L
H-H_	0	-12.61559600	-0.35381600	-2.34866100 L
H-H_	0	-12.60415200	-2.22478700	-0.89171000 L
H-H_	0	-12.61321300	-1.87610400	1.45550800 L
H-H_	0	-12.62234000	0.35306900	2.35044700 L
H-H_	0	12.76784200	-0.58142800	-5.36981900 L
H-H_	0	12.80512900	-4.97928200	-2.19640700 L
H-H_	0	-12.60038100	2.22050600	0.89003300 L
H-H_	0	-12.61833300	1.87636800	-1.45858700 L
H-H_	0	12.81145700	-4.37589300	3.21780700 L
H-H_	0	12.76900400	0.58493900	5.37223400 L
H-H_	0	12.80071100	4.98919500	2.20485200 L
H-H_	0	12.81456700	4.37756600	-3.20673500 L
C-C_3	0	-0.26749800	0.02817500	0.39246800 H
H-H_	0	-1.54932300	-0.62955700	-1.20767400 H
H-H_	0	-2.24316300	-0.80026900	0.41316800 H
C-C_3	0	-1.32629100	-0.89845300	-0.17563200 H
H-H_	0	-0.99562900	-1.91882300	-0.12953300 H
N-N_3	0	-0.67960800	1.39737700	0.23614500 H
H-H_	0	-0.00413900	1.83376700	-0.37567900 H
H-H_	0	-1.60089400	1.45725400	-0.18003300 H
C-C_R	0	1.14014200	-0.12463100	-0.16854800 H
O-O_R	0	1.75712800	0.75424800	-0.73475100 H
O-O_R	0	1.69862000	-1.31450600	0.11412200 H
H-H_	0	2.61180500	-1.28389600	-0.21850000 H
H-H_	0	-0.13790500	-0.22641200	1.44531800 H

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B-B_2	0	-10.29151100	2.46461800	-3.35196800 L
N-N_3	0	-11.56452400	1.98218300	-4.03519800 L
B-	0	-12.84823400	2.63126200	-3.45834900 L
B-B_2	0	-5.15059500	2.43367900	-3.20885200 L
N-N_3	0	-6.42411000	1.95610800	-3.90810400 L
B-B_2	0	-7.72344000	2.42638000	-3.25399300 L
B-B_2	0	-8.99790300	0.42735700	-4.00097400 L
N-N_3	0	-8.98613900	1.96899700	-3.97892800 L
N-N_3	0	-10.29225300	-0.30333200	-4.39622200 L
B-B_2	0	-11.53641800	0.46105400	-3.90490500 L
B-	0	-12.83363700	-1.67901100	-4.00156600 L
N-N_3	0	-12.74835600	-0.28786800	-3.35135100 L
B-B_2	0	-0.00460400	2.46902900	-3.18200200 L
N-N_3	0	-1.28910600	1.96800600	-3.84193100 L
B-B_2	0	-2.57774300	2.45869900	-3.18609700 L
B-B_2	0	-3.85348200	0.42647900	-3.86329100 L
N-N_3	0	-3.85560700	1.95974500	-3.86587000 L
N-N_3	0	-5.12801000	-0.30970600	-4.27770600 L
B-B_2	0	-6.42452600	0.42296400	-3.92737200 L
B-B_2	0	-7.71021400	-1.67962400	-3.65010900 L
N-N_3	0	-7.70082900	-0.31342000	-4.34606100 L
N-N_3	0	-8.98520000	-2.51812200	-3.67467600 L
B-B_2	0	-10.27716400	-1.70398300	-3.76936400 L

B-B_2	0	-11.55819600	-3.20574100	-2.36882500 L
N-N_3	0	-11.56114000	-2.52210100	-3.73322700 L
N-N_3	0	-12.76388800	-3.07335800	-1.43873400 L
B-B_2	0	5.14273200	2.43298200	-3.21931000 L
N-N_3	0	3.84668300	1.96056300	-3.87772200 L
B-B_2	0	2.56880900	2.44974500	-3.19139300 L
B-B_2	0	1.27683800	0.43283000	-3.82991800 L
N-N_3	0	1.27763000	1.96643400	-3.84837400 L
N-N_3	0	-0.00670300	-0.30340000	-4.20547800 L
B-B_2	0	-1.28888300	0.43239400	-3.82530900 L
B-B_2	0	-2.57018800	-1.69094400	-3.57260100 L
N-N_3	0	-2.56418600	-0.30499800	-4.23181500 L
N-N_3	0	-3.85586800	-2.51570200	-3.58870200 L
B-B_2	0	-5.13831400	-1.68062200	-3.59387300 L
B-B_2	0	-6.44142300	-3.38528600	-2.35964400 L
N-N_3	0	-6.42357800	-2.50642200	-3.61476500 L
N-N_3	0	-7.73936600	-4.08645500	-1.94675400 L
B-B_2	0	-9.01806300	-3.36592200	-2.38815100 L
B-B_2	0	-10.31371700	-4.21203000	-0.43489500 L
N-N_3	0	-10.33159000	-4.04441900	-1.96082600 L
N-N_3	0	-11.60381800	-4.53394500	0.30854900 L
B-	0	-12.87251200	-4.32681000	-0.55555000 L
B-B_2	0	10.29073800	2.40722000	-3.25730500 L
N-N_3	0	9.00035400	1.95299000	-3.95259200 L
B-B_2	0	7.71818100	2.42004700	-3.25158300 L
B-B_2	0	6.41498000	0.42393800	-3.92687000 L
N-N_3	0	6.41985800	1.95551800	-3.91560600 L
N-N_3	0	5.12030400	-0.30817200	-4.28450000 L
B-B_2	0	3.84487200	0.42863700	-3.87324900 L
B-B_2	0	2.56022700	-1.67785000	-3.55232800 L
N-N_3	0	2.55318300	-0.30476200	-4.23216700 L
N-N_3	0	1.27756200	-2.51092200	-3.56110000 L
B-B_2	0	-0.00639500	-1.68393100	-3.53695200 L
B-B_2	0	-1.29080600	-3.45359100	-2.35466100 L
N-N_3	0	-1.28502800	-2.52085800	-3.57485000 L
N-N_3	0	-2.58679300	-4.15864600	-1.94445300 L
B-B_2	0	-3.86460500	-3.41286800	-2.34543300 L
B-B_2	0	-5.16488100	-4.22572100	-0.41256600 L
N-N_3	0	-5.16179200	-4.11402300	-1.93888300 L
N-N_3	0	-6.46196900	-4.57467500	0.31846300 L
B-B_2	0	-7.74168300	-4.17837100	-0.41781700 L
B-B_2	0	-9.03106900	-3.80550700	1.66358500 L
N-N_3	0	-9.02602600	-4.55337600	0.31644900 L
N-N_3	0	-10.33276400	-3.72760600	2.47975400 L

B-B_2	0	-11.56905700	-3.66223500	1.56241500 L
B-	0	-12.84723200	-2.63270200	3.45915800 L
N-N_3	0	-12.77257600	-2.79344400	1.93129200 L
B-	0	12.81596200	2.19196300	-2.96273300 L
B-B_2	0	11.54990200	0.41713300	-4.10840000 L
N-N_3	0	11.60706600	1.93450700	-3.90229500 L
N-N_3	0	10.24808400	-0.31862200	-4.42158900 L
B-B_2	0	8.98660000	0.42049300	-3.99144800 L
B-B_2	0	7.70351300	-1.68302500	-3.65241700 L
N-N_3	0	7.68950200	-0.31177000	-4.34016200 L
N-N_3	0	6.41406700	-2.50808700	-3.62027900 L
B-B_2	0	5.12992300	-1.67775600	-3.59836500 L
B-B_2	0	3.85500900	-3.40275600	-2.34119600 L
N-N_3	0	3.84325100	-2.50637600	-3.58267000 L
N-N_3	0	2.57691700	-4.14445400	-1.93765800 L
B-B_2	0	1.28177100	-3.43612000	-2.33857500 L
B-B_2	0	-0.00298100	-4.33329200	-0.41438500 L
N-N_3	0	-0.00173200	-4.17363900	-1.94320000 L
N-N_3	0	-1.29831400	-4.69777800	0.32453800 L
B-B_2	0	-2.58685400	-4.31125100	-0.41566400 L
B-B_2	0	-3.87450900	-3.88238900	1.65615900 L
N-N_3	0	-3.88757400	-4.63853700	0.32305300 L
N-N_3	0	-5.16322500	-3.77522300	2.47689300 L
B-B_2	0	-6.45381900	-3.83428200	1.65910400 L
B-B_2	0	-7.72226700	-2.42574700	3.25454000 L
N-N_3	0	-7.74048700	-3.75274500	2.48768100 L
N-N_3	0	-8.98535500	-1.96908000	3.97941000 L
B-B_2	0	-10.29055100	-2.46505000	3.35243400 L
B-B_2	0	-11.53619900	-0.46191700	3.90520100 L
N-N_3	0	-11.56372200	-1.98303500	4.03570200 L
N-N_3	0	-12.74809900	0.28654000	3.35093800 L
B-	0	12.80999100	-1.51907200	-3.40923400 L
N-N_3	0	12.83024200	-0.34417200	-4.39272200 L
N-N_3	0	11.59851700	-2.46016700	-3.64758600 L
B-B_2	0	10.27525400	-1.67202800	-3.69001200 L
B-B_2	0	9.00030700	-3.36809500	-2.38940600 L
N-N_3	0	8.99308200	-2.51355800	-3.66108300 L
N-N_3	0	7.72079500	-4.07842100	-1.94853100 L
B-B_2	0	6.42787400	-3.37601600	-2.35945000 L
B-B_2	0	5.15648600	-4.22130400	-0.41354100 L
N-N_3	0	5.15087700	-4.10714400	-1.93963700 L
N-N_3	0	3.87755400	-4.62555100	0.32278200 L
B-B_2	0	2.57828500	-4.28581400	-0.41175600 L
B-B_2	0	1.28740900	-3.92648200	1.66239700 L

N-N_3	0	1.29390900	-4.68119500	0.32552200 L
N-N_3	0	-0.00069500	-3.82594200	2.48282800 L
B-B_2	0	-1.29465300	-3.95693400	1.67408100 L
B-B_2	0	-2.57639300	-2.45280000	3.18897200 L
N-N_3	0	-2.58875600	-3.81617100	2.48223800 L
N-N_3	0	-3.85441400	-1.95779600	3.86991600 L
B-B_2	0	-5.14879600	-2.43116500	3.21028000 L
B-B_2	0	-6.42454200	-0.42250100	3.92903100 L
N-N_3	0	-6.42324400	-1.95546300	3.90925800 L
N-N_3	0	-7.70118600	0.31369900	4.34684500 L
B-B_2	0	-8.99778100	-0.42747600	4.00151500 L
B-B_2	0	-10.27756400	1.70349100	3.76931500 L
N-N_3	0	-10.29235400	0.30292600	4.39646600 L
N-N_3	0	-11.56175900	2.52125700	3.73304800 L
B-	0	-12.83404700	1.67770000	4.00106500 L
N-N_3	0	12.85910300	-4.01729100	-1.93352200 L
B-B_2	0	11.56582600	-3.41943300	-2.45314100 L
B-B_2	0	10.30607700	-4.11733500	-0.43483600 L
N-N_3	0	10.27881700	-4.08434800	-1.97229800 L
N-N_3	0	9.03310500	-4.52940200	0.31369000 L
B-B_2	0	7.73336300	-4.17409200	-0.41874400 L
B-B_2	0	6.44278900	-3.82043100	1.65194700 L
N-N_3	0	6.45361400	-4.57150700	0.31878000 L
N-N_3	0	5.15520300	-3.76589600	2.47393800 L
B-B_2	0	3.86727000	-3.86637700	1.65215000 L
B-B_2	0	2.56917500	-2.43883800	3.18308600 L
N-N_3	0	2.58031900	-3.79794400	2.47435500 L
N-N_3	0	1.27772900	-1.95580200	3.84033900 L
B-B_2	0	-0.00427800	-2.45141400	3.16912200 L
B-B_2	0	-1.28650100	-0.42515200	3.83890800 L
N-N_3	0	-1.28585400	-1.96064100	3.84196800 L
N-N_3	0	-2.56515600	0.30988200	4.23475600 L
B-B_2	0	-3.85330400	-0.42477100	3.86747300 L
B-B_2	0	-5.13938500	1.67936200	3.59160000 L
N-N_3	0	-5.12875400	0.31085700	4.27941000 L
N-N_3	0	-6.42396900	2.50617500	3.61401800 L
B-B_2	0	-7.71071300	1.67952000	3.65005100 L
B-B_2	0	-9.01878200	3.36559800	2.38783800 L
N-N_3	0	-8.98575100	2.51793300	3.67447600 L
N-N_3	0	-10.33242800	4.04403500	1.96081800 L
B-B_2	0	-11.55885700	3.20498100	2.36868500 L
B-	0	-12.87356500	4.32652200	0.55591200 L
N-N_3	0	-12.76482200	3.07297300	1.43890900 L
B-	0	12.83649800	-3.73771500	-0.42653100 L

B-B_2	0	11.58287800	-3.83378400	1.69451300 L
N-N_3	0	11.63593000	-4.42399900	0.28025100 L
N-N_3	0	10.28648000	-3.74314700	2.49827900 L
B-B_2	0	9.01620800	-3.79622200	1.65880500 L
B-B_2	0	7.71799800	-2.41607600	3.25119600 L
N-N_3	0	7.72666900	-3.74056900	2.47774500 L
N-N_3	0	6.41930300	-1.95123000	3.91465900 L
B-B_2	0	5.14245200	-2.42622200	3.21588500 L
B-B_2	0	3.84507900	-0.42187400	3.87842800 L
N-N_3	0	3.84593800	-1.95382000	3.87394800 L
N-N_3	0	2.55453800	0.31103000	4.24387300 L
B-B_2	0	1.27690500	-0.42211000	3.83952500 L
B-B_2	0	-0.00552000	1.69810700	3.57362900 L
N-N_3	0	-0.00552600	0.31003000	4.22916700 L
N-N_3	0	-1.29050000	2.52800700	3.58489900 L
B-B_2	0	-2.57029600	1.68944600	3.56401600 L
B-B_2	0	-3.86552400	3.41206900	2.34323700 L
N-N_3	0	-3.85632600	2.51302800	3.58365900 L
N-N_3	0	-5.16264100	4.11339000	1.93766700 L
B-B_2	0	-6.44224600	3.38506000	2.35901000 L
B-B_2	0	-7.74244300	4.17901700	0.41747500 L
N-N_3	0	-7.74017400	4.08636300	1.94643800 L
N-N_3	0	-9.02711600	4.55400900	-0.31649300 L
B-B_2	0	-10.31470800	4.21226900	0.43496000 L
B-B_2	0	-11.57022500	3.66168500	-1.56202000 L
N-N_3	0	-11.60503700	4.53367900	-0.30837100 L
N-N_3	0	-12.77332700	2.79212200	-1.93048300 L
B-	0	12.81660900	-2.19159500	2.96501300 L
N-N_3	0	12.86819000	-3.64432400	2.47749600 L
N-N_3	0	11.60714600	-1.93244400	3.90347500 L
B-B_2	0	10.29075400	-2.40489900	3.25831600 L
B-B_2	0	8.98720600	-0.41752400	3.99262400 L
N-N_3	0	9.00021000	-1.94996800	3.95305300 L
N-N_3	0	7.69068200	0.31475400	4.34297500 L
B-B_2	0	6.41541400	-0.41973900	3.92968900 L
B-B_2	0	5.13121500	1.68259200	3.60680800 L
N-N_3	0	5.12162700	0.31214100	4.29072300 L
N-N_3	0	3.84541500	2.51210700	3.59157700 L
B-B_2	0	2.56098800	1.68622800	3.56863500 L
B-B_2	0	1.28043200	3.42549100	2.33645500 L
N-N_3	0	1.27982000	2.52229100	3.57651400 L
N-N_3	0	-0.00050300	4.17356200	1.94805000 L
B-B_2	0	-1.29138500	3.45613500	2.35935700 L
B-B_2	0	-2.58536600	4.29249900	0.41163600 L

N-N_3	0	-2.58707500	4.15582300	1.94063600 L
N-N_3	0	-3.88632900	4.63273900	-0.32234500 L
B-B_2	0	-5.16557700	4.22212600	0.41160000 L
B-B_2	0	-6.45522900	3.83720900	-1.66034100 L
N-N_3	0	-6.46229000	4.57539500	-0.31864900 L
N-N_3	0	-7.74232500	3.75398200	-2.48797200 L
B-B_2	0	-9.03240100	3.80608200	-1.66352900 L
N-N_3	0	-10.33415700	3.72737200	-2.47949900 L
N-N_3	0	12.83143500	0.34628400	4.39064300 L
B-B_2	0	11.55061600	-0.41483400	4.10764400 L
B-B_2	0	10.27620200	1.67489600	3.69123500 L
N-N_3	0	10.24926200	0.32111600	4.42220000 L
N-N_3	0	8.99430300	2.51667500	3.66355500 L
B-B_2	0	7.70464600	1.68649200	3.65629300 L
B-B_2	0	6.42825600	3.37716800	2.36255900 L
N-N_3	0	6.41575900	2.51205200	3.62536300 L
N-N_3	0	5.15004800	4.10531800	1.94070900 L
B-B_2	0	3.85546400	3.39903800	2.34379900 L
B-B_2	0	2.57688600	4.27013600	0.40930800 L
N-N_3	0	2.57497200	4.13377000	1.93436500 L
N-N_3	0	1.29676900	4.68302000	-0.32479200 L
B-B_2	0	-0.00358000	4.35514900	0.41972800 L
B-B_2	0	-1.29618000	3.97853700	-1.68200700 L
N-N_3	0	-1.30244600	4.70387800	-0.32272900 L
N-N_3	0	-2.59133100	3.82676800	-2.48836200 L
B-B_2	0	-3.87584600	3.88899800	-1.66121000 L
N-N_3	0	-5.16587100	3.77967000	-2.47932100 L
B-	0	12.81025700	1.52154700	3.40761100 L
B-B_2	0	11.56607300	3.42375400	2.45506100 L
N-N_3	0	11.59950000	2.46286900	3.64825400 L
N-N_3	0	10.27857600	4.08755500	1.97395900 L
B-B_2	0	9.00060300	3.37080400	2.39155000 L
B-B_2	0	7.73280100	4.17392900	0.42018600 L
N-N_3	0	7.72051600	4.07994300	1.95013300 L
N-N_3	0	6.45238200	4.57042600	-0.31700300 L
B-B_2	0	5.15598200	4.21537000	0.41454300 L
B-B_2	0	3.86732800	3.86856600	-1.65448900 L
N-N_3	0	3.87632800	4.61850500	-0.32076500 L
N-N_3	0	2.58027300	3.80515700	-2.47666100 L
B-B_2	0	1.28753800	3.92934000	-1.66263000 L
N-N_3	0	0.00062100	3.84137900	-2.48746300 L
B-	0	12.83683800	3.74255600	0.42873800 L
N-N_3	0	12.85886500	4.02268800	1.93564600 L
N-N_3	0	11.63544200	4.42684700	-0.27872700 L

B-B_2	0	10.30571800	4.11975300	0.43649600 L
B-B_2	0	9.01604900	3.79834300	-1.65763300 L
N-N_3	0	9.03232900	4.53079500	-0.31213600 L
N-N_3	0	7.72702100	3.74401600	-2.47730000 L
B-B_2	0	6.44255900	3.82324900	-1.65239300 L
N-N_3	0	5.15567800	3.77146400	-2.47568600 L
N-N_3	0	12.86839100	3.64443500	-2.47454600 L
B-B_2	0	11.58277500	3.83473900	-1.69215800 L
N-N_3	0	10.28674200	3.74512200	-2.49658800 L
H-H_	0	-12.59644100	-0.41137800	-2.32632500 L
H-H_	0	-12.59186500	-2.24962000	-0.82183900 L
H-H_	0	-12.61674000	-1.85051800	1.51205000 L
H-H_	0	-12.59564100	0.41009900	2.32599200 L
H-H_	0	12.76748600	-0.72868700	-5.36263900 L
H-H_	0	12.81481000	-5.05209000	-2.07406800 L
H-H_	0	-12.59318400	2.24922200	0.82193400 L
H-H_	0	-12.61673200	1.84928000	-1.51132100 L
H-H_	0	12.83040600	-4.27039100	3.31362500 L
H-H_	0	12.76996200	0.73041400	5.36079500 L
H-H_	0	12.81347100	5.05749800	2.07576100 L
H-H_	0	12.83167100	4.27094900	-3.31038900 L
C-C_R	0	-0.57871200	-0.04035900	0.29234500 H
H-H_	0	-2.12696200	-0.76080400	-1.00489200 H
H-H_	0	-2.49673900	-0.95987800	0.71186000 H
C-C_3	0	-1.68380200	-0.97763800	-0.02062300 H
H-H_	0	-1.26570000	-1.96652400	-0.05243200 H
N-N_R	0	-1.02068900	1.41153900	0.02050300 H
H-H_	0	-0.18900700	1.84113700	-0.38711400 H
H-H_	0	-1.89582600	1.46424600	-0.49216000 H
C-C_R	0	0.80776600	-0.12768100	-0.03427700 H
O-O_R	0	1.50789100	0.86098900	-0.31273500 H
O-O_R	0	1.35957800	-1.36328300	0.03204800 H
H-H_	0	2.30558900	-1.23959600	-0.14641100 H
H-H_	0	-0.89361000	0.98691000	1.09459200 H

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B-B_2	0	-10.32855600	-1.73551700	3.77526300 L
N-N_3	0	-11.60053000	-1.13765500	4.36147600 L
B-	0	-12.88383900	-1.89135500	3.92880200 L
B-B_2	0	-5.18917300	-1.71021300	3.60851200 L
N-N_3	0	-6.46232900	-1.11847800	4.21379300 L
B-B_2	0	-7.76135800	-1.70604800	3.66113000 L
B-B_2	0	-9.04131100	0.39229900	4.02523000 L

N-N_3	0	-9.02360900	-1.12594700	4.29261000 L
N-N_3	0	-10.33919000	1.18056400	4.27163200 L
B-B_2	0	-11.58146800	0.33030300	3.94244500 L
B-	0	-12.88492200	2.44398100	3.60951300 L
N-N_3	0	-12.79697400	0.95053700	3.25400200 L
B-B_2	0	-0.04708300	-1.74472700	3.57744900 L
N-N_3	0	-1.32827500	-1.12849800	4.14024100 L
B-B_2	0	-2.61713000	-1.72397700	3.57725600 L
B-B_2	0	-3.89559400	0.38568100	3.88863500 L
N-N_3	0	-3.89396200	-1.12116100	4.16597500 L
N-N_3	0	-5.17250700	1.18201800	4.16011500 L
B-B_2	0	-6.46727000	0.39242000	3.95312900 L
B-B_2	0	-7.75913800	2.39537000	3.27690600 L
N-N_3	0	-7.74695900	1.18985800	4.22387800 L
N-N_3	0	-9.03875600	3.21403700	3.12692400 L
B-B_2	0	-10.32784900	2.43012100	3.38102300 L
B-B_2	0	-11.60941400	3.60387600	1.69774800 L
N-N_3	0	-11.61488400	3.21736000	3.17412100 L
N-N_3	0	-12.80233100	3.26107600	0.80574300 L
B-B_2	0	5.09552000	-1.71415200	3.56668900 L
N-N_3	0	3.80313600	-1.12056700	4.12324600 L
B-B_2	0	2.52300200	-1.72920400	3.54870200 L
B-B_2	0	1.23682400	0.37717200	3.82101200 L
N-N_3	0	1.24086500	-1.12845300	4.12043600 L
N-N_3	0	-0.04248900	1.17147900	4.07479500 L
B-B_2	0	-1.32753100	0.37788400	3.84518500 L
B-B_2	0	-2.61499100	2.40117400	3.18433100 L
N-N_3	0	-2.60465200	1.17574000	4.10553800 L
N-N_3	0	-3.90325400	3.21298900	3.05291200 L
B-B_2	0	-5.18614800	2.39498400	3.22522400 L
B-B_2	0	-6.49358000	3.80887400	1.67352100 L
N-N_3	0	-6.47509300	3.20417300	3.08099100 L
N-N_3	0	-7.79377800	4.39788400	1.11640200 L
B-B_2	0	-9.07040800	3.77839300	1.69344700 L
B-B_2	0	-10.36148700	4.19448100	-0.39850400 L
N-N_3	0	-10.38483300	4.34623700	1.12943700 L
N-N_3	0	-11.65024800	4.35656200	-1.19554500 L
B-	0	-12.92106000	4.31136600	-0.31044100 L
B-B_2	0	10.24124400	-1.70058400	3.62435400 L
N-N_3	0	8.95031800	-1.11300000	4.20993300 L
B-B_2	0	7.66962300	-1.70492000	3.60753800 L
B-B_2	0	6.37134500	0.39194400	3.88897400 L
N-N_3	0	6.37166700	-1.11524300	4.16275200 L
N-N_3	0	5.07939000	1.17994800	4.11184300 L

B-B_2	0	3.80311500	0.38496600	3.83910700 L
B-B_2	0	2.51903100	2.40961200	3.16510500 L
N-N_3	0	2.51571400	1.17374200	4.07214000 L
N-N_3	0	1.23614300	3.23233000	3.02970000 L
B-B_2	0	-0.04679100	2.41206400	3.17006700 L
B-B_2	0	-1.33938900	3.89966800	1.65402000 L
N-N_3	0	-1.33380400	3.22581800	3.03357200 L
N-N_3	0	-2.63988800	4.49640000	1.11240900 L
B-B_2	0	-3.91621400	3.84815500	1.65978800 L
B-B_2	0	-5.21604200	4.21429800	-0.39958500 L
N-N_3	0	-5.21683000	4.43989500	1.11314900 L
N-N_3	0	-6.50849900	4.39745100	-1.19523600 L
B-B_2	0	-7.79041700	4.16350600	-0.39752400 L
B-B_2	0	-9.07062500	3.37383400	-2.36816100 L
N-N_3	0	-9.07119900	4.37824500	-1.19914900 L
N-N_3	0	-10.36772600	3.14337700	-3.16169700 L
B-B_2	0	-11.60802600	3.25613100	-2.25450100 L
B-	0	-12.88085400	1.89791600	-3.94102700 L
N-N_3	0	-12.82161900	2.35088000	-2.47200800 L
B-	0	12.76526800	-1.55459200	3.29835300 L
B-B_2	0	11.50405200	0.41655600	4.06531900 L
N-N_3	0	11.55690300	-1.11117700	4.16588600 L
N-N_3	0	10.20537300	1.20169700	4.24210900 L
B-B_2	0	8.94165800	0.39919000	3.95531000 L
B-B_2	0	7.66250200	2.41457100	3.24574000 L
N-N_3	0	7.64687400	1.18673800	4.16529700 L
N-N_3	0	6.37511800	3.22561000	3.06914400 L
B-B_2	0	5.08864600	2.40976000	3.19864100 L
B-B_2	0	3.81157000	3.88985100	1.66084900 L
N-N_3	0	3.80344200	3.22784100	3.04242900 L
N-N_3	0	2.53025800	4.53426900	1.11748700 L
B-B_2	0	1.23538100	3.92011900	1.65624100 L
B-B_2	0	-0.05648500	4.45284200	-0.41416800 L
N-N_3	0	-0.05676200	4.55652200	1.12411800 L
N-N_3	0	-1.36119100	4.54217200	-1.21682200 L
B-B_2	0	-2.63813300	4.30315300	-0.40703400 L
B-B_2	0	-3.91835600	3.42253600	-2.33044300 L
N-N_3	0	-3.93762500	4.45582300	-1.20103500 L
N-N_3	0	-5.19790700	3.16420500	-3.13068300 L
B-B_2	0	-6.49439200	3.39214400	-2.35142600 L
B-B_2	0	-7.75893900	1.70530100	-3.65666100 L
N-N_3	0	-7.77528500	3.15488700	-3.15789900 L
N-N_3	0	-9.02049100	1.12678100	-4.29130300 L
B-B_2	0	-10.32629700	1.73762100	-3.77697900 L

B-B_2	0	-11.58092300	-0.32598900	-3.94500800 L
N-N_3	0	-11.59708600	1.14108500	-4.36644900 L
N-N_3	0	-12.79155500	-0.93988000	-3.24281600 L
B-	0	12.76643500	2.18879200	3.01993500 L
N-N_3	0	12.78720400	1.21343900	4.20113300 L
N-N_3	0	11.55979000	3.16270000	3.08831500 L
B-B_2	0	10.23410000	2.40046200	3.27770900 L
B-B_2	0	8.95987100	3.83078000	1.69249600 L
N-N_3	0	8.95468700	3.22774200	3.10041600 L
N-N_3	0	7.68143400	4.44308600	1.12234600 L
B-B_2	0	6.38662000	3.84669900	1.67068500 L
B-B_2	0	5.11171500	4.27078500	-0.39807400 L
N-N_3	0	5.11082600	4.48556600	1.11713500 L
N-N_3	0	3.83163700	4.49817800	-1.20265200 L
B-B_2	0	2.53044700	4.35759500	-0.40629800 L
B-B_2	0	1.23805900	3.46819200	-2.30222400 L
N-N_3	0	1.24664000	4.55846300	-1.21779300 L
N-N_3	0	-0.04801000	3.18961400	-3.08230100 L
B-B_2	0	-1.34085900	3.46588300	-2.31378800 L
B-B_2	0	-2.61505200	1.70824800	-3.53945300 L
N-N_3	0	-2.62264800	3.17831900	-3.10393100 L
N-N_3	0	-3.88850800	1.11353500	-4.14389400 L
B-B_2	0	-5.18635400	1.70434700	-3.59273600 L
B-B_2	0	-6.46629500	-0.39574700	-3.95130100 L
N-N_3	0	-6.45820200	1.11621400	-4.20542400 L
N-N_3	0	-7.74753900	-1.19018000	-4.22457400 L
B-B_2	0	-9.04058200	-0.39145000	-4.02468500 L
B-B_2	0	-10.33008900	-2.42711100	-3.37949000 L
N-N_3	0	-10.33944600	-1.17831700	-4.27138500 L
N-N_3	0	-11.61882800	-3.21143100	-3.17004400 L
B-	0	-12.88777600	-2.43252400	-3.59907000 L
N-N_3	0	12.81852100	4.37228500	1.10919300 L
B-B_2	0	11.52630400	3.89177100	1.74070700 L
B-B_2	0	10.26263400	4.15793100	-0.37341700 L
N-N_3	0	10.23858700	4.44427600	1.13720600 L
N-N_3	0	8.98728100	4.40112300	-1.18890700 L
B-B_2	0	7.68934600	4.21562800	-0.39312300 L
B-B_2	0	6.39249200	3.40991500	-2.32523800 L
N-N_3	0	6.40729700	4.44196900	-1.19498700 L
N-N_3	0	5.10020500	3.17199900	-3.10673000 L
B-B_2	0	3.81735300	3.44467700	-2.31540400 L
B-B_2	0	2.52098100	1.70879800	-3.51202400 L
N-N_3	0	2.52362500	3.18213900	-3.08604500 L
N-N_3	0	1.23643000	1.11125100	-4.08038600 L

B-B_2	0	-0.04638400	1.71408600	-3.51226300 L
B-B_2	0	-1.32643500	-0.40074100	-3.83836500 L
N-N_3	0	-1.32412400	1.11228200	-4.09570300 L
N-N_3	0	-2.60581000	-1.18778100	-4.11570200 L
B-B_2	0	-3.89432700	-0.39673400	-3.88475400 L
B-B_2	0	-5.18886300	-2.40540500	-3.23752000 L
N-N_3	0	-5.17339300	-1.18656600	-4.16413400 L
N-N_3	0	-6.47992000	-3.20928600	-3.08702500 L
B-B_2	0	-7.76157700	-2.39736400	-3.27994900 L
B-B_2	0	-9.07248500	-3.77719000	-1.69350200 L
N-N_3	0	-9.04238900	-3.21351000	-3.12740800 L
N-N_3	0	-10.38635200	-4.34497800	-1.12867200 L
B-B_2	0	-11.61105700	-3.60049400	-1.69413100 L
B-	0	-12.92082300	-4.32227800	0.31318200 L
N-N_3	0	-12.80941200	-3.27188800	-0.80379800 L
B-	0	12.79602100	3.78831100	-0.30842500 L
B-B_2	0	11.53340100	3.42704500	-2.39593600 L
N-N_3	0	11.59055300	4.30612100	-1.14053300 L
N-N_3	0	10.23383700	3.16721900	-3.15796300 L
B-B_2	0	8.96665500	3.39296000	-2.34236600 L
B-B_2	0	7.66717500	1.70178600	-3.60274300 L
N-N_3	0	7.67284800	3.15883000	-3.12292800 L
N-N_3	0	6.36762700	1.11135800	-4.15521100 L
B-B_2	0	5.09248700	1.70600900	-3.55149800 L
B-B_2	0	3.80126900	-0.39818200	-3.84080300 L
N-N_3	0	3.79784700	1.11135200	-4.10404700 L
N-N_3	0	2.51593600	-1.18825500	-4.08758300 L
B-B_2	0	1.23484400	-0.40141600	-3.82201200 L
B-B_2	0	-0.04777600	-2.45737500	-3.23245900 L
N-N_3	0	-0.04402300	-1.19009800	-4.10016800 L
N-N_3	0	-1.33983700	-3.26180000	-3.07594900 L
B-B_2	0	-2.61675200	-2.42790300	-3.21515300 L
B-B_2	0	-3.91945900	-3.84976100	-1.67179100 L
N-N_3	0	-3.90990000	-3.22931200	-3.07123700 L
N-N_3	0	-5.21829800	-4.43483500	-1.11436100 L
B-B_2	0	-6.49611000	-3.80826400	-1.67706400 L
B-B_2	0	-7.78990300	-4.15874100	0.39715500 L
N-N_3	0	-7.79510500	-4.39584000	-1.11648600 L
N-N_3	0	-9.07010500	-4.37631700	1.19929400 L
B-B_2	0	-10.36151000	-4.19507600	0.39933300 L
B-B_2	0	-11.60878500	-3.25750100	2.25385000 L
N-N_3	0	-11.64912300	-4.35991000	1.19718500 L
N-N_3	0	-12.81741900	-2.34323200	2.45986800 L
B-	0	12.76507400	1.55789800	-3.30292700 L

N-N_3	0	12.81664000	3.07995100	-3.12670100 L
N-N_3	0	11.55508300	1.11158200	-4.16697500 L
B-B_2	0	10.23943600	1.70037100	-3.62439400 L
B-B_2	0	8.94099500	-0.40069500	-3.95477000 L
N-N_3	0	8.94776500	1.11158300	-4.20799700 L
N-N_3	0	7.64740600	-1.18903700	-4.16730400 L
B-B_2	0	6.37003900	-0.39723000	-3.88978000 L
B-B_2	0	5.09036900	-2.41956100	-3.21157200 L
N-N_3	0	5.08002100	-1.18646100	-4.11939500 L
N-N_3	0	3.80838100	-3.24176700	-3.05750300 L
B-B_2	0	2.51885800	-2.43525900	-3.19643500 L
B-B_2	0	1.23671100	-3.93723100	-1.68934300 L
N-N_3	0	1.24054700	-3.26862700	-3.07390700 L
N-N_3	0	-0.05767000	-4.53880800	-1.12674800 L
B-B_2	0	-1.34232200	-3.91075700	-1.68345300 L
B-B_2	0	-2.63582200	-4.25434600	0.39833900 L
N-N_3	0	-2.64206600	-4.48671300	-1.11647300 L
N-N_3	0	-3.93120600	-4.43269000	1.19551100 L
B-B_2	0	-5.21442900	-4.19692500	0.39697100 L
B-B_2	0	-6.49470000	-3.38933200	2.35442500 L
N-N_3	0	-6.50560500	-4.38930200	1.19388300 L
N-N_3	0	-7.77705400	-3.15465200	3.15961300 L
B-B_2	0	-9.07122300	-3.37231100	2.36846000 L
N-N_3	0	-10.36901500	-3.14197600	3.16123000 L
N-N_3	0	12.78795600	-1.21173700	-4.19520100 L
B-B_2	0	11.50371500	-0.41578500	-4.06229600 L
B-B_2	0	10.23488200	-2.40120100	-3.27682700 L
N-N_3	0	10.20598800	-1.20198800	-4.24075900 L
N-N_3	0	8.95636800	-3.22951900	-3.10131000 L
B-B_2	0	7.66390100	-2.41788600	-3.24940500 L
B-B_2	0	6.38766900	-3.84348700	-1.67240500 L
N-N_3	0	6.37841100	-3.23080900	-3.07452700 L
N-N_3	0	5.11011600	-4.47577500	-1.11591200 L
B-B_2	0	3.81300000	-3.88252600	-1.66674900 L
B-B_2	0	2.52816500	-4.31039100	0.40058100 L
N-N_3	0	2.53301000	-4.52341100	-1.11986400 L
N-N_3	0	1.23923700	-4.51728500	1.20481500 L
B-B_2	0	-0.05552500	-4.33892300	0.40025100 L
B-B_2	0	-1.34086400	-3.46658400	2.34637400 L
N-N_3	0	-1.35384900	-4.49153700	1.20190300 L
N-N_3	0	-2.62773000	-3.19009500	3.12923600 L
B-B_2	0	-3.91792900	-3.41872400	2.34230400 L
N-N_3	0	-5.20086900	-3.16733500	3.13863500 L
B-	0	12.76561800	-2.18731400	-3.01419800 L

B-B_2	0	11.52617400	-3.89579300	-1.74106200 L
N-N_3	0	11.56071300	-3.16279000	-3.08667300 L
N-N_3	0	10.23770700	-4.44631200	-1.13721300 L
B-B_2	0	8.96007300	-3.83137200	-1.69271000 L
B-B_2	0	7.68799600	-4.21226500	0.39361200 L
N-N_3	0	7.68057500	-4.44122800	-1.12178300 L
N-N_3	0	6.40407100	-4.43623400	1.19494700 L
B-B_2	0	5.10924700	-4.25329400	0.39820400 L
B-B_2	0	3.81606500	-3.44428500	2.33052300 L
N-N_3	0	3.82496800	-4.47788000	1.19976600 L
N-N_3	0	2.52982500	-3.20232600	3.12030100 L
B-B_2	0	1.23773800	-3.48908400	2.34995400 L
N-N_3	0	-0.05102100	-3.21750100	3.13264400 L
B-	0	12.79709200	-3.79475900	0.30707800 L
N-N_3	0	12.81760600	-4.37906800	-1.11042500 L
N-N_3	0	11.59023500	-4.30832100	1.14011700 L
B-B_2	0	10.26211000	-4.15944900	0.37324200 L
B-B_2	0	8.96749800	-3.39342600	2.34309100 L
N-N_3	0	8.98617500	-4.40077100	1.18907900 L
N-N_3	0	7.67508100	-3.16130000	3.12589400 L
B-B_2	0	6.39298600	-3.41033900	2.33013200 L
N-N_3	0	5.10338900	-3.17779800	3.11642800 L
N-N_3	0	12.81869100	-3.07651300	3.12129600 L
B-B_2	0	11.53445900	-3.42566100	2.39291900 L
N-N_3	0	10.23593700	-3.16725100	3.15705000 L
H-H_	0	-12.64916900	0.86453400	2.22469800 L
H-H_	0	-12.60631200	2.33524400	0.36564100 L
H-H_	0	-12.69135300	1.50579100	-1.87388600 L
H-H_	0	-12.63088500	-0.85588400	-2.21518100 L
H-H_	0	12.72967600	1.76841900	5.08500400 L
H-H_	0	12.77166700	5.41367700	1.03294400 L
H-H_	0	-12.62555400	-2.34337800	-0.36432700 L
H-H_	0	-12.67433900	-1.49844400	1.86412800 L
H-H_	0	12.77590700	3.51965600	-4.07406700 L
H-H_	0	12.73301000	-1.76654800	-5.07934500 L
H-H_	0	12.76836200	-5.42032300	-1.03380900 L
H-H_	0	12.78076400	-3.51683000	4.06849700 L
C-C_R	0	0.84809000	0.06978500	-0.12649000 H
H-H_	0	-0.88307700	0.83719300	0.90115700 H
H-H_	0	-0.99163000	0.95450300	-0.85350300 H
C-C_3	0	-0.28424200	1.00202200	-0.01226800 H
H-H_	0	0.12558800	1.99036700	0.03766800 H
N-N_R	0	0.44186800	-1.31534100	0.03249500 H
H-H_	0	1.40399900	-1.76558600	0.05789100 H

H-H_	0	-0.08310600	-1.45653600	0.89600300 H
C-C_R	0	2.22772300	0.11096400	-0.03180200 H
O-O_R	0	2.92511200	-0.95312800	0.05691200 H
O-O_R	0	2.85923400	1.31666900	-0.04967500 H
H-H_	0	3.80524000	1.11094600	-0.00453500 H
H-H_	0	-0.15722000	-1.63612500	-0.72092400 H

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B-B_2	0	-10.34184600	-3.25087900	2.64184500 L
N-N_3	0	-11.61794100	-2.95189700	3.41799600 L
B-	0	-12.89899300	-3.42482400	2.68554000 L
B-B_2	0	-5.19798000	-3.22412900	2.55134400 L
N-N_3	0	-6.47636100	-2.93247200	3.33861200 L
B-B_2	0	-7.77226600	-3.20762200	2.57557000 L

B-B_2	0	-9.04423900	-1.45617500	3.79310700 L
N-N_3	0	-9.03942000	-2.94228500	3.38349800 L
N-N_3	0	-10.33750000	-0.83858400	4.35160900 L
B-B_2	0	-11.58365500	-1.44768600	3.68048000 L
B-	0	-12.86819400	0.60787400	4.32831500 L
N-N_3	0	-12.80088200	-0.58146000	3.35520800 L
B-B_2	0	-0.04530000	-3.30287600	2.55082000 L
N-N_3	0	-1.33279100	-2.96587200	3.30898900 L
B-B_2	0	-2.62185500	-3.25423500	2.54002700 L
B-B_2	0	-3.89664900	-1.45794300	3.68406700 L
N-N_3	0	-3.90473900	-2.94450800	3.31634900 L
N-N_3	0	-5.17069100	-0.82931200	4.25166900 L
B-B_2	0	-6.46947000	-1.45222800	3.73666100 L
B-B_2	0	-7.74649300	0.66268500	3.95851200 L
N-N_3	0	-7.74523000	-0.82918900	4.31246400 L
N-N_3	0	-9.01571400	1.47844900	4.18840300 L
B-B_2	0	-10.31333200	0.67336200	4.09021700 L
B-B_2	0	-11.58827500	2.47873400	3.10586500 L
N-N_3	0	-11.59104300	1.48318000	4.26244200 L
N-N_3	0	-12.78758200	2.56931900	2.16326800 L
B-B_2	0	5.10930000	-3.24144500	2.53118300 L
N-N_3	0	3.81772200	-2.94973000	3.29413500 L
B-B_2	0	2.53090900	-3.26989300	2.52656000 L
B-B_2	0	1.24440100	-1.47879600	3.65823300 L
N-N_3	0	1.24736900	-2.97466100	3.30335900 L
N-N_3	0	-0.04009600	-0.83721600	4.18091500 L
B-B_2	0	-1.32528400	-1.47002300	3.65228400 L
B-B_2	0	-2.60604100	0.65684000	3.83574000 L
N-N_3	0	-2.60259000	-0.83187300	4.20060800 L
N-N_3	0	-3.88463400	1.46343000	4.06027400 L
B-B_2	0	-5.17494600	0.65912000	3.89011600 L
B-B_2	0	-6.47240500	2.61882400	3.10064800 L
N-N_3	0	-6.45384400	1.46664700	4.11124400 L
N-N_3	0	-7.76596700	3.41169900	2.88766600 L
B-B_2	0	-9.04800100	2.61251600	3.14510100 L
B-B_2	0	-10.34695900	3.93062400	1.47515200 L
N-N_3	0	-10.35778700	3.38531100	2.91015200 L
N-N_3	0	-11.64035100	4.43670300	0.84832400 L
B-	0	-12.90676600	4.00603200	1.62992700 L
B-B_2	0	10.25993000	-3.19959100	2.53598200 L
N-N_3	0	8.97379000	-2.92807500	3.32748600 L
B-B_2	0	7.68635500	-3.22271200	2.54622600 L
B-B_2	0	6.38438300	-1.45062900	3.67798000 L
N-N_3	0	6.39231600	-2.93710700	3.31069400 L

N-N_3	0	5.09123000	-0.82763800	4.20272200 L
B-B_2	0	3.81274100	-1.45970500	3.64996100 L
B-B_2	0	2.52459900	0.65362000	3.80709000 L
N-N_3	0	2.52659300	-0.83339200	4.18287200 L
N-N_3	0	1.24096900	1.45853900	4.00205400 L
B-B_2	0	-0.04102800	0.65219600	3.80723400 L
B-B_2	0	-1.32611500	2.64483200	3.04537800 L
N-N_3	0	-1.31959200	1.46096600	4.02141100 L
N-N_3	0	-2.61708000	3.44011400	2.85183500 L
B-B_2	0	-3.89784000	2.62784900	3.06525100 L
B-B_2	0	-5.20128800	3.92661400	1.42163300 L
N-N_3	0	-5.18988800	3.42109300	2.86583900 L
N-N_3	0	-6.49832000	4.47310800	0.82468800 L
B-B_2	0	-7.77595300	3.89497100	1.43364600 L
B-B_2	0	-9.07482300	4.10028300	-0.66523000 L
N-N_3	0	-9.06206100	4.45731500	0.83371300 L
N-N_3	0	-10.38157100	4.23743400	-1.46527300 L
B-B_2	0	-11.61168000	3.92742900	-0.59111600 L
B-	0	-12.89824500	3.42550300	-2.68449900 L
N-N_3	0	-12.81481600	3.18047400	-1.16848500 L
B-	0	12.78777500	-2.92209400	2.29014500 L
B-B_2	0	11.52047200	-1.45665300	3.81240300 L
N-N_3	0	11.57988600	-2.88725300	3.26583700 L
N-N_3	0	10.21952600	-0.82690000	4.31084100 L
B-B_2	0	8.95654300	-1.44733600	3.72432300 L
B-B_2	0	7.66500600	0.67108400	3.90286800 L
N-N_3	0	7.65949700	-0.82498600	4.24401300 L
N-N_3	0	6.37027400	1.47106400	4.07126800 L
B-B_2	0	5.09272500	0.66198200	3.84521500 L
B-B_2	0	3.80867000	2.63704800	3.03988000 L
N-N_3	0	3.80215300	1.46280300	4.02419900 L
N-N_3	0	2.52580200	3.45048800	2.84524900 L
B-B_2	0	1.23980000	2.64347500	3.02660600 L
B-B_2	0	-0.04806200	4.06542000	1.44156500 L
N-N_3	0	-0.04353800	3.45943300	2.85384000 L
N-N_3	0	-1.35005100	4.59529600	0.82985600 L
B-B_2	0	-2.62489100	3.98244100	1.41887800 L
B-B_2	0	-3.92063600	4.19178800	-0.67093300 L
N-N_3	0	-3.92586500	4.52355200	0.82318100 L
N-N_3	0	-5.21352900	4.31632500	-1.48049500 L
B-B_2	0	-6.49814800	4.13809100	-0.66987500 L
B-B_2	0	-7.77152700	3.20769500	-2.57611000 L
N-N_3	0	-7.79031100	4.27937300	-1.48073600 L
N-N_3	0	-9.03888500	2.94267800	-3.38379200 L

B-B_2	0	-10.34109300	3.25146100	-2.64178000 L
B-B_2	0	-11.58347700	1.44855300	-3.68036900 L
N-N_3	0	-11.61747500	2.95273000	-3.41759000 L
N-N_3	0	-12.80140600	0.58280000	-3.35637600 L
B-	0	12.76127500	0.60580000	3.60516500 L
N-N_3	0	12.80254300	-0.77947500	4.25868200 L
N-N_3	0	11.55438100	1.44590000	4.10038500 L
B-B_2	0	10.23545000	0.66688500	3.93888400 L
B-B_2	0	8.95113800	2.63811300	3.11966900 L
N-N_3	0	8.94830600	1.48098500	4.12469800 L
N-N_3	0	7.66624200	3.43115600	2.87801300 L
B-B_2	0	6.37972300	2.63102200	3.07172600 L
B-B_2	0	5.10704700	3.98076200	1.42373000 L
N-N_3	0	5.09689800	3.43806100	2.85520900 L
N-N_3	0	3.82935900	4.58041500	0.82966600 L
B-B_2	0	2.52972500	4.03584500	1.42752900 L
B-B_2	0	1.24346500	4.29830200	-0.67105400 L
N-N_3	0	1.24471300	4.62277500	0.83256000 L
N-N_3	0	-0.05063000	4.41419800	-1.48757300 L
B-B_2	0	-1.34181400	4.27289100	-0.67256900 L
B-B_2	0	-2.62127600	3.25611200	-2.54048900 L
N-N_3	0	-2.63736300	4.36795100	-1.48497300 L
N-N_3	0	-3.90372200	2.94421200	-3.31718900 L
B-B_2	0	-5.19725500	3.22387600	-2.55218700 L
B-B_2	0	-6.46912800	1.45205900	-3.73717100 L
N-N_3	0	-6.47567500	2.93228600	-3.33936600 L
N-N_3	0	-7.74516000	0.82920300	-4.31263800 L
B-B_2	0	-9.04404300	1.45658000	-3.79334400 L
B-B_2	0	-10.31367300	-0.67263700	-4.09045200 L
N-N_3	0	-10.33750500	0.83931200	-4.35174800 L
N-N_3	0	-11.59152200	-1.48217200	-4.26281600 L
B-	0	-12.86846200	-0.60664100	-4.32937500 L
N-N_3	0	12.80362800	3.42326400	2.88747600 L
B-B_2	0	11.51503800	2.69305800	3.21173300 L
B-B_2	0	10.25750200	3.90383500	1.45201600 L
N-N_3	0	10.22353000	3.45229100	2.92155200 L
N-N_3	0	8.98512900	4.49790500	0.83690800 L
B-B_2	0	7.68431300	3.94834300	1.43513700 L
B-B_2	0	6.40266100	4.18616700	-0.65982900 L
N-N_3	0	6.40512500	4.53129400	0.83057000 L
N-N_3	0	5.12127900	4.35706000	-1.47609600 L
B-B_2	0	3.82549300	4.25074300	-0.66712100 L
B-B_2	0	2.53197700	3.27697500	-2.52851600 L
N-N_3	0	2.53905800	4.40154900	-1.48391200 L

N-N_3	0	1.24601700	2.96475300	-3.29449200 L
B-B_2	0	-0.04558100	3.29665000	-2.54516000 L
B-B_2	0	-1.32585300	1.47177600	-3.66050000 L
N-N_3	0	-1.33184500	2.96672000	-3.30891500 L
N-N_3	0	-2.60239700	0.83058000	-4.20594600 L
B-B_2	0	-3.89556900	1.45767800	-3.68727300 L
B-B_2	0	-5.17514300	-0.65956500	-3.88936600 L
N-N_3	0	-5.17064300	0.82860800	-4.25224900 L
N-N_3	0	-6.45423500	-1.46689000	-4.11082900 L
B-B_2	0	-7.74678700	-0.66260500	-3.95843300 L
B-B_2	0	-9.04899100	-2.61199900	-3.14501500 L
N-N_3	0	-9.01622900	-1.47804300	-4.18840400 L
N-N_3	0	-10.35902300	-3.38438500	-2.91008000 L
B-B_2	0	-11.58920000	-2.47747200	-3.10603700 L
B-	0	-12.90828500	-4.00320300	-1.62940700 L
N-N_3	0	-12.78796000	-2.56654300	-2.16263400 L
B-	0	12.79486500	3.56320800	1.36126800 L
B-B_2	0	11.54484600	4.20291000	-0.66698500 L
N-N_3	0	11.58834000	4.39930200	0.85335400 L
N-N_3	0	10.25239400	4.31082100	-1.47357900 L
B-B_2	0	8.97699900	4.15491200	-0.65551300 L
B-B_2	0	7.68684700	3.22128300	-2.54340100 L
N-N_3	0	7.69328400	4.31446200	-1.46836400 L
N-N_3	0	6.39242300	2.93428900	-3.30630900 L
B-B_2	0	5.10971400	3.24475100	-2.52865800 L
B-B_2	0	3.81291500	1.45471200	-3.63196200 L
N-N_3	0	3.81889700	2.94875200	-3.29084600 L
N-N_3	0	2.52412400	0.82600400	-4.15629800 L
B-B_2	0	1.24314800	1.46483600	-3.62129700 L
B-B_2	0	-0.04024900	-0.65930700	-3.79605000 L
N-N_3	0	-0.03515100	0.83054500	-4.16570300 L
N-N_3	0	-1.31969500	-1.46353100	-4.01549300 L
B-B_2	0	-2.60607300	-0.65734500	-3.83366700 L
B-B_2	0	-3.89895700	-2.62980700	-3.06470600 L
N-N_3	0	-3.88472200	-1.46415600	-4.05849200 L
N-N_3	0	-5.19147800	-3.42241700	-2.86641700 L
B-B_2	0	-6.47342900	-2.61924900	-3.10047100 L
B-B_2	0	-7.77748700	-3.89536000	-1.43381100 L
N-N_3	0	-7.76731700	-3.41166700	-2.88770400 L
N-N_3	0	-9.06375300	-4.45711700	-0.83379000 L
B-B_2	0	-10.34841100	-3.92962500	-1.47503100 L
B-B_2	0	-11.61292700	-3.92615600	0.59143000 L
N-N_3	0	-11.64204000	-4.43505700	-0.84814200 L
N-N_3	0	-12.81626600	-3.17998700	1.16945500 L

B-	0	12.78697300	2.91489400	-2.28787200 L
N-N_3	0	12.83372000	4.20926600	-1.46672400 L
N-N_3	0	11.57971900	2.88330600	-3.26439300 L
B-B_2	0	10.26018100	3.19611100	-2.53414200 L
B-B_2	0	8.95545800	1.44397600	-3.72124500 L
N-N_3	0	8.97356600	2.92494900	-3.32505400 L
N-N_3	0	7.65738900	0.82139600	-4.23878700 L
B-B_2	0	6.38337300	1.44645000	-3.66948700 L
B-B_2	0	5.09131500	-0.66855000	-3.84030700 L
N-N_3	0	5.08871800	0.82294800	-4.19102600 L
N-N_3	0	3.80137200	-1.47004700	-4.02427600 L
B-B_2	0	2.52374000	-0.66463600	-3.79830700 L
B-B_2	0	1.23864300	-2.66324800	-3.04177100 L
N-N_3	0	1.23979700	-1.46708400	-4.00310800 L
N-N_3	0	-0.04766500	-3.47340700	-2.86022400 L
B-B_2	0	-1.32756900	-2.65114700	-3.04389800 L
B-B_2	0	-2.62691500	-3.98918500	-1.42131500 L
N-N_3	0	-2.61933700	-3.44423100	-2.85303000 L
N-N_3	0	-3.92817400	-4.52671700	-0.82394700 L
B-B_2	0	-5.20308300	-3.92933200	-1.42272400 L
B-B_2	0	-6.49921400	-4.13879200	0.66937200 L
N-N_3	0	-6.50024300	-4.47441700	-0.82512700 L
N-N_3	0	-7.79132800	-4.27964500	1.48059400 L
B-B_2	0	-9.07605600	-4.10032100	0.66523300 L
N-N_3	0	-10.38282200	-4.23686000	1.46539400 L
N-N_3	0	12.80067100	0.77731000	-4.26295700 L
B-B_2	0	11.51934300	1.45385300	-3.81386700 L
B-B_2	0	10.23446000	-0.66976600	-3.93824200 L
N-N_3	0	10.21758200	0.82396100	-4.31000700 L
N-N_3	0	8.94751400	-1.48419500	-4.12365700 L
B-B_2	0	7.66380500	-0.67522800	-3.90017300 L
B-B_2	0	6.37977900	-2.63861800	-3.07476000 L
N-N_3	0	6.36945100	-1.47550500	-4.07045900 L
N-N_3	0	5.09814900	-3.44773000	-2.85964300 L
B-B_2	0	3.80848500	-2.65031300	-3.04732500 L
B-B_2	0	2.52919700	-4.03733800	-1.42792500 L
N-N_3	0	2.52636300	-3.46563900	-2.85177200 L
N-N_3	0	1.24556700	-4.63320900	-0.83457700 L
B-B_2	0	-0.04978700	-4.08124000	-1.44698800 L
B-B_2	0	-1.34075800	-4.25528200	0.66846200 L
N-N_3	0	-1.35185700	-4.59902100	-0.82832900 L
N-N_3	0	-2.63603500	-4.36042400	1.48043800 L
B-B_2	0	-3.92164900	-4.18873200	0.66845100 L
N-N_3	0	-5.21370100	-4.31613200	1.47941800 L

B-	0	12.76142600	-0.60765700	-3.60872000 L
B-B_2	0	11.51520600	-2.69384100	-3.20917400 L
N-N_3	0	11.55355400	-1.44852400	-4.10040800 L
N-N_3	0	10.22441800	-3.45470100	-2.92011600 L
B-B_2	0	8.95124600	-2.64200200	-3.11951100 L
B-B_2	0	7.68462100	-3.95144700	-1.43545200 L
N-N_3	0	7.66730400	-3.43656300	-2.87912800 L
N-N_3	0	6.40495900	-4.53204100	-0.82978600 L
B-B_2	0	5.10744400	-3.98321600	-1.42576800 L
B-B_2	0	3.82425700	-4.23419100	0.66525500 L
N-N_3	0	3.82882700	-4.57666700	-0.82751100 L
N-N_3	0	2.54114600	-4.39711300	1.48451300 L
B-B_2	0	1.24241200	-4.31667800	0.67322400 L
N-N_3	0	-0.05433000	-4.41557900	1.48719300 L
B-	0	12.79391900	-3.56282300	-1.35708100 L
N-N_3	0	12.80446400	-3.42227500	-2.88323500 L
N-N_3	0	11.58826100	-4.40140000	-0.85137500 L
B-B_2	0	10.25761500	-3.90609100	-1.45042400 L
B-B_2	0	8.97623100	-4.15581600	0.65658200 L
N-N_3	0	8.98504000	-4.50009600	-0.83563100 L
N-N_3	0	7.69159000	-4.31352300	1.46871000 L
B-B_2	0	6.40215800	-4.18063600	0.65898200 L
N-N_3	0	5.11951100	-4.34820600	1.47381500 L
N-N_3	0	12.83243000	-4.21700100	1.46976100 L
B-B_2	0	11.54404900	-4.20820000	0.66939100 L
N-N_3	0	10.25093500	-4.31402200	1.47524700 L
H-H_	0	-12.66882300	-0.20881300	2.38956800 L
H-H_	0	-12.59903600	1.93326500	1.35766900 L
H-H_	0	-12.65436800	2.16150600	-1.01019400 L
H-H_	0	-12.67061500	0.21024000	-2.39053800 L
H-H_	0	12.75607500	-0.65396200	5.29532000 L
H-H_	0	12.74490100	4.38047800	3.30319200 L
H-H_	0	-12.59799900	-1.93082500	-1.35709000 L
H-H_	0	-12.65668300	-2.16092900	1.01091500 L
H-H_	0	12.79665000	5.01666800	-2.12946300 L
H-H_	0	12.75174300	0.65126400	-5.29941800 L
H-H_	0	12.74781600	-4.37940000	-3.29944800 L
H-H_	0	12.79320100	-5.02392600	2.13295600 L
C-C_R	0	0.69208800	0.04944100	0.29284300 H
H-H_	0	-1.22663600	0.98493400	0.67222200 H
H-H_	0	-0.84646200	0.73232500	-1.03535100 H
C-C_3	0	-0.40920700	0.97862000	-0.05547600 H
H-H_	0	0.01058900	1.96539800	-0.11551200 H
N-N_R	0	0.24736400	-1.40927300	0.06462500 H

H-H_	0	1.07969000	-1.85428800	-0.32458500 H
H-H_	0	0.36962200	-0.95114300	1.12531200 H
C-C_R	0	2.08051600	0.12354200	-0.02903500 H
O-O_R	0	2.77990600	-0.87485500	-0.27230300 H
O-O_R	0	2.63450000	1.35979600	0.00117800 H
H-H_	0	3.58156300	1.22885900	-0.16621500 H
H-H_	0	-0.62503900	-1.47560600	-0.45109700 H

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B-B_2	0	10.35121000	3.20804700	2.70040900 L
N-N_3	0	11.62841200	2.90013600	3.47086100 L
B-	0	12.90814700	3.38821500	2.74626700 L
B-B_2	0	5.20696500	3.17347800	2.61669800 L
N-N_3	0	6.48678700	2.87671300	3.39968800 L
B-B_2	0	7.78142800	3.16132900	2.63731300 L

B-B_2	0	9.05738500	1.39649000	3.82906900 L
N-N_3	0	9.05029700	2.88789500	3.43977000 L
N-N_3	0	10.35300700	0.77013500	4.37264800 L
B-B_2	0	11.59714500	1.39200700	3.70941300 L
B-	0	12.88426800	-0.67492100	4.30998600 L
N-N_3	0	12.81111300	0.53128500	3.35851900 L
B-B_2	0	0.05436800	3.23737500	2.60789700 L
N-N_3	0	1.34032900	2.89943300	3.36894100 L
B-B_2	0	2.63103300	3.19730300	2.60512200 L
B-B_2	0	3.90762900	1.39649500	3.73774200 L
N-N_3	0	3.91395900	2.88553000	3.38051000 L
N-N_3	0	5.18472700	0.76226600	4.29324500 L
B-B_2	0	6.48179100	1.39253200	3.78220600 L
B-B_2	0	7.76101100	-0.72386500	3.96277500 L
N-N_3	0	7.76040700	0.76128300	4.34324200 L
N-N_3	0	9.03129900	-1.54389000	4.17091200 L
B-B_2	0	10.32845900	-0.73691800	4.08389800 L
B-B_2	0	11.59952600	-2.52340200	3.05954400 L
N-N_3	0	11.60728400	-1.54962800	4.23472100 L
N-N_3	0	12.79882700	-2.60323300	2.11581200 L
B-B_2	0	-5.09948400	3.17723500	2.58181700 L
N-N_3	0	-3.80863300	2.87970300	3.34437800 L
B-B_2	0	-2.52194700	3.20678200	2.58011500 L
B-B_2	0	-1.23394000	1.40718700	3.70791600 L
N-N_3	0	-1.23865200	2.90415000	3.35603000 L
N-N_3	0	0.04999100	0.76856200	4.23864600 L
B-B_2	0	1.33456100	1.40246400	3.70724100 L
B-B_2	0	2.61883300	-0.72010200	3.87009000 L
N-N_3	0	2.61425400	0.76410100	4.25096200 L
N-N_3	0	3.90095500	-1.52837700	4.06622400 L
B-B_2	0	5.18902200	-0.71959500	3.90711300 L
B-B_2	0	6.48453100	-2.65881700	3.06631100 L
N-N_3	0	6.46951100	-1.53091200	4.10406500 L
N-N_3	0	7.77647500	-3.44820600	2.83243300 L
B-B_2	0	9.05989700	-2.65609900	3.10412100 L
B-B_2	0	10.35390500	-3.94565800	1.40720900 L
N-N_3	0	10.36805500	-3.42574700	2.85160300 L
N-N_3	0	11.64514400	-4.44669900	0.77213000 L
B-	0	12.91351200	-4.03164600	1.55927200 L
B-B_2	0	-10.24921200	3.14418900	2.58515600 L
N-N_3	0	-8.96379400	2.86296700	3.37447200 L
B-B_2	0	-7.67599300	3.16267100	2.59601300 L
B-B_2	0	-6.37553100	1.38082300	3.71775900 L
N-N_3	0	-6.38258900	2.86929200	3.35905000 L

N-N_3	0	-5.08349600	0.75396200	4.24195200 L
B-B_2	0	-3.80310700	1.38826100	3.69574300 L
B-B_2	0	-2.51540800	-0.72738000	3.86193400 L
N-N_3	0	-2.51771400	0.76181400	4.23270300 L
N-N_3	0	-1.23123500	-1.53625300	4.04343500 L
B-B_2	0	0.05241700	-0.72339000	3.87148700 L
B-B_2	0	1.33840500	-2.67464800	3.02258000 L
N-N_3	0	1.33614400	-1.53200500	4.04644600 L
N-N_3	0	2.62802300	-3.46530500	2.80200400 L
B-B_2	0	3.91062500	-2.66332800	3.03806400 L
B-B_2	0	5.20894800	-3.92193200	1.35768300 L
N-N_3	0	5.20069200	-3.45329300	2.81441700 L
N-N_3	0	6.50307800	-4.46318900	0.74987900 L
B-B_2	0	7.78330200	-3.90066000	1.36833500 L
B-B_2	0	9.07989300	-4.07904000	-0.73539700 L
N-N_3	0	9.06678300	-4.45791600	0.75825100 L
N-N_3	0	10.38594400	-4.21013400	-1.53766400 L
B-B_2	0	11.61736100	-3.91642300	-0.65963500 L
B-	0	12.90512300	-3.38789100	-2.74606500 L
N-N_3	0	12.82293400	-3.16555300	-1.22653400 L
B-	0	-12.77620100	2.87119700	2.33402300 L
B-B_2	0	-11.51208800	1.38817600	3.84146400 L
N-N_3	0	-11.56978400	2.82464800	3.31072500 L
N-N_3	0	-10.21249900	0.75258700	4.33540100 L
B-B_2	0	-8.94801000	1.37884000	3.75834300 L
B-B_2	0	-7.65762700	-0.74057700	3.91735100 L
N-N_3	0	-7.65238700	0.75123500	4.27528800 L
N-N_3	0	-6.36424400	-1.54367000	4.07732900 L
B-B_2	0	-5.08441900	-0.73268500	3.87315700 L
B-B_2	0	-3.79916200	-2.68525100	3.03060800 L
N-N_3	0	-3.79677900	-1.53848400	4.04809100 L
N-N_3	0	-2.51464200	-3.48905900	2.80889200 L
B-B_2	0	-1.22937600	-2.68783900	3.02581200 L
B-B_2	0	0.05776700	-4.03378300	1.37313400 L
N-N_3	0	0.05758700	-3.48647300	2.80898200 L
N-N_3	0	1.35629900	-4.55863400	0.75325400 L
B-B_2	0	2.63337400	-3.96394700	1.35403100 L
B-B_2	0	3.92622000	-4.14668400	-0.74019800 L
N-N_3	0	3.93085300	-4.50168000	0.74837800 L
N-N_3	0	5.21748400	-4.27205800	-1.55176100 L
B-B_2	0	6.50317900	-4.10597400	-0.73970900 L
B-B_2	0	7.77842100	-3.16135100	-2.63735300 L
N-N_3	0	7.79435200	-4.24385000	-1.55267100 L
N-N_3	0	9.04724900	-2.88838000	-3.44003800 L

B-B_2	0	10.34813900	-3.20848000	-2.70076200 L
B-B_2	0	11.59420200	-1.39273000	-3.71082500 L
N-N_3	0	11.62540600	-2.90077100	-3.47136800 L
N-N_3	0	12.81014900	-0.53273100	-3.36481100 L
B-	0	-12.75360700	-0.67102100	3.60714300 L
N-N_3	0	-12.79525400	0.70627600	4.27735100 L
N-N_3	0	-11.54751800	-1.51756100	4.09335200 L
B-B_2	0	-10.22817100	-0.73649800	3.94542800 L
B-B_2	0	-8.94224600	-2.69214000	3.09699800 L
N-N_3	0	-8.94175200	-1.55328000	4.12251700 L
N-N_3	0	-7.65624000	-3.47793800	2.83836600 L
B-B_2	0	-6.37078000	-2.68161100	3.05288500 L
B-B_2	0	-5.09503800	-3.98289900	1.36997100 L
N-N_3	0	-5.08674100	-3.48103300	2.81687000 L
N-N_3	0	-3.81524600	-4.56550100	0.76270900 L
B-B_2	0	-2.51770800	-4.02361200	1.36951100 L
B-B_2	0	-1.23510500	-4.26769500	-0.74177900 L
N-N_3	0	-1.23223700	-4.59558500	0.76228800 L
N-N_3	0	0.06035300	-4.36343300	-1.55935900 L
B-B_2	0	1.34761700	-4.21088400	-0.74182300 L
B-B_2	0	2.62795600	-3.20073100	-2.60896700 L
N-N_3	0	2.64178100	-4.31249500	-1.55454100 L
N-N_3	0	3.91154600	-2.88772800	-3.38282800 L
B-B_2	0	5.20397200	-3.17369000	-2.61743500 L
B-B_2	0	6.47899200	-1.39300900	-3.78226400 L
N-N_3	0	6.48399300	-2.87719600	-3.39999800 L
N-N_3	0	7.75741200	-0.76139400	-4.34300700 L
B-B_2	0	9.05446500	-1.39704200	-3.82960000 L
B-B_2	0	10.32572500	0.73606800	-4.08549400 L
N-N_3	0	10.34988800	-0.77104600	-4.37389000 L
N-N_3	0	11.60440400	1.54855900	-4.23784400 L
B-	0	12.88114600	0.67379400	-4.31610700 L
N-N_3	0	-12.79360500	-3.47878900	2.84959200 L
B-B_2	0	-11.50629500	-2.75309500	3.18829100 L
B-B_2	0	-10.24680900	-3.92157300	1.40200900 L
N-N_3	0	-10.21341400	-3.50328000	2.88127600 L
N-N_3	0	-8.97302500	-4.49855900	0.77310300 L
B-B_2	0	-7.67300300	-3.95947500	1.38317300 L
B-B_2	0	-6.39206100	-4.15088400	-0.71827400 L
N-N_3	0	-6.39200500	-4.52491600	0.76520300 L
N-N_3	0	-5.11256600	-4.30979500	-1.53911800 L
B-B_2	0	-3.81517300	-4.21890500	-0.73131300 L
B-B_2	0	-2.52469600	-3.21427500	-2.58125000 L
N-N_3	0	-2.53115200	-4.35580700	-1.55359500 L

N-N_3	0	-1.24219700	-2.90233800	-3.35420200 L
B-B_2	0	0.05220600	-3.24174600	-2.61270800 L
B-B_2	0	1.33300300	-1.40963500	-3.71577300 L
N-N_3	0	1.33808500	-2.90691000	-3.37600700 L
N-N_3	0	2.61170900	-0.76411300	-4.25257600 L
B-B_2	0	3.90459800	-1.39855400	-3.74061100 L
B-B_2	0	5.18624000	0.71886700	-3.90141100 L
N-N_3	0	5.18208100	-0.76191100	-4.29228600 L
N-N_3	0	6.46637000	1.53073800	-4.10009100 L
B-B_2	0	7.75831300	0.72349200	-3.96136700 L
B-B_2	0	9.05873300	2.65518800	-3.10358200 L
N-N_3	0	9.02853700	1.54334700	-4.17067400 L
N-N_3	0	10.36753100	3.42428600	-2.85231300 L
B-B_2	0	11.59842700	2.52158100	-3.06210300 L
B-	0	12.91483200	4.02565000	-1.56093400 L
N-N_3	0	12.79691900	2.59739800	-2.11709500 L
B-	0	-12.78576800	-3.58550400	1.32055000 L
B-B_2	0	-11.53419600	-4.17287600	-0.72224100 L
N-N_3	0	-11.57688400	-4.40612800	0.79277500 L
N-N_3	0	-10.24233000	-4.26822200	-1.53167900 L
B-B_2	0	-8.96659700	-4.12363500	-0.71162500 L
B-B_2	0	-7.67869200	-3.16103200	-2.58842900 L
N-N_3	0	-7.68325600	-4.26828100	-1.52771700 L
N-N_3	0	-6.38543600	-2.86584600	-3.35028200 L
B-B_2	0	-5.10213300	-3.18287500	-2.57676900 L
B-B_2	0	-3.80626300	-1.38493300	-3.67689500 L
N-N_3	0	-3.81272300	-2.88019800	-3.33886200 L
N-N_3	0	-2.51977900	-0.75584200	-4.20737700 L
B-B_2	0	-1.23763800	-1.40131300	-3.68131200 L
B-B_2	0	0.04812300	0.72221300	-3.83221500 L
N-N_3	0	0.04261100	-0.76365000	-4.21941200 L
N-N_3	0	1.33132400	1.52819200	-4.02072600 L
B-B_2	0	2.61616600	0.71658800	-3.85529700 L
B-B_2	0	3.90937500	2.66422900	-3.02928600 L
N-N_3	0	3.89680800	1.52719600	-4.05540600 L
N-N_3	0	5.20024100	3.45417800	-2.81032500 L
B-B_2	0	6.48330100	2.65864000	-3.06237300 L
B-B_2	0	7.78463500	3.90177200	-1.36720100 L
N-N_3	0	7.77592000	3.44784800	-2.83082400 L
N-N_3	0	9.06912600	4.45781600	-0.75818100 L
B-B_2	0	10.35515700	3.94389800	-1.40778300 L
B-B_2	0	11.61992700	3.91413000	0.65859400 L
N-N_3	0	11.64749200	4.44348000	-0.77357300 L
N-N_3	0	12.82695300	3.16630700	1.22657300 L

B-	0	-12.77707300	-2.86098500	-2.32357600 L
N-N_3	0	-12.82377200	-4.16679100	-1.52102200 L
N-N_3	0	-11.57198000	-2.81797000	-3.30197600 L
B-B_2	0	-10.25159100	-3.13893900	-2.57691400 L
B-B_2	0	-8.94913900	-1.37311400	-3.74780600 L
N-N_3	0	-8.96609100	-2.85789500	-3.36606500 L
N-N_3	0	-7.65245700	-0.74551100	-4.26262600 L
B-B_2	0	-6.37703500	-1.37529600	-3.70232200 L
B-B_2	0	-5.08450500	0.74067500	-3.86151800 L
N-N_3	0	-5.08435800	-0.74818300	-4.22451500 L
N-N_3	0	-3.79563800	1.54534200	-4.04093400 L
B-B_2	0	-2.51659100	0.73354200	-3.83931400 L
B-B_2	0	-1.22932400	2.70238800	-3.01993900 L
N-N_3	0	-1.23045600	1.53777200	-4.02068800 L
N-N_3	0	0.06002200	3.49752800	-2.80230000 L
B-B_2	0	1.33800600	2.67938100	-3.00735800 L
B-B_2	0	2.63535100	3.97648000	-1.35044800 L
N-N_3	0	2.62848900	3.46933500	-2.79537900 L
N-N_3	0	3.93424100	4.51059800	-0.74554400 L
B-B_2	0	5.21052800	3.92749600	-1.35510400 L
B-B_2	0	6.50610300	4.10900300	0.74115800 L
N-N_3	0	6.50585000	4.46657900	-0.74835500 L
N-N_3	0	7.79771000	4.24486500	1.55364200 L
B-B_2	0	9.08270400	4.07934200	0.73558700 L
N-N_3	0	10.38924700	4.20944200	1.53710900 L
N-N_3	0	-12.79527300	-0.70129400	-4.27454000 L
B-B_2	0	-11.51299700	-1.38250100	-3.83539400 L
B-B_2	0	-10.22872800	0.74215800	-3.93878200 L
N-N_3	0	-10.21250300	-0.74718700	-4.32743700 L
N-N_3	0	-8.94234200	1.55905800	-4.11652600 L
B-B_2	0	-7.65778600	0.74745500	-3.90880500 L
B-B_2	0	-6.37122200	2.69477100	-3.05455600 L
N-N_3	0	-6.36416100	1.55046500	-4.07198500 L
N-N_3	0	-5.08871500	3.49808500	-2.82183100 L
B-B_2	0	-3.79946900	2.70663500	-3.03879700 L
B-B_2	0	-2.51764000	4.04169800	-1.37109200 L
N-N_3	0	-2.51328000	3.50795000	-2.81174400 L
N-N_3	0	-1.23159800	4.61740600	-0.76061600 L
B-B_2	0	0.05960200	4.05368300	-1.36933700 L
B-B_2	0	1.34942900	4.21496700	0.74406600 L
N-N_3	0	1.35911700	4.57271300	-0.74809900 L
N-N_3	0	2.64430000	4.31359500	1.55635100 L
B-B_2	0	3.92930300	4.15199500	0.74194300 L
N-N_3	0	5.22068100	4.27459400	1.55386300 L

B-	0	-12.75544400	0.67602100	-3.60439100 L
B-B_2	0	-11.50778600	2.75675000	-3.18014500 L
N-N_3	0	-11.54827600	1.52294500	-4.08748100 L
N-N_3	0	-10.21556600	3.50860500	-2.87480600 L
B-B_2	0	-8.94340800	2.69953600	-3.09305500 L
B-B_2	0	-7.67384200	3.96499700	-1.38039800 L
N-N_3	0	-7.65850400	3.48738300	-2.83676500 L
N-N_3	0	-6.39249100	4.52734400	-0.76138200 L
B-B_2	0	-5.09580700	3.99127400	-1.37181900 L
B-B_2	0	-3.81328400	4.19559500	0.72830200 L
N-N_3	0	-3.81645600	4.56821000	-0.75829200 L
N-N_3	0	-2.53383400	4.35083300	1.55475600 L
B-B_2	0	-1.23275800	4.29509500	0.74695400 L
N-N_3	0	0.06441000	4.36946700	1.56451400 L
B-	0	-12.78492600	3.58662300	-1.30927500 L
N-N_3	0	-12.79571800	3.48013000	-2.83836100 L
N-N_3	0	-11.57668000	4.40981700	-0.78426600 L
B-B_2	0	-10.24728900	3.92569500	-1.39508300 L
B-B_2	0	-8.96473600	4.12447200	0.71725300 L
N-N_3	0	-8.97298600	4.50209800	-0.76696000 L
N-N_3	0	-7.67956800	4.26638600	1.53151900 L
B-B_2	0	-6.39081700	4.14255200	0.71919700 L
N-N_3	0	-5.10894300	4.29628000	1.53709200 L
N-N_3	0	-12.82060500	4.17709700	1.53159900 L
B-B_2	0	-11.53214900	4.17944500	0.73120900 L
N-N_3	0	-10.23895500	4.27247200	1.53896300 L
H-H_	0	12.67038800	0.17534800	2.38777700 L
H-H_	0	12.61288600	-1.95365100	1.32043500 L
H-H_	0	12.66670500	-2.14859300	-1.05226800 L
H-H_	0	12.67380100	-0.17707600	-2.39336500 L
H-H_	0	-12.75062600	0.56815800	5.31246500 L
H-H_	0	-12.73217100	-4.44477700	3.24407000 L
H-H_	0	12.60778900	1.94869700	-1.32171400 L
H-H_	0	12.67372300	2.14901300	1.05173100 L
H-H_	0	-12.78808900	-4.96488200	-2.19502400 L
H-H_	0	-12.74812400	-0.56324300	-5.30955200 L
H-H_	0	-12.73691500	4.44628000	-3.23284700 L
H-H_	0	-12.78174700	4.97505900	2.20558000 L
C-C_3	0	-0.96921800	0.01645400	0.39220400 H
H-H_	0	1.00675400	-0.81141000	0.38889100 H
H-H_	0	0.31371800	-0.59211200	-1.22628900 H
C-C_3	0	0.09016900	-0.89220200	-0.20297000 H
H-H_	0	-0.24003600	-1.91374200	-0.18837200 H
N-N_3	0	-0.55736700	1.38981700	0.27729200 H

H-H_	0	-1.24037700	1.84691600	-0.31066900 H
H-H_	0	-1.09851000	-0.26943700	1.43707600 H
C-C_R	0	-2.37770700	-0.12036000	-0.17118500 H
O-O_R	0	-2.99833800	0.77674300	-0.70402500 H
O-O_R	0	-2.93280900	-1.32060600	0.07119000 H
H-H_	0	-3.84733700	-1.28011100	-0.25662300 H
H-H_	0	0.35828100	1.46287800	-0.14902500 H

aRTS4@ B

B-B_2	0	10.35394800	3.25251200	2.64676400 L
N-N_3	0	11.63033100	2.95468700	3.42260900 L
B-	0	12.91091100	3.42887600	2.69019900 L
B-B_2	0	5.20983700	3.22509000	2.55852300 L
N-N_3	0	6.48823600	2.93483900	3.34643900 L
B-B_2	0	7.78422700	3.20895900	2.58233600 L

B-B_2	0	9.05704900	1.45890000	3.79999700 L
N-N_3	0	9.05194200	2.94468400	3.38961700 L
N-N_3	0	10.35108000	0.84072500	4.35651400 L
B-B_2	0	11.59687100	1.45052400	3.68515300 L
B-	0	12.88169500	-0.60627800	4.32771700 L
N-N_3	0	12.81319000	0.58432400	3.35635500 L
B-B_2	0	0.05606100	3.28717700	2.53310100 L
N-N_3	0	1.34049000	2.95659600	3.30076500 L
B-B_2	0	2.63396700	3.25156800	2.54050000 L
B-B_2	0	3.90767300	1.45885100	3.69313700 L
N-N_3	0	3.91482600	2.94454500	3.32192800 L
N-N_3	0	5.18278800	0.83230400	4.26184700 L
B-B_2	0	6.48158400	1.45511600	3.74602300 L
B-B_2	0	7.75951200	-0.65940800	3.96446700 L
N-N_3	0	7.75832900	0.83190800	4.32027800 L
N-N_3	0	9.02895400	-1.47578500	4.19107500 L
B-B_2	0	10.32654400	-0.67084000	4.09303000 L
B-B_2	0	11.59987300	-2.47489400	3.10381800 L
N-N_3	0	11.60437300	-1.48125500	4.26212100 L
N-N_3	0	12.79814500	-2.56495300	2.15984800 L
B-B_2	0	-5.09809200	3.23610300	2.52221500 L
N-N_3	0	-3.80540400	2.94233800	3.28315400 L
B-B_2	0	-2.52001700	3.26469700	2.51351200 L
B-B_2	0	-1.23236300	1.47084000	3.65589100 L
N-N_3	0	-1.23549700	2.96365600	3.28732400 L
N-N_3	0	0.05073100	0.83804600	4.19465800 L
B-B_2	0	1.33518200	1.46369000	3.65513000 L
B-B_2	0	2.61844000	-0.65709500	3.85596600 L
N-N_3	0	2.61323300	0.83352600	4.21136700 L
N-N_3	0	3.89928400	-1.46156400	4.07304500 L
B-B_2	0	5.18786500	-0.65606200	3.90089400 L
B-B_2	0	6.48461500	-2.61285100	3.10350800 L
N-N_3	0	6.46747100	-1.46358200	4.11757000 L
N-N_3	0	7.77746500	-3.40574500	2.88711000 L
B-B_2	0	9.05992700	-2.60767100	3.14528500 L
B-B_2	0	10.35694100	-3.92477900	1.47271200 L
N-N_3	0	10.36898600	-3.38084800	2.90826600 L
N-N_3	0	11.64966400	-4.43255700	0.84588000 L
B-	0	12.91683500	-4.00171400	1.62634500 L
B-B_2	0	-10.24861500	3.19922300	2.53115200 L
N-N_3	0	-8.96230500	2.92602200	3.32217400 L
B-B_2	0	-7.67500100	3.22016700	2.54037200 L
B-B_2	0	-6.37305900	1.44729800	3.67411600 L
N-N_3	0	-6.38028400	2.93296200	3.30371900 L

N-N_3	0	-5.08026500	0.82626800	4.20282000 L
B-B_2	0	-3.80065900	1.45365700	3.64672900 L
B-B_2	0	-2.51407700	-0.66149800	3.84232000 L
N-N_3	0	-2.51559900	0.83332100	4.19039600 L
N-N_3	0	-1.23050500	-1.46749900	4.03855600 L
B-B_2	0	0.05288500	-0.65906500	3.85008600 L
B-B_2	0	1.33872400	-2.63247100	3.05093300 L
N-N_3	0	1.33514500	-1.46481100	4.04628600 L
N-N_3	0	2.62858300	-3.42836600	2.85253500 L
B-B_2	0	3.91070600	-2.61995000	3.07120800 L
B-B_2	0	5.21170400	-3.91341900	1.42086200 L
N-N_3	0	5.20164300	-3.41369600	2.86711500 L
N-N_3	0	6.50744100	-4.46218100	0.82319100 L
B-B_2	0	7.78614700	-3.88603300	1.43199100 L
B-B_2	0	9.08389000	-4.09526400	-0.66766300 L
N-N_3	0	9.07122000	-4.45041700	0.83178400 L
N-N_3	0	10.39040200	-4.23535500	-1.46761400 L
B-B_2	0	11.62087900	-3.92493800	-0.59408600 L
B-	0	12.90772600	-3.42711000	-2.68825500 L
N-N_3	0	12.82457900	-3.17989400	-1.17261600 L
B-	0	-12.77640200	2.92315900	2.28456100 L
B-B_2	0	-11.50975600	1.45435100	3.80393200 L
N-N_3	0	-11.56868500	2.88599200	3.26038100 L
N-N_3	0	-10.20945400	0.82589300	4.30589400 L
B-B_2	0	-8.94570200	1.44540600	3.71950300 L
B-B_2	0	-7.65478100	-0.67285000	3.90471400 L
N-N_3	0	-7.64898800	0.82402400	4.24143500 L
N-N_3	0	-6.36124400	-1.47288000	4.07722500 L
B-B_2	0	-5.08213100	-0.66571800	3.85576200 L
B-B_2	0	-3.79784400	-2.63647200	3.05147500 L
N-N_3	0	-3.79491500	-1.46864100	4.04468900 L
N-N_3	0	-2.51398200	-3.44661700	2.85007600 L
B-B_2	0	-1.22837100	-2.64130000	3.04692600 L
B-B_2	0	0.05938300	-4.03900200	1.43686300 L
N-N_3	0	0.05740500	-3.44879800	2.85601300 L
N-N_3	0	1.35976700	-4.57070400	0.82691100 L
B-B_2	0	2.63568700	-3.96204800	1.41710400 L
B-B_2	0	3.93014900	-4.17605200	-0.67192900 L
N-N_3	0	3.93507200	-4.50712600	0.82201200 L
N-N_3	0	5.22196900	-4.30898700	-1.48163500 L
B-B_2	0	6.50718600	-4.12909700	-0.67192200 L
B-B_2	0	7.78098800	-3.20749500	-2.58190300 L
N-N_3	0	7.79895000	-4.27511500	-1.48259200 L
N-N_3	0	9.04891900	-2.94423300	-3.38922600 L

B-B_2	0	10.35066100	-3.25177700	-2.64609100 L
B-B_2	0	11.59403000	-1.45030700	-3.68584000 L
N-N_3	0	11.62732800	-2.95430300	-3.42188200 L
N-N_3	0	12.81284400	-0.58510300	-3.36337600 L
B-	0	-12.74911700	-0.60975300	3.59933900 L
N-N_3	0	-12.79258000	0.77734100	4.24875300 L
N-N_3	0	-11.54367900	-1.44765200	4.10118900 L
B-B_2	0	-10.22485500	-0.66893800	3.93796800 L
B-B_2	0	-8.93984200	-2.64183000	3.12510400 L
N-N_3	0	-8.93802200	-1.48222300	4.12734400 L
N-N_3	0	-7.65427200	-3.43390000	2.88350300 L
B-B_2	0	-6.36888500	-2.63239600	3.07711400 L
B-B_2	0	-5.09425000	-3.97715800	1.42598700 L
N-N_3	0	-5.08517000	-3.43761300	2.85920300 L
N-N_3	0	-3.81495000	-4.57597900	0.83299900 L
B-B_2	0	-2.51682800	-4.02018800	1.42595300 L
B-B_2	0	-1.23313900	-4.31698800	-0.67683700 L
N-N_3	0	-1.23168200	-4.61041200	0.83497900 L
N-N_3	0	0.06498500	-4.41301400	-1.49032100 L
B-B_2	0	1.35075900	-4.24556600	-0.67323500 L
B-B_2	0	2.63071200	-3.25429400	-2.55036400 L
N-N_3	0	2.64598900	-4.35422600	-1.48387100 L
N-N_3	0	3.91357300	-2.94742700	-3.32792100 L
B-B_2	0	5.20661000	-3.22343800	-2.56031500 L
B-B_2	0	6.47911700	-1.45524700	-3.74784000 L
N-N_3	0	6.48575600	-2.93461800	-3.34713800 L
N-N_3	0	7.75584300	-0.83133200	-4.32067500 L
B-B_2	0	9.05433300	-1.45869400	-3.80053100 L
B-B_2	0	10.32387400	0.67074100	-4.09442500 L
N-N_3	0	10.34823600	-0.84091300	-4.35745700 L
N-N_3	0	11.60141200	1.48101300	-4.26509500 L
B-	0	12.87853200	0.60603700	-4.33439800 L
N-N_3	0	-12.79116300	-3.43299800	2.89907400 L
B-B_2	0	-11.50343900	-2.69996900	3.21973500 L
B-B_2	0	-10.24596700	-3.91021000	1.46011100 L
N-N_3	0	-10.21123100	-3.45765700	2.92919700 L
N-N_3	0	-8.97316000	-4.50245500	0.84361000 L
B-B_2	0	-7.67220800	-3.95139300	1.44071300 L
B-B_2	0	-6.39205600	-4.19073000	-0.65597900 L
N-N_3	0	-6.39194300	-4.53228800	0.83520000 L
N-N_3	0	-5.11306600	-4.36355000	-1.47500100 L
B-B_2	0	-3.81454300	-4.26649800	-0.66927300 L
B-B_2	0	-2.52283900	-3.28093500	-2.52758000 L
N-N_3	0	-2.52936400	-4.41328000	-1.48899000 L

N-N_3	0	-1.23923800	-2.96938200	-3.29891800 L
B-B_2	0	0.05485800	-3.30063200	-2.55347000 L
B-B_2	0	1.33411000	-1.47535800	-3.67194800 L
N-N_3	0	1.34046900	-2.96968400	-3.31946800 L
N-N_3	0	2.61110100	-0.83430700	-4.21795500 L
B-B_2	0	3.90511000	-1.46198000	-3.70112100 L
B-B_2	0	5.18517000	0.65495800	-3.89476600 L
N-N_3	0	5.18089400	-0.83162500	-4.26358900 L
N-N_3	0	6.46412900	1.46383500	-4.11220500 L
B-B_2	0	7.75691700	0.65953100	-3.96275300 L
B-B_2	0	9.05869100	2.60709200	-3.14363500 L
N-N_3	0	9.02613000	1.47599200	-4.19019400 L
N-N_3	0	10.36843600	3.37977600	-2.90807400 L
B-B_2	0	11.59879300	2.47351900	-3.10591400 L
B-	0	12.91854100	3.99476200	-1.62687900 L
N-N_3	0	12.79568700	2.55822700	-2.15982500 L
B-	0	-12.78520400	-3.57441800	1.37294100 L
B-B_2	0	-11.53490100	-4.20645500	-0.65762900 L
N-N_3	0	-11.57691200	-4.40665000	0.86226200 L
N-N_3	0	-10.24306900	-4.31166500	-1.46551600 L
B-B_2	0	-8.96683400	-4.15788500	-0.64826700 L
B-B_2	0	-7.67840800	-3.21992200	-2.53467600 L
N-N_3	0	-7.68418000	-4.31600200	-1.46257300 L
N-N_3	0	-6.38478000	-2.93189700	-3.29835200 L
B-B_2	0	-5.10129400	-3.24652300	-2.52341400 L
B-B_2	0	-3.80486400	-1.45438300	-3.62922000 L
N-N_3	0	-3.81124500	-2.94877400	-3.28633900 L
N-N_3	0	-2.51849400	-0.82777400	-4.16141300 L
B-B_2	0	-1.23608900	-1.46973300	-3.63326800 L
B-B_2	0	0.04835700	0.65486200	-3.80578500 L
N-N_3	0	0.04263200	-0.83484500	-4.17821100 L
N-N_3	0	1.32937700	1.45912700	-4.01420200 L
B-B_2	0	2.61561000	0.65158900	-3.83970100 L
B-B_2	0	3.90926000	2.61835200	-3.05709400 L
N-N_3	0	3.89460000	1.45979100	-4.05906100 L
N-N_3	0	5.20057700	3.41340000	-2.85981900 L
B-B_2	0	6.48320300	2.61216200	-3.09706500 L
B-B_2	0	7.78773300	3.88809100	-1.42964600 L
N-N_3	0	7.77663000	3.40545900	-2.88394700 L
N-N_3	0	9.07412100	4.45115600	-0.83092200 L
B-B_2	0	10.35851100	3.92330700	-1.47236400 L
B-B_2	0	11.62391500	3.92300400	0.59404900 L
N-N_3	0	11.65257700	4.42926200	-0.84647100 L
N-N_3	0	12.82951400	3.18222700	1.17429000 L

B-	0	-12.77788800	-2.91247800	-2.27311700 L
N-N_3	0	-12.82446400	-4.20967500	-1.45637800 L
N-N_3	0	-11.57172000	-2.87849000	-3.25083800 L
B-B_2	0	-10.25163100	-3.19375900	-2.52274000 L
B-B_2	0	-8.94753900	-1.43943800	-3.70811900 L
N-N_3	0	-8.96577900	-2.92110900	-3.31428600 L
N-N_3	0	-7.64963600	-0.81775800	-4.22715800 L
B-B_2	0	-6.37549700	-1.44326400	-3.65867500 L
B-B_2	0	-5.08252900	0.67186600	-3.83535300 L
N-N_3	0	-5.08189300	-0.82079100	-4.18309600 L
N-N_3	0	-3.79298000	1.47260400	-4.02479400 L
B-B_2	0	-2.51562900	0.66424600	-3.80444700 L
B-B_2	0	-1.22904800	2.65441100	-3.03203500 L
N-N_3	0	-1.23110700	1.46595800	-4.00419900 L
N-N_3	0	0.06019200	3.45614500	-2.84106100 L
B-B_2	0	1.33807500	2.63265300	-3.02654900 L
B-B_2	0	2.63798500	3.97634000	-1.40959800 L
N-N_3	0	2.62849400	3.42896300	-2.83981200 L
N-N_3	0	3.93915800	4.52016000	-0.81825900 L
B-B_2	0	5.21344600	3.92060800	-1.41612600 L
B-B_2	0	6.51101400	4.13563400	0.67449600 L
N-N_3	0	6.51084100	4.46756600	-0.82082300 L
N-N_3	0	7.80328200	4.27820400	1.48453200 L
B-B_2	0	9.08735000	4.09691400	0.66874500 L
N-N_3	0	10.39433300	4.23566100	1.46793600 L
N-N_3	0	-12.79304300	-0.77094700	-4.24425400 L
B-B_2	0	-11.51124300	-1.44756500	-3.79639300 L
B-B_2	0	-10.22533100	0.67556100	-3.92951300 L
N-N_3	0	-10.20993400	-0.81947200	-4.29651300 L
N-N_3	0	-8.93799400	1.48859300	-4.11890000 L
B-B_2	0	-7.65489800	0.67979400	-3.89222400 L
B-B_2	0	-6.36877600	2.64665300	-3.07509400 L
N-N_3	0	-6.36017500	1.47900700	-4.06590200 L
N-N_3	0	-5.08639200	3.45647200	-2.86259700 L
B-B_2	0	-3.79762900	2.65766800	-3.05116300 L
B-B_2	0	-2.51661300	4.05506900	-1.43119500 L
N-N_3	0	-2.51221400	3.46763900	-2.85098500 L
N-N_3	0	-1.22826900	4.64283700	-0.83431700 L
B-B_2	0	0.06188100	4.05762000	-1.42656100 L
B-B_2	0	1.35448200	4.27113000	0.67906400 L
N-N_3	0	1.36340700	4.59128000	-0.82160100 L
N-N_3	0	2.65093900	4.36569000	1.48920800 L
B-B_2	0	3.93439100	4.19078000	0.67584200 L
N-N_3	0	5.22687000	4.31619300	1.48533100 L

B-	0	-12.75082600	0.61626400	-3.59514300 L
B-B_2	0	-11.50471500	2.70524000	-3.21111200 L
N-N_3	0	-11.54412000	1.45420300	-4.09420200 L
N-N_3	0	-10.21321000	3.46456800	-2.92225200 L
B-B_2	0	-8.94063500	2.65067500	-3.11977900 L
B-B_2	0	-7.67335200	3.96160300	-1.43835300 L
N-N_3	0	-7.65614900	3.44514100	-2.88127400 L
N-N_3	0	-6.39369700	4.54115600	-0.83191100 L
B-B_2	0	-5.09508300	3.99577500	-1.42928300 L
B-B_2	0	-3.81293100	4.24729300	0.66355700 L
N-N_3	0	-3.81698200	4.59133200	-0.82995700 L
N-N_3	0	-2.53344200	4.40984800	1.48866700 L
B-B_2	0	-1.22990800	4.36230000	0.68266000 L
N-N_3	0	0.06874000	4.42685800	1.49829100 L
B-	0	-12.78458500	3.57677200	-1.36127300 L
N-N_3	0	-12.79316600	3.43596300	-2.88749100 L
N-N_3	0	-11.57712500	4.41153300	-0.85309300 L
B-B_2	0	-10.24670700	3.91633600	-1.45287700 L
B-B_2	0	-8.96514300	4.15980800	0.65379100 L
N-N_3	0	-8.97391500	4.50873700	-0.83725300 L
N-N_3	0	-7.68037300	4.31423000	1.46598400 L
B-B_2	0	-6.39123500	4.18441100	0.65543800 L
N-N_3	0	-5.10958300	4.34932400	1.47114200 L
N-N_3	0	-12.82113700	4.22027800	1.46771600 L
B-B_2	0	-11.53287900	4.21348300	0.66713900 L
N-N_3	0	-10.23953600	4.31637200	1.47318800 L
H-H_	0	12.67895900	0.21270800	2.39061600 L
H-H_	0	12.60845900	-1.92896100	1.35443000 L
H-H_	0	12.66518100	-2.16061400	-1.01538000 L
H-H_	0	12.68435400	-0.21394900	-2.39671100 L
H-H_	0	-12.74885600	0.65495300	5.28588500 L
H-H_	0	-12.72951400	-4.38974900	3.31542900 L
H-H_	0	12.60150500	1.92345600	-1.35446300 L
H-H_	0	12.67430700	2.16245800	1.01624000 L
H-H_	0	-12.78816600	-5.01481100	-2.12191100 L
H-H_	0	-12.74699300	-0.64881800	-5.28131600 L
H-H_	0	-12.73405400	4.39297100	-3.30362300 L
H-H_	0	-12.78170900	5.02540700	2.13307800 L
C-C_3	0	-1.00017900	0.02573600	0.34666900 H
H-H_	0	0.94919400	-0.86589400	0.45153700 H
H-H_	0	0.31123400	-0.68825000	-1.18855000 H
C-C_3	0	0.04812200	-0.94337600	-0.16469300 H
H-H_	0	-0.32244700	-1.94913900	-0.11043100 H
N-N_3	0	-0.59805900	1.34573900	0.05117200 H

H-H_	0	-1.33859300	1.95638500	-0.21557100 H
H-H_	0	-1.13277600	-0.17815000	1.41872400 H
C-C_R	0	-2.42735200	-0.12592600	-0.16260800 H
O-O_R	0	-3.11340600	0.79154100	-0.56607800 H
O-O_R	0	-2.92372900	-1.36509300	-0.00354500 H
H-H_	0	-3.85995400	-1.32466700	-0.26290300 H
H-H_	0	0.35061300	1.63958600	0.17123000 H

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B-B_2	0	10.36416200	3.46735000	2.35867700 L
N-N_3	0	11.64201100	3.23393800	3.15436700 L
B-	0	12.92171700	3.63584200	2.37839600 L
B-B_2	0	5.21997200	3.44939500	2.28518700 L
N-N_3	0	6.49957000	3.22321900	3.09162700 L
B-B_2	0	7.79427800	3.42623100	2.30387900 L
B-B_2	0	9.06527500	1.78415700	3.66496700 L

N-N_3	0	9.06319100	3.22912900	3.12828900 L
N-N_3	0	10.35838700	1.21328000	4.27169100 L
B-B_2	0	11.60494300	1.75864700	3.54832300 L
B-	0	12.88472500	-0.23564700	4.37929700 L
N-N_3	0	12.82475400	0.86790100	3.30935700 L
B-B_2	0	0.06506600	3.53442800	2.26861500 L
N-N_3	0	1.35079000	3.25935900	3.05700400 L
B-B_2	0	2.64400500	3.48530600	2.27267000 L
B-B_2	0	3.91555800	1.78862900	3.56187400 L
N-N_3	0	3.92631700	3.23970500	3.07299800 L
N-N_3	0	5.18953200	1.20573800	4.17804200 L
B-B_2	0	6.48965400	1.78219300	3.61365700 L
B-B_2	0	7.76381000	-0.30980800	4.00525400 L
N-N_3	0	7.76545800	1.20580300	4.23667000 L
N-N_3	0	9.03104800	-1.10660100	4.30237400 L
B-B_2	0	10.33060000	-0.31529900	4.13993400 L
B-B_2	0	11.60290100	-2.19858100	3.31128300 L
N-N_3	0	11.60586600	-1.11075700	4.38154600 L
N-N_3	0	12.80069900	-2.36563400	2.37740100 L
B-B_2	0	-5.09234000	3.47777900	2.25415200 L
N-N_3	0	-3.80055700	3.24701300	3.03781400 L
B-B_2	0	-2.51295900	3.51327300	2.24932600 L
B-B_2	0	-1.22667500	1.80725600	3.51734900 L
N-N_3	0	-1.22825800	3.27047900	3.04325600 L
N-N_3	0	0.05566600	1.21305800	4.09972300 L
B-B_2	0	1.34242000	1.79708400	3.52110500 L
B-B_2	0	2.62287900	-0.30554300	3.88149800 L
N-N_3	0	2.61907000	1.20744000	4.12450200 L
N-N_3	0	3.90105600	-1.09296300	4.16788400 L
B-B_2	0	5.19214100	-0.30656700	3.93568600 L
B-B_2	0	6.48713600	-2.32646200	3.30677600 L
N-N_3	0	6.46961000	-1.09621600	4.22108500 L
N-N_3	0	7.77892900	-3.13769700	3.16351900 L
B-B_2	0	9.06237700	-2.32275600	3.35592800 L
B-B_2	0	10.36107100	-3.77926900	1.80494800 L
N-N_3	0	10.37061900	-3.11558600	3.18916200 L
N-N_3	0	11.65480700	-4.33907700	1.22621200 L
B-	0	12.92118500	-3.84230400	1.96781700 L
B-B_2	0	-10.24389400	3.43256000	2.25531700 L
N-N_3	0	-8.95878300	3.22430000	3.06765600 L
B-B_2	0	-7.66984000	3.45786800	2.26813100 L
B-B_2	0	-6.36826100	1.78060600	3.53497400 L
N-N_3	0	-6.37628200	3.23416200	3.05395900 L
N-N_3	0	-5.07529600	1.20182900	4.10874200 L

B-B_2	0	-3.79527800	1.78860900	3.50952500 L
B-B_2	0	-2.50933300	-0.30666500	3.86261600 L
N-N_3	0	-2.51036000	1.21048300	4.09748400 L
N-N_3	0	-1.22536600	-1.09461100	4.11695000 L
B-B_2	0	0.05690400	-0.30410000	3.86114400 L
B-B_2	0	1.34254100	-2.34001300	3.23542600 L
N-N_3	0	1.33692200	-1.09290800	4.12849600 L
N-N_3	0	2.63056200	-3.15352200	3.11524700 L
B-B_2	0	3.91349800	-2.33111800	3.26617700 L
B-B_2	0	5.21603100	-3.77024900	1.74150000 L
N-N_3	0	5.20316600	-3.14252300	3.13706300 L
N-N_3	0	6.51267200	-4.37147500	1.19874300 L
B-B_2	0	7.79035700	-3.74330100	1.75592300 L
B-B_2	0	9.09135500	-4.13700900	-0.31484400 L
N-N_3	0	9.07635100	-4.35871100	1.21005900 L
N-N_3	0	10.39933600	-4.34460300	-1.09746900 L
B-B_2	0	11.62782000	-3.95787100	-0.25220000 L
B-	0	12.91762600	-3.63742500	-2.37755900 L
N-N_3	0	12.82869400	-3.25809300	-0.88987400 L
B-	0	-12.77441200	3.14243000	2.03075800 L
B-B_2	0	-11.50595500	1.79070200	3.65492800 L
N-N_3	0	-11.56502200	3.17761100	3.00518900 L
N-N_3	0	-10.20583200	1.20429600	4.20696100 L
B-B_2	0	-8.94143700	1.77855000	3.57711100 L
B-B_2	0	-7.64907500	-0.31829200	3.92273800 L
N-N_3	0	-7.64458800	1.19976600	4.14567200 L
N-N_3	0	-6.35481500	-1.10066800	4.15744000 L
B-B_2	0	-5.07649100	-0.31195300	3.87330000 L
B-B_2	0	-3.79182200	-2.34061300	3.22807900 L
N-N_3	0	-3.78957200	-1.09695900	4.12506600 L
N-N_3	0	-2.50822300	-3.16458400	3.09849200 L
B-B_2	0	-1.22350200	-2.34513600	3.22464100 L
B-B_2	0	0.06463600	-3.88314900	1.74898000 L
N-N_3	0	0.06071500	-3.16813700	3.10893700 L
N-N_3	0	1.36482700	-4.47725200	1.20184700 L
B-B_2	0	2.64044800	-3.81642700	1.73479900 L
B-B_2	0	3.93836900	-4.22714900	-0.32076000 L
N-N_3	0	3.94043800	-4.41676200	1.19742300 L
N-N_3	0	5.23180500	-4.43034500	-1.11276900 L
B-B_2	0	6.51494000	-4.17539400	-0.32040700 L
B-B_2	0	7.79028000	-3.42437200	-2.30208400 L
N-N_3	0	7.80832600	-4.39065000	-1.11270500 L
N-N_3	0	9.05922000	-3.22895000	-3.12689400 L
B-B_2	0	10.36011700	-3.46767400	-2.35747600 L

B-B_2	0	11.60185800	-1.76021700	-3.54828200 L
N-N_3	0	11.63800200	-3.23535400	-3.15355800 L
N-N_3	0	12.82321300	-0.87078400	-3.31215700 L
B-	0	-12.74072300	-0.28636000	3.60906700 L
N-N_3	0	-12.78934600	1.14767300	4.14661800 L
N-N_3	0	-11.53677900	-1.07904000	4.18228800 L
B-B_2	0	-10.21887000	-0.31486200	3.95669500 L
B-B_2	0	-8.93212200	-2.34932100	3.30995600 L
N-N_3	0	-8.93105300	-1.10885400	4.21075600 L
N-N_3	0	-7.64535000	-3.15842700	3.14011400 L
B-B_2	0	-6.36178900	-2.33938100	3.25684600 L
B-B_2	0	-5.08612700	-3.83396200	1.73575900 L
N-N_3	0	-5.07704400	-3.15888600	3.11065600 L
N-N_3	0	-3.80614200	-4.48913500	1.20577000 L
B-B_2	0	-2.50987000	-3.86814100	1.73378300 L
B-B_2	0	-1.22504200	-4.40251200	-0.32468800 L
N-N_3	0	-1.22461600	-4.52005900	1.21132700 L
N-N_3	0	0.07720900	-4.55380400	-1.12306000 L
B-B_2	0	1.35880400	-4.30104500	-0.32191500 L
B-B_2	0	2.64031000	-3.48145300	-2.27495600 L
N-N_3	0	2.65635200	-4.48155000	-1.11514200 L
N-N_3	0	3.92356700	-3.23851800	-3.07396400 L
B-B_2	0	5.21599000	-3.44522800	-2.28384400 L
B-B_2	0	6.48680000	-1.78137200	-3.61424100 L
N-N_3	0	6.49592600	-3.22163200	-3.09019300 L
N-N_3	0	7.76293000	-1.20530100	-4.23637000 L
B-B_2	0	9.06224600	-1.78433000	-3.66450600 L
B-B_2	0	10.32855500	0.31424900	-4.14002800 L
N-N_3	0	10.35551400	-1.21438600	-4.27157000 L
N-N_3	0	11.60405200	1.10896800	-4.38237400 L
B-	0	12.88236300	0.23303100	-4.38193600 L
N-N_3	0	-12.78227900	-3.16176500	3.15977600 L
B-B_2	0	-11.49503700	-2.40067900	3.40920400 L
B-B_2	0	-10.23727500	-3.77414100	1.77303500 L
N-N_3	0	-10.20234300	-3.18207900	3.19179900 L
N-N_3	0	-8.96430700	-4.42257000	1.21623500 L
B-B_2	0	-7.66374700	-3.81264300	1.75377200 L
B-B_2	0	-6.38521600	-4.26142700	-0.31109600 L
N-N_3	0	-6.38304200	-4.44936600	1.20702900 L
N-N_3	0	-5.10801200	-4.51201300	-1.11280300 L
B-B_2	0	-3.80741100	-4.34719700	-0.32179700 L
B-B_2	0	-2.51552100	-3.52636500	-2.25737600 L
N-N_3	0	-2.52192400	-4.56702400	-1.12571600 L
N-N_3	0	-1.23048300	-3.27188800	-3.04829100 L

B-B_2	0	0.06354800	-3.53518800	-2.27571200 L
B-B_2	0	1.34079600	-1.80259700	-3.53367900 L
N-N_3	0	1.34958700	-3.26390300	-3.06477800 L
N-N_3	0	2.61692600	-1.20638700	-4.13121100 L
B-B_2	0	3.91261800	-1.78876300	-3.56742400 L
B-B_2	0	5.19004700	0.30731100	-3.93234300 L
N-N_3	0	5.18753100	-1.20425400	-4.17953800 L
N-N_3	0	6.46754200	1.09743400	-4.21720300 L
B-B_2	0	7.76182700	0.31014300	-4.00374700 L
B-B_2	0	9.06200300	2.32192300	-3.35375500 L
N-N_3	0	9.02927200	1.10647100	-4.30104700 L
N-N_3	0	10.37093800	3.11395200	-3.18802100 L
B-B_2	0	11.60257900	2.19618300	-3.31153400 L
B-	0	12.92330900	3.83699300	-1.96774000 L
N-N_3	0	12.80019600	2.36049600	-2.37699200 L
B-	0	-12.77585700	-3.44954400	1.65461200 L
B-B_2	0	-11.52826700	-4.28157000	-0.30446400 L
N-N_3	0	-11.56819400	-4.32828100	1.22795600 L
N-N_3	0	-10.23679100	-4.45220400	-1.10059200 L
B-B_2	0	-8.95994900	-4.22607400	-0.30204500 L
B-B_2	0	-7.67366900	-3.45877400	-2.26301400 L
N-N_3	0	-7.67876500	-4.45785100	-1.10019100 L
N-N_3	0	-6.38091800	-3.23442000	-3.04924800 L
B-B_2	0	-5.09572700	-3.49061700	-2.25496300 L
B-B_2	0	-3.79930000	-1.78877500	-3.49320200 L
N-N_3	0	-3.80510800	-3.25358400	-3.03896000 L
N-N_3	0	-2.51383700	-1.20201700	-4.07093800 L
B-B_2	0	-1.22989900	-1.80312100	-3.50117300 L
B-B_2	0	0.05321200	0.30599600	-3.83573300 L
N-N_3	0	0.04881800	-1.20821900	-4.09161300 L
N-N_3	0	1.33254100	1.09387100	-4.10944900 L
B-B_2	0	2.62033000	0.30485600	-3.87364700 L
B-B_2	0	3.91298200	2.33071700	-3.25486600 L
N-N_3	0	3.89806900	1.09439100	-4.15924800 L
N-N_3	0	5.20292900	3.14256100	-3.12973700 L
B-B_2	0	6.48664200	2.32630800	-3.30105700 L
B-B_2	0	7.79237500	3.74424700	-1.75287200 L
N-N_3	0	7.77896700	3.13738400	-3.15990100 L
N-N_3	0	9.07950100	4.35864400	-1.20840000 L
B-B_2	0	10.36313200	3.77746300	-1.80374600 L
B-B_2	0	11.63138200	3.95549300	0.25274300 L
N-N_3	0	11.65793500	4.33592600	-1.22589500 L
N-N_3	0	12.83281300	3.25677000	0.89059600 L
B-	0	-12.77658800	-3.13079600	-2.02019800 L

N-N_3	0	-12.81795200	-4.35660000	-1.09917900 L
N-N_3	0	-11.56869200	-3.16942100	-2.99623200 L
B-B_2	0	-10.24753500	-3.42698600	-2.24746500 L
B-B_2	0	-8.94354400	-1.77234300	-3.56564600 L
N-N_3	0	-8.96283800	-3.21962400	-3.06035600 L
N-N_3	0	-7.64538800	-1.19314400	-4.13093700 L
B-B_2	0	-6.37084600	-1.77683500	-3.51943500 L
B-B_2	0	-5.07727400	0.31804700	-3.85031800 L
N-N_3	0	-5.07738000	-1.19590500	-4.08894900 L
N-N_3	0	-3.78775800	1.10059200	-4.10087500 L
B-B_2	0	-2.51054000	0.31171100	-3.82074700 L
B-B_2	0	-1.22451300	2.35880100	-3.21476600 L
N-N_3	0	-1.22853600	1.09695800	-4.08936300 L
N-N_3	0	0.06362300	3.17480200	-3.09549100 L
B-B_2	0	1.34226800	2.34152300	-3.21736000 L
B-B_2	0	2.64299500	3.82432300	-1.72609700 L
N-N_3	0	2.63101300	3.15403400	-3.10304100 L
N-N_3	0	3.94415700	4.42525000	-1.19296100 L
B-B_2	0	5.21809400	3.77448900	-1.73598700 L
B-B_2	0	6.51913200	4.18100600	0.32370000 L
N-N_3	0	6.51604600	4.37492800	-1.19567900 L
N-N_3	0	7.81325200	4.39344800	1.11523700 L
B-B_2	0	9.09527400	4.13789700	0.31662200 L
N-N_3	0	10.40386400	4.34402800	1.09848400 L
N-N_3	0	-12.78994000	-1.14031300	-4.14203300 L
B-B_2	0	-11.50772500	-1.78320100	-3.64749600 L
B-B_2	0	-10.21910000	0.32204700	-3.94785700 L
N-N_3	0	-10.20640900	-1.19722500	-4.19744100 L
N-N_3	0	-8.93055900	1.11544600	-4.20174000 L
B-B_2	0	-7.64909400	0.32541200	-3.90924800 L
B-B_2	0	-6.36115700	2.35287100	-3.25451600 L
N-N_3	0	-6.35342700	1.10651400	-4.14463500 L
N-N_3	0	-5.07746900	3.17617300	-3.11458100 L
B-B_2	0	-3.79120800	2.36003700	-3.22623200 L
B-B_2	0	-2.50808300	3.89941000	-1.74181300 L
N-N_3	0	-2.50642300	3.18461600	-3.10162900 L
N-N_3	0	-1.21880000	4.54600500	-1.21191100 L
B-B_2	0	0.06747400	3.89335000	-1.73708400 L
B-B_2	0	1.36314600	4.32538600	0.32895200 L
N-N_3	0	1.36858400	4.49035600	-1.19585700 L
N-N_3	0	2.66205200	4.49537800	1.12172300 L
B-B_2	0	3.94285800	4.24044500	0.32571700 L
N-N_3	0	5.23730300	4.43808500	1.11709700 L
B-	0	-12.74210000	0.29373300	-3.60459900 L

B-B_2	0	-11.49559900	2.40704400	-3.40068600 L
N-N_3	0	-11.53673500	1.08634900	-4.17516300 L
N-N_3	0	-10.20348700	3.18973200	-3.18521400 L
B-B_2	0	-8.93224800	2.35842700	-3.30465300 L
B-B_2	0	-7.66400600	3.82364100	-1.75236000 L
N-N_3	0	-7.64639000	3.16950100	-3.13846000 L
N-N_3	0	-6.38373500	4.45882200	-1.20441100 L
B-B_2	0	-5.08591100	3.85200900	-1.74038900 L
B-B_2	0	-3.80448200	4.32231100	0.31854800 L
N-N_3	0	-3.80632500	4.50309500	-1.20332100 L
N-N_3	0	-2.52540500	4.56340600	1.12621100 L
B-B_2	0	-1.21972600	4.44703800	0.32805600 L
N-N_3	0	0.08179700	4.57330800	1.13235600 L
B-	0	-12.77460700	3.45381400	-1.64319600 L
N-N_3	0	-12.78343200	3.16645700	-3.14846200 L
N-N_3	0	-11.56761000	4.33450900	-1.21907800 L
B-B_2	0	-10.23721600	3.78144600	-1.76627500 L
B-B_2	0	-8.95745200	4.22823200	0.30741900 L
N-N_3	0	-8.96424500	4.42988200	-1.21034000 L
N-N_3	0	-7.67405800	4.45539500	1.10381200 L
B-B_2	0	-6.38350200	4.25376300	0.31105700 L
N-N_3	0	-5.10343000	4.49505100	1.11009900 L
N-N_3	0	-12.81381000	4.36822500	1.10971900 L
B-B_2	0	-11.52543200	4.28952000	0.31346400 L
N-N_3	0	-10.23241800	4.45725500	1.10800300 L
H-H_	0	12.70205900	0.41516800	2.37735900 L
H-H_	0	12.60891800	-1.80081500	1.52101700 L
H-H_	0	12.66185300	-2.23003600	-0.82329500 L
H-H_	0	12.70337600	-0.41820400	-2.37972600 L
H-H_	0	-12.74976300	1.10782400	5.19035100 L
H-H_	0	-12.72083500	-4.07377000	3.66673000 L
H-H_	0	12.60655000	1.79629800	-1.52059600 L
H-H_	0	12.66701500	2.22857500	0.82375900 L
H-H_	0	-12.77786500	-5.21340700	-1.69647700 L
H-H_	0	-12.74807500	-1.10059200	-5.18568100 L
H-H_	0	-12.72419800	4.07866900	-3.65530700 L
H-H_	0	-12.77055600	5.22494900	1.70691500 L
C-C_3	0	-1.19036000	0.05786100	0.29511100 H
H-H_	0	0.74061300	-0.85231300	0.50811100 H
H-H_	0	0.13106100	-0.80027300	-1.14815400 H
C-C_3	0	-0.15392500	-0.96444400	-0.11223200 H
H-H_	0	-0.54618600	-1.95422300	0.01925700 H
N-N_3	0	-0.77763800	1.33971600	-0.19976000 H
H-H_	0	-1.55656200	1.96362100	-0.07017800 H

H-H_	0	-1.28461900	0.01049900	1.38942900 H
C-C_R	0	-2.63964600	-0.12992600	-0.12997600 H
O-O_R	0	-3.38353100	0.78805100	-0.41307800 H
O-O_R	0	-3.07931200	-1.39517200	-0.03221600 H
H-H_	0	-4.03335900	-1.37205200	-0.22004600 H
H-H_	0	0.05903300	1.66316600	0.26628700 H

Coordinates of all stationary points in the pathway a of α -Ala chiral transformation confined in SWBNNT(7,7)

S α -Ala @C

B-B_2	0	10.32156600	-0.32791100	4.85255600 L
N-N_3	0	11.61754200	-1.10863700	5.05713600 L
B-	0	12.89201600	-0.23825400	4.90784200 L
B-B_2	0	5.18363700	-0.32812700	4.74388800 L
N-N_3	0	6.46608000	-1.11328500	5.02039900 L
B-B_2	0	7.75617000	-0.32936600	4.77342100 L
B-B_2	0	9.04296100	-2.38025100	4.17952900 L
N-N_3	0	9.02890800	-1.12061900	5.06995700 L
N-N_3	0	10.34519400	-3.18848400	4.07025100 L
B-B_2	0	11.56252700	-2.25058500	4.04999900 L
B-	0	12.89414900	-3.99926500	2.88623100 L
N-N_3	0	12.71621500	-2.48416400	3.07525800 L
B-B_2	0	0.04334700	-0.32730900	4.73175500 L
N-N_3	0	1.32759800	-1.11118200	5.00337400 L
B-B_2	0	2.61314600	-0.32764000	4.73565400 L
B-B_2	0	3.89861300	-2.36887500	4.13599100 L
N-N_3	0	3.89725100	-1.11171600	5.00881700 L
N-N_3	0	5.18347100	-3.19375300	4.04625000 L
B-B_2	0	6.47146700	-2.37419700	4.14903600 L
B-B_2	0	7.75811700	-3.96290100	2.73033800 L
N-N_3	0	7.75609100	-3.20378400	4.06338100 L
N-N_3	0	9.03328500	-4.68398700	2.29710800 L
B-B_2	0	10.32413400	-4.01534600	2.77949200 L
B-B_2	0	11.56658700	-4.58217500	0.77628700 L
N-N_3	0	11.62124300	-4.65972600	2.29703800 L
N-N_3	0	12.71684500	-3.95702900	-0.01238400 L
B-B_2	0	-5.09705400	-0.32644700	4.74293300 L
N-N_3	0	-3.81056600	-1.11019400	5.00737600 L
B-B_2	0	-2.52628900	-0.32663800	4.73420100 L
B-B_2	0	-1.24195000	-2.36771400	4.13066900 L
N-N_3	0	-1.24132600	-1.11062000	5.00302600 L
N-N_3	0	0.04284100	-3.19203800	4.03944200 L
B-B_2	0	1.32788900	-2.36789400	4.13044700 L
B-B_2	0	2.61345500	-3.95116000	2.71218400 L
N-N_3	0	2.61274500	-3.19195000	4.04080400 L
N-N_3	0	3.90006800	-4.65178400	2.27293400 L
B-B_2	0	5.18503100	-3.94916000	2.71518900 L
B-B_2	0	6.47429200	-4.75592500	0.74670200 L
N-N_3	0	6.47005700	-4.65151300	2.27555700 L
N-N_3	0	7.76049400	-5.19598100	0.04068200 L

B-B_2	0	9.04651600	-4.77158500	0.75721300 L
B-B_2	0	10.32535600	-4.68007500	-1.39445700 L
N-N_3	0	10.34974500	-5.18221600	0.05398300 L
N-N_3	0	11.62143800	-4.69576600	-2.20120900 L
B-	0	12.89560000	-4.74585900	-1.31947500 L
B-B_2	0	-10.23766200	-0.31682000	4.77054400 L
N-N_3	0	-8.95656400	-1.11480100	5.04074700 L
B-B_2	0	-7.67034000	-0.32817500	4.76213800 L
B-B_2	0	-6.38274400	-2.36645600	4.14087500 L
N-N_3	0	-6.38091400	-1.11157100	5.01765000 L
N-N_3	0	-5.09742700	-3.18999600	4.04425500 L
B-B_2	0	-3.81213100	-2.36644500	4.13348800 L
B-B_2	0	-2.52795700	-3.95017800	2.71137900 L
N-N_3	0	-2.52721900	-3.19083000	4.03985100 L
N-N_3	0	-1.24349100	-4.65591200	2.27317900 L
B-B_2	0	0.04261300	-3.95388500	2.71223300 L
B-B_2	0	1.32788100	-4.76256500	0.74636200 L
N-N_3	0	1.32848700	-4.65590900	2.27297700 L
N-N_3	0	2.61521200	-5.19499000	0.04223500 L
B-B_2	0	3.90032900	-4.75517400	0.74624100 L
B-B_2	0	5.18571000	-4.60258000	-1.37266600 L
N-N_3	0	5.18728200	-5.18799700	0.04120600 L
N-N_3	0	6.46980400	-4.68258500	-2.19918800 L
B-B_2	0	7.75902000	-4.61518600	-1.37901000 L
B-B_2	0	9.04258300	-3.55816700	-3.23542700 L
N-N_3	0	9.03300100	-4.71589400	-2.21603200 L
N-N_3	0	10.34312400	-3.26108800	-3.99783000 L
B-B_2	0	11.56192000	-3.45334800	-3.08150900 L
B-	0	12.88838500	-1.91620300	-4.51762900 L
N-N_3	0	12.71210800	-2.44683800	-3.08570200 L
B-	0	-12.74330700	-0.27781000	4.37281100 L
B-B_2	0	-11.51351900	-2.39950300	4.20908900 L
N-N_3	0	-11.56046300	-1.07662800	4.97523900 L
N-N_3	0	-10.22554000	-3.21383700	4.09135800 L
B-B_2	0	-8.95378600	-2.37518500	4.16660600 L
B-B_2	0	-7.67322400	-3.96017600	2.72706300 L
N-N_3	0	-7.66579000	-3.19262900	4.05488500 L
N-N_3	0	-6.38523900	-4.65450600	2.27852000 L
B-B_2	0	-5.09961900	-3.95055500	2.71613100 L
B-B_2	0	-3.81509700	-4.75815300	0.74732700 L
N-N_3	0	-3.81408900	-4.65226600	2.27385900 L
N-N_3	0	-2.53099400	-5.20176500	0.04386400 L
B-B_2	0	-1.24392400	-4.76573800	0.74659700 L
B-B_2	0	0.04128100	-4.62421400	-1.37382900 L

N-N_3	0	0.04233100	-5.20339100	0.04306800 L
N-N_3	0	1.32848500	-4.69482900	-2.19733500 L
B-B_2	0	2.61350900	-4.61120400	-1.37212400 L
B-B_2	0	3.89750400	-3.53814100	-3.20891900 L
N-N_3	0	3.90005100	-4.68572100	-2.19658700 L
N-N_3	0	5.18112300	-3.24819700	-3.98934200 L
B-B_2	0	6.47081100	-3.53943300	-3.21995800 L
B-B_2	0	7.75237200	-1.78238700	-4.43252900 L
N-N_3	0	7.75391900	-3.25648300	-4.00732000 L
N-N_3	0	9.02396400	-1.19362600	-5.04108600 L
B-B_2	0	10.31792900	-1.81456400	-4.50522600 L
B-B_2	0	11.55636700	0.26790600	-4.60989900 L
N-N_3	0	11.61291900	-1.19650300	-5.02682000 L
N-N_3	0	12.71060700	0.90088400	-3.83351300 L
B-	0	-12.74895300	-3.61944200	2.52643300 L
N-N_3	0	-12.80798700	-3.15999000	3.98554300 L
N-N_3	0	-11.56507800	-4.58824600	2.27952800 L
B-B_2	0	-10.24091100	-3.95346600	2.74134000 L
B-B_2	0	-8.95854300	-4.77088700	0.75991600 L
N-N_3	0	-8.96134000	-4.66742100	2.28986100 L
N-N_3	0	-7.67169100	-5.19272300	0.04920700 L
B-B_2	0	-6.38688000	-4.75378300	0.75125500 L
B-B_2	0	-5.10324900	-4.61395800	-1.37103300 L
N-N_3	0	-5.10274600	-5.19277600	0.04556000 L
N-N_3	0	-3.81835000	-4.69732200	-2.19661000 L
B-B_2	0	-2.53083300	-4.62395600	-1.37330000 L
B-B_2	0	-1.24564900	-3.54625800	-3.20310000 L
N-N_3	0	-1.24502300	-4.70082500	-2.19824900 L
N-N_3	0	0.03960400	-3.25117600	-3.97759000 L
B-B_2	0	1.32582500	-3.54193100	-3.20358900 L
B-B_2	0	2.60881100	-1.77499800	-4.39167500 L
N-N_3	0	2.60998800	-3.24929700	-3.98172700 L
N-N_3	0	3.89173800	-1.17972600	-4.97407900 L
B-B_2	0	5.17963000	-1.77456100	-4.40303800 L
B-B_2	0	6.46561600	0.33152200	-4.74135800 L
N-N_3	0	6.46092800	-1.18101700	-4.98968800 L
N-N_3	0	7.74863500	1.11861800	-5.02484900 L
B-B_2	0	9.03694600	0.32651000	-4.77848100 L
B-B_2	0	10.31779100	2.40790000	-4.22590900 L
N-N_3	0	10.33781200	1.10394800	-5.03172000 L
N-N_3	0	11.61492000	3.19870400	-4.07510700 L
B-	0	12.88788700	2.34818700	-4.32026100 L
N-N_3	0	-12.81348600	-5.11143900	0.03167900 L
B-B_2	0	-11.51916000	-4.81771100	0.76786300 L

B-B_2	0	-10.24593400	-4.61685200	-1.35837700 L
N-N_3	0	-10.23129700	-5.22732700	0.05456200 L
N-N_3	0	-8.96633100	-4.70017500	-2.19892600 L
B-B_2	0	-7.67763200	-4.61738200	-1.37219700 L
B-B_2	0	-6.38891700	-3.54092100	-3.20465200 L
N-N_3	0	-6.39000700	-4.69148000	-2.19535800 L
N-N_3	0	-5.10316300	-3.25137800	-3.98015600 L
B-B_2	0	-3.81737800	-3.54633500	-3.20536900 L
B-B_2	0	-2.53146100	-1.77672300	-4.38234300 L
N-N_3	0	-2.53114600	-3.25277700	-3.97852000 L
N-N_3	0	-1.24678300	-1.17966300	-4.95699200 L
B-B_2	0	0.03862000	-1.77578700	-4.38322000 L
B-B_2	0	1.32275400	0.32854700	-4.70465200 L
N-N_3	0	1.32182800	-1.17955200	-4.96301800 L
N-N_3	0	2.60583600	1.11281200	-4.98131900 L
B-B_2	0	3.89297000	0.32945300	-4.71934300 L
B-B_2	0	5.17949100	2.37068600	-4.12174600 L
N-N_3	0	5.17613300	1.11453900	-4.99638700 L
N-N_3	0	6.46365000	3.19609900	-4.03635000 L
B-B_2	0	7.75222800	2.37958900	-4.15095900 L
B-B_2	0	9.04323700	3.96959600	-2.73132300 L
N-N_3	0	9.02669600	3.21886800	-4.07870300 L
N-N_3	0	10.34737100	4.64680100	-2.28182800 L
B-B_2	0	11.56321200	3.79167000	-2.67257000 L
B-	0	12.89681800	4.85465100	-0.86238900 L
N-N_3	0	12.71620000	3.57411800	-1.69326200 L
B-	0	-12.75582100	-4.24203900	-1.22731400 L
B-B_2	0	-11.52131300	-3.58096900	-3.24808500 L
N-N_3	0	-11.57003100	-4.63815900	-2.14337000 L
N-N_3	0	-10.23265600	-3.27585200	-4.01185400 L
B-B_2	0	-8.96082100	-3.55322200	-3.21686700 L
B-B_2	0	-7.67616400	-1.77820500	-4.40681000 L
N-N_3	0	-7.67225100	-3.25252600	-3.98396700 L
N-N_3	0	-6.38582800	-1.17963600	-4.97071500 L
B-B_2	0	-5.10258200	-1.77640200	-4.38895500 L
B-B_2	0	-3.81597900	0.32832000	-4.70045800 L
N-N_3	0	-3.81555500	-1.17985200	-4.95959000 L
N-N_3	0	-2.53071500	1.11172900	-4.96902000 L
B-B_2	0	-1.24668600	0.32811500	-4.69741900 L
B-B_2	0	0.03875500	2.37059600	-4.10045200 L
N-N_3	0	0.03713800	1.11193700	-4.97029300 L
N-N_3	0	1.32372400	3.19506700	-4.01690400 L
B-B_2	0	2.60873700	2.37058100	-4.10963000 L
B-B_2	0	3.89776700	3.95717800	-2.69807000 L

N-N_3	0	3.89415600	3.19452800	-4.02480300 L
N-N_3	0	5.18542700	4.65685400	-2.25963000 L
B-B_2	0	6.47131000	3.95873200	-2.70707000 L
B-B_2	0	7.76058900	4.76576200	-0.73882300 L
N-N_3	0	7.75830800	4.66452100	-2.26936600 L
N-N_3	0	9.03674300	5.22120300	-0.03342200 L
B-B_2	0	10.32686600	4.82845000	-0.75962500 L
B-B_2	0	11.56834100	4.46002700	1.29020500 L
N-N_3	0	11.62475700	5.19426800	-0.04386700 L
N-N_3	0	12.71832300	3.55365300	1.72846100 L
B-	0	-12.74982500	-1.65084200	-4.03085700 L
N-N_3	0	-12.81540300	-3.17720800	-3.93126800 L
N-N_3	0	-11.56616500	-1.18688700	-4.91656900 L
B-B_2	0	-10.24373600	-1.78810700	-4.40788100 L
B-B_2	0	-8.95731500	0.32965700	-4.74082200 L
N-N_3	0	-8.96197600	-1.18332700	-4.99334700 L
N-N_3	0	-7.66789500	1.11418200	-4.98965800 L
B-B_2	0	-6.38619600	0.32903600	-4.71111700 L
B-B_2	0	-5.10102300	2.37267100	-4.10693500 L
N-N_3	0	-5.09960100	1.11245900	-4.97538500 L
N-N_3	0	-3.81492200	3.19591000	-4.01515200 L
B-B_2	0	-2.53044000	2.37124800	-4.10038500 L
B-B_2	0	-1.24418400	3.96765700	-2.69304200 L
N-N_3	0	-1.24540300	3.19603900	-4.01447900 L
N-N_3	0	0.04222500	4.67273200	-2.25820500 L
B-B_2	0	1.32592800	3.96307400	-2.69339300 L
B-B_2	0	2.61505400	4.76765200	-0.73062800 L
N-N_3	0	2.61387300	4.66297800	-2.25716700 L
N-N_3	0	3.90397400	5.19508500	-0.02640400 L
B-B_2	0	5.18734400	4.75510000	-0.73251900 L
B-B_2	0	6.47665900	4.60784200	1.38993100 L
N-N_3	0	6.47366500	5.18821600	-0.02838900 L
N-N_3	0	7.76225200	4.69250200	2.21852600 L
B-B_2	0	9.04877300	4.62500600	1.38914800 L
B-B_2	0	10.32650400	3.60270800	3.28614800 L
N-N_3	0	10.35157600	4.68622100	2.20168200 L
N-N_3	0	11.62226400	3.26741800	4.02075300 L
B-	0	12.89688900	3.69508100	3.24865000 L
N-N_3	0	-12.81100700	1.12056200	-4.91080400 L
B-B_2	0	-11.51703800	0.33639500	-4.78797300 L
B-B_2	0	-10.24164100	2.37122200	-4.13498700 L
N-N_3	0	-10.22820700	1.12098000	-5.03328200 L
N-N_3	0	-8.96118100	3.20903300	-4.03845300 L
B-B_2	0	-7.67427200	2.38004500	-4.12351700 L

B-B_2	0	-6.38652100	3.95776900	-2.69234000 L
N-N_3	0	-6.38539800	3.19888100	-4.02145800 L
N-N_3	0	-5.10200500	4.66202000	-2.25215100 L
B-B_2	0	-3.81520500	3.96151100	-2.69042600 L
B-B_2	0	-2.52911400	4.77533200	-0.72788600 L
N-N_3	0	-2.53062800	4.66892600	-2.25438000 L
N-N_3	0	-1.24384700	5.21450400	-0.02347600 L
B-B_2	0	0.04324600	4.78632200	-0.73160000 L
B-B_2	0	1.33035500	4.61650500	1.38598700 L
N-N_3	0	1.33202400	5.21037600	-0.02477200 L
N-N_3	0	2.61690800	4.68837100	2.21114700 L
B-B_2	0	3.90289200	4.60855300	1.38694900 L
B-B_2	0	5.18712700	3.53565800	3.22397600 L
N-N_3	0	5.18896800	4.68422500	2.21244800 L
N-N_3	0	6.47001000	3.24953100	4.00568700 L
B-B_2	0	7.76036200	3.54849100	3.24054900 L
B-B_2	0	9.04413600	1.79147000	4.45730800 L
N-N_3	0	9.03341600	3.27663900	4.04019600 L
N-N_3	0	10.34467500	1.19596100	5.01836200 L
B-B_2	0	11.56320300	1.76631200	4.27565500 L
N-N_3	0	12.71430500	0.85789700	3.84484100 L
B-	0	-12.74804200	2.16484700	-3.79328200 L
B-B_2	0	-11.51802300	4.00994800	-2.73363200 L
N-N_3	0	-11.56493000	3.14478000	-3.99405800 L
N-N_3	0	-10.23006000	4.69181400	-2.27401800 L
B-B_2	0	-8.95784400	3.97112200	-2.70762000 L
B-B_2	0	-7.67592400	4.77191800	-0.72540800 L
N-N_3	0	-7.67061800	4.66186300	-2.25491400 L
N-N_3	0	-6.38789500	5.20052500	-0.01935600 L
B-B_2	0	-5.10186800	4.76685800	-0.72559800 L
B-B_2	0	-3.81432400	4.61446600	1.39044100 L
N-N_3	0	-3.81634900	5.20425300	-0.02146900 L
N-N_3	0	-2.52801700	4.69272500	2.21403100 L
B-B_2	0	-1.24217200	4.62115200	1.38779200 L
B-B_2	0	0.04431300	3.53896200	3.21742000 L
N-N_3	0	0.04480200	4.69260100	2.21148000 L
N-N_3	0	1.32928800	3.24841800	3.99449200 L
B-B_2	0	2.61550800	3.53742300	3.21973100 L
B-B_2	0	3.89963500	1.77535100	4.41547500 L
N-N_3	0	3.90017000	3.24792000	3.99841300 L
N-N_3	0	5.18306800	1.18121000	4.99853900 L
B-B_2	0	6.47260600	1.77693700	4.43071700 L
N-N_3	0	7.75553800	1.18462400	5.02194000 L
B-	0	-12.75333300	4.37175500	-0.68757100 L

N-N_3	0	-12.81209100	4.59736800	-2.20073700 L
N-N_3	0	-11.56761400	5.13174700	-0.04075400 L
B-B_2	0	-10.24396100	4.76624200	-0.73659100 L
B-B_2	0	-8.95794800	4.62775100	1.39910100 L
N-N_3	0	-8.96402400	5.21086600	-0.01914400 L
N-N_3	0	-7.66919800	4.69230400	2.22016100 L
B-B_2	0	-6.38618700	4.61086700	1.39296900 L
B-B_2	0	-5.09889400	3.54131500	3.22823100 L
N-N_3	0	-5.09993800	4.68972600	2.21649800 L
N-N_3	0	-3.81108700	3.25046800	4.00008100 L
B-B_2	0	-2.52692800	3.53988800	3.22049200 L
B-B_2	0	-1.24113700	1.77556900	4.40746400 L
N-N_3	0	-1.24068200	3.24902600	3.99437800 L
N-N_3	0	0.04358800	1.18157100	4.98555700 L
B-B_2	0	1.32890500	1.77517700	4.40835100 L
N-N_3	0	2.61274700	1.18145900	4.98959400 L
N-N_3	0	-12.81175000	4.60806300	2.20940000 L
B-B_2	0	-11.51863700	4.67037200	1.41706000 L
B-B_2	0	-10.24098300	3.55670200	3.23746100 L
N-N_3	0	-10.22919900	4.72569600	2.23589400 L
N-N_3	0	-8.95919700	3.26352400	4.02647100 L
B-B_2	0	-7.67285500	3.54855200	3.24194000 L
B-B_2	0	-6.38242700	1.77867400	4.42186700 L
N-N_3	0	-6.38265100	3.25298900	4.00970400 L
N-N_3	0	-5.09562000	1.18332300	4.99504300 L
B-B_2	0	-3.81146700	1.77695900	4.41343400 L
N-N_3	0	-2.52538900	1.18230800	4.98818500 L
B-	0	-12.74985200	3.27491100	2.95982400 L
B-B_2	0	-11.51410100	1.80160400	4.49156500 L
N-N_3	0	-11.56340500	3.23359200	3.95600500 L
N-N_3	0	-10.22500200	1.19740600	5.04879500 L
B-B_2	0	-8.95402800	1.78848600	4.44692300 L
N-N_3	0	-7.66445700	1.18602900	5.00720100 L
N-N_3	0	-12.80804500	1.14403600	4.93648200 L
H-H_	0	12.44604500	-2.06275800	2.15819300 L
H-H_	0	12.44268000	-2.97704000	-0.24918900 L
H-H_	0	12.43874300	-1.65074000	-2.46667200 L
H-H_	0	12.44111600	0.91890800	-2.82421500 L
H-H_	0	-12.79380600	-4.00681000	4.59814700 L
H-H_	0	-12.79710500	-6.11490100	-0.26051600 L
H-H_	0	12.44410100	2.79565800	-1.05173900 L
H-H_	0	12.44388000	2.56827700	1.51543700 L
H-H_	0	-12.80464900	-3.57097400	-4.89947000 L
H-H_	0	-12.79896600	1.61977200	-5.82908500 L

H-H_	0	12.44120900	0.40652100	2.94297100 L
H-H_	0	-12.79651700	5.62690600	-2.38073000 L
H-H_	0	-12.79646400	5.38197800	2.91182800 L
H-H_	0	-12.79704200	1.08539500	5.98004800 L
C-C_3	0	-0.55088500	0.04300800	-0.51342700 H
H-H_	0	-0.36798700	-0.94193500	1.41222800 H
H-H_	0	1.13722700	-0.86212300	0.48608400 H
C-C_3	0	0.05716900	-1.02175300	0.40796100 H
H-H_	0	-0.11683000	-2.02595400	0.01996600 H
N-N_3	0	-0.27608100	1.38279300	-0.00479200 H
H-H_	0	-0.95478500	2.04264800	-0.37151400 H
H-H_	0	0.65841100	1.69080500	-0.25155400 H
C-C_R	0	-2.05907200	-0.09276600	-0.68949800 H
O-O_R	0	-2.82728900	0.84089100	-0.80197400 H
O-O_R	0	-2.46812400	-1.37912600	-0.76607200 H
H-H_	0	-3.42641200	-1.36487800	-0.93035800 H
H-H_	0	-0.15573000	-0.12205200	-1.53512700 H

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B-B_2	0	-10.28568600	2.62161000	4.11261800 L
N-N_3	0	-11.58226900	3.40460800	3.92200700 L
B-	0	-12.85566400	2.56707900	4.20674600 L
B-B_2	0	-5.14762400	2.57813800	4.01910800 L
N-N_3	0	-6.43122900	3.39848000	3.89030700 L
B-B_2	0	-7.72021100	2.58898700	4.04322400 L
B-B_2	0	-9.00849300	4.10713500	2.54494700 L
N-N_3	0	-8.99415700	3.42404400	3.92783300 L
N-N_3	0	-10.31160000	4.76219200	2.06093400 L
B-B_2	0	-11.52887300	3.92865100	2.49228200 L
B-	0	-12.85911600	4.90591500	0.63103300 L
N-N_3	0	-12.68341700	3.66811100	1.52532200 L
B-B_2	0	-0.00698900	2.57724800	4.01418400 L
N-N_3	0	-1.29164200	3.39646000	3.88263400 L
B-B_2	0	-2.57679800	2.57764100	4.01412200 L
B-B_2	0	-3.86278700	4.08739100	2.51822700 L
N-N_3	0	-3.86196700	3.39573200	3.88312300 L
N-N_3	0	-5.14909000	4.76496600	2.04263200 L
B-B_2	0	-6.43648700	4.09258000	2.52411000 L
B-B_2	0	-7.72293000	4.79989200	0.51630700 L
N-N_3	0	-7.72225700	4.77669300	2.04994500 L
N-N_3	0	-8.99788000	5.22058300	-0.21247700 L
B-B_2	0	-10.28930600	4.86755900	0.53160300 L
B-B_2	0	-11.52986400	4.39636400	-1.49711500 L

N-N_3	0	-11.58570900	5.19904100	-0.20307500 L
N-N_3	0	-12.67777100	3.46485500	-1.88508500 L
B-B_2	0	5.13462300	2.57500200	4.02291300 L
N-N_3	0	3.84903000	3.39244200	3.88451700 L
B-B_2	0	2.56340400	2.57511700	4.01649700 L
B-B_2	0	1.27927300	4.08484400	2.51599600 L
N-N_3	0	1.27869700	3.39420600	3.88156600 L
N-N_3	0	-0.00482300	4.76818700	2.04262500 L
B-B_2	0	-1.29129800	4.09092600	2.51893200 L
B-B_2	0	-2.57718100	4.78988000	0.51232800 L
N-N_3	0	-2.57754700	4.76746100	2.04242400 L
N-N_3	0	-3.86439600	5.18475100	-0.21380100 L
B-B_2	0	-5.14948400	4.78406200	0.51260100 L
B-B_2	0	-6.43760100	4.53184900	-1.60049600 L
N-N_3	0	-6.43458800	5.18343500	-0.21358500 L
N-N_3	0	-7.72265000	4.57580500	-2.43325600 L
B-B_2	0	-9.00976900	4.55217100	-1.60253100 L
B-B_2	0	-10.28732600	3.43367500	-3.44431600 L
N-N_3	0	-10.31203100	4.57258500	-2.41814600 L
N-N_3	0	-11.58333900	3.06052100	-4.16023400 L
B-	0	-12.85804100	3.52585900	-3.41035500 L
B-B_2	0	10.27562900	2.57115100	4.04929400 L
N-N_3	0	8.99568200	3.40326000	3.90721700 L
B-B_2	0	7.70809800	2.58113200	4.03735300 L
B-B_2	0	6.42179900	4.07788600	2.52114800 L
N-N_3	0	6.41987900	3.39402300	3.89065700 L
N-N_3	0	5.13743600	4.75658500	2.04208500 L
B-B_2	0	3.85065600	4.08045200	2.51753700 L
B-B_2	0	2.56616800	4.78561500	0.51064900 L
N-N_3	0	2.56620000	4.76086600	2.04066800 L
N-N_3	0	1.28181600	5.19106100	-0.21469900 L
B-B_2	0	-0.00498800	4.79592300	0.51217900 L
B-B_2	0	-1.29126900	4.53459900	-1.59660500 L
N-N_3	0	-1.29197100	5.19154800	-0.21419700 L
N-N_3	0	-2.57786200	4.56835500	-2.42336600 L
B-B_2	0	-3.86366800	4.52884200	-1.59615700 L
B-B_2	0	-5.14822100	3.36819900	-3.37778900 L
N-N_3	0	-5.14939600	4.56552700	-2.42484100 L
N-N_3	0	-6.43104000	3.04349400	-4.14424100 L
B-B_2	0	-7.72128100	3.38118100	-3.39555900 L
B-B_2	0	-9.00506000	1.56469600	-4.52170300 L
N-N_3	0	-8.99426300	3.06919700	-4.18062000 L
N-N_3	0	-10.30541400	0.94194400	-5.05248200 L
B-B_2	0	-11.52360000	1.54842500	-4.33859400 L

B-	0	-12.85291200	-0.48430800	-4.87188100 L
N-N_3	0	-12.67494300	0.66253900	-3.86375500 L
B-	0	12.78269500	2.34581200	3.72137500 L
B-B_2	0	11.55337800	4.13064500	2.56187700 L
N-N_3	0	11.59940900	3.33530900	3.86758800 L
N-N_3	0	10.26591100	4.78823100	2.06628900 L
B-B_2	0	8.99318000	4.09194000	2.53687000 L
B-B_2	0	7.71246100	4.78755400	0.51358600 L
N-N_3	0	7.70617900	4.75746300	2.04692500 L
N-N_3	0	6.42478900	5.18017000	-0.21406700 L
B-B_2	0	5.13850800	4.78102100	0.51178200 L
B-B_2	0	3.85226100	4.52928500	-1.59834400 L
N-N_3	0	3.85324700	5.18227400	-0.21435500 L
N-N_3	0	2.56693200	4.57263500	-2.42652600 L
B-B_2	0	1.28059400	4.53711400	-1.59862600 L
B-B_2	0	-0.00574300	3.37558500	-3.37813100 L
N-N_3	0	-0.00597000	4.57326900	-2.42516400 L
N-N_3	0	-1.29164200	3.04526900	-4.13712600 L
B-B_2	0	-2.57670100	3.37030900	-3.37507100 L
B-B_2	0	-3.86120000	1.55053400	-4.47792600 L
N-N_3	0	-3.86175000	3.04223300	-4.13717400 L
N-N_3	0	-5.14439400	0.92731200	-5.02992400 L
B-B_2	0	-6.43387300	1.55123400	-4.49361700 L
B-B_2	0	-7.71737700	-0.56972600	-4.73077600 L
N-N_3	0	-7.71649800	0.92998300	-5.05474100 L
N-N_3	0	-8.98987400	-1.37454100	-4.98927400 L
B-B_2	0	-10.28254400	-0.57189700	-4.81162800 L
B-B_2	0	-11.52441300	-2.45315900	-3.91727200 L
N-N_3	0	-11.57863500	-1.36134100	-4.97856000 L
N-N_3	0	-12.68019400	-2.64081500	-2.93509800 L
B-	0	12.78892100	4.38386700	0.49955300 L
N-N_3	0	12.84813700	4.68780800	1.99888600 L
N-N_3	0	11.60472600	5.11176300	-0.18559200 L
B-B_2	0	10.28047100	4.78268200	0.52700900 L
B-B_2	0	8.99596300	4.53934300	-1.60112400 L
N-N_3	0	9.00106100	5.19083300	-0.21287700 L
N-N_3	0	7.70807300	4.56594100	-2.42566300 L
B-B_2	0	6.42411900	4.52423200	-1.59700100 L
B-B_2	0	5.13772600	3.37242400	-3.38313300 L
N-N_3	0	5.13887400	4.56599500	-2.42511500 L
N-N_3	0	3.85102800	3.04658500	-4.14292800 L
B-B_2	0	2.56569000	3.37708400	-3.38212200 L
B-B_2	0	1.27946500	1.55472100	-4.47616000 L
N-N_3	0	1.27912900	3.04799900	-4.14060800 L

N-N_3	0	-0.00568800	0.92937200	-5.01908400 L
B-B_2	0	-1.29063400	1.55279100	-4.47405900 L
B-B_2	0	-2.57491500	-0.56479200	-4.68627000 L
N-N_3	0	-2.57472200	0.92816800	-5.02101100 L
N-N_3	0	-3.85823600	-1.36225600	-4.92125800 L
B-B_2	0	-5.14513200	-0.56678800	-4.69803500 L
B-B_2	0	-6.43320600	-2.58176000	-4.00539900 L
N-N_3	0	-6.42696800	-1.36492600	-4.93725400 L
N-N_3	0	-7.71791000	-3.40638000	-3.88154200 L
B-B_2	0	-9.00470000	-2.58935400	-4.03862600 L
B-B_2	0	-10.28728400	-4.15436100	-2.56190700 L
N-N_3	0	-10.30720300	-3.39113200	-3.89125500 L
N-N_3	0	-11.58464100	-4.77451900	-2.04948000 L
B-	0	-12.85697800	-4.14509800	-2.67278600 L
N-N_3	0	12.85052900	4.47673100	-2.40551200 L
B-B_2	0	11.55657800	4.57823600	-1.61848000 L
B-B_2	0	10.27980200	3.38173800	-3.38623400 L
N-N_3	0	10.26812200	4.59635700	-2.44049100 L
N-N_3	0	8.99856600	3.05277400	-4.16167900 L
B-B_2	0	7.71182700	3.37569100	-3.39281700 L
B-B_2	0	6.42118400	1.55225800	-4.48615800 L
N-N_3	0	6.42239000	3.04506600	-4.14727500 L
N-N_3	0	5.13410500	0.92935200	-5.02852200 L
B-B_2	0	3.85006700	1.55350600	-4.47928500 L
B-B_2	0	2.56416700	-0.56324400	-4.68694000 L
N-N_3	0	2.56389300	0.92991400	-5.02222300 L
N-N_3	0	1.27864500	-1.35957800	-4.91323500 L
B-B_2	0	-0.00536700	-0.56312200	-4.68204300 L
B-B_2	0	-1.29014700	-2.57257400	-3.97924000 L
N-N_3	0	-1.28934900	-1.36038700	-4.91277900 L
N-N_3	0	-2.57465500	-3.39244000	-3.85325500 L
B-B_2	0	-3.86043200	-2.57488100	-3.98781600 L
B-B_2	0	-5.14796800	-4.08706800	-2.49669000 L
N-N_3	0	-5.14504900	-3.39516800	-3.86165700 L
N-N_3	0	-6.43388900	-4.76607900	-2.02448500 L
B-B_2	0	-7.72122600	-4.09997500	-2.51338700 L
B-B_2	0	-9.01148600	-4.80837200	-0.50376100 L
N-N_3	0	-8.99696700	-4.79829300	-2.04602700 L
N-N_3	0	-10.31525500	-5.18249700	0.21859300 L
B-B_2	0	-11.53188100	-4.62082200	-0.53441600 L
B-	0	-12.86192900	-4.67699700	1.56660500 L
N-N_3	0	-12.68318600	-3.95696000	0.22039300 L
B-	0	12.78757000	3.11016400	-3.09303800 L
B-B_2	0	11.55273100	1.56961500	-4.55755700 L

N-N_3	0	11.60250600	3.02455800	-4.08789000 L
N-N_3	0	10.26319000	0.93912700	-5.08340200 L
B-B_2	0	8.99265100	1.55931500	-4.51095800 L
B-B_2	0	7.70823100	-0.56946700	-4.71994400 L
N-N_3	0	7.70290800	0.93047600	-5.04093400 L
N-N_3	0	6.41819900	-1.36428100	-4.93454000 L
B-B_2	0	5.13486700	-0.56545400	-4.69885500 L
B-B_2	0	3.84925700	-2.57247900	-3.98672800 L
N-N_3	0	3.84754600	-1.36078900	-4.92154200 L
N-N_3	0	2.56396900	-3.39104500	-3.85284900 L
B-B_2	0	1.27918300	-2.57210300	-3.97993200 L
B-B_2	0	-0.00629800	-4.09455600	-2.49160000 L
N-N_3	0	-0.00555900	-3.39174800	-3.85091500 L
N-N_3	0	-1.29204300	-4.77864000	-2.02227200 L
B-B_2	0	-2.57623500	-4.09245500	-2.49248200 L
B-B_2	0	-3.86494800	-4.79739800	-0.49093600 L
N-N_3	0	-3.86398400	-4.76937200	-2.02080600 L
N-N_3	0	-5.15320700	-5.18922000	0.23525100 L
B-B_2	0	-6.43926300	-4.79346300	-0.49251000 L
B-B_2	0	-7.72532700	-4.54130700	1.62169900 L
N-N_3	0	-7.72611000	-5.19568700	0.23443400 L
N-N_3	0	-8.99970300	-4.59857200	2.46220800 L
B-B_2	0	-10.29172800	-4.60616600	1.63919400 L
B-B_2	0	-11.52933100	-3.29350000	3.25913400 L
N-N_3	0	-11.58818400	-4.58023600	2.44499500 L
N-N_3	0	-12.67737600	-2.28596700	3.20658200 L
B-	0	12.78283800	-0.50058700	-4.33792100 L
N-N_3	0	12.84608300	0.89146700	-4.97185200 L
N-N_3	0	11.59837700	-1.32885300	-4.89623900 L
B-B_2	0	10.27578100	-0.55924600	-4.72984300 L
B-B_2	0	8.99137400	-2.58313100	-4.02049800 L
N-N_3	0	8.99425900	-1.36961400	-4.95850000 L
N-N_3	0	7.70336400	-3.39370500	-3.86675200 L
B-B_2	0	6.42003300	-2.57327200	-3.99546200 L
B-B_2	0	5.13676800	-4.08446700	-2.49337300 L
N-N_3	0	5.13462100	-3.39095500	-3.85768200 L
N-N_3	0	3.85186900	-4.76455900	-2.01715700 L
B-B_2	0	2.56487300	-4.08767200	-2.49062600 L
B-B_2	0	1.27947500	-4.80054800	-0.48845000 L
N-N_3	0	1.28056800	-4.77197000	-2.01833600 L
N-N_3	0	-0.00510100	-5.20510200	0.23750100 L
B-B_2	0	-1.29288100	-4.81617800	-0.49183700 L
B-B_2	0	-2.57960000	-4.53517200	1.61400800 L
N-N_3	0	-2.58149400	-5.20247500	0.23640000 L

N-N_3	0	-3.86599000	-4.56495500	2.44203100 L
B-B_2	0	-5.15194100	-4.52781500	1.61512900 L
B-B_2	0	-6.43836900	-3.36949400	3.40396000 L
N-N_3	0	-6.43622200	-4.56461900	2.44463800 L
N-N_3	0	-7.72193300	-3.04786200	4.17583800 L
B-B_2	0	-9.01018400	-3.38929600	3.41989500 L
B-B_2	0	-10.28693400	-1.58313900	4.59770800 L
N-N_3	0	-10.31132100	-3.05377500	4.16521300 L
N-N_3	0	-11.58295300	-0.93950200	5.08507500 L
B-	0	-12.85776100	-1.68260300	4.60884100 L
N-N_3	0	12.84578500	-3.35704300	-3.79702900 L
B-B_2	0	11.55138800	-2.60971200	-4.06167400 L
B-B_2	0	10.27827300	-4.08260000	-2.51296800 L
N-N_3	0	10.26330000	-3.41643500	-3.90068700 L
N-N_3	0	8.99893600	-4.77250900	-2.02522500 L
B-B_2	0	7.71051000	-4.09089100	-2.50070000 L
B-B_2	0	6.42326700	-4.78091100	-0.48751800 L
N-N_3	0	6.42307400	-4.76249000	-2.01798600 L
N-N_3	0	5.13887400	-5.18295000	0.23890200 L
B-B_2	0	3.85179100	-4.78836000	-0.48730600 L
B-B_2	0	2.56507400	-4.53262400	1.61908900 L
N-N_3	0	2.56735500	-5.19208700	0.23840700 L
N-N_3	0	1.27854600	-4.56927500	2.44524700 L
B-B_2	0	-0.00711900	-4.53936900	1.61611700 L
B-B_2	0	-1.29358100	-3.36626500	3.38897200 L
N-N_3	0	-1.29407900	-4.56895200	2.44227000 L
N-N_3	0	-2.57838900	-3.03796500	4.15095000 L
B-B_2	0	-3.86493900	-3.36546700	3.39234600 L
B-B_2	0	-5.14870000	-1.54677600	4.49935900 L
N-N_3	0	-5.14894200	-3.03862900	4.15755300 L
N-N_3	0	-6.43074600	-0.92635900	5.05558000 L
B-B_2	0	-7.72135900	-1.55435000	4.52684600 L
B-B_2	0	-9.00620800	0.56908500	4.76755500 L
N-N_3	0	-8.99377600	-0.93641400	5.10418800 L
N-N_3	0	-10.30731500	1.35801900	4.98035100 L
B-B_2	0	-11.52491000	0.50259600	4.59678600 L
N-N_3	0	-12.67846400	1.09797000	3.79019200 L
B-	0	12.78626200	-3.73648800	-2.31510300 L
B-B_2	0	11.55517600	-4.83752700	-0.49456000 L
N-N_3	0	11.60243800	-4.69065900	-2.01645600 L
N-N_3	0	10.26726200	-5.21340500	0.23734500 L
B-B_2	0	8.99476100	-4.79512300	-0.49184900 L
B-B_2	0	7.71137400	-4.53378700	1.62877400 L
N-N_3	0	7.70758200	-5.18096200	0.23836500 L

N-N_3	0	6.42226900	-4.56607700	2.45259000 L
B-B_2	0	5.13740700	-4.52874100	1.62251800 L
B-B_2	0	3.84888700	-3.36838200	3.40015900 L
N-N_3	0	3.85044000	-4.56669200	2.44821700 L
N-N_3	0	2.56157800	-3.04086700	4.15798900 L
B-B_2	0	1.27751700	-3.36775900	3.39313200 L
B-B_2	0	-0.00829100	-1.54716400	4.49243000 L
N-N_3	0	-0.00886300	-3.03892000	4.15133200 L
N-N_3	0	-1.29302100	-0.92578500	5.04095400 L
B-B_2	0	-2.57812000	-1.54632400	4.49237700 L
B-B_2	0	-3.86264400	0.56995900	4.71891500 L
N-N_3	0	-3.86209000	-0.92539500	5.04401400 L
N-N_3	0	-5.14637400	1.36697700	4.95469000 L
B-B_2	0	-6.43510500	0.57241300	4.73490300 L
N-N_3	0	-7.71844300	1.37222500	4.97763300 L
B-	0	12.78759200	-4.16160700	1.47234000 L
N-N_3	0	12.84940300	-5.09068600	0.25695200 L
N-N_3	0	11.60249400	-4.51772200	2.40530300 L
B-B_2	0	10.27941400	-4.53409900	1.61870400 L
B-B_2	0	8.99212300	-3.38309400	3.42352300 L
N-N_3	0	8.99863000	-4.57681500	2.46067100 L
N-N_3	0	7.70246000	-3.04588200	4.17372900 L
B-B_2	0	6.42034800	-3.36842800	3.40596500 L
B-B_2	0	5.13330200	-1.55062400	4.51031000 L
N-N_3	0	5.13316900	-3.04189600	4.16480800 L
N-N_3	0	3.84578900	-0.92811400	5.05262600 L
B-B_2	0	2.56197800	-1.54914800	4.49982400 L
B-B_2	0	1.27711800	0.56808500	4.71729700 L
N-N_3	0	1.27578300	-0.92682000	5.04426100 L
N-N_3	0	-0.00766700	1.36461400	4.94745600 L
B-B_2	0	-1.29252600	0.56913100	4.71499400 L
N-N_3	0	-2.57673800	1.36535600	4.94777700 L
N-N_3	0	12.84557600	-2.97904600	4.12809400 L
B-B_2	0	11.55254000	-3.41189500	3.46115400 L
B-B_2	0	10.27485600	-1.56560800	4.53288700 L
N-N_3	0	10.26274300	-3.07020600	4.20709500 L
N-N_3	0	8.99300600	-0.93267300	5.08746400 L
B-B_2	0	7.70703500	-1.55378700	4.52916200 L
B-B_2	0	6.41812700	0.56593700	4.73298300 L
N-N_3	0	6.41685300	-0.92871500	5.06433400 L
N-N_3	0	5.13221800	1.36296000	4.95782400 L
B-B_2	0	3.84733900	0.56687800	4.72451300 L
N-N_3	0	2.56175400	1.36367800	4.95149200 L
B-	0	12.78270400	-1.44959000	4.15520000 L

B-B_2	0	11.54943900	0.57346100	4.80988600 L
N-N_3	0	11.59717200	-0.94164500	5.01402000 L
N-N_3	0	10.26090300	1.37039000	5.01266100 L
B-B_2	0	8.98951200	0.56602400	4.76110700 L
N-N_3	0	7.70081100	1.36317400	4.96967100 L
N-N_3	0	12.84369400	1.36231200	4.89293800 L
H-H_	0	-12.41540600	2.85704900	0.92376400 L
H-H_	0	-12.40015900	2.49276200	-1.62112600 L
H-H_	0	-12.40195600	0.25579600	-2.94085300 L
H-H_	0	-12.41286800	-2.17472100	-2.03908500 L
H-H_	0	12.83400300	5.72532700	2.12513700 L
H-H_	0	12.83749800	5.21711200	-3.14324400 L
H-H_	0	-12.41016800	-2.96572500	0.40617900 L
H-H_	0	-12.39976300	-1.52302300	2.54886200 L
H-H_	0	12.83292700	0.78080700	-6.01116400 L
H-H_	0	12.83157800	-4.23591300	-4.36269600 L
H-H_	0	-12.40835600	1.06735100	2.78136300 L
H-H_	0	12.83604200	-6.07891800	0.59725100 L
H-H_	0	12.83132900	-3.32654000	5.11380800 L
H-H_	0	12.83052100	1.90965900	5.78334700 L
C-C_3	0	-0.78247300	-0.01723400	-0.57715800 H
H-H_	0	-0.79516800	0.75163000	1.46635800 H
H-H_	0	-2.32070000	0.96658500	0.59263900 H
C-C_3	0	-1.23105500	1.00159900	0.49402600 H
H-H_	0	-0.94260300	2.01695600	0.21536600 H
N-N_3	0	-1.18814000	-1.36074600	-0.29096900 H
H-H_	0	-0.47942400	-2.06415300	-0.18089700 H
H-H_	0	-2.15637900	-1.60391700	-0.19272800 H
C-C_R	0	0.73295400	-0.00999400	-0.73050500 H
O-O_R	0	1.45920100	-0.97361400	-0.59972400 H
O-O_R	0	1.20764000	1.21881800	-1.04056300 H
H-H_	0	2.17233100	1.14052900	-1.13015900 H
H-H_	0	-1.16980100	0.33449600	-1.55049300 H

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B-B_2	0	-10.28646600	2.09627200	4.40929500 L
N-N_3	0	-11.58302000	2.89644200	4.31186800 L
B-	0	-12.85671900	2.03095200	4.49219900 L
B-B_2	0	-5.14797600	2.06289000	4.31568100 L
N-N_3	0	-6.43151800	2.89307200	4.28334300 L
B-B_2	0	-7.72074200	2.07164900	4.33870600 L
B-B_2	0	-9.00791100	3.75838700	3.03106300 L
N-N_3	0	-8.99458500	2.91478000	4.32243500 L

N-N_3	0	-10.31033400	4.46819800	2.62978200 L
B-B_2	0	-11.52756200	3.58816200	2.95538700 L
B-	0	-12.85789100	4.78389100	1.22734200 L
N-N_3	0	-12.68001600	3.44528500	1.96177800 L
B-B_2	0	-0.00661200	2.06242500	4.31152500 L
N-N_3	0	-1.29188500	2.89028000	4.27565900 L
B-B_2	0	-2.57702700	2.06212700	4.31155900 L
B-B_2	0	-3.86292000	3.73711400	3.00236600 L
N-N_3	0	-3.86220500	2.89026000	4.27687100 L
N-N_3	0	-5.14830900	4.46846500	2.61166700 L
B-B_2	0	-6.43616200	3.74421800	3.00889300 L
B-B_2	0	-7.72179000	4.69292000	1.10131600 L
N-N_3	0	-7.72115600	4.48188600	2.62070800 L
N-N_3	0	-8.99610800	5.20307600	0.43082700 L
B-B_2	0	-10.28780100	4.76037900	1.12495300 L
B-B_2	0	-11.52818400	4.54932400	-0.94772900 L
N-N_3	0	-11.58432400	5.18139100	0.43760600 L
N-N_3	0	-12.67939300	3.68054100	-1.45352700 L
B-B_2	0	5.13536700	2.06548600	4.32108400 L
N-N_3	0	3.84890900	2.89215700	4.28099000 L
B-B_2	0	2.56399200	2.06341200	4.31529000 L
B-B_2	0	1.27881900	3.73730000	3.00238300 L
N-N_3	0	1.27825500	2.89086900	4.27714000 L
N-N_3	0	-0.00643000	4.46876900	2.61171500 L
B-B_2	0	-1.29174200	3.73716200	3.00140100 L
B-B_2	0	-2.57707000	4.67628200	1.09493900 L
N-N_3	0	-2.57729400	4.46751800	2.61068300 L
N-N_3	0	-3.86333800	5.16103500	0.42426000 L
B-B_2	0	-5.14869400	4.67418000	1.09525900 L
B-B_2	0	-6.43650900	4.69219600	-1.03365200 L
N-N_3	0	-6.43299400	5.16291200	0.42469900 L
N-N_3	0	-7.72122600	4.84408900	-1.85383100 L
B-B_2	0	-9.00838800	4.71586200	-1.03267600 L
B-B_2	0	-10.28675900	3.84367100	-3.00261100 L
N-N_3	0	-10.31048600	4.84151600	-1.83888300 L
N-N_3	0	-11.58278300	3.56656600	-3.76050700 L
B-	0	-12.85706600	3.93674200	-2.95873400 L
B-B_2	0	10.27682000	2.06265800	4.34419900 L
N-N_3	0	8.99613200	2.90478100	4.30323500 L
B-B_2	0	7.70903400	2.07211800	4.33477700 L
B-B_2	0	6.42112400	3.73763500	3.00829200 L
N-N_3	0	6.42008000	2.89556100	4.28667400 L
N-N_3	0	5.13596200	4.46732200	2.61398400 L
B-B_2	0	3.84991900	3.73759300	3.00524500 L

B-B_2	0	2.56506500	4.67641300	1.09656900 L
N-N_3	0	2.56454600	4.46806900	2.61250000 L
N-N_3	0	1.28011500	5.16441400	0.42536800 L
B-B_2	0	-0.00618400	4.67994200	1.09620600 L
B-B_2	0	-1.29141600	4.69057600	-1.02961200 L
N-N_3	0	-1.29202300	5.16565900	0.42502600 L
N-N_3	0	-2.57719700	4.83065500	-1.84584200 L
B-B_2	0	-3.86295200	4.68610700	-1.03027500 L
B-B_2	0	-5.14770700	3.76583400	-2.94698800 L
N-N_3	0	-5.14830800	4.83002100	-1.84725700 L
N-N_3	0	-6.43089200	3.54389900	-3.74854200 L
B-B_2	0	-7.72074300	3.78319500	-2.96185800 L
B-B_2	0	-9.00617000	2.12596600	-4.30861600 L
N-N_3	0	-8.99421700	3.57498700	-3.77967400 L
N-N_3	0	-10.30765200	1.57415400	-4.91088700 L
B-B_2	0	-11.52560400	2.08882000	-4.12753300 L
B-	0	-12.85503600	0.13551200	-4.90254800 L
N-N_3	0	-12.67627700	1.15138800	-3.76282100 L
B-	0	12.78493800	1.88077300	3.99261200 L
B-B_2	0	11.55290200	3.78924600	3.05348700 L
N-N_3	0	11.60002300	2.84415200	4.25527200 L
N-N_3	0	10.26477600	4.50121800	2.64133100 L
B-B_2	0	8.99266500	3.75228900	3.02500700 L
B-B_2	0	7.71087000	4.68554800	1.10008700 L
N-N_3	0	7.70483400	4.47044500	2.61863200 L
N-N_3	0	6.42266200	5.16263800	0.42600400 L
B-B_2	0	5.13704100	4.67600000	1.09769000 L
B-B_2	0	3.85145100	4.68419200	-1.02813000 L
N-N_3	0	3.85134900	5.16129900	0.42590500 L
N-N_3	0	2.56611900	4.82867400	-1.84433200 L
B-B_2	0	1.28002900	4.68718800	-1.02853100 L
B-B_2	0	-0.00528400	3.76461100	-2.94266700 L
N-N_3	0	-0.00513400	4.83100000	-1.84513800 L
N-N_3	0	-1.29045300	3.53899700	-3.74009000 L
B-B_2	0	-2.57625700	3.76454100	-2.94345900 L
B-B_2	0	-3.86125200	2.10513500	-4.27438800 L
N-N_3	0	-3.86111700	3.53979900	-3.74238300 L
N-N_3	0	-5.14568400	1.55800300	-4.89967900 L
B-B_2	0	-6.43447400	2.10893900	-4.28661300 L
B-B_2	0	-7.71896600	0.03511500	-4.78226300 L
N-N_3	0	-7.71845300	1.56310900	-4.91891300 L
N-N_3	0	-8.99232100	-0.73281400	-5.13256300 L
B-B_2	0	-10.28463600	0.04217300	-4.85715500 L
B-B_2	0	-11.52467100	-1.93302300	-4.19241000 L

N-N_3	0	-11.58093900	-0.72198700	-5.11538300 L
N-N_3	0	-12.67778200	-2.23665900	-3.23639600 L
B-	0	12.78652000	4.29101100	1.03566400 L
N-N_3	0	12.84725500	4.41046100	2.56075500 L
N-N_3	0	11.60241100	5.09789500	0.44572300 L
B-B_2	0	10.27871300	4.68254300	1.11267700 L
B-B_2	0	8.99426000	4.70300300	-1.03010800 L
N-N_3	0	8.99869300	5.17684900	0.42850700 L
N-N_3	0	7.70619200	4.83176400	-1.84477500 L
B-B_2	0	6.42272800	4.68338300	-1.02777900 L
B-B_2	0	5.13740500	3.76642000	-2.94722200 L
N-N_3	0	5.13735500	4.82742100	-1.84399900 L
N-N_3	0	3.85060800	3.54016200	-3.74261800 L
B-B_2	0	2.56570800	3.76424400	-2.94365600 L
B-B_2	0	1.28013100	2.10414800	-4.27211800 L
N-N_3	0	1.27996400	3.53894500	-3.74037300 L
N-N_3	0	-0.00512600	1.55779800	-4.89478300 L
B-B_2	0	-1.29015400	2.10406100	-4.27103000 L
B-B_2	0	-2.57522600	0.03406500	-4.75404000 L
N-N_3	0	-2.57503600	1.55747600	-4.89448900 L
N-N_3	0	-3.86041500	-0.72819400	-5.07924100 L
B-B_2	0	-5.14624500	0.03433400	-4.75716200 L
B-B_2	0	-6.43380900	-2.04711800	-4.30496400 L
N-N_3	0	-6.42938600	-0.72896800	-5.08673300 L
N-N_3	0	-7.71802400	-2.88125300	-4.27597200 L
B-B_2	0	-9.00528000	-2.05224200	-4.33343500 L
B-B_2	0	-10.28498800	-3.78344200	-3.05209100 L
N-N_3	0	-10.30711800	-2.86669600	-4.28067400 L
N-N_3	0	-11.58150000	-4.46235900	-2.61763500 L
B-	0	-12.85504600	-3.76154200	-3.15684000 L
N-N_3	0	12.84865500	4.74621300	-1.83550000 L
B-B_2	0	11.55455000	4.74616400	-1.04219800 L
B-B_2	0	10.27902400	3.78327300	-2.94859300 L
N-N_3	0	10.26617700	4.86734200	-1.85562000 L
N-N_3	0	8.99827700	3.55529000	-3.76031300 L
B-B_2	0	7.71115900	3.77521300	-2.95658800 L
B-B_2	0	6.42201400	2.10735300	-4.27812900 L
N-N_3	0	6.42199900	3.54335100	-3.74785000 L
N-N_3	0	5.13604700	1.55889200	-4.89856600 L
B-B_2	0	3.85078700	2.10528900	-4.27478800 L
B-B_2	0	2.56545700	0.03422400	-4.75989900 L
N-N_3	0	2.56507200	1.55831600	-4.89686100 L
N-N_3	0	1.28009300	-0.72858600	-5.08382300 L
B-B_2	0	-0.00471900	0.03389700	-4.75783200 L

B-B_2	0	-1.29001100	-2.04031300	-4.29292600 L
N-N_3	0	-1.29046900	-0.72843000	-5.08003200 L
N-N_3	0	-2.57505500	-2.86826800	-4.25508000 L
B-B_2	0	-3.86090400	-2.04133200	-4.29392500 L
B-B_2	0	-5.14630500	-3.71350900	-2.98152700 L
N-N_3	0	-5.14545700	-2.87087400	-4.25896000 L
N-N_3	0	-6.43004500	-4.44727200	-2.59246400 L
B-B_2	0	-7.71918400	-3.73095700	-2.99874200 L
B-B_2	0	-9.00682800	-4.68202900	-1.08887000 L
N-N_3	0	-8.99321900	-4.48322500	-2.61845500 L
N-N_3	0	-10.30943500	-5.14655800	-0.41899700 L
B-B_2	0	-11.52676200	-4.49613200	-1.09529400 L
B-	0	-12.85723100	-4.81993100	0.98086900 L
N-N_3	0	-12.67903100	-3.93454900	-0.26297900 L
B-	0	12.78669700	3.47830300	-2.69135900 L
B-B_2	0	11.55386700	2.13665500	-4.34125600 L
N-N_3	0	11.60222500	3.51971100	-3.68963600 L
N-N_3	0	10.26510900	1.57636600	-4.94251900 L
B-B_2	0	8.99361300	2.11896700	-4.29805300 L
B-B_2	0	7.71060500	0.03393100	-4.77456900 L
N-N_3	0	7.70500600	1.56206900	-4.90545300 L
N-N_3	0	6.42174200	-0.72905200	-5.08777800 L
B-B_2	0	5.13687900	0.03451500	-4.76122900 L
B-B_2	0	3.85113000	-2.04021500	-4.29583400 L
N-N_3	0	3.85092500	-0.72823800	-5.08365000 L
N-N_3	0	2.56592500	-2.86838300	-4.25700900 L
B-B_2	0	1.28038100	-2.04116300	-4.29704300 L
B-B_2	0	-0.00468800	-3.70939400	-2.97742700 L
N-N_3	0	-0.00511700	-2.86831800	-4.25563300 L
N-N_3	0	-1.28957700	-4.44096800	-2.58641900 L
B-B_2	0	-2.57514200	-3.71101400	-2.97818800 L
B-B_2	0	-3.86136100	-4.65100700	-1.07189500 L
N-N_3	0	-3.86041100	-4.44210400	-2.58762100 L
N-N_3	0	-5.14710500	-5.13907500	-0.40197800 L
B-B_2	0	-6.43491200	-4.65994500	-1.07487000 L
B-B_2	0	-7.72101800	-4.68324800	1.05508400 L
N-N_3	0	-7.72013600	-5.15499400	-0.40451300 L
N-N_3	0	-8.99540000	-4.85075300	1.88072200 L
B-B_2	0	-10.28708600	-4.75458200	1.06299500 L
B-B_2	0	-11.52750500	-3.66240800	2.83718600 L
N-N_3	0	-11.58373200	-4.83432200	1.86494100 L
N-N_3	0	-12.67823500	-2.65952500	2.91423300 L
B-	0	12.78597600	0.05669200	-4.38015700 L
N-N_3	0	12.84773200	1.51664600	-4.83685400 L

N-N_3	0	11.60144900	-0.69740500	-5.03536200 L
B-B_2	0	10.27832900	0.04580300	-4.77765200 L
B-B_2	0	8.99358700	-2.04811200	-4.32048000 L
N-N_3	0	8.99762200	-0.73073600	-5.10582400 L
N-N_3	0	7.70530400	-2.87075100	-4.26506000 L
B-B_2	0	6.42222700	-2.04056800	-4.29844100 L
B-B_2	0	5.13744700	-3.71258200	-2.98153300 L
N-N_3	0	5.13661500	-2.86807100	-4.25797800 L
N-N_3	0	3.85106400	-4.44017000	-2.58696800 L
B-B_2	0	2.56587300	-3.70942100	-2.97860800 L
B-B_2	0	1.28066100	-4.65049700	-1.07064200 L
N-N_3	0	1.28062300	-4.43971100	-2.58621900 L
N-N_3	0	-0.00455400	-5.13952800	-0.40096700 L
B-B_2	0	-1.28990300	-4.65179700	-1.07100400 L
B-B_2	0	-2.57625600	-4.66545700	1.05366000 L
N-N_3	0	-2.57594400	-5.13859900	-0.40140000 L
N-N_3	0	-3.86266300	-4.80894700	1.86858500 L
B-B_2	0	-5.14785400	-4.66340900	1.05243600 L
B-B_2	0	-6.43616900	-3.75234500	2.97662700 L
N-N_3	0	-6.43225500	-4.81126700	1.86888000 L
N-N_3	0	-7.72087600	-3.53304100	3.78145400 L
B-B_2	0	-9.00796100	-3.77511900	2.98630500 L
B-B_2	0	-10.28690100	-2.13402300	4.38193600 L
N-N_3	0	-10.31007800	-3.53824000	3.76701500 L
N-N_3	0	-11.58330200	-1.55628100	4.94458000 L
B-	0	-12.85728400	-2.23714300	4.38135000 L
N-N_3	0	12.84776600	-2.84418000	-4.18824500 L
B-B_2	0	11.55370700	-2.07014100	-4.36225500 L
B-B_2	0	10.27896400	-3.71720400	-3.00162600 L
N-N_3	0	10.26523600	-2.88999200	-4.29988100 L
N-N_3	0	8.99857800	-4.45902500	-2.59984700 L
B-B_2	0	7.71116100	-3.72343200	-2.99019400 L
B-B_2	0	6.42298700	-4.64776000	-1.07265900 L
N-N_3	0	6.42235200	-4.44493500	-2.58984300 L
N-N_3	0	5.13776100	-5.13395800	-0.40095500 L
B-B_2	0	3.85162500	-4.64745100	-1.07083400 L
B-B_2	0	2.56621100	-4.66475600	1.05491500 L
N-N_3	0	2.56673300	-5.13670200	-0.40069300 L
N-N_3	0	1.28074500	-4.81177500	1.87071700 L
B-B_2	0	-0.00511100	-4.66797200	1.05482200 L
B-B_2	0	-1.29115100	-3.74896500	2.97075500 L
N-N_3	0	-1.29120800	-4.81194700	1.87005600 L
N-N_3	0	-2.57702700	-3.52187700	3.76721400 L
B-B_2	0	-3.86275000	-3.74712300	2.97032000 L

B-B_2	0	-5.14812100	-2.08593700	4.29776400 L
N-N_3	0	-5.14802300	-3.52207600	3.76902700 L
N-N_3	0	-6.43143300	-1.53891400	4.92390900 L
B-B_2	0	-7.72103900	-2.09618800	4.31886900 L
B-B_2	0	-9.00714700	-0.01939100	4.81540600 L
N-N_3	0	-8.99461300	-1.55460900	4.96588300 L
N-N_3	0	-10.30887700	0.73803900	5.11992500 L
B-B_2	0	-11.52638900	-0.06525700	4.63591400 L
N-N_3	0	-12.67832000	0.62216300	3.90356800 L
B-	0	12.78684500	-3.39908900	-2.76270200 L
B-B_2	0	11.55490700	-4.71185600	-1.08907500 L
N-N_3	0	11.60245500	-4.38180600	-2.58191400 L
N-N_3	0	10.26667400	-5.17442900	-0.40895000 L
B-B_2	0	8.99458000	-4.66723400	-1.08041200 L
B-B_2	0	7.71199100	-4.67141700	1.05820700 L
N-N_3	0	7.70666100	-5.13792400	-0.40280300 L
N-N_3	0	6.42351200	-4.80844100	1.87214700 L
B-B_2	0	5.13811300	-4.66277500	1.05520100 L
B-B_2	0	3.85140300	-3.74618600	2.97220800 L
N-N_3	0	3.85219200	-4.80840600	1.87056500 L
N-N_3	0	2.56561000	-3.52197700	3.76941700 L
B-B_2	0	1.28009500	-3.74924900	2.97208100 L
B-B_2	0	-0.00609000	-2.08572400	4.29435600 L
N-N_3	0	-0.00588600	-3.52259900	3.76816700 L
N-N_3	0	-1.29151400	-1.53686100	4.91503600 L
B-B_2	0	-2.57695000	-2.08552600	4.29455000 L
B-B_2	0	-3.86259600	-0.01342600	4.77523000 L
N-N_3	0	-3.86200500	-1.53709200	4.91694700 L
N-N_3	0	-5.14710500	0.75007700	5.10233800 L
B-B_2	0	-6.43558400	-0.01237600	4.78778300 L
N-N_3	0	-7.71973400	0.75265600	5.12215000 L
B-	0	12.78766700	-4.28628200	0.94662000 L
N-N_3	0	12.84912200	-5.05678400	-0.37490600 L
N-N_3	0	11.60332300	-4.75678700	1.82821500 L
B-B_2	0	10.27987700	-4.67319300	1.04652800 L
B-B_2	0	8.99436900	-3.76063000	2.98472400 L
N-N_3	0	8.99958300	-4.82138400	1.87707000 L
N-N_3	0	7.70585600	-3.52303100	3.77384000 L
B-B_2	0	6.42278700	-3.74476700	2.97291700 L
B-B_2	0	5.13648500	-2.08531300	4.30299200 L
N-N_3	0	5.13693200	-3.52014600	3.76994400 L
N-N_3	0	3.84937500	-1.53669500	4.92093500 L
B-B_2	0	2.56487100	-2.08573000	4.29770400 L
B-B_2	0	1.27881500	-0.01339500	4.77333000 L

N-N_3	0	1.27864900	-1.53688100	4.91663300 L
N-N_3	0	-0.00676800	0.74905200	5.09639400 L
B-B_2	0	-1.29166700	-0.01361700	4.77138700 L
N-N_3	0	-2.57654900	0.74902600	5.09696000 L
N-N_3	0	12.84844200	-3.44806900	3.73013800 L
B-B_2	0	11.55464900	-3.79313100	3.01518400 L
B-B_2	0	10.27806800	-2.09870600	4.31448400 L
N-N_3	0	10.26591400	-3.54970300	3.80021000 L
N-N_3	0	8.99684000	-1.54148800	4.94623000 L
B-B_2	0	7.71025700	-2.08849000	4.31655600 L
B-B_2	0	6.42055800	-0.01252700	4.78346500 L
N-N_3	0	6.42067400	-1.53652600	4.92809600 L
N-N_3	0	5.13431400	0.75033400	5.10436000 L
B-B_2	0	3.84950000	-0.01287200	4.77816300 L
N-N_3	0	2.56338200	0.74962400	5.10002800 L
B-	0	12.78551600	-1.93444800	3.95127400 L
B-B_2	0	11.55221300	-0.01086700	4.85713600 L
N-N_3	0	11.60081600	-1.53966700	4.86874400 L
N-N_3	0	10.26313100	0.75435500	5.15543400 L
B-B_2	0	8.99205600	-0.01397700	4.80840100 L
N-N_3	0	7.70312600	0.75087600	5.11378500 L
N-N_3	0	12.84579700	0.76272100	5.03665700 L
H-H_	0	-12.40854100	2.71583700	1.26477200 L
H-H_	0	-12.40663600	2.68147800	-1.31527900 L
H-H_	0	-12.40231400	0.63563300	-2.89643800 L
H-H_	0	-12.40724300	-1.88248100	-2.29141700 L
H-H_	0	12.83363200	5.42493700	2.81223100 L
H-H_	0	12.83544800	5.57451700	-2.47293500 L
H-H_	0	-12.40718400	-2.97456900	0.04711000 L
H-H_	0	-12.40425500	-1.81951900	2.35656400 L
H-H_	0	12.83412700	1.53547300	-5.88186600 L
H-H_	0	12.83388900	-3.64866900	-4.85547200 L
H-H_	0	-12.40593400	0.71249700	2.89893000 L
H-H_	0	12.83569500	-6.07971500	-0.16039400 L
H-H_	0	12.83548000	-3.91789700	4.66377600 L
H-H_	0	12.83115800	1.19839000	5.98669300 L
C-C_3	0	-0.74355800	-0.19996700	-0.70920600 H
H-H_	0	-0.68659100	0.98566900	1.13057400 H
H-H_	0	-1.85195100	1.56435700	-0.07933400 H
C-C_3	0	-0.85187700	1.13976400	0.05864300 H
H-H_	0	-0.12108100	1.86750900	-0.30900200 H
N-N_3	0	-1.66515300	-1.24838700	-0.28349800 H
H-H_	0	-1.38258500	-1.62505700	0.61807100 H
H-H_	0	-2.61349800	-0.89391200	-0.20711200 H

C-C_R	0	0.67367100	-0.72882200	-0.54929000 H
O-O_R	0	1.03835100	-1.48438700	0.32635800 H
O-O_R	0	1.52200000	-0.21150700	-1.46900600 H
H-H_	0	2.40810800	-0.56342400	-1.27619100 H
H-H_	0	-0.90557700	-0.00278200	-1.77413700 H

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B-B_2	0	-10.31082000	1.99408000	4.44540100 L
N-N_3	0	-11.60740800	2.79641800	4.36924300 L
B-	0	-12.88105600	1.92686900	4.52992200 L
B-B_2	0	-5.17292500	1.96282400	4.34403100 L
N-N_3	0	-6.45620300	2.79374400	4.33490200 L
B-B_2	0	-7.74540800	1.97109600	4.37088000 L
B-B_2	0	-9.03367100	3.69052200	3.10775200 L
N-N_3	0	-9.01908900	2.81454300	4.37735800 L
N-N_3	0	-10.33682600	4.40907400	2.72462700 L
B-B_2	0	-11.55362200	3.52116000	3.03011500 L
B-	0	-12.88495800	4.75666600	1.33086200 L
N-N_3	0	-12.70697200	3.40168000	2.03450400 L
B-B_2	0	-0.03263600	1.96194500	4.33520500 L
N-N_3	0	-1.31732400	2.79097900	4.32217100 L
B-B_2	0	-2.60242200	1.96207800	4.33697200 L
B-B_2	0	-3.88852700	3.67340400	3.07521600 L
N-N_3	0	-3.88717500	2.79112200	4.32566000 L
N-N_3	0	-5.17450100	4.41441600	2.70538800 L
B-B_2	0	-6.46183400	3.67871300	3.08363700 L
B-B_2	0	-7.74864300	4.67401800	1.20173600 L
N-N_3	0	-7.74756700	4.42517500	2.71530500 L
N-N_3	0	-9.02406000	5.19662900	0.54303700 L
B-B_2	0	-10.31499500	4.73674900	1.22713000 L
B-B_2	0	-11.55556900	4.56806900	-0.84898600 L
N-N_3	0	-11.61195900	5.17124500	0.54920000 L
N-N_3	0	-12.70466400	3.70621400	-1.37127500 L
B-B_2	0	5.10817600	1.96373400	4.34810100 L
N-N_3	0	3.82182700	2.79132700	4.32842300 L
B-B_2	0	2.53731300	1.96201400	4.33895900 L
B-B_2	0	1.25279000	3.67322000	3.07249800 L
N-N_3	0	1.25208200	2.79075000	4.32268400 L
N-N_3	0	-0.03190700	4.41760400	2.70463700 L
B-B_2	0	-1.31725700	3.67424100	3.07251800 L
B-B_2	0	-2.60289500	4.66757900	1.19416700 L
N-N_3	0	-2.60307000	4.41521000	2.70344200 L
N-N_3	0	-3.89056500	5.16647900	0.53624300 L

B-B_2	0	-5.17522200	4.66064900	1.19503100 L
B-B_2	0	-6.46339000	4.72362100	-0.93174000 L
N-N_3	0	-6.46076300	5.16243300	0.53643000 L
N-N_3	0	-7.74879000	4.88744300	-1.74870000 L
B-B_2	0	-9.03560600	4.74041100	-0.93033600 L
B-B_2	0	-10.31228500	3.90327500	-2.91635200 L
N-N_3	0	-10.33802400	4.87911100	-1.73403400 L
N-N_3	0	-11.60763200	3.63807000	-3.67979700 L
B-	0	-12.88272100	3.99049200	-2.87135700 L
B-B_2	0	10.24885800	1.96089900	4.37846600 L
N-N_3	0	8.96822400	2.80382200	4.35877200 L
B-B_2	0	7.68147700	1.97024500	4.36607000 L
B-B_2	0	6.39476600	3.67198500	3.08368200 L
N-N_3	0	6.39247100	2.79465300	4.33808800 L
N-N_3	0	5.10999000	4.41262700	2.70845800 L
B-B_2	0	3.82376500	3.67200800	3.07687400 L
B-B_2	0	2.53988400	4.66736500	1.19538500 L
N-N_3	0	2.53888200	4.41420700	2.70446500 L
N-N_3	0	1.25597500	5.17734000	0.53803800 L
B-B_2	0	-0.03145000	4.67699000	1.19622200 L
B-B_2	0	-1.31676500	4.73780600	-0.92877500 L
N-N_3	0	-1.31839200	5.17741400	0.53738300 L
N-N_3	0	-2.60389300	4.88863800	-1.74174100 L
B-B_2	0	-3.88930300	4.72539300	-0.92889200 L
B-B_2	0	-5.17298400	3.83410900	-2.85944200 L
N-N_3	0	-5.17570900	4.88030700	-1.74260500 L
N-N_3	0	-6.45555800	3.62169600	-3.66474600 L
B-B_2	0	-7.74614100	3.84622900	-2.87517900 L
B-B_2	0	-9.02860400	2.21084600	-4.25196100 L
N-N_3	0	-9.01881700	3.65031200	-3.69726300 L
N-N_3	0	-10.32852000	1.67018300	-4.86730400 L
B-B_2	0	-11.54772600	2.16762200	-4.07491000 L
B-	0	-12.87540700	0.23128000	-4.89446700 L
N-N_3	0	-12.69885300	1.22228500	-3.73263300 L
B-	0	12.75541600	1.78751100	4.02076000 L
B-B_2	0	11.52612600	3.72379700	3.13757800 L
N-N_3	0	11.57207100	2.74437300	4.31147100 L
N-N_3	0	10.23831500	4.44560200	2.74273400 L
B-B_2	0	8.96603300	3.68631000	3.10441400 L
B-B_2	0	7.68625800	4.67147300	1.20437600 L
N-N_3	0	7.67870800	4.41548900	2.71644400 L
N-N_3	0	6.39896400	5.16642000	0.54130800 L
B-B_2	0	5.11230200	4.66373500	1.19878400 L
B-B_2	0	3.82769700	4.72755500	-0.92637600 L

N-N_3	0	3.82745400	5.16803600	0.53902900 L
N-N_3	0	2.54357600	4.89351600	-1.74083300 L
B-B_2	0	1.25611000	4.73894800	-0.92859800 L
B-B_2	0	-0.02915300	3.84613800	-2.85615700 L
N-N_3	0	-0.03019500	4.89574600	-1.74192700 L
N-N_3	0	-1.31498400	3.62517200	-3.65439700 L
B-B_2	0	-2.60111800	3.83934900	-2.85555100 L
B-B_2	0	-3.88419400	2.19348100	-4.20713700 L
N-N_3	0	-3.88586300	3.62158400	-3.65721300 L
N-N_3	0	-5.16670900	1.65489800	-4.84393500 L
B-B_2	0	-6.45711700	2.19508200	-4.22494600 L
B-B_2	0	-7.73962200	0.12927000	-4.76362700 L
N-N_3	0	-7.73930300	1.65986200	-4.86984100 L
N-N_3	0	-9.01166800	-0.63093600	-5.13510200 L
B-B_2	0	-10.30495000	0.13746400	-4.84557700 L
B-B_2	0	-11.54607600	-1.85292000	-4.22986300 L
N-N_3	0	-11.60049800	-0.62073800	-5.12434900 L
N-N_3	0	-12.70089800	-2.17854600	-3.28327600 L
B-	0	12.76369500	4.27861400	1.13667100 L
N-N_3	0	12.82060600	4.35948100	2.66443600 L
N-N_3	0	11.57886800	5.09695700	0.56376400 L
B-B_2	0	10.25429400	4.66621500	1.21939700 L
B-B_2	0	8.97149200	4.73574000	-0.92218400 L
N-N_3	0	8.97521900	5.17765100	0.54619600 L
N-N_3	0	7.68444200	4.88187200	-1.73528100 L
B-B_2	0	6.39966200	4.72063400	-0.92280800 L
B-B_2	0	5.11471500	3.84037600	-2.85726700 L
N-N_3	0	5.11540600	4.88326100	-1.73728000 L
N-N_3	0	3.82878200	3.62752400	-3.65721300 L
B-B_2	0	2.54256300	3.84813400	-2.85868900 L
B-B_2	0	1.25698600	2.19730100	-4.19715300 L
N-N_3	0	1.25628000	3.62903400	-3.65624500 L
N-N_3	0	-0.02761300	1.65535100	-4.82440800 L
B-B_2	0	-1.31335700	2.19463300	-4.19752300 L
B-B_2	0	-2.59677400	0.12913900	-4.71508500 L
N-N_3	0	-2.59639900	1.65491900	-4.83107200 L
N-N_3	0	-3.87976300	-0.62648400	-5.06355300 L
B-B_2	0	-5.16711700	0.12853600	-4.72953000 L
B-B_2	0	-6.45512200	-1.96527000	-4.33234700 L
N-N_3	0	-6.44872100	-0.62771700	-5.08079100 L
N-N_3	0	-7.73948800	-2.79968000	-4.32853400 L
B-B_2	0	-9.02650200	-1.96916400	-4.36781100 L
B-B_2	0	-10.30919600	-3.73099100	-3.13223500 L
N-N_3	0	-10.32856400	-2.78446600	-4.33798800 L

N-N_3	0	-11.60687000	-4.41891300	-2.71592000 L
B-	0	-12.87908700	-3.70477800	-3.24052300 L
N-N_3	0	12.82671200	4.79041700	-1.72399700 L
B-B_2	0	11.53219000	4.77735600	-0.93152800 L
B-B_2	0	10.25694700	3.84705100	-2.85353700 L
N-N_3	0	10.24438300	4.91335800	-1.74331900 L
N-N_3	0	8.97642800	3.63285100	-3.66929400 L
B-B_2	0	7.68890700	3.84327700	-2.86360300 L
B-B_2	0	6.39885600	2.19509500	-4.20601900 L
N-N_3	0	6.40018600	3.62462000	-3.65882000 L
N-N_3	0	5.11199300	1.65589000	-4.83186900 L
B-B_2	0	3.82773700	2.19690700	-4.20096800 L
B-B_2	0	2.54196300	0.13062500	-4.70637300 L
N-N_3	0	2.54157700	1.65619200	-4.82616700 L
N-N_3	0	1.25723600	-0.62489100	-5.04639600 L
B-B_2	0	-0.02734100	0.12998700	-4.70518800 L
B-B_2	0	-1.31207500	-1.95949800	-4.30225300 L
N-N_3	0	-1.31044500	-0.62559600	-5.05159200 L
N-N_3	0	-2.59654500	-2.78868000	-4.29565100 L
B-B_2	0	-3.88241100	-1.96048100	-4.31352400 L
B-B_2	0	-5.17049100	-3.67078700	-3.05398000 L
N-N_3	0	-5.16697700	-2.79055700	-4.30596100 L
N-N_3	0	-6.45593700	-4.41241200	-2.68629900 L
B-B_2	0	-7.74338900	-3.68318600	-3.07444500 L
B-B_2	0	-9.03434200	-4.67850800	-1.19032900 L
N-N_3	0	-9.01895000	-4.44286100	-2.71458300 L
N-N_3	0	-10.33846900	-5.15494100	-0.53173800 L
B-B_2	0	-11.55446000	-4.48831600	-1.19469300 L
B-	0	-12.88608100	-4.85414600	0.87400500 L
N-N_3	0	-12.70676200	-3.94353800	-0.35130100 L
B-	0	12.76487100	3.53635600	-2.60021700 L
B-B_2	0	11.53052200	2.21989900	-4.26964600 L
N-N_3	0	11.58027800	3.59327800	-3.59777100 L
N-N_3	0	10.24131100	1.67182300	-4.88186300 L
B-B_2	0	8.97041300	2.20440300	-4.22775100 L
B-B_2	0	7.68566500	0.12762800	-4.73877600 L
N-N_3	0	7.68084500	1.65798400	-4.84271700 L
N-N_3	0	6.39532300	-0.62758700	-5.06499600 L
B-B_2	0	5.11241000	0.12959700	-4.71672000 L
B-B_2	0	3.82643600	-1.95926400	-4.30163500 L
N-N_3	0	3.82534400	-0.62526800	-5.05156300 L
N-N_3	0	2.54146300	-2.78865100	-4.29051300 L
B-B_2	0	1.25718100	-1.95926700	-4.29778600 L
B-B_2	0	-0.02843300	-3.67842400	-3.04527500 L

N-N_3	0	-0.02728100	-2.78851400	-4.28999500 L
N-N_3	0	-1.31523300	-4.41900500	-2.67829700 L
B-B_2	0	-2.59914900	-3.67358800	-3.04737900 L
B-B_2	0	-3.88839600	-4.66436900	-1.17084000 L
N-N_3	0	-3.88628700	-4.41328000	-2.68021900 L
N-N_3	0	-5.17625800	-5.16260700	-0.51247700 L
B-B_2	0	-6.46223400	-4.66414300	-1.17472500 L
B-B_2	0	-7.74964400	-4.72843600	0.95270800 L
N-N_3	0	-7.74930900	-5.17007100	-0.51621700 L
N-N_3	0	-9.02480400	-4.90843000	1.77443400 L
B-B_2	0	-10.31605200	-4.79430600	0.95827800 L
B-B_2	0	-11.55519600	-3.73383700	2.75236500 L
N-N_3	0	-11.61306700	-4.88719600	1.75816200 L
N-N_3	0	-12.70437900	-2.73075200	2.84820900 L
B-	0	12.75914100	0.13840400	-4.34821200 L
N-N_3	0	12.82421400	1.60718400	-4.77500900 L
N-N_3	0	11.57546100	-0.59974500	-5.02239200 L
B-B_2	0	10.25304900	0.13815400	-4.74707400 L
B-B_2	0	8.96798600	-1.96726300	-4.33871600 L
N-N_3	0	8.97128900	-0.63029700	-5.09049000 L
N-N_3	0	7.67958400	-2.79106200	-4.30489600 L
B-B_2	0	6.39683600	-1.95987400	-4.31103800 L
B-B_2	0	5.11289300	-3.67589800	-3.04736000 L
N-N_3	0	5.11115100	-2.78839100	-4.29416200 L
N-N_3	0	3.82789100	-4.41923700	-2.67732400 L
B-B_2	0	2.54148300	-3.67952800	-3.04633300 L
B-B_2	0	1.25551800	-4.68130900	-1.17037500 L
N-N_3	0	1.25614500	-4.42349600	-2.67912700 L
N-N_3	0	-0.03149200	-5.18214100	-0.51096000 L
B-B_2	0	-1.31601800	-4.67474800	-1.16956300 L
B-B_2	0	-2.60386600	-4.72473600	0.95254600 L
N-N_3	0	-2.60443800	-5.17098400	-0.51110600 L
N-N_3	0	-3.89140300	-4.87721400	1.76479200 L
B-B_2	0	-5.17626700	-4.71572100	0.95106900 L
B-B_2	0	-6.46377100	-3.83364100	2.88951200 L
N-N_3	0	-6.46147500	-4.87424900	1.76444200 L
N-N_3	0	-7.74817000	-3.62620800	3.69821200 L
B-B_2	0	-9.03579000	-3.85295300	2.89929900 L
B-B_2	0	-10.31287000	-2.23639600	4.32553300 L
N-N_3	0	-10.33756400	-3.62880400	3.68434400 L
N-N_3	0	-11.60867100	-1.66913500	4.90032800 L
B-	0	-12.88347800	-2.33677300	4.32320400 L
N-N_3	0	12.82201500	-2.76693000	-4.23144500 L
B-B_2	0	11.52783700	-1.98844400	-4.38332600 L

B-B_2	0	10.25432600	-3.67314100	-3.06833000 L
N-N_3	0	10.23951400	-2.80974200	-4.34273200 L
N-N_3	0	8.97479900	-4.42699600	-2.68745600 L
B-B_2	0	7.68663600	-3.68206500	-3.05661900 L
B-B_2	0	6.39924000	-4.66145100	-1.16725700 L
N-N_3	0	6.39897100	-4.41718300	-2.67807400 L
N-N_3	0	5.11484600	-5.16593800	-0.50769600 L
B-B_2	0	3.82740100	-4.66933500	-1.16769600 L
B-B_2	0	2.54074100	-4.72718100	0.95385900 L
N-N_3	0	2.54296300	-5.17637300	-0.50916200 L
N-N_3	0	1.25528300	-4.88628900	1.76768500 L
B-B_2	0	-0.03175000	-4.73789900	0.95421200 L
B-B_2	0	-1.31810900	-3.83410300	2.87888200 L
N-N_3	0	-1.31934300	-4.88618400	1.76721600 L
N-N_3	0	-2.60331700	-3.61744700	3.68016800 L
B-B_2	0	-3.89011100	-3.83134900	2.88188900 L
B-B_2	0	-5.17408400	-2.18936500	4.23642600 L
N-N_3	0	-5.17494200	-3.61701900	3.68473700 L
N-N_3	0	-6.45642900	-1.65328600	4.87411800 L
B-B_2	0	-7.74704900	-2.19888000	4.26064600 L
B-B_2	0	-9.03167300	-0.13117300	4.80082300 L
N-N_3	0	-9.01962300	-1.66926000	4.91959200 L
N-N_3	0	-10.33255000	0.61970700	5.12417700 L
B-B_2	0	-11.55055900	-0.17203100	4.62304400 L
N-N_3	0	-12.70321100	0.53227600	3.90812200 L
B-	0	12.76224400	-3.36067600	-2.82169100 L
B-B_2	0	11.53125000	-4.71838400	-1.18374200 L
N-N_3	0	11.57831000	-4.34830100	-2.66722800 L
N-N_3	0	10.24321500	-5.19595700	-0.51424600 L
B-B_2	0	8.97078200	-4.67524300	-1.17421200 L
B-B_2	0	7.68768700	-4.72610400	0.96149400 L
N-N_3	0	7.68365900	-5.16376100	-0.50826400 L
N-N_3	0	6.39879400	-4.87784200	1.77206300 L
B-B_2	0	5.11358100	-4.72103100	0.95651000 L
B-B_2	0	3.82517600	-3.83111400	2.88303800 L
N-N_3	0	3.82702300	-4.87943300	1.76821400 L
N-N_3	0	2.53832800	-3.61712900	3.68091500 L
B-B_2	0	1.25360100	-3.83352400	2.87885000 L
B-B_2	0	-0.03257500	-2.18897100	4.22692000 L
N-N_3	0	-0.03233000	-3.61753700	3.67801000 L
N-N_3	0	-1.31726600	-1.65157700	4.85863600 L
B-B_2	0	-2.60298700	-2.18925200	4.22982100 L
B-B_2	0	-3.88781300	-0.12535400	4.75227200 L
N-N_3	0	-3.88717600	-1.65176900	4.86355400 L

N-N_3	0	-5.17144400	0.63093800	5.09830500 L
B-B_2	0	-6.46041900	-0.12416800	4.76871700 L
N-N_3	0	-7.74358800	0.63358900	5.12252400 L
B-	0	12.76491200	-4.33619400	0.85953600 L
N-N_3	0	12.82528600	-5.07962800	-0.47758400 L
N-N_3	0	11.57908500	-4.82132200	1.73157800 L
B-B_2	0	10.25584700	-4.72426300	0.95097800 L
B-B_2	0	8.96854200	-3.84533700	2.90242400 L
N-N_3	0	8.97524300	-4.88834700	1.77814400 L
N-N_3	0	7.67899500	-3.61986500	3.69351100 L
B-B_2	0	6.39672200	-3.83002500	2.88787700 L
B-B_2	0	5.10915000	-2.18990700	4.24054500 L
N-N_3	0	5.10972200	-3.61658100	3.68598000 L
N-N_3	0	3.82150700	-1.65200000	4.86620600 L
B-B_2	0	2.53781600	-2.18923900	4.23131500 L
B-B_2	0	1.25214200	-0.12558600	4.74673700 L
N-N_3	0	1.25172700	-1.65161800	4.85943100 L
N-N_3	0	-0.03282900	0.62957000	5.08750500 L
B-B_2	0	-1.31751100	-0.12558100	4.74572100 L
N-N_3	0	-2.60161200	0.62975200	5.08973500 L
N-N_3	0	12.82217700	-3.54319100	3.65586400 L
B-B_2	0	11.52906200	-3.87765000	2.93461500 L
B-B_2	0	10.25062100	-2.20418200	4.25954200 L
N-N_3	0	10.23936700	-3.64685100	3.72219800 L
N-N_3	0	8.96857800	-1.65794000	4.89929000 L
B-B_2	0	7.68283300	-2.19378300	4.25822900 L
B-B_2	0	6.39281800	-0.12579200	4.76274300 L
N-N_3	0	6.39245900	-1.65242600	4.87735900 L
N-N_3	0	5.10630600	0.62983000	5.09895500 L
B-B_2	0	3.82217800	-0.12567500	4.75363400 L
N-N_3	0	2.53618200	0.62963800	5.09154600 L
B-	0	12.75798300	-2.03331700	3.90110600 L
B-B_2	0	11.52392300	-0.12584000	4.83982100 L
N-N_3	0	11.57272300	-1.65452200	4.82450500 L
N-N_3	0	10.23498700	0.63251500	5.15660000 L
B-B_2	0	8.96411700	-0.12788100	4.79122200 L
N-N_3	0	7.67481200	0.63005100	5.11217300 L
N-N_3	0	12.81785800	0.64338000	5.03592600 L
H-H_	0	-12.43654600	2.68797300	1.32102500 L
H-H_	0	-12.42947200	2.70533900	-1.25218500 L
H-H_	0	-12.42628200	0.68783000	-2.87720000 L
H-H_	0	-12.43173900	-1.84701900	-2.32973700 L
H-H_	0	12.80448400	5.36725200	2.94143200 L
H-H_	0	12.81363100	5.62880100	-2.34811500 L

H-H_	0	-12.43458300	-2.99027700	-0.02144900 L
H-H_	0	-12.42867300	-1.88034300	2.30737500 L
H-H_	0	12.81290200	1.64734600	-5.81944600 L
H-H_	0	12.80779800	-3.55278000	-4.92052500 L
H-H_	0	-12.43178200	0.64615200	2.90561700 L
H-H_	0	12.81047800	-6.10668400	-0.28387900 L
H-H_	0	12.80887000	-4.02787700	4.58187100 L
H-H_	0	12.80537600	1.05467100	5.99679800 L
C-C_R	0	0.22341700	0.01677100	-0.62665300 H
H-H_	0	-0.36116800	1.12610300	1.15187200 H
H-H_	0	-1.52779000	1.22707600	-0.18901600 H
C-C_3	0	-0.46065400	1.16368000	0.05259400 H
H-H_	0	0.00476200	2.08846100	-0.28870700 H
N-N_3	0	-0.31861500	-1.40054700	-0.21440400 H
H-H_	0	0.48189700	-2.02605600	-0.10092200 H
H-H_	0	-0.99222800	-1.38862000	0.54678100 H
C-C_R	0	1.63824800	-0.08825500	-0.80904900 H
O-O_R	0	2.27131600	-1.15364300	-0.80883700 H
O-O_R	0	2.26853500	1.10373500	-1.02863500 H
H-H_	0	3.19617600	0.88526400	-1.21207300 H
H-H_	0	-0.50270500	-0.93804500	-1.27713200 H

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B-B_2	0	-10.30456300	2.52330300	4.16900100 L
N-N_3	0	-11.60151300	3.30981200	3.99580700 L
B-	0	-12.87476300	2.46551300	4.26059500 L
B-B_2	0	-5.16658600	2.48282000	4.07330400 L
N-N_3	0	-6.45028000	3.30585600	3.96370200 L
B-B_2	0	-7.73910500	2.49287200	4.09846700 L
B-B_2	0	-9.02781000	4.04553000	2.63587500 L
N-N_3	0	-9.01323700	3.33016800	4.00240500 L
N-N_3	0	-10.33121700	4.71128000	2.16760000 L
B-B_2	0	-11.54777600	3.86662600	2.57859400 L
B-	0	-12.87881700	4.88599900	0.74114100 L
N-N_3	0	-12.70115000	3.62698400	1.60490100 L
B-B_2	0	-0.02630500	2.48300800	4.06567100 L
N-N_3	0	-1.31121800	3.30433700	3.95341600 L
B-B_2	0	-2.59604000	2.48252600	4.06682600 L
B-B_2	0	-3.88240300	4.02843300	2.60787900 L
N-N_3	0	-3.88115400	3.30354200	3.95561700 L
N-N_3	0	-5.16883000	4.71761400	2.14988800 L
B-B_2	0	-6.45588600	4.03263100	2.61446100 L
B-B_2	0	-7.74250800	4.78930900	0.62474800 L

N-N_3	0	-7.74194700	4.72768300	2.15735500 L
N-N_3	0	-9.01782700	5.22657300	-0.09359200 L
B-B_2	0	-10.30892400	4.85382000	0.64130200 L
B-B_2	0	-11.54883100	4.43165400	-1.39884200 L
N-N_3	0	-11.60570000	5.20176600	-0.08517900 L
N-N_3	0	-12.69803200	3.51266400	-1.81216300 L
B-B_2	0	5.11483900	2.48720400	4.08101400 L
N-N_3	0	3.82840000	3.30648100	3.96151700 L
B-B_2	0	2.54382700	2.48438300	4.07134900 L
B-B_2	0	1.25918600	4.03083900	2.60773100 L
N-N_3	0	1.25823900	3.30483200	3.95485600 L
N-N_3	0	-0.02551800	4.72533200	2.15187100 L
B-B_2	0	-1.31095000	4.03203000	2.60715700 L
B-B_2	0	-2.59650400	4.78565700	0.62044100 L
N-N_3	0	-2.59734800	4.72081700	2.14935500 L
N-N_3	0	-3.88433400	5.19769400	-0.09496400 L
B-B_2	0	-5.16901700	4.77656100	0.62079500 L
B-B_2	0	-6.45659500	4.57544000	-1.49770500 L
N-N_3	0	-6.45454100	5.19255100	-0.09514600 L
N-N_3	0	-7.74158500	4.63740200	-2.32928500 L
B-B_2	0	-9.02881100	4.59256300	-1.49964800 L
B-B_2	0	-10.30488100	3.51809500	-3.36847700 L
N-N_3	0	-10.33086600	4.63164800	-2.31486000 L
N-N_3	0	-11.59996900	3.16197400	-4.09444600 L
B-	0	-12.87535600	3.61096700	-3.33587000 L
B-B_2	0	10.25578300	2.48702600	4.11160500 L
N-N_3	0	8.97526000	3.32150000	3.98978300 L
B-B_2	0	7.68826300	2.49531900	4.09813700 L
B-B_2	0	6.40175600	4.02855700	2.61882700 L
N-N_3	0	6.39935600	3.31055000	3.97070400 L
N-N_3	0	5.11723800	4.71809000	2.15567700 L
B-B_2	0	3.83052400	4.02921700	2.61257300 L
B-B_2	0	2.54681700	4.78512000	0.62332200 L
N-N_3	0	2.54575600	4.72070500	2.15208500 L
N-N_3	0	1.26304400	5.20876600	-0.09302400 L
B-B_2	0	-0.02498800	4.79738100	0.62290300 L
B-B_2	0	-1.31009300	4.59104500	-1.49384300 L
N-N_3	0	-1.31203100	5.21093000	-0.09405500 L
N-N_3	0	-2.59677300	4.63819400	-2.32010100 L
B-B_2	0	-3.88243000	4.57755400	-1.49376700 L
B-B_2	0	-5.16567200	3.45372100	-3.29972900 L
N-N_3	0	-5.16849700	4.63016400	-2.32102500 L
N-N_3	0	-6.44779200	3.14499300	-4.07406100 L
B-B_2	0	-7.73880400	3.46538000	-3.31898100 L

B-B_2	0	-9.02130800	1.67450300	-4.48672100 L
N-N_3	0	-9.01108300	3.17091300	-4.11180200 L
N-N_3	0	-10.32120700	1.06355100	-5.03237800 L
B-B_2	0	-11.54040000	1.65427800	-4.30691000 L
B-	0	-12.86888100	-0.36694100	-4.88365500 L
N-N_3	0	-12.69133700	0.75794700	-3.85108500 L
B-	0	12.76314000	2.27193300	3.77929000 L
B-B_2	0	11.53342500	4.08518900	2.66554000 L
N-N_3	0	11.57912000	3.25655500	3.95038700 L
N-N_3	0	10.24563300	4.75240400	2.18422900 L
B-B_2	0	8.97316400	4.04406100	2.63705900 L
B-B_2	0	7.69344600	4.78638600	0.63025300 L
N-N_3	0	7.68605900	4.72029800	2.16238700 L
N-N_3	0	6.40630100	5.19538300	-0.08906800 L
B-B_2	0	5.11944400	4.77990000	0.62653300 L
B-B_2	0	3.83470000	4.57588300	-1.48872500 L
N-N_3	0	3.83476800	5.19823600	-0.09087600 L
N-N_3	0	2.55020400	4.63733600	-2.31670200 L
B-B_2	0	1.26276900	4.58626600	-1.49139500 L
B-B_2	0	-0.02223200	3.46093800	-3.29277000 L
N-N_3	0	-0.02261500	4.64197600	-2.31895500 L
N-N_3	0	-1.30744200	3.14573200	-4.05935000 L
B-B_2	0	-2.59392700	3.45775700	-3.29409100 L
B-B_2	0	-3.87709800	1.65964800	-4.43648000 L
N-N_3	0	-3.87810300	3.14402600	-4.06423600 L
N-N_3	0	-5.15952300	1.04909500	-5.00470800 L
B-B_2	0	-6.44991600	1.66073600	-4.45624700 L
B-B_2	0	-7.73307800	-0.45458200	-4.74232200 L
N-N_3	0	-7.73201100	1.05201600	-5.03248700 L
N-N_3	0	-9.00549700	-1.25351000	-5.01925400 L
B-B_2	0	-10.29835000	-0.45515400	-4.82451700 L
B-B_2	0	-11.54010000	-2.35579500	-3.97195200 L
N-N_3	0	-11.59430700	-1.24098100	-5.00904100 L
N-N_3	0	-12.69476000	-2.56386700	-2.99259600 L
B-	0	12.77119900	4.38686400	0.61144800 L
N-N_3	0	12.82789700	4.65735300	2.11730300 L
N-N_3	0	11.58612600	5.12699600	-0.05913800 L
B-B_2	0	10.26154600	4.78180200	0.64529800 L
B-B_2	0	8.97833400	4.58427600	-1.48812000 L
N-N_3	0	8.98251600	5.20576100	-0.08621500 L
N-N_3	0	7.69099600	4.62863000	-2.31268300 L
B-B_2	0	6.40652600	4.56969600	-1.48586900 L
B-B_2	0	5.12105200	3.45558200	-3.29574100 L
N-N_3	0	5.12191100	4.62929900	-2.31360900 L

N-N_3	0	3.83462900	3.14599000	-4.06253800 L
B-B_2	0	2.54914400	3.46072400	-3.29520900 L
B-B_2	0	1.26341700	1.66144500	-4.42669500 L
N-N_3	0	1.26302500	3.14737300	-4.06052700 L
N-N_3	0	-0.02127600	1.04941200	-4.98490500 L
B-B_2	0	-1.30654500	1.66013700	-4.42616200 L
B-B_2	0	-2.59047900	-0.45170300	-4.69435000 L
N-N_3	0	-2.58957900	1.04941000	-4.99100000 L
N-N_3	0	-3.87381200	-1.24272500	-4.95010100 L
B-B_2	0	-5.16067300	-0.45255000	-4.70826700 L
B-B_2	0	-6.44925300	-2.48279100	-4.06273500 L
N-N_3	0	-6.44259900	-1.24481500	-4.96635200 L
N-N_3	0	-7.73407700	-3.30974300	-3.95733300 L
B-B_2	0	-9.02063000	-2.48926800	-4.09597200 L
B-B_2	0	-10.30341500	-4.08744000	-2.65518500 L
N-N_3	0	-10.32308200	-3.29420500	-3.96689500 L
N-N_3	0	-11.60108100	-4.71895300	-2.15746400 L
B-	0	-12.87323800	-4.07357300	-2.76477300 L
N-N_3	0	12.83353700	4.53685600	-2.29066200 L
B-B_2	0	11.53897500	4.62280700	-1.50270600 L
B-B_2	0	10.26298500	3.46447200	-3.29659200 L
N-N_3	0	10.25111400	4.65872000	-2.32519500 L
N-N_3	0	8.98210500	3.15263700	-4.07973700 L
B-B_2	0	7.69507600	3.45893600	-3.30459600 L
B-B_2	0	6.40478800	1.65958900	-4.43787500 L
N-N_3	0	6.40588400	3.14459500	-4.06639000 L
N-N_3	0	5.11778700	1.04920900	-4.99443600 L
B-B_2	0	3.83384300	1.66061000	-4.43110000 L
B-B_2	0	2.54808700	-0.45139300	-4.68949500 L
N-N_3	0	2.54767800	1.04956400	-4.98776600 L
N-N_3	0	1.26308700	-1.24159900	-4.93769800 L
B-B_2	0	-0.02105000	-0.45119300	-4.68629300 L
B-B_2	0	-1.30606300	-2.47709400	-4.03710700 L
N-N_3	0	-1.30466600	-1.24177700	-4.93966400 L
N-N_3	0	-2.59113400	-3.29852700	-3.93018600 L
B-B_2	0	-3.87656000	-2.47755900	-4.04619700 L
B-B_2	0	-5.16459200	-4.02161600	-2.58853400 L
N-N_3	0	-5.16158200	-3.29977200	-3.93796700 L
N-N_3	0	-6.45024100	-4.71152300	-2.13177800 L
B-B_2	0	-7.73754400	-4.03439600	-2.60527300 L
B-B_2	0	-9.02776800	-4.79083400	-0.61289300 L
N-N_3	0	-9.01322200	-4.74363900	-2.15452900 L
N-N_3	0	-10.33158200	-5.18277700	0.09979400 L
B-B_2	0	-11.54797200	-4.60218800	-0.63912300 L

B-	0	-12.87841100	-4.71349300	1.45972400 L
N-N_3	0	-12.70056000	-3.95964500	0.13200600 L
B-	0	12.77003700	3.18527700	-3.00717700 L
B-B_2	0	11.53621600	1.67820300	-4.50697800 L
N-N_3	0	11.58603700	3.12225900	-4.00491800 L
N-N_3	0	10.24693800	1.06071500	-5.04885700 L
B-B_2	0	8.97623300	1.66730600	-4.46229600 L
B-B_2	0	7.69183200	-0.45630000	-4.72226200 L
N-N_3	0	7.68653400	1.05094700	-5.00697600 L
N-N_3	0	6.40171600	-1.24549000	-4.95637200 L
B-B_2	0	5.11855700	-0.45292200	-4.70021800 L
B-B_2	0	3.83282800	-2.47855000	-4.04088300 L
N-N_3	0	3.83154600	-1.24256700	-4.94341200 L
N-N_3	0	2.54804700	-3.30141600	-3.93078800 L
B-B_2	0	1.26341100	-2.47888800	-4.03737700 L
B-B_2	0	-0.02227400	-4.03251700	-2.58451500 L
N-N_3	0	-0.02182500	-3.30005700	-3.92795500 L
N-N_3	0	-1.30922800	-4.72151500	-2.12763400 L
B-B_2	0	-2.59312500	-4.02629300	-2.58433800 L
B-B_2	0	-3.88167400	-4.77530300	-0.59876500 L
N-N_3	0	-3.88059800	-4.71370900	-2.12761900 L
N-N_3	0	-5.16915900	-5.18753000	0.11738400 L
B-B_2	0	-6.45561000	-4.77507800	-0.60073600 L
B-B_2	0	-7.74196100	-4.57638100	1.51911300 L
N-N_3	0	-7.74232000	-5.19582000	0.11587700 L
N-N_3	0	-9.01658100	-4.65459100	2.35753700 L
B-B_2	0	-10.30840700	-4.64224600	1.53437000 L
B-B_2	0	-11.54712300	-3.37026800	3.18549400 L
N-N_3	0	-11.60489600	-4.63696900	2.34043400 L
N-N_3	0	-12.69610000	-2.36279600	3.15719100 L
B-	0	12.76558300	-0.39738200	-4.33734900 L
N-N_3	0	12.82984200	1.00996600	-4.93637600 L
N-N_3	0	11.58181600	-1.21110700	-4.91787600 L
B-B_2	0	10.25923200	-0.44594200	-4.73227300 L
B-B_2	0	8.97482300	-2.48732700	-4.07459900 L
N-N_3	0	8.97768900	-1.25026100	-4.98128900 L
N-N_3	0	7.68686800	-3.30160700	-3.94148800 L
B-B_2	0	6.40355400	-2.47827000	-4.04885200 L
B-B_2	0	5.12009800	-4.02813300	-2.58670400 L
N-N_3	0	5.11830600	-3.29960400	-3.93261100 L
N-N_3	0	3.83553400	-4.72078500	-2.12764200 L
B-B_2	0	2.54842100	-4.03482500	-2.58750500 L
B-B_2	0	1.26265100	-4.78936600	-0.59948200 L
N-N_3	0	1.26272100	-4.72592100	-2.12887300 L

N-N_3	0	-0.02372200	-5.20281000	0.11869400 L
B-B_2	0	-1.30928000	-4.78673100	-0.59873400 L
B-B_2	0	-2.59611000	-4.56776000	1.51403800 L
N-N_3	0	-2.59729700	-5.19528100	0.11834000 L
N-N_3	0	-3.88275400	-4.62063400	2.34037500 L
B-B_2	0	-5.16848900	-4.56218000	1.51405000 L
B-B_2	0	-6.45565900	-3.44925700	3.33043300 L
N-N_3	0	-6.45311700	-4.62019100	2.34173800 L
N-N_3	0	-7.73974000	-3.14542100	4.10861800 L
B-B_2	0	-9.02763400	-3.46899100	3.34430600 L
B-B_2	0	-10.30498100	-1.69080700	4.56290900 L
N-N_3	0	-10.32910500	-3.15118700	4.09686400 L
N-N_3	0	-11.60099100	-1.05831900	5.06456300 L
B-	0	-12.87568300	-1.79139300	4.57286700 L
N-N_3	0	12.82904900	-3.26747700	-3.87216000 L
B-B_2	0	11.53480000	-2.51328100	-4.11706000 L
B-B_2	0	10.26187600	-4.02387800	-2.60543200 L
N-N_3	0	10.24665500	-3.32348800	-3.97613400 L
N-N_3	0	8.98259700	-4.72536800	-2.13442900 L
B-B_2	0	7.69405000	-4.03288300	-2.59348600 L
B-B_2	0	6.40668000	-4.76937500	-0.59769800 L
N-N_3	0	6.40676400	-4.71626900	-2.12724200 L
N-N_3	0	5.12209300	-5.18702000	0.11955300 L
B-B_2	0	3.83478000	-4.77755700	-0.59833900 L
B-B_2	0	2.54812900	-4.56671000	1.51372200 L
N-N_3	0	2.55022700	-5.19665500	0.11892300 L
N-N_3	0	1.26242600	-4.62326400	2.34040500 L
B-B_2	0	-0.02407200	-4.57406300	1.51442000 L
B-B_2	0	-1.31034300	-3.44813200	3.31901500 L
N-N_3	0	-1.31063600	-4.62543700	2.34100100 L
N-N_3	0	-2.59550600	-3.13656800	4.08799600 L
B-B_2	0	-3.88197200	-3.44612900	3.32136100 L
B-B_2	0	-5.16647200	-1.65238200	4.46691600 L
N-N_3	0	-5.16669500	-3.13643600	4.09257200 L
N-N_3	0	-6.44883300	-1.04367100	5.03549200 L
B-B_2	0	-7.73928800	-1.66020300	4.49306900 L
B-B_2	0	-9.02460600	0.45728000	4.77913000 L
N-N_3	0	-9.01190800	-1.05510100	5.08336100 L
N-N_3	0	-10.32580000	1.24122200	5.00918400 L
B-B_2	0	-11.54336800	0.39404500	4.60757800 L
N-N_3	0	-12.69616800	1.00594100	3.81236600 L
B-	0	12.77043300	-3.68354700	-2.40005500 L
B-B_2	0	11.53885600	-4.82642500	-0.60579200 L
N-N_3	0	11.58605700	-4.64387800	-2.12386600 L

N-N_3	0	10.25077100	-5.21740000	0.11779900 L
B-B_2	0	8.97829800	-4.78328600	-0.60206400 L
B-B_2	0	7.69479700	-4.56756100	1.52314500 L
N-N_3	0	7.69105000	-5.18505200	0.11936500 L
N-N_3	0	6.40564200	-4.61764300	2.34588700 L
B-B_2	0	5.12068900	-4.56236500	1.51670000 L
B-B_2	0	3.83226100	-3.44224800	3.32014200 L
N-N_3	0	3.83387100	-4.61864700	2.34136000 L
N-N_3	0	2.54565900	-3.13361000	4.08666200 L
B-B_2	0	1.26095100	-3.44463900	3.31670500 L
B-B_2	0	-0.02529900	-1.65119700	4.45776900 L
N-N_3	0	-0.02444200	-3.13549500	4.08529600 L
N-N_3	0	-1.31018700	-1.04193600	5.01969500 L
B-B_2	0	-2.59556200	-1.65216700	4.46024700 L
B-B_2	0	-3.88094300	0.45941900	4.72963100 L
N-N_3	0	-3.87983000	-1.04238900	5.02432100 L
N-N_3	0	-5.16475800	1.25137700	4.98231800 L
B-B_2	0	-6.45344000	0.46152200	4.74616600 L
N-N_3	0	-7.73687600	1.25589600	5.00606800 L
B-	0	12.77163600	-4.19253500	1.37452400 L
N-N_3	0	12.83292700	-5.09623400	0.14009600 L
N-N_3	0	11.58608500	-4.56687000	2.29985100 L
B-B_2	0	10.26296300	-4.56727500	1.51308600 L
B-B_2	0	8.97541700	-3.45488300	3.34198700 L
N-N_3	0	8.98216100	-4.62786800	2.35396100 L
N-N_3	0	7.68576300	-3.13507300	4.09971800 L
B-B_2	0	6.40364600	-3.44109900	3.32512700 L
B-B_2	0	5.11603900	-1.64950200	4.47072500 L
N-N_3	0	5.11666000	-3.13247100	4.09143000 L
N-N_3	0	3.82846500	-1.04055500	5.02770300 L
B-B_2	0	2.54492400	-1.65005600	4.46181300 L
B-B_2	0	1.25890500	0.46020900	4.72563000 L
N-N_3	0	1.25877500	-1.04118000	5.02100800 L
N-N_3	0	-0.02645600	1.25047000	4.97238000 L
B-B_2	0	-1.31077200	0.45926800	4.72340400 L
N-N_3	0	-2.59506500	1.25009400	4.97393500 L
N-N_3	0	12.82903900	-3.06240600	4.05249300 L
B-B_2	0	11.53580700	-3.48226000	3.37747300 L
B-B_2	0	10.25720200	-1.66165100	4.49204800 L
N-N_3	0	10.24619300	-3.15845800	4.13185000 L
N-N_3	0	8.97512700	-1.04284600	5.06175600 L
B-B_2	0	7.68958000	-1.65141700	4.48898000 L
B-B_2	0	6.39949500	0.46229300	4.74288900 L
N-N_3	0	6.39919600	-1.03978800	5.03880500 L

N-N_3	0	5.11291800	1.25279900	4.98620600 L
B-B_2	0	3.82891500	0.46138600	4.73343700 L
N-N_3	0	2.54264700	1.25162900	4.97803800 L
B-	0	12.76387700	-1.53409400	4.11481800 L
B-B_2	0	11.53048100	0.47129400	4.82120300 L
N-N_3	0	11.57921200	-1.04837800	4.98737200 L
N-N_3	0	10.24145200	1.26203700	5.04398300 L
B-B_2	0	8.97071100	0.46339300	4.77189000 L
N-N_3	0	7.68143100	1.25438200	4.99967300 L
N-N_3	0	12.82423000	1.25848500	4.92502300 L
H-H_	0	-12.43093300	2.83146700	0.98386300 L
H-H_	0	-12.42327500	2.53382900	-1.57121500 L
H-H_	0	-12.41806700	0.33145100	-2.93722700 L
H-H_	0	-12.42533700	-2.11901100	-2.08644900 L
H-H_	0	12.81144000	5.69177100	2.26662300 L
H-H_	0	12.82180700	5.29279800	-3.01246400 L
H-H_	0	-12.42938500	-2.97286500	0.34250500 L
H-H_	0	-12.41988800	-1.58493400	2.51659600 L
H-H_	0	12.81797200	0.92523500	-5.97813800 L
H-H_	0	12.81397300	-4.13205000	-4.45942200 L
H-H_	0	-12.42456600	0.99756900	2.80349800 L
H-H_	0	12.81874900	-6.09129200	0.45984600 L
H-H_	0	12.81679500	-3.43252700	5.02996400 L
H-H_	0	12.81047000	1.78261200	5.82928800 L
C-C_R	0	0.04086500	-0.02339900	-0.37232100 H
H-H_	0	-1.05520200	1.33692100	0.92969000 H
H-H_	0	-1.69959500	1.24833400	-0.72213300 H
C-C_3	0	-0.77240600	1.19675700	-0.12862700 H
H-H_	0	-0.16407400	2.05709300	-0.41080400 H
N-N_R	0	-0.48103400	-1.34894800	0.02597900 H
H-H_	0	0.38821200	-1.92673600	-0.19334700 H
H-H_	0	-0.72012400	-1.43672500	1.02065700 H
C-C_R	0	1.35747700	-0.20223400	-0.75842700 H
O-O_R	0	1.91634100	-1.34713000	-0.78391700 H
O-O_R	0	2.07424500	0.90474700	-1.12825700 H
H-H_	0	2.94413600	0.56912400	-1.39242500 H
H-H_	0	-1.28112400	-1.68156300	-0.52076700 H

Coordinates of all stationary points in the pathway a of α -Ala chiral transformation confined in SWBNNT(8,8)

S α -Ala @D

B-B_2	0	10.26448500	-4.90639900	2.57043800 L
N-N_3	0	11.57223100	-5.46413700	2.00867200 L
B-	0	12.84041700	-4.82006200	2.62792500 L
B-B_2	0	5.12956300	-4.83729700	2.51728300 L
N-N_3	0	6.41281800	-5.48841200	2.00064300 L
B-B_2	0	7.70213900	-4.86148200	2.53495200 L
B-B_2	0	8.98623100	-5.48267600	0.48037100 L
N-N_3	0	8.97674200	-5.53213900	2.02275100 L
N-N_3	0	10.28933300	-5.84524400	-0.24579100 L
B-B_2	0	11.48954500	-5.25383000	0.50421400 L
B-	0	12.84210400	-5.26741000	-1.57344200 L
N-N_3	0	12.60418300	-4.52734500	-0.24746800 L
B-B_2	0	-0.01050900	-4.84579100	2.51844200 L
N-N_3	0	1.27518800	-5.49137700	1.99900600 L
B-B_2	0	2.55867600	-4.84003000	2.51600200 L
B-B_2	0	3.84466600	-5.44672800	0.46721100 L
N-N_3	0	3.84487800	-5.48353300	1.99653500 L
N-N_3	0	5.13018100	-5.84090900	-0.26179600 L
B-B_2	0	6.41784900	-5.45487400	0.46830900 L
B-B_2	0	7.70299600	-5.23605500	-1.66350200 L
N-N_3	0	7.70098300	-5.86198000	-0.26184700 L
N-N_3	0	8.97718300	-5.33960400	-2.50166400 L
B-B_2	0	10.26578900	-5.29060800	-1.67249600 L
B-B_2	0	11.48733100	-4.05909200	-3.36991300 L
N-N_3	0	11.57287600	-5.27917400	-2.46517800 L
N-N_3	0	12.59576000	-3.00724400	-3.37427800 L
B-B_2	0	-5.15153400	-4.84899800	2.52237100 L
N-N_3	0	-3.86546400	-5.49182400	2.00013600 L
B-B_2	0	-2.58030000	-4.84507300	2.51881500 L
B-B_2	0	-1.29580100	-5.45648900	0.47019200 L
N-N_3	0	-1.29551200	-5.49290400	1.99980000 L
N-N_3	0	-0.01081800	-5.85076100	-0.26022800 L
B-B_2	0	1.27485500	-5.45759400	0.46916600 L
B-B_2	0	2.55900500	-5.21879600	-1.65560400 L
N-N_3	0	2.56087200	-5.84790400	-0.26081800 L
N-N_3	0	3.84470700	-5.29373800	-2.48097700 L
B-B_2	0	5.12993100	-5.21130300	-1.65630900 L
B-B_2	0	6.41634300	-4.17774100	-3.53244700 L
N-N_3	0	6.41305600	-5.29577900	-2.48391300 L
N-N_3	0	7.69824500	-3.94249500	-4.33699300 L

B-B_2	0	8.98472000	-4.20494700	-3.54773900 L
B-B_2	0	10.26211100	-2.53720500	-4.92557400 L
N-N_3	0	10.28676100	-3.94175100	-4.31713000 L
N-N_3	0	11.56974900	-1.96597000	-5.47483100 L
B-	0	12.83913900	-2.58375200	-4.83161000 L
B-B_2	0	-10.28841400	-4.86717800	2.54776000 L
N-N_3	0	-9.00958500	-5.52206200	2.01361500 L
B-B_2	0	-7.72461300	-4.86623800	2.53194500 L
B-B_2	0	-6.43731000	-5.45362000	0.47280300 L
N-N_3	0	-6.43550800	-5.49850700	2.00290500 L
N-N_3	0	-5.15209600	-5.84438400	-0.25824400 L
B-B_2	0	-3.86634500	-5.45109900	0.47084400 L
B-B_2	0	-2.58183000	-5.21314700	-1.65168800 L
N-N_3	0	-2.58205400	-5.84681700	-0.25926800 L
N-N_3	0	-1.29720900	-5.29406700	-2.47743500 L
B-B_2	0	-0.01113700	-5.21715300	-1.65321200 L
B-B_2	0	1.27238700	-4.17415100	-3.51944800 L
N-N_3	0	1.27314100	-5.29708800	-2.47988900 L
N-N_3	0	2.55716500	-3.92776900	-4.31178600 L
B-B_2	0	3.84328400	-4.17190000	-3.52142000 L
B-B_2	0	5.12689700	-2.49182800	-4.84777400 L
N-N_3	0	5.12716100	-3.92706300	-4.31662900 L
N-N_3	0	6.40827200	-1.96618300	-5.49646600 L
B-B_2	0	7.69964900	-2.50569000	-4.87822300 L
B-B_2	0	8.97996400	-0.44303800	-5.48652100 L
N-N_3	0	8.97286500	-1.98536600	-5.54585100 L
N-N_3	0	10.28166700	0.28535400	-5.84848900 L
B-B_2	0	11.48079200	-0.46347100	-5.25468300 L
B-	0	12.83433600	1.61220000	-5.26393500 L
N-N_3	0	12.59053700	0.28867700	-4.52133500 L
B-	0	-12.77635400	-4.47231500	2.35317700 L
B-B_2	0	-11.56396000	-5.49795500	0.48066200 L
N-N_3	0	-11.61284400	-5.43081900	2.00567500 L
N-N_3	0	-10.28165300	-5.89319300	-0.25315100 L
B-B_2	0	-9.00802300	-5.48025900	0.47946800 L
B-B_2	0	-7.72614800	-5.23054200	-1.65859500 L
N-N_3	0	-7.71996000	-5.85374800	-0.25668700 L
N-N_3	0	-6.43723500	-5.29883600	-2.48033600 L
B-B_2	0	-5.15310400	-5.21476100	-1.65293800 L
B-B_2	0	-3.86777500	-4.17298600	-3.51901100 L
N-N_3	0	-3.86713500	-5.29329400	-2.47710800 L
N-N_3	0	-2.58256400	-3.92992100	-4.31120100 L
B-B_2	0	-1.29739600	-4.17274700	-3.51823400 L
B-B_2	0	-0.01357800	-2.49586200	-4.84488300 L

N-N_3	0	-0.01286300	-3.92999100	-4.31157000 L
N-N_3	0	1.27122100	-1.96716800	-5.48344200 L
B-B_2	0	2.55608300	-2.49267500	-4.84227000 L
B-B_2	0	3.83968700	-0.43534900	-5.43466200 L
N-N_3	0	3.84019400	-1.96459700	-5.48373400 L
N-N_3	0	5.12266600	0.29606400	-5.83308700 L
B-B_2	0	6.41214900	-0.43367700	-5.45256800 L
B-B_2	0	7.69547800	1.70298600	-5.24046700 L
N-N_3	0	7.69333700	0.29884200	-5.86199300 L
N-N_3	0	8.96891300	2.54168000	-5.35190700 L
B-B_2	0	10.25761700	1.71291400	-5.29662900 L
B-B_2	0	11.47835300	3.42185700	-4.07813300 L
N-N_3	0	11.56559100	2.50481300	-5.28869000 L
N-N_3	0	12.59555700	3.45169000	-3.03584200 L
B-	0	-12.77732600	-4.82087900	-1.50256900 L
N-N_3	0	-12.86514800	-5.72264400	-0.27022200 L
N-N_3	0	-11.61469900	-5.24968100	-2.42874000 L
B-B_2	0	-10.28996000	-5.23974900	-1.64741100 L
B-B_2	0	-9.00941500	-4.20182500	-3.53877200 L
N-N_3	0	-9.01141400	-5.32158600	-2.48910200 L
N-N_3	0	-7.72082900	-3.94195700	-4.32173700 L
B-B_2	0	-6.43863300	-4.17781600	-3.52287500 L
B-B_2	0	-5.15430600	-2.49937800	-4.85110400 L
N-N_3	0	-5.15263800	-3.93216800	-4.31337900 L
N-N_3	0	-3.86809900	-1.97149600	-5.48835900 L
B-B_2	0	-2.58340600	-2.49632400	-4.84526400 L
B-B_2	0	-1.29998400	-0.44026800	-5.43448800 L
N-N_3	0	-1.29861100	-1.96937000	-5.48543100 L
N-N_3	0	-0.01546300	0.29036500	-5.82742700 L
B-B_2	0	1.26962500	-0.43810400	-5.43203700 L
B-B_2	0	2.55249900	1.69011300	-5.20401300 L
N-N_3	0	2.55350900	0.29282900	-5.82703500 L
N-N_3	0	3.83650200	2.51604100	-5.29381200 L
B-B_2	0	5.12300100	1.69339800	-5.20862200 L
B-B_2	0	6.40877500	3.58394600	-4.19780700 L
N-N_3	0	6.40463900	2.52204500	-5.30361700 L
N-N_3	0	7.69052200	4.39158600	-3.97377500 L
B-B_2	0	8.97673400	3.59922100	-4.22780400 L
B-B_2	0	10.25517500	4.99874700	-2.57791300 L
N-N_3	0	10.27877900	4.37158800	-3.97409500 L
N-N_3	0	11.56183500	5.55861400	-2.01570500 L
B-	0	12.83119400	4.91678400	-2.63487600 L
N-N_3	0	-12.86668100	-3.83877300	-4.23787600 L
B-B_2	0	-11.56524700	-4.21367700	-3.54984800 L

B-B_2	0	-10.29091800	-2.52482400	-4.87098100 L
N-N_3	0	-10.28295700	-3.97329200	-4.34837300 L
N-N_3	0	-9.01213300	-1.98748200	-5.52362600 L
B-B_2	0	-7.72730500	-2.50889200	-4.86988000 L
B-B_2	0	-6.44050800	-0.44525500	-5.44804500 L
N-N_3	0	-6.43795300	-1.97545400	-5.49795200 L
N-N_3	0	-5.15478700	0.28641700	-5.83655000 L
B-B_2	0	-3.86991500	-0.44219000	-5.43942500 L
B-B_2	0	-2.58688600	1.68563100	-5.20770200 L
N-N_3	0	-2.58481500	0.28846400	-5.83122300 L
N-N_3	0	-1.30254700	2.51133500	-5.29492800 L
B-B_2	0	-0.01715000	1.68771800	-5.20445800 L
B-B_2	0	1.26567800	3.56974800	-4.18658000 L
N-N_3	0	1.26692100	2.51354300	-5.29342800 L
N-N_3	0	2.54994000	4.36701300	-3.95401700 L
B-B_2	0	3.83613000	3.57271900	-4.18719000 L
B-B_2	0	5.12017800	4.92222400	-2.52780300 L
N-N_3	0	5.11975100	4.37168100	-3.95585100 L
N-N_3	0	6.40232000	5.57430000	-2.00906300 L
B-B_2	0	7.69279200	4.94980000	-2.54348900 L
B-B_2	0	8.97547500	5.57165600	-0.48783800 L
N-N_3	0	8.96620100	5.62199700	-2.03025300 L
N-N_3	0	10.27773700	5.93667800	0.23861400 L
B-B_2	0	11.47924100	5.34775600	-0.51130000 L
B-	0	12.83170300	5.36525200	1.56655400 L
N-N_3	0	12.59584100	4.62447900	0.24060000 L
B-	0	-12.77698800	-2.32980900	-4.47112800 L
B-B_2	0	-11.56678500	-0.45520300	-5.49562100 L
N-N_3	0	-11.61558900	-1.98021700	-5.43123600 L
N-N_3	0	-10.28492900	0.27834900	-5.89346000 L
B-B_2	0	-9.01116700	-0.45321700	-5.47861200 L
B-B_2	0	-7.73051500	1.68810200	-5.23380100 L
N-N_3	0	-7.72283400	0.28339900	-5.85105400 L
N-N_3	0	-6.44200400	2.51033100	-5.30614200 L
B-B_2	0	-5.15757100	1.68450600	-5.21391700 L
B-B_2	0	-3.87439600	3.56440600	-4.18962400 L
N-N_3	0	-3.87225900	2.50944100	-5.29800800 L
N-N_3	0	-2.59033800	4.36186000	-3.95555800 L
B-B_2	0	-1.30428800	3.56727400	-4.18769100 L
B-B_2	0	-0.02108800	4.91588900	-2.52723700 L
N-N_3	0	-0.02016100	4.36476500	-3.95459900 L
N-N_3	0	1.26339300	5.56250800	-2.00608200 L
B-B_2	0	2.54925600	4.91813600	-2.52670500 L
B-B_2	0	3.83414000	5.52374200	-0.47614200 L

N-N_3	0	3.83387600	5.56441900	-2.00575400 L
N-N_3	0	5.11831100	5.92082200	0.25412500 L
B-B_2	0	6.40707900	5.53891800	-0.47646000 L
B-B_2	0	7.69261600	5.32156900	1.65621200 L
N-N_3	0	7.68931000	5.94779600	0.25449100 L
N-N_3	0	8.96655700	5.42816800	2.49442400 L
B-B_2	0	10.25530500	5.38196900	1.66530600 L
B-B_2	0	11.47965100	4.15371400	3.36295700 L
N-N_3	0	11.56232400	5.37386600	2.45809900 L
N-N_3	0	12.58949400	3.10338700	3.36598700 L
B-	0	-12.77990500	1.53094000	-4.82470700 L
N-N_3	0	-12.86866300	0.29456700	-5.72066600 L
N-N_3	0	-11.61926000	2.45570400	-5.26106800 L
B-B_2	0	-10.29402800	1.67542700	-5.24594100 L
B-B_2	0	-9.01565900	3.57564100	-4.22026400 L
N-N_3	0	-9.01600500	2.51742100	-5.33198200 L
N-N_3	0	-7.72830500	4.36247800	-3.96649100 L
B-B_2	0	-6.44503200	3.56349700	-4.19497000 L
B-B_2	0	-5.16241600	4.91025200	-2.52944900 L
N-N_3	0	-5.16044100	4.35891200	-3.95713800 L
N-N_3	0	-3.87766200	5.55530300	-2.00680600 L
B-B_2	0	-2.59143300	4.91237200	-2.52792300 L
B-B_2	0	-1.30738300	5.51731600	-0.47685900 L
N-N_3	0	-1.30724500	5.55942400	-2.00644600 L
N-N_3	0	-0.02270700	5.91303400	0.25308900 L
B-B_2	0	1.26318600	5.52068200	-0.47656300 L
B-B_2	0	2.54865600	5.28575100	1.64770100 L
N-N_3	0	2.54806000	5.91572400	0.25331400 L
N-N_3	0	3.83387800	5.36827600	2.47304000 L
B-B_2	0	5.11979600	5.29029900	1.64870000 L
B-B_2	0	6.40838100	4.26184000	3.52704700 L
N-N_3	0	6.40249200	5.37852700	2.47668300 L
N-N_3	0	7.69108300	4.02978500	4.33121200 L
B-B_2	0	8.97670600	4.29411200	3.54121100 L
B-B_2	0	10.25786200	2.62931300	4.91901300 L
N-N_3	0	10.27950700	4.03383500	4.31036100 L
N-N_3	0	11.56691400	2.06029300	5.46729400 L
B-	0	12.83477300	2.68016100	4.82306100 L
N-N_3	0	-12.87341600	4.27470900	-3.86509700 L
B-B_2	0	-11.57139500	3.58460900	-4.23371600 L
B-B_2	0	-10.29924600	4.91690600	-2.55283600 L
N-N_3	0	-10.29005900	4.38558000	-3.99802900 L
N-N_3	0	-9.02167800	5.57445700	-2.01889500 L
B-B_2	0	-7.73549000	4.92148700	-2.53772100 L

B-B_2	0	-6.44886100	5.51068500	-0.47842000 L
N-N_3	0	-6.44761900	5.55623700	-2.00863900 L
N-N_3	0	-5.16408300	5.90361500	0.25254500 L
B-B_2	0	-3.87795700	5.51240600	-0.47719600 L
B-B_2	0	-2.59258700	5.27868100	1.64732100 L
N-N_3	0	-2.59355300	5.90864800	0.25286200 L
N-N_3	0	-1.30753100	5.36231100	2.47269400 L
B-B_2	0	-0.02196300	5.28305600	1.64755700 L
B-B_2	0	1.26456200	4.24646400	3.51594300 L
N-N_3	0	1.26325400	5.36590300	2.47286800 L
N-N_3	0	2.54999200	4.00523700	4.30903100 L
B-B_2	0	3.83545400	4.24971200	3.51718000 L
B-B_2	0	5.12260400	2.57532200	4.84628600 L
N-N_3	0	5.12006700	4.00975200	4.31248000 L
N-N_3	0	6.40551800	2.05184500	5.49350000 L
B-B_2	0	7.69536400	2.59340700	4.87376100 L
B-B_2	0	8.97975500	0.53297500	5.48060100 L
N-N_3	0	8.97005600	2.07528100	5.54027000 L
N-N_3	0	10.28287500	-0.19328800	5.84170300 L
B-B_2	0	11.48041900	0.55759800	5.24727400 L
B-	0	12.83754600	-1.51597500	5.25764700 L
N-N_3	0	12.59191900	-0.19288900	4.51482900 L
B-	0	-12.78605400	4.51633400	-2.35732700 L
B-B_2	0	-11.57570800	5.54569700	-0.48557400 L
N-N_3	0	-11.62474200	5.47775200	-2.01054400 L
N-N_3	0	-10.29397800	5.94325900	0.24800900 L
B-B_2	0	-9.01970200	5.53257500	-0.48472800 L
B-B_2	0	-7.73703800	5.28559100	1.65341300 L
N-N_3	0	-7.73215700	5.90839200	0.25129400 L
N-N_3	0	-6.44826500	5.35694900	2.47518500 L
B-B_2	0	-5.16379600	5.27519300	1.64802300 L
B-B_2	0	-3.87643000	4.23855100	3.51634200 L
N-N_3	0	-3.87811800	5.35752400	2.47255100 L
N-N_3	0	-2.59076800	3.99856300	4.30923000 L
B-B_2	0	-1.30592600	4.24300600	3.51603200 L
B-B_2	0	-0.01847500	2.56802900	4.84201400 L
N-N_3	0	-0.02034400	4.00218700	4.30885400 L
N-N_3	0	1.26720900	2.04242400	5.48197800 L
B-B_2	0	2.55171800	2.57111800	4.84217700 L
B-B_2	0	3.83928400	0.51637600	5.43145900 L
N-N_3	0	3.83706700	2.04556700	5.48319600 L
N-N_3	0	5.12377500	-0.21338300	5.82776100 L
B-B_2	0	6.41191500	0.51936900	5.44820800 L
B-B_2	0	7.69897900	-1.61475300	5.23290900 L

N-N_3	0	7.69456500	-0.21138600	5.85614400 L
N-N_3	0	8.97361200	-2.45160200	5.34425100 L
B-B_2	0	10.26106800	-1.62082000	5.28962400 L
B-B_2	0	11.48477000	-3.32766600	4.07114100 L
N-N_3	0	11.57026000	-2.41067400	5.28187400 L
N-N_3	0	12.60215700	-3.35542000	3.02900300 L
B-	0	-12.78774500	4.86678500	1.49771500 L
N-N_3	0	-12.87716100	5.76840500	0.26539000 L
N-N_3	0	-11.62566100	5.29737800	2.42376100 L
B-B_2	0	-10.30095600	5.28992200	1.64231000 L
B-B_2	0	-9.01825400	4.25486000	3.53386000 L
N-N_3	0	-9.02250200	5.37433400	2.48390400 L
N-N_3	0	-7.72928100	3.99809900	4.31717300 L
B-B_2	0	-6.44734600	4.23676000	3.51872300 L
B-B_2	0	-5.15952700	2.56183900	4.84802900 L
N-N_3	0	-5.16112700	3.99467000	4.31004700 L
N-N_3	0	-3.87238100	2.03651800	5.48572200 L
B-B_2	0	-2.58864900	2.56481100	4.84366600 L
B-B_2	0	-1.30060500	0.51028500	5.43097400 L
N-N_3	0	-1.30249200	2.03945400	5.48296200 L
N-N_3	0	-0.01471700	-0.21827800	5.82370300 L
B-B_2	0	1.26882900	0.51341400	5.42911300 L
B-B_2	0	2.55594700	-1.61061900	5.19430100 L
N-N_3	0	2.55441300	-0.21547400	5.82181500 L
N-N_3	0	3.84141300	-2.43389300	5.28243400 L
B-B_2	0	5.12656100	-1.60899800	5.19967400 L
B-B_2	0	6.41558600	-3.49655000	4.18766100 L
N-N_3	0	6.40930400	-2.43578400	5.29441000 L
N-N_3	0	7.69838500	-4.30274400	3.96493300 L
B-B_2	0	8.98340700	-3.50867800	4.21973100 L
N-N_3	0	10.28665400	-4.27918200	3.96659000 L
N-N_3	0	-12.87483800	3.88317000	4.23230300 L
B-B_2	0	-11.57412800	4.26116400	3.54456900 L
B-B_2	0	-10.29625200	2.57501900	4.86574600 L
N-N_3	0	-10.29144000	4.02353900	4.34325500 L
N-N_3	0	-9.01641900	2.04052000	5.51862300 L
B-B_2	0	-7.73260300	2.56505900	4.86541000 L
B-B_2	0	-6.44128000	0.50431400	5.44289000 L
N-N_3	0	-6.44227500	2.03449200	5.49386600 L
N-N_3	0	-5.15394200	-0.22481000	5.83076500 L
B-B_2	0	-3.87066100	0.50716000	5.43489600 L
B-B_2	0	-2.58286700	-1.61736600	5.19924900 L
N-N_3	0	-2.58405700	-0.22153600	5.82569400 L
N-N_3	0	-1.29703000	-2.44076200	5.28560000 L

B-B_2	0	-0.01344000	-1.61457400	5.19840600 L
B-B_2	0	1.27308600	-3.49186000	4.17486000 L
N-N_3	0	1.27263100	-2.43738700	5.28336300 L
N-N_3	0	2.55872400	-4.28604500	3.94196800 L
B-B_2	0	3.84303100	-3.48878400	4.17446000 L
N-N_3	0	5.12774200	-4.28582500	3.94461800 L
B-	0	-12.78176000	2.37437300	4.46532800 L
B-B_2	0	-11.56752100	0.50239600	5.48991700 L
N-N_3	0	-11.61978900	2.02731200	5.42564700 L
N-N_3	0	-10.28402500	-0.22826500	5.88785200 L
B-B_2	0	-9.01193400	0.50627100	5.47316800 L
B-B_2	0	-7.72643300	-1.63199800	5.22748500 L
N-N_3	0	-7.72193800	-0.22754300	5.84536200 L
N-N_3	0	-6.43587500	-2.45113400	5.29897600 L
B-B_2	0	-5.15357600	-1.62211100	5.20639800 L
B-B_2	0	-3.86621200	-3.49809800	4.17989100 L
N-N_3	0	-3.86622900	-2.44401000	5.28891800 L
N-N_3	0	-2.58018400	-4.29227800	3.94529800 L
B-B_2	0	-1.29615500	-3.49471600	4.17649000 L
N-N_3	0	-0.01065500	-4.28989500	3.94393300 L
B-	0	-12.77607600	-1.48668300	4.81926000 L
N-N_3	0	-12.86772000	-0.25030100	5.71492200 L
N-N_3	0	-11.61334900	-2.40869600	5.25591000 L
B-B_2	0	-10.28993200	-1.62538400	5.24035600 L
B-B_2	0	-9.00738500	-3.52277300	4.21451900 L
N-N_3	0	-9.00989300	-2.46439400	5.32608800 L
N-N_3	0	-7.71819600	-4.30657400	3.96041800 L
B-B_2	0	-6.43680600	-3.50424300	4.18777400 L
N-N_3	0	-5.15018600	-4.29634800	3.94936600 L
N-N_3	0	-12.86361500	-4.23116600	3.86101400 L
B-B_2	0	-11.56312800	-3.53787800	4.22899700 L
N-N_3	0	-10.27995600	-4.33577000	3.99290500 L
H-H_	0	12.26855600	-3.56078000	-0.46062300 L
H-H_	0	12.25198900	-2.17785200	-2.83917600 L
H-H_	0	12.24773200	0.50531400	-3.55802700 L
H-H_	0	12.26318600	2.92557700	-2.19616300 L
H-H_	0	-12.88460700	-6.71778300	-0.58952900 L
H-H_	0	-12.88824000	-4.31628500	-5.16747600 L
H-H_	0	12.26288000	3.65700800	0.45381600 L
H-H_	0	12.24630500	2.27357700	2.83115600 L
H-H_	0	-12.89048300	0.60929300	-6.71721800 L
H-H_	0	-12.89410300	5.20165000	-4.34779000 L
H-H_	0	12.25012000	-0.41019800	3.55131800 L
H-H_	0	12.26896800	-2.82981500	2.18933200 L

H-H_	0	-12.89811500	6.76351500	0.58469600 L
H-H_	0	-12.89766500	4.36048700	5.16197400 L
H-H_	0	-12.88898000	-0.56484600	6.71154200 L
H-H_	0	-12.88172000	-5.15823600	4.34356500 L
C-C_3	0	0.29262800	-1.69409200	0.24484500 H
H-H_	0	-0.09372600	-0.03712400	-1.11000400 H
H-H_	0	-1.46893300	-1.12641900	-0.86714200 H
C-C_3	0	-0.38202700	-1.08530700	-0.99135500 H
H-H_	0	-0.11820500	-1.63598300	-1.89668000 H
N-N_3	0	-0.08630700	-0.98009600	1.46191200 H
H-H_	0	0.58511100	-1.15873000	2.20356200 H
H-H_	0	-1.00910400	-1.25848500	1.77931700 H
C-C_R	0	1.81404300	-1.72312800	0.16373400 H
O-O_R	0	2.55742800	-1.59641800	1.11526900 H
O-O_R	0	2.27222000	-1.96954900	-1.08516300 H
H-H_	0	3.24067600	-2.03436100	-1.02660300 H
H-H_	0	0.01832700	-2.76361700	0.27551300 H

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B-B_2	0	-10.27032000	-5.26628600	-1.74697600 L
N-N_3	0	-11.57788300	-5.72675300	-1.10280800 L
B-	0	-12.84624200	-5.19233400	-1.81835800 L
B-B_2	0	-5.13491000	-5.19239900	-1.70551000 L
N-N_3	0	-6.41881300	-5.75144700	-1.09160100 L
B-B_2	0	-7.70772600	-5.21686600	-1.71895700 L
B-B_2	0	-8.99206600	-5.49781900	0.40829000 L
N-N_3	0	-8.98268800	-5.79585600	-1.10579000 L
N-N_3	0	-10.29517400	-5.73702100	1.18391700 L
B-B_2	0	-11.49560600	-5.27569800	0.34784400 L
B-	0	-12.84746300	-4.94638600	2.39941100 L
N-N_3	0	-12.60811200	-4.43319600	0.97049600 L
B-B_2	0	0.00560600	-5.20456100	-1.70494300 L
N-N_3	0	-1.28039400	-5.76015400	-1.09060600 L
B-B_2	0	-2.56385500	-5.19729400	-1.70374600 L
B-B_2	0	-3.85036700	-5.46752400	0.41424000 L
N-N_3	0	-3.85070400	-5.74947300	-1.08919400 L
N-N_3	0	-5.13631800	-5.73473300	1.19818800 L
B-B_2	0	-6.42356800	-5.47123300	0.41516900 L
B-B_2	0	-7.70818700	-4.90597000	2.48271900 L
N-N_3	0	-7.70697400	-5.75242000	1.20204700 L
N-N_3	0	-8.98202400	-4.87137500	3.32712800 L
B-B_2	0	-10.27096500	-4.95717100	2.50118000 L
B-B_2	0	-11.49078200	-3.46552600	3.97695600 L
N-N_3	0	-11.57804900	-4.81568500	3.28135800 L
N-N_3	0	-12.59824800	-2.42565000	3.81216900 L
B-B_2	0	5.14680300	-5.20041800	-1.70785100 L
N-N_3	0	3.86154400	-5.75484000	-1.09075900 L
B-B_2	0	2.57538900	-5.19994000	-1.70458100 L
B-B_2	0	1.29147100	-5.48268400	0.41375500 L
N-N_3	0	1.29136900	-5.76106000	-1.09088600 L
N-N_3	0	0.00603300	-5.75162700	1.19859500 L
B-B_2	0	-1.27954500	-5.48233300	0.41420500 L
B-B_2	0	-2.56396300	-4.88845400	2.46702300 L
N-N_3	0	-2.56654800	-5.74350800	1.19819200 L
N-N_3	0	-3.84913900	-4.82718300	3.29452300 L
B-B_2	0	-5.13530300	-4.88307800	2.46935200 L
B-B_2	0	-6.42056100	-3.55716900	4.15393200 L
N-N_3	0	-6.41767500	-4.83091200	3.30101200 L
N-N_3	0	-7.70174900	-3.19609600	4.91169600 L

B-B_2	0	-8.98876200	-3.58227000	4.17580100 L
B-B_2	0	-10.26561900	-1.71518400	5.27002400 L
N-N_3	0	-10.29038300	-3.19875100	4.89344900 L
N-N_3	0	-11.57343600	-1.06425000	5.72174500 L
B-	0	-12.84275900	-1.77542100	5.18324000 L
B-B_2	0	10.28379400	-5.21713000	-1.73112400 L
N-N_3	0	9.00557000	-5.78013700	-1.09979200 L
B-B_2	0	7.71993800	-5.21598000	-1.71519000 L
B-B_2	0	6.43328100	-5.46967300	0.41058300 L
N-N_3	0	6.43156900	-5.75809100	-1.09264300 L
N-N_3	0	5.14858100	-5.73909000	1.19518400 L
B-B_2	0	3.86213800	-5.47109000	0.41241900 L
B-B_2	0	2.57746200	-4.89080000	2.46590300 L
N-N_3	0	2.57848800	-5.74579400	1.19713200 L
N-N_3	0	1.29238900	-4.83325100	3.29292200 L
B-B_2	0	0.00654600	-4.89470700	2.46688200 L
B-B_2	0	-1.27713200	-3.55352800	4.13374700 L
N-N_3	0	-1.27869800	-4.83240900	3.29373000 L
N-N_3	0	-2.56106000	-3.18282600	4.87760500 L
B-B_2	0	-3.84764500	-3.55073100	4.13788100 L
B-B_2	0	-5.13065000	-1.68137900	5.18273400 L
N-N_3	0	-5.13058000	-3.18274700	4.88581500 L
N-N_3	0	-6.41166000	-1.06036700	5.74151600 L
B-B_2	0	-7.70328400	-1.69130500	5.21727700 L
B-B_2	0	-8.98372200	0.44170300	5.49344200 L
N-N_3	0	-8.97628800	-1.07206000	5.79493800 L
N-N_3	0	-10.28546200	1.21764800	5.73696100 L
B-B_2	0	-11.48432300	0.38478700	5.26776000 L
B-	0	-12.83857900	2.43691700	4.95641300 L
N-N_3	0	-12.59636300	1.01351800	4.42918200 L
B-	0	12.77196300	-4.79569300	-1.60238300 L
B-B_2	0	11.56004200	-5.51113600	0.40942000 L
N-N_3	0	11.60867400	-5.68713600	-1.10695600 L
N-N_3	0	10.27783500	-5.78351400	1.19720400 L
B-B_2	0	9.00400300	-5.49428300	0.40799200 L
B-B_2	0	7.72204900	-4.90372200	2.47714500 L
N-N_3	0	7.71632500	-5.74574700	1.19472200 L
N-N_3	0	6.43296000	-4.83769200	3.29878200 L
B-B_2	0	5.14895200	-4.89043800	2.46846200 L
B-B_2	0	3.86315900	-3.55650400	4.13722100 L
N-N_3	0	3.86265500	-4.83296300	3.29374900 L
N-N_3	0	2.57735300	-3.18680200	4.87757000 L
B-B_2	0	1.29277400	-3.55448600	4.13303400 L
B-B_2	0	0.00940000	-1.68402100	5.17221700 L

N-N_3	0	0.00823200	-3.18489400	4.87548800 L
N-N_3	0	-1.27456700	-1.06188100	5.72204500 L
B-B_2	0	-2.56005400	-1.68186400	5.17357600 L
B-B_2	0	-3.84357300	0.44272200	5.43815000 L
N-N_3	0	-3.84346300	-1.05996600	5.72619500 L
N-N_3	0	-5.12654900	1.22714200	5.71782500 L
B-B_2	0	-6.41600300	0.44626200	5.45724900 L
B-B_2	0	-7.70000600	2.52279600	4.91285100 L
N-N_3	0	-7.69719600	1.23367600	5.74718000 L
N-N_3	0	-8.97357500	3.36831500	4.89156900 L
B-B_2	0	-10.26208500	2.54117900	4.96841200 L
B-B_2	0	-11.48474600	4.03666300	3.49753300 L
N-N_3	0	-11.57001300	3.32221800	4.83784900 L
N-N_3	0	-12.60388400	3.90186000	2.46564000 L
B-	0	12.77374200	-4.52405500	2.25759500 L
N-N_3	0	12.86119700	-5.61263600	1.18658000 L
N-N_3	0	11.61060200	-4.79701500	3.24057200 L
B-B_2	0	10.28595100	-4.91370400	2.46777700 L
B-B_2	0	9.00492400	-3.58295900	4.16538500 L
N-N_3	0	9.00725600	-4.85831800	3.31148500 L
N-N_3	0	7.71593000	-3.19930100	4.89514500 L
B-B_2	0	6.43405400	-3.56150000	4.14434600 L
B-B_2	0	5.14953800	-1.68936800	5.18294500 L
N-N_3	0	5.14750300	-3.19017200	4.88324700 L
N-N_3	0	3.86325400	-1.06623800	5.72713700 L
B-B_2	0	2.57885600	-1.68603400	5.17448200 L
B-B_2	0	1.29574600	0.43833700	5.43341700 L
N-N_3	0	1.29420200	-1.06391600	5.72256100 L
N-N_3	0	0.01164500	1.22152700	5.70886100 L
B-B_2	0	-1.27360400	0.44034600	5.43302800 L
B-B_2	0	-2.55704700	2.50615500	4.87637800 L
N-N_3	0	-2.55727900	1.22370800	5.71055000 L
N-N_3	0	-3.84131000	3.33548800	4.83582600 L
B-B_2	0	-5.12756900	2.50920200	4.88181200 L
B-B_2	0	-6.41443600	4.21585400	3.58605200 L
N-N_3	0	-6.40946500	3.34199900	4.84571900 L
N-N_3	0	-7.69662900	4.97716500	3.23720300 L
B-B_2	0	-8.98248100	4.23494300	3.61454200 L
B-B_2	0	-10.26222500	5.35347900	1.76392500 L
N-N_3	0	-10.28489200	4.95717900	3.24235300 L
N-N_3	0	-11.56896200	5.81645600	1.11996500 L
B-	0	-12.83811800	5.28436300	1.83587100 L
N-N_3	0	12.86214300	-3.11133100	4.79722800 L
B-B_2	0	11.56082100	-3.59295000	4.17892400 L

B-B_2	0	10.28613300	-1.71247600	5.20932500 L
N-N_3	0	10.27826300	-3.22638200	4.92769400 L
N-N_3	0	9.00725500	-1.07706000	5.76680600 L
B-B_2	0	7.72253400	-1.69648100	5.20468000 L
B-B_2	0	6.43588600	0.43387100	5.44631100 L
N-N_3	0	6.43302100	-1.06905100	5.73852000 L
N-N_3	0	5.15043700	1.21794100	5.71495800 L
B-B_2	0	3.86541700	0.43625300	5.43770000 L
B-B_2	0	2.58236100	2.50209000	4.87642200 L
N-N_3	0	2.58073500	1.21971600	5.71083300 L
N-N_3	0	1.29812900	3.33161100	4.83414600 L
B-B_2	0	0.01264700	2.50419900	4.87513400 L
B-B_2	0	-1.27118200	4.20187000	3.57461800 L
N-N_3	0	-1.27154300	3.33364900	4.83430500 L
N-N_3	0	-2.55589900	4.95172400	3.21918400 L
B-B_2	0	-3.84175000	4.20411300	3.57617900 L
B-B_2	0	-5.12706600	5.27133800	1.72393300 L
N-N_3	0	-5.12583500	4.95567600	3.22151000 L
N-N_3	0	-6.40980300	5.83111700	1.10794800 L
B-B_2	0	-7.69972500	5.29983400	1.73620400 L
B-B_2	0	-8.98371100	5.58203200	-0.39164500 L
N-N_3	0	-8.97362900	5.88046500	1.12243300 L
N-N_3	0	-10.28651300	5.82412400	-1.16695300 L
B-B_2	0	-11.48778200	5.36521900	-0.33068400 L
B-	0	-12.84090900	5.03935900	-2.38200100 L
N-N_3	0	-12.60237100	4.52540800	-0.95324300 L
B-	0	12.77203900	-1.58455500	4.78323700 L
B-B_2	0	11.56198700	0.43070600	5.49269500 L
N-N_3	0	11.61078500	-1.08473800	5.67454300 L
N-N_3	0	10.28055800	1.21843500	5.77030600 L
B-B_2	0	9.00650800	0.43040500	5.47745700 L
B-B_2	0	7.72582100	2.50685500	4.89792500 L
N-N_3	0	7.71835800	1.21693000	5.72881400 L
N-N_3	0	6.43752200	3.33062900	4.84101100 L
B-B_2	0	5.15294700	2.50097900	4.88059600 L
B-B_2	0	3.86913000	4.19678700	3.57467400 L
N-N_3	0	3.86788700	3.32941000	4.83525000 L
N-N_3	0	2.58486100	4.94743700	3.21841400 L
B-B_2	0	1.29893700	4.19979900	3.57434000 L
B-B_2	0	0.01444400	5.26702800	1.72176400 L
N-N_3	0	0.01444000	4.95017800	3.21866300 L
N-N_3	0	-1.27063700	5.82144400	1.10454200 L
B-B_2	0	-2.55605600	5.26829000	1.72226300 L
B-B_2	0	-3.84215400	5.53598000	-0.39802900 L

N-N_3	0	-3.84128200	5.82215500	1.10512500 L
N-N_3	0	-5.12696700	5.80905400	-1.18219400 L
B-B_2	0	-6.41517900	5.54933800	-0.39891500 L
B-B_2	0	-7.70152300	4.98871200	-2.46740500 L
N-N_3	0	-7.69806100	5.83377800	-1.18568100 L
N-N_3	0	-8.97601200	4.95704300	-3.31102600 L
B-B_2	0	-10.26433900	5.04462900	-2.48440400 L
B-B_2	0	-11.48761000	3.55572200	-3.95984500 L
N-N_3	0	-11.57196000	4.90598100	-3.26416000 L
N-N_3	0	-12.59502800	2.51638500	-3.79159900 L
B-	0	12.77403100	2.28563600	4.51389400 L
N-N_3	0	12.86422100	1.20647900	5.59389500 L
N-N_3	0	11.61452100	3.26821400	4.80106000 L
B-B_2	0	10.28920000	2.49568100	4.91017900 L
B-B_2	0	9.01034400	4.21122000	3.59921100 L
N-N_3	0	9.01140800	3.34104400	4.86354800 L
N-N_3	0	7.72292900	4.94857100	3.22555800 L
B-B_2	0	6.43976200	4.19594400	3.57805600 L
B-B_2	0	5.15604000	5.26234100	1.72166500 L
N-N_3	0	5.15507900	4.94425000	3.21866500 L
N-N_3	0	3.87082000	5.81576000	1.10368200 L
B-B_2	0	2.58495100	5.26412300	1.72145700 L
B-B_2	0	1.29963100	5.53240900	-0.39896700 L
N-N_3	0	1.30021400	5.81928900	1.10407200 L
N-N_3	0	0.01432800	5.80476100	-1.18239600 L
B-B_2	0	-1.27108100	5.53449200	-0.39840900 L
B-B_2	0	-2.55736800	4.95869600	-2.45590900 L
N-N_3	0	-2.55659400	5.80588300	-1.18177100 L
N-N_3	0	-3.84307800	4.90545000	-3.28299500 L
B-B_2	0	-5.12859300	4.96107700	-2.45628500 L
B-B_2	0	-6.41720900	3.64097100	-4.14270900 L
N-N_3	0	-6.41176700	4.91296300	-3.28693300 L
N-N_3	0	-7.69994700	3.28147600	-4.89851600 L
B-B_2	0	-8.98547300	3.66863400	-4.16073700 L
B-B_2	0	-10.26580200	1.80302700	-5.25311700 L
N-N_3	0	-10.28833700	3.28683100	-4.87712100 L
N-N_3	0	-11.57502900	1.15311800	-5.70247300 L
B-	0	-12.84276500	1.86546700	-5.16174300 L
N-N_3	0	12.86777800	4.84573500	3.13641800 L
B-B_2	0	11.56604900	4.22196800	3.60939500 L
B-B_2	0	10.29298100	5.27247500	1.74041600 L
N-N_3	0	10.28458700	4.97586400	3.25132800 L
N-N_3	0	9.01498500	5.83690000	1.10972800 L
B-B_2	0	7.72915700	5.27461300	1.72639900 L

B-B_2	0	6.44130600	5.52759400	-0.39930000 L
N-N_3	0	6.44088700	5.81717700	1.10392300 L
N-N_3	0	5.15600400	5.79765100	-1.18314900 L
B-B_2	0	3.87033100	5.52848900	-0.39931200 L
B-B_2	0	2.58406400	4.95491900	-2.45736100 L
N-N_3	0	2.58534100	5.80166700	-1.18284900 L
N-N_3	0	1.29850900	4.90324100	-3.28458900 L
B-B_2	0	0.01334400	4.95780400	-2.45678200 L
B-B_2	0	-1.27337100	3.63139200	-4.13163200 L
N-N_3	0	-1.27238300	4.90508400	-3.28383800 L
N-N_3	0	-2.55896500	3.26410800	-4.87452900 L
B-B_2	0	-3.84426600	3.63247700	-4.13205400 L
B-B_2	0	-5.13072200	1.76463400	-5.17369300 L
N-N_3	0	-5.12895600	3.26627700	-4.87760900 L
N-N_3	0	-6.41318800	1.14380500	-5.72918900 L
B-B_2	0	-7.70342300	1.77663300	-5.20386600 L
B-B_2	0	-8.98646600	-0.35526100	-5.47649500 L
N-N_3	0	-8.97782200	1.15823300	-5.77933500 L
N-N_3	0	-10.28906000	-1.12997300	-5.71903400 L
B-B_2	0	-11.48665800	-0.29602600	-5.24848000 L
B-	0	-12.84301000	-2.34795400	-4.94127400 L
N-N_3	0	-12.60070900	-0.92502400	-4.41268300 L
B-	0	12.78006900	4.84680600	1.60941800 L
B-B_2	0	11.56833800	5.56618000	-0.40094300 L
N-N_3	0	11.61807200	5.74079300	1.11553400 L
N-N_3	0	10.28580600	5.83942200	-1.18789700 L
B-B_2	0	9.01218600	5.55088400	-0.39806200 L
B-B_2	0	7.72864000	4.96261100	-2.46741900 L
N-N_3	0	7.72411500	5.80329700	-1.18407400 L
N-N_3	0	6.43945300	4.89971800	-3.28918500 L
B-B_2	0	5.15535300	4.95239600	-2.45899700 L
B-B_2	0	3.86765800	3.62649400	-4.13388700 L
N-N_3	0	3.86921400	4.89979200	-3.28520400 L
N-N_3	0	2.58173500	3.26070300	-4.87663300 L
B-B_2	0	1.29713100	3.62967200	-4.13272300 L
B-B_2	0	0.01010400	1.76142000	-5.16927900 L
N-N_3	0	0.01130700	3.26288400	-4.87526600 L
N-N_3	0	-1.27534200	1.13898500	-5.71597300 L
B-B_2	0	-2.55995000	1.76276400	-5.16911900 L
B-B_2	0	-3.84630200	-0.36101400	-5.42307000 L
N-N_3	0	-3.84490000	1.14047500	-5.71755200 L
N-N_3	0	-5.13006800	-1.14495900	-5.69983800 L
B-B_2	0	-6.41878600	-0.36213200	-5.44137200 L
B-B_2	0	-7.70475100	-2.43692700	-4.89392400 L

N-N_3	0	-7.70075300	-1.14879100	-5.72975300 L
N-N_3	0	-8.97876300	-3.28172000	-4.87346800 L
B-B_2	0	-10.26670900	-2.45373600	-4.95088200 L
B-B_2	0	-11.49124300	-3.94870200	-3.48133500 L
N-N_3	0	-11.57510500	-3.23405200	-4.82159500 L
N-N_3	0	-12.60938400	-3.81064600	-2.44884800 L
B-	0	12.78062100	4.57851200	-2.24941200 L
N-N_3	0	12.86906400	5.66734500	-1.17877700 L
N-N_3	0	11.61700000	4.85154500	-3.23182300 L
B-B_2	0	10.29268900	4.96980600	-2.45857000 L
B-B_2	0	9.00956500	3.64150900	-4.15666600 L
N-N_3	0	9.01373800	4.91630000	-3.30196500 L
N-N_3	0	7.72032900	3.26083500	-4.88736500 L
B-B_2	0	6.43861300	3.62526000	-4.13743500 L
B-B_2	0	5.15101600	1.75675200	-5.17733800 L
N-N_3	0	5.15213100	3.25775000	-4.87833200 L
N-N_3	0	3.86382200	1.13504100	-5.72112900 L
B-B_2	0	2.58020000	1.75939000	-5.17182600 L
B-B_2	0	1.29310600	-0.36344700	-5.41982800 L
N-N_3	0	1.29410300	1.13724800	-5.71728200 L
N-N_3	0	0.00769100	-1.14600600	-5.69067900 L
B-B_2	0	-1.27636400	-0.36171900	-5.41886700 L
B-B_2	0	-2.56215300	-2.42405000	-4.85379600 L
N-N_3	0	-2.56098000	-1.14461500	-5.69250900 L
N-N_3	0	-3.84686100	-3.25185900	-4.81232200 L
B-B_2	0	-5.13242100	-2.42469500	-4.86041400 L
B-B_2	0	-6.42098500	-4.13097700	-3.56592600 L
N-N_3	0	-6.41465400	-3.25676600	-4.82520200 L
N-N_3	0	-7.70379000	-4.89223200	-3.21937100 L
B-B_2	0	-8.98894700	-4.14874400	-3.59673700 L
N-N_3	0	-10.29216700	-4.87004800	-3.22539600 L
N-N_3	0	12.86615600	3.16213800	-4.78651300 L
B-B_2	0	11.56545400	3.64673500	-4.16911300 L
B-B_2	0	10.28760300	1.76863000	-5.20001400 L
N-N_3	0	10.28258100	3.28257300	-4.91845300 L
N-N_3	0	9.00772300	1.13557700	-5.75777700 L
B-B_2	0	7.72404300	1.75798600	-5.19669900 L
B-B_2	0	6.43338800	-0.36958600	-5.43509000 L
N-N_3	0	6.43362000	1.13267900	-5.73065700 L
N-N_3	0	5.14607100	-1.15156000	-5.70073500 L
B-B_2	0	3.86294100	-0.36622200	-5.42520300 L
B-B_2	0	2.57625400	-2.42700500	-4.85384100 L
N-N_3	0	2.57650000	-1.14830900	-5.69367300 L
N-N_3	0	1.29074500	-3.25402800	-4.80931200 L

B-B_2	0	0.00690000	-2.42496500	-4.85141800 L
B-B_2	0	-1.27830400	-4.12241500	-3.55086300 L
N-N_3	0	-1.27777100	-3.25282500	-4.80958300 L
N-N_3	0	-2.56379100	-4.87139200	-3.19841900 L
B-B_2	0	-3.84833000	-4.12030500	-3.55277200 L
N-N_3	0	-5.13294900	-4.87204900	-3.20167300 L
B-	0	12.77281400	1.63553400	-4.77257100 L
B-B_2	0	11.55935600	-0.37719400	-5.48343600 L
N-N_3	0	11.61114700	1.13825500	-5.66471300 L
N-N_3	0	10.27619200	-1.16239700	-5.76041000 L
B-B_2	0	9.00393000	-0.37167500	-5.46726200 L
B-B_2	0	7.71939800	-2.44498400	-4.88492500 L
N-N_3	0	7.71400600	-1.15583300	-5.71709400 L
N-N_3	0	6.42906500	-3.26556300	-4.82572500 L
B-B_2	0	5.14668400	-2.43248800	-4.86317500 L
B-B_2	0	3.86044500	-4.12577000	-3.55475900 L
N-N_3	0	3.85951500	-3.25740800	-4.81441300 L
N-N_3	0	2.57505600	-4.87498800	-3.19941900 L
B-B_2	0	1.29052700	-4.12370800	-3.55075300 L
N-N_3	0	0.00568300	-4.87491100	-3.19906600 L
B-	0	12.76831400	-2.23481500	-4.50591100 L
N-N_3	0	12.85998100	-1.15548900	-5.58562900 L
N-N_3	0	11.60654900	-3.21493900	-4.79249000 L
B-B_2	0	10.28275900	-2.43960700	-4.90017500 L
B-B_2	0	9.00149600	-4.15289500	-3.58821200 L
N-N_3	0	9.00308700	-3.28218500	-4.85218500 L
N-N_3	0	7.71288800	-4.88790200	-3.21382600 L
B-B_2	0	6.43097400	-4.13179300	-3.56342600 L
N-N_3	0	5.14490000	-4.87771100	-3.20359400 L
N-N_3	0	12.85811700	-4.79543600	-3.12944900 L
B-B_2	0	11.55723200	-4.16898000	-3.60113100 L
N-N_3	0	10.27457800	-4.92026700	-3.24194600 L
H-H_	0	-12.26989100	-3.44568500	1.02317600 L
H-H_	0	-12.25308100	-1.69222100	3.15234900 L
H-H_	0	-12.25633700	1.07684200	3.44289300 L
H-H_	0	-12.27399100	3.24754900	1.72042200 L
H-H_	0	12.88015800	-6.54333000	1.66206500 L
H-H_	0	12.88378200	-3.43214500	5.79183900 L
H-H_	0	-12.26644200	3.53713100	-1.00613700 L
H-H_	0	-12.24857400	1.78323000	-3.13213900 L
H-H_	0	12.88789200	1.67477000	6.52812600 L
H-H_	0	12.88825100	5.83715500	3.46703400 L
H-H_	0	-12.26262300	-0.98927800	-3.42579500 L
H-H_	0	-12.27750400	-3.15673400	-1.70416100 L

H-H_	0	12.88789200	6.59791000	-1.65452200 L
H-H_	0	12.88922300	3.48289700	-5.78111000 L
H-H_	0	12.88216600	-1.62354900	-6.52001200 L
H-H_	0	12.87603600	-5.78702500	-3.45970900 L
C-C_3	0	-0.07379300	-1.78386000	-0.05570500 H
H-H_	0	-0.08010100	0.11099200	1.03999700 H
H-H_	0	1.09879700	-1.07633100	1.62590500 H
C-C_3	0	0.08112600	-0.95252200	1.24164300 H
H-H_	0	-0.61903400	-1.28790000	2.01268500 H
N-N_3	0	0.83963100	-1.42387200	-1.10156700 H
H-H_	0	0.48397900	-1.04493800	-1.96270400 H
H-H_	0	1.82978000	-1.52901600	-0.97818900 H
C-C_R	0	-1.49103100	-1.67107800	-0.59784700 H
O-O_R	0	-1.80246800	-1.19014500	-1.66735700 H
O-O_R	0	-2.40441700	-2.17919100	0.26443000 H
H-H_	0	-3.27815200	-2.07726700	-0.14927200 H
H-H_	0	0.04178000	-2.83847400	0.23048100 H

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B-B_2	0	-10.26991900	-5.39284100	-1.34307000 L
N-N_3	0	-11.57717400	-5.80405700	-0.66596700 L
B-	0	-12.84568900	-5.32696400	-1.42059000 L
B-B_2	0	-5.13419400	-5.31916900	-1.30824100 L
N-N_3	0	-6.41854000	-5.82865500	-0.65350000 L
B-B_2	0	-7.70717900	-5.34194000	-1.31910400 L
B-B_2	0	-8.99146700	-5.45923500	0.82298100 L
N-N_3	0	-8.98227300	-5.87228300	-0.66379800 L
N-N_3	0	-10.29446600	-5.63782000	1.61501700 L
B-B_2	0	-11.49548800	-5.24339600	0.74603700 L
B-	0	-12.84658100	-4.75488700	2.76617500 L
N-N_3	0	-12.60772200	-4.35480600	1.30149500 L
B-B_2	0	0.00645000	-5.33192200	-1.30875400 L
N-N_3	0	-1.27900800	-5.84028800	-0.65335500 L
B-B_2	0	-2.56316100	-5.32741700	-1.30766800 L
B-B_2	0	-3.84948200	-5.43183000	0.82497500 L
N-N_3	0	-3.85036100	-5.82989300	-0.65216100 L
N-N_3	0	-5.13542100	-5.63530800	1.62814200 L
B-B_2	0	-6.42277500	-5.43336100	0.82721900 L
B-B_2	0	-7.70709900	-4.70757800	2.84424500 L
N-N_3	0	-7.70622000	-5.65171800	1.63380700 L
N-N_3	0	-8.98067300	-4.60748000	3.68386500 L
B-B_2	0	-10.26995500	-4.75770500	2.86755100 L
B-B_2	0	-11.48926500	-3.15574000	4.22306900 L

N-N_3	0	-11.57682100	-4.55591100	3.63471200 L
N-N_3	0	-12.59464000	-2.13031500	3.97506400 L
B-B_2	0	5.14819400	-5.32188600	-1.31170100 L
N-N_3	0	3.86339000	-5.82828600	-0.65399400 L
B-B_2	0	2.57669500	-5.32382200	-1.30895300 L
B-B_2	0	1.29292400	-5.43975000	0.82397700 L
N-N_3	0	1.29315800	-5.83689800	-0.65365000 L
N-N_3	0	0.00796100	-5.64739300	1.62765000 L
B-B_2	0	-1.27828800	-5.44418800	0.82483800 L
B-B_2	0	-2.56276100	-4.68896300	2.82401300 L
N-N_3	0	-2.56496200	-5.64317300	1.62777400 L
N-N_3	0	-3.84752200	-4.56368000	3.64504300 L
B-B_2	0	-5.13412000	-4.68528000	2.82771800 L
B-B_2	0	-6.41927700	-3.23202300	4.40490900 L
N-N_3	0	-6.41618400	-4.56824000	3.65346700 L
N-N_3	0	-7.70028400	-2.81431200	5.13340900 L
B-B_2	0	-8.98743300	-3.25633100	4.42988600 L
B-B_2	0	-10.26446500	-1.31079600	5.37768800 L
N-N_3	0	-10.28894700	-2.81888300	5.11617400 L
N-N_3	0	-11.57285300	-0.62752100	5.77738600 L
B-	0	-12.84179100	-1.37632200	5.29140800 L
B-B_2	0	10.28518600	-5.33678200	-1.33318000 L
N-N_3	0	9.00724600	-5.85038400	-0.66055900 L
B-B_2	0	7.72131400	-5.33588300	-1.31744100 L
B-B_2	0	6.43473900	-5.42582800	0.82116300 L
N-N_3	0	6.43332200	-5.82956700	-0.65529300 L
N-N_3	0	5.15000800	-5.63401400	1.62405600 L
B-B_2	0	3.86370200	-5.42804400	0.82243200 L
B-B_2	0	2.57872800	-4.68918000	2.82392500 L
N-N_3	0	2.57991400	-5.64050400	1.62579300 L
N-N_3	0	1.29323400	-4.56732100	3.64302900 L
B-B_2	0	0.00787800	-4.69210300	2.82334500 L
B-B_2	0	-1.27612600	-3.22680800	4.38183600 L
N-N_3	0	-1.27720600	-4.56659200	3.64299500 L
N-N_3	0	-2.55989100	-2.80184500	5.09610300 L
B-B_2	0	-3.84647100	-3.22559000	4.38698100 L
B-B_2	0	-5.12963600	-1.28266100	5.28866100 L
N-N_3	0	-5.12917900	-2.80217600	5.10538300 L
N-N_3	0	-6.41072500	-0.62195700	5.79965800 L
B-B_2	0	-7.70221500	-1.29061400	5.32408800 L
B-B_2	0	-8.98276800	0.85729200	5.44026100 L
N-N_3	0	-8.97542300	-0.62988500	5.85351700 L
N-N_3	0	-10.28466700	1.64890800	5.62510100 L
B-B_2	0	-11.48273600	0.78361100	5.21684500 L

B-	0	-12.83741800	2.80779600	4.75802200 L
N-N_3	0	-12.59540600	1.34979300	4.33558000 L
B-	0	12.77348600	-4.90624700	-1.23746100 L
B-B_2	0	11.56148000	-5.46478700	0.82350900 L
N-N_3	0	11.61026300	-5.75703100	-0.67484600 L
N-N_3	0	10.27935600	-5.67660900	1.62991900 L
B-B_2	0	9.00544700	-5.44941700	0.82078400 L
B-B_2	0	7.72311200	-4.70174700	2.83827900 L
N-N_3	0	7.71777600	-5.64001800	1.62445600 L
N-N_3	0	6.43376900	-4.57290900	3.65207300 L
B-B_2	0	5.15004000	-4.68921500	2.82777900 L
B-B_2	0	3.86388200	-3.23105200	4.38929000 L
N-N_3	0	3.86344600	-4.56818600	3.64566500 L
N-N_3	0	2.57773500	-2.80611900	5.09877500 L
B-B_2	0	1.29366400	-3.22816500	4.38280900 L
B-B_2	0	0.01006800	-1.28479700	5.27832100 L
N-N_3	0	0.00883000	-2.80344900	5.09435400 L
N-N_3	0	-1.27391000	-0.62411200	5.78093700 L
B-B_2	0	-2.55923100	-1.28303500	5.27947600 L
B-B_2	0	-3.84279700	0.85513100	5.38682900 L
N-N_3	0	-3.84265800	-0.62229900	5.78463800 L
N-N_3	0	-5.12591800	1.65775800	5.60761800 L
B-B_2	0	-6.41516200	0.85955800	5.40474000 L
B-B_2	0	-7.69909900	2.89037500	4.70867100 L
N-N_3	0	-7.69648700	1.66603300	5.63547600 L
N-N_3	0	-8.97266000	3.73198200	4.62490100 L
B-B_2	0	-10.26111300	2.91272500	4.76193000 L
B-B_2	0	-11.48398100	4.29634000	3.18540700 L
N-N_3	0	-11.56898300	3.68219300	4.57460100 L
N-N_3	0	-12.60512300	4.08889100	2.16778600 L
B-	0	12.77437500	-4.33833400	2.59090000 L
N-N_3	0	12.86269500	-5.50548200	1.60615600 L
N-N_3	0	11.61151300	-4.53648800	3.59193300 L
B-B_2	0	10.28698600	-4.71206300	2.83019600 L
B-B_2	0	9.00556400	-3.25612600	4.42170500 L
N-N_3	0	9.00811400	-4.59263700	3.66703000 L
N-N_3	0	7.71632600	-2.81839200	5.11999300 L
B-B_2	0	6.43470200	-3.23603200	4.39809400 L
B-B_2	0	5.15002700	-1.29069700	5.29292800 L
N-N_3	0	5.14788100	-2.80974800	5.10629300 L
N-N_3	0	3.86363900	-0.62861300	5.78886100 L
B-B_2	0	2.57945200	-1.28739600	5.28292900 L
B-B_2	0	1.29643900	0.85075200	5.38416500 L
N-N_3	0	1.29457000	-0.62619900	5.78266400 L

N-N_3	0	0.01231100	1.65217500	5.60098300 L
B-B_2	0	-1.27288700	0.85284600	5.38277000 L
B-B_2	0	-2.55617500	2.87177100	4.67529500 L
N-N_3	0	-2.55668300	1.65427100	5.60164600 L
N-N_3	0	-3.84047300	3.69568000	4.57311100 L
B-B_2	0	-5.12670000	2.87486700	4.67959800 L
B-B_2	0	-6.41330200	4.48074200	3.26091200 L
N-N_3	0	-6.40862300	3.70257100	4.58180500 L
N-N_3	0	-7.69539700	5.21398400	2.85613400 L
B-B_2	0	-8.98138600	4.50202400	3.28744900 L
B-B_2	0	-10.26085200	5.48009700	1.35882500 L
N-N_3	0	-10.28368000	5.19492400	2.86266300 L
N-N_3	0	-11.56701400	5.89489800	0.68195600 L
B-	0	-12.83658300	5.42128700	1.43703300 L
N-N_3	0	12.86264600	-2.73806800	5.01694400 L
B-B_2	0	11.56141000	-3.26487000	4.43642600 L
B-B_2	0	10.28654800	-1.31244300	5.32295500 L
N-N_3	0	10.27870800	-2.84318700	5.15539100 L
N-N_3	0	9.00757000	-0.63713500	5.83110000 L
B-B_2	0	7.72299800	-1.29659200	5.31617100 L
B-B_2	0	6.43651700	0.84616700	5.39850900 L
N-N_3	0	6.43337800	-0.63096500	5.80132800 L
N-N_3	0	5.15116700	1.64822300	5.60812700 L
B-B_2	0	3.86607800	0.84841300	5.38924700 L
B-B_2	0	2.58336100	2.86730100	4.67658700 L
N-N_3	0	2.58148200	1.65018600	5.60359300 L
N-N_3	0	1.29923800	3.69162900	4.57261200 L
B-B_2	0	0.01358400	2.86976400	4.67486500 L
B-B_2	0	-1.26996600	4.46566100	3.25133100 L
N-N_3	0	-1.27060100	3.69390800	4.57230700 L
N-N_3	0	-2.55458800	5.18683600	2.84047500 L
B-B_2	0	-3.84060000	4.46823100	3.25238000 L
B-B_2	0	-5.12566200	5.39318800	1.32525000 L
N-N_3	0	-5.12458800	5.19121500	2.84232600 L
N-N_3	0	-6.40826700	5.90489300	0.66856200 L
B-B_2	0	-7.69830900	5.42303500	1.33519700 L
B-B_2	0	-8.98237900	5.54284700	-0.80758800 L
N-N_3	0	-8.97196700	5.95598600	0.67926000 L
N-N_3	0	-10.28513100	5.72523400	-1.59925200 L
B-B_2	0	-11.48705800	5.33399500	-0.73002700 L
B-	0	-12.84000500	4.84773700	-2.74927300 L
N-N_3	0	-12.60108400	4.44724400	-1.28475000 L
B-	0	12.77234500	-1.21663800	4.88885200 L
B-B_2	0	11.56255100	0.84588200	5.44650300 L

N-N_3	0	11.61111400	-0.65184900	5.74044400 L
N-N_3	0	10.28114400	1.65216800	5.66428700 L
B-B_2	0	9.00709800	0.84465400	5.43049300 L
B-B_2	0	7.72681500	2.87240100	4.69794000 L
N-N_3	0	7.71902300	1.64784000	5.62243400 L
N-N_3	0	6.43870900	3.68991500	4.57962000 L
B-B_2	0	5.15395500	2.86584500	4.68091100 L
B-B_2	0	3.87050400	4.45942500	3.25192700 L
N-N_3	0	3.86908400	3.68892500	4.57393500 L
N-N_3	0	2.58640200	5.18143500	2.84011200 L
B-B_2	0	1.30024700	4.46310800	3.25137500 L
B-B_2	0	0.01595200	5.38747400	1.32357900 L
N-N_3	0	0.01586500	5.18481700	2.84016500 L
N-N_3	0	-1.26901700	5.89365700	0.66596000 L
B-B_2	0	-2.55462000	5.38945900	1.32392900 L
B-B_2	0	-3.84071000	5.49494300	-0.81042100 L
N-N_3	0	-3.83972900	5.89513500	0.66646600 L
N-N_3	0	-5.12550200	5.70728500	-1.61324800 L
B-B_2	0	-6.41376100	5.50884700	-0.81235200 L
B-B_2	0	-7.70038600	4.79063200	-2.83115500 L
N-N_3	0	-7.69663600	5.73224400	-1.61861900 L
N-N_3	0	-8.97502800	4.69385400	-3.66960100 L
B-B_2	0	-10.26328100	4.84553600	-2.85206800 L
B-B_2	0	-11.48647600	3.24628400	-4.20710500 L
N-N_3	0	-11.57105000	4.64646700	-3.61840500 L
N-N_3	0	-12.59185100	2.22167400	-3.95584400 L
B-	0	12.77528300	2.62255500	4.33278600 L
N-N_3	0	12.86480800	1.62693400	5.49030000 L
N-N_3	0	11.61563900	3.62385000	4.54511200 L
B-B_2	0	10.29020100	2.86174700	4.71136900 L
B-B_2	0	9.01174300	4.47412100	3.27532500 L
N-N_3	0	9.01255900	3.70143200	4.60145500 L
N-N_3	0	7.72454000	5.18146400	2.84699000 L
B-B_2	0	6.44115400	4.45802900	3.25532000 L
B-B_2	0	5.15768300	5.38107500	1.32370900 L
N-N_3	0	5.15668400	5.17748700	2.84052000 L
N-N_3	0	3.87261000	5.88622200	0.66538800 L
B-B_2	0	2.58653700	5.38376100	1.32346100 L
B-B_2	0	1.30119000	5.48964800	-0.81106800 L
N-N_3	0	1.30191800	5.89066900	0.66561700 L
N-N_3	0	0.01592300	5.70148800	-1.61305500 L
B-B_2	0	-1.26958600	5.49264700	-0.81065100 L
B-B_2	0	-2.55613600	4.76063500	-2.81759500 L
N-N_3	0	-2.55506600	5.70347600	-1.61253500 L

N-N_3	0	-3.84194000	4.64399000	-3.63806100 L
B-B_2	0	-5.12740400	4.76352700	-2.81809800 L
B-B_2	0	-6.41640000	3.31714400	-4.39731100 L
N-N_3	0	-6.41070100	4.65150200	-3.64244700 L
N-N_3	0	-7.69928700	2.90058900	-5.12302700 L
B-B_2	0	-8.98465100	3.34350100	-4.41701500 L
B-B_2	0	-10.26522600	1.39924400	-5.36228800 L
N-N_3	0	-10.28766600	2.90755700	-5.10145900 L
N-N_3	0	-11.57498700	0.71695500	-5.75942900 L
B-	0	-12.84228700	1.46714300	-5.27124900 L
N-N_3	0	12.86928800	5.07169900	2.76661800 L
B-B_2	0	11.56750800	4.48547500	3.28518900 L
B-B_2	0	10.29473500	5.39061000	1.34158900 L
N-N_3	0	10.28614200	5.20998800	2.87069300 L
N-N_3	0	9.01690200	5.90557300	0.66957000 L
B-B_2	0	7.73084000	5.39261600	1.32740700 L
B-B_2	0	6.44298000	5.48271100	-0.81122600 L
N-N_3	0	6.44274900	5.88661200	0.66538300 L
N-N_3	0	5.15773100	5.69234300	-1.61342600 L
B-B_2	0	3.87195000	5.48472600	-0.81119700 L
B-B_2	0	2.58537600	4.75514000	-2.81890200 L
N-N_3	0	2.58700400	5.69743400	-1.61332700 L
N-N_3	0	1.29974300	4.64039500	-3.63961000 L
B-B_2	0	0.01461900	4.75893800	-2.81843600 L
B-B_2	0	-1.27252900	3.30776800	-4.38593600 L
N-N_3	0	-1.27118400	4.64302300	-3.63892000 L
N-N_3	0	-2.55826300	2.88472600	-5.09829400 L
B-B_2	0	-3.84343500	3.30926300	-4.38626900 L
B-B_2	0	-5.13023100	1.36699200	-5.28145900 L
N-N_3	0	-5.12827100	2.88690100	-5.10131000 L
N-N_3	0	-6.41273700	0.70581800	-5.78821900 L
B-B_2	0	-7.70292300	1.37675100	-5.31238100 L
B-B_2	0	-8.98587700	-0.77007200	-5.42371000 L
N-N_3	0	-8.97747700	0.71651500	-5.83911700 L
N-N_3	0	-10.28845700	-1.56058100	-5.60787200 L
B-B_2	0	-11.48544300	-0.69419300	-5.19861600 L
B-	0	-12.84217700	-2.71877500	-4.74476800 L
N-N_3	0	-12.60052300	-1.26110500	-4.32078200 L
B-	0	12.78210200	4.95617800	1.24395100 L
B-B_2	0	11.57011300	5.51850300	-0.81581100 L
N-N_3	0	11.61996800	5.80939900	0.68273000 L
N-N_3	0	10.28768800	5.73126100	-1.62147400 L
B-B_2	0	9.01392400	5.50481500	-0.81184800 L
B-B_2	0	7.73001000	4.76003600	-2.82991600 L

N-N_3	0	7.72590700	5.69674700	-1.61487800 L
N-N_3	0	6.44071300	4.63483000	-3.64432600 L
B-B_2	0	5.15669400	4.75151600	-2.82052100 L
B-B_2	0	3.86847700	3.30141400	-4.38860000 L
N-N_3	0	3.87046400	4.63607200	-3.64012900 L
N-N_3	0	2.58233900	2.88021800	-5.10090200 L
B-B_2	0	1.29796800	3.30534600	-4.38717800 L
B-B_2	0	0.01051700	1.36350100	-5.27740400 L
N-N_3	0	0.01198100	2.88300700	-5.09920400 L
N-N_3	0	-1.27508700	0.70158600	-5.77491500 L
B-B_2	0	-2.55948400	1.36526400	-5.27686000 L
B-B_2	0	-3.84601900	-0.77167300	-5.36917800 L
N-N_3	0	-3.84450600	0.70321300	-5.77629100 L
N-N_3	0	-5.12961600	-1.57410400	-5.58712400 L
B-B_2	0	-6.41837700	-0.77423700	-5.38795400 L
B-B_2	0	-7.70418300	-2.80347000	-4.68914700 L
N-N_3	0	-7.70018300	-1.58023400	-5.61744400 L
N-N_3	0	-8.97809200	-3.64462800	-4.60716300 L
B-B_2	0	-10.26602200	-2.82463700	-4.74507100 L
B-B_2	0	-11.49109700	-4.20808600	-3.17060500 L
N-N_3	0	-11.57431200	-3.59365500	-4.55970500 L
N-N_3	0	-12.61051100	-3.99574900	-2.15218400 L
B-	0	12.78155500	4.39104600	-2.58316100 L
N-N_3	0	12.87091600	5.55863100	-1.59908700 L
N-N_3	0	11.61826900	4.58920200	-3.58371500 L
B-B_2	0	10.29404800	4.76682500	-2.82178600 L
B-B_2	0	9.01035200	3.31341200	-4.41383000 L
N-N_3	0	9.01501100	4.64956100	-3.65858200 L
N-N_3	0	7.72083000	2.87875700	-5.11326400 L
B-B_2	0	6.43941900	3.29927400	-4.39272500 L
B-B_2	0	5.15127000	1.35735300	-5.28760000 L
N-N_3	0	5.15266200	2.87669700	-5.10311500 L
N-N_3	0	3.86373600	0.69663600	-5.78231500 L
B-B_2	0	2.58053800	1.36080000	-5.28085700 L
B-B_2	0	1.29327300	-0.77464200	-5.36764200 L
N-N_3	0	1.29417700	0.69940600	-5.77706300 L
N-N_3	0	0.00757000	-1.57483400	-5.57837900 L
B-B_2	0	-1.27614400	-0.77224500	-5.36515300 L
B-B_2	0	-2.56187900	-2.78700700	-4.64818300 L
N-N_3	0	-2.56078800	-1.57321700	-5.57922900 L
N-N_3	0	-3.84637700	-3.60990500	-4.54730100 L
B-B_2	0	-5.13200600	-2.78855600	-4.65573800 L
B-B_2	0	-6.42040600	-4.39643400	-3.24098600 L
N-N_3	0	-6.41404800	-3.61606000	-4.56045300 L

N-N_3	0	-7.70340700	-5.12974200	-2.83940800 L
B-B_2	0	-8.98844700	-4.41578800	-3.27038700 L
N-N_3	0	-10.29178000	-5.10763500	-2.84687100 L
N-N_3	0	12.86673300	2.78650600	-5.00583000 L
B-B_2	0	11.56616400	3.31668300	-4.42672900 L
B-B_2	0	10.28771100	1.36688900	-5.31407000 L
N-N_3	0	10.28312600	2.89768200	-5.14662500 L
N-N_3	0	9.00750300	0.69415200	-5.82245500 L
B-B_2	0	7.72423700	1.35685600	-5.30860000 L
B-B_2	0	6.43329600	-0.78274500	-5.38695200 L
N-N_3	0	6.43344000	0.69341100	-5.79341900 L
N-N_3	0	5.14571700	-1.58215100	-5.59309300 L
B-B_2	0	3.86293500	-0.77839900	-5.37521500 L
B-B_2	0	2.57636000	-2.79192900	-4.65293900 L
N-N_3	0	2.57617300	-1.57799400	-5.58401500 L
N-N_3	0	1.29056900	-3.61318000	-4.54728700 L
B-B_2	0	0.00718700	-2.78834100	-4.64709300 L
B-B_2	0	-1.27793600	-4.38801000	-3.22715700 L
N-N_3	0	-1.27768500	-3.61059800	-4.54466600 L
N-N_3	0	-2.56335300	-5.11022100	-2.82198100 L
B-B_2	0	-3.84774200	-4.38579900	-3.22875500 L
N-N_3	0	-5.13256000	-5.10957200	-2.82387200 L
B-	0	12.77262400	1.26525300	-4.87806900 L
B-B_2	0	11.55921100	-0.79436800	-5.43833800 L
N-N_3	0	11.61098600	0.70351700	-5.73106000 L
N-N_3	0	10.27581100	-1.59778100	-5.65524600 L
B-B_2	0	9.00379200	-0.78736000	-5.42074200 L
B-B_2	0	7.71952500	-2.81185100	-4.68565600 L
N-N_3	0	7.71367200	-1.58780700	-5.61090800 L
N-N_3	0	6.42931600	-3.62598600	-4.56540800 L
B-B_2	0	5.14675200	-2.79814100	-4.66371600 L
B-B_2	0	3.86105600	-4.39112700	-3.23406500 L
N-N_3	0	3.85959600	-3.61741700	-4.55397900 L
N-N_3	0	2.57610400	-5.11286900	-2.82405100 L
B-B_2	0	1.29102800	-4.39033300	-3.22958300 L
N-N_3	0	0.00612300	-5.11369600	-2.82309500 L
B-	0	12.76908900	-2.57398500	-4.32643400 L
N-N_3	0	12.85967100	-1.57823900	-5.48374900 L
N-N_3	0	11.60685700	-3.57255700	-4.53766300 L
B-B_2	0	10.28296200	-2.80740300	-4.70236100 L
B-B_2	0	9.00230500	-4.41756500	-3.26545800 L
N-N_3	0	9.00339000	-3.64410800	-4.59111900 L
N-N_3	0	7.71408900	-5.12279400	-2.83666400 L
B-B_2	0	6.43172400	-4.39594300	-3.24223600 L

N-N_3	0	5.14613600	-5.11364300	-2.82759000 L
N-N_3	0	12.85916200	-5.02276500	-2.76012300 L
B-B_2	0	11.55810800	-4.43410900	-3.27776400 L
N-N_3	0	10.27569000	-5.15607300	-2.86223700 L
H-H_	0	-12.26946300	-3.36621100	1.27682700 L
H-H_	0	-12.24645300	-1.45021800	3.26184600 L
H-H_	0	-12.25604800	1.34123200	3.34707100 L
H-H_	0	-12.27832800	3.37987200	1.47296900 L
H-H_	0	12.88242500	-6.39712000	2.15134500 L
H-H_	0	12.88437400	-2.98363100	6.03275300 L
H-H_	0	-12.26447500	3.45808600	-1.26022400 L
H-H_	0	-12.24243100	1.54175900	-3.24304900 L
H-H_	0	12.88802600	2.16358800	6.38702100 L
H-H_	0	12.88934000	6.08547200	3.02058900 L
H-H_	0	-12.26366100	-1.25339000	-3.33142100 L
H-H_	0	-12.28056100	-3.28745900	-1.45810700 L
H-H_	0	12.89054300	6.44999900	-2.14472100 L
H-H_	0	12.89029100	3.03216200	-6.02157600 L
H-H_	0	12.88073800	-2.11470500	-6.38063400 L
H-H_	0	12.87689100	-6.03671000	-3.01358400 L
C-C_3	0	-0.11435100	-1.77173700	-0.01378300 H
H-H_	0	-0.12673100	0.22396700	0.89928900 H
H-H_	0	1.04610400	-0.90684000	1.60648200 H
C-C_3	0	0.03414300	-0.81786800	1.19683400 H
H-H_	0	-0.67360600	-1.07402600	1.99196500 H
N-N_3	0	0.81412300	-1.55356300	-1.11639100 H
H-H_	0	0.48222000	-0.81472600	-1.73100600 H
H-H_	0	1.74256300	-1.31929200	-0.78124900 H
C-C_R	0	-1.53090000	-1.68066800	-0.56017400 H
O-O_R	0	-1.85622000	-1.09867600	-1.57349400 H
O-O_R	0	-2.42602500	-2.30061500	0.24537300 H
H-H_	0	-3.30525500	-2.18285200	-0.15270200 H
H-H_	0	0.01584000	-2.79215600	0.35897000 H

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B-B_2	0	-10.27752400	-5.50088600	-0.65560600 L
N-N_3	0	-11.58500000	-5.81846400	0.07010200 L
B-	0	-12.85372900	-5.43931600	-0.73802300 L
B-B_2	0	-5.14238400	-5.41693100	-0.63444400 L
N-N_3	0	-6.42510300	-5.83811600	0.08344200 L
B-B_2	0	-7.71501800	-5.44610900	-0.63996500 L
B-B_2	0	-8.99794100	-5.28700100	1.50158800 L
N-N_3	0	-8.98923500	-5.88758700	0.07997600 L

N-N_3	0	-10.30055500	-5.36557600	2.31010200 L
B-B_2	0	-11.50074000	-5.08151600	1.39833500 L
B-	0	-12.85359400	-4.34690700	3.34085900 L
N-N_3	0	-12.61256400	-4.13004100	1.83841600 L
B-B_2	0	-0.00183300	-5.42583600	-0.63706100 L
N-N_3	0	-1.28731400	-5.83564600	0.08296500 L
B-B_2	0	-2.57137800	-5.41788900	-0.63490600 L
B-B_2	0	-3.85655700	-5.24268200	1.49607100 L
N-N_3	0	-3.85692200	-5.83016900	0.08359700 L
N-N_3	0	-5.14096000	-5.35132100	2.31977200 L
B-B_2	0	-6.42959900	-5.25490300	1.50099400 L
B-B_2	0	-7.71435900	-4.28897900	3.41572600 L
N-N_3	0	-7.71206900	-5.37412400	2.32970100 L
N-N_3	0	-8.98827400	-4.08896800	4.23691600 L
B-B_2	0	-10.27694500	-4.33762600	3.44425500 L
B-B_2	0	-11.49783000	-2.58340300	4.59510200 L
N-N_3	0	-11.58455000	-4.04441800	4.18024300 L
N-N_3	0	-12.60795200	-1.59811700	4.23190500 L
B-B_2	0	5.13982200	-5.42337300	-0.63484000 L
N-N_3	0	3.85356800	-5.83463200	0.08323000 L
B-B_2	0	2.56858100	-5.42131700	-0.63589500 L
B-B_2	0	1.28342700	-5.24339800	1.49376400 L
N-N_3	0	1.28375100	-5.83556600	0.08284300 L
N-N_3	0	-0.00087100	-5.35187700	2.31674200 L
B-B_2	0	-1.28609300	-5.24568800	1.49487200 L
B-B_2	0	-2.57043800	-4.26615700	3.39652500 L
N-N_3	0	-2.57115100	-5.35087700	2.31765200 L
N-N_3	0	-3.85574600	-4.04751400	4.19624900 L
B-B_2	0	-5.14147500	-4.26507600	3.39750600 L
B-B_2	0	-6.42809600	-2.63593100	4.78962100 L
N-N_3	0	-6.42397500	-4.05215300	4.20284200 L
N-N_3	0	-7.70988500	-2.13355300	5.46066700 L
B-B_2	0	-8.99611500	-2.65771500	4.81445600 L
B-B_2	0	-10.27432300	-0.61208400	5.51854600 L
N-N_3	0	-10.29823300	-2.14077600	5.44177700 L
N-N_3	0	-11.58221700	0.11477600	5.83306900 L
B-	0	-12.85106900	-0.69089200	5.44861300 L
B-B_2	0	10.27651700	-5.44680900	-0.64928700 L
N-N_3	0	8.99761100	-5.86820200	0.08323400 L
B-B_2	0	7.71278500	-5.44170400	-0.63589600 L
B-B_2	0	6.42469600	-5.25155200	1.49629200 L
N-N_3	0	6.42347700	-5.84241700	0.08414100 L
N-N_3	0	5.13844300	-5.35336100	2.31754800 L
B-B_2	0	3.85380800	-5.24407400	1.49448700 L

B-B_2	0	2.56886500	-4.26665000	3.39611400 L
N-N_3	0	2.56848400	-5.35023400	2.31623100 L
N-N_3	0	1.28461800	-4.05303600	4.19830500 L
B-B_2	0	-0.00058200	-4.26863900	3.39746200 L
B-B_2	0	-1.28474600	-2.63478400	4.77675600 L
N-N_3	0	-1.28564800	-4.05085700	4.19735500 L
N-N_3	0	-2.56982700	-2.12600400	5.43144500 L
B-B_2	0	-3.85533000	-2.63160800	4.77572000 L
B-B_2	0	-5.13942800	-0.59426900	5.43048500 L
N-N_3	0	-5.13909900	-2.12470400	5.43535700 L
N-N_3	0	-6.42113900	0.12495800	5.85299800 L
B-B_2	0	-7.71200500	-0.59808800	5.46318600 L
B-B_2	0	-8.99347700	1.54583200	5.30724400 L
N-N_3	0	-8.98553500	0.12302300	5.90535500 L
N-N_3	0	-10.29555200	2.35454100	5.38952800 L
B-B_2	0	-11.49494200	1.44421900	5.09889800 L
B-	0	-12.84862600	3.39332000	4.38237100 L
N-N_3	0	-12.60923000	1.89224700	4.15396800 L
B-	0	12.76400600	-5.00652500	-0.60749000 L
B-B_2	0	11.55142300	-5.29840800	1.50735400 L
N-N_3	0	11.60092000	-5.77916200	0.05855300 L
N-N_3	0	10.26870900	-5.40590800	2.33340000 L
B-B_2	0	8.99544700	-5.28089300	1.50116200 L
B-B_2	0	7.71315900	-4.28466000	3.40965300 L
N-N_3	0	7.70673500	-5.36612900	2.32147300 L
N-N_3	0	6.42405500	-4.05617700	4.20162800 L
B-B_2	0	5.13999100	-4.26948700	3.39767700 L
B-B_2	0	3.85509300	-2.63602400	4.77747100 L
N-N_3	0	3.85421400	-4.05135900	4.19658600 L
N-N_3	0	2.57089000	-2.12995300	5.43558400 L
B-B_2	0	1.28526200	-2.63844600	4.78174100 L
B-B_2	0	0.00108200	-0.59893100	5.42584700 L
N-N_3	0	-0.00023200	-2.12908200	5.43494900 L
N-N_3	0	-1.28330500	0.12120600	5.83907800 L
B-B_2	0	-2.56876700	-0.59612400	5.42514500 L
B-B_2	0	-3.85288200	1.53740800	5.25645000 L
N-N_3	0	-3.85286100	0.12335100	5.84091800 L
N-N_3	0	-5.13632200	2.36180300	5.37052600 L
B-B_2	0	-6.42551400	1.54394600	5.27249000 L
B-B_2	0	-7.70994700	3.46565300	4.31774100 L
N-N_3	0	-7.70719200	2.37308300	5.39658300 L
N-N_3	0	-8.98361000	4.28874800	4.12423700 L
B-B_2	0	-10.27225600	3.49515000	4.36893000 L
B-B_2	0	-11.49547200	4.65813700	2.62429600 L

N-N_3	0	-11.57971000	4.23409200	4.08282800 L
N-N_3	0	-12.61114800	4.30716900	1.64075900 L
B-	0	12.76439300	-3.95954700	3.11976700 L
N-N_3	0	12.85237500	-5.24105600	2.28941700 L
N-N_3	0	11.60161100	-4.03058300	4.13768500 L
B-B_2	0	10.27697700	-4.29880100	3.40356600 L
B-B_2	0	8.99668900	-2.65644000	4.80345300 L
N-N_3	0	8.99824000	-4.07562200	4.21895100 L
N-N_3	0	7.70838300	-2.13623300	5.44414300 L
B-B_2	0	6.42599700	-2.63904200	4.78053800 L
B-B_2	0	5.14190500	-0.59983200	5.43114500 L
N-N_3	0	5.14052300	-2.13014600	5.43421500 L
N-N_3	0	3.85582900	0.11897600	5.84155600 L
B-B_2	0	2.57105900	-0.59992500	5.42663100 L
B-B_2	0	1.28714900	1.53256600	5.25236200 L
N-N_3	0	1.28625300	0.11949100	5.83918200 L
N-N_3	0	0.00285100	2.35534500	5.36341500 L
B-B_2	0	-1.28254600	1.53438000	5.25281800 L
B-B_2	0	-2.56661600	3.44308900	4.28671100 L
N-N_3	0	-2.56662200	2.35762800	5.36500500 L
N-N_3	0	-3.85119100	4.24623300	4.07692600 L
B-B_2	0	-5.13735000	3.44664700	4.29085100 L
B-B_2	0	-6.42458000	4.85104000	2.67276500 L
N-N_3	0	-6.41951700	4.25407400	4.08485900 L
N-N_3	0	-7.70697200	5.52422000	2.17495400 L
B-B_2	0	-8.99277900	4.87521900	2.69670000 L
B-B_2	0	-10.27266500	5.58832800	0.65574500 L
N-N_3	0	-10.29530000	5.50557100	2.18416800 L
N-N_3	0	-11.58004400	5.90672600	-0.06980800 L
B-	0	-12.84896600	5.52860600	0.73846800 L
N-N_3	0	12.85408700	-2.06903600	5.32681100 L
B-B_2	0	11.55239800	-2.66370400	4.81716600 L
B-B_2	0	10.27833900	-0.61637300	5.45553400 L
N-N_3	0	10.27044300	-2.15605800	5.47936800 L
N-N_3	0	8.99984300	0.11703200	5.87674800 L
B-B_2	0	7.71482800	-0.60193400	5.45042000 L
B-B_2	0	6.42770700	1.53253100	5.26221700 L
N-N_3	0	6.42571000	0.11900800	5.85025800 L
N-N_3	0	5.14200700	2.35423800	5.36746700 L
B-B_2	0	3.85706600	1.53218100	5.25501400 L
B-B_2	0	2.57315600	3.43998500	4.28618700 L
N-N_3	0	2.57217200	2.35428700	5.36426500 L
N-N_3	0	1.28864900	4.24301500	4.07567800 L
B-B_2	0	0.00330000	3.44130900	4.28561200 L

B-B_2	0	-1.28113000	4.83637900	2.66496300 L
N-N_3	0	-1.28119400	4.24458600	4.07594000 L
N-N_3	0	-2.56611400	5.49695600	2.16319100 L
B-B_2	0	-3.85178700	4.83813600	2.66585700 L
B-B_2	0	-5.13732200	5.50253400	0.63378000 L
N-N_3	0	-5.13610100	5.50055100	2.16430800 L
N-N_3	0	-6.42019900	5.92406200	-0.08385600 L
B-B_2	0	-7.71008200	5.53209100	0.63965200 L
B-B_2	0	-8.99359300	5.37370100	-1.50171600 L
N-N_3	0	-8.98426600	5.97420100	-0.08003800 L
N-N_3	0	-10.29632600	5.45282400	-2.30998300 L
B-B_2	0	-11.49647400	5.16955400	-1.39795700 L
B-	0	-12.85011400	4.43518300	-3.33994400 L
N-N_3	0	-12.60870900	4.21834000	-1.83755800 L
B-	0	12.76388900	-0.57529100	5.01067800 L
B-B_2	0	11.55398500	1.54050100	5.30671600 L
N-N_3	0	11.60316500	0.09133400	5.78595600 L
N-N_3	0	10.27212100	2.36723300	5.41951100 L
B-B_2	0	8.99835200	1.53605400	5.29167700 L
B-B_2	0	7.71684400	3.45119600	4.30477100 L
N-N_3	0	7.71005800	2.35675700	5.38007800 L
N-N_3	0	6.42815200	4.24548200	4.08143200 L
B-B_2	0	5.14387200	3.44081700	4.28969700 L
B-B_2	0	3.85929200	4.83312900	2.66516800 L
N-N_3	0	3.85842900	4.24191800	4.07652000 L
N-N_3	0	2.57470200	5.49440100	2.16302800 L
B-B_2	0	1.28904900	4.83503900	2.66476500 L
B-B_2	0	0.00419400	5.50000800	0.63290500 L
N-N_3	0	0.00427000	5.49620100	2.16304500 L
N-N_3	0	-1.28106600	5.91607300	-0.08457400 L
B-B_2	0	-2.56628400	5.50022700	0.63308700 L
B-B_2	0	-3.85223100	5.32936400	-1.49779200 L
N-N_3	0	-3.85165900	5.91570400	-0.08439000 L
N-N_3	0	-5.13693700	5.43744500	-2.32126100 L
B-B_2	0	-6.42521800	5.34132600	-1.50183200 L
B-B_2	0	-7.71090300	4.37483900	-3.41605300 L
N-N_3	0	-7.70795100	5.46029800	-2.33018700 L
N-N_3	0	-8.98509500	4.17515900	-4.23689300 L
B-B_2	0	-10.27350300	4.42471600	-3.44404500 L
B-B_2	0	-11.49562300	2.67110500	-4.59471800 L
N-N_3	0	-11.58144800	4.13215100	-4.17972800 L
N-N_3	0	-12.60736600	1.68696300	-4.23330300 L
B-	0	12.76645300	3.15979900	3.97483700 L
N-N_3	0	12.85568300	2.32158200	5.25104500 L

N-N_3	0	11.60539100	4.17880900	4.05476300 L
B-B_2	0	10.28042900	3.44377600	4.31855200 L
B-B_2	0	9.00066200	4.85475000	2.68544700 L
N-N_3	0	9.00216500	4.26129400	4.10087700 L
N-N_3	0	7.71284300	5.49933100	2.16894000 L
B-B_2	0	6.42999000	4.83423100	2.66822600 L
B-B_2	0	5.14577800	5.49752600	0.63306100 L
N-N_3	0	5.14493600	5.49247400	2.16348600 L
N-N_3	0	3.86031100	5.91256600	-0.08467000 L
B-B_2	0	2.57468200	5.49813000	0.63291600 L
B-B_2	0	1.28934000	5.32799400	-1.49778200 L
N-N_3	0	1.28973700	5.91501200	-0.08466900 L
N-N_3	0	0.00402900	5.43522900	-2.32012800 L
B-B_2	0	-1.28125600	5.32899800	-1.49761000 L
B-B_2	0	-2.56700400	4.34847600	-3.39684200 L
N-N_3	0	-2.56671200	5.43536100	-2.31985000 L
N-N_3	0	-3.85230100	4.13030900	-4.19693100 L
B-B_2	0	-5.13807000	4.35024400	-3.39854300 L
B-B_2	0	-6.42582100	2.72017500	-4.78938700 L
N-N_3	0	-6.42080200	4.13691800	-4.20341900 L
N-N_3	0	-7.70799100	2.21841800	-5.46016800 L
B-B_2	0	-8.99389000	2.74377500	-4.81416500 L
B-B_2	0	-10.27367600	0.69917600	-5.51875200 L
N-N_3	0	-10.29635900	2.22785200	-5.44155800 L
N-N_3	0	-11.58201100	-0.02642300	-5.83415600 L
B-	0	-12.85034600	0.78047200	-5.45060300 L
N-N_3	0	12.85789800	5.38293300	2.10217400 L
B-B_2	0	11.55649400	4.86880300	2.69322200 L
B-B_2	0	10.28275300	5.51340800	0.64868000 L
N-N_3	0	10.27456200	5.53258900	2.18832700 L
N-N_3	0	9.00451200	5.93658800	-0.08392700 L
B-B_2	0	7.71891500	5.51160800	0.63477000 L
B-B_2	0	6.43091600	5.32559800	-1.49802700 L
N-N_3	0	6.43038800	5.91508400	-0.08517800 L
N-N_3	0	5.14542100	5.43056900	-2.32006700 L
B-B_2	0	3.85996100	5.32524700	-1.49767500 L
B-B_2	0	2.57399800	4.34648700	-3.39726400 L
N-N_3	0	2.57486800	5.43327400	-2.32013400 L
N-N_3	0	1.28857800	4.12903800	-4.19710600 L
B-B_2	0	0.00348700	4.34824300	-3.39709500 L
B-B_2	0	-1.28244200	2.71273000	-4.77321000 L
N-N_3	0	-1.28192500	4.13012000	-4.19693000 L
N-N_3	0	-2.56742100	2.20529600	-5.42931200 L
B-B_2	0	-3.85306700	2.71365900	-4.77539000 L

B-B_2	0	-5.13882500	0.67660800	-5.42888200 L
N-N_3	0	-5.13714200	2.20721000	-5.43469100 L
N-N_3	0	-6.42100800	-0.04138000	-5.85186900 L
B-B_2	0	-7.71138000	0.68290500	-5.46249700 L
B-B_2	0	-8.99482900	-1.45991400	-5.30735500 L
N-N_3	0	-8.98539400	-0.03700400	-5.90519000 L
N-N_3	0	-10.29769300	-2.26739000	-5.38989400 L
B-B_2	0	-11.49636100	-1.35590900	-5.09991100 L
B-	0	-12.85193700	-3.30267600	-4.38127300 L
N-N_3	0	-12.61038700	-1.80184000	-4.15371300 L
B-	0	12.76996200	5.07074200	0.60743200 L
B-B_2	0	11.55777700	5.36305100	-1.50763500 L
N-N_3	0	11.60766200	5.84423500	-0.05898500 L
N-N_3	0	10.27543200	5.47253600	-2.33396500 L
B-B_2	0	9.00178800	5.34965200	-1.50200400 L
B-B_2	0	7.71830500	4.35529200	-3.41047100 L
N-N_3	0	7.71353900	5.43723900	-2.32268100 L
N-N_3	0	6.42896200	4.12813600	-4.20246800 L
B-B_2	0	5.14512600	4.34525300	-3.39912100 L
B-B_2	0	3.85805400	2.70991600	-4.77478200 L
N-N_3	0	3.85894000	4.12707800	-4.19756000 L
N-N_3	0	2.57228400	2.20293700	-5.42951200 L
B-B_2	0	1.28778000	2.71158500	-4.77336100 L
B-B_2	0	0.00164800	0.67411900	-5.41998700 L
N-N_3	0	0.00239700	2.20410100	-5.42842600 L
N-N_3	0	-1.28325300	-0.04394200	-5.83447700 L
B-B_2	0	-2.56822400	0.67526800	-5.42194400 L
B-B_2	0	-3.85422700	-1.45701800	-5.25436000 L
N-N_3	0	-3.85272100	-0.04268900	-5.83836100 L
N-N_3	0	-5.13838200	-2.27974700	-5.36995000 L
B-B_2	0	-6.42684900	-1.46058600	-5.27184600 L
B-B_2	0	-7.71328100	-3.38113800	-4.31814400 L
N-N_3	0	-7.70931500	-2.28837400	-5.39668900 L
N-N_3	0	-8.98785900	-4.20279900	-4.12449100 L
B-B_2	0	-10.27562100	-3.40773900	-4.36898100 L
B-B_2	0	-11.49971000	-4.56914000	-2.62374300 L
N-N_3	0	-11.58393100	-4.14500800	-4.08227100 L
N-N_3	0	-12.61518600	-4.21782600	-1.64008400 L
B-	0	12.76886800	4.02212800	-3.11989600 L
N-N_3	0	12.85880400	5.30345500	-2.28944100 L
N-N_3	0	11.60640900	4.09514600	-4.13804000 L
B-B_2	0	10.28212900	4.36531700	-3.40405000 L
B-B_2	0	8.99956400	2.72430700	-4.80336000 L
N-N_3	0	9.00312700	4.14377400	-4.21948400 L

N-N_3	0	7.71036700	2.20525600	-5.44334300 L
B-B_2	0	6.42879900	2.71013800	-4.77967900 L
B-B_2	0	5.14217100	0.67132700	-5.42854300 L
N-N_3	0	5.14232600	2.20181900	-5.43212900 L
N-N_3	0	3.85522300	-0.04644700	-5.83841000 L
B-B_2	0	2.57151000	0.67290200	-5.42207800 L
B-B_2	0	1.28524500	-1.45869000	-5.24905800 L
N-N_3	0	1.28582300	-0.04515200	-5.83446200 L
N-N_3	0	0.00019700	-2.27996200	-5.36197500 L
B-B_2	0	-1.28411200	-1.45753900	-5.24924500 L
B-B_2	0	-2.56974600	-3.36670000	-4.28797400 L
N-N_3	0	-2.56883200	-2.27882800	-5.36366000 L
N-N_3	0	-3.85563700	-4.16704500	-4.07811900 L
B-B_2	0	-5.14061300	-3.36528400	-4.29120000 L
B-B_2	0	-6.42932300	-4.76719200	-2.67331600 L
N-N_3	0	-6.42376400	-4.17103700	-4.08552900 L
N-N_3	0	-7.71217200	-5.43909600	-2.17519800 L
B-B_2	0	-8.99739800	-4.78900000	-2.69687200 L
N-N_3	0	-10.30041200	-5.41799500	-2.18402900 L
N-N_3	0	12.85611600	2.13240400	-5.32802000 L
B-B_2	0	11.55530300	2.72847500	-4.81782700 L
B-B_2	0	10.27863700	0.68258600	-5.45566100 L
N-N_3	0	10.27250200	2.22228000	-5.47956600 L
N-N_3	0	8.99911700	-0.04937600	-5.87637900 L
B-B_2	0	7.71508700	0.67090400	-5.44927000 L
B-B_2	0	6.42567200	-1.46266200	-5.26157400 L
N-N_3	0	6.42497600	-0.04865500	-5.84855900 L
N-N_3	0	5.13908000	-2.28312100	-5.36720900 L
B-B_2	0	3.85511800	-1.46015000	-5.25296100 L
B-B_2	0	2.56893100	-3.36882600	-4.28689700 L
N-N_3	0	2.56929100	-2.28110900	-5.36272700 L
N-N_3	0	1.28429100	-4.17293100	-4.08020600 L
B-B_2	0	-0.00036000	-3.36978200	-4.28811300 L
B-B_2	0	-1.28561700	-4.76553200	-2.66982200 L
N-N_3	0	-1.28576100	-4.17152600	-4.07985600 L
N-N_3	0	-2.57229700	-5.41959000	-2.16476400 L
B-B_2	0	-3.85639400	-4.75774000	-2.66693700 L
N-N_3	0	-5.14151600	-5.41750900	-2.16461400 L
B-	0	12.76436000	0.63875700	-5.01189900 L
B-B_2	0	11.55195100	-1.47565600	-5.30746100 L
N-N_3	0	11.60254500	-0.02655400	-5.78669200 L
N-N_3	0	10.26923300	-2.30105000	-5.42016700 L
B-B_2	0	8.99630500	-1.46863100	-5.29186400 L
B-B_2	0	7.71296400	-3.38306300	-4.30588400 L

N-N_3	0	7.70716400	-2.28801300	-5.38050400 L
N-N_3	0	6.42361400	-4.17642400	-4.08305700 L
B-B_2	0	5.13994300	-3.37072800	-4.29067000 L
B-B_2	0	3.85389700	-4.76258800	-2.66746900 L
N-N_3	0	3.85383900	-4.17119800	-4.07834600 L
N-N_3	0	2.56952700	-5.42436200	-2.16580000 L
B-B_2	0	1.28362300	-4.76872400	-2.67094300 L
N-N_3	0	-0.00172800	-5.42741000	-2.16748800 L
B-	0	12.76293200	-3.09605700	-3.97565800 L
N-N_3	0	12.85285400	-2.25807000	-5.25195600 L
N-N_3	0	11.60087400	-4.11393500	-4.05538500 L
B-B_2	0	10.27657700	-3.37774300	-4.31937200 L
B-B_2	0	8.99541600	-4.78743800	-2.68648600 L
N-N_3	0	8.99762600	-4.19420300	-4.10197100 L
N-N_3	0	7.70699300	-5.43071200	-2.17003000 L
B-B_2	0	6.42483000	-4.76478000	-2.66988300 L
N-N_3	0	5.13926400	-5.42158100	-2.16497000 L
N-N_3	0	12.85206800	-5.31862700	-2.10225900 L
B-B_2	0	11.55118600	-4.80355100	-2.69367000 L
N-N_3	0	10.26862100	-5.46624800	-2.18894800 L
H-H_	0	-12.27296500	-3.15234200	1.69299900 L
H-H_	0	-12.26583400	-1.00850300	3.43962300 L
H-H_	0	-12.27254200	1.75370500	3.17427000 L
H-H_	0	-12.27648400	3.51449100	1.04746700 L
H-H_	0	12.87156300	-6.05724000	2.94219200 L
H-H_	0	12.87653700	-2.18643900	6.36525000 L
H-H_	0	-12.26933700	3.24055300	-1.69219400 L
H-H_	0	-12.26685900	1.09662400	-3.44087200 L
H-H_	0	12.87748700	2.96931400	6.07117400 L
H-H_	0	12.87788200	6.42109600	2.22242000 L
H-H_	0	-12.27261100	-1.66332100	-3.17438300 L
H-H_	0	-12.28006900	-3.42547000	-1.04661600 L
H-H_	0	12.87955400	6.11964100	-2.94216700 L
H-H_	0	12.87826700	2.24981800	-6.36646300 L
H-H_	0	12.87385700	-2.90589400	-6.07203100 L
H-H_	0	12.87137300	-6.35679100	-2.22259600 L
C-C_R	0	0.21784700	-1.78770700	0.16965400 H
H-H_	0	0.91878400	-0.08149900	1.32665100 H
H-H_	0	1.81489900	-1.58881500	1.63024400 H
C-C_3	0	0.82492600	-1.17925400	1.39810900 H
H-H_	0	0.17499500	-1.39527600	2.24832900 H
N-N_3	0	1.00760700	-1.50337100	-1.16329600 H
H-H_	0	0.33697200	-1.32662300	-1.91511400 H
H-H_	0	1.76536200	-0.83272500	-1.06899800 H

C-C_R	0	-1.17917400	-1.80187900	-0.13114700 H
O-O_R	0	-1.65603800	-1.75421500	-1.27394700 H
O-O_R	0	-1.98868200	-1.92054900	0.96453800 H
H-H_	0	-2.89191700	-2.00387200	0.61953600 H
H-H_	0	0.98579100	-2.55695800	-0.65205500 H

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B-B_2	0	-10.26822800	-5.52897200	-0.24056100 L
N-N_3	0	-11.57561300	-5.79055500	0.50729800 L
B-	0	-12.84447700	-5.47407000	-0.32715200 L
B-B_2	0	-5.13301000	-5.44207800	-0.22648200 L
N-N_3	0	-6.41550600	-5.80765900	0.52172400 L
B-B_2	0	-7.70571700	-5.47259900	-0.22936600 L
B-B_2	0	-8.98851400	-5.15165000	1.89416700 L
N-N_3	0	-8.97976500	-5.85834100	0.52222300 L
N-N_3	0	-10.29113100	-5.16902500	2.70632100 L
B-B_2	0	-11.49123500	-4.95479500	1.77563200 L
B-	0	-12.84433500	-4.07364600	3.65573800 L
N-N_3	0	-12.60206200	-3.97125400	2.14139400 L
B-B_2	0	0.00737900	-5.44079800	-0.22891700 L
N-N_3	0	-1.27731100	-5.79773600	0.52006300 L
B-B_2	0	-2.56249000	-5.44108600	-0.22779100 L
B-B_2	0	-3.84719400	-5.10672000	1.88546800 L
N-N_3	0	-3.84725500	-5.79859800	0.52090300 L
N-N_3	0	-5.13155700	-5.15386700	2.71492900 L
B-B_2	0	-6.42012700	-5.11895200	1.89112800 L
B-B_2	0	-7.70506800	-4.01265400	3.72827000 L
N-N_3	0	-7.70262000	-5.17594200	2.72644300 L
N-N_3	0	-8.97915600	-3.75159600	4.53192000 L
B-B_2	0	-10.26761500	-4.05839900	3.75960400 L
B-B_2	0	-11.48810300	-2.22227600	4.77547400 L
N-N_3	0	-11.57546300	-3.71014300	4.47085500 L
N-N_3	0	-12.59823500	-1.26650900	4.34046700 L
B-B_2	0	5.14852400	-5.45079300	-0.22572300 L
N-N_3	0	3.86141900	-5.80409400	0.52132500 L
B-B_2	0	2.57758100	-5.44362800	-0.22782500 L
B-B_2	0	1.29210700	-5.10563100	1.88407700 L
N-N_3	0	1.29174600	-5.79843600	0.52002000 L
N-N_3	0	0.00759300	-5.15396400	2.71243600 L
B-B_2	0	-1.27707100	-5.10545500	1.88448100 L
B-B_2	0	-2.56124700	-3.99387500	3.71135800 L
N-N_3	0	-2.56174800	-5.15304000	2.71281400 L
N-N_3	0	-3.84705400	-3.71597400	4.49128200 L

B-B_2	0	-5.13213500	-3.99087900	3.70940500 L
B-B_2	0	-6.41866500	-2.26251700	4.97598000 L
N-N_3	0	-6.41492900	-3.71835600	4.49602000 L
N-N_3	0	-7.70049600	-1.71095900	5.60704400 L
B-B_2	0	-8.98663600	-2.28125800	5.00107800 L
B-B_2	0	-10.26415200	-0.18823400	5.55016400 L
N-N_3	0	-10.28875200	-1.71839300	5.58749600 L
N-N_3	0	-11.57171700	0.56068700	5.80931300 L
B-	0	-12.84081100	-0.27117600	5.48635400 L
B-B_2	0	10.28515400	-5.47918800	-0.23729600 L
N-N_3	0	9.00589000	-5.84307100	0.52494800 L
B-B_2	0	7.72143700	-5.47158000	-0.22475700 L
B-B_2	0	6.43313900	-5.12008400	1.88740800 L
N-N_3	0	6.43160400	-5.81525700	0.52349100 L
N-N_3	0	5.14680400	-5.15988200	2.71398600 L
B-B_2	0	3.86225300	-5.11055300	1.88506600 L
B-B_2	0	2.57794600	-3.99623600	3.71106700 L
N-N_3	0	2.57676900	-5.15509000	2.71240500 L
N-N_3	0	1.29371500	-3.72297200	4.49525500 L
B-B_2	0	0.00809600	-3.99690500	3.71336900 L
B-B_2	0	-1.27552700	-2.26613200	4.96816100 L
N-N_3	0	-1.27687900	-3.72133200	4.49533800 L
N-N_3	0	-2.56063700	-1.70844100	5.58150500 L
B-B_2	0	-3.84591500	-2.26093500	4.96410700 L
B-B_2	0	-5.12928100	-0.17961200	5.46279900 L
N-N_3	0	-5.12985800	-1.70528900	5.58273800 L
N-N_3	0	-6.41073900	0.57001300	5.82954400 L
B-B_2	0	-7.70184200	-0.17963900	5.49469700 L
B-B_2	0	-8.98227600	1.94693600	5.17763200 L
N-N_3	0	-8.97512400	0.57318900	5.88111700 L
N-N_3	0	-10.28394600	2.76023100	5.19851500 L
B-B_2	0	-11.48394900	1.83128000	4.97743500 L
B-	0	-12.83633000	3.72214000	4.11642100 L
N-N_3	0	-12.59850600	2.20784600	4.00211500 L
B-	0	12.77238700	-5.03711600	-0.22855900 L
B-B_2	0	11.55986500	-5.16852300	1.90228700 L
N-N_3	0	11.60932800	-5.75721100	0.49393400 L
N-N_3	0	10.27712500	-5.21379800	2.73405500 L
B-B_2	0	9.00394300	-5.15065300	1.89466500 L
B-B_2	0	7.72209300	-4.01466700	3.72416300 L
N-N_3	0	7.71510800	-5.17368300	2.71893800 L
N-N_3	0	6.43325400	-3.72787600	4.49734600 L
B-B_2	0	5.14896400	-3.99961400	3.71171700 L
B-B_2	0	3.86485700	-2.26814000	4.96685400 L

N-N_3	0	3.86356800	-3.72285400	4.49295600 L
N-N_3	0	2.58052000	-1.71350400	5.58459100 L
B-B_2	0	1.29466400	-2.26838000	4.96988000 L
B-B_2	0	0.01139000	-0.18684000	5.46071400 L
N-N_3	0	0.00974000	-1.71196200	5.58485600 L
N-N_3	0	-1.27290000	0.56282700	5.81768400 L
B-B_2	0	-2.55857000	-0.18338800	5.45892800 L
B-B_2	0	-3.84163900	1.93191700	5.12842100 L
N-N_3	0	-3.84245700	0.56623800	5.81835200 L
N-N_3	0	-5.12465300	2.76327200	5.17951600 L
B-B_2	0	-6.41428300	1.94106800	5.14354400 L
B-B_2	0	-7.69761500	3.78543900	4.04577700 L
N-N_3	0	-7.69553800	2.77788100	5.20437900 L
N-N_3	0	-8.97076700	4.59219400	3.79022700 L
B-B_2	0	-10.25993500	3.82038800	4.09457300 L
B-B_2	0	-11.48254500	4.84811800	2.26671100 L
N-N_3	0	-11.56681500	4.53651900	3.75333700 L
N-N_3	0	-12.59776000	4.42245900	1.31260400 L
B-	0	12.77313100	-3.71369400	3.41082800 L
N-N_3	0	12.86088700	-5.05327100	2.67785400 L
N-N_3	0	11.61058800	-3.70910000	4.43141600 L
B-B_2	0	10.28584300	-4.03034300	3.71913300 L
B-B_2	0	9.00632500	-2.28841500	4.99374800 L
N-N_3	0	9.00726800	-3.74693400	4.51577700 L
N-N_3	0	7.71831800	-1.72155000	5.59417600 L
B-B_2	0	6.43567600	-2.27178900	4.96995400 L
B-B_2	0	5.15240000	-0.18932900	5.46666000 L
N-N_3	0	5.15043100	-1.71516500	5.58415100 L
N-N_3	0	3.86659500	0.55895800	5.82171700 L
B-B_2	0	2.58147600	-0.18844700	5.46185500 L
B-B_2	0	1.29845100	1.92490000	5.12659700 L
N-N_3	0	1.29682300	0.56040900	5.81887900 L
N-N_3	0	0.01437600	2.75407900	5.17413600 L
B-B_2	0	-1.27131400	1.92746000	5.12582400 L
B-B_2	0	-2.55432900	3.75769100	4.01701400 L
N-N_3	0	-2.55503200	2.75737800	5.17472400 L
N-N_3	0	-3.83844200	4.54322600	3.74656300 L
B-B_2	0	-5.12503800	3.76296000	4.02058100 L
B-B_2	0	-6.41143200	5.04075600	2.30024000 L
N-N_3	0	-6.40672900	4.55311300	3.75370300 L
N-N_3	0	-7.69342000	5.67478500	1.75250100 L
B-B_2	0	-8.97962400	5.06825200	2.32217300 L
B-B_2	0	-10.25908100	5.62416300	0.23274500 L
N-N_3	0	-10.28176200	5.65851300	1.76303200 L

N-N_3	0	-11.56638200	5.88666100	-0.51504100 L
B-	0	-12.83549800	5.57119600	0.31940400 L
N-N_3	0	12.86390100	-1.66581500	5.47290100 L
B-B_2	0	11.56202700	-2.29584200	5.00828000 L
B-B_2	0	10.28894800	-0.20620100	5.49209300 L
N-N_3	0	10.28027000	-1.73980000	5.63068700 L
N-N_3	0	9.01073600	0.55730600	5.85691900 L
B-B_2	0	7.72537600	-0.19108400	5.48586300 L
B-B_2	0	6.43918300	1.92339400	5.13698900 L
N-N_3	0	6.43657200	0.55845500	5.83037200 L
N-N_3	0	5.15385900	2.75134500	5.17929900 L
B-B_2	0	3.86849100	1.92372200	5.12984200 L
B-B_2	0	2.58549100	3.75238000	4.01788400 L
N-N_3	0	2.58385800	2.75228100	5.17585100 L
N-N_3	0	1.30134500	4.53745400	3.74626400 L
B-B_2	0	0.01557600	3.75469700	4.01664300 L
B-B_2	0	-1.26801400	5.02251300	2.29397200 L
N-N_3	0	-1.26850400	4.54018400	3.74600900 L
N-N_3	0	-2.55259000	5.64362600	1.74315000 L
B-B_2	0	-3.83865800	5.02582800	2.29449400 L
B-B_2	0	-5.12377200	5.53411100	0.21761100 L
N-N_3	0	-5.12256600	5.64884500	1.74382600 L
N-N_3	0	-6.40638300	5.90057200	-0.53011000 L
B-B_2	0	-7.69652200	5.56558700	0.22106400 L
B-B_2	0	-8.98003300	5.24563500	-1.90224700 L
N-N_3	0	-8.97047100	5.95233600	-0.53024900 L
N-N_3	0	-10.28269400	5.26404700	-2.71423100 L
B-B_2	0	-11.48282100	5.05077200	-1.78337100 L
B-	0	-12.83702300	4.17258700	-3.66423300 L
N-N_3	0	-12.59531300	4.06935400	-2.14983500 L
B-	0	12.77487700	-0.19970200	5.04632700 L
B-B_2	0	11.56561200	1.93271000	5.18187000 L
N-N_3	0	11.61405700	0.52368700	5.76886500 L
N-N_3	0	10.28395500	2.76595200	5.23061400 L
B-B_2	0	9.00988100	1.92797800	5.16620800 L
B-B_2	0	7.72930000	3.76244600	4.03576500 L
N-N_3	0	7.72194300	2.75357200	5.19171500 L
N-N_3	0	6.44100800	4.53788200	3.75207100 L
B-B_2	0	5.15627500	3.75225200	4.02150100 L
B-B_2	0	3.87243100	5.01643700	2.29483300 L
N-N_3	0	3.87121300	4.53524600	3.74741300 L
N-N_3	0	2.58821800	5.63802200	1.74346400 L
B-B_2	0	1.30216600	5.01975200	2.29415100 L
B-B_2	0	0.01772600	5.52828600	0.21727200 L

N-N_3	0	0.01778200	5.64133300	1.74323700 L
N-N_3	0	-1.26725500	5.88931900	-0.52988000 L
B-B_2	0	-2.55273800	5.53014000	0.21727200 L
B-B_2	0	-3.83874800	5.19854400	-1.89457700 L
N-N_3	0	-3.83783700	5.89060200	-0.52983600 L
N-N_3	0	-5.12334000	5.24482200	-2.72397300 L
B-B_2	0	-6.41171400	5.21181200	-1.89973000 L
B-B_2	0	-7.69788400	4.10438200	-3.73583600 L
N-N_3	0	-7.69432500	5.26858400	-2.73482800 L
N-N_3	0	-8.97214800	3.84445000	-4.53951800 L
B-B_2	0	-10.26040200	4.15342100	-3.76760200 L
B-B_2	0	-11.48341000	2.31910400	-4.78372800 L
N-N_3	0	-11.56857700	3.80711700	-4.47917000 L
N-N_3	0	-12.59605800	1.36542500	-4.35055400 L
B-	0	12.77932900	3.44465700	3.73061300 L
N-N_3	0	12.86752100	2.70696400	5.06753100 L
N-N_3	0	11.61828200	4.46688500	3.73096200 L
B-B_2	0	10.29296200	3.75486800	4.05034000 L
B-B_2	0	9.01390300	5.03661500	2.31339200 L
N-N_3	0	9.01507300	4.55379900	3.77028300 L
N-N_3	0	7.72641900	5.64038400	1.74891800 L
B-B_2	0	6.44316900	5.01631300	2.29779600 L
B-B_2	0	5.15928200	5.52260400	0.21770500 L
N-N_3	0	5.15846900	5.63461300	1.74405400 L
N-N_3	0	3.87405500	5.88257400	-0.52954500 L
B-B_2	0	2.58819400	5.52480100	0.21752200 L
B-B_2	0	1.30274800	5.19399500	-1.89423400 L
N-N_3	0	1.30351600	5.88662200	-0.52977200 L
N-N_3	0	0.01751100	5.23950000	-2.72235400 L
B-B_2	0	-1.26780300	5.19655500	-1.89419900 L
B-B_2	0	-2.55407700	4.07618400	-3.71412200 L
N-N_3	0	-2.55315500	5.24120500	-2.72220300 L
N-N_3	0	-3.83943200	3.79942200	-4.49570100 L
B-B_2	0	-5.12509800	4.07948300	-3.71620500 L
B-B_2	0	-6.41369600	2.35063800	-4.98142900 L
N-N_3	0	-6.40787400	3.80721700	-4.50298600 L
N-N_3	0	-7.69610600	1.80107900	-5.61309800 L
B-B_2	0	-8.98171000	2.37390100	-5.00812100 L
B-B_2	0	-10.26261300	0.28313400	-5.55823900 L
N-N_3	0	-10.28447700	1.81330400	-5.59524600 L
N-N_3	0	-11.57130000	-0.46331000	-5.81862100 L
B-	0	-12.83919700	0.37085600	-5.49698600 L
N-N_3	0	12.87154200	5.51508900	1.69089200 L
B-B_2	0	11.56974800	5.04931800	2.32002600 L

B-B_2	0	10.29623000	5.53648900	0.23199200 L
N-N_3	0	10.28825400	5.67342700	1.76567600 L
N-N_3	0	9.01823500	5.90358600	-0.53068700 L
B-B_2	0	7.73243300	5.53525100	0.21828600 L
B-B_2	0	6.44424700	5.18881600	-1.89449100 L
N-N_3	0	6.44410700	5.88351300	-0.53026600 L
N-N_3	0	5.15873900	5.23224800	-2.72203900 L
B-B_2	0	3.87331800	5.18981900	-1.89397300 L
B-B_2	0	2.58678700	4.07154700	-3.71468700 L
N-N_3	0	2.58826200	5.23617300	-2.72221600 L
N-N_3	0	1.30119300	3.79543400	-4.49587400 L
B-B_2	0	0.01635200	4.07447100	-3.71435700 L
B-B_2	0	-1.27041400	2.34125100	-4.96439000 L
N-N_3	0	-1.26917000	3.79769800	-4.49555700 L
N-N_3	0	-2.55565000	1.78717200	-5.58092600 L
B-B_2	0	-3.84099100	2.34351100	-4.96665500 L
B-B_2	0	-5.12775900	0.26429900	-5.46720100 L
N-N_3	0	-5.12528000	1.79023400	-5.58661300 L
N-N_3	0	-6.41038100	-0.48233800	-5.83560400 L
B-B_2	0	-7.70030600	0.26966900	-5.50106700 L
B-B_2	0	-8.98488900	-1.85461300	-5.18584500 L
N-N_3	0	-8.97477900	-0.48055000	-5.88863400 L
N-N_3	0	-10.28824800	-2.66528000	-5.20696000 L
B-B_2	0	-11.48650100	-1.73394400	-4.98659100 L
B-	0	-12.84267700	-3.62015300	-4.12235900 L
N-N_3	0	-12.60054000	-2.10649200	-4.00918300 L
B-	0	12.78274000	5.08945400	0.22447700 L
B-B_2	0	11.57100400	5.22197700	-1.90685900 L
N-N_3	0	11.62133100	5.81138500	-0.49881200 L
N-N_3	0	10.28879700	5.27062800	-2.73925900 L
B-B_2	0	9.01510500	5.21117900	-1.90040400 L
B-B_2	0	7.73098600	4.07752900	-3.72940900 L
N-N_3	0	7.72683200	5.23760000	-2.72530800 L
N-N_3	0	6.44139400	3.79254700	-4.50210200 L
B-B_2	0	5.15784400	4.06920500	-3.71685500 L
B-B_2	0	3.86995700	2.33649000	-4.96719800 L
N-N_3	0	3.87144700	3.79257800	-4.49662600 L
N-N_3	0	2.58383100	1.78280900	-5.58225900 L
B-B_2	0	1.29975200	2.33902000	-4.96505800 L
B-B_2	0	0.01268700	0.25963900	-5.45898400 L
N-N_3	0	0.01402300	1.78483600	-5.58033500 L
N-N_3	0	-1.27265400	-0.48644000	-5.81908200 L
B-B_2	0	-2.55716900	0.26189700	-5.46032700 L
B-B_2	0	-3.84405000	-1.85136200	-5.13543400 L

N-N_3	0	-3.84208200	-0.48412000	-5.82242600 L
N-N_3	0	-5.12891500	-2.67937400	-5.18841600 L
B-B_2	0	-6.41681300	-1.85426600	-5.15133700 L
B-B_2	0	-7.70404200	-3.69600900	-4.05480000 L
N-N_3	0	-7.69988700	-2.68819600	-5.21302800 L
N-N_3	0	-8.97897000	-4.49978500	-3.79865100 L
B-B_2	0	-10.26645100	-3.72508400	-4.10263800 L
B-B_2	0	-11.49059100	-4.74974800	-2.27377200 L
N-N_3	0	-11.57498400	-4.43786100	-3.76037000 L
N-N_3	0	-12.60611800	-4.32480300	-1.31964800 L
B-	0	12.78086000	3.76375700	-3.41516600 L
N-N_3	0	12.87208600	5.10292300	-2.68181200 L
N-N_3	0	11.61878900	3.76273600	-4.43629300 L
B-B_2	0	10.29473000	4.08698800	-3.72418400 L
B-B_2	0	9.01137500	2.34745800	-4.99815000 L
N-N_3	0	9.01552000	3.80620800	-4.52081300 L
N-N_3	0	7.72187900	1.78280000	-5.59763700 L
B-B_2	0	6.44065000	2.33570000	-4.97279100 L
B-B_2	0	5.15324500	0.25476200	-5.46904700 L
N-N_3	0	5.15386200	1.78084600	-5.58558400 L
N-N_3	0	3.86600300	-0.49109200	-5.82453700 L
B-B_2	0	2.58258100	0.25743300	-5.46213200 L
B-B_2	0	1.29545000	-1.85538500	-5.13199500 L
N-N_3	0	1.29643800	-0.48871700	-5.81988400 L
N-N_3	0	0.01007500	-2.68248400	-5.18402000 L
B-B_2	0	-1.27391800	-1.85330800	-5.13167600 L
B-B_2	0	-2.56024400	-3.68455200	-4.03059800 L
N-N_3	0	-2.55925400	-2.68003700	-5.18448200 L
N-N_3	0	-3.84694700	-4.46474800	-3.75821400 L
B-B_2	0	-5.13123600	-3.68022300	-4.03076500 L
B-B_2	0	-6.42024600	-4.95217000	-2.30922300 L
N-N_3	0	-6.41494200	-4.46665000	-3.76315000 L
N-N_3	0	-7.70309800	-5.58345200	-1.76060400 L
B-B_2	0	-8.98833700	-4.97510100	-2.33040200 L
N-N_3	0	-10.29135100	-5.56287200	-1.77084300 L
N-N_3	0	12.86749900	1.71778000	-5.47984700 L
B-B_2	0	11.56712200	2.34997200	-5.01409900 L
B-B_2	0	10.28983200	0.26279500	-5.49733800 L
N-N_3	0	10.28391900	1.79641400	-5.63577400 L
N-N_3	0	9.01005600	-0.49824900	-5.86188900 L
B-B_2	0	7.72619100	0.25224000	-5.48980800 L
B-B_2	0	6.43617400	-1.86078700	-5.14316900 L
N-N_3	0	6.43587500	-0.49474400	-5.83442100 L
N-N_3	0	5.14954600	-2.68680000	-5.18709600 L

B-B_2	0	3.86550600	-1.85751300	-5.13582500 L
B-B_2	0	2.57877000	-3.68761800	-4.02917800 L
N-N_3	0	2.57947300	-2.68424500	-5.18409900 L
N-N_3	0	1.29411800	-4.47354800	-3.76153300 L
B-B_2	0	0.00930600	-3.68928500	-4.03195100 L
B-B_2	0	-1.27666100	-4.95203800	-2.30893900 L
N-N_3	0	-1.27662100	-4.47176300	-3.76169500 L
N-N_3	0	-2.56323800	-5.56400300	-1.75288500 L
B-B_2	0	-3.84736200	-4.94381700	-2.30527300 L
N-N_3	0	-5.13252300	-5.56152700	-1.75208500 L
B-	0	12.77620400	0.25184600	-5.05318800 L
B-B_2	0	11.56263200	-1.87824700	-5.18724100 L
N-N_3	0	11.61349400	-0.46953500	-5.77473500 L
N-N_3	0	10.27964900	-2.70937300	-5.23635300 L
B-B_2	0	9.00688900	-1.86934600	-5.17205200 L
B-B_2	0	7.72300700	-3.70225000	-4.04312600 L
N-N_3	0	7.71765900	-2.69285800	-5.19854300 L
N-N_3	0	6.43360200	-4.47600200	-3.76034200 L
B-B_2	0	5.14993900	-3.68902400	-4.03064600 L
B-B_2	0	3.86343800	-4.94965800	-2.30489200 L
N-N_3	0	3.86389600	-4.47090200	-3.75793200 L
N-N_3	0	2.57866200	-5.56867100	-1.75268700 L
B-B_2	0	1.29318900	-4.95506100	-2.30918700 L
N-N_3	0	0.00750200	-5.56907100	-1.75372200 L
B-	0	12.77333900	-3.39190600	-3.73519400 L
N-N_3	0	12.86324100	-2.65462400	-5.07223100 L
N-N_3	0	11.61070900	-4.41230700	-3.73587800 L
B-B_2	0	10.28665900	-3.69830900	-4.05610000 L
B-B_2	0	9.00478200	-4.97740300	-2.31957500 L
N-N_3	0	9.00750000	-4.49531600	-3.77669600 L
N-N_3	0	7.71598800	-5.57842100	-1.75528800 L
B-B_2	0	6.43424300	-4.95271400	-2.30564700 L
N-N_3	0	5.14832500	-5.56769200	-1.75155100 L
N-N_3	0	12.86120300	-5.46243800	-1.69508200 L
B-B_2	0	11.56050800	-4.99441400	-2.32482600 L
N-N_3	0	10.27767100	-5.61628800	-1.77099900 L
H-H_	0	-12.26100600	-3.00779000	1.92277100 L
H-H_	0	-12.25634100	-0.73756500	3.50636900 L
H-H_	0	-12.26270100	1.99521900	3.03548300 L
H-H_	0	-12.26266600	3.58679500	0.78183300 L
H-H_	0	12.88015100	-5.81878600	3.38937000 L
H-H_	0	12.88576900	-1.70554100	6.51721100 L
H-H_	0	-12.25605300	3.10521400	-1.93139800 L
H-H_	0	-12.25635600	0.83560400	-3.51612100 L

H-H_	0	12.88875800	3.41580200	5.83547600 L
H-H_	0	12.89282000	6.55938600	1.73129400 L
H-H_	0	-12.26257000	-1.89428800	-3.04320500 L
H-H_	0	-12.27114200	-3.48949700	-0.78824500 L
H-H_	0	12.89402700	5.86853300	-3.39314900 L
H-H_	0	12.88851600	1.75745800	-6.52417700 L
H-H_	0	12.88362700	-3.36363800	-5.84003600 L
H-H_	0	12.88082400	-6.50675500	-1.73578700 L
C-C_R	0	-0.27675700	-1.53320300	0.28410800 H
H-H_	0	0.92167800	-0.10734500	1.41827700 H
H-H_	0	1.34246900	-1.80315700	1.71883500 H
C-C_3	0	0.50433900	-1.12742500	1.48393800 H
H-H_	0	-0.16637000	-1.13654200	2.34610800 H
N-N_R	0	0.36833200	-1.53337000	-1.04906400 H
H-H_	0	-0.48572500	-1.78922600	-1.63491000 H
H-H_	0	0.73740400	-0.62470900	-1.35404600 H
C-C_R	0	-1.62280400	-1.78338500	0.08407800 H
O-O_R	0	-2.11628400	-2.00723400	-1.06961800 H
O-O_R	0	-2.44490000	-1.79255300	1.17965300 H
H-H_	0	-3.32194200	-2.02169400	0.83685000 H
H-H_	0	1.11185200	-2.22753700	-1.16700800 H

Coordinates of all stationary points in the pathway b of α -Ala chiral transformation confined in SWBNNT(6,6)

bSTS1@B

B-B_2	0	-10.32232300	0.21766400	-4.13830000 L
N-N_3	0	-11.59682100	-0.54245600	-4.47855000 L
B-	0	-12.87667700	0.32349800	-4.36070700 L
B-B_2	0	-5.18384600	0.21118800	-3.93316700 L
N-N_3	0	-6.45942200	-0.54092100	-4.31338100 L
B-B_2	0	-7.75557000	0.21091000	-4.00429700 L
B-B_2	0	-9.05094400	-1.87079900	-3.61331800 L
N-N_3	0	-9.02130200	-0.54494100	-4.39893400 L
N-N_3	0	-10.35734100	-2.68162800	-3.55350400 L
B-B_2	0	-11.59141100	-1.75894400	-3.55703500 L
B-	0	-12.90839400	-3.57260200	-2.44845200 L
N-N_3	0	-12.79489500	-2.05464500	-2.66306900 L
B-B_2	0	-0.04869500	0.21560800	-3.84033000 L
N-N_3	0	-1.32601100	-0.53832300	-4.20620800 L
B-B_2	0	-2.61454100	0.21281100	-3.87424700 L
B-B_2	0	-3.90224600	-1.87861100	-3.50998400 L
N-N_3	0	-3.89014800	-0.53942200	-4.25401100 L
N-N_3	0	-5.19017400	-2.70232200	-3.48844300 L
B-B_2	0	-6.47582300	-1.87423400	-3.55720500 L
B-B_2	0	-7.77880400	-3.48409900	-2.20602700 L
N-N_3	0	-7.76550300	-2.70055600	-3.52297400 L
N-N_3	0	-9.06443700	-4.16933800	-1.75024300 L
B-B_2	0	-10.34910000	-3.51989600	-2.26768200 L
B-B_2	0	-11.62128600	-3.96855500	-0.25647900 L
N-N_3	0	-11.64215700	-4.15496600	-1.77176900 L
N-N_3	0	-12.82214300	-3.35085600	0.46087400 L
B-B_2	0	5.08473100	0.20971000	-3.88361600 L
N-N_3	0	3.79283100	-0.53957200	-4.21107500 L
B-B_2	0	2.51607500	0.21415800	-3.84261600 L
B-B_2	0	1.23204700	-1.89291900	-3.46745600 L
N-N_3	0	1.23282700	-0.53796800	-4.18945600 L
N-N_3	0	-0.05052300	-2.72733200	-3.45827400 L
B-B_2	0	-1.33257400	-1.89027600	-3.47994900 L
B-B_2	0	-2.62927600	-3.54950600	-2.17940800 L
N-N_3	0	-2.61932000	-2.71294100	-3.46307400 L
N-N_3	0	-3.92897900	-4.21840300	-1.73040700 L
B-B_2	0	-5.20469900	-3.50661400	-2.18645900 L
B-B_2	0	-6.50727100	-4.18906200	-0.20165700 L
N-N_3	0	-6.50099800	-4.17823700	-1.73333700 L
N-N_3	0	-7.80296200	-4.50746100	0.55141300 L

B-B_2	0	-9.08399000	-4.15099200	-0.20954600 L
B-B_2	0	-10.35836900	-3.74954500	1.89769000 L
N-N_3	0	-10.39423100	-4.45839800	0.53596500 L
N-N_3	0	-11.63868500	-3.61569300	2.71239600 L
B-	0	-12.91646500	-3.91445700	1.88846900 L
B-B_2	0	10.22884300	0.20695900	-3.97698000 L
N-N_3	0	8.93924600	-0.55094500	-4.31956700 L
B-B_2	0	7.65785500	0.20341100	-3.94272200 L
B-B_2	0	6.36856400	-1.87917400	-3.51054300 L
N-N_3	0	6.36066800	-0.54460400	-4.26174300 L
N-N_3	0	5.08378800	-2.70940100	-3.46170200 L
B-B_2	0	3.79902000	-1.88360400	-3.47450600 L
B-B_2	0	2.51761900	-3.57900700	-2.17389600 L
N-N_3	0	2.51654400	-2.71840100	-3.44429100 L
N-N_3	0	1.23694400	-4.30916700	-1.74981500 L
B-B_2	0	-0.05383400	-3.61486100	-2.20149100 L
B-B_2	0	-1.34934500	-4.31021000	-0.20234000 L
N-N_3	0	-1.35384200	-4.27598800	-1.73703400 L
N-N_3	0	-2.64909400	-4.60053600	0.55459500 L
B-B_2	0	-3.93002000	-4.23858800	-0.20045600 L
B-B_2	0	-5.21329500	-3.73006100	1.84546700 L
N-N_3	0	-5.22577300	-4.54840200	0.55262600 L
N-N_3	0	-6.49625000	-3.60891500	2.66891900 L
B-B_2	0	-7.78793000	-3.70532500	1.85695500 L
B-B_2	0	-9.06175100	-2.24756900	3.41025300 L
N-N_3	0	-9.05977800	-3.61312700	2.69532200 L
N-N_3	0	-10.35592700	-1.75419300	4.07915500 L
B-B_2	0	-11.60058000	-2.20161200	3.28871600 L
B-	0	-12.87999100	-0.32589200	4.35801800 L
N-N_3	0	-12.81569200	-1.28283500	3.15532800 L
B-	0	12.75432900	0.19351500	-3.63564800 L
B-B_2	0	11.50277400	-1.92666200	-3.66792200 L
N-N_3	0	11.54593400	-0.52757700	-4.28990100 L
N-N_3	0	10.20933200	-2.72858200	-3.54808200 L
B-B_2	0	8.93954800	-1.88617400	-3.56647400 L
B-B_2	0	7.67002100	-3.52575400	-2.19635500 L
N-N_3	0	7.65170600	-2.70781500	-3.49301000 L
N-N_3	0	6.38912400	-4.22580700	-1.73537600 L
B-B_2	0	5.09384600	-3.54423800	-2.17829800 L
B-B_2	0	3.81421100	-4.30515600	-0.20190900 L
N-N_3	0	3.81406700	-4.25893800	-1.73256900 L
N-N_3	0	2.53414500	-4.66547000	0.55857300 L
B-B_2	0	1.23282800	-4.40768800	-0.21233500 L
B-B_2	0	-0.05917200	-3.85176400	1.85738900 L

N-N_3	0	-0.06923900	-4.67913800	0.55690200 L
N-N_3	0	-1.34994600	-3.66719800	2.66368000 L
B-B_2	0	-2.63650100	-3.77435800	1.84435800 L
B-B_2	0	-3.91150100	-2.25537000	3.33248300 L
N-N_3	0	-3.92392400	-3.63140900	2.66061500 L
N-N_3	0	-5.18773100	-1.74723900	4.00737200 L
B-B_2	0	-6.48609200	-2.24654600	3.37080700 L
B-B_2	0	-7.75861000	-0.21546100	4.00984900 L
N-N_3	0	-7.76354200	-1.74800500	4.05440000 L
N-N_3	0	-9.02444000	0.54131400	4.40225900 L
B-B_2	0	-10.32530300	-0.22098500	4.14052200 L
B-B_2	0	-11.59293300	1.75651900	3.55774900 L
N-N_3	0	-11.60009000	0.53964600	4.47888500 L
N-N_3	0	-12.79753000	2.05585600	2.66643800 L
B-	0	12.77777000	-3.18292800	-2.04982400 L
N-N_3	0	12.78997400	-2.71206900	-3.50795000 L
N-N_3	0	11.57237500	-4.11261900	-1.74351200 L
B-B_2	0	10.24258400	-3.49091400	-2.21260500 L
B-B_2	0	8.96523900	-4.21198600	-0.21209400 L
N-N_3	0	8.96888300	-4.20365600	-1.74339800 L
N-N_3	0	7.68390200	-4.55290800	0.54633200 L
B-B_2	0	6.39174900	-4.23945600	-0.20599300 L
B-B_2	0	5.10311600	-3.76110200	1.83314600 L
N-N_3	0	5.11337900	-4.59792300	0.55184100 L
N-N_3	0	3.81298300	-3.64230100	2.64396800 L
B-B_2	0	2.52307200	-3.80714900	1.83290500 L
B-B_2	0	1.23287100	-2.27180000	3.28862200 L
N-N_3	0	1.23771700	-3.67300800	2.65276800 L
N-N_3	0	-0.04867000	-1.75452500	3.94221000 L
B-B_2	0	-1.33804700	-2.27171700	3.30604700 L
B-B_2	0	-2.61665500	-0.21843900	3.89702000 L
N-N_3	0	-2.61620900	-1.74977100	3.96705300 L
N-N_3	0	-3.89484800	0.53384600	4.26759000 L
B-B_2	0	-5.18691000	-0.21714100	3.94446300 L
B-B_2	0	-6.47784600	1.86770300	3.56035200 L
N-N_3	0	-6.46308400	0.53619000	4.31993300 L
N-N_3	0	-7.76635200	2.69558100	3.52553700 L
B-B_2	0	-9.05260300	1.86681200	3.61579300 L
B-B_2	0	-10.34889300	3.51768100	2.27049200 L
N-N_3	0	-10.35832800	2.67857100	3.55570500 L
N-N_3	0	-11.64123400	4.15406100	1.77459600 L
B-	0	-12.90817500	3.57405200	2.45188600 L
N-N_3	0	12.82247400	-4.45801500	0.55624800 L
B-B_2	0	11.53256800	-4.26882300	-0.21866800 L

B-B_2	0	10.25422400	-3.69980300	1.82749400 L
N-N_3	0	10.24179600	-4.55084100	0.54611100 L
N-N_3	0	8.97072400	-3.60916000	2.66316600 L
B-B_2	0	7.68056300	-3.73388000	1.84218200 L
B-B_2	0	6.37789900	-2.24518200	3.32034800 L
N-N_3	0	6.38875800	-3.62363700	2.65428100 L
N-N_3	0	5.08327700	-1.74211100	3.95919300 L
B-B_2	0	3.80474600	-2.25308800	3.29075500 L
B-B_2	0	2.51406600	-0.21296200	3.87663500 L
N-N_3	0	2.51606400	-1.74621100	3.93485400 L
N-N_3	0	1.23214000	0.53586100	4.23849500 L
B-B_2	0	-0.04978300	-0.21868300	3.88484300 L
B-B_2	0	-1.33422500	1.87730900	3.49381700 L
N-N_3	0	-1.33109200	0.53428300	4.23610100 L
N-N_3	0	-2.62172900	2.69949300	3.46433800 L
B-B_2	0	-3.90515100	1.86785600	3.51491500 L
B-B_2	0	-5.20394800	3.49781700	2.18749500 L
N-N_3	0	-5.19125700	2.69404200	3.49019200 L
N-N_3	0	-6.49937400	4.17316800	1.73689500 L
B-B_2	0	-7.77836100	3.47975500	2.20884700 L
B-B_2	0	-9.08302700	4.14895200	0.21299400 L
N-N_3	0	-9.06352800	4.16639900	1.75361100 L
N-N_3	0	-10.39315300	4.45602100	-0.53298600 L
B-B_2	0	-11.62048900	3.96707000	0.25945100 L
B-	0	-12.91507700	3.90872400	-1.88499000 L
N-N_3	0	-12.81948900	3.34529500	-0.45742900 L
B-	0	12.78400700	-3.37559400	1.64197300 L
B-B_2	0	11.51635500	-2.26735700	3.44163300 L
N-N_3	0	11.57637800	-3.54951800	2.60350600 L
N-N_3	0	10.21489300	-1.75224100	4.05688300 L
B-B_2	0	8.95119800	-2.24454700	3.36079700 L
B-B_2	0	7.65709600	-0.20888700	3.95601700 L
N-N_3	0	7.65390400	-1.74250500	3.99716800 L
N-N_3	0	6.36186800	0.53980300	4.27916900 L
B-B_2	0	5.08368000	-0.21137800	3.90331400 L
B-B_2	0	3.79895100	1.87947300	3.50091700 L
N-N_3	0	3.79421300	0.53748900	4.24043600 L
N-N_3	0	2.51835700	2.71635500	3.47032000 L
B-B_2	0	1.23099800	1.89424900	3.51870800 L
B-B_2	0	-0.05532800	3.57405400	2.19845100 L
N-N_3	0	-0.05630800	2.71895600	3.47593600 L
N-N_3	0	-1.35043300	4.25293200	1.73939600 L
B-B_2	0	-2.62903100	3.53007600	2.17682600 L
B-B_2	0	-3.92789500	4.24168300	0.20271300 L

N-N_3	0	-3.92601400	4.20811900	1.73282400 L
N-N_3	0	-5.22514900	4.54989400	-0.54860800 L
B-B_2	0	-6.50605700	4.18826200	0.20537400 L
B-B_2	0	-7.78672700	3.70322200	-1.85263100 L
N-N_3	0	-7.80212000	4.50595200	-0.54750700 L
N-N_3	0	-9.05813800	3.60977600	-2.69142500 L
B-B_2	0	-10.35693400	3.74624300	-1.89428300 L
B-B_2	0	-11.59815500	2.19770800	-3.28614000 L
N-N_3	0	-11.63707700	3.61163300	-2.70926100 L
N-N_3	0	-12.81504000	1.28050600	-3.15789900 L
B-	0	12.75413800	-0.20330300	3.64800800 L
N-N_3	0	12.79817100	-1.69111500	4.01287700 L
N-N_3	0	11.54564900	0.51954700	4.30007400 L
B-B_2	0	10.22807000	-0.21450200	3.98788800 L
B-B_2	0	8.94010100	1.87875700	3.57674500 L
N-N_3	0	8.93957100	0.54425600	4.33117600 L
N-N_3	0	7.65280300	2.70089200	3.50297200 L
B-B_2	0	6.36954300	1.87286300	3.52582000 L
B-B_2	0	5.09374700	3.52669600	2.18440000 L
N-N_3	0	5.08551000	2.70307800	3.47515700 L
N-N_3	0	3.81175300	4.23522100	1.73638600 L
B-B_2	0	2.51851100	3.54768300	2.18037400 L
B-B_2	0	1.23509200	4.34068400	0.20538000 L
N-N_3	0	1.23610400	4.26277900	1.74231700 L
N-N_3	0	-0.05963800	4.66699700	-0.55311000 L
B-B_2	0	-1.34828500	4.31700800	0.20416500 L
B-B_2	0	-2.63509800	3.78234600	-1.84258800 L
N-N_3	0	-2.64770700	4.60919100	-0.55232800 L
N-N_3	0	-3.92363600	3.63171300	-2.65600700 L
B-B_2	0	-5.21235900	3.73099000	-1.84091300 L
B-B_2	0	-6.48408400	2.24216800	-3.36260500 L
N-N_3	0	-6.49510200	3.60633900	-2.66403600 L
N-N_3	0	-7.76037900	1.74356700	-4.04800600 L
B-B_2	0	-9.05936400	2.24369300	-3.40552300 L
N-N_3	0	-10.35284200	1.75078900	-4.07593700 L
N-N_3	0	12.79063200	2.70222100	3.51454400 L
B-B_2	0	11.50308300	1.91760800	3.67552500 L
B-B_2	0	10.24253000	3.48266700	2.22077900 L
N-N_3	0	10.21009500	2.72054200	3.55653200 L
N-N_3	0	8.96808900	4.19466700	1.75126500 L
B-B_2	0	7.66985300	3.51492700	2.20361900 L
B-B_2	0	6.39089700	4.22886700	0.21113400 L
N-N_3	0	6.38733900	4.21190600	1.74087300 L
N-N_3	0	5.11266200	4.59124700	-0.54622200 L

B-B_2	0	3.81409600	4.28816300	0.20489700 L
B-B_2	0	2.52481700	3.82292700	-1.84939800 L
N-N_3	0	2.53152000	4.64552300	-0.55269600 L
N-N_3	0	1.23897500	3.68721400	-2.66763600 L
B-B_2	0	-0.05584300	3.86428300	-1.86804300 L
B-B_2	0	-1.33773100	2.27354000	-3.29591800 L
N-N_3	0	-1.35061300	3.67416200	-2.66523200 L
N-N_3	0	-2.61494400	1.74415100	-3.95210500 L
B-B_2	0	-3.91022600	2.25214300	-3.32096300 L
N-N_3	0	-5.18496200	1.74160500	-3.99640100 L
B-	0	12.77721400	3.17420400	2.05679900 L
B-B_2	0	11.53276700	4.26417900	0.22793200 L
N-N_3	0	11.57221100	4.10508600	1.75240800 L
N-N_3	0	10.24202300	4.54498400	-0.53719300 L
B-B_2	0	8.96510000	4.20459600	0.21997400 L
B-B_2	0	7.68230000	3.73101000	-1.83695300 L
N-N_3	0	7.68382400	4.54603700	-0.53869700 L
N-N_3	0	6.39285700	3.62455400	-2.65237200 L
B-B_2	0	5.10460100	3.76686200	-1.83655400 L
B-B_2	0	3.80782600	2.26269500	-3.29595000 L
N-N_3	0	3.81790400	3.65507600	-2.65415400 L
N-N_3	0	2.51741900	1.74609600	-3.92917100 L
B-B_2	0	1.23522300	2.28027800	-3.28816400 L
N-N_3	0	-0.04846200	1.74946400	-3.92595500 L
B-	0	12.78597100	3.37072200	-1.63126000 L
N-N_3	0	12.82285400	4.45419100	-0.54651500 L
N-N_3	0	11.57860200	3.54265200	-2.59341900 L
B-B_2	0	10.25589200	3.69413300	-1.81854300 L
B-B_2	0	8.95358700	2.23897500	-3.35178700 L
N-N_3	0	8.97363300	3.60432100	-2.65556800 L
N-N_3	0	7.65664500	1.73707300	-3.98861900 L
B-B_2	0	6.38049200	2.24478500	-3.31620100 L
N-N_3	0	5.08659800	1.74040100	-3.95496300 L
N-N_3	0	12.80045700	1.68158400	-3.99920300 L
B-B_2	0	11.51853100	2.25897200	-3.42937300 L
N-N_3	0	10.21732900	1.74480800	-4.04617400 L
H-H_	0	-12.61475100	-1.60353000	-1.73945200 L
H-H_	0	-12.65197600	-2.32323200	0.52515200 L
H-H_	0	-12.68283900	-0.71418200	2.29055100 L
H-H_	0	-12.62086700	1.60407600	1.74251100 L
H-H_	0	12.73207700	-3.55454400	-4.12392100 L
H-H_	0	12.78161300	-5.39106100	1.02555900 L
H-H_	0	-12.64575000	2.31825600	-0.52196200 L
H-H_	0	-12.68676200	0.71190300	-2.29243100 L

H-H_	0	12.75216100	-1.77408700	5.05380000 L
H-H_	0	12.73408000	3.54425900	4.13123500 L
H-H_	0	12.78113800	5.38674800	-1.01672200 L
H-H_	0	12.75606600	1.76548300	-5.04012100 L
C-C_3	0	0.92199600	0.18238200	0.25331900 H
H-H_	0	0.00126500	-1.24689100	-0.99467100 H
H-H_	0	-0.62370000	-1.24544500	0.65613600 H
C-C_3	0	0.28116900	-1.15866600	0.05091300 H
H-H_	0	0.99663400	-1.91792200	0.30722100 H
N-N_3	0	0.12727800	1.15448300	-0.46890400 H
H-H_	0	0.00883200	1.98113000	0.08002500 H
H-H_	0	-0.79855000	0.78278700	-0.64977200 H
C-C_R	0	2.40577500	0.25509200	-0.12278500 H
O-O_R	0	3.04167900	1.27897200	-0.21277600 H
O-O_R	0	2.99845900	-0.96140200	-0.24002900 H
H-H_	0	3.94285400	-0.79523900	-0.40332600 H
H-H_	0	0.94807600	0.38988700	1.32594100 H

bSINT1@B

B-B_2	0	-10.25063700	1.56910600	3.85681300 L
N-N_3	0	-11.53261300	2.39042700	3.83872100 L
B-	0	-12.80671300	1.54210100	4.08055200 L
B-B_2	0	-5.11033400	1.53846300	3.71735000 L
N-N_3	0	-6.39413900	2.36730600	3.74077500 L
B-B_2	0	-7.68279800	1.54325100	3.75329700 L
B-B_2	0	-8.98222400	3.25874500	2.52196600 L
N-N_3	0	-8.95654100	2.38267000	3.78958800 L
N-N_3	0	-10.29143900	3.95593100	2.11176900 L
B-B_2	0	-11.52291600	3.11155700	2.49345800 L
B-	0	-12.83083800	4.29519300	0.71615600 L
N-N_3	0	-12.72783000	3.01307100	1.55803300 L
B-B_2	0	0.03218900	1.54639600	3.72707700 L
N-N_3	0	-1.25480600	2.37146100	3.71812000 L
B-B_2	0	-2.53841900	1.53941400	3.71370200 L
B-B_2	0	-3.82885200	3.26238100	2.47865700 L
N-N_3	0	-3.82441700	2.36692000	3.72209300 L
N-N_3	0	-5.11931600	3.98426200	2.08549300 L
B-B_2	0	-6.40512300	3.26066200	2.49582500 L
B-B_2	0	-7.70041900	4.11181800	0.57093900 L
N-N_3	0	-7.69803800	3.98032700	2.09727000 L
N-N_3	0	-8.98176900	4.52706200	-0.14748500 L
B-B_2	0	-10.27193500	4.16745700	0.59150200 L
B-B_2	0	-11.53075700	3.70409100	-1.42520100 L

N-N_3	0	-11.55990100	4.52652800	-0.13874200 L
N-N_3	0	-12.73148100	2.84275100	-1.81827500 L
B-B_2	0	5.17132600	1.53233100	3.70270200 L
N-N_3	0	3.88524100	2.36037900	3.70810800 L
B-B_2	0	2.59990800	1.53455200	3.68924700 L
B-B_2	0	1.31486800	3.27205100	2.46925900 L
N-N_3	0	1.31961000	2.37022700	3.71233200 L
N-N_3	0	0.02933000	4.01105200	2.08478200 L
B-B_2	0	-1.25397800	3.26808200	2.46979700 L
B-B_2	0	-2.54659800	4.17178000	0.55295700 L
N-N_3	0	-2.54341800	3.99179200	2.07617500 L
N-N_3	0	-3.84487300	4.56148800	-0.15669700 L
B-B_2	0	-5.12430600	4.12764100	0.56192700 L
B-B_2	0	-6.41742600	3.85370600	-1.52710600 L
N-N_3	0	-6.41763700	4.52542900	-0.15075700 L
N-N_3	0	-7.70602900	3.82055100	-2.35480700 L
B-B_2	0	-8.99342000	3.83718000	-1.52533900 L
B-B_2	0	-10.26096300	2.57965300	-3.27019600 L
N-N_3	0	-10.29655500	3.80217900	-2.34179700 L
N-N_3	0	-11.53869900	2.12853300	-3.96611600 L
B-	0	-12.81851400	2.74980200	-3.35102900 L
B-B_2	0	10.31679500	1.52593700	3.75145700 L
N-N_3	0	9.03440700	2.36757300	3.75400100 L
B-B_2	0	7.74508500	1.53721600	3.73352300 L
B-B_2	0	6.46150500	3.25154100	2.48202600 L
N-N_3	0	6.45570100	2.36209500	3.72807100 L
N-N_3	0	5.17874500	3.98273300	2.07918000 L
B-B_2	0	3.88851700	3.26064400	2.46928400 L
B-B_2	0	2.60487400	4.17061800	0.55199000 L
N-N_3	0	2.60392600	3.99549800	2.07439600 L
N-N_3	0	1.32537300	4.61472300	-0.16367300 L
B-B_2	0	0.02851100	4.24362400	0.56329400 L
B-B_2	0	-1.26361100	3.97867500	-1.55860400 L
N-N_3	0	-1.26902900	4.62625900	-0.16128500 L
N-N_3	0	-2.55907700	3.88456800	-2.36977100 L
B-B_2	0	-3.84028300	3.89443400	-1.53471100 L
B-B_2	0	-5.12017400	2.54039400	-3.16108400 L
N-N_3	0	-5.13174600	3.84026200	-2.35343300 L
N-N_3	0	-6.39765500	2.09999900	-3.87644500 L
B-B_2	0	-7.69272000	2.53553500	-3.19035300 L
B-B_2	0	-8.97170200	0.57513600	-4.02066900 L
N-N_3	0	-8.96011600	2.11398100	-3.92843300 L
N-N_3	0	-10.26928000	-0.13976000	-4.43458200 L
B-B_2	0	-11.51078700	0.60305000	-3.90424200 L

B-	0	-12.80509200	-1.53646500	-4.08805700 L
N-N_3	0	-12.72595000	-0.16862500	-3.38961100 L
B-	0	12.84736800	1.38100700	3.44366600 L
B-B_2	0	11.59929700	3.31465600	2.56339900 L
N-N_3	0	11.63963100	2.31503900	3.72414700 L
N-N_3	0	10.30821100	3.99168100	2.10988200 L
B-B_2	0	9.03405500	3.25556200	2.50510600 L
B-B_2	0	7.75965400	4.11757500	0.56112400 L
N-N_3	0	7.74972000	3.97214000	2.08728500 L
N-N_3	0	6.47556500	4.53545700	-0.15847400 L
B-B_2	0	5.18293800	4.13603500	0.55647200 L
B-B_2	0	3.89571600	3.88687300	-1.53449800 L
N-N_3	0	3.90065700	4.56247000	-0.16104900 L
N-N_3	0	2.61084600	3.87271000	-2.36389000 L
B-B_2	0	1.31712100	3.94273200	-1.54627100 L
B-B_2	0	0.02784800	2.60190000	-3.18606900 L
N-N_3	0	0.03063600	3.91314600	-2.37854800 L
N-N_3	0	-1.26201300	2.12200200	-3.85326100 L
B-B_2	0	-2.54597900	2.56576800	-3.15392100 L
B-B_2	0	-3.82412400	0.57396000	-3.92150000 L
N-N_3	0	-3.82849100	2.10438800	-3.85073000 L
N-N_3	0	-5.10144300	-0.14745200	-4.35452900 L
B-B_2	0	-6.39688800	0.56991100	-3.96822900 L
B-B_2	0	-7.68041400	-1.53879300	-3.75508100 L
N-N_3	0	-7.67656900	-0.15035700	-4.40475800 L
N-N_3	0	-8.95514300	-2.37716300	-3.79544900 L
B-B_2	0	-10.24892300	-1.56326900	-3.86165800 L
B-B_2	0	-11.52284300	-3.10621900	-2.50026300 L
N-N_3	0	-11.53117400	-2.38447200	-3.84514600 L
N-N_3	0	-12.72726800	-3.00643500	-1.56425900 L
B-	0	12.86421100	3.71920800	0.54836200 L
N-N_3	0	12.88896500	3.93792300	2.06526000 L
N-N_3	0	11.65981800	4.42938000	-0.12743600 L
B-B_2	0	10.33265900	4.08316900	0.57456500 L
B-B_2	0	9.04395600	3.84762800	-1.53348600 L
N-N_3	0	9.05571000	4.51693200	-0.15542600 L
N-N_3	0	7.75594600	3.82721700	-2.35617700 L
B-B_2	0	6.47066000	3.85613500	-1.52974300 L
B-B_2	0	5.17755200	2.55201700	-3.17779700 L
N-N_3	0	5.18524000	3.84460100	-2.35737400 L
N-N_3	0	3.88572200	2.11423000	-3.86842800 L
B-B_2	0	2.60172000	2.56818000	-3.16912800 L
B-B_2	0	1.31341200	0.59221100	-3.92365300 L
N-N_3	0	1.31537400	2.12787600	-3.86763600 L

N-N_3	0	0.02727300	-0.13644000	-4.31039600 L
B-B_2	0	-1.25566100	0.58622100	-3.90264500 L
B-B_2	0	-2.53650500	-1.54113700	-3.69284000 L
N-N_3	0	-2.53421500	-0.14145000	-4.32052400 L
N-N_3	0	-3.82157600	-2.36887900	-3.72811300 L
B-B_2	0	-5.10694000	-1.53773600	-3.71205100 L
B-B_2	0	-6.40565100	-3.26769300	-2.50934400 L
N-N_3	0	-6.39227600	-2.36420300	-3.74666900 L
N-N_3	0	-7.70055700	-3.98095900	-2.10727600 L
B-B_2	0	-8.98251900	-3.25618500	-2.53011800 L
B-B_2	0	-10.27185900	-4.16140500	-0.59806800 L
N-N_3	0	-10.29228100	-3.95136800	-2.11872600 L
N-N_3	0	-11.55926100	-4.51989800	0.13311500 L
B-	0	-12.83054000	-4.28808200	-0.72142200 L
N-N_3	0	12.89654500	3.75402400	-2.35632900 L
B-B_2	0	11.61032500	3.90207200	-1.56616500 L
B-B_2	0	10.32616000	2.53681000	-3.19143600 L
N-N_3	0	10.31500800	3.84013000	-2.37345700 L
N-N_3	0	9.03976000	2.10942900	-3.91009700 L
B-B_2	0	7.75337000	2.54427800	-3.19639400 L
B-B_2	0	6.45552000	0.58042700	-3.96303400 L
N-N_3	0	6.45932900	2.10986800	-3.88826200 L
N-N_3	0	5.16412200	-0.13989600	-4.35416000 L
B-B_2	0	3.88356700	0.58373700	-3.93418400 L
B-B_2	0	2.59790300	-1.52442900	-3.67114500 L
N-N_3	0	2.59494000	-0.13821500	-4.32740100 L
N-N_3	0	1.31620400	-2.35859700	-3.69887000 L
B-B_2	0	0.03043900	-1.53207800	-3.66870700 L
B-B_2	0	-1.25322200	-3.31601300	-2.50122900 L
N-N_3	0	-1.24931800	-2.36822800	-3.71029700 L
N-N_3	0	-2.54727000	-4.03025900	-2.10596900 L
B-B_2	0	-3.82884800	-3.28981300	-2.50294900 L
B-B_2	0	-5.12597100	-4.12978800	-0.57854200 L
N-N_3	0	-5.12391300	-3.99910500	-2.10332200 L
N-N_3	0	-6.41795100	-4.51622400	0.14219200 L
B-B_2	0	-7.70111300	-4.10693200	-0.58043400 L
B-B_2	0	-8.99120300	-3.82631600	1.51750200 L
N-N_3	0	-8.98119200	-4.51941100	0.14100200 L
N-N_3	0	-10.29381300	-3.79391300	2.33517800 L
B-B_2	0	-11.52908200	-3.69695000	1.41928400 L
B-	0	-12.81734900	-2.74533800	3.34589300 L
N-N_3	0	-12.73058400	-2.83717800	1.81320900 L
B-	0	12.85438600	2.32214800	-2.90264800 L
B-B_2	0	11.59231600	0.58233500	-4.10674500 L

N-N_3	0	11.64577900	2.09232600	-3.85004300 L
N-N_3	0	10.29326100	-0.14473300	-4.45036600 L
B-B_2	0	9.02792200	0.57977200	-4.00707000 L
B-B_2	0	7.74418100	-1.52998300	-3.73658100 L
N-N_3	0	7.73407900	-0.14138900	-4.38827200 L
N-N_3	0	6.45444400	-2.35478500	-3.72959700 L
B-B_2	0	5.16962400	-1.52488100	-3.69995600 L
B-B_2	0	3.88988300	-3.26713400	-2.47646900 L
N-N_3	0	3.88239200	-2.35240200	-3.70491700 L
N-N_3	0	2.61186600	-4.01561300	-2.08953900 L
B-B_2	0	1.31785400	-3.30835500	-2.49198500 L
B-B_2	0	0.03017100	-4.25758100	-0.58429600 L
N-N_3	0	0.03314100	-4.05264200	-2.11040100 L
N-N_3	0	-1.26828800	-4.60837100	0.14941100 L
B-B_2	0	-2.54862000	-4.18928600	-0.58000900 L
B-B_2	0	-3.83848500	-3.84969700	1.50503600 L
N-N_3	0	-3.84647300	-4.55271400	0.14439900 L
N-N_3	0	-5.12439100	-3.81052700	2.33417600 L
B-B_2	0	-6.41479300	-3.83208200	1.51303700 L
B-B_2	0	-7.69068300	-2.52418700	3.18536700 L
N-N_3	0	-7.70139000	-3.80593800	2.34496500 L
N-N_3	0	-8.95956800	-2.10703100	3.92410900 L
B-B_2	0	-10.25968500	-2.57237900	3.26456900 L
B-B_2	0	-11.51190200	-0.59748400	3.89950600 L
N-N_3	0	-11.53810900	-2.12298400	3.96068300 L
N-N_3	0	-12.72663000	0.17370400	3.38298000 L
B-	0	12.84845100	-1.37305500	-3.45454300 L
N-N_3	0	12.87543000	-0.16983300	-4.40329900 L
N-N_3	0	11.63943300	-2.30727000	-3.72961000 L
B-B_2	0	10.31638700	-1.51834500	-3.75724500 L
B-B_2	0	9.03504200	-3.24691400	-2.50787100 L
N-N_3	0	9.03397800	-2.36008700	-3.75751600 L
N-N_3	0	7.75183500	-3.96535300	-2.09099300 L
B-B_2	0	6.46274500	-3.24639600	-2.48533800 L
B-B_2	0	5.18507500	-4.13589400	-0.56244700 L
N-N_3	0	5.18287000	-3.98230500	-2.08532900 L
N-N_3	0	3.90247100	-4.56175200	0.15522500 L
B-B_2	0	2.60754500	-4.17969600	-0.56498300 L
B-B_2	0	1.31746900	-3.92873600	1.52863200 L
N-N_3	0	1.32652300	-4.61725200	0.15271800 L
N-N_3	0	0.02239900	-3.86128500	2.34485000 L
B-B_2	0	-1.26124200	-3.89292200	1.51003100 L
B-B_2	0	-2.54350200	-2.52919800	3.14890600 L
N-N_3	0	-2.55187300	-3.82660100	2.33102800 L

N-N_3	0	-3.82693500	-2.09190600	3.85722200 L
B-B_2	0	-5.11692100	-2.51967600	3.15690500 L
B-B_2	0	-6.39864000	-0.56230300	3.97904800 L
N-N_3	0	-6.39669100	-2.09115000	3.87551300 L
N-N_3	0	-7.68067400	0.15724100	4.40815200 L
B-B_2	0	-8.97326800	-0.56860600	4.01981600 L
N-N_3	0	-10.27171500	0.14592800	4.43109300 L
N-N_3	0	12.89066800	-3.92327800	-2.06576200 L
B-B_2	0	11.60017900	-3.30229700	-2.56494700 L
B-B_2	0	10.33378000	-4.07529600	-0.57721600 L
N-N_3	0	10.30996900	-3.98184900	-2.11255600 L
N-N_3	0	9.05706400	-4.51120900	0.15184700 L
B-B_2	0	7.76119300	-4.11260000	-0.56490700 L
B-B_2	0	6.47050700	-3.84966600	1.52430700 L
N-N_3	0	6.47730700	-4.53173400	0.15438900 L
N-N_3	0	5.18337700	-3.83471400	2.35014300 L
B-B_2	0	3.89469200	-3.87809800	1.52534400 L
B-B_2	0	2.60012500	-2.54855400	3.15362300 L
N-N_3	0	2.60735000	-3.85688100	2.35228300 L
N-N_3	0	1.31377500	-2.10727100	3.85358000 L
B-B_2	0	0.02579900	-2.55726200	3.16254700 L
B-B_2	0	-1.25543900	-0.57541500	3.97878200 L
N-N_3	0	-1.25929600	-2.10797400	3.86352100 L
N-N_3	0	-2.54005100	0.15384400	4.37326400 L
B-B_2	0	-3.82462100	-0.56354600	3.95821400 L
N-N_3	0	-5.10772400	0.15590200	4.37485900 L
B-	0	12.86376700	-3.70657300	-0.54864300 L
B-B_2	0	11.61049900	-3.89986200	1.56534700 L
N-N_3	0	11.66093300	-4.42156000	0.12455500 L
N-N_3	0	10.31439100	-3.83577500	2.37114600 L
B-B_2	0	9.04405000	-3.84273400	1.53031100 L
B-B_2	0	7.75281500	-2.53717900	3.19105900 L
N-N_3	0	7.75509300	-3.82078700	2.35194800 L
N-N_3	0	6.45837400	-2.10209600	3.88212600 L
B-B_2	0	5.17639900	-2.54121500	3.16924900 L
B-B_2	0	3.88429400	-0.57351200	3.93617900 L
N-N_3	0	3.88382900	-2.10316300	3.85916300 L
N-N_3	0	2.59911800	0.14743100	4.34079900 L
B-B_2	0	1.31270000	-0.57406400	3.94032000 L
N-N_3	0	0.03457900	0.14861800	4.36936300 L
B-	0	12.85571100	-2.32070500	2.90099700 L
N-N_3	0	12.89601000	-3.75344700	2.35675500 L
N-N_3	0	11.64574700	-2.08657800	3.84580600 L
B-B_2	0	10.32606600	-2.53155200	3.18743500 L

B-B_2	0	9.02858800	-0.57295800	4.00098900 L
N-N_3	0	9.03948400	-2.10263200	3.90500100 L
N-N_3	0	7.73555300	0.14806100	4.38412100 L
B-B_2	0	6.45619700	-0.57294600	3.95983400 L
N-N_3	0	5.16654000	0.14691000	4.35541300 L
N-N_3	0	12.87677300	0.17661500	4.39081800 L
B-B_2	0	11.59299400	-0.57566000	4.09681700 L
N-N_3	0	10.29459300	0.15140800	4.44307700 L
H-H_	0	-12.55702300	2.21004500	0.91396800 L
H-H_	0	-12.56394900	1.88390600	-1.44167000 L
H-H_	0	-12.58397800	-0.32756500	-2.36817300 L
H-H_	0	-12.55548800	-2.20331900	-0.92054400 L
H-H_	0	12.84108700	4.96602900	2.24754700 L
H-H_	0	12.85407700	4.41342100	-3.16620600 L
H-H_	0	-12.56434800	-1.87801300	1.43687900 L
H-H_	0	-12.58332800	0.33233500	2.36166700 L
H-H_	0	12.82023700	-0.52605000	-5.38441500 L
H-H_	0	12.84549300	-4.95123500	-2.24957700 L
H-H_	0	12.85111200	-4.41150600	3.16758500 L
H-H_	0	12.82422200	0.53147900	5.37256900 L
C-C_3	0	-0.41637100	-0.11194300	0.48111700 H
H-H_	0	0.49541200	0.67348400	-1.26795100 H
H-H_	0	1.16735400	1.33311900	0.22455100 H
C-C_3	0	0.24490300	1.02154600	-0.26838400 H
H-H_	0	-0.44648800	1.84351900	-0.33341900 H
N-N_3	0	0.26897900	-1.35212600	0.26136700 H
H-H_	0	0.19775700	-1.56157400	-0.72409600 H
H-H_	0	1.25331700	-1.23677100	0.47944700 H
C-C_R	0	-1.86907700	-0.21315300	0.07506100 H
O-O_R	0	-2.35566200	-1.05192000	-0.63774400 H
O-O_R	0	-2.59529300	0.80727900	0.57487800 H
H-H_	0	-3.50240000	0.70519200	0.24563200 H
H-H_	0	-0.41892900	0.11652600	1.53666800 H

bTS2@B

B-B_2	0	-10.26189400	-1.32489200	3.94984900 L
N-N_3	0	-11.53572300	-0.66928300	4.46551100 L
B-	0	-12.81726300	-1.47022300	4.12279100 L
B-B_2	0	-5.12120700	-1.30101000	3.78306800 L
N-N_3	0	-6.39696700	-0.65443200	4.32441800 L
B-B_2	0	-7.69405400	-1.30007000	3.83516300 L
B-B_2	0	-8.97998600	0.82079900	3.96893700 L
N-N_3	0	-8.95909000	-0.65937800	4.39931800 L

N-N_3	0	-10.28088200	1.62773300	4.12145100 L
B-B_2	0	-11.51935200	0.74227000	3.88460600 L
B-	0	-12.82782400	2.78964600	3.29643500 L
N-N_3	0	-12.72074400	1.26844500	3.10039600 L
B-B_2	0	0.02141700	-1.30503500	3.73160900 L
N-N_3	0	-1.26096200	-0.65250000	4.24550700 L
B-B_2	0	-2.54955000	-1.30770200	3.74953100 L
B-B_2	0	-3.83353100	0.81840700	3.85639600 L
N-N_3	0	-3.82760700	-0.65448400	4.27845100 L
N-N_3	0	-5.11492900	1.63225900	4.03975000 L
B-B_2	0	-6.40571700	0.82115000	3.90887500 L
B-B_2	0	-7.69999300	2.73414000	3.01444300 L
N-N_3	0	-7.68917200	1.63878300	4.08676900 L
N-N_3	0	-8.98042900	3.52791000	2.76808400 L
B-B_2	0	-10.26881100	2.77184700	3.09832800 L
B-B_2	0	-11.54282400	3.75923400	1.29041600 L
N-N_3	0	-11.55829700	3.52621500	2.79902700 L
N-N_3	0	-12.74997800	3.36687300	0.43820100 L
B-B_2	0	5.16067500	-1.27705200	3.75631000 L
N-N_3	0	3.86710000	-0.63823200	4.26270500 L
B-B_2	0	2.58973700	-1.28810500	3.72936500 L
B-B_2	0	1.29964600	0.83563400	3.84309900 L
N-N_3	0	1.30261200	-0.64624800	4.24373000 L
N-N_3	0	0.01344000	1.64387600	4.01153300 L
B-B_2	0	-1.26452300	0.82444800	3.82849700 L
B-B_2	0	-2.55547000	2.76131900	2.96881200 L
N-N_3	0	-2.54802700	1.63284900	4.00546400 L
N-N_3	0	-3.84827100	3.53948800	2.72857900 L
B-B_2	0	-5.12724600	2.73886600	2.98198000 L
B-B_2	0	-6.42891600	3.95604400	1.26870700 L
N-N_3	0	-6.41771500	3.51996600	2.73710500 L
N-N_3	0	-7.72453100	4.48206100	0.64396800 L
B-B_2	0	-9.00496700	3.93261600	1.28127400 L
B-B_2	0	-10.28751900	4.13497300	-0.84793400 L
N-N_3	0	-10.31553500	4.44119800	0.65634700 L
N-N_3	0	-11.57149900	4.22667700	-1.66210000 L
B-	0	-12.84539100	4.29615500	-0.78313400 L
B-B_2	0	10.30619000	-1.27244300	3.81087100 L
N-N_3	0	9.01704500	-0.63434600	4.34528800 L
B-B_2	0	7.73460700	-1.27214500	3.79636500 L
B-B_2	0	6.43855500	0.84264300	3.90096600 L
N-N_3	0	6.43767200	-0.63532000	4.30242600 L
N-N_3	0	5.14882000	1.65292400	4.05127300 L
B-B_2	0	3.86766800	0.84084900	3.86193700 L

B-B_2	0	2.58398700	2.79098600	2.99752200 L
N-N_3	0	2.58000300	1.65107300	4.02441900 L
N-N_3	0	1.30044500	3.59353300	2.75857300 L
B-B_2	0	0.01343000	2.79841700	2.99795200 L
B-B_2	0	-1.27666800	4.06263400	1.28552600 L
N-N_3	0	-1.27937800	3.57637400	2.74251000 L
N-N_3	0	-2.57418100	4.56509600	0.64770700 L
B-B_2	0	-3.85268200	3.99478900	1.26735000 L
B-B_2	0	-5.14152700	4.10752300	-0.83222700 L
N-N_3	0	-5.14876800	4.51339000	0.64287300 L
N-N_3	0	-6.42926700	4.22228900	-1.64890100 L
B-B_2	0	-7.71668000	4.08352400	-0.83547400 L
B-B_2	0	-8.99849500	3.10560100	-2.71861800 L
N-N_3	0	-8.99349400	4.22459100	-1.65911800 L
N-N_3	0	-10.29750000	2.79934100	-3.48401000 L
B-B_2	0	-11.53815400	3.01913700	-2.59671600 L
B-	0	-12.81875400	1.47930800	-4.10855400 L
N-N_3	0	-12.74912600	2.09073000	-2.69898100 L
B-	0	12.83056300	-1.16017100	3.47237300 L
B-B_2	0	11.57376600	0.87271400	4.06530300 L
N-N_3	0	11.62357800	-0.64071900	4.29835100 L
N-N_3	0	10.27627800	1.67299100	4.15212100 L
B-B_2	0	9.01020000	0.84816300	3.95548900 L
B-B_2	0	7.73396700	2.77146000	3.03573600 L
N-N_3	0	7.71830100	1.65622800	4.08816600 L
N-N_3	0	6.44913800	3.55820800	2.76457200 L
B-B_2	0	5.15811700	2.77548900	3.00966500 L
B-B_2	0	3.88068700	4.01951700	1.28960900 L
N-N_3	0	3.87536600	3.57199300	2.75442000 L
N-N_3	0	2.60255100	4.58263800	0.66099700 L
B-B_2	0	1.30330600	4.08752100	1.30169800 L
B-B_2	0	0.01650600	4.22305000	-0.82872400 L
N-N_3	0	0.01135700	4.61560300	0.66125500 L
N-N_3	0	-1.27715300	4.29239000	-1.64891700 L
B-B_2	0	-2.56352500	4.15692800	-0.82972000 L
B-B_2	0	-3.84394200	3.12387700	-2.68417000 L
N-N_3	0	-3.85529500	4.25121200	-1.64758100 L
N-N_3	0	-5.12620100	2.80457400	-3.45768900 L
B-B_2	0	-6.42110600	3.10925300	-2.70170400 L
B-B_2	0	-7.69457300	1.30987800	-3.83285700 L
N-N_3	0	-7.70416700	2.80170700	-3.48150200 L
N-N_3	0	-8.96102900	0.66981800	-4.39485200 L
B-B_2	0	-10.26287400	1.33499600	-3.94279700 L
B-B_2	0	-11.52034200	-0.73287000	-3.87608800 L

N-N_3	0	-11.53794900	0.67925100	-4.45593200 L
N-N_3	0	-12.72461800	-1.26335600	-3.09895500 L
B-	0	12.84304200	2.50924000	2.82706200 L
N-N_3	0	12.85746100	1.67827100	4.11458800 L
N-N_3	0	11.63326200	3.48108700	2.76950500 L
B-B_2	0	10.30661900	2.75108600	3.05532600 L
B-B_2	0	9.02960700	3.96751100	1.30632900 L
N-N_3	0	9.02876200	3.55318300	2.78094900 L
N-N_3	0	7.74852200	4.50046400	0.66628600 L
B-B_2	0	6.45642700	3.97946500	1.29362100 L
B-B_2	0	5.17563200	4.11451300	-0.81010600 L
N-N_3	0	5.17808100	4.53251000	0.66217500 L
N-N_3	0	3.89054200	4.24568600	-1.62863500 L
B-B_2	0	2.59620200	4.15965200	-0.81390500 L
B-B_2	0	1.30766900	3.14941300	-2.66685600 L
N-N_3	0	1.31418500	4.29446100	-1.64124800 L
N-N_3	0	0.02129900	2.81228000	-3.42158000 L
B-B_2	0	-1.26790700	3.14568100	-2.67100300 L
B-B_2	0	-2.54926200	1.31545700	-3.76882300 L
N-N_3	0	-2.55132700	2.81401600	-3.44002100 L
N-N_3	0	-3.82980700	0.66514100	-4.29465300 L
B-B_2	0	-5.12077200	1.30964100	-3.78932700 L
B-B_2	0	-6.40715000	-0.80990900	-3.90965500 L
N-N_3	0	-6.39915600	0.66506600	-4.32667300 L
N-N_3	0	-7.69073600	-1.62813000	-4.08206200 L
B-B_2	0	-8.98131300	-0.81022300	-3.96413700 L
B-B_2	0	-10.26835600	-2.76153400	-3.09144800 L
N-N_3	0	-10.28191400	-1.61767700	-4.11487900 L
N-N_3	0	-11.55653200	-3.51818100	-2.79363600 L
B-	0	-12.82693300	-2.78514800	-3.29412700 L
N-N_3	0	12.88761400	4.42575600	0.64911500 L
B-B_2	0	11.59624300	4.02843000	1.33808000 L
B-B_2	0	10.32605200	4.04489100	-0.79139900 L
N-N_3	0	10.30686100	4.50734300	0.67557900 L
N-N_3	0	9.04734700	4.19312500	-1.62532700 L
B-B_2	0	7.75274600	4.08510300	-0.80940100 L
B-B_2	0	6.45644900	3.08323200	-2.65621800 L
N-N_3	0	6.46650500	4.21629100	-1.62711800 L
N-N_3	0	5.16637100	2.78011200	-3.41789100 L
B-B_2	0	3.88226600	3.10600400	-2.65139200 L
B-B_2	0	2.58839900	1.29565100	-3.72690800 L
N-N_3	0	2.59596800	2.79759900	-3.41570900 L
N-N_3	0	1.30267900	0.65638100	-4.24670200 L
B-B_2	0	0.02034800	1.30703400	-3.72837000 L

B-B_2	0	-1.26493300	-0.81547900	-3.84619000 L
N-N_3	0	-1.25857800	0.66175300	-4.26066000 L
N-N_3	0	-2.55002600	-1.62320500	-4.01437800 L
B-B_2	0	-3.83456800	-0.80685800	-3.86825100 L
B-B_2	0	-5.12774500	-2.71967100	-2.97323800 L
N-N_3	0	-5.11717600	-1.62156100	-4.04003000 L
N-N_3	0	-6.41646800	-3.50277900	-2.72592900 L
B-B_2	0	-7.69998100	-2.71979100	-3.00584700 L
B-B_2	0	-9.00376800	-3.92081800	-1.27305600 L
N-N_3	0	-8.97898200	-3.51560600	-2.75979600 L
N-N_3	0	-10.31465800	-4.43062700	-0.64936300 L
B-B_2	0	-11.54215400	-3.75011800	-1.28497700 L
B-	0	-12.84626300	-4.27887700	0.78768000 L
N-N_3	0	-12.74606300	-3.34891300	-0.43254700 L
B-	0	12.85563500	3.68216800	-0.69134300 L
B-B_2	0	11.59531600	3.10869700	-2.73047100 L
N-N_3	0	11.65174800	4.11257100	-1.57322100 L
N-N_3	0	10.29700500	2.78227500	-3.46820200 L
B-B_2	0	9.02969800	3.07582300	-2.67411100 L
B-B_2	0	7.73378700	1.28096400	-3.79372200 L
N-N_3	0	7.73673100	2.77177300	-3.43177400 L
N-N_3	0	6.43695100	0.64427300	-4.29981100 L
B-B_2	0	5.15971300	1.28572400	-3.75370400 L
B-B_2	0	3.86725700	-0.83213400	-3.86336700 L
N-N_3	0	3.86649100	0.64774400	-4.26148300 L
N-N_3	0	2.58125700	-1.64342800	-4.02900200 L
B-B_2	0	1.29978600	-0.82804100	-3.85637700 L
B-B_2	0	0.01294600	-2.77633700	-2.99090800 L
N-N_3	0	0.01326000	-1.63657300	-4.02050800 L
N-N_3	0	-1.27999700	-3.54819200	-2.72595600 L
B-B_2	0	-2.55674100	-2.73871500	-2.96383000 L
B-B_2	0	-3.85157000	-3.96628900	-1.25186100 L
N-N_3	0	-3.84810800	-3.51668400	-2.71536300 L
N-N_3	0	-5.14564800	-4.49698900	-0.63293900 L
B-B_2	0	-6.42731700	-3.93925400	-1.25727600 L
B-B_2	0	-7.71675700	-4.07727000	0.84492200 L
N-N_3	0	-7.72282700	-4.47024800	-0.63582700 L
N-N_3	0	-8.99498900	-4.21651900	1.66699400 L
B-B_2	0	-10.28804200	-4.12463100	0.85493900 L
B-B_2	0	-11.53861200	-3.00712600	2.60374500 L
N-N_3	0	-11.57316400	-4.21399600	1.66807100 L
N-N_3	0	-12.75234200	-2.08293600	2.71339000 L
B-	0	12.83036300	1.16957800	-3.47195600 L
N-N_3	0	12.87936300	2.70091600	-3.42783500 L

N-N_3	0	11.62263700	0.64895600	-4.29616700 L
B-B_2	0	10.30543000	1.28114500	-3.80871200 L
B-B_2	0	9.00936300	-0.83944500	-3.95170900 L
N-N_3	0	9.01619600	0.64283200	-4.34242800 L
N-N_3	0	7.71753300	-1.64740200	-4.08443200 L
B-B_2	0	6.43796100	-0.83357100	-3.89802300 L
B-B_2	0	5.15693300	-2.76513800	-3.00557800 L
N-N_3	0	5.14882200	-1.64400300	-4.04898700 L
N-N_3	0	3.87335800	-3.56028600	-2.74920100 L
B-B_2	0	2.58307900	-2.77795700	-2.99549000 L
B-B_2	0	1.30148100	-4.06859500	-1.29510400 L
N-N_3	0	1.29764100	-3.57647600	-2.75269900 L
N-N_3	0	0.00677100	-4.57820400	-0.64831900 L
B-B_2	0	-1.27619600	-4.01063900	-1.26309900 L
B-B_2	0	-2.56308700	-4.16466800	0.85099400 L
N-N_3	0	-2.57073000	-4.53635900	-0.63648600 L
N-N_3	0	-3.85649800	-4.25934800	1.66539500 L
B-B_2	0	-5.14061700	-4.10766200	0.84691400 L
B-B_2	0	-6.42247900	-3.10580400	2.71094400 L
N-N_3	0	-6.43100700	-4.22005300	1.65979900 L
N-N_3	0	-7.70528700	-2.79322600	3.48866900 L
B-B_2	0	-8.99940600	-3.09717400	2.72607300 L
N-N_3	0	-10.29794000	-2.78931600	3.49127600 L
N-N_3	0	12.85649200	-1.66974300	-4.10972000 L
B-B_2	0	11.57279300	-0.86413200	-4.06077700 L
B-B_2	0	10.30527300	-2.74310500	-3.05183700 L
N-N_3	0	10.27532600	-1.66445700	-4.14818900 L
N-N_3	0	9.02712800	-3.54499000	-2.77769200 L
B-B_2	0	7.73268500	-2.76256200	-3.03181400 L
B-B_2	0	6.45458700	-3.97012600	-1.28923200 L
N-N_3	0	6.44734900	-3.54863700	-2.76015900 L
N-N_3	0	5.17576900	-4.52270900	-0.65760200 L
B-B_2	0	3.87830500	-4.00763900	-1.28386300 L
B-B_2	0	2.59588700	-4.15561800	0.82211700 L
N-N_3	0	2.59953300	-4.57105400	-0.65589300 L
N-N_3	0	1.31184700	-4.28159400	1.64861400 L
B-B_2	0	0.01491600	-4.18697200	0.83906500 L
B-B_2	0	-1.26720000	-3.16794900	2.70870500 L
N-N_3	0	-1.27254100	-4.29606600	1.66557400 L
N-N_3	0	-2.55485000	-2.81428800	3.45816600 L
B-B_2	0	-3.84479100	-3.13006900	2.70038100 L
N-N_3	0	-5.12854600	-2.79919300	3.46632400 L
B-	0	12.84135600	-2.50152700	-2.82274600 L
B-B_2	0	11.59480200	-4.02319800	-1.33619200 L

N-N_3	0	11.63174900	-3.47363900	-2.76676200 L
N-N_3	0	10.30526200	-4.50076100	-0.67309500 L
B-B_2	0	9.02806100	-3.96017400	-1.30332700 L
B-B_2	0	7.75203800	-4.07749300	0.81287000 L
N-N_3	0	7.74674300	-4.49239700	-0.66286600 L
N-N_3	0	6.46653800	-4.20889300	1.63141600 L
B-B_2	0	5.17460300	-4.10817600	0.81584600 L
B-B_2	0	3.88315800	-3.10041200	2.65813600 L
N-N_3	0	3.89065800	-4.24125500	1.63598600 L
N-N_3	0	2.59895300	-2.79131800	3.42523700 L
B-B_2	0	1.30835300	-3.14604800	2.68400200 L
N-N_3	0	0.02526000	-2.81511700	3.44725800 L
B-	0	12.85547800	-3.67678300	0.69228700 L
N-N_3	0	12.88611100	-4.42139400	-0.64765400 L
N-N_3	0	11.65140100	-4.10507700	1.57497000 L
B-B_2	0	10.32541700	-4.03761100	0.79358100 L
B-B_2	0	9.03013500	-3.06714800	2.67623900 L
N-N_3	0	9.04713400	-4.18509900	1.62811400 L
N-N_3	0	7.73763800	-2.76304600	3.43452900 L
B-B_2	0	6.45711300	-3.07516800	2.65976800 L
N-N_3	0	5.16785600	-2.77197900	3.42220900 L
N-N_3	0	12.88015500	-2.69144200	3.42719500 L
B-B_2	0	11.59565000	-3.09948600	2.73078100 L
N-N_3	0	10.29782700	-2.77346800	3.46965600 L
H-H_	0	-12.54069500	1.07834300	2.09007500 L
H-H_	0	-12.58844300	2.39332200	0.09921400 L
H-H_	0	-12.60698300	1.31654500	-2.01392100 L
H-H_	0	-12.55163000	-1.07185600	-2.08771800 L
H-H_	0	12.79561600	2.33332500	4.92675100 L
H-H_	0	12.84549400	5.45168800	0.45366800 L
H-H_	0	-12.57670400	-2.37696800	-0.09262800 L
H-H_	0	-12.61772800	-1.30887500	2.02673000 L
H-H_	0	12.83934300	3.05756000	-4.40952800 L
H-H_	0	12.79516900	-2.32424100	-4.92237100 L
H-H_	0	12.84297700	-5.44712800	-0.45139200 L
H-H_	0	12.84129300	-3.04878900	4.40867700 L
C-C_R	0	-0.06479200	-0.22462600	0.18205100 H
H-H_	0	1.21621200	1.21205600	-0.75350500 H
H-H_	0	1.46524000	1.04089000	0.97467300 H
C-C_3	0	0.69505500	1.05529900	0.19989900 H
H-H_	0	0.01023100	1.87066400	0.37169400 H
N-N_R	0	0.73589700	-1.33712300	-0.26478300 H
H-H_	0	1.28418800	-1.04274200	-1.07196500 H
H-H_	0	1.42145700	-1.55277800	0.44872100 H

C-C_R	0	-1.44839900	-0.20536700	-0.18626700 H
O-O_R	0	-2.12641400	-1.17552800	0.32454000 H
O-O_R	0	-2.08043800	0.80273100	-0.76602000 H
H-H_	0	-3.03653900	0.69555300	-0.62429200 H
H-H_	0	-1.03111100	-1.12098100	0.95636900 H

bINT2@B

B-B_2	0	-10.21182800	-3.66760100	2.12249100 L
N-N_3	0	-11.48855700	-3.46824800	2.92825200 L
B-	0	-12.76873600	-3.85502200	2.14723000 L
B-B_2	0	-5.06204100	-3.64337100	2.05827400 L
N-N_3	0	-6.34761500	-3.44522500	2.86467700 L
B-B_2	0	-7.64000600	-3.61782500	2.06856600 L
B-B_2	0	-8.91665700	-2.03194100	3.48954900 L
N-N_3	0	-8.91060500	-3.45564400	2.89861300 L
N-N_3	0	-10.20990000	-1.49102200	4.12170200 L
B-B_2	0	-11.45295400	-2.00747300	3.37301200 L
B-	0	-12.74517600	-0.05384400	4.23856800 L
N-N_3	0	-12.64092500	-1.08483100	3.10188300 L
B-B_2	0	0.09558800	-3.64870000	2.06720700 L
N-N_3	0	-1.19279600	-3.47617300	2.87535000 L
B-B_2	0	-2.48367200	-3.69038100	2.07579900 L
B-B_2	0	-3.76945300	-2.03336700	3.41586100 L
N-N_3	0	-3.77579500	-3.46687900	2.86555200 L
N-N_3	0	-5.04984600	-1.47595000	4.03965900 L
B-B_2	0	-6.34313600	-2.02450100	3.44016600 L
B-B_2	0	-7.62061300	0.04728900	3.94004900 L
N-N_3	0	-7.61991400	-1.47916300	4.08842200 L
N-N_3	0	-8.88769400	0.82268100	4.29104000 L
B-B_2	0	-10.18551700	0.04294300	4.06555200 L
B-B_2	0	-11.45117100	1.99210600	3.37422400 L
N-N_3	0	-11.46705600	0.81762100	4.34883100 L
N-N_3	0	-12.67445800	2.28597700	2.50658200 L
B-B_2	0	5.24757100	-3.56594900	2.07080100 L
N-N_3	0	3.95681800	-3.41908300	2.87741800 L
B-B_2	0	2.67271600	-3.59809900	2.06440700 L
B-B_2	0	1.37230900	-2.02178500	3.44780300 L
N-N_3	0	1.38332500	-3.44178000	2.87040600 L
N-N_3	0	0.08205400	-1.47846300	4.05955300 L
B-B_2	0	-1.19880400	-2.04641900	3.44542000 L
B-B_2	0	-2.48378700	0.04702100	3.87529200 L
N-N_3	0	-2.48794800	-1.48075200	4.03770900 L
N-N_3	0	-3.76660100	0.81708500	4.18433400 L

B-B_2	0	-5.05094300	0.04782700	3.88045800 L
B-B_2	0	-6.34060300	2.11364300	3.39423700 L
N-N_3	0	-6.32824700	0.81726000	4.21197400 L
N-N_3	0	-7.62879500	2.93677300	3.32133300 L
B-B_2	0	-8.91411700	2.10975700	3.44248400 L
B-B_2	0	-10.20636500	3.70664200	2.02973500 L
N-N_3	0	-10.21953800	2.91682100	3.34545700 L
N-N_3	0	-11.49535800	4.32284700	1.50433200 L
B-	0	-12.76245400	3.79460400	2.22207300 L
B-B_2	0	10.39528600	-3.50863700	2.06837200 L
N-N_3	0	9.11097900	-3.38903900	2.89886700 L
B-B_2	0	7.82316800	-3.54110400	2.08000400 L
B-B_2	0	6.51774500	-2.00186400	3.50886900 L
N-N_3	0	6.53093500	-3.40144300	2.88786900 L
N-N_3	0	5.22225400	-1.47215500	4.12691100 L
B-B_2	0	3.94539600	-2.01063600	3.47837700 L
B-B_2	0	2.64964700	0.05189400	3.94162500 L
N-N_3	0	2.64971100	-1.47325500	4.08729100 L
N-N_3	0	1.35816900	0.82064800	4.22749700 L
B-B_2	0	0.07928400	0.04899600	3.90045400 L
B-B_2	0	-1.20188600	2.14073600	3.42779000 L
N-N_3	0	-1.20619600	0.81717400	4.20867600 L
N-N_3	0	-2.49087600	2.95992100	3.31882200 L
B-B_2	0	-3.76912200	2.12291700	3.38108200 L
B-B_2	0	-5.06043600	3.69818700	1.97021000 L
N-N_3	0	-5.05716300	2.94235600	3.30317600 L
N-N_3	0	-6.35557500	4.33887400	1.47100500 L
B-B_2	0	-7.63557200	3.66715800	1.97414300 L
B-B_2	0	-8.93806300	4.22205200	-0.05395800 L
N-N_3	0	-8.92008200	4.32716700	1.48240300 L
N-N_3	0	-10.24920700	4.47597200	-0.82029100 L
B-B_2	0	-11.48115300	4.04923200	0.00240300 L
B-	0	-12.76914500	3.85039100	-2.14550100 L
N-N_3	0	-12.69506000	3.41002600	-0.67436100 L
B-	0	12.91630500	-3.17120900	1.86835400 L
B-B_2	0	11.65486100	-2.02944000	3.64944400 L
N-N_3	0	11.71621300	-3.32966600	2.84008000 L
N-N_3	0	10.35163000	-1.48095300	4.22731900 L
B-B_2	0	9.09030000	-2.00172500	3.55003700 L
B-B_2	0	7.79721200	0.05757200	4.04494400 L
N-N_3	0	7.79315400	-1.47176100	4.16315300 L
N-N_3	0	6.50210200	0.82700000	4.31899200 L
B-B_2	0	5.22197200	0.05382000	3.99372400 L
B-B_2	0	3.93976700	2.10549100	3.43620800 L

N-N_3	0	3.92838400	0.82290400	4.27266000 L
N-N_3	0	2.65744100	2.93340600	3.32739000 L
B-B_2	0	1.36679300	2.11887700	3.41240200 L
B-B_2	0	0.09182200	3.70585400	1.98870700 L
N-N_3	0	0.08839800	2.95691700	3.33046300 L
N-N_3	0	-1.19265600	4.37421400	1.48223000 L
B-B_2	0	-2.48633700	3.72341200	1.98435200 L
B-B_2	0	-3.77327000	4.31331400	-0.05744500 L
N-N_3	0	-3.77682600	4.37514000	1.47755000 L
N-N_3	0	-5.07033900	4.55990600	-0.83719800 L
B-B_2	0	-6.35657500	4.26176500	-0.05974800 L
B-B_2	0	-7.63966300	3.61563100	-2.07120200 L
N-N_3	0	-7.65373400	4.52082300	-0.83575500 L
N-N_3	0	-8.91143500	3.45360900	-2.89970700 L
B-B_2	0	-10.21203000	3.66438900	-2.12256700 L
B-B_2	0	-11.45366200	2.00452800	-3.37353200 L
N-N_3	0	-11.48932800	3.46501800	-2.92769500 L
N-N_3	0	-12.64248400	1.08211700	-3.10503600 L
B-	0	12.90613200	0.03173400	3.75662100 L
N-N_3	0	12.93352700	-1.43361700	4.20563900 L
N-N_3	0	11.68899000	0.80087000	4.33858400 L
B-B_2	0	10.37003900	0.04979000	4.07383900 L
B-B_2	0	9.08460600	2.10330000	3.51082000 L
N-N_3	0	9.08251500	0.83156300	4.36553100 L
N-N_3	0	7.79869400	2.91740900	3.36660300 L
B-B_2	0	6.51205100	2.09874300	3.46663000 L
B-B_2	0	5.24122600	3.62440100	1.98432500 L
N-N_3	0	5.22902200	2.92280200	3.34499800 L
N-N_3	0	3.96284200	4.29110600	1.47324500 L
B-B_2	0	2.66681500	3.65493400	1.97699400 L
B-B_2	0	1.38592100	4.23389200	-0.05563500 L
N-N_3	0	1.38933200	4.33210200	1.47407300 L
N-N_3	0	0.10568800	4.54813400	-0.83437900 L
B-B_2	0	-1.19243800	4.30803000	-0.05509100 L
B-B_2	0	-2.48343700	3.67048800	-2.07832700 L
N-N_3	0	-2.48175000	4.58108800	-0.83854900 L
N-N_3	0	-3.77499000	3.46535900	-2.87285200 L
B-B_2	0	-5.06203600	3.64305000	-2.06623200 L
B-B_2	0	-6.34420700	2.02588400	-3.44747300 L
N-N_3	0	-6.34874600	3.44629900	-2.87052600 L
N-N_3	0	-7.62159600	1.47830500	-4.09202800 L
B-B_2	0	-8.91759400	2.03038500	-3.49169400 L
B-B_2	0	-10.18565800	-0.04512900	-4.06682100 L
N-N_3	0	-10.21088900	1.48888700	-4.12300300 L

N-N_3	0	-11.46661500	-0.82038800	-4.35046700 L
B-	0	-12.74511100	0.05077200	-4.24165900 L
N-N_3	0	12.93843200	2.90934000	3.36924000 L
B-B_2	0	11.64945500	2.14612900	3.60568700 L
B-B_2	0	10.38886300	3.56981300	2.01178900 L
N-N_3	0	10.35705700	2.93610500	3.41311000 L
N-N_3	0	9.11497800	4.23892200	1.48191200 L
B-B_2	0	7.81638800	3.60512000	1.99619800 L
B-B_2	0	6.53669800	4.14536700	-0.05024800 L
N-N_3	0	6.53601900	4.26127100	1.47593900 L
N-N_3	0	5.25606500	4.45452600	-0.82664700 L
B-B_2	0	3.96310600	4.18711900	-0.05369200 L
B-B_2	0	2.67113700	3.59702200	-2.07080500 L
N-N_3	0	2.68089500	4.49354500	-0.82982700 L
N-N_3	0	1.38428400	3.44786600	-2.88268500 L
B-B_2	0	0.09516500	3.65175000	-2.08223400 L
B-B_2	0	-1.19932100	2.05767900	-3.47744000 L
N-N_3	0	-1.19546700	3.48026900	-2.88907900 L
N-N_3	0	-2.49029900	1.48431100	-4.05942100 L
B-B_2	0	-3.77032800	2.03675000	-3.43380700 L
B-B_2	0	-5.05184300	-0.04579300	-3.88119200 L
N-N_3	0	-5.05262200	1.47700100	-4.04987400 L
N-N_3	0	-6.32787100	-0.81799100	-4.21005500 L
B-B_2	0	-7.62097300	-0.04798400	-3.94092200 L
B-B_2	0	-8.91333000	-2.11087600	-3.44141000 L
N-N_3	0	-8.88734600	-0.82457600	-4.29121500 L
N-N_3	0	-10.21853500	-2.91857800	-3.34518700 L
B-B_2	0	-11.45063800	-1.99429700	-3.37520100 L
B-	0	-12.76230900	-3.79436400	-2.22136200 L
N-N_3	0	-12.67267000	-2.28578800	-2.50510700 L
B-	0	12.92176600	3.24240700	1.87328900 L
B-B_2	0	11.67584500	4.16200800	-0.04518500 L
N-N_3	0	11.71847500	4.14470600	1.48694000 L
N-N_3	0	10.38646500	4.41645900	-0.82413600 L
B-B_2	0	9.10965400	4.12247000	-0.04590700 L
B-B_2	0	7.82245800	3.54132400	-2.08011700 L
N-N_3	0	7.82687800	4.41886600	-0.82258300 L
N-N_3	0	6.53079300	3.40178100	-2.88860900 L
B-B_2	0	5.24663200	3.56503900	-2.07245000 L
B-B_2	0	3.94620700	2.01318600	-3.48465900 L
N-N_3	0	3.95714100	3.42037600	-2.88111400 L
N-N_3	0	2.65198900	1.47618500	-4.09614300 L
B-B_2	0	1.37267400	2.02918800	-3.46452600 L
B-B_2	0	0.08026900	-0.04159900	-3.90141500 L

N-N_3	0	0.08428800	1.48413100	-4.07966400 L
N-N_3	0	-1.20585200	-0.81388300	-4.19681600 L
B-B_2	0	-2.48429700	-0.04087600	-3.87618200 L
B-B_2	0	-3.76763200	-2.11667600	-3.36533300 L
N-N_3	0	-3.76611400	-0.81598200	-4.17742500 L
N-N_3	0	-5.05436100	-2.93799900	-3.29197400 L
B-B_2	0	-6.33970700	-2.11170000	-3.38801800 L
B-B_2	0	-7.63514700	-3.66827500	-1.97210300 L
N-N_3	0	-7.62706200	-2.93674800	-3.31843200 L
N-N_3	0	-8.92002000	-4.32963000	-1.48252400 L
B-B_2	0	-10.20602100	-3.70827500	-2.02942600 L
B-B_2	0	-11.48139300	-4.05145000	-0.00214400 L
N-N_3	0	-11.49550900	-4.32409500	-1.50428300 L
N-N_3	0	-12.69649600	-3.41543800	0.67565000 L
B-	0	12.91650300	3.17569100	-1.86783700 L
N-N_3	0	12.96718200	4.30180900	-0.82901200 L
N-N_3	0	11.71581100	3.33119000	-2.83937200 L
B-B_2	0	10.39469500	3.51015800	-2.06791100 L
B-B_2	0	9.09068200	2.00195300	-3.54919700 L
N-N_3	0	9.11065300	3.38952000	-2.89852800 L
N-N_3	0	7.79413000	1.47209000	-4.16336100 L
B-B_2	0	6.51832600	2.00258000	-3.51039700 L
B-B_2	0	5.22267200	-0.05261000	-3.99409200 L
N-N_3	0	5.22380200	1.47315900	-4.13000100 L
N-N_3	0	3.92850500	-0.82170200	-4.27069500 L
B-B_2	0	2.65051700	-0.04818300	-3.94229700 L
B-B_2	0	1.36683300	-2.11030900	-3.39819000 L
N-N_3	0	1.35818000	-0.81754500	-4.22199700 L
N-N_3	0	0.08658800	-2.94530400	-3.31041100 L
B-B_2	0	-1.20194900	-2.12754600	-3.39934200 L
B-B_2	0	-2.48538800	-3.74218700	-1.98485000 L
N-N_3	0	-2.48844700	-2.95309200	-3.30538700 L
N-N_3	0	-3.77887700	-4.38861700	-1.47829300 L
B-B_2	0	-5.05899700	-3.69716300	-1.96130100 L
B-B_2	0	-6.35751300	-4.27000200	0.06051700 L
N-N_3	0	-6.35529100	-4.34072400	-1.46960800 L
N-N_3	0	-7.65525400	-4.52621600	0.83580100 L
B-B_2	0	-8.93872200	-4.22643000	0.05384800 L
N-N_3	0	-10.24988000	-4.47936400	0.82023100 L
N-N_3	0	12.93433600	1.43337800	-4.20118800 L
B-B_2	0	11.65518200	2.02933400	-3.64616200 L
B-B_2	0	10.37053500	-0.04974100	-4.07300900 L
N-N_3	0	10.35247000	1.48116500	-4.22561600 L
N-N_3	0	9.08298700	-0.83133300	-4.36549100 L

B-B_2	0	7.79778800	-0.05727600	-4.04489100 L
B-B_2	0	6.51204200	-2.09799600	-3.46545600 L
N-N_3	0	6.50242300	-0.82667900	-4.31853600 L
N-N_3	0	5.22825400	-2.92129200	-3.34271700 L
B-B_2	0	3.93954700	-2.10239400	-3.43113100 L
B-B_2	0	2.66694400	-3.65521900	-1.97227800 L
N-N_3	0	2.65575800	-2.92838200	-3.31966300 L
N-N_3	0	1.38975700	-4.33595900	-1.47251000 L
B-B_2	0	0.09105500	-3.70231200	-1.97423100 L
B-B_2	0	-1.19077700	-4.35095000	0.05556200 L
N-N_3	0	-1.18931700	-4.39100600	-1.48373500 L
N-N_3	0	-2.48320600	-4.61110100	0.84091500 L
B-B_2	0	-3.77387500	-4.34050800	0.05784700 L
N-N_3	0	-5.07312000	-4.57148400	0.83847800 L
B-	0	12.90595300	-0.03230600	-3.75340100 L
B-B_2	0	11.64977300	-2.14723300	-3.60765800 L
N-N_3	0	11.68955000	-0.80057100	-4.33794400 L
N-N_3	0	10.35713000	-2.93648200	-3.41404000 L
B-B_2	0	9.08481600	-2.10340500	-3.51128200 L
B-B_2	0	7.81692700	-3.60510500	-1.99625000 L
N-N_3	0	7.79858200	-2.91714700	-3.36646300 L
N-N_3	0	6.53701300	-4.26201100	-1.47613100 L
B-B_2	0	5.24153200	-3.62521600	-1.98327500 L
B-B_2	0	3.96515600	-4.19497500	0.05366800 L
N-N_3	0	3.96370300	-4.29398600	-1.47338700 L
N-N_3	0	2.68492400	-4.50407100	0.83067800 L
B-B_2	0	1.38822100	-4.25363700	0.05714600 L
N-N_3	0	0.10957400	-4.56885900	0.83755900 L
B-	0	12.92300100	-3.24272700	-1.87565700 L
N-N_3	0	12.93855200	-2.91093300	-3.37191700 L
N-N_3	0	11.71930800	-4.14367600	-1.48727700 L
B-B_2	0	10.38952100	-3.56935700	-2.01244000 L
B-B_2	0	9.11086000	-4.12120700	0.04577800 L
N-N_3	0	9.11590300	-4.23833400	-1.48198900 L
N-N_3	0	7.82857400	-4.41879600	0.82247900 L
B-B_2	0	6.53823000	-4.14694100	0.05006300 L
N-N_3	0	5.25869600	-4.45795500	0.82664200 L
N-N_3	0	12.96850900	-4.29639200	0.82861100 L
B-B_2	0	11.67690400	-4.15804500	0.04488600 L
N-N_3	0	10.38791700	-4.41422600	0.82398200 L
H-H_	0	-12.44289600	-0.57289200	2.21365300 L
H-H_	0	-12.54196900	1.78258200	1.60256400 L
H-H_	0	-12.55547300	2.37641000	-0.65275100 L
H-H_	0	-12.44659100	0.57030200	-2.21628300 L

H-H_	0	12.87174800	-1.45624100	5.24879900 L
H-H_	0	12.88452500	3.80584200	3.90394400 L
H-H_	0	-12.53702500	-1.78317500	-1.60110200 L
H-H_	0	-12.56005100	-2.38143300	0.65334300 L
H-H_	0	12.93841000	5.21539600	-1.33601000 L
H-H_	0	12.87396000	1.45693200	-5.24440800 L
H-H_	0	12.88356800	-3.80788600	-3.90575200 L
H-H_	0	12.94125000	-5.21046100	1.33482400 L
C-C_R	0	-2.33497300	-0.03148800	0.00446100 H
H-H_	0	-1.21760900	1.57559600	-0.88722500 H
H-H_	0	-0.25895900	0.41951700	-0.00075400 H
C-C_3	0	-1.21463800	0.95176700	-0.00764500 H
H-H_	0	-1.21826700	1.59780000	0.85566700 H
N-N_R	0	-1.94355000	-1.40892100	0.01288400 H
H-H_	0	-1.33646200	-1.55858900	-0.78514600 H
H-H_	0	-1.32494400	-1.54630400	0.80430400 H
C-C_R	0	-3.66130600	0.17092000	0.00561000 H
O-O_R	0	-4.55830100	-0.84927100	0.01787700 H
O-O_R	0	-4.26353500	1.37513600	-0.00610100 H
H-H_	0	-5.21994800	1.22916600	0.00605900 H
H-H_	0	-3.99289100	-1.64510700	0.02543900 H

bTS3@B

B-B_2	0	-10.22566900	3.78005100	-1.93060600 L
N-N_3	0	-11.50313000	3.62368500	-2.74488700 L
B-	0	-12.78272000	3.96154000	-1.94067100 L
B-B_2	0	-5.07527700	3.76330100	-1.87507000 L
N-N_3	0	-6.36173700	3.61376700	-2.69038700 L
B-B_2	0	-7.65350000	3.73507400	-1.88357800 L
B-B_2	0	-8.92840000	2.22894800	-3.38858400 L
N-N_3	0	-8.92522500	3.61740200	-2.71939100 L
N-N_3	0	-10.22060900	1.71857500	-4.04756900 L
B-B_2	0	-11.46525100	2.19062000	-3.27256300 L
B-	0	-12.75055900	0.28536200	-4.25793500 L
N-N_3	0	-12.65952200	1.25814600	-3.06965400 L
B-B_2	0	0.08469100	3.79992700	-1.88815900 L
N-N_3	0	-1.20506200	3.66649400	-2.70464000 L
B-B_2	0	-2.49567400	3.81829900	-1.89108000 L
B-B_2	0	-3.78013800	2.24546000	-3.32385300 L
N-N_3	0	-3.78887000	3.64353800	-2.69304800 L
N-N_3	0	-5.06061700	1.71182500	-3.96909300 L
B-B_2	0	-6.35460000	2.22808100	-3.34416700 L
B-B_2	0	-7.62807400	0.17886300	-3.93573600 L

N-N_3	0	-7.63091200	1.71048300	-4.01531500 L
N-N_3	0	-8.89173900	-0.58200400	-4.32732300 L
B-B_2	0	-10.19236000	0.18379200	-4.07082800 L
B-B_2	0	-11.45684300	-1.79764900	-3.48200000 L
N-N_3	0	-11.47015500	-0.57808100	-4.39936400 L
N-N_3	0	-12.67134500	-2.11832100	-2.61218900 L
B-B_2	0	5.23955800	3.70122400	-1.87797100 L
N-N_3	0	3.95044900	3.59737200	-2.69319500 L
B-B_2	0	2.66305700	3.74139900	-1.87744500 L
B-B_2	0	1.36392900	2.23881200	-3.33704400 L
N-N_3	0	1.37591200	3.63103500	-2.69521900 L
N-N_3	0	0.07657400	1.72199100	-3.97592100 L
B-B_2	0	-1.20839200	2.27096800	-3.35407900 L
B-B_2	0	-2.49306200	0.19314600	-3.84063800 L
N-N_3	0	-2.49703000	1.72324500	-3.96605500 L
N-N_3	0	-3.77086000	-0.57055300	-4.18427000 L
B-B_2	0	-5.05934800	0.18366300	-3.86508300 L
B-B_2	0	-6.34620800	-1.90736400	-3.47407900 L
N-N_3	0	-6.33251400	-0.57582600	-4.23424300 L
N-N_3	0	-7.63199700	-2.73825700	-3.45642100 L
B-B_2	0	-8.91917700	-1.90861900	-3.54155300 L
B-B_2	0	-10.21593400	-3.57782100	-2.21865600 L
N-N_3	0	-10.22390300	-2.72151300	-3.49216000 L
N-N_3	0	-11.50865600	-4.21746700	-1.72937300 L
B-	0	-12.77344200	-3.63915200	-2.41178400 L
B-B_2	0	10.38818200	3.62716700	-1.86956800 L
N-N_3	0	9.10483200	3.54999500	-2.70628900 L
B-B_2	0	7.81576300	3.66792300	-1.88350500 L
B-B_2	0	6.50952500	2.20009300	-3.38165700 L
N-N_3	0	6.52482700	3.57051500	-2.69884900 L
N-N_3	0	5.21397300	1.70170100	-4.02329700 L
B-B_2	0	3.93753400	2.21698300	-3.35541500 L
B-B_2	0	2.64006100	0.17962200	-3.89693700 L
N-N_3	0	2.64323400	1.70899000	-3.98883000 L
N-N_3	0	1.34721500	-0.57342300	-4.20862700 L
B-B_2	0	0.07209600	0.19157100	-3.85489000 L
B-B_2	0	-1.21110300	-1.90297900	-3.42131800 L
N-N_3	0	-1.21303900	-0.56727600	-4.17745600 L
N-N_3	0	-2.49366500	-2.73275100	-3.38802300 L
B-B_2	0	-3.77673400	-1.90236100	-3.42563600 L
B-B_2	0	-5.06911400	-3.57269700	-2.13200000 L
N-N_3	0	-5.05866400	-2.73390300	-3.41374300 L
N-N_3	0	-6.36672200	-4.25058900	-1.69168400 L
B-B_2	0	-7.64474800	-3.54607600	-2.15412000 L

B-B_2	0	-8.95322600	-4.22150100	-0.16707300 L
N-N_3	0	-8.93227000	-4.23310200	-1.70686500 L
N-N_3	0	-10.26562300	-4.51416000	0.58219500 L
B-B_2	0	-11.49409300	-4.03280500	-0.21388800 L
B-	0	-12.78198200	-3.96539700	1.94446400 L
N-N_3	0	-12.71070100	-3.44122300	0.50063000 L
B-	0	12.90982100	3.27797200	-1.68377200 L
B-B_2	0	11.64623200	2.21870000	-3.51387300 L
N-N_3	0	11.70970800	3.48152000	-2.64732700 L
N-N_3	0	10.34246900	1.70493300	-4.12267900 L
B-B_2	0	9.08179600	2.19419800	-3.42086700 L
B-B_2	0	7.78456800	0.16374000	-4.01642200 L
N-N_3	0	7.78388500	1.69732200	-4.05924700 L
N-N_3	0	6.48661200	-0.58766200	-4.32617900 L
B-B_2	0	5.21040500	0.17113800	-3.95606500 L
B-B_2	0	3.92454500	-1.90618700	-3.49850600 L
N-N_3	0	3.91423500	-0.58063400	-4.26648300 L
N-N_3	0	2.63781500	-2.73377500	-3.43259200 L
B-B_2	0	1.35491600	-1.90395000	-3.44682800 L
B-B_2	0	0.07638300	-3.59463900	-2.12847900 L
N-N_3	0	0.07060300	-2.73458000	-3.40019500 L
N-N_3	0	-1.20794800	-4.31963700	-1.70332900 L
B-B_2	0	-2.49439100	-3.59390500	-2.11746800 L
B-B_2	0	-3.79138900	-4.37629800	-0.16075300 L
N-N_3	0	-3.78817900	-4.29231900	-1.69164700 L
N-N_3	0	-5.09489900	-4.63699400	0.60027100 L
B-B_2	0	-6.37369800	-4.28121500	-0.16061600 L
B-B_2	0	-7.65370400	-3.73746300	1.88001200 L
N-N_3	0	-7.67325700	-4.57383200	0.59688100 L
N-N_3	0	-8.92361200	-3.61590400	2.71746000 L
B-B_2	0	-10.22536000	-3.78151700	1.93076400 L
B-B_2	0	-11.46333300	-2.19065800	3.27131600 L
N-N_3	0	-11.50154500	-3.62462200	2.74634300 L
N-N_3	0	-12.65602300	-1.25750100	3.06345300 L
B-	0	12.89028000	0.16103500	-3.73172800 L
N-N_3	0	12.92456000	1.64901700	-4.09798300 L
N-N_3	0	11.67364400	-0.56910800	-4.36226400 L
B-B_2	0	10.35676000	0.16775900	-4.05209100 L
B-B_2	0	9.06855600	-1.91394400	-3.60595000 L
N-N_3	0	9.06673300	-0.59395500	-4.38435600 L
N-N_3	0	7.78099600	-2.73287500	-3.50610300 L
B-B_2	0	6.49611700	-1.90638300	-3.54777200 L
B-B_2	0	5.22697000	-3.52828800	-2.16281100 L
N-N_3	0	5.21034900	-2.73340700	-3.47113100 L

N-N_3	0	3.95021600	-4.23166300	-1.69644000 L
B-B_2	0	2.65146700	-3.55830400	-2.14202600 L
B-B_2	0	1.37755000	-4.32757000	-0.16206600 L
N-N_3	0	1.37395900	-4.27707900	-1.69300700 L
N-N_3	0	0.10272100	-4.69091000	0.60497300 L
B-B_2	0	-1.20520200	-4.47953900	-0.17108200 L
B-B_2	0	-2.49680400	-3.80140500	1.85028300 L
N-N_3	0	-2.50799600	-4.70831700	0.60830900 L
N-N_3	0	-3.78344100	-3.62353500	2.66422300 L
B-B_2	0	-5.07736200	-3.76947200	1.86264500 L
B-B_2	0	-6.35172600	-2.21801700	3.32641000 L
N-N_3	0	-6.35952200	-3.60938300	2.68291400 L
N-N_3	0	-7.62648200	-1.70487700	4.00525500 L
B-B_2	0	-8.92597500	-2.22534500	3.38248800 L
B-B_2	0	-10.19170400	-0.18216300	4.06865600 L
N-N_3	0	-10.21773400	-1.71675400	4.04426900 L
N-N_3	0	-11.47096400	0.57799500	4.39689000 L
B-	0	-12.75041600	-0.28614200	4.25235500 L
N-N_3	0	12.92057600	-2.73710200	-3.53168900 L
B-B_2	0	11.63297200	-1.95757000	-3.71539700 L
B-B_2	0	10.37557500	-3.46913200	-2.20294700 L
N-N_3	0	10.33930800	-2.75394300	-3.56405800 L
N-N_3	0	9.10335800	-4.16835400	-1.70997600 L
B-B_2	0	7.80280800	-3.50629000	-2.18239500 L
B-B_2	0	6.52882900	-4.17476500	-0.17162400 L
N-N_3	0	6.52440400	-4.19552900	-1.70170400 L
N-N_3	0	5.25263500	-4.53341500	0.58849600 L
B-B_2	0	3.95580600	-4.23856100	-0.16670500 L
B-B_2	0	2.66355500	-3.74334300	1.86459200 L
N-N_3	0	2.68009000	-4.59789300	0.59459800 L
N-N_3	0	1.37119100	-3.61550900	2.67134000 L
B-B_2	0	0.08508400	-3.79775200	1.85636500 L
B-B_2	0	-1.20899900	-2.22607200	3.27901400 L
N-N_3	0	-1.20745700	-3.63242100	2.65826400 L
N-N_3	0	-2.49197600	-1.69773200	3.91744600 L
B-B_2	0	-3.77833300	-2.22006200	3.28280500 L
B-B_2	0	-5.05761100	-0.16874100	3.86289800 L
N-N_3	0	-5.05477800	-1.69861100	3.94498500 L
N-N_3	0	-6.33303900	0.58209800	4.24022000 L
B-B_2	0	-7.62678400	-0.17283700	3.93426500 L
B-B_2	0	-8.92117400	1.91282700	3.54668400 L
N-N_3	0	-8.89235100	0.58414700	4.32848500 L
N-N_3	0	-10.22668100	2.72397100	3.49442800 L
B-B_2	0	-11.45834700	1.79905500	3.48146200 L

B-	0	-12.77397500	3.64505300	2.41390600 L
N-N_3	0	-12.67527200	2.12402000	2.61633500 L
B-	0	12.91164300	-3.15523900	-2.05723400 L
B-B_2	0	11.66738200	-4.16951400	-0.18516300 L
N-N_3	0	11.70650600	-4.07283200	-1.71451000 L
N-N_3	0	10.38036200	-4.46862100	0.58157100 L
B-B_2	0	9.10117500	-4.13922600	-0.17820200 L
B-B_2	0	7.81477500	-3.66866100	1.88300400 L
N-N_3	0	7.82145200	-4.48214100	0.58307100 L
N-N_3	0	6.52269300	-3.56975500	2.69711700 L
B-B_2	0	5.23907300	-3.70262300	1.87432100 L
B-B_2	0	3.93406500	-2.20779000	3.34007300 L
N-N_3	0	3.94726200	-3.59209100	2.68530800 L
N-N_3	0	2.63654800	-1.69724300	3.96706400 L
B-B_2	0	1.36127400	-2.21611900	3.29826100 L
B-B_2	0	0.07045400	-0.16502600	3.85584700 L
N-N_3	0	0.07051300	-1.69837200	3.92855000 L
N-N_3	0	-1.21321600	0.58595900	4.20555800 L
B-B_2	0	-2.49139900	-0.16528600	3.83840800 L
B-B_2	0	-3.77666200	1.92996900	3.46382900 L
N-N_3	0	-3.77157900	0.58478100	4.19817000 L
N-N_3	0	-5.06444800	2.75095900	3.43657600 L
B-B_2	0	-6.34815500	1.91892700	3.49045400 L
B-B_2	0	-7.64669700	3.54525400	2.15854400 L
N-N_3	0	-7.63632900	2.74497200	3.46527700 L
N-N_3	0	-8.93227500	4.23217000	1.70720100 L
B-B_2	0	-10.21694300	3.57951200	2.22024100 L
B-B_2	0	-11.49345500	4.03362200	0.21492800 L
N-N_3	0	-11.50836600	4.22029500	1.73013600 L
N-N_3	0	-12.70766500	3.43556400	-0.49793500 L
B-	0	12.90670500	-3.27216200	1.68407500 L
N-N_3	0	12.96059600	-4.34346800	0.58883800 L
N-N_3	0	11.70826000	-3.48245100	2.64807000 L
B-B_2	0	10.38690400	-3.62687900	1.87001400 L
B-B_2	0	9.07962600	-2.19617700	3.42249700 L
N-N_3	0	9.10315700	-3.55126200	2.70663100 L
N-N_3	0	7.78073800	-1.69774500	4.05848100 L
B-B_2	0	6.50679700	-2.19822900	3.37782000 L
B-B_2	0	5.20914100	-0.16697200	3.95537100 L
N-N_3	0	5.20921500	-1.69769700	4.01557900 L
N-N_3	0	3.91508700	0.58551600	4.27216700 L
B-B_2	0	2.63804600	-0.16647400	3.89628200 L
B-B_2	0	1.35626000	1.92835200	3.48311600 L
N-N_3	0	1.34833100	0.58638700	4.22421700 L

N-N_3	0	0.07672700	2.76813200	3.45104300 L
B-B_2	0	-1.21095700	1.94430300	3.48987200 L
B-B_2	0	-2.49677800	3.62080900	2.16596000 L
N-N_3	0	-2.49813500	2.77017800	3.44563800 L
N-N_3	0	-3.79255600	4.28889900	1.69743300 L
B-B_2	0	-5.07132500	3.57253200	2.14455100 L
B-B_2	0	-6.37109400	4.25903800	0.16049800 L
N-N_3	0	-6.36755300	4.24394600	1.69184400 L
N-N_3	0	-7.66897100	4.56445300	-0.59642700 L
B-B_2	0	-8.95167100	4.21641300	0.16722000 L
N-N_3	0	-10.26381600	4.51217600	-0.58190400 L
N-N_3	0	12.92194800	-1.65623400	4.10804600 L
B-B_2	0	11.64424300	-2.22418900	3.52116800 L
B-B_2	0	10.35626600	-0.17138500	4.05335600 L
N-N_3	0	10.33971900	-1.70823000	4.12623900 L
N-N_3	0	9.06704200	0.59206000	4.38391400 L
B-B_2	0	7.78378900	-0.16430000	4.01631400 L
B-B_2	0	6.49858400	1.90804200	3.55118100 L
N-N_3	0	6.48715200	0.58821500	4.32741300 L
N-N_3	0	5.21552400	2.73807100	3.47810700 L
B-B_2	0	3.92729900	1.91568300	3.51301600 L
B-B_2	0	2.65535400	3.55936000	2.15542000 L
N-N_3	0	2.64477900	2.74883600	3.45442700 L
N-N_3	0	1.37777000	4.26905600	1.69689200 L
B-B_2	0	0.08006400	3.60796000	2.16488500 L
B-B_2	0	-1.20493600	4.35431400	0.16852700 L
N-N_3	0	-1.20541400	4.31010500	1.70751700 L
N-N_3	0	-2.50013300	4.65318100	-0.59864800 L
B-B_2	0	-3.78837900	4.31651200	0.16315900 L
N-N_3	0	-5.08647800	4.60723300	-0.59750200 L
B-	0	12.89151400	-0.16893200	3.73852300 L
B-B_2	0	11.63485000	1.95016800	3.70882400 L
N-N_3	0	11.67374500	0.56496800	4.36275100 L
N-N_3	0	10.34250700	2.74944200	3.56062800 L
B-B_2	0	9.07058800	1.91125600	3.60419000 L
B-B_2	0	7.80514300	3.50500000	2.18211500 L
N-N_3	0	7.78459600	2.73221500	3.50636400 L
N-N_3	0	6.52613800	4.19357000	1.70141300 L
B-B_2	0	5.22997100	3.52721500	2.16626300 L
B-B_2	0	3.95440100	4.22043400	0.16676700 L
N-N_3	0	3.95242200	4.22668100	1.69705600 L
N-N_3	0	2.67321400	4.57285000	-0.59224500 L
B-B_2	0	1.37552000	4.27440600	0.16412400 L
N-N_3	0	0.09476900	4.63304700	-0.59680000 L

B-	0	12.91175500	3.14856500	2.04923500 L
N-N_3	0	12.92367400	2.72730600	3.52273400 L
N-N_3	0	11.70847200	4.07058500	1.71241700 L
B-B_2	0	10.37756700	3.46665300	2.20032800 L
B-B_2	0	9.10183600	4.14001700	0.17746900 L
N-N_3	0	9.10518900	4.16732700	1.70928600 L
N-N_3	0	7.82094600	4.48099100	-0.58352200 L
B-B_2	0	6.52868500	4.17059200	0.17118200 L
N-N_3	0	5.24977700	4.52562500	-0.58835100 L
N-N_3	0	12.96092500	4.35179800	-0.59081900 L
B-B_2	0	11.66845700	4.17513700	0.18361000 L
N-N_3	0	10.38046300	4.47082800	-0.58261300 L
H-H_	0	-12.47768600	0.70132000	-2.20546500 L
H-H_	0	-12.51554400	-1.66886000	-1.68360700 L
H-H_	0	-12.57830300	-2.40711300	0.53734000 L
H-H_	0	-12.46984700	-0.70008800	2.20052500 L
H-H_	0	12.86692900	1.73040600	-5.13844700 L
H-H_	0	12.86004600	-3.60137200	-4.11641400 L
H-H_	0	-12.52542800	1.67278400	1.68766900 L
H-H_	0	-12.56891100	2.40231300	-0.53614300 L
H-H_	0	12.93658600	-5.28190600	1.04848100 L
H-H_	0	12.86078300	-1.73513600	5.14849800 L
H-H_	0	12.86694300	3.59039600	4.10958100 L
H-H_	0	12.93362900	5.28910000	-1.05259300 L
C-C_R	0	-2.00739900	-0.08983700	-0.01563700 H
H-H_	0	-1.18809000	-1.99011400	0.07870400 H
H-H_	0	-0.19447900	-0.79768800	0.90013000 H
C-C_3	0	-0.83642500	-0.98008500	0.02389600 H
H-H_	0	-0.18761800	-0.88522300	-0.86014800 H
N-N_R	0	-1.68640300	1.32451000	0.00105400 H
H-H_	0	-1.15132400	1.56819600	0.82784600 H
H-H_	0	-1.12135500	1.58954500	-0.79756800 H
C-C_R	0	-3.37711100	-0.15681300	-0.00765300 H
O-O_R	0	-4.04825400	0.95670000	-0.00830800 H
O-O_R	0	-4.05872200	-1.32390900	-0.00030300 H
H-H_	0	-4.99769200	-1.08575800	0.00050800 H
H-H_	0	-2.81809800	1.63415800	-0.00660100 H

bINT3@SWBNNT(6.6)

B-B_2	0	-10.22461800	-3.82236900	1.85801900 L
N-N_3	0	-11.50203700	-3.68130900	2.67496600 L
B-	0	-12.78151900	-4.00531300	1.86503500 L
B-B_2	0	-5.07397500	-3.80818200	1.80526500 L
N-N_3	0	-6.36099400	-3.67228400	2.62210300 L
B-B_2	0	-7.65238400	-3.77749900	1.81262900 L
B-B_2	0	-8.92725700	-2.29918200	3.34460600 L
N-N_3	0	-8.92435400	-3.67506100	2.64995800 L
N-N_3	0	-10.21949600	-1.80047500	4.01246400 L
B-B_2	0	-11.46417300	-2.25815800	3.22886500 L
B-	0	-12.74932100	-0.37044000	4.24666300 L
N-N_3	0	-12.65714600	-1.32097800	3.04061400 L
B-B_2	0	0.08711700	-3.84740400	1.82099300 L
N-N_3	0	-1.20296600	-3.72835000	2.63929300 L
B-B_2	0	-2.49391000	-3.86846800	1.82391300 L
B-B_2	0	-3.77879900	-2.31654900	3.27976800 L
N-N_3	0	-3.78817400	-3.70453900	2.62651100 L
N-N_3	0	-5.05917600	-1.79359200	3.93421700 L
B-B_2	0	-6.35339700	-2.29847000	3.30051800 L
B-B_2	0	-7.62654600	-0.25969800	3.92853500 L

N-N_3	0	-7.62966900	-1.79248500	3.98070900 L
N-N_3	0	-8.89000600	0.49418200	4.33425200 L
B-B_2	0	-10.19087300	-0.26636100	4.06350200 L
B-B_2	0	-11.45447300	1.72664400	3.51215300 L
N-N_3	0	-11.46866500	0.48959300	4.40579700 L
N-N_3	0	-12.66903900	2.06549800	2.64939100 L
B-B_2	0	5.24205000	-3.74070600	1.80815200 L
N-N_3	0	3.95353600	-3.65448400	2.62625700 L
B-B_2	0	2.66562000	-3.78396000	1.80904100 L
B-B_2	0	1.36603200	-2.30976200	3.29508400 L
N-N_3	0	1.37895000	-3.69092800	2.62969100 L
N-N_3	0	0.07788700	-1.80384600	3.94123800 L
B-B_2	0	-1.20684900	-2.34247900	3.30940300 L
B-B_2	0	-2.49154000	-0.27304200	3.83363900 L
N-N_3	0	-2.49556400	-1.80539800	3.93072600 L
N-N_3	0	-3.76934500	0.48430800	4.19086300 L
B-B_2	0	-5.05774800	-0.26377200	3.85753300 L
B-B_2	0	-6.34431700	1.83459500	3.50548900 L
N-N_3	0	-6.33078800	0.48905900	4.24059200 L
N-N_3	0	-7.62970900	2.66614000	3.50447700 L
B-B_2	0	-8.91710500	1.83546500	3.57372000 L
B-B_2	0	-10.21346800	3.53199100	2.28528500 L
N-N_3	0	-10.22136900	2.64978400	3.54099400 L
N-N_3	0	-11.50609100	4.18261400	1.81049500 L
B-	0	-12.77086500	3.59025200	2.48090000 L
B-B_2	0	10.39046300	-3.66304000	1.79799200 L
N-N_3	0	9.10758700	-3.60359400	2.63680900 L
B-B_2	0	7.81814600	-3.70552700	1.81256200 L
B-B_2	0	6.51189400	-2.26891600	3.34025300 L
N-N_3	0	6.52774300	-3.62559200	2.63054400 L
N-N_3	0	5.21619800	-1.78329100	3.99145900 L
B-B_2	0	3.93982500	-2.28685400	3.31443700 L
B-B_2	0	2.64160200	-0.26001400	3.89170400 L
N-N_3	0	2.64504800	-1.79079100	3.95652100 L
N-N_3	0	1.34834800	0.48687800	4.21625900 L
B-B_2	0	0.07345800	-0.27143800	3.84745700 L
B-B_2	0	-1.20963000	1.83165200	3.45532800 L
N-N_3	0	-1.21159300	0.48105000	4.18478800 L
N-N_3	0	-2.49225300	2.66177000	3.43733400 L
B-B_2	0	-3.77495500	1.83038500	3.45762900 L
B-B_2	0	-5.06706600	3.52604600	2.19642800 L
N-N_3	0	-5.05679800	2.66197200	3.46130400 L
N-N_3	0	-6.36430300	4.21378900	1.77086900 L
B-B_2	0	-7.64251400	3.50021200	2.21877100 L

B-B_2	0	-8.95129800	4.21957100	0.24736300 L
N-N_3	0	-8.92973600	4.19755600	1.78703700 L
N-N_3	0	-10.26414100	4.52816100	-0.49488400 L
B-B_2	0	-11.49243900	4.03045000	0.29143400 L
B-	0	-12.78100600	4.00873400	-1.86812200 L
N-N_3	0	-12.71061000	3.45650900	-0.43478000 L
B-	0	12.91166800	-3.30862100	1.61794100 L
B-B_2	0	11.64866300	-2.28776200	3.47016000 L
N-N_3	0	11.71231500	-3.53252600	2.57786000 L
N-N_3	0	10.34488800	-1.78653200	4.08928700 L
B-B_2	0	9.08418200	-2.26243000	3.37847100 L
B-B_2	0	7.78637700	-0.24451100	4.01314200 L
N-N_3	0	7.78627900	-1.77861900	4.02685400 L
N-N_3	0	6.48805000	0.50048500	4.33668800 L
B-B_2	0	5.21209200	-0.25176000	3.95225500 L
B-B_2	0	3.92582800	1.83348000	3.53295000 L
N-N_3	0	3.91547000	0.49371000	4.27587200 L
N-N_3	0	2.63902600	2.66194100	3.48270600 L
B-B_2	0	1.35621300	1.83189800	3.48032900 L
B-B_2	0	0.07801200	3.54836400	2.19550100 L
N-N_3	0	0.07205300	2.66348600	3.45019500 L
N-N_3	0	-1.20599600	4.28137900	1.78405700 L
B-B_2	0	-2.49255800	3.54811600	2.18402300 L
B-B_2	0	-3.78897600	4.36993000	0.24193800 L
N-N_3	0	-3.78615600	4.25442200	1.77097600 L
N-N_3	0	-5.09246900	4.65062400	-0.51226000 L
B-B_2	0	-6.37153400	4.27811600	0.24078900 L
B-B_2	0	-7.65258800	3.77993300	-1.81024200 L
N-N_3	0	-7.67141000	4.58818100	-0.50933800 L
N-N_3	0	-8.92317800	3.67387600	-2.64872300 L
B-B_2	0	-10.22446800	3.82377300	-1.85836300 L
B-B_2	0	-11.46276500	2.25810600	-3.22765400 L
N-N_3	0	-11.50090200	3.68213900	-2.67623300 L
N-N_3	0	-12.65436600	1.32028100	-3.03500200 L
B-	0	12.89218400	-0.23444300	3.72828900 L
N-N_3	0	12.92695200	-1.72936400	4.06512500 L
N-N_3	0	11.67532500	0.48280900	4.37308100 L
B-B_2	0	10.35864600	-0.24828100	4.04865500 L
B-B_2	0	9.06985600	1.84107300	3.64238300 L
N-N_3	0	9.06832400	0.50648100	4.39545900 L
N-N_3	0	7.78199800	2.66123800	3.55786300 L
B-B_2	0	6.49740300	1.83358500	3.58317300 L
B-B_2	0	5.22826400	3.48185600	2.22948200 L
N-N_3	0	5.21141000	2.66147000	3.52198300 L

N-N_3	0	3.95157800	4.19431100	1.77712100 L
B-B_2	0	2.65293700	3.51180300	2.20868900 L
B-B_2	0	1.37937600	4.32004700	0.24424600 L
N-N_3	0	1.37555200	4.23929600	1.77385600 L
N-N_3	0	0.10474100	4.69986700	-0.51503900 L
B-B_2	0	-1.20274000	4.46941100	0.25508700 L
B-B_2	0	-2.49533100	3.85058700	-1.78671400 L
N-N_3	0	-2.50542000	4.72163300	-0.51857500 L
N-N_3	0	-3.78289000	3.68636100	-2.60205600 L
B-B_2	0	-5.07583900	3.81434600	-1.79563300 L
B-B_2	0	-6.35108100	2.28955100	-3.28553500 L
N-N_3	0	-6.35920300	3.66889200	-2.61674600 L
N-N_3	0	-7.62609600	1.78731500	-3.97209000 L
B-B_2	0	-8.92540500	2.29595800	-3.33946900 L
B-B_2	0	-10.19064400	0.26479700	-4.06138800 L
N-N_3	0	-10.21731200	1.79872600	-4.00955900 L
N-N_3	0	-11.46971600	-0.48965300	-4.40341500 L
B-	0	-12.74954700	0.37091400	-4.24150000 L
N-N_3	0	12.92158800	2.66713700	3.58542800 L
B-B_2	0	11.63424700	1.88365300	3.75350700 L
B-B_2	0	10.37672800	3.42381700	2.27026000 L
N-N_3	0	10.34028400	2.68225400	3.61718300 L
N-N_3	0	9.10443600	4.13220800	1.79080100 L
B-B_2	0	7.80400100	3.46033500	2.24948400 L
B-B_2	0	6.53039400	4.16929600	0.25212800 L
N-N_3	0	6.52557500	4.15871100	1.78233400 L
N-N_3	0	5.25436400	4.54374900	-0.50065800 L
B-B_2	0	3.95746400	4.23260700	0.24783000 L
B-B_2	0	2.66564500	3.78136500	-1.79425300 L
N-N_3	0	2.68182000	4.60785700	-0.50592900 L
N-N_3	0	1.37352000	3.67140500	-2.60403100 L
B-B_2	0	0.08682700	3.83574000	-1.78634500 L
B-B_2	0	-1.20749900	2.30027200	-3.24514900 L
N-N_3	0	-1.20443700	3.69376600	-2.59532400 L
N-N_3	0	-2.49144500	1.78177200	-3.88961300 L
B-B_2	0	-3.77726800	2.29348300	-3.24500400 L
B-B_2	0	-5.05662300	0.25045100	-3.85604300 L
N-N_3	0	-5.05436800	1.78149200	-3.91367100 L
N-N_3	0	-6.33171500	-0.49459300	-4.24589900 L
B-B_2	0	-7.62577900	0.25429100	-3.92714000 L
B-B_2	0	-8.91920000	-1.83926200	-3.57823300 L
N-N_3	0	-8.89090800	-0.49613900	-4.33509600 L
N-N_3	0	-10.22415000	-2.65208700	-3.54305100 L
B-B_2	0	-11.45611400	-1.72804800	-3.51158600 L

B-	0	-12.77163400	-3.59556000	-2.48277000 L
N-N_3	0	-12.67273800	-2.07058500	-2.65293100 L
B-	0	12.91296100	3.11383900	2.11937500 L
B-B_2	0	11.66887600	4.16397100	0.26702700 L
N-N_3	0	11.70758600	4.03747800	1.79419300 L
N-N_3	0	10.38210500	4.47857900	-0.49388400 L
B-B_2	0	9.10270200	4.13388900	0.25873800 L
B-B_2	0	7.81678700	3.70593400	-1.81218500 L
N-N_3	0	7.82318400	4.49234200	-0.49570600 L
N-N_3	0	6.52501800	3.62427100	-2.62868300 L
B-B_2	0	5.24109500	3.74050500	-1.80386400 L
B-B_2	0	3.93609500	2.27711400	-3.30082400 L
N-N_3	0	3.94957800	3.64750200	-2.61753800 L
N-N_3	0	2.63870600	1.77950100	-3.93839000 L
B-B_2	0	1.36308000	2.28608600	-3.26088100 L
B-B_2	0	0.07162300	0.24739300	-3.85438300 L
N-N_3	0	0.07237600	1.78179700	-3.90222200 L
N-N_3	0	-1.21270200	-0.49754700	-4.21424200 L
B-B_2	0	-2.49039500	0.24794500	-3.83373800 L
B-B_2	0	-3.77518300	-1.85475900	-3.49336900 L
N-N_3	0	-3.77065000	-0.49684900	-4.20424100 L
N-N_3	0	-5.06235200	-2.67704100	-3.48234900 L
B-B_2	0	-6.34639700	-1.84476900	-3.52027700 L
B-B_2	0	-7.64443900	-3.50000200	-2.22305500 L
N-N_3	0	-7.63388200	-2.67214000	-3.51258800 L
N-N_3	0	-8.92999300	-4.19723800	-1.78763000 L
B-B_2	0	-10.21462800	-3.53384300	-2.28687300 L
B-B_2	0	-11.49201300	-4.03131900	-0.29237000 L
N-N_3	0	-11.50612900	-4.18533600	-1.81121700 L
N-N_3	0	-12.70799500	-3.45159700	0.43264100 L
B-	0	12.90856800	3.30402300	-1.61944500 L
N-N_3	0	12.96230700	4.35321600	-0.50302100 L
N-N_3	0	11.71048600	3.53379800	-2.57941500 L
B-B_2	0	10.38889800	3.66305100	-1.79907100 L
B-B_2	0	9.08170400	2.26438100	-3.38043600 L
N-N_3	0	9.10546000	3.60480600	-2.63751200 L
N-N_3	0	7.78292500	1.77914000	-4.02667000 L
B-B_2	0	6.50886800	2.26686600	-3.33707200 L
B-B_2	0	5.21066600	0.24795200	-3.95346100 L
N-N_3	0	5.21143900	1.77951000	-3.98516600 L
N-N_3	0	3.91630800	-0.49820900	-4.28358800 L
B-B_2	0	2.63946200	0.24780400	-3.89506100 L
B-B_2	0	1.35717900	-1.85225000	-3.51549500 L
N-N_3	0	1.34921800	-0.49872000	-4.23516100 L

N-N_3	0	0.07740800	-2.69168300	-3.49633500 L
B-B_2	0	-1.21008500	-1.86751100	-3.52074200 L
B-B_2	0	-2.49479500	-3.57097200	-2.22908200 L
N-N_3	0	-2.49665200	-2.69473400	-3.49150900 L
N-N_3	0	-3.78993100	-4.25196000	-1.77695200 L
B-B_2	0	-5.06910700	-3.52623200	-2.20807700 L
B-B_2	0	-6.36929000	-4.25939900	-0.24080600 L
N-N_3	0	-6.36513600	-4.20858600	-1.77143700 L
N-N_3	0	-7.66774600	-4.58016300	0.50873800 L
B-B_2	0	-8.95006300	-4.21546900	-0.24772700 L
N-N_3	0	-10.26262100	-4.52655000	0.49455500 L
N-N_3	0	12.92409200	1.73639900	-4.07488300 L
B-B_2	0	11.64636300	2.29318100	-3.47741300 L
B-B_2	0	10.35780100	0.25184500	-4.05044300 L
N-N_3	0	10.34188800	1.78984400	-4.09310800 L
N-N_3	0	9.06828900	-0.50456200	-4.39574800 L
B-B_2	0	7.78533600	0.24517600	-4.01389700 L
B-B_2	0	6.49940700	-1.83462700	-3.58680300 L
N-N_3	0	6.48841900	-0.50090100	-4.33894200 L
N-N_3	0	5.21580900	-2.66501000	-3.52826300 L
B-B_2	0	3.92817400	-1.84109500	-3.54717700 L
B-B_2	0	2.65617900	-3.50869800	-2.21864000 L
N-N_3	0	2.64511900	-2.67411500	-3.50234400 L
N-N_3	0	1.37839200	-4.22711800	-1.77461700 L
B-B_2	0	0.08107200	-3.55328800	-2.22487800 L
B-B_2	0	-1.20268200	-4.35225200	-0.24824100 L
N-N_3	0	-1.20298300	-4.26857300	-1.78551100 L
N-N_3	0	-2.49777700	-4.67194200	0.51113100 L
B-B_2	0	-3.78649100	-4.31888600	-0.24348300 L
N-N_3	0	-5.08514800	-4.62500300	0.51004800 L
B-	0	12.89286500	0.24203200	-3.73504700 L
B-B_2	0	11.63557700	-1.87684700	-3.74830700 L
N-N_3	0	11.67501300	-0.47875500	-4.37421200 L
N-N_3	0	10.34280100	-2.67799900	-3.61469000 L
B-B_2	0	9.07137800	-1.83839500	-3.64131900 L
B-B_2	0	7.80579900	-3.45857000	-2.24928500 L
N-N_3	0	7.78491700	-2.66032300	-3.55836500 L
N-N_3	0	6.52666300	-4.15603600	-1.78178200 L
B-B_2	0	5.23061900	-3.47920800	-2.23175700 L
B-B_2	0	3.95598300	-4.21571200	-0.24625500 L
N-N_3	0	3.95286400	-4.18748000	-1.77629800 L
N-N_3	0	2.67559200	-4.58616400	0.50546100 L
B-B_2	0	1.37731600	-4.27063900	-0.24260500 L
N-N_3	0	0.09728200	-4.64907400	0.50989000 L

B-	0	12.91291700	-3.10786200	-2.11322000 L
N-N_3	0	12.92399700	-2.65828600	-3.57833700 L
N-N_3	0	11.70916600	-4.03526900	-1.79317100 L
B-B_2	0	10.37827300	-3.42135000	-2.26852200 L
B-B_2	0	9.10332900	-4.13438300	-0.25851200 L
N-N_3	0	9.10580600	-4.13091000	-1.79056700 L
N-N_3	0	7.82292000	-4.49128400	0.49590200 L
B-B_2	0	6.53019600	-4.16530800	-0.25141300 L
N-N_3	0	5.25190700	-4.53704800	0.50105000 L
N-N_3	0	12.96284400	-4.36016300	0.50356100 L
B-B_2	0	11.66992300	-4.16867400	-0.26662100 L
N-N_3	0	10.38242400	-4.48030200	0.49410200 L
H-H_	0	-12.47277900	-0.74814300	2.18746300 L
H-H_	0	-12.51342200	1.63538400	1.71164900 L
H-H_	0	-12.58134800	2.42294300	-0.49153000 L
H-H_	0	-12.46620000	0.74698900	-2.18294900 L
H-H_	0	12.86952900	-1.83123200	5.10379500 L
H-H_	0	12.86049300	3.51986400	4.18680600 L
H-H_	0	-12.52224700	-1.63896200	-1.71507900 L
H-H_	0	-12.57309600	-2.41879700	0.49065900 L
H-H_	0	12.93852500	5.30065900	-0.94381700 L
H-H_	0	12.86344400	1.83600900	-5.11358800 L
H-H_	0	12.86615200	-3.50987800	-4.18164200 L
H-H_	0	12.93631500	-5.30661400	0.94632500 L
C-C_R	0	-2.07182700	0.07469300	0.11548200 H
H-H_	0	-1.34053000	1.99014700	-0.08968900 H
H-H_	0	-0.33084700	0.81274900	-0.91682400 H
C-C_3	0	-0.93615100	1.00127100	-0.01233900 H
H-H_	0	-0.23539300	0.97104300	0.83534000 H
N-N_R	0	-1.66734200	-1.31478100	-0.00496200 H
H-H_	0	-1.13987600	-1.47984500	-0.86246300 H
H-H_	0	-1.07148300	-1.61577700	0.75912500 H
C-C_R	0	-3.45133200	0.11393900	0.02171200 H
O-O_R	0	-4.14845500	-0.95252800	-0.04152700 H
O-O_R	0	-4.08388800	1.31895300	0.01235100 H
H-H_	0	-5.02955200	1.11112100	-0.03025600 H
H-H_	0	-2.63103700	-1.76356200	-0.02092100 H

Coordinates of all stationary points in the pathway b of α -Ala chiral transformation confined in SWBNNT(7,7)

bSTS1@C

B-B_2	0	-10.28975500	-0.22879300	-4.85092700 L
N-N_3	0	-11.58617500	-1.00578500	-5.06735700 L
B-	0	-12.86042100	-0.13832900	-4.90001100 L
B-B_2	0	-5.15174600	-0.23076000	-4.74521000 L
N-N_3	0	-6.43428500	-1.01097500	-5.03500900 L
B-B_2	0	-7.72429400	-0.23157700	-4.77385900 L
B-B_2	0	-9.01063500	-2.29280000	-4.21533100 L
N-N_3	0	-8.99726200	-1.01759500	-5.08334700 L
N-N_3	0	-10.31257100	-3.10319900	-4.12039200 L
B-B_2	0	-11.52973400	-2.16580800	-4.08115400 L
B-	0	-12.86076400	-3.93824500	-2.95279200 L
N-N_3	0	-12.68383500	-2.41954100	-3.11191100 L
B-B_2	0	-0.01151100	-0.23055700	-4.73647300 L
N-N_3	0	-1.29614000	-1.00909000	-5.02149200 L
B-B_2	0	-2.58119100	-0.23047200	-4.73795800 L
B-B_2	0	-3.86650300	-2.28136500	-4.17347000 L
N-N_3	0	-3.86549400	-1.00946800	-5.02424000 L
N-N_3	0	-5.15126600	-3.10755300	-4.09751800 L
B-B_2	0	-6.43930200	-2.28662300	-4.18554700 L
B-B_2	0	-7.72513700	-3.90119400	-2.79543500 L
N-N_3	0	-7.72359500	-3.11798300	-4.11446800 L
N-N_3	0	-8.99963400	-4.63150600	-2.37615900 L
B-B_2	0	-10.29091100	-3.95468200	-2.84575300 L
B-B_2	0	-11.53344500	-4.56183000	-0.85430800 L
N-N_3	0	-11.58758100	-4.60943500	-2.37632600 L
N-N_3	0	-12.68626800	-3.95655000	-0.05394500 L
B-B_2	0	5.12944700	-0.23085900	-4.75307200 L
N-N_3	0	3.84242500	-1.00945300	-5.03079600 L
B-B_2	0	2.55842700	-0.23054800	-4.74245700 L
B-B_2	0	1.27395800	-2.28217300	-4.17460100 L
N-N_3	0	1.27270200	-1.00916400	-5.02361100 L
N-N_3	0	-0.01119000	-3.10742700	-4.09630900 L
B-B_2	0	-1.29602400	-2.28177200	-4.17227100 L
B-B_2	0	-2.58105700	-3.88794400	-2.77916100 L
N-N_3	0	-2.58121600	-3.10655300	-4.09474600 L
N-N_3	0	-3.86718800	-4.59568700	-2.35049100 L
B-B_2	0	-5.15228100	-3.88579400	-2.77984500 L
B-B_2	0	-6.44081700	-4.72974800	-0.82660000 L
N-N_3	0	-6.43661900	-4.59701000	-2.35320300 L
N-N_3	0	-7.72654900	-5.18505800	-0.12957200 L

B-B_2	0	-9.01301700	-4.74865700	-0.83824800 L
B-B_2	0	-10.29245800	-4.70004200	1.31430400 L
N-N_3	0	-10.31595700	-5.17429900	-0.14346700 L
N-N_3	0	-11.58843000	-4.73292600	2.12050900 L
B-	0	-12.86246500	-4.77045400	1.23805200 L
B-B_2	0	10.27056700	-0.22095500	-4.78165300 L
N-N_3	0	8.98926800	-1.01394400	-5.06553700 L
B-B_2	0	7.70292900	-0.23249000	-4.77295100 L
B-B_2	0	6.41518200	-2.28067500	-4.18697600 L
N-N_3	0	6.41325700	-1.01105600	-5.04225500 L
N-N_3	0	5.12998700	-3.10601300	-4.10388000 L
B-B_2	0	3.84418900	-2.28150400	-4.17980600 L
B-B_2	0	2.56051400	-3.89020100	-2.78555200 L
N-N_3	0	2.55915200	-3.10754600	-4.10051500 L
N-N_3	0	1.27536900	-4.59963200	-2.35466300 L
B-B_2	0	-0.01050000	-3.89019500	-2.78149600 L
B-B_2	0	-1.29535100	-4.73096800	-0.82812800 L
N-N_3	0	-1.29604400	-4.59961500	-2.35278300 L
N-N_3	0	-2.58150200	-5.17816900	-0.13055700 L
B-B_2	0	-3.86687200	-4.72568100	-0.82580400 L
B-B_2	0	-5.15249000	-4.61576700	1.29592400 L
N-N_3	0	-5.15322800	-5.17335500	-0.12912700 L
N-N_3	0	-6.43700300	-4.71286300	2.12002500 L
B-B_2	0	-7.72609500	-4.63143500	1.30083600 L
B-B_2	0	-9.01156100	-3.61045700	3.17566700 L
N-N_3	0	-9.00024000	-4.74931100	2.13533100 L
N-N_3	0	-10.31292900	-3.32783400	3.94234400 L
B-B_2	0	-11.53127500	-3.50613200	3.02255000 L
B-	0	-12.85981400	-1.99115600	4.47929400 L
N-N_3	0	-12.68017300	-2.49833200	3.03938300 L
B-	0	12.77822100	-0.18885100	-4.38797600 L
B-B_2	0	11.54668000	-2.31186200	-4.25552800 L
N-N_3	0	11.59331500	-0.97703100	-5.00085600 L
N-N_3	0	10.25860600	-3.12751600	-4.14849100 L
B-B_2	0	8.98659100	-2.28825500	-4.21205500 L
B-B_2	0	7.70612200	-3.89312600	-2.79566000 L
N-N_3	0	7.69873500	-3.10745300	-4.11278100 L
N-N_3	0	6.41861300	-4.59448800	-2.35758300 L
B-B_2	0	5.13225200	-3.88673200	-2.78747500 L
B-B_2	0	3.84798500	-4.71788300	-0.83041700 L
N-N_3	0	3.84737400	-4.59590900	-2.35577800 L
N-N_3	0	2.56372100	-5.16826100	-0.13237100 L
B-B_2	0	1.27615200	-4.72623200	-0.82962400 L
B-B_2	0	-0.00863700	-4.61499700	1.29260200 L

N-N_3	0	-0.00843900	-5.17575200	-0.13130300 L
N-N_3	0	-1.29337800	-4.71332400	2.11713500 L
B-B_2	0	-2.58072500	-4.62273300	1.29566400 L
B-B_2	0	-3.86597800	-3.58489000	3.15214800 L
N-N_3	0	-3.86695700	-4.71378100	2.11879300 L
N-N_3	0	-5.15054800	-3.31147900	3.93724000 L
B-B_2	0	-6.43965500	-3.58911200	3.16192400 L
B-B_2	0	-7.72341500	-1.85582000	4.40546900 L
N-N_3	0	-7.72358600	-3.32190100	3.95367100 L
N-N_3	0	-8.99612500	-1.27821400	5.02251000 L
B-B_2	0	-10.28910000	-1.88998200	4.47390600 L
B-B_2	0	-11.52768300	0.19062900	4.61200400 L
N-N_3	0	-11.58519800	-1.28078500	5.00339500 L
N-N_3	0	-12.68021100	0.83736100	3.84444300 L
B-	0	12.78213700	-3.55297600	-2.58875100 L
N-N_3	0	12.84112400	-3.07528600	-4.04204700 L
N-N_3	0	11.59814300	-4.52467900	-2.35391100 L
B-B_2	0	10.27393000	-3.88461600	-2.80822200 L
B-B_2	0	8.99103900	-4.72970500	-0.83831100 L
N-N_3	0	8.99454400	-4.60505000	-2.36680800 L
N-N_3	0	7.70382900	-5.16297400	-0.13509000 L
B-B_2	0	6.41951300	-4.71350400	-0.83162900 L
B-B_2	0	5.13491600	-4.60515500	1.29232800 L
N-N_3	0	5.13498100	-5.16207000	-0.13320000 L
N-N_3	0	3.84878300	-4.70213600	2.11432600 L
B-B_2	0	2.56293300	-4.60736300	1.29122800 L
B-B_2	0	1.27694900	-3.58111000	3.15108800 L
N-N_3	0	1.27807800	-4.70672800	2.11457600 L
N-N_3	0	-0.00892300	-3.30967800	3.93258200 L
B-B_2	0	-1.29412200	-3.58416000	3.15019600 L
B-B_2	0	-2.57982100	-1.84534200	4.37365100 L
N-N_3	0	-2.57957800	-3.31049200	3.93228800 L
N-N_3	0	-3.86430700	-1.26256400	4.96466900 L
B-B_2	0	-5.15063800	-1.84633300	4.37949500 L
B-B_2	0	-6.43781000	0.25218400	4.75433000 L
N-N_3	0	-6.43306900	-1.26448100	4.97534600 L
N-N_3	0	-7.72133900	1.03405700	5.04923900 L
B-B_2	0	-9.00895300	0.24630900	4.78659000 L
B-B_2	0	-10.28900000	2.33747100	4.26927500 L
N-N_3	0	-10.31024000	1.01907500	5.05129300 L
N-N_3	0	-11.58601900	3.13087900	4.13132000 L
B-	0	-12.85918700	2.27532700	4.35763300 L
N-N_3	0	12.84599800	-5.07619600	-0.11311600 L
B-B_2	0	11.55143200	-4.77272300	-0.84518400 L

B-B_2	0	10.27675700	-4.61349600	1.28478400 L
N-N_3	0	10.26371000	-5.19699000	-0.13970500 L
N-N_3	0	8.99651400	-4.71425800	2.12261700 L
B-B_2	0	7.70878400	-4.61277600	1.29648400 L
B-B_2	0	6.41911600	-3.57634200	3.15362600 L
N-N_3	0	6.42017100	-4.70244900	2.11682200 L
N-N_3	0	5.13301500	-3.30627200	3.93600600 L
B-B_2	0	3.84774500	-3.57748400	3.15207100 L
B-B_2	0	2.56110000	-1.84567700	4.38314600 L
N-N_3	0	2.56197300	-3.30898900	3.93523200 L
N-N_3	0	1.27431400	-1.26209500	4.96783300 L
B-B_2	0	-0.00944200	-1.84507800	4.37539700 L
B-B_2	0	-1.29511300	0.25067200	4.73380500 L
N-N_3	0	-1.29503700	-1.26202900	4.96252700 L
N-N_3	0	-2.57957400	1.02978400	5.01788100 L
B-B_2	0	-3.86536100	0.25085600	4.73831500 L
B-B_2	0	-5.15101200	2.30076500	4.17167600 L
N-N_3	0	-5.14925000	1.03071500	5.02575900 L
N-N_3	0	-6.43460100	3.12804500	4.09842500 L
B-B_2	0	-7.72353300	2.31009000	4.19744500 L
B-B_2	0	-9.01233000	3.92627500	2.80528500 L
N-N_3	0	-8.99761900	3.15090700	4.13869300 L
N-N_3	0	-10.31558100	4.61295900	2.36793200 L
B-B_2	0	-11.53221900	3.75082400	2.74053900 L
B-	0	-12.86369400	4.85482800	0.95270400 L
N-N_3	0	-12.68681300	3.55749300	1.75800500 L
B-	0	12.78465200	-4.23182600	1.16255100 L
B-B_2	0	11.55116600	-3.62064800	3.19915800 L
N-N_3	0	11.60035700	-4.65122000	2.06978100 L
N-N_3	0	10.26226100	-3.33333700	3.96910100 L
B-B_2	0	8.99081100	-3.59111200	3.16695200 L
B-B_2	0	7.70615100	-1.84552800	4.40073800 L
N-N_3	0	7.70202100	-3.30871000	3.94078700 L
N-N_3	0	6.41642300	-1.26019200	4.97990200 L
B-B_2	0	5.13238000	-1.84354600	4.38675900 L
B-B_2	0	3.84521300	0.25193300	4.74362200 L
N-N_3	0	3.84546000	-1.26128300	4.97328500 L
N-N_3	0	2.55902400	1.03101300	5.02206400 L
B-B_2	0	1.27480500	0.25086700	4.73830900 L
B-B_2	0	-0.01043200	2.29905000	4.16215300 L
N-N_3	0	-0.01074200	1.03014600	5.01707400 L
N-N_3	0	-1.29522100	3.12468500	4.08520100 L
B-B_2	0	-2.58044400	2.29965000	4.16434800 L
B-B_2	0	-3.86701900	3.90755400	2.77418900 L

N-N_3	0	-3.86531900	3.12532900	4.08937000 L
N-N_3	0	-5.15323700	4.61703100	2.34751900 L
B-B_2	0	-6.44044800	3.91309900	2.78225900 L
B-B_2	0	-7.72770300	4.75841600	0.82859800 L
N-N_3	0	-7.72632600	4.62838600	2.35695600 L
N-N_3	0	-9.00292900	5.22923600	0.13169400 L
B-B_2	0	-10.29394200	4.82456900	0.84966900 L
B-B_2	0	-11.53554200	4.49760800	-1.20682100 L
N-N_3	0	-11.59077100	5.20676000	0.14077600 L
N-N_3	0	-12.68576200	3.59931800	-1.66074100 L
B-	0	12.78082200	-1.71079800	4.02806500 L
N-N_3	0	12.84488500	-3.23446300	3.89298600 L
N-N_3	0	11.59633000	-1.26593900	4.92249700 L
B-B_2	0	10.27386000	-1.85544400	4.40016900 L
B-B_2	0	8.98748400	0.25374500	4.77723600 L
N-N_3	0	8.99237500	-1.26388000	4.99927900 L
N-N_3	0	7.69825800	1.03390600	5.03987300 L
B-B_2	0	6.41614400	0.25336800	4.75049400 L
B-B_2	0	5.13082400	2.30355100	4.17541000 L
N-N_3	0	5.12953100	1.03235600	5.02817200 L
N-N_3	0	3.84417300	3.12669000	4.09125400 L
B-B_2	0	2.55972600	2.30025200	4.16699800 L
B-B_2	0	1.27453100	3.90821900	2.77129700 L
N-N_3	0	1.27412100	3.12478300	4.08587200 L
N-N_3	0	-0.01041800	4.62173000	2.34678200 L
B-B_2	0	-1.29550000	3.90851300	2.77107500 L
B-B_2	0	-2.58212200	4.75021500	0.82098600 L
N-N_3	0	-2.58171600	4.61805900	2.34538600 L
N-N_3	0	-3.86987600	5.19494900	0.12549200 L
B-B_2	0	-5.15438300	4.74335100	0.82249600 L
B-B_2	0	-6.44321300	4.64045300	-1.30266900 L
N-N_3	0	-6.43979300	5.19253600	0.12681400 L
N-N_3	0	-7.72861900	4.74242200	-2.12961300 L
B-B_2	0	-9.01537800	4.66042700	-1.30198800 L
B-B_2	0	-10.29361700	3.67410800	-3.21715800 L
N-N_3	0	-10.31796100	4.73816800	-2.11358700 L
N-N_3	0	-11.58954200	3.35206900	-3.95734400 L
B-	0	-12.86406300	3.76701200	-3.17825000 L
N-N_3	0	12.84099100	1.04204800	4.96418100 L
B-B_2	0	11.54746900	0.25983500	4.82633400 L
B-B_2	0	10.27211300	2.30313200	4.20298100 L
N-N_3	0	10.25828000	1.03994600	5.08285400 L
N-N_3	0	8.99136200	3.14178500	4.11686700 L
B-B_2	0	7.70440100	2.31166600	4.19138300 L

B-B_2	0	6.41688900	3.90587700	2.77880800 L
N-N_3	0	6.41524800	3.13118100	4.09905800 L
N-N_3	0	5.13212600	4.61481000	2.34693000 L
B-B_2	0	3.84563500	3.90673300	2.77453700 L
B-B_2	0	2.56098700	4.74970900	0.82115900 L
N-N_3	0	2.56072000	4.61776400	2.34564400 L
N-N_3	0	1.27673700	5.20377600	0.12480000 L
B-B_2	0	-0.01051700	4.76137100	0.82262000 L
B-B_2	0	-1.29705800	4.64648200	-1.29990000 L
N-N_3	0	-1.29793600	5.20542100	0.12512100 L
N-N_3	0	-2.58360200	4.73610000	-2.12290800 L
B-B_2	0	-3.86927700	4.63875800	-1.30000200 L
B-B_2	0	-5.15424600	3.60384700	-3.15721700 L
N-N_3	0	-5.15543300	4.73220900	-2.12340900 L
N-N_3	0	-6.43741900	3.33284200	-3.94378700 L
B-B_2	0	-7.72745500	3.61790900	-3.17295700 L
B-B_2	0	-9.01195600	1.88337800	-4.42024200 L
N-N_3	0	-9.00078900	3.36096600	-3.97706400 L
N-N_3	0	-10.31287300	1.29770800	-4.99073800 L
B-B_2	0	-11.53094100	1.85552900	-4.23785400 L
N-N_3	0	-12.68027000	0.93942500	-3.81881400 L
B-	0	12.78008100	2.10284700	3.86206900 L
B-B_2	0	11.54870600	3.95925500	2.82334400 L
N-N_3	0	11.59531000	3.07890200	4.07330700 L
N-N_3	0	10.26076900	4.64764900	2.37277300 L
B-B_2	0	8.98842400	3.92065500	2.79573300 L
B-B_2	0	7.70723000	4.75016100	0.82375900 L
N-N_3	0	7.70095800	4.61668500	2.35157400 L
N-N_3	0	6.41961900	5.19129200	0.12463200 L
B-B_2	0	5.13333200	4.74407600	0.82191400 L
B-B_2	0	3.84725000	4.63595800	-1.29976400 L
N-N_3	0	3.84829800	5.19437100	0.12498700 L
N-N_3	0	2.56148900	4.73347700	-2.12243900 L
B-B_2	0	1.27515100	4.64226800	-1.29907400 L
B-B_2	0	-0.01116100	3.60707000	-3.15426300 L
N-N_3	0	-0.01054700	4.73760900	-2.12248400 L
N-N_3	0	-1.29679200	3.33171600	-3.93560100 L
B-B_2	0	-2.58249200	3.60556000	-3.15430700 L
B-B_2	0	-3.86740500	1.86605600	-4.38076200 L
N-N_3	0	-3.86763700	3.33072700	-3.93738500 L
N-N_3	0	-5.15115600	1.28257700	-4.97381100 L
B-B_2	0	-6.44043400	1.86819900	-4.39514500 L
N-N_3	0	-7.72371400	1.28646200	-4.99610500 L
B-	0	12.78359500	4.34981000	0.78215900 L

N-N_3	0	12.84312100	4.55322100	2.29839200 L
N-N_3	0	11.59919800	5.12171400	0.14748200 L
B-B_2	0	10.27517300	4.74512900	0.83656100 L
B-B_2	0	8.99047100	4.64640100	-1.30339600 L
N-N_3	0	8.99562500	5.20191000	0.12604200 L
N-N_3	0	7.70247900	4.72960000	-2.12401100 L
B-B_2	0	6.41879300	4.63094900	-1.29979700 L
B-B_2	0	5.13218500	3.60403700	-3.16059100 L
N-N_3	0	5.13341900	4.72908100	-2.12279300 L
N-N_3	0	3.84486100	3.33107800	-3.94002900 L
B-B_2	0	2.56018800	3.60488300	-3.15586800 L
B-B_2	0	1.27371400	1.86598500	-4.37709200 L
N-N_3	0	1.27399400	3.33145300	-3.93645500 L
N-N_3	0	-0.01167200	1.28249100	-4.96435800 L
B-B_2	0	-1.29663500	1.86625200	-4.37626600 L
N-N_3	0	-2.58099700	1.28256700	-4.96622800 L
N-N_3	0	12.84494700	4.63833300	-2.11009400 L
B-B_2	0	11.55091600	4.68575000	-1.31802700 L
B-B_2	0	10.27397100	3.61557100	-3.16527600 L
N-N_3	0	10.26253400	4.76122700	-2.13699700 L
N-N_3	0	8.99260100	3.34166800	-3.96171000 L
B-B_2	0	7.70607700	3.60937600	-3.17160700 L
B-B_2	0	6.41538600	1.86690500	-4.39098300 L
N-N_3	0	6.41632500	3.33196000	-3.94692600 L
N-N_3	0	5.12841400	1.28354600	-4.97628200 L
B-B_2	0	3.84438200	1.86626200	-4.38348200 L
N-N_3	0	2.55776300	1.28289600	-4.96893200 L
B-	0	12.78121100	3.32328100	-2.89153400 L
B-B_2	0	11.54699400	1.89081100	-4.46215700 L
N-N_3	0	11.59660800	3.30871400	-3.89040900 L
N-N_3	0	10.25741700	1.29832400	-5.03017000 L
B-B_2	0	8.98689000	1.87654700	-4.41540500 L
N-N_3	0	7.69724800	1.28620600	-4.98820700 L
N-N_3	0	12.84026300	1.24389200	-4.92379800 L
H-H_	0	-12.41457400	-2.01604200	-2.18655800 L
H-H_	0	-12.41608500	-2.98009500	0.20121600 L
H-H_	0	-12.40382700	-1.69248900	2.43442700 L
H-H_	0	-12.40811100	0.87434500	2.83634500 L
H-H_	0	12.82655000	-3.91438500	-4.66517600 L
H-H_	0	12.83287900	-6.08527000	0.15925200 L
H-H_	0	-12.41825300	2.79079300	1.10104600 L
H-H_	0	-12.41166000	2.61033500	-1.46470600 L
H-H_	0	12.83262500	-3.65069000	4.85173100 L
H-H_	0	12.82645600	1.52769100	5.88967000 L

H-H_	0	-12.40412000	0.47268800	-2.92571400 L
H-H_	0	12.82862400	5.58001700	2.49350200 L
H-H_	0	12.83274900	5.42854900	-2.79419500 L
H-H_	0	12.82610200	1.20562000	-5.96827100 L
C-C_3	0	-0.52159300	-0.05484400	0.38200200 H
H-H_	0	-1.37013400	-1.31145600	-1.17415200 H
H-H_	0	-2.56649700	-0.60694600	-0.05626900 H
C-C_3	0	-1.56703500	-1.04784400	-0.13083100 H
H-H_	0	-1.55716900	-1.96743900	0.45876700 H
N-N_3	0	-0.45822200	1.15793600	-0.44517100 H
H-H_	0	-0.53982600	2.00169200	0.10566800 H
H-H_	0	-1.15439400	1.16636900	-1.18130000 H
C-C_R	0	0.88445500	-0.66211400	0.41808300 H
O-O_R	0	1.64488300	-0.58432600	1.36080700 H
O-O_R	0	1.22072800	-1.28366200	-0.73642200 H
H-H_	0	2.14228800	-1.57865400	-0.64378400 H
H-H_	0	-0.74013400	0.20202800	1.42470200 H

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B-B_2	0	-10.25598600	-4.60671600	-1.62479400 L
N-N_3	0	-11.55308700	-5.10001700	-0.98861400 L
B-	0	-12.82590900	-4.61869200	-1.73144800 L
B-B_2	0	-5.11679400	-4.52770300	-1.58188800 L
N-N_3	0	-6.40194800	-5.08708100	-0.97093000 L
B-B_2	0	-7.68991300	-4.54389600	-1.59205400 L
B-B_2	0	-8.97805100	-4.79932700	0.52516700 L
N-N_3	0	-8.96509300	-5.12377300	-0.98271100 L
N-N_3	0	-10.28086500	-5.00990700	1.31237900 L
B-B_2	0	-11.49800700	-4.62260200	0.45738200 L
B-	0	-12.82707900	-4.22835100	2.52228300 L
N-N_3	0	-12.64879000	-3.81232700	1.05329300 L
B-B_2	0	0.02589400	-4.53919900	-1.58143000 L
N-N_3	0	-1.26080100	-5.09605800	-0.96933500 L
B-B_2	0	-2.54500700	-4.53178900	-1.57966900 L
B-B_2	0	-3.83224500	-4.77732000	0.52915900 L
N-N_3	0	-3.83222200	-5.08782200	-0.96889400 L
N-N_3	0	-5.11865100	-5.00644900	1.32477900 L
B-B_2	0	-6.40602500	-4.77953000	0.53016500 L
B-B_2	0	-7.69066800	-4.08067400	2.54312400 L
N-N_3	0	-7.69163300	-5.01719600	1.32828100 L
N-N_3	0	-8.96423900	-3.95932500	3.37806000 L
B-B_2	0	-10.25679200	-4.14277100	2.57656700 L
B-B_2	0	-11.49452400	-2.51685100	3.88206600 L

N-N_3	0	-11.55285000	-3.94697600	3.35938700 L
N-N_3	0	-12.64467700	-1.54504300	3.62013100 L
B-B_2	0	5.16930000	-4.53118100	-1.58219700 L
N-N_3	0	3.88389400	-5.08953400	-0.96885100 L
B-B_2	0	2.59711300	-4.53324400	-1.58045500 L
B-B_2	0	1.31183700	-4.78429100	0.52930200 L
N-N_3	0	1.31245300	-5.09558700	-0.96909400 L
N-N_3	0	0.02602300	-5.01539900	1.32528800 L
B-B_2	0	-1.26028400	-4.78648300	0.52935500 L
B-B_2	0	-2.54573600	-4.06726800	2.52884200 L
N-N_3	0	-2.54717700	-5.01152000	1.32492000 L
N-N_3	0	-3.83116100	-3.92452600	3.34580700 L
B-B_2	0	-5.11755700	-4.06486600	2.53091000 L
B-B_2	0	-6.40369400	-2.55616000	4.03603300 L
N-N_3	0	-6.40091300	-3.92694200	3.35088100 L
N-N_3	0	-7.68702900	-2.08002700	4.72356600 L
B-B_2	0	-8.97529300	-2.57455100	4.05769900 L
B-B_2	0	-10.25280700	-0.56090100	4.82706700 L
N-N_3	0	-10.27628900	-2.08976900	4.71598500 L
N-N_3	0	-11.54886700	0.17089500	5.16740400 L
B-	0	-12.82334300	-0.65792700	4.86274600 L
B-B_2	0	10.31112400	-4.53364200	-1.59904800 L
N-N_3	0	9.03143400	-5.10096200	-0.97349500 L
B-B_2	0	7.74319700	-4.53910400	-1.58635800 L
B-B_2	0	6.45529700	-4.77255700	0.52830500 L
N-N_3	0	6.45535500	-5.08891800	-0.96929300 L
N-N_3	0	5.17031400	-5.00552100	1.32434100 L
B-B_2	0	3.88370500	-4.77695000	0.52911200 L
B-B_2	0	2.59740100	-4.06875500	2.53083900 L
N-N_3	0	2.59861700	-5.01084900	1.32497500 L
N-N_3	0	1.31143400	-3.92785000	3.34647000 L
B-B_2	0	0.02584900	-4.07159000	2.53013500 L
B-B_2	0	-1.25952400	-2.55258700	4.01805800 L
N-N_3	0	-1.26021000	-3.92672300	3.34514600 L
N-N_3	0	-2.54399900	-2.07248800	4.69511300 L
B-B_2	0	-3.83056900	-2.55222300	4.02238000 L
B-B_2	0	-5.11467100	-0.54282800	4.72200800 L
N-N_3	0	-5.11431900	-2.07300600	4.70245900 L
N-N_3	0	-6.39705700	0.18039000	5.13444900 L
B-B_2	0	-7.68728500	-0.54614500	4.75085800 L
B-B_2	0	-8.97340300	1.57833900	4.53369000 L
N-N_3	0	-8.96004000	0.17949300	5.18389200 L
N-N_3	0	-10.27514700	2.39371900	4.57178300 L
B-B_2	0	-11.49263300	1.47531100	4.38202400 L

B-	0	-12.82380900	3.40613000	3.55433200 L
N-N_3	0	-12.64603500	1.88181600	3.46542000 L
B-	0	12.81960500	-4.15377600	-1.48045300 L
B-B_2	0	11.58742900	-4.83285900	0.53526900 L
N-N_3	0	11.63507800	-5.01984600	-0.98224100 L
N-N_3	0	10.29912300	-5.04059800	1.33096700 L
B-B_2	0	9.02694800	-4.78949600	0.52809500 L
B-B_2	0	7.74352000	-4.07396000	2.54189100 L
N-N_3	0	7.73923500	-5.00647900	1.32424800 L
N-N_3	0	6.45433400	-3.92765000	3.35314100 L
B-B_2	0	5.16957500	-4.06762500	2.53387800 L
B-B_2	0	3.88210900	-2.55415600	4.02508000 L
N-N_3	0	3.88266300	-3.92686200	3.34842700 L
N-N_3	0	2.59566700	-2.07397200	4.69822400 L
B-B_2	0	1.31119300	-2.55400800	4.02048400 L
B-B_2	0	0.02582200	-0.54321100	4.71339400 L
N-N_3	0	0.02547100	-2.07306100	4.69398600 L
N-N_3	0	-1.25881100	0.17982300	5.11922700 L
B-B_2	0	-2.54412600	-0.54275300	4.71500000 L
B-B_2	0	-3.82939900	1.57205200	4.48796900 L
N-N_3	0	-3.82831900	0.18011700	5.12322400 L
N-N_3	0	-5.11378000	2.40023500	4.54708000 L
B-B_2	0	-6.40206500	1.57634100	4.50206200 L
B-B_2	0	-7.68809500	3.39497900	3.39212200 L
N-N_3	0	-7.68613400	2.40861100	4.56698500 L
N-N_3	0	-8.96249600	4.18428700	3.09796200 L
B-B_2	0	-10.25378700	3.44025900	3.45174000 L
B-B_2	0	-11.49652000	4.36396000	1.58592300 L
N-N_3	0	-11.55063700	4.16254200	3.09527600 L
N-N_3	0	-12.64906000	3.89711400	0.69734600 L
B-	0	12.81956400	-3.74762200	2.30970500 L
N-N_3	0	12.88149000	-4.91756500	1.32405600 L
N-N_3	0	11.63460200	-3.89404500	3.29760200 L
B-B_2	0	10.31152800	-4.07872200	2.53283700 L
B-B_2	0	9.02505700	-2.56647300	4.04958300 L
N-N_3	0	9.03067300	-3.93845000	3.36405600 L
N-N_3	0	7.73581900	-2.07717000	4.71153100 L
B-B_2	0	6.45338500	-2.55448300	4.02977600 L
B-B_2	0	5.16724900	-0.54368900	4.72632100 L
N-N_3	0	5.16677600	-2.07425900	4.70297400 L
N-N_3	0	3.88026300	0.17959500	5.12623600 L
B-B_2	0	2.59604600	-0.54382500	4.71813700 L
B-B_2	0	1.31099100	1.57093800	4.48395300 L
N-N_3	0	1.31030300	0.17951300	5.12042300 L

N-N_3	0	0.02598900	2.39795900	4.53993700 L
B-B_2	0	-1.25892900	1.57107700	4.48305500 L
B-B_2	0	-2.54430900	3.38101100	3.36868400 L
N-N_3	0	-2.54355300	2.39824200	4.54119400 L
N-N_3	0	-3.83009300	4.15021900	3.06296500 L
B-B_2	0	-5.11531700	3.38079600	3.37228700 L
B-B_2	0	-6.40450700	4.53310300	1.58368700 L
N-N_3	0	-6.39944900	4.15279600	3.06807700 L
N-N_3	0	-7.69023200	5.09757400	0.97176800 L
B-B_2	0	-8.97646100	4.55098000	1.59978300 L
B-B_2	0	-10.25673300	4.85721400	-0.53109500 L
N-N_3	0	-10.27951300	5.08510300	0.98484500 L
N-N_3	0	-11.55323400	5.02222500	-1.32007800 L
B-	0	-12.82677500	4.91255000	-0.44286600 L
N-N_3	0	12.87891400	-2.02226200	4.64933600 L
B-B_2	0	11.58531000	-2.58706000	4.09089200 L
B-B_2	0	10.30851500	-0.55507700	4.74817000 L
N-N_3	0	10.29611800	-2.09456900	4.74834900 L
N-N_3	0	9.02717300	0.18110800	5.15725300 L
B-B_2	0	7.74084900	-0.54364400	4.74359400 L
B-B_2	0	6.45218600	1.57146600	4.49554600 L
N-N_3	0	6.45118000	0.18077900	5.13560800 L
N-N_3	0	5.16647400	2.39841800	4.54683000 L
B-B_2	0	3.88137600	1.57121700	4.48918900 L
B-B_2	0	2.59670500	3.38156400	3.36996800 L
N-N_3	0	2.59578900	2.39812600	4.54235600 L
N-N_3	0	1.31149100	4.15190100	3.06248100 L
B-B_2	0	0.02607700	3.38192300	3.36834900 L
B-B_2	0	-1.25923100	4.53076400	1.57981500 L
N-N_3	0	-1.25933100	4.15185500	3.06222400 L
N-N_3	0	-2.54573300	5.08703900	0.96783000 L
B-B_2	0	-3.83094400	4.52726900	1.58018400 L
B-B_2	0	-5.11728300	4.77060500	-0.52942600 L
N-N_3	0	-5.11715800	5.08492200	0.96803500 L
N-N_3	0	-6.40180200	5.00426900	-1.32543300 L
B-B_2	0	-7.69050400	4.78784000	-0.53049300 L
B-B_2	0	-8.97656900	4.09116400	-2.54786300 L
N-N_3	0	-8.96503900	5.04208000	-1.33337500 L
N-N_3	0	-10.27836700	3.93805400	-3.34980100 L
B-B_2	0	-11.49623800	3.96145800	-2.41252500 L
B-	0	-12.82456700	2.70783500	-4.10004700 L
N-N_3	0	-12.64583000	2.97118300	-2.59620200 L
B-	0	12.81555500	-0.52183000	4.35189600 L
B-B_2	0	11.58351000	1.59420100	4.56652400 L

N-N_3	0	11.63118600	0.15623000	5.08558600 L
N-N_3	0	10.29505500	2.41593700	4.59511000 L
B-B_2	0	9.02353100	1.57674600	4.52108000 L
B-B_2	0	7.74182800	3.39108000	3.38545600 L
N-N_3	0	7.73510800	2.40037200	4.55634900 L
N-N_3	0	6.45354600	4.15377700	3.06836300 L
B-B_2	0	5.16817500	3.38279600	3.37463500 L
B-B_2	0	3.88321200	4.52782200	1.58112100 L
N-N_3	0	3.88230900	4.15139300	3.06447900 L
N-N_3	0	2.59823200	5.08791900	0.96829900 L
B-B_2	0	1.31168000	4.53079200	1.57986700 L
B-B_2	0	0.02642900	4.78475200	-0.53060700 L
N-N_3	0	0.02625600	5.09161600	0.96871600 L
N-N_3	0	-1.26052600	5.01105300	-1.32585600 L
B-B_2	0	-2.54523300	4.77507700	-0.52992400 L
B-B_2	0	-3.83115900	4.06549300	-2.53296200 L
N-N_3	0	-3.83199400	5.00407300	-1.32472400 L
N-N_3	0	-5.11606200	3.92538200	-3.35152200 L
B-B_2	0	-6.40466200	4.06967900	-2.53983500 L
B-B_2	0	-7.68818900	2.56431100	-4.05045000 L
N-N_3	0	-7.68907300	3.93609800	-3.36379400 L
N-N_3	0	-8.96101800	2.09425800	-4.75257500 L
B-B_2	0	-10.25404300	2.60742500	-4.11098500 L
B-B_2	0	-11.49200000	0.57689600	-4.58615900 L
N-N_3	0	-11.54992000	2.09242100	-4.73279800 L
N-N_3	0	-12.64417100	-0.18636400	-3.93366400 L
B-	0	12.81731500	3.09315900	3.12545500 L
N-N_3	0	12.87765500	2.38275100	4.48019300 L
N-N_3	0	11.63330800	4.09025000	3.05529400 L
B-B_2	0	10.30955300	3.38303800	3.39742800 L
B-B_2	0	9.02624000	4.54184800	1.59396600 L
N-N_3	0	9.02955900	4.16543600	3.08064700 L
N-N_3	0	7.73893200	5.08523600	0.97203700 L
B-B_2	0	6.45465700	4.52540500	1.58343900 L
B-B_2	0	5.17047500	4.77392200	-0.52962100 L
N-N_3	0	5.16999400	5.08395900	0.96916500 L
N-N_3	0	3.88477500	5.00650200	-1.32503000 L
B-B_2	0	2.59801900	4.77746300	-0.53009500 L
B-B_2	0	1.31242500	4.07097900	-2.53267400 L
N-N_3	0	1.31310300	5.01256000	-1.32611200 L
N-N_3	0	0.02633100	3.92763200	-3.34783200 L
B-B_2	0	-1.25930100	4.06887500	-2.53158500 L
B-B_2	0	-2.54408000	2.55245100	-4.02237400 L
N-N_3	0	-2.54482500	3.92578800	-3.34812600 L

N-N_3	0	-3.82844800	2.07256000	-4.70025700 L
B-B_2	0	-5.11528300	2.55278300	-4.02808400 L
B-B_2	0	-6.40164500	0.54244500	-4.73682300 L
N-N_3	0	-6.39781100	2.07477000	-4.70990500 L
N-N_3	0	-7.68487500	-0.18239900	-5.15387200 L
B-B_2	0	-8.97297400	0.55171400	-4.76737200 L
B-B_2	0	-10.25186800	-1.59623300	-4.59510800 L
N-N_3	0	-10.27393700	-0.16873200	-5.15363300 L
N-N_3	0	-11.54834500	-2.40240700	-4.58776400 L
B-	0	-12.82213500	-1.52246100	-4.67276900 L
N-N_3	0	12.88099000	5.00716300	0.93758200 L
B-B_2	0	11.58662300	4.58530100	1.60874700 L
B-B_2	0	10.31255800	4.77931100	-0.51841500 L
N-N_3	0	10.29870800	5.11932900	0.98286300 L
N-N_3	0	9.03262100	5.01651900	-1.32860200 L
B-B_2	0	7.74450400	4.78062200	-0.53104200 L
B-B_2	0	6.45552500	4.06403800	-2.53320200 L
N-N_3	0	6.45639900	5.00507500	-1.32591800 L
N-N_3	0	5.16976800	3.92495500	-3.34959400 L
B-B_2	0	3.88397600	4.06681500	-2.53289200 L
B-B_2	0	2.59745800	2.55387200	-4.02379300 L
N-N_3	0	2.59816300	3.92747200	-3.34917600 L
N-N_3	0	1.31140900	2.07290300	-4.69676600 L
B-B_2	0	0.02658400	2.55337800	-4.02082100 L
B-B_2	0	-1.25837200	0.54291800	-4.71451000 L
N-N_3	0	-1.25832000	2.07262800	-4.69640500 L
N-N_3	0	-2.54259400	-0.18054600	-5.12097100 L
B-B_2	0	-3.82888300	0.54262600	-4.72032100 L
B-B_2	0	-5.11396900	-1.57179600	-4.49021700 L
N-N_3	0	-5.11253100	-0.18142300	-5.12963200 L
N-N_3	0	-6.39691400	-2.40102500	-4.55214400 L
B-B_2	0	-7.68644200	-1.57888800	-4.51868000 L
B-B_2	0	-8.97440800	-3.40041700	-3.40716700 L
N-N_3	0	-8.95985600	-2.41914200	-4.59728500 L
N-N_3	0	-10.27719900	-4.15018000	-3.08816000 L
B-B_2	0	-11.49415300	-3.23951400	-3.31584600 L
N-N_3	0	-12.64785300	-3.20738000	-2.31399800 L
B-	0	12.82115200	4.38474500	-0.45992700 L
B-B_2	0	11.58770100	4.11431900	-2.56909300 L
N-N_3	0	11.63634200	4.94613400	-1.28618200 L
N-N_3	0	10.29896200	3.95543300	-3.37558500 L
B-B_2	0	9.02725400	4.07956800	-2.54270900 L
B-B_2	0	7.74289200	2.55743300	-4.04306300 L
N-N_3	0	7.73881400	3.92705900	-3.35266500 L

N-N_3	0	6.45316000	2.07335500	-4.70925200 L
B-B_2	0	5.16911300	2.55364900	-4.02965700 L
B-B_2	0	3.88200400	0.54276700	-4.72049100 L
N-N_3	0	3.88186100	2.07313900	-4.70143700 L
N-N_3	0	2.59585800	-0.18063500	-5.12182300 L
B-B_2	0	1.31162200	0.54290900	-4.71469200 L
B-B_2	0	0.02649100	-1.57086700	-4.48052400 L
N-N_3	0	0.02656400	-0.18039400	-5.11852700 L
N-N_3	0	-1.25843300	-2.39753600	-4.53684200 L
B-B_2	0	-2.54346200	-1.57063900	-4.48216300 L
B-B_2	0	-3.82976000	-3.38170600	-3.36940000 L
N-N_3	0	-3.82799600	-2.39798200	-4.54126200 L
N-N_3	0	-5.11517500	-4.15280100	-3.06538400 L
B-B_2	0	-6.40277400	-3.38863100	-3.38033500 L
N-N_3	0	-7.68800600	-4.16512600	-3.07845100 L
B-	0	12.81798000	2.36422300	-3.69581000 L
N-N_3	0	12.88153700	3.84607300	-3.31622100 L
N-N_3	0	11.63337400	2.06909100	-4.65013300 L
B-B_2	0	10.31072600	2.56671800	-4.03997400 L
B-B_2	0	9.02433200	0.54614200	-4.75290100 L
N-N_3	0	9.02935500	2.07972400	-4.72711200 L
N-N_3	0	7.73511200	-0.18106200	-5.13870700 L
B-B_2	0	6.45288400	0.54255000	-4.72726300 L
B-B_2	0	5.16749500	-1.57388000	-4.49249300 L
N-N_3	0	5.16637800	-0.18114000	-5.12774300 L
N-N_3	0	3.88086400	-2.39966600	-4.54336500 L
B-B_2	0	2.59649900	-1.57182100	-4.48447800 L
B-B_2	0	1.31119900	-3.38231800	-3.36635300 L
N-N_3	0	1.31089400	-2.39829200	-4.53808200 L
N-N_3	0	0.02594600	-4.15375300	-3.06223000 L
B-B_2	0	-1.25875800	-3.38115500	-3.36512700 L
N-N_3	0	-2.54429600	-4.15151200	-3.06150000 L
N-N_3	0	12.87804600	-0.20208600	-5.06222500 L
B-B_2	0	11.58435500	0.54771000	-4.80069400 L
B-B_2	0	10.30856200	-1.56989200	-4.51855700 L
N-N_3	0	10.29527800	-0.18036400	-5.18127400 L
N-N_3	0	9.02769200	-2.41113500	-4.57072600 L
B-B_2	0	7.74096600	-1.57965800	-4.50886500 L
B-B_2	0	6.45308600	-3.38306800	-3.37538800 L
N-N_3	0	6.45175300	-2.40309500	-4.55144100 L
N-N_3	0	5.16792900	-4.15249000	-3.06514000 L
B-B_2	0	3.88203800	-3.38288800	-3.37054300 L
N-N_3	0	2.59661800	-4.15309600	-3.06261500 L
B-	0	12.81576100	-1.42814400	-4.14760100 L

B-B_2	0	11.58466600	-3.43036300	-3.42876900 L
N-N_3	0	11.63160300	-2.35659900	-4.51703700 L
N-N_3	0	10.29656200	-4.18342300	-3.09798900 L
B-B_2	0	9.02451100	-3.39608900	-3.39509400 L
N-N_3	0	7.73675600	-4.15519200	-3.07119300 L
N-N_3	0	12.87894700	-4.10331500	-3.00942300 L
H-H_	0	-12.37533700	-2.80438400	1.02313500 L
H-H_	0	-12.37014600	-0.93889600	2.81457400 L
H-H_	0	-12.37554300	1.63386700	2.48717100 L
H-H_	0	-12.37782500	2.97634200	0.28479600 L
H-H_	0	12.86795600	-5.80882100	1.87000800 L
H-H_	0	12.86609900	-2.15310900	5.68630400 L
H-H_	0	-12.37074900	2.07663400	-2.13165700 L
H-H_	0	-12.37214900	-0.38590600	-2.94479800 L
H-H_	0	12.86371000	3.10778300	5.23300300 L
H-H_	0	12.86653100	6.04732400	0.83540200 L
H-H_	0	-12.37766000	-2.55876500	-1.54077400 L
H-H_	0	12.86894300	4.41175500	-4.19510200 L
H-H_	0	12.86480200	-0.53054100	-6.05446200 L
H-H_	0	12.86426600	-5.08361900	-3.37188200 L
C-C_3	0	-0.58434300	0.03496900	-0.49546900 H
H-H_	0	0.26178900	-0.86291400	1.31222800 H
H-H_	0	1.27654800	-1.03223600	-0.13726500 H
C-C_3	0	0.24582400	-1.04559800	0.23235200 H
H-H_	0	-0.16611700	-2.04245500	0.05348600 H
N-N_3	0	-0.12797200	1.41217500	-0.30639000 H
H-H_	0	-0.13443400	1.66583600	0.67811400 H
H-H_	0	0.81964700	1.52435600	-0.65571900 H
C-C_R	0	-2.04164500	-0.09194200	-0.07038400 H
O-O_R	0	-2.89277400	-0.71362200	-0.66876200 H
O-O_R	0	-2.28499800	0.52722200	1.11345700 H
H-H_	0	-3.22225400	0.38687300	1.32980500 H
H-H_	0	-0.57930800	-0.17691700	-1.56881800 H

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B-B_2	0	10.26394500	3.55886300	-3.32696600 L
N-N_3	0	11.56125400	4.26732300	-2.94524500 L
B-	0	12.83402900	3.52707700	-3.43087200 L
B-B_2	0	5.12528300	3.50036800	-3.24871400 L
N-N_3	0	6.41011900	4.26052500	-2.91877500 L
B-B_2	0	7.69813100	3.51321000	-3.26864000 L
B-B_2	0	8.98740200	4.60467500	-1.43712500 L
N-N_3	0	8.97317200	4.29084000	-2.94725300 L

N-N_3	0	10.29081900	5.11549500	-0.80348100 L
B-B_2	0	11.50727200	4.41517700	-1.42969700 L
B-	0	12.83772700	4.88951500	0.61745200 L
N-N_3	0	12.65889600	3.91533100	-0.55804100 L
B-B_2	0	-0.01641600	3.50682300	-3.24348000 L
N-N_3	0	1.26990600	4.26534700	-2.91369400 L
B-B_2	0	2.55406900	3.50231100	-3.24340900 L
B-B_2	0	3.84186100	4.58748300	-1.41936200 L
N-N_3	0	3.84065300	4.26018300	-2.91379700 L
N-N_3	0	5.12884800	5.12056100	-0.78746600 L
B-B_2	0	6.41547500	4.58923700	-1.42213200 L
B-B_2	0	7.70139600	4.76641800	0.69985100 L
N-N_3	0	7.70171300	5.12997700	-0.79031000 L
N-N_3	0	8.97587100	4.99089000	1.51161400 L
B-B_2	0	10.26762700	4.83386100	0.70343300 L
B-B_2	0	11.50609700	3.87130700	2.55246600 L
N-N_3	0	11.56419400	4.96972000	1.49790600 L
N-N_3	0	12.65624000	2.87613800	2.70343200 L
B-B_2	0	-5.15807300	3.50660800	-3.24997200 L
N-N_3	0	-3.87248300	4.26583000	-2.91580600 L
B-B_2	0	-2.58643700	3.50666100	-3.24482200 L
B-B_2	0	-1.30182000	4.60507900	-1.42281800 L
N-N_3	0	-1.30151200	4.26901300	-2.91597300 L
N-N_3	0	-0.01493300	5.13854300	-0.78965300 L
B-B_2	0	1.26978700	4.59720600	-1.42011200 L
B-B_2	0	2.55611700	4.75859800	0.69682200 L
N-N_3	0	2.55753500	5.12750200	-0.78788000 L
N-N_3	0	3.84280700	4.95560500	1.50037700 L
B-B_2	0	5.12820300	4.75126700	0.69736300 L
B-B_2	0	6.41464100	3.97608400	2.68118000 L
N-N_3	0	6.41259900	4.95452900	1.50181800 L
N-N_3	0	7.69855500	3.81336800	3.50069800 L
B-B_2	0	8.98656200	3.99726200	2.69144600 L
B-B_2	0	10.26322100	2.45986000	4.20280900 L
N-N_3	0	10.28796300	3.81596300	3.48807300 L
N-N_3	0	11.55870900	1.92416100	4.80764600 L
B-	0	12.83369400	2.56138300	4.19754100 L
B-B_2	0	-10.29959600	3.50601100	-3.27354200 L
N-N_3	0	-9.01981200	4.27759100	-2.93070700 L
B-B_2	0	-7.73182200	3.51426000	-3.26110200 L
B-B_2	0	-6.44501600	4.58792000	-1.42268000 L
N-N_3	0	-6.44381700	4.26663400	-2.91914800 L
N-N_3	0	-5.16086600	5.12555900	-0.78935200 L
B-B_2	0	-3.87329800	4.59417600	-1.42122300 L

B-B_2	0	-2.58802700	4.76357800	0.69530100 L
N-N_3	0	-2.58925900	5.13490000	-0.78937600 L
N-N_3	0	-1.30275700	4.96518300	1.49992800 L
B-B_2	0	-0.01579200	4.77065600	0.69629100 L
B-B_2	0	1.26929500	3.97409000	2.66791600 L
N-N_3	0	1.27112000	4.96354900	1.50066600 L
N-N_3	0	2.55408000	3.80211700	3.48036100 L
B-B_2	0	3.84112000	3.97179500	2.67208400 L
B-B_2	0	5.12449000	2.40687900	4.11415400 L
N-N_3	0	5.12540000	3.80239500	3.48618000 L
N-N_3	0	6.40665900	1.90619200	4.78023400 L
B-B_2	0	7.69743000	2.41837500	4.13892500 L
B-B_2	0	8.98211800	0.38260700	4.78766500 L
N-N_3	0	8.96983800	1.92475200	4.82548000 L
N-N_3	0	10.28308400	-0.35043600	5.14955000 L
B-B_2	0	11.50134200	0.41458800	4.60893200 L
B-	0	12.83171000	-1.68631500	4.62257100 L
N-N_3	0	12.65373200	-0.32530300	3.93045600 L
B-	0	-12.80777300	3.20748300	-3.01241700 L
B-B_2	0	-11.57697400	4.64653000	-1.44529400 L
N-N_3	0	-11.62347700	4.20125200	-2.90797200 L
N-N_3	0	-10.28911100	5.15798900	-0.80087500 L
B-B_2	0	-9.01655900	4.60293200	-1.43209500 L
B-B_2	0	-7.73470400	4.76539600	0.69932400 L
N-N_3	0	-7.72954000	5.12468300	-0.79159900 L
N-N_3	0	-6.44635100	4.95991000	1.50162800 L
B-B_2	0	-5.16069900	4.75923600	0.69657100 L
B-B_2	0	-3.87372600	3.97404200	2.66956800 L
N-N_3	0	-3.87453600	4.96044600	1.49957900 L
N-N_3	0	-2.58750400	3.80329000	3.47891600 L
B-B_2	0	-1.30223200	3.97528800	2.66722600 L
B-B_2	0	-0.01702300	2.40614900	4.10279400 L
N-N_3	0	-0.01668300	3.80267000	3.47744100 L
N-N_3	0	1.26733100	1.90359500	4.76328800 L
B-B_2	0	2.55344200	2.40634700	4.10700000 L
B-B_2	0	3.83804900	0.37404800	4.73859500 L
N-N_3	0	3.83743900	1.90393000	4.76904100 L
N-N_3	0	5.12170000	-0.36299500	5.12410400 L
B-B_2	0	6.41077200	0.37379400	4.75579100 L
B-B_2	0	7.69596500	-1.73857700	4.46640200 L
N-N_3	0	7.69403100	-0.36443600	5.14856900 L
N-N_3	0	8.96969000	-2.58058300	4.51561600 L
B-B_2	0	10.26145400	-1.75776500	4.54198800 L
B-B_2	0	11.50414400	-3.35485400	3.20598800 L

N-N_3	0	11.55808800	-2.56292200	4.50653600 L
N-N_3	0	12.65753300	-3.28666500	2.20558300 L
B-	0	-12.81164900	4.37218400	0.61473300 L
N-N_3	0	-12.87129800	5.04438100	-0.75958400 L
N-N_3	0	-11.62645800	4.90279300	1.46067000 L
B-B_2	0	-10.30278400	4.76406700	0.68716300 L
B-B_2	0	-9.01707200	3.99008800	2.68382600 L
N-N_3	0	-9.02268700	4.97143900	1.50530800 L
N-N_3	0	-7.72822000	3.80720500	3.48695000 L
B-B_2	0	-6.44528300	3.97365600	2.67226000 L
B-B_2	0	-5.15895100	2.40852400	4.11229100 L
N-N_3	0	-5.15895000	3.80332900	3.48181700 L
N-N_3	0	-3.87186200	1.90465100	4.76688900 L
B-B_2	0	-2.58753800	2.40713900	4.10534900 L
B-B_2	0	-1.30234700	0.37407400	4.73065200 L
N-N_3	0	-1.30191000	1.90380400	4.76231000 L
N-N_3	0	-0.01749900	-0.36207900	5.11132400 L
B-B_2	0	1.26759300	0.37402700	4.73128900 L
B-B_2	0	2.55279900	-1.73106400	4.43175500 L
N-N_3	0	2.55167500	-0.36210000	5.11499800 L
N-N_3	0	3.83768500	-2.55957700	4.46261000 L
B-B_2	0	5.12340400	-1.73159000	4.43914400 L
B-B_2	0	6.41264300	-3.50814400	3.26657300 L
N-N_3	0	6.40677300	-2.56188000	4.47205500 L
N-N_3	0	7.69816800	-4.27271200	2.93668700 L
B-B_2	0	8.98435900	-3.51960200	3.29189600 L
B-B_2	0	10.26592600	-4.66138100	1.46759900 L
N-N_3	0	10.28734300	-4.25714900	2.94628400 L
N-N_3	0	11.56304400	-5.13130100	0.81397800 L
B-	0	12.83590700	-4.67628200	1.57313100 L
N-N_3	0	-12.87128000	3.72930100	3.44936700 L
B-B_2	0	-11.57756200	4.02451000	2.71225900 L
B-B_2	0	-10.30049300	2.42396000	4.12556300 L
N-N_3	0	-10.28855700	3.83590200	3.51204700 L
N-N_3	0	-9.01908500	1.91238200	4.79456100 L
B-B_2	0	-7.73267800	2.41341800	4.12723300 L
B-B_2	0	-6.44324700	0.37515200	4.74160000 L
N-N_3	0	-6.44292300	1.90570400	4.77552200 L
N-N_3	0	-5.15713200	-0.36193300	5.11812900 L
B-B_2	0	-3.87251300	0.37451400	4.73527900 L
B-B_2	0	-2.58737200	-1.73164400	4.43098900 L
N-N_3	0	-2.58682500	-0.36205100	5.11347500 L
N-N_3	0	-1.30204400	-2.55990000	4.45819600 L
B-B_2	0	-0.01733400	-1.73117000	4.42853900 L

B-B_2	0	1.26823900	-3.50238800	3.25345700 L
N-N_3	0	1.26757200	-2.55944400	4.45824100 L
N-N_3	0	2.55408700	-4.26080000	2.92199000 L
B-B_2	0	3.83949400	-3.50229000	3.25734700 L
B-B_2	0	5.12663100	-4.58217300	1.42889400 L
N-N_3	0	5.12528100	-4.26123800	2.92511500 L
N-N_3	0	6.41173900	-5.11890200	0.79770500 L
B-B_2	0	7.69978000	-4.59813200	1.43766900 L
B-B_2	0	8.98757200	-4.77768800	-0.68769200 L
N-N_3	0	8.97498500	-5.15554600	0.80772600 L
N-N_3	0	10.29030300	-4.96010600	-1.48205800 L
B-B_2	0	11.50742300	-4.60278900	-0.61410300 L
B-	0	12.83631600	-4.13555300	-2.66365600 L
N-N_3	0	12.65758400	-3.77114700	-1.18107500 L
B-	0	-12.80771000	2.23462400	3.77474000 L
B-B_2	0	-11.57452900	0.37938400	4.81388700 L
N-N_3	0	-11.62315100	1.90514100	4.71776400 L
N-N_3	0	-10.28587100	-0.36152000	5.17045600 L
B-B_2	0	-9.01461700	0.37878200	4.76720700 L
B-B_2	0	-7.73175700	-1.73831500	4.45249100 L
N-N_3	0	-7.72570100	-0.36142900	5.12847800 L
N-N_3	0	-6.44282600	-2.56313200	4.46802300 L
B-B_2	0	-5.15836200	-1.73288700	4.43722200 L
B-B_2	0	-3.87297600	-3.50334500	3.25576200 L
N-N_3	0	-3.87207800	-2.56043500	4.46122400 L
N-N_3	0	-2.58772800	-4.26285100	2.92186200 L
B-B_2	0	-1.30219400	-3.50402200	3.25403600 L
B-B_2	0	-0.01666800	-4.59192000	1.42724700 L
N-N_3	0	-0.01661300	-4.26306100	2.92171300 L
N-N_3	0	1.27022900	-5.12518200	0.79551300 L
B-B_2	0	2.55482500	-4.58543500	1.42691600 L
B-B_2	0	3.84178200	-4.75452000	-0.68988400 L
N-N_3	0	3.84182600	-5.11920100	0.79598700 L
N-N_3	0	5.12786400	-4.95645300	-1.49343500 L
B-B_2	0	6.41549400	-4.75786900	-0.69153200 L
B-B_2	0	7.69986500	-3.98869500	-2.67913400 L
N-N_3	0	7.70100900	-4.96718200	-1.49779700 L
N-N_3	0	8.97332500	-3.83812500	-3.50950100 L
B-B_2	0	10.26598100	-4.04914400	-2.71502700 L
B-B_2	0	11.50334100	-2.37869900	-3.96375500 L
N-N_3	0	11.56199700	-3.82598200	-3.49064400 L
N-N_3	0	12.65464000	-1.41706700	-3.67101300 L
B-	0	-12.80573100	-1.57352500	4.09402500 L
N-N_3	0	-12.86861600	-0.37857200	5.04885000 L

N-N_3	0	-11.62241400	-2.51412100	4.43397100 L
B-B_2	0	-10.29921500	-1.72823800	4.46183200 L
B-B_2	0	-9.01534300	-3.51638000	3.27874700 L
N-N_3	0	-9.01861100	-2.57108100	4.48648200 L
N-N_3	0	-7.72765200	-4.26425400	2.92946300 L
B-B_2	0	-6.44400500	-3.50304100	3.25973900 L
B-B_2	0	-5.15996800	-4.58886600	1.42844800 L
N-N_3	0	-5.15889900	-4.26162900	2.92361900 L
N-N_3	0	-3.87422300	-5.12508800	0.79596700 L
B-B_2	0	-2.58770100	-4.58991200	1.42689100 L
B-B_2	0	-1.30229300	-4.76867700	-0.69113200 L
N-N_3	0	-1.30244800	-5.12946400	0.79628000 L
N-N_3	0	-0.01538100	-4.96754500	-1.49423800 L
B-B_2	0	1.26948200	-4.76032300	-0.69038500 L
B-B_2	0	2.55499500	-3.97721800	-2.66545800 L
N-N_3	0	2.55631000	-4.95989900	-1.49292100 L
N-N_3	0	3.84055300	-3.80600800	-3.47650100 L
B-B_2	0	5.12672100	-3.97390400	-2.66651000 L
B-B_2	0	6.41261400	-2.41326500	-4.11795800 L
N-N_3	0	6.41010600	-3.80713800	-3.48101000 L
N-N_3	0	7.69573000	-1.91318800	-4.78858800 L
B-B_2	0	8.98415100	-2.43058100	-4.14067700 L
B-B_2	0	10.26141600	-0.39157700	-4.84079900 L
N-N_3	0	10.28489500	-1.92335900	-4.78225500 L
N-N_3	0	11.55721200	0.35132100	-5.15695100 L
B-	0	12.83181000	-0.48789800	-4.88276600 L
N-N_3	0	-12.86961700	-4.21117300	2.87043800 L
B-B_2	0	-11.57548600	-3.55214100	3.31156800 L
B-B_2	0	-10.30205600	-4.59182000	1.44526700 L
N-N_3	0	-10.28732500	-4.29323500	2.95529500 L
N-N_3	0	-9.02234300	-5.13690300	0.80021600 L
B-B_2	0	-7.73399000	-4.59705300	1.43236500 L
B-B_2	0	-6.44600900	-4.75564400	-0.68892700 L
N-N_3	0	-6.44604200	-5.12493400	0.79644800 L
N-N_3	0	-5.16109800	-4.96003400	-1.49290900 L
B-B_2	0	-3.87407600	-4.76071000	-0.69032900 L
B-B_2	0	-2.58806300	-3.98157900	-2.66547500 L
N-N_3	0	-2.58913100	-4.96682600	-1.49435900 L
N-N_3	0	-1.30239600	-3.81044900	-3.47597600 L
B-B_2	0	-0.01617300	-3.98385600	-2.66672200 L
B-B_2	0	1.26849800	-2.41249300	-4.09983100 L
N-N_3	0	1.26958600	-3.80987800	-3.47673200 L
N-N_3	0	2.55269300	-1.90685000	-4.75868100 L
B-B_2	0	3.83954600	-2.41073500	-4.10437700 L

B-B_2	0	5.12341300	-0.37700600	-4.73142300 L
N-N_3	0	5.12314400	-1.90699000	-4.76676800 L
N-N_3	0	6.40544000	0.36035300	-5.11938100 L
B-B_2	0	7.69596100	-0.37923900	-4.76234200 L
B-B_2	0	8.98249000	1.73640100	-4.47264700 L
N-N_3	0	8.96847100	0.36087200	-5.17082800 L
N-N_3	0	10.28448100	2.55231700	-4.48308000 L
B-B_2	0	11.50200900	1.62763300	-4.32664100 L
N-N_3	0	12.65546100	2.00069900	-3.39601600 L
B-	0	-12.81119100	-4.20916500	1.34059000 L
B-B_2	0	-11.57845900	-4.81518500	-0.69797200 L
N-N_3	0	-11.62605200	-5.05627700	0.81191600 L
N-N_3	0	-10.29009400	-4.99346600	-1.50067800 L
B-B_2	0	-9.01783300	-4.77204400	-0.68923400 L
B-B_2	0	-7.73438500	-3.98343300	-2.67514800 L
N-N_3	0	-7.73015700	-4.96015500	-1.49271100 L
N-N_3	0	-6.44531400	-3.80770800	-3.48052000 L
B-B_2	0	-5.16038500	-3.97855800	-2.66730000 L
B-B_2	0	-3.87301300	-2.41104400	-4.10068600 L
N-N_3	0	-3.87374400	-3.80832600	-3.47641000 L
N-N_3	0	-2.58681100	-1.90645400	-4.75565900 L
B-B_2	0	-1.30215600	-2.41203900	-4.09748200 L
B-B_2	0	-0.01699500	-0.37729400	-4.71499600 L
N-N_3	0	-0.01728200	-1.90673800	-4.75437900 L
N-N_3	0	1.26708600	0.35958500	-5.09619200 L
B-B_2	0	2.55288700	-0.37736000	-4.72072800 L
B-B_2	0	3.83836100	1.72894300	-4.42153200 L
N-N_3	0	3.83645100	0.35981100	-5.10477800 L
N-N_3	0	5.12267500	2.55878300	-4.45501000 L
B-B_2	0	6.41107200	1.73374100	-4.43918900 L
N-N_3	0	7.69530400	2.56758500	-4.47653800 L
B-	0	-12.81052200	-3.66500600	-2.43095200 L
N-N_3	0	-12.87248900	-4.87074400	-1.48939700 L
N-N_3	0	-11.62546400	-3.77462800	-3.42350900 L
B-B_2	0	-10.30241600	-3.98781100	-2.66614600 L
B-B_2	0	-9.01569900	-2.42098100	-4.12639600 L
N-N_3	0	-9.02157700	-3.81722400	-3.49165000 L
N-N_3	0	-7.72628500	-1.90842600	-4.77014400 L
B-B_2	0	-6.44413100	-2.41038100	-4.10574600 L
B-B_2	0	-5.15766100	-0.37572500	-4.72874700 L
N-N_3	0	-5.15740800	-1.90614900	-4.76062100 L
N-N_3	0	-3.87036700	0.36077000	-5.10237100 L
B-B_2	0	-2.58684600	-0.37670400	-4.71872700 L
B-B_2	0	-1.30146200	1.72903000	-4.41223000 L

N-N_3	0	-1.30119400	0.35997900	-5.09531600 L
N-N_3	0	-0.01651500	2.55707600	-4.44302400 L
B-B_2	0	1.26799800	1.72806900	-4.41237500 L
N-N_3	0	2.55242000	2.55657600	-4.44592100 L
N-N_3	0	-12.86950100	-1.85413300	-4.70499400 L
B-B_2	0	-11.57584000	-2.43904600	-4.16764900 L
B-B_2	0	-10.29851600	-0.38548700	-4.75434700 L
N-N_3	0	-10.28665600	-1.92411400	-4.80791200 L
N-N_3	0	-9.01690600	0.36396500	-5.13781400 L
B-B_2	0	-7.73102400	-0.37466200	-4.74812100 L
B-B_2	0	-6.44205700	1.73134100	-4.42848300 L
N-N_3	0	-6.44096900	0.36257900	-5.11424300 L
N-N_3	0	-5.15606500	2.55933600	-4.45223000 L
B-B_2	0	-3.87145200	1.73031500	-4.41924700 L
N-N_3	0	-2.58565200	2.55822800	-4.44568600 L
B-	0	-12.80482900	-0.36490100	-4.35610200 L
B-B_2	0	-11.57323200	1.75711300	-4.50160400 L
N-N_3	0	-11.62097600	0.33704300	-5.06766200 L
N-N_3	0	-10.28469000	2.57910600	-4.50254000 L
B-B_2	0	-9.01330900	1.73775000	-4.45564800 L
N-N_3	0	-7.72475500	2.56199500	-4.46340100 L
N-N_3	0	-12.86725500	2.54263800	-4.39010800 L
H-H_	0	12.38616900	2.98095300	-0.17835200 L
H-H_	0	12.38235600	1.99788600	2.20811000 L
H-H_	0	12.38193900	-0.49024500	2.93517500 L
H-H_	0	12.38689100	-2.61105500	1.45599100 L
H-H_	0	-12.85654100	6.08019600	-0.62010300 L
H-H_	0	-12.85849000	4.26262900	4.34824600 L
H-H_	0	12.38322700	-2.76510100	-1.11585900 L
H-H_	0	12.38205300	-0.83878300	-2.84459500 L
H-H_	0	-12.85655700	-0.73981200	6.02964200 L
H-H_	0	-12.85399200	-5.20332500	3.19903600 L
H-H_	0	12.38465700	1.71839700	-2.42721200 L
H-H_	0	-12.85880000	-5.74111200	-2.06806400 L
H-H_	0	-12.85783400	-1.94922100	-5.74586500 L
H-H_	0	-12.85254900	3.29235000	-5.11833000 L
C-C_R	0	0.23166200	-0.08289200	-0.43771000 H
H-H_	0	-1.07799700	1.13719900	0.82178300 H
H-H_	0	-1.57129800	1.01240700	-0.87600400 H
C-C_3	0	-0.70110900	1.08962700	-0.21397700 H
H-H_	0	-0.20693300	2.04003800	-0.43077100 H
N-N_R	0	-0.26288400	-1.40499700	-0.07545200 H
H-H_	0	-0.70453500	-1.41092100	0.84482000 H
H-H_	0	-0.94075100	-1.74407100	-0.74806200 H

C-C_R	0	1.62774100	0.08382000	-0.11942300 H
O-O_R	0	2.39072700	-0.62579200	-0.87795700 H
O-O_R	0	2.14245000	0.96298400	0.72812800 H
H-H_	0	3.10143600	1.03501600	0.58240000 H
H-H_	0	1.27783200	-0.67930500	-1.44056100 H

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B-B_2	0	-10.26507200	-3.72262000	-3.13250500 L
N-N_3	0	-11.56253000	-4.41158500	-2.71712400 L
B-	0	-12.83507800	-3.69452400	-3.23697500 L
B-B_2	0	-5.12614900	-3.66562600	-3.06124100 L
N-N_3	0	-6.41169300	-4.40734000	-2.69443000 L
B-B_2	0	-7.69924100	-3.67599800	-3.07789000 L
B-B_2	0	-8.98806400	-4.67769000	-1.19596800 L
N-N_3	0	-8.97460000	-4.43658700	-2.71934600 L
N-N_3	0	-10.29135600	-5.15642100	-0.53743100 L
B-B_2	0	-11.50818500	-4.48715500	-1.19623300 L
B-	0	-12.83700100	-4.86372600	0.87283300 L
N-N_3	0	-12.66082000	-3.94835400	-0.34940700 L
B-B_2	0	0.01539100	-3.67166400	-3.05822100 L
N-N_3	0	-1.26966000	-4.41688500	-2.69433700 L
B-B_2	0	-2.55502600	-3.67316100	-3.06201800 L
B-B_2	0	-3.84200200	-4.66393200	-1.18406100 L
N-N_3	0	-3.84232100	-4.41158400	-2.69326800 L
N-N_3	0	-5.12900700	-5.16300800	-0.52447600 L
B-B_2	0	-6.41595700	-4.66332500	-1.18374900 L
B-B_2	0	-7.70071000	-4.73356100	0.94498200 L
N-N_3	0	-7.70212500	-5.17127600	-0.52504700 L
N-N_3	0	-8.97461800	-4.91691700	1.76787400 L
B-B_2	0	-10.26705100	-4.80116200	0.95383900 L
B-B_2	0	-11.50465700	-3.74723100	2.75261000 L
N-N_3	0	-11.56279800	-4.89780200	1.75520800 L
N-N_3	0	-12.65339700	-2.74391300	2.85098500 L
B-B_2	0	5.15728000	-3.66629200	-3.06582200 L
N-N_3	0	3.87241800	-4.40952600	-2.69520000 L
B-B_2	0	2.58573600	-3.66791900	-3.05944300 L
B-B_2	0	1.30228300	-4.67776500	-1.18677300 L
N-N_3	0	1.30165800	-4.41501300	-2.69446300 L
N-N_3	0	0.01610100	-5.18118500	-0.52808500 L
B-B_2	0	-1.26947900	-4.67459900	-1.18576800 L
B-B_2	0	-2.55508600	-4.72622400	0.93777300 L
N-N_3	0	-2.55722900	-5.17105600	-0.52637700 L
N-N_3	0	-3.84143600	-4.88161500	1.75122600 L

B-B_2	0	-5.12735300	-4.71865500	0.93972400 L
B-B_2	0	-6.41285500	-3.84379200	2.88287000 L
N-N_3	0	-6.41129500	-4.88070300	1.75446100 L
N-N_3	0	-7.69635000	-3.63996000	3.69393000 L
B-B_2	0	-8.98483500	-3.86484500	2.89590500 L
B-B_2	0	-10.26095400	-2.25282400	4.32781800 L
N-N_3	0	-10.28580000	-3.64363500	3.68319200 L
N-N_3	0	-11.55645900	-1.68706100	4.90481000 L
B-	0	-12.83168100	-2.35318100	4.32690800 L
B-B_2	0	10.29865200	-3.66486700	-3.09289400 L
N-N_3	0	9.01939800	-4.41923200	-2.71205600 L
B-B_2	0	7.73092100	-3.67328300	-3.07820700 L
B-B_2	0	6.44562900	-4.65718300	-1.18936900 L
N-N_3	0	6.44354600	-4.40890500	-2.69965300 L
N-N_3	0	5.16210500	-5.16385400	-0.52978500 L
B-B_2	0	3.87395500	-4.66504100	-1.18650900 L
B-B_2	0	2.58949500	-4.72983300	0.93592600 L
N-N_3	0	2.59040500	-5.17465000	-0.52834400 L
N-N_3	0	1.30447300	-4.89105000	1.74999300 L
B-B_2	0	0.01706100	-4.73874400	0.93757600 L
B-B_2	0	-1.26751800	-3.84165700	2.86636600 L
N-N_3	0	-1.26979800	-4.88954100	1.75088400 L
N-N_3	0	-2.55189400	-3.62915000	3.66990000 L
B-B_2	0	-3.83934200	-3.83973300	2.87193200 L
B-B_2	0	-5.12223800	-2.20431200	4.23495600 L
N-N_3	0	-5.12321000	-3.62957300	3.67732500 L
N-N_3	0	-6.40421800	-1.67087000	4.87555100 L
B-B_2	0	-7.69516300	-2.21455400	4.26112400 L
B-B_2	0	-8.97964700	-0.14874300	4.80810800 L
N-N_3	0	-8.96738100	-1.68714700	4.92255500 L
N-N_3	0	-10.28040400	0.60118700	5.13406700 L
B-B_2	0	-11.49849800	-0.18927500	4.63125800 L
B-	0	-12.82932400	1.90938000	4.54347500 L
N-N_3	0	-12.65083500	0.51672800	3.91751200 L
B-	0	12.80720000	-3.35379800	-2.84904700 L
B-B_2	0	11.57757900	-4.71388000	-1.21190500 L
N-N_3	0	11.62297500	-4.34116800	-2.69479400 L
N-N_3	0	10.29034400	-5.19345700	-0.54222000 L
B-B_2	0	9.01713800	-4.67099000	-1.19935300 L
B-B_2	0	7.73639300	-4.72848700	0.93795300 L
N-N_3	0	7.73078600	-5.16136900	-0.53327300 L
N-N_3	0	6.44847200	-4.88334600	1.74957700 L
B-B_2	0	5.16231300	-4.72405100	0.93605000 L
B-B_2	0	3.87573500	-3.84088700	2.86721600 L

N-N_3	0	3.87648800	-4.88521900	1.74862500 L
N-N_3	0	2.58960200	-3.62974000	3.66714000 L
B-B_2	0	1.30410000	-3.84287400	2.86539800 L
B-B_2	0	0.01917100	-2.20356700	4.22141300 L
N-N_3	0	0.01870100	-3.62956900	3.66605000 L
N-N_3	0	-1.26495400	-1.66892500	4.85673400 L
B-B_2	0	-2.55121500	-2.20377100	4.22651700 L
B-B_2	0	-3.83578600	-0.14248100	4.75767000 L
N-N_3	0	-3.83499100	-1.66919000	4.86347800 L
N-N_3	0	-5.11939700	0.61272600	5.10624700 L
B-B_2	0	-6.40842600	-0.14148800	4.77502400 L
B-B_2	0	-7.69380800	1.95458300	4.38311300 L
N-N_3	0	-7.69152100	0.61519900	5.13137500 L
N-N_3	0	-8.96740500	2.79813600	4.39277600 L
B-B_2	0	-10.25910300	1.97744600	4.45906700 L
B-B_2	0	-11.50261100	3.50951000	3.04942500 L
N-N_3	0	-11.55587700	2.77985700	4.38592600 L
N-N_3	0	-12.65799500	3.39645400	2.05540600 L
B-	0	12.81317700	-4.33695900	0.83125200 L
N-N_3	0	12.87247300	-5.07656900	-0.50801900 L
N-N_3	0	11.62865900	-4.82539800	1.70316400 L
B-B_2	0	10.30451600	-4.72613900	0.92441600 L
B-B_2	0	9.01929400	-3.85421100	2.88056300 L
N-N_3	0	9.02491600	-4.89321900	1.75254600 L
N-N_3	0	7.73060900	-3.63193800	3.67401700 L
B-B_2	0	6.44741000	-3.83948900	2.86914500 L
B-B_2	0	5.16107800	-2.20439900	4.22922500 L
N-N_3	0	5.16120700	-3.62906800	3.66946900 L
N-N_3	0	3.87405000	-1.66884100	4.85820300 L
B-B_2	0	2.58963300	-2.20389900	4.22286300 L
B-B_2	0	1.30442500	-0.14232200	4.74742900 L
N-N_3	0	1.30423300	-1.66874200	4.85454100 L
N-N_3	0	0.01972900	0.61165400	5.09190100 L
B-B_2	0	-1.26541000	-0.14258400	4.74956300 L
B-B_2	0	-2.55088100	1.94536500	4.34657100 L
N-N_3	0	-2.54940900	0.61164900	5.09668300 L
N-N_3	0	-3.83570700	2.77435100	4.33723100 L
B-B_2	0	-5.12138000	1.94613700	4.35483200 L
B-B_2	0	-6.41109000	3.66500000	3.09904300 L
N-N_3	0	-6.40459600	2.77716700	4.34826600 L
N-N_3	0	-7.69669200	4.41349400	2.73462100 L
B-B_2	0	-8.98274900	3.67807600	3.12589200 L
B-B_2	0	-10.26542800	4.73250900	1.25060900 L
N-N_3	0	-10.28594500	4.39854300	2.74671300 L

N-N_3	0	-11.56276000	5.17087600	0.57600900 L
B-	0	-12.83516000	4.75469300	1.35779300 L
N-N_3	0	12.87378500	-3.55374000	3.63031700 L
B-B_2	0	11.57983900	-3.88584000	2.90944400 L
B-B_2	0	10.30263200	-2.21789600	4.24251200 L
N-N_3	0	10.29106700	-3.65846300	3.69955100 L
N-N_3	0	9.02119300	-1.67433400	4.88573600 L
B-B_2	0	7.73483500	-2.20796200	4.24404500 L
B-B_2	0	6.44513200	-0.14196900	4.75740300 L
N-N_3	0	6.44504500	-1.66902700	4.86652500 L
N-N_3	0	5.15892900	0.61240300	5.09753900 L
B-B_2	0	3.87448000	-0.14208700	4.75115300 L
B-B_2	0	2.58904600	1.94678000	4.34471300 L
N-N_3	0	2.58883900	0.61196800	5.09310400 L
N-N_3	0	1.30355200	2.77515200	4.33173600 L
B-B_2	0	0.01914500	1.94563500	4.34252000 L
B-B_2	0	-1.26691100	3.65831600	3.08302500 L
N-N_3	0	-1.26582100	2.77423000	4.33187700 L
N-N_3	0	-2.55284200	4.40023200	2.71660400 L
B-B_2	0	-3.83802800	3.65819900	3.08797400 L
B-B_2	0	-5.12592300	4.65235700	1.21191800 L
N-N_3	0	-5.12379800	4.40099200	2.72144100 L
N-N_3	0	-6.41165500	5.15851900	0.55728200 L
B-B_2	0	-7.69919200	4.66814200	1.22199900 L
B-B_2	0	-8.98843800	4.74429300	-0.90816800 L
N-N_3	0	-8.97497200	5.19442900	0.56700600 L
N-N_3	0	-10.29184000	4.88603300	-1.70985100 L
B-B_2	0	-11.50864000	4.57289400	-0.82447200 L
B-	0	-12.83796800	4.00073200	-2.84694900 L
N-N_3	0	-12.65834300	3.71250200	-1.34783100 L
B-	0	12.80940900	-2.04489500	3.88171900 L
B-B_2	0	11.57630400	-0.14168400	4.83009900 L
N-N_3	0	11.62526400	-1.67028100	4.80822000 L
N-N_3	0	10.28750900	0.61535100	5.15040100 L
B-B_2	0	9.01644500	-0.14388600	4.78338300 L
B-B_2	0	7.73324900	1.95547600	4.36652400 L
N-N_3	0	7.72738200	0.61278900	5.10816300 L
N-N_3	0	6.44416600	2.77989600	4.34225200 L
B-B_2	0	5.15991500	1.94886400	4.35112600 L
B-B_2	0	3.87415900	3.66085600	3.08617100 L
N-N_3	0	3.87346100	2.77640900	4.33521400 L
N-N_3	0	2.58868500	4.40347900	2.71644600 L
B-B_2	0	1.30338500	3.66074400	3.08375200 L
B-B_2	0	0.01705300	4.66353600	1.20783600 L

N-N_3	0	0.01755300	4.40311700	2.71595000 L
N-N_3	0	-1.26979900	5.16875400	0.55272500 L
B-B_2	0	-2.55397500	4.65674300	1.20810300 L
B-B_2	0	-3.84187900	4.72776800	-0.91372100 L
N-N_3	0	-3.84159400	5.16023600	0.55397000 L
N-N_3	0	-5.12933000	4.88718900	-1.72473800 L
B-B_2	0	-6.41609800	4.72683500	-0.91292500 L
B-B_2	0	-7.70140200	3.85673700	-2.85716900 L
N-N_3	0	-7.70256100	4.89425600	-1.72747400 L
N-N_3	0	-8.97510300	3.66260100	-3.67802700 L
B-B_2	0	-10.26761200	3.91361800	-2.89501500 L
B-B_2	0	-11.50429200	2.18059000	-4.05618500 L
N-N_3	0	-11.56381600	3.65016100	-3.65761000 L
N-N_3	0	-12.65473300	1.23425700	-3.71436200 L
B-	0	12.80726900	1.77446500	4.01702100 L
N-N_3	0	12.87023800	0.62694400	5.02833800 L
N-N_3	0	11.62375300	2.73015700	4.31107800 L
B-B_2	0	10.30068000	1.94630000	4.37667200 L
B-B_2	0	9.01657400	3.67510600	3.10867400 L
N-N_3	0	9.01994000	2.78914600	4.36056900 L
N-N_3	0	7.72887200	4.40523300	2.72370200 L
B-B_2	0	6.44521300	3.66089600	3.09036100 L
B-B_2	0	5.16093800	4.65773100	1.20923100 L
N-N_3	0	5.16003800	4.40255000	2.71834100 L
N-N_3	0	3.87527400	5.16332900	0.55179200 L
B-B_2	0	2.58849000	4.65978800	1.20774600 L
B-B_2	0	1.30240400	4.73738900	-0.91607400 L
N-N_3	0	1.30327000	5.16936000	0.55217400 L
N-N_3	0	0.01635000	4.90051100	-1.72872000 L
B-B_2	0	-1.26963000	4.73879900	-0.91608100 L
B-B_2	0	-2.55621900	3.85538400	-2.84866900 L
N-N_3	0	-2.55737000	4.89672200	-1.72719400 L
N-N_3	0	-3.84260900	3.63632900	-3.64699500 L
B-B_2	0	-5.12802600	3.84579500	-2.84581600 L
B-B_2	0	-6.41404900	2.20847100	-4.21053600 L
N-N_3	0	-6.41200500	3.63439800	-3.64901200 L
N-N_3	0	-7.69663800	1.67435400	-4.85546300 L
B-B_2	0	-8.98541800	2.22424900	-4.23556100 L
B-B_2	0	-10.26222900	0.15216400	-4.83264900 L
N-N_3	0	-10.28585400	1.68493500	-4.85090100 L
N-N_3	0	-11.55810300	-0.60519300	-5.11225200 L
B-	0	-12.83283900	0.24601400	-4.87831800 L
N-N_3	0	12.87076400	4.34964300	2.66704000 L
B-B_2	0	11.57676100	3.71276900	3.13986700 L

B-B_2	0	10.30315600	4.65917100	1.22482500 L
N-N_3	0	10.28852400	4.43527700	2.74769200 L
N-N_3	0	9.02350300	5.17218800	0.55391600 L
B-B_2	0	7.73502500	4.66483800	1.21222000 L
B-B_2	0	6.44656000	4.71939500	-0.91372100 L
N-N_3	0	6.44718600	5.16161400	0.55156300 L
N-N_3	0	5.16162900	4.88437500	-1.72653900 L
B-B_2	0	3.87461800	4.72653800	-0.91474900 L
B-B_2	0	2.58764400	3.85004300	-2.84712800 L
N-N_3	0	2.58976200	4.89346800	-1.72777100 L
N-N_3	0	1.30167100	3.63803000	-3.64702400 L
B-B_2	0	0.01553600	3.85685400	-2.84838900 L
B-B_2	0	-1.27009400	2.20886500	-4.18998600 L
N-N_3	0	-1.27029900	3.63992800	-3.64770200 L
N-N_3	0	-2.55429000	1.66893100	-4.82060200 L
B-B_2	0	-3.84109400	2.20754200	-4.19508600 L
B-B_2	0	-5.12458300	0.14258500	-4.71776500 L
N-N_3	0	-5.12413000	1.66889300	-4.83071900 L
N-N_3	0	-6.40606400	-0.61243000	-5.07177100 L
B-B_2	0	-7.69694200	0.14359300	-4.75213400 L
B-B_2	0	-8.98339700	-1.95631900	-4.36273700 L
N-N_3	0	-8.96913600	-0.61547600	-5.12543600 L
N-N_3	0	-10.28554300	-2.77152500	-4.33461000 L
B-B_2	0	-11.50264000	-1.84009000	-4.22165800 L
N-N_3	0	-12.65590300	-2.16826600	-3.27408400 L
B-	0	12.81259100	4.27187600	1.13915300 L
B-B_2	0	11.57904100	4.77446300	-0.92698400 L
N-N_3	0	11.62715600	5.09119600	0.56887500 L
N-N_3	0	10.29059500	4.91356300	-1.73733800 L
B-B_2	0	9.01839200	4.73379400	-0.91555500 L
B-B_2	0	7.73384600	3.84769600	-2.85902100 L
N-N_3	0	7.73062900	4.88250000	-1.72705400 L
N-N_3	0	6.44431100	3.63226900	-3.65390600 L
B-B_2	0	5.15990600	3.84477500	-2.84977300 L
B-B_2	0	3.87117200	2.20655500	-4.19990500 L
N-N_3	0	3.87285600	3.63418900	-3.64850700 L
N-N_3	0	2.58392000	1.66926200	-4.82623500 L
B-B_2	0	1.30045400	2.20823900	-4.19255300 L
B-B_2	0	0.01457400	0.14346400	-4.70319900 L
N-N_3	0	0.01448800	1.66907700	-4.81921300 L
N-N_3	0	-1.26963500	-0.61064500	-5.04800900 L
B-B_2	0	-2.55462000	0.14313600	-4.70553900 L
B-B_2	0	-3.83945600	-1.94909600	-4.31237400 L
N-N_3	0	-3.83772100	-0.61123600	-5.05522800 L

N-N_3	0	-5.12407400	-2.77874700	-4.30825700 L
B-B_2	0	-6.41203800	-1.95299900	-4.32897700 L
N-N_3	0	-7.69648500	-2.78718500	-4.32808400 L
B-	0	12.80950400	3.53836700	-2.60112600 L
N-N_3	0	12.87295100	4.78922000	-1.72047600 L
N-N_3	0	11.62443700	3.60012000	-3.59775800 L
B-B_2	0	10.30183100	3.85116500	-2.85137300 L
B-B_2	0	9.01381600	2.21432300	-4.23155300 L
N-N_3	0	9.02052600	3.64035600	-3.66682900 L
N-N_3	0	7.72369100	1.67072400	-4.84797600 L
B-B_2	0	6.44225600	2.20519500	-4.20797800 L
B-B_2	0	5.15498100	0.14190700	-4.72773900 L
N-N_3	0	5.15468100	1.66890700	-4.83530400 L
N-N_3	0	3.86703800	-0.61182000	-5.06318900 L
B-B_2	0	2.58418300	0.14321800	-4.71287800 L
B-B_2	0	1.29927900	-1.94719000	-4.30635600 L
N-N_3	0	1.29789300	-0.61078500	-5.05125700 L
N-N_3	0	0.01483600	-2.77675300	-4.29920200 L
B-B_2	0	-1.27003100	-1.94812100	-4.30514000 L
N-N_3	0	-2.55406700	-2.77809000	-4.30313600 L
N-N_3	0	12.86705700	1.61929300	-4.78509100 L
B-B_2	0	11.57391300	2.22979800	-4.27571900 L
B-B_2	0	10.29590900	0.15023200	-4.76053200 L
N-N_3	0	10.28410000	1.68442300	-4.88900700 L
N-N_3	0	9.01383300	-0.61687600	-5.10571600 L
B-B_2	0	7.72839100	0.13986700	-4.75074200 L
B-B_2	0	6.43984200	-1.94854700	-4.32835400 L
N-N_3	0	6.43779800	-0.61424000	-5.07893800 L
N-N_3	0	5.15402500	-2.77694800	-4.31150200 L
B-B_2	0	3.86924600	-1.94760200	-4.31623200 L
N-N_3	0	2.58376500	-2.77635000	-4.30297200 L
B-	0	12.80256600	0.14878400	-4.36422700 L
B-B_2	0	11.57094700	-1.97771000	-4.40568800 L
N-N_3	0	11.61803900	-0.58672100	-5.03984300 L
N-N_3	0	10.28246200	-2.79872000	-4.36540900 L
B-B_2	0	9.01106700	-1.95609000	-4.35797100 L
N-N_3	0	7.72261700	-2.77981300	-4.32479900 L
N-N_3	0	12.86509000	-2.75694900	-4.25759300 L
H-H_	0	-12.39052900	-2.99565100	-0.01644800 L
H-H_	0	-12.37752500	-1.89240200	2.31197100 L
H-H_	0	-12.37868200	0.63377800	2.91555600 L
H-H_	0	-12.39014600	2.68526400	1.33846600 L
H-H_	0	12.85830700	-6.10418200	-0.31724300 L
H-H_	0	12.86192600	-4.04216300	4.55437600 L

H-H_	0	-12.38309300	2.71130200	-1.23168100 L
H-H_	0	-12.38074100	0.69775400	-2.86066000 L
H-H_	0	12.85804900	1.03503600	5.99057700 L
H-H_	0	12.85468000	5.35684300	2.94610400 L
H-H_	0	-12.38462300	-1.84063700	-2.31979000 L
H-H_	0	12.86011300	5.62986600	-2.34154900 L
H-H_	0	12.85452800	1.66371600	-5.82934100 L
H-H_	0	12.84950000	-3.54128600	-4.94836600 L
C-C_R	0	-0.23490100	0.03721100	-0.37551700 H
H-H_	0	1.13603700	-1.11622600	0.83778300 H
H-H_	0	1.51703800	-1.12578400	-0.89066100 H
C-C_3	0	0.68871400	-1.12586600	-0.16697500 H
H-H_	0	0.14681800	-2.06556000	-0.28086400 H
N-N_R	0	0.23007900	1.40104800	-0.25287300 H
H-H_	0	0.58941600	1.59980900	0.67926700 H
H-H_	0	0.97845700	1.60743700	-0.91181700 H
C-C_R	0	-1.54232300	-0.07222400	-0.67768700 H
O-O_R	0	-2.35412000	1.00135700	-0.85975600 H
O-O_R	0	-2.19438400	-1.25121600	-0.82281500 H
H-H_	0	-3.10177500	-1.06098800	-1.09927600 H
H-H_	0	-1.76375300	1.77027700	-0.71684100 H

bTS3@C

B-B_2	0	10.22805600	3.08873000	-3.74498500 L
N-N_3	0	11.52495100	3.84347800	-3.46387600 L
B-	0	12.79811000	3.04369400	-3.84268500 L
B-B_2	0	5.08995700	3.03903500	-3.66127600 L
N-N_3	0	6.37400500	3.83790700	-3.43833700 L
B-B_2	0	7.66249900	3.05009000	-3.68155200 L
B-B_2	0	8.95030600	4.38334700	-2.01721500 L
N-N_3	0	8.93689600	3.86531700	-3.46986000 L
N-N_3	0	10.25330000	4.97642100	-1.45868700 L
B-B_2	0	11.47067900	4.19818600	-1.98306000 L
B-	0	12.79894700	4.95270000	-0.01916700 L
N-N_3	0	12.62513800	3.82795700	-1.05240300 L
B-B_2	0	-0.05002000	3.03854200	-3.66109300 L
N-N_3	0	1.23420000	3.83890600	-3.43811400 L
B-B_2	0	2.51937700	3.03962100	-3.65876300 L
B-B_2	0	3.80422700	4.36949400	-2.00066600 L
N-N_3	0	3.80471000	3.83713700	-3.43521100 L
N-N_3	0	5.09110100	4.98303200	-1.44641200 L
B-B_2	0	6.37811100	4.36932000	-2.00131400 L
B-B_2	0	7.66291100	4.83316400	0.07651000 L

N-N_3	0	7.66402900	4.99156000	-1.44889300 L
N-N_3	0	8.93692600	5.16431500	0.85152100 L
B-B_2	0	10.22927700	4.90198800	0.07244300 L
B-B_2	0	11.46785100	4.19486400	2.03267800 L
N-N_3	0	11.52470300	5.14484900	0.84255000 L
N-N_3	0	12.61630400	3.22518500	2.30968200 L
B-B_2	0	-5.19220400	3.03640600	-3.67851700 L
N-N_3	0	-3.90705100	3.83298700	-3.44536000 L
B-B_2	0	-2.62073600	3.03671800	-3.66893000 L
B-B_2	0	-1.33844000	4.36562400	-2.00420900 L
N-N_3	0	-1.33616300	3.83527700	-3.43955000 L
N-N_3	0	-0.05507600	4.98939400	-1.45228300 L
B-B_2	0	1.23282900	4.37603600	-2.00514800 L
B-B_2	0	2.51717400	4.83046700	0.07185600 L
N-N_3	0	2.51908300	4.99105200	-1.45037100 L
N-N_3	0	3.80391500	5.13057100	0.84286100 L
B-B_2	0	5.08933600	4.81906800	0.07481500 L
B-B_2	0	6.37531700	4.31309800	2.14342500 L
N-N_3	0	6.37380700	5.12707200	0.84528600 L
N-N_3	0	7.65900500	4.25882100	2.97774400 L
B-B_2	0	8.94744000	4.33534200	2.15218300 L
B-B_2	0	10.22350700	3.00768300	3.85048400 L
N-N_3	0	10.24857000	4.26001200	2.96636500 L
N-N_3	0	11.51889800	2.55385400	4.51932200 L
B-	0	12.79431900	3.10538900	3.83172900 L
B-B_2	0	-10.33363700	3.03346900	-3.70999200 L
N-N_3	0	-9.05414900	3.84335500	-3.46960900 L
B-B_2	0	-7.76588700	3.04291300	-3.69445100 L
B-B_2	0	-6.48156000	4.35172400	-2.01237300 L
N-N_3	0	-6.47822100	3.83369400	-3.45277400 L
N-N_3	0	-5.19831600	4.97033500	-1.45561300 L
B-B_2	0	-3.91021400	4.35768200	-2.00774500 L
B-B_2	0	-2.62761800	4.81800000	0.06867900 L
N-N_3	0	-2.62682600	4.97855300	-1.45304000 L
N-N_3	0	-1.34349600	5.13042700	0.83894700 L
B-B_2	0	-0.05544200	4.82991100	0.07005600 L
B-B_2	0	1.22918600	4.31342600	2.13175200 L
N-N_3	0	1.23021200	5.13636700	0.84091400 L
N-N_3	0	2.51456800	4.24730500	2.95826200 L
B-B_2	0	3.80138100	4.30929300	2.13411400 L
B-B_2	0	5.08461700	2.94446800	3.76743300 L
N-N_3	0	5.08578000	4.24654000	2.96348600 L
N-N_3	0	6.36651000	2.53422200	4.49341300 L
B-B_2	0	7.65759300	2.95863000	3.79172800 L

B-B_2	0	8.94162000	1.02398000	4.69978100 L
N-N_3	0	8.92977000	2.55802200	4.53693400 L
N-N_3	0	10.24216900	0.34428800	5.15494500 L
B-B_2	0	11.46020100	1.03131900	4.51809400 L
B-	0	12.79103600	-1.04877900	4.80476000 L
N-N_3	0	12.61010800	0.20820400	3.93851800 L
B-	0	-12.84229400	2.77191000	-3.41612300 L
B-B_2	0	-11.61338700	4.40385100	-2.04910200 L
N-N_3	0	-11.65788700	3.77071300	-3.44082400 L
N-N_3	0	-10.32674200	4.99846200	-1.47755900 L
B-B_2	0	-9.05306900	4.36467100	-2.02733400 L
B-B_2	0	-7.77391400	4.81397000	0.06494500 L
N-N_3	0	-7.76700300	4.96820600	-1.46091800 L
N-N_3	0	-6.48694900	5.11730200	0.83506700 L
B-B_2	0	-5.19997400	4.81059200	0.06657700 L
B-B_2	0	-3.91471600	4.30409900	2.13005100 L
N-N_3	0	-3.91538600	5.12185100	0.83644800 L
N-N_3	0	-2.62903100	4.24499700	2.95639100 L
B-B_2	0	-1.34273000	4.30891300	2.13020900 L
B-B_2	0	-0.05734000	2.94497500	3.75998400 L
N-N_3	0	-0.05740400	4.24776700	2.95678200 L
N-N_3	0	1.22779600	2.53096100	4.47764500 L
B-B_2	0	2.51343200	2.94400700	3.76032600 L
B-B_2	0	3.79795700	1.01011800	4.64994700 L
N-N_3	0	3.79745600	2.53101300	4.48160100 L
N-N_3	0	5.08126700	0.32947900	5.12874600 L
B-B_2	0	6.37049600	1.01162600	4.66801500 L
B-B_2	0	7.65536300	-1.12127000	4.65952500 L
N-N_3	0	7.65330100	0.33082600	5.15474600 L
N-N_3	0	8.92858700	-1.94974500	4.82202300 L
B-B_2	0	10.22050700	-1.13088900	4.73830700 L
B-B_2	0	11.46292700	-2.89460400	3.62981100 L
N-N_3	0	11.51747900	-1.93333700	4.81069000 L
N-N_3	0	12.62049700	-2.97003600	2.63473400 L
B-	0	-12.84962800	4.40658300	0.02841900 L
N-N_3	0	-12.90896900	4.88792900	-1.42374200 L
N-N_3	0	-11.66663200	5.04891200	0.79615900 L
B-B_2	0	-10.34186600	4.80846400	0.04998500 L
B-B_2	0	-9.05808200	4.31349100	2.13469500 L
N-N_3	0	-9.06308300	5.12604500	0.83403300 L
N-N_3	0	-7.77023500	4.24232000	2.95681500 L
B-B_2	0	-6.48630400	4.29933500	2.12894300 L
B-B_2	0	-5.20018000	2.94310000	3.76661800 L
N-N_3	0	-5.20101000	4.24156300	2.95596800 L

N-N_3	0	-3.91309500	2.53077700	4.48271600 L
B-B_2	0	-2.62834400	2.94398200	3.76230100 L
B-B_2	0	-1.34237000	1.00983700	4.64587100 L
N-N_3	0	-1.34229400	2.53115400	4.47917900 L
N-N_3	0	-0.05699000	0.32922400	5.11731800 L
B-B_2	0	1.22765200	1.00984000	4.64377300 L
B-B_2	0	2.51272400	-1.11711500	4.62081000 L
N-N_3	0	2.51174200	0.32948900	5.11915300 L
N-N_3	0	3.79732800	-1.93432600	4.76102200 L
B-B_2	0	5.08307900	-1.11699400	4.62897100 L
B-B_2	0	6.37227300	-3.03525600	3.70545300 L
N-N_3	0	6.36581900	-1.93604100	4.77326300 L
N-N_3	0	7.65714600	-3.83888000	3.48491100 L
B-B_2	0	8.94358100	-3.04531400	3.73614400 L
B-B_2	0	10.22605200	-4.42772400	2.08700500 L
N-N_3	0	10.24620900	-3.82394200	3.49597100 L
N-N_3	0	11.52306600	-4.98508300	1.50641100 L
B-	0	12.79543500	-4.43412800	2.20002700 L
N-N_3	0	-12.91289600	4.15500900	2.92440800 L
B-B_2	0	-11.61858500	4.34871100	2.15541000 L
B-B_2	0	-10.34202600	2.95463700	3.77266300 L
N-N_3	0	-10.33044100	4.27112000	2.97467100 L
N-N_3	0	-9.06083000	2.53804100	4.50498300 L
B-B_2	0	-7.77411800	2.94694400	3.77810900 L
B-B_2	0	-6.48385000	1.00903900	4.65652700 L
N-N_3	0	-6.48452600	2.53079200	4.48905400 L
N-N_3	0	-5.19731800	0.32823500	5.12622600 L
B-B_2	0	-3.91284700	1.00940400	4.65098000 L
B-B_2	0	-2.62693600	-1.11849100	4.62365700 L
N-N_3	0	-2.62661300	0.32884400	5.12136600 L
N-N_3	0	-1.34121600	-1.93567900	4.75833900 L
B-B_2	0	-0.05684300	-1.11773300	4.61945300 L
B-B_2	0	1.22886700	-3.03085800	3.68999800 L
N-N_3	0	1.22805800	-1.93496300	4.75783100 L
N-N_3	0	2.51462400	-3.82661300	3.46253800 L
B-B_2	0	3.79945700	-3.02922900	3.69220400 L
B-B_2	0	5.08717500	-4.34943900	2.02921400 L
N-N_3	0	5.08474400	-3.82680300	3.46737700 L
N-N_3	0	6.37239400	-4.96922600	1.48025800 L
B-B_2	0	7.66017300	-4.36645400	2.04459200 L
B-B_2	0	8.95052300	-4.83560100	-0.03373000 L
N-N_3	0	8.93549100	-5.00615700	1.49904900 L
N-N_3	0	10.25448400	-5.12326700	-0.79450300 L
B-B_2	0	11.47138900	-4.65514100	0.01972100 L

B-	0	12.80204200	-4.46362400	-2.07291600 L
N-N_3	0	12.62325000	-3.90746400	-0.65120400 L
B-	0	-12.84902900	2.71796500	3.44868300 L
B-B_2	0	-11.61546400	1.01991700	4.72809000 L
N-N_3	0	-11.66486800	2.51901000	4.42815800 L
N-N_3	0	-10.32622600	0.33303300	5.17828900 L
B-B_2	0	-9.05538200	1.01438600	4.68097300 L
B-B_2	0	-7.77152100	-1.12476600	4.64643300 L
N-N_3	0	-7.76607000	0.32877900	5.13634500 L
N-N_3	0	-6.48218600	-1.93977800	4.76981100 L
B-B_2	0	-5.19800000	-1.12008900	4.63034700 L
B-B_2	0	-3.91207100	-3.03102200	3.69232000 L
N-N_3	0	-3.91136400	-1.93679000	4.76259700 L
N-N_3	0	-2.62662900	-3.82798000	3.46243800 L
B-B_2	0	-1.34131700	-3.03107900	3.68959000 L
B-B_2	0	-0.05505900	-4.35593400	2.02539100 L
N-N_3	0	-0.05594600	-3.82838100	3.46207200 L
N-N_3	0	1.23129500	-4.97421700	1.47431300 L
B-B_2	0	2.51574500	-4.35248100	2.02554500 L
B-B_2	0	3.80394400	-4.81513900	-0.04707600 L
N-N_3	0	3.80275500	-4.96872700	1.47526300 L
N-N_3	0	5.09161400	-5.12334600	-0.81348100 L
B-B_2	0	6.37810200	-4.81646400	-0.04426700 L
B-B_2	0	7.66533700	-4.32037700	-2.11345200 L
N-N_3	0	7.66496400	-5.13268700	-0.81259900 L
N-N_3	0	8.94024300	-4.27851300	-2.95406500 L
B-B_2	0	10.23186400	-4.38363600	-2.13728600 L
B-B_2	0	11.47044800	-2.88885900	-3.59002500 L
N-N_3	0	11.52864300	-4.26298600	-2.93394700 L
N-N_3	0	12.61794900	-1.89426000	-3.41703000 L
B-	0	-12.84641500	-1.01068200	4.27190100 L
N-N_3	0	-12.90898200	0.29911400	5.06194800 L
N-N_3	0	-11.66196600	-1.89815400	4.73043200 L
B-B_2	0	-10.33912400	-1.11474000	4.65490400 L
B-B_2	0	-9.05448900	-3.04217000	3.71618900 L
N-N_3	0	-9.05806200	-1.94649000	4.78939300 L
N-N_3	0	-7.76656700	-3.82933600	3.46900400 L
B-B_2	0	-6.48307900	-3.03076900	3.69586900 L
B-B_2	0	-5.19853100	-4.35135400	2.02557500 L
N-N_3	0	-5.19783100	-3.82704900	3.46365500 L
N-N_3	0	-3.91284600	-4.96832000	1.47152600 L
B-B_2	0	-2.62647700	-4.35315100	2.02495500 L
B-B_2	0	-1.33963900	-4.81530600	-0.04982100 L
N-N_3	0	-1.34101000	-4.97231400	1.47250100 L

N-N_3	0	-0.05429700	-5.13060600	-0.81748400 L
B-B_2	0	1.23214600	-4.82312600	-0.04877700 L
B-B_2	0	2.51975200	-4.31728900	-2.11212300 L
N-N_3	0	2.51957400	-5.13103900	-0.81590800 L
N-N_3	0	3.80715500	-4.25022500	-2.93598900 L
B-B_2	0	5.09166500	-4.30787500	-2.10809800 L
B-B_2	0	6.37976200	-2.94639200	-3.74474200 L
N-N_3	0	6.37697500	-4.24680000	-2.93431800 L
N-N_3	0	7.66369700	-2.53527300	-4.47196800 L
B-B_2	0	8.95147600	-2.96432300	-3.76159200 L
B-B_2	0	10.22874200	-1.03165400	-4.71678100 L
N-N_3	0	10.25280800	-2.54319500	-4.46162800 L
N-N_3	0	11.52505900	-0.33545500	-5.12464600 L
B-	0	12.79969500	-1.12917600	-4.73786700 L
N-N_3	0	-12.90872600	-3.78428700	3.40088000 L
B-B_2	0	-11.61462700	-3.07329600	3.75253000 L
B-B_2	0	-10.34041300	-4.35119900	2.04053000 L
N-N_3	0	-10.32637800	-3.85510100	3.49771000 L
N-N_3	0	-9.06061500	-4.97784000	1.47463200 L
B-B_2	0	-7.77245700	-4.35837800	2.02944100 L
B-B_2	0	-6.48356700	-4.80173800	-0.05106900 L
N-N_3	0	-6.48446700	-4.96713100	1.47064800 L
N-N_3	0	-5.19848100	-5.11402300	-0.81936300 L
B-B_2	0	-3.91189700	-4.80808400	-0.05043600 L
B-B_2	0	-2.62426900	-4.30683600	-2.11351500 L
N-N_3	0	-2.62654600	-5.12169400	-0.81828000 L
N-N_3	0	-1.33822700	-4.24861700	-2.93908400 L
B-B_2	0	-0.05229900	-4.31586800	-2.11316300 L
B-B_2	0	1.23522400	-2.94558400	-3.73464900 L
N-N_3	0	1.23423000	-4.25233000	-2.93806200 L
N-N_3	0	2.52049300	-2.52848100	-4.45060900 L
B-B_2	0	3.80655400	-2.94649100	-3.73738300 L
B-B_2	0	5.09099400	-1.00606000	-4.61248800 L
N-N_3	0	5.09132300	-2.52824700	-4.45483300 L
N-N_3	0	6.37271700	-0.32447900	-5.09229100 L
B-B_2	0	7.66343500	-1.01068400	-4.64226100 L
B-B_2	0	8.94834100	1.12626300	-4.63340800 L
N-N_3	0	8.93568000	-0.32950700	-5.14373000 L
N-N_3	0	10.24961300	1.93421500	-4.75318700 L
B-B_2	0	11.46671600	1.03957600	-4.47104700 L
N-N_3	0	12.61960100	1.53633800	-3.59943000 L
B-	0	-12.84885200	-3.98455000	1.88428300 L
B-B_2	0	-11.61581300	-4.85816500	-0.05456600 L
N-N_3	0	-11.66423900	-4.89541500	1.47392600 L

N-N_3	0	-10.32738800	-5.14462900	-0.82521700 L
B-B_2	0	-9.05530100	-4.81652400	-0.05040400 L
B-B_2	0	-7.77042500	-4.30480800	-2.12434100 L
N-N_3	0	-7.76745200	-5.11236500	-0.82048000 L
N-N_3	0	-6.48095400	-4.24036800	-2.94552900 L
B-B_2	0	-5.19649100	-4.30114100	-2.11626500 L
B-B_2	0	-3.90708700	-2.94179800	-3.74657700 L
N-N_3	0	-3.90959600	-4.24299500	-2.94069200 L
N-N_3	0	-2.61950200	-2.52849600	-4.46074500 L
B-B_2	0	-1.33598200	-2.94428000	-3.73959900 L
B-B_2	0	-0.04884400	-1.00650500	-4.61201700 L
N-N_3	0	-0.04898600	-2.52833300	-4.45260600 L
N-N_3	0	1.23692300	-0.32473900	-5.08001900 L
B-B_2	0	2.52092100	-1.00640600	-4.60721200 L
B-B_2	0	3.80552500	1.12267900	-4.58403200 L
N-N_3	0	3.80500400	-0.32464700	-5.08044600 L
N-N_3	0	5.08907300	1.94124400	-4.72733500 L
B-B_2	0	6.37738100	1.12644500	-4.59905000 L
N-N_3	0	7.66069000	1.94855300	-4.74910400 L
B-	0	-12.84601800	-3.95203300	-1.92821500 L
N-N_3	0	-12.90965100	-5.01885400	-0.83187300 L
N-N_3	0	-11.66090400	-4.19672700	-2.89622900 L
B-B_2	0	-10.33838500	-4.30612700	-2.11620800 L
B-B_2	0	-9.04990000	-2.95162200	-3.77348500 L
N-N_3	0	-9.05706800	-4.24962000	-2.95648600 L
N-N_3	0	-7.75977900	-2.53005000	-4.47887900 L
B-B_2	0	-6.47830200	-2.93969300	-3.75286300 L
B-B_2	0	-5.19022300	-1.00624300	-4.63827300 L
N-N_3	0	-5.19080800	-2.52763400	-4.46821800 L
N-N_3	0	-3.90191300	-0.32512300	-5.10310900 L
B-B_2	0	-2.61901300	-1.00679700	-4.62464900 L
B-B_2	0	-1.33361700	1.12166700	-4.59110600 L
N-N_3	0	-1.33168700	-0.32511400	-5.08979900 L
N-N_3	0	-0.04796800	1.93874500	-4.72489000 L
B-B_2	0	1.23602500	1.12150400	-4.58115100 L
N-N_3	0	2.52005900	1.93906000	-4.72167600 L
N-N_3	0	-12.90280400	-2.46748800	-4.42809300 L
B-B_2	0	-11.61009200	-2.97478900	-3.81509800 L
B-B_2	0	-10.33157900	-1.01794200	-4.66768500 L
N-N_3	0	-10.31995900	-2.55001000	-4.51649200 L
N-N_3	0	-9.04919100	-0.32571900	-5.14483400 L
B-B_2	0	-7.76387600	-1.00689500	-4.66006700 L
B-B_2	0	-6.47469500	1.12225000	-4.61699200 L
N-N_3	0	-6.47305600	-0.32434000	-5.11823000 L

N-N_3	0	-5.18841200	1.93988400	-4.74663400 L
B-B_2	0	-3.90380800	1.12206700	-4.60441200 L
N-N_3	0	-2.61755800	1.93945800	-4.73575900 L
B-	0	-12.83914700	-0.94501000	-4.28025700 L
B-B_2	0	-11.60607200	1.13914400	-4.70094500 L
N-N_3	0	-11.65343800	-0.34302100	-5.07561400 L
N-N_3	0	-10.31713400	1.95370700	-4.80712100 L
B-B_2	0	-9.04610800	1.12554300	-4.64849500 L
N-N_3	0	-7.75719600	1.94143000	-4.76178900 L
N-N_3	0	-12.89997000	1.93272700	-4.69520100 L
H-H_	0	12.35800100	2.95167700	-0.55013000 L
H-H_	0	12.34027200	2.29086600	1.93212100 L
H-H_	0	12.33410400	-0.08769100	2.97518100 L
H-H_	0	12.35607200	-2.40257500	1.79832400 L
H-H_	0	-12.89612500	5.93311900	-1.42475700 L
H-H_	0	-12.90122000	4.80479200	3.74308400 L
H-H_	0	12.35078500	-2.90109000	-0.71876700 L
H-H_	0	12.33910400	-1.21449200	-2.67410900 L
H-H_	0	-12.89561000	0.06948800	6.08159600 L
H-H_	0	-12.89409100	-4.72427800	3.85781700 L
H-H_	0	12.34818300	1.38906100	-2.60129400 L
H-H_	0	-12.89695600	-5.95969100	-1.28712200 L
H-H_	0	-12.88885800	-2.70010800	-5.44705300 L
H-H_	0	-12.88379600	2.58083100	-5.51513400 L
C-C_R	0	1.64200100	0.02564000	-0.27163800 H
H-H_	0	1.33683700	2.09944400	-0.13421700 H
H-H_	0	0.38206700	1.20431000	1.04581500 H
C-C_3	0	0.75651700	1.18672500	0.00986700 H
H-H_	0	-0.12018600	1.25038000	-0.65453200 H
N-N_R	0	1.21021800	-1.36851700	-0.05901800 H
H-H_	0	0.97606000	-1.60139000	0.90833400 H
H-H_	0	0.44426100	-1.67881500	-0.66022400 H
C-C_R	0	2.94051100	-0.06576100	-0.70576700 H
O-O_R	0	3.47922600	-1.24231000	-0.83429700 H
O-O_R	0	3.67665600	1.03643100	-1.00087700 H
H-H_	0	4.54103500	0.71411200	-1.29621200 H
H-H_	0	2.27563000	-1.77816900	-0.39942900 H

bINT3@SWBNNT(7.7)

B-B_2	0	10.26060500	4.37684000	-2.15793800 L
N-N_3	0	11.55759400	4.94519100	-1.58765300 L
B-	0	12.83046100	4.37550300	-2.26502300 L
B-B_2	0	5.12123900	4.30694000	-2.10809100 L
N-N_3	0	6.40669600	4.93660700	-1.57058400 L
B-B_2	0	7.69453700	4.31950300	-2.11853800 L
B-B_2	0	8.98206500	4.83481300	-0.04915100 L
N-N_3	0	8.96976700	4.97006900	-1.58555200 L
N-N_3	0	10.28474100	5.14015100	0.70668900 L
B-B_2	0	11.50230100	4.65055000	-0.09364500 L
B-	0	12.82995600	4.51331500	2.00526600 L
N-N_3	0	12.65324500	3.92058100	0.59807200 L
B-B_2	0	-0.02141200	4.31762600	-2.10985000 L
N-N_3	0	1.26437600	4.94918400	-1.57294100 L
B-B_2	0	2.54945800	4.31546800	-2.10930200 L
B-B_2	0	3.83584700	4.81724100	-0.04537400 L
N-N_3	0	3.83701000	4.94081800	-1.57056500 L
N-N_3	0	5.12226800	5.14095600	0.71694400 L
B-B_2	0	6.40987800	4.81724900	-0.04300800 L
B-B_2	0	7.69343700	4.36979300	2.04075400 L

N-N_3	0	7.69539300	5.15048400	0.72041300 L
N-N_3	0	8.96664900	4.35046100	2.88478000 L
B-B_2	0	10.25970400	4.43459700	2.06767700 L
B-B_2	0	11.49625900	2.97931000	3.56172800 L
N-N_3	0	11.55516700	4.33543500	2.86938200 L
N-N_3	0	12.64516700	1.98165200	3.41838400 L
B-B_2	0	-5.16466300	4.30648600	-2.11309400 L
N-N_3	0	-3.88000200	4.93821000	-1.57369100 L
B-B_2	0	-2.59263200	4.30988900	-2.10921200 L
B-B_2	0	-1.30878400	4.82625500	-0.04725700 L
N-N_3	0	-1.30868500	4.94584800	-1.57301600 L
N-N_3	0	-0.02316100	5.15425500	0.71461000 L
B-B_2	0	1.26359000	4.82875900	-0.04700400 L
B-B_2	0	2.54812400	4.35899300	2.02639300 L
N-N_3	0	2.55065600	5.14834000	0.71528700 L
N-N_3	0	3.83347500	4.31527700	2.85500600 L
B-B_2	0	5.12015600	4.35432700	2.02949200 L
B-B_2	0	6.40517900	3.03893500	3.70737000 L
N-N_3	0	6.40329600	4.31632100	2.86063100 L
N-N_3	0	7.68813600	2.64881500	4.44789500 L
B-B_2	0	8.97688300	3.05850800	3.72762600 L
B-B_2	0	10.25336100	1.15254500	4.73604800 L
N-N_3	0	10.27740600	2.65670000	4.44050700 L
N-N_3	0	11.54917300	0.46717000	5.16324100 L
B-	0	12.82406500	1.25180200	4.75937000 L
B-B_2	0	-10.30628100	4.30552700	-2.13543900 L
N-N_3	0	-9.02731000	4.94682800	-1.58441200 L
B-B_2	0	-7.73844200	4.31307300	-2.12094900 L
B-B_2	0	-6.45250500	4.80957300	-0.05105100 L
N-N_3	0	-6.45134600	4.93634200	-1.57638700 L
N-N_3	0	-5.16840000	5.14025100	0.71114600 L
B-B_2	0	-3.88081600	4.81601000	-0.04839800 L
B-B_2	0	-2.59571200	4.36091000	2.02574800 L
N-N_3	0	-2.59653300	5.14799300	0.71338400 L
N-N_3	0	-1.31031600	4.32090500	2.85359600 L
B-B_2	0	-0.02379200	4.36596600	2.02690100 L
B-B_2	0	1.26064100	3.03621700	3.68756800 L
N-N_3	0	1.26224900	4.31940900	2.85360000 L
N-N_3	0	2.54471100	2.64014000	4.41812100 L
B-B_2	0	3.83195600	3.03522100	3.69351400 L
B-B_2	0	5.11518600	1.12379500	4.63117500 L
N-N_3	0	5.11536100	2.64060900	4.42690100 L
N-N_3	0	6.39710300	0.45511000	5.12867800 L
B-B_2	0	7.68784200	1.12946900	4.66078500 L

B-B_2	0	8.97339600	-1.00641100	4.70495100 L
N-N_3	0	8.96010000	0.46139400	5.17958400 L
N-N_3	0	10.27469500	-1.81129600	4.84435400 L
B-B_2	0	11.49241100	-0.92352800	4.54338400 L
B-	0	12.82404500	-2.94234400	3.96324700 L
N-N_3	0	12.64683900	-1.44075800	3.68575100 L
B-	0	-12.81483700	3.94304500	-1.97285200 L
B-B_2	0	-11.58467400	4.86827000	-0.05632400 L
N-N_3	0	-11.63085700	4.86465700	-1.58536300 L
N-N_3	0	-10.29710800	5.17248800	0.70879800 L
B-B_2	0	-9.02413500	4.82477700	-0.05576300 L
B-B_2	0	-7.74232800	4.36327700	2.03142600 L
N-N_3	0	-7.73733200	5.13929900	0.70860200 L
N-N_3	0	-6.45383600	4.31756600	2.85556900 L
B-B_2	0	-5.16824700	4.35795500	2.02660400 L
B-B_2	0	-3.88147700	3.03667000	3.69015400 L
N-N_3	0	-3.88192700	4.31793800	2.85322200 L
N-N_3	0	-2.59549400	2.64121900	4.41696700 L
B-B_2	0	-1.31034900	3.03805000	3.68830000 L
B-B_2	0	-0.02546800	1.12386200	4.61690900 L
N-N_3	0	-0.02499300	2.64073100	4.41495600 L
N-N_3	0	1.25859500	0.45465000	5.10802500 L
B-B_2	0	2.54454200	1.12356500	4.62167700 L
B-B_2	0	3.82960100	-1.00420400	4.65300800 L
N-N_3	0	3.82819000	0.45464800	5.11524600 L
N-N_3	0	5.11354200	-1.81944000	4.81437900 L
B-B_2	0	6.40218900	-1.00749700	4.67055500 L
B-B_2	0	7.68866300	-2.95005200	3.79432000 L
N-N_3	0	7.68576500	-1.82601100	4.83841100 L
N-N_3	0	8.96299000	-3.77029700	3.60231000 L
B-B_2	0	10.25413500	-2.98833500	3.86237400 L
B-B_2	0	11.49883800	-4.13762000	2.12778600 L
N-N_3	0	11.55109500	-3.74973900	3.60032600 L
N-N_3	0	12.65297500	-3.78568300	1.18974600 L
B-	0	-12.81874300	4.00917900	1.83649500 L
N-N_3	0	-12.87934800	5.04961700	0.71488200 L
N-N_3	0	-11.63416500	4.27447700	2.79989700 L
B-B_2	0	-10.31044200	4.36517500	2.01944500 L
B-B_2	0	-9.02470600	3.04898500	3.70924400 L
N-N_3	0	-9.03029900	4.32785700	2.86268400 L
N-N_3	0	-7.73575700	2.64367900	4.42622300 L
B-B_2	0	-6.45293200	3.03608800	3.69288800 L
B-B_2	0	-5.16679700	1.12407400	4.62631200 L
N-N_3	0	-5.16663100	2.64081100	4.41965700 L

N-N_3	0	-3.87983400	0.45468800	5.11080800 L
B-B_2	0	-2.59562500	1.12426400	4.61922200 L
B-B_2	0	-1.31038400	-1.00364000	4.64308000 L
N-N_3	0	-1.31023300	0.45479200	5.10637600 L
N-N_3	0	-0.02565600	-1.81755500	4.80116700 L
B-B_2	0	1.25920000	-1.00357700	4.64465400 L
B-B_2	0	2.54522400	-2.93747900	3.76206400 L
N-N_3	0	2.54346400	-1.81766100	4.80480400 L
N-N_3	0	3.83088900	-3.73924200	3.55623500 L
B-B_2	0	5.11608700	-2.93768800	3.76945800 L
B-B_2	0	6.40663600	-4.30535900	2.14015600 L
N-N_3	0	6.40009100	-3.74200800	3.56531100 L
N-N_3	0	7.69296100	-4.94207200	1.60538200 L
B-B_2	0	8.97857600	-4.32115300	2.16162500 L
B-B_2	0	10.26114000	-4.89004100	0.08705400 L
N-N_3	0	10.28229200	-4.92773500	1.61956500 L
N-N_3	0	11.55839900	-5.15073000	-0.67429700 L
B-	0	12.83100300	-4.93456500	0.18421000 L
N-N_3	0	-12.87895800	2.57940600	4.36733400 L
B-B_2	0	-11.58507100	3.07323500	3.74578800 L
B-B_2	0	-10.30802300	1.13618500	4.64500800 L
N-N_3	0	-10.29617300	2.66442300	4.45895500 L
N-N_3	0	-9.02663100	0.45546600	5.14088200 L
B-B_2	0	-7.74038000	1.12516200	4.64276800 L
B-B_2	0	-6.45116000	-1.00437700	4.65367800 L
N-N_3	0	-6.45063600	0.45388900	5.11982500 L
N-N_3	0	-5.16518900	-1.81833500	4.80611000 L
B-B_2	0	-3.88049200	-1.00396900	4.64722600 L
B-B_2	0	-2.59512500	-2.93912100	3.76036800 L
N-N_3	0	-2.59489100	-1.81781500	4.80181700 L
N-N_3	0	-1.30986200	-3.74196100	3.55244800 L
B-B_2	0	-0.02494800	-2.93933600	3.76047300 L
B-B_2	0	1.26152800	-4.30311500	2.12963900 L
N-N_3	0	1.26067700	-3.74086200	3.55288200 L
N-N_3	0	2.54842400	-4.93263500	1.59426900 L
B-B_2	0	3.83314500	-4.29984100	2.13244700 L
B-B_2	0	5.12130900	-4.80766500	0.07184800 L
N-N_3	0	5.11983200	-4.93030900	1.59709500 L
N-N_3	0	6.40712200	-5.13749200	-0.68709300 L
B-B_2	0	7.69474100	-4.82266600	0.07621700 L
B-B_2	0	8.98283500	-4.37876000	-2.00953500 L
N-N_3	0	8.97043900	-5.17327400	-0.68753100 L
N-N_3	0	10.28550300	-4.32313800	-2.82275400 L
B-B_2	0	11.50260500	-4.23182600	-1.88858000 L

B-	0	12.83151200	-3.19035600	-3.71424400 L
N-N_3	0	12.65141900	-3.26979000	-2.18975600 L
B-	0	-12.81454900	1.05401400	4.25391600 L
B-B_2	0	-11.58233500	-1.01980200	4.72573400 L
N-N_3	0	-11.63065900	0.47067700	5.06562000 L
N-N_3	0	-10.29375900	-1.83152400	4.85629400 L
B-B_2	0	-9.02244700	-1.00740700	4.67968600 L
B-B_2	0	-7.73995000	-2.94832800	3.77703000 L
N-N_3	0	-7.73373200	-1.82004400	4.81607400 L
N-N_3	0	-6.45135900	-3.74426000	3.55767300 L
B-B_2	0	-5.16639900	-2.94049000	3.76499300 L
B-B_2	0	-3.88058400	-4.30208400	2.12944900 L
N-N_3	0	-3.88028600	-3.74156500	3.55353100 L
N-N_3	0	-2.59537600	-4.93529200	1.59257600 L
B-B_2	0	-1.30921700	-4.30529900	2.12940600 L
B-B_2	0	-0.02252400	-4.82554800	0.06759900 L
N-N_3	0	-0.02318500	-4.93803000	1.59413500 L
N-N_3	0	1.26504800	-5.15138700	-0.69207900 L
B-B_2	0	2.54904700	-4.81505600	0.06867500 L
B-B_2	0	3.83669100	-4.36062800	-2.00576200 L
N-N_3	0	3.83710300	-5.14071300	-0.68948400 L
N-N_3	0	5.12326000	-4.31753300	-2.83258000 L
B-B_2	0	6.41068200	-4.36003600	-2.00749000 L
B-B_2	0	7.69500500	-3.04645800	-3.68635100 L
N-N_3	0	7.69627500	-4.32559300	-2.83968400 L
N-N_3	0	8.96799300	-2.66327200	-4.43909900 L
B-B_2	0	10.26094500	-3.09447500	-3.73954700 L
B-B_2	0	11.49772500	-1.13522100	-4.45615700 L
N-N_3	0	11.55701600	-2.65732700	-4.41804800 L
N-N_3	0	12.64914400	-0.29738200	-3.90112300 L
B-	0	-12.81487100	-2.68621900	3.48057100 L
N-N_3	0	-12.87636900	-1.81321500	4.73660000 L
N-N_3	0	-11.63107400	-3.68438500	3.53611500 L
B-B_2	0	-10.30757800	-2.93975300	3.78780300 L
B-B_2	0	-9.02358500	-4.31455800	2.14328700 L
N-N_3	0	-9.02732200	-3.75519100	3.57122500 L
N-N_3	0	-7.73615000	-4.93149300	1.59452600 L
B-B_2	0	-6.45202800	-4.29945200	2.13118200 L
B-B_2	0	-5.16706400	-4.81158600	0.06645100 L
N-N_3	0	-5.16719700	-4.93089800	1.59225900 L
N-N_3	0	-3.88125100	-5.14227300	-0.69343600 L
B-B_2	0	-2.59430400	-4.81678200	0.06686100 L
B-B_2	0	-1.30754600	-4.36794400	-2.00815300 L
N-N_3	0	-1.30922400	-5.15112800	-0.69312100 L

N-N_3	0	-0.02133300	-4.32531700	-2.83493700 L
B-B_2	0	1.26472300	-4.37016800	-2.00831700 L
B-B_2	0	2.55052100	-3.04024500	-3.66739200 L
N-N_3	0	2.55165500	-4.32404500	-2.83436400 L
N-N_3	0	3.83565400	-2.63931700	-4.39368300 L
B-B_2	0	5.12188200	-3.03547200	-3.66801600 L
B-B_2	0	6.40784500	-1.12188700	-4.60896600 L
N-N_3	0	6.40482200	-2.64017100	-4.40025000 L
N-N_3	0	7.69041500	-0.45226200	-5.11162700 L
B-B_2	0	8.97904500	-1.13369700	-4.63962800 L
B-B_2	0	10.25704200	1.02004700	-4.73118300 L
N-N_3	0	10.27959000	-0.46502400	-5.11083300 L
N-N_3	0	11.55338500	1.82122600	-4.82357800 L
B-	0	12.82748500	0.93790600	-4.79856800 L
N-N_3	0	-12.87802000	-4.85898800	1.54924900 L
B-B_2	0	-11.58396300	-4.35640000	2.16286900 L
B-B_2	0	-10.30933800	-4.81274500	0.07678900 L
N-N_3	0	-10.29584500	-4.96380700	1.60861700 L
N-N_3	0	-9.02929900	-5.14872200	-0.69743000 L
B-B_2	0	-7.74120000	-4.81685600	0.06523200 L
B-B_2	0	-6.45129100	-4.35336200	-2.00897100 L
N-N_3	0	-6.45305400	-5.13888600	-0.69527800 L
N-N_3	0	-5.16538000	-4.31564700	-2.83585100 L
B-B_2	0	-3.87956600	-4.35900300	-2.00802400 L
B-B_2	0	-2.59181200	-3.03754400	-3.66816000 L
N-N_3	0	-2.59379100	-4.32133000	-2.83521400 L
N-N_3	0	-1.30508000	-2.63969000	-4.39193300 L
B-B_2	0	-0.02051200	-3.03910600	-3.66440300 L
B-B_2	0	1.26495600	-1.12238100	-4.58540600 L
N-N_3	0	1.26456600	-2.64018400	-4.39107100 L
N-N_3	0	2.54891200	-0.45208900	-5.07516900 L
B-B_2	0	3.83516400	-1.12178700	-4.59114700 L
B-B_2	0	5.11929900	1.00723800	-4.62053500 L
N-N_3	0	5.11813900	-0.45106500	-5.08492200 L
N-N_3	0	6.40178500	1.82269600	-4.78630200 L
B-B_2	0	7.69172700	1.01147000	-4.65197900 L
B-B_2	0	8.97926100	2.95780800	-3.77613500 L
N-N_3	0	8.96473800	1.83603300	-4.83484400 L
N-N_3	0	10.28199400	3.74152500	-3.55298400 L
B-B_2	0	11.49887400	2.80958500	-3.66536600 L
N-N_3	0	12.65269600	2.90264200	-2.66749400 L
B-	0	-12.81839200	-4.41441100	0.08541600 L
B-B_2	0	-11.58357300	-4.40445800	-2.04027000 L
N-N_3	0	-11.63295200	-5.07269900	-0.66502500 L

N-N_3	0	-10.29443200	-4.34525900	-2.85947000 L
B-B_2	0	-9.02304800	-4.36783800	-2.01726400 L
B-B_2	0	-7.73734300	-3.03972400	-3.69007200 L
N-N_3	0	-7.73435100	-4.31591500	-2.83929200 L
N-N_3	0	-6.44696700	-2.63983700	-4.40874900 L
B-B_2	0	-5.16355800	-3.03596400	-3.67567000 L
B-B_2	0	-3.87517900	-1.12232900	-4.59962600 L
N-N_3	0	-3.87558600	-2.63963200	-4.39887200 L
N-N_3	0	-2.58812100	-0.45250200	-5.08251400 L
B-B_2	0	-1.30491700	-1.12226800	-4.58914800 L
B-B_2	0	-0.01969000	1.00561900	-4.61003800 L
N-N_3	0	-0.01920600	-0.45222700	-5.07409400 L
N-N_3	0	1.26450200	1.81954800	-4.77015500 L
B-B_2	0	2.54950200	1.00634900	-4.61227100 L
B-B_2	0	3.83478500	2.94630200	-3.73853900 L
N-N_3	0	3.83342000	1.82045700	-4.77501500 L
N-N_3	0	5.12041200	3.74857100	-3.53281300 L
B-B_2	0	6.40762500	2.94988400	-3.74806700 L
N-N_3	0	7.69296200	3.75774300	-3.54579900 L
B-	0	-12.81265100	-2.80366500	-3.37165200 L
N-N_3	0	-12.87697100	-4.22851600	-2.81507600 L
N-N_3	0	-11.62731900	-2.62671800	-4.35395200 L
B-B_2	0	-10.30522000	-3.04730200	-3.68728100 L
B-B_2	0	-9.01753500	-1.12815800	-4.63831500 L
N-N_3	0	-9.02321700	-2.64742000	-4.42747200 L
N-N_3	0	-7.72753900	-0.45334800	-5.10788100 L
B-B_2	0	-6.44605700	-1.12221900	-4.61026700 L
B-B_2	0	-5.16027500	1.00727500	-4.63192900 L
N-N_3	0	-5.15866000	-0.45238800	-5.09318100 L
N-N_3	0	-3.87328300	1.82028600	-4.78207300 L
B-B_2	0	-2.58946700	1.00582100	-4.61885700 L
B-B_2	0	-1.30527400	2.94324000	-3.73431800 L
N-N_3	0	-1.30370500	1.81927400	-4.77245400 L
N-N_3	0	-0.02098000	3.74831000	-3.53022000 L
B-B_2	0	1.26441500	2.94529200	-3.73394200 L
N-N_3	0	2.54928200	3.74921100	-3.53104000 L
N-N_3	0	-12.87080700	-0.42205500	-5.03942000 L
B-B_2	0	-11.57752100	-1.13477500	-4.68763600 L
B-B_2	0	-10.30121500	1.00135700	-4.66520800 L
N-N_3	0	-10.28783100	-0.45879100	-5.15310600 L
N-N_3	0	-9.01995600	1.82953600	-4.81879200 L
B-B_2	0	-7.73368800	1.01161500	-4.65315100 L
B-B_2	0	-6.44668500	2.94176100	-3.74951600 L
N-N_3	0	-6.44405000	1.82326500	-4.79474100 L

N-N_3	0	-5.16184200	3.74402900	-3.53651400 L
B-B_2	0	-3.87584700	2.94215100	-3.74111100 L
N-N_3	0	-2.59102100	3.74548700	-3.53139800 L
B-	0	-12.80840400	0.90667500	-4.28168400 L
B-B_2	0	-11.57797500	2.98242800	-3.81458000 L
N-N_3	0	-11.62398500	1.78251700	-4.76191200 L
N-N_3	0	-10.29017900	3.77090100	-3.57890900 L
B-B_2	0	-9.01797100	2.95254200	-3.77416900 L
N-N_3	0	-7.73045700	3.74605600	-3.54594300 L
N-N_3	0	-12.87261800	3.70233400	-3.48363300 L
H-H_	0	12.38077000	2.91624400	0.69120100 L
H-H_	0	12.36911100	1.28240200	2.69272800 L
H-H_	0	12.37765900	-1.31598300	2.68395500 L
H-H_	0	12.38337400	-2.92270000	0.66617600 L
H-H_	0	-12.86573100	6.00101500	1.14759500 L
H-H_	0	-12.86724200	2.83492300	5.38082300 L
H-H_	0	12.37491300	-2.32582200	-1.83738100 L
H-H_	0	12.37610700	0.02205400	-2.94451200 L
H-H_	0	-12.86317900	-2.43918900	5.57360200 L
H-H_	0	-12.86288100	-5.90378700	1.57667100 L
H-H_	0	12.38281300	2.35505900	-1.81962500 L
H-H_	0	-12.86412500	-4.89664400	-3.61883300 L
H-H_	0	-12.85710100	-0.21751300	-6.06439100 L
H-H_	0	-12.85756600	4.62978200	-3.96550800 L
C-C_R	0	0.49096700	0.02265700	-0.27429300 H
H-H_	0	-0.69640300	1.14855300	1.16287900 H
H-H_	0	-1.32762600	1.21050000	-0.49479400 H
C-C_3	0	-0.40066600	1.15233600	0.09924900 H
H-H_	0	0.14635200	2.08015700	-0.07321600 H
N-N_R	0	0.04869400	-1.36967700	-0.04484400 H
H-H_	0	-0.17217700	-1.59503600	0.93153400 H
H-H_	0	-0.73908900	-1.67567600	-0.62447400 H
C-C_R	0	1.80100300	-0.03425400	-0.71459100 H
O-O_R	0	2.41659500	-1.13640300	-0.89518600 H
O-O_R	0	2.44879100	1.14633700	-0.96216400 H
H-H_	0	3.32923800	0.89332200	-1.27816300 H
H-H_	0	0.94645000	-1.86433600	-0.34423000 H

Coordinates of all stationary points in the pathway b of α -Ala chiral transformation confined in SWBNNT(8,8)

bSTS1@D

B-B_2	0	-10.26984400	-5.21623200	-1.90046100 L
N-N_3	0	-11.57721200	-5.69682700	-1.27084400 L
B-	0	-12.84566200	-5.14167100	-1.97026400 L
B-B_2	0	-5.13436900	-5.14375600	-1.85700300 L
N-N_3	0	-6.41831900	-5.72105600	-1.26040600 L
B-B_2	0	-7.70723300	-5.16737300	-1.87102600 L
B-B_2	0	-8.99156800	-5.51264600	0.24655700 L
N-N_3	0	-8.98213500	-5.76485200	-1.27578700 L
N-N_3	0	-10.29464700	-5.77501000	1.01478300 L
B-B_2	0	-11.49546800	-5.28979300	0.19281300 L
B-	0	-12.84695000	-5.02263000	2.25389100 L
N-N_3	0	-12.60896700	-4.46765500	0.84045100 L
B-B_2	0	0.00578800	-5.15095500	-1.85675200 L
N-N_3	0	-1.27921900	-5.72745400	-1.25975800 L
B-B_2	0	-2.56358000	-5.14884200	-1.85606300 L
B-B_2	0	-3.84967000	-5.48349800	0.25312300 L
N-N_3	0	-3.85013700	-5.71994400	-1.25831000 L
N-N_3	0	-5.13566700	-5.77316700	1.02906800 L
B-B_2	0	-6.42293300	-5.48652700	0.25414200 L
B-B_2	0	-7.70764400	-4.98160100	2.33697400 L
N-N_3	0	-7.70642400	-5.79057900	1.03236100 L
N-N_3	0	-8.98141800	-4.97141700	3.18210700 L
B-B_2	0	-10.27048400	-5.03404900	2.35431900 L
B-B_2	0	-11.49068100	-3.58569800	3.87203000 L
N-N_3	0	-11.57732100	-4.91577300	3.13866600 L
N-N_3	0	-12.59702300	-2.54076000	3.73411100 L
B-B_2	0	5.14714300	-5.14793200	-1.86152900 L
N-N_3	0	3.86203200	-5.72005600	-1.26062600 L
B-B_2	0	2.57591100	-5.14788300	-1.85837100 L
B-B_2	0	1.29200100	-5.48996900	0.25184500 L
N-N_3	0	1.29174900	-5.72491300	-1.26001300 L
N-N_3	0	0.00748100	-5.78563900	1.02841600 L
B-B_2	0	-1.27867600	-5.49503000	0.25270100 L
B-B_2	0	-2.56319500	-4.96285300	2.32186100 L
N-N_3	0	-2.56533400	-5.78085200	1.02869800 L
N-N_3	0	-3.84852700	-4.92549100	3.15053200 L
B-B_2	0	-5.13468600	-4.95818400	2.32410900 L
B-B_2	0	-6.42019900	-3.68072800	4.04565700 L
N-N_3	0	-6.41709200	-4.92978000	3.15696100 L
N-N_3	0	-7.70145300	-3.34138400	4.81333800 L

B-B_2	0	-8.98843300	-3.70686800	4.06693300 L
B-B_2	0	-10.26554400	-1.87137300	5.21278200 L
N-N_3	0	-10.29008800	-3.34395100	4.79521400 L
N-N_3	0	-11.57365200	-1.23323300	5.68174900 L
B-	0	-12.84280600	-1.92829300	5.12221200 L
B-B_2	0	10.28409000	-5.16362300	-1.88550300 L
N-N_3	0	9.00595700	-5.74477500	-1.27065900 L
B-B_2	0	7.72025800	-5.16303500	-1.86934100 L
B-B_2	0	6.43377500	-5.47864600	0.24829900 L
N-N_3	0	6.43198700	-5.72306100	-1.26273400 L
N-N_3	0	5.14908000	-5.77106600	1.02463700 L
B-B_2	0	3.86272800	-5.47963100	0.25013700 L
B-B_2	0	2.57810200	-4.96209000	2.32105300 L
N-N_3	0	2.57908300	-5.77720700	1.02641900 L
N-N_3	0	1.29330300	-4.93077000	3.14991100 L
B-B_2	0	0.00737600	-4.96841300	2.32254800 L
B-B_2	0	-1.27672500	-3.67613100	4.02647700 L
N-N_3	0	-1.27811100	-4.93052700	3.15030600 L
N-N_3	0	-2.56090600	-3.32680900	4.78011300 L
B-B_2	0	-3.84729400	-3.67355500	4.02993200 L
B-B_2	0	-5.13058200	-1.83479100	5.12745300 L
N-N_3	0	-5.13033300	-3.32710200	4.78790700 L
N-N_3	0	-6.41169900	-1.23004500	5.70359400 L
B-B_2	0	-7.70320200	-1.84583500	5.16139100 L
B-B_2	0	-8.98369900	0.27850100	5.49824200 L
N-N_3	0	-8.97638100	-1.24331900	5.75617800 L
N-N_3	0	-10.28553400	1.04700500	5.76366100 L
B-B_2	0	-11.48389700	0.22814200	5.26941500 L
B-	0	-12.83845500	2.28801100	5.01717000 L
N-N_3	0	-12.59508700	0.88093600	4.44828600 L
B-	0	12.77223900	-4.74594400	-1.74489200 L
B-B_2	0	11.56049300	-5.51924800	0.24555400 L
N-N_3	0	11.60904900	-5.65136700	-1.27527200 L
N-N_3	0	10.27845200	-5.81513500	1.02512700 L
B-B_2	0	9.00448100	-5.50306400	0.24484600 L
B-B_2	0	7.72258900	-4.97416000	2.33078600 L
N-N_3	0	7.71686800	-5.77772500	1.02391400 L
N-N_3	0	6.43360600	-4.93296400	3.15417800 L
B-B_2	0	5.14951300	-4.96106500	2.32285000 L
B-B_2	0	3.86362400	-3.67827900	4.03106000 L
N-N_3	0	3.86345200	-4.92894700	3.14984000 L
N-N_3	0	2.57772300	-3.33079600	4.78201700 L
B-B_2	0	1.29322500	-3.67720100	4.02710000 L
B-B_2	0	0.00941400	-1.83721700	5.11850200 L

N-N_3	0	0.00831900	-3.32902000	4.77917300 L
N-N_3	0	-1.27476000	-1.23096500	5.68523400 L
B-B_2	0	-2.56002100	-1.83494100	5.11879400 L
B-B_2	0	-3.84364000	0.28115300	5.44400700 L
N-N_3	0	-3.84355100	-1.22917200	5.68871200 L
N-N_3	0	-5.12663800	1.05711900	5.74624500 L
B-B_2	0	-6.41603600	0.28415800	5.46281900 L
B-B_2	0	-7.69992700	2.37599400	4.97934000 L
N-N_3	0	-7.69728700	1.06280500	5.77530900 L
N-N_3	0	-8.97350600	3.22180600	4.98297800 L
B-B_2	0	-10.26196300	2.39260100	5.03446600 L
B-B_2	0	-11.48415700	3.93176500	3.60863800 L
N-N_3	0	-11.57006000	3.17690800	4.92657400 L
N-N_3	0	-12.60437100	3.83088000	2.57400300 L
B-	0	12.77391900	-4.58660500	2.12207700 L
N-N_3	0	12.86179700	-5.64293200	1.01928200 L
N-N_3	0	11.61115800	-4.88935000	3.09670000 L
B-B_2	0	10.28645800	-4.98334100	2.32091600 L
B-B_2	0	9.00533800	-3.70407600	4.05757700 L
N-N_3	0	9.00784900	-4.95339800	3.16601300 L
N-N_3	0	7.71636000	-3.34254600	4.79854400 L
B-B_2	0	6.43449300	-3.68261700	4.03750700 L
B-B_2	0	5.14968400	-1.84224600	5.13060600 L
N-N_3	0	5.14797600	-3.33366800	4.78730600 L
N-N_3	0	3.86317100	-1.23527500	5.69228700 L
B-B_2	0	2.57894300	-1.83914900	5.12176800 L
B-B_2	0	1.29560900	0.27687100	5.44071400 L
N-N_3	0	1.29400500	-1.23302400	5.68681600 L
N-N_3	0	0.01138500	1.05170900	5.73814700 L
B-B_2	0	-1.27371100	0.27886700	5.43931600 L
B-B_2	0	-2.55702500	2.36014800	4.94302800 L
N-N_3	0	-2.55741400	1.05384400	5.73923500 L
N-N_3	0	-3.84120000	3.19041800	4.92701400 L
B-B_2	0	-5.12750700	2.36320900	4.94830300 L
B-B_2	0	-6.41407300	4.10805000	3.70394900 L
N-N_3	0	-6.40934300	3.19679800	4.93684200 L
N-N_3	0	-7.69610300	4.87974200	3.37814700 L
B-B_2	0	-8.98206800	4.12654900	3.73265500 L
B-B_2	0	-10.26145800	5.30150100	1.91686400 L
N-N_3	0	-10.28435300	4.85984600	3.38236600 L
N-N_3	0	-11.56786200	5.78490600	1.28752000 L
B-	0	-12.83722900	5.23255400	1.98752700 L
N-N_3	0	12.86245700	-3.25100100	4.70328500 L
B-B_2	0	11.56122000	-3.71399900	4.07076000 L

B-B_2	0	10.28630200	-1.86524800	5.15659300 L
N-N_3	0	10.27863000	-3.37012000	4.83011400 L
N-N_3	0	9.00728800	-1.24670000	5.73243500 L
B-B_2	0	7.72269300	-1.84951500	5.15227000 L
B-B_2	0	6.43577300	0.27262000	5.45556800 L
N-N_3	0	6.43303000	-1.23813300	5.70409700 L
N-N_3	0	5.15012200	1.04842100	5.74634500 L
B-B_2	0	3.86528300	0.27491000	5.44612300 L
B-B_2	0	2.58225000	2.35610700	4.94441700 L
N-N_3	0	2.58040100	1.05001600	5.74118300 L
N-N_3	0	1.29801300	3.18644000	4.92609900 L
B-B_2	0	0.01260100	2.35812900	4.94222900 L
B-B_2	0	-1.27092500	4.09374400	3.69244700 L
N-N_3	0	-1.27152200	3.18846300	4.92571800 L
N-N_3	0	-2.55547400	4.85408200	3.35955100 L
B-B_2	0	-3.84143000	4.09626200	3.69388700 L
B-B_2	0	-5.12642000	5.21894600	1.87452600 L
N-N_3	0	-5.12534800	4.85834000	3.36191400 L
N-N_3	0	-6.40895200	5.79736300	1.27567300 L
B-B_2	0	-7.69901400	5.24771800	1.88760800 L
B-B_2	0	-8.98291400	5.59428000	-0.23068100 L
N-N_3	0	-8.97266200	5.84708400	1.29166100 L
N-N_3	0	-10.28561400	5.85993400	-0.99845300 L
B-B_2	0	-11.48737000	5.37753100	-0.17611500 L
B-	0	-12.84027600	5.11336000	-2.23658700 L
N-N_3	0	-12.60284800	4.55777000	-0.82331500 L
B-	0	12.77230300	-1.72448000	4.73483400 L
B-B_2	0	11.56191500	0.26873800	5.50344300 L
N-N_3	0	11.61083200	-1.25143200	5.64038000 L
N-N_3	0	10.28026800	1.04786700	5.80339900 L
B-B_2	0	9.00640600	0.26857400	5.48730800 L
B-B_2	0	7.72566400	2.36079800	4.96795600 L
N-N_3	0	7.71807800	1.04730100	5.76105600 L
N-N_3	0	6.43729300	3.18573300	4.93459900 L
B-B_2	0	5.15280200	2.35513400	4.94956100 L
B-B_2	0	3.86924000	4.08844600	3.69342200 L
N-N_3	0	3.86768800	3.18440600	4.92796900 L
N-N_3	0	2.58509000	4.84934200	3.35923700 L
B-B_2	0	1.29911600	4.09150300	3.69254900 L
B-B_2	0	0.01497700	5.21357200	1.87242200 L
N-N_3	0	0.01476700	4.85224800	3.35918500 L
N-N_3	0	-1.26991100	5.78645100	1.27195600 L
B-B_2	0	-2.55546700	5.21534800	1.87280700 L
B-B_2	0	-3.84138100	5.54667600	-0.23849100 L

N-N_3	0	-3.84049700	5.78779000	1.27254000 L
N-N_3	0	-5.12607200	5.84336400	-1.01418100 L
B-B_2	0	-6.41437400	5.56088300	-0.23895000 L
B-B_2	0	-7.70085400	5.06193700	-2.32284700 L
N-N_3	0	-7.69715000	5.86899000	-1.01688900 L
N-N_3	0	-8.97538700	5.05506000	-3.16692100 L
B-B_2	0	-10.26371500	5.11934000	-2.33817900 L
B-B_2	0	-11.48759000	3.67393600	-3.85549200 L
N-N_3	0	-11.57121200	5.00398900	-3.12182700 L
N-N_3	0	-12.59390600	2.62946600	-3.71415200 L
B-	0	12.77418400	2.15143200	4.57960900 L
N-N_3	0	12.86398900	1.04137200	5.62786500 L
N-N_3	0	11.61432500	3.12509000	4.89449900 L
B-B_2	0	10.28906000	2.34955500	4.98073600 L
B-B_2	0	9.01039400	4.10229800	3.71968900 L
N-N_3	0	9.01117500	3.19577000	4.95822400 L
N-N_3	0	7.72304800	4.85019300	3.36738100 L
B-B_2	0	6.43983000	4.08755400	3.69743900 L
B-B_2	0	5.15646900	5.20812100	1.87288100 L
N-N_3	0	5.15523700	4.84607600	3.35986500 L
N-N_3	0	3.87143000	5.77976200	1.27134000 L
B-B_2	0	2.58542800	5.21025600	1.87233500 L
B-B_2	0	1.30036000	5.54161300	-0.23930900 L
N-N_3	0	1.30087800	5.78375300	1.27157300 L
N-N_3	0	0.01520500	5.83744400	-1.01441700 L
B-B_2	0	-1.27033100	5.54439900	-0.23886400 L
B-B_2	0	-2.55666800	5.03023700	-2.31250700 L
N-N_3	0	-2.55570800	5.83934900	-1.01385500 L
N-N_3	0	-3.84241100	5.00165200	-3.14077100 L
B-B_2	0	-5.12791500	5.03335200	-2.31272900 L
B-B_2	0	-6.41690500	3.76303700	-4.03643500 L
N-N_3	0	-6.41115900	5.00979000	-3.14432400 L
N-N_3	0	-7.69989700	3.42530600	-4.80183800 L
B-B_2	0	-8.98525200	3.79149200	-4.05312300 L
B-B_2	0	-10.26600300	1.95749000	-5.19694200 L
N-N_3	0	-10.28830900	3.43028300	-4.77981800 L
N-N_3	0	-11.57556000	1.32023000	-5.66330400 L
B-	0	-12.84304200	2.01645600	-5.10139200 L
N-N_3	0	12.86791200	4.74994200	3.27625800 L
B-B_2	0	11.56609300	4.11279200	3.73079600 L
B-B_2	0	10.29336200	5.21711800	1.89278200 L
N-N_3	0	10.28469900	4.87674500	3.39444400 L
N-N_3	0	9.01553600	5.79987400	1.27863300 L
B-B_2	0	7.72955600	5.21994400	1.87839500 L

B-B_2	0	6.44200200	5.53556800	-0.23917300 L
N-N_3	0	6.44145800	5.78074000	1.27193200 L
N-N_3	0	5.15685900	5.82895200	-1.01487800 L
B-B_2	0	3.87104000	5.53706700	-0.23949000 L
B-B_2	0	2.58481100	5.02492300	-2.31373000 L
N-N_3	0	2.58620600	5.83363100	-1.01474900 L
N-N_3	0	1.29931800	4.99806300	-3.14227100 L
B-B_2	0	0.01407100	5.02858600	-2.31332100 L
B-B_2	0	-1.27290600	3.75241800	-4.02650500 L
N-N_3	0	-1.27163800	5.00065500	-3.14163800 L
N-N_3	0	-2.55869400	3.40709000	-4.77960000 L
B-B_2	0	-3.84388700	3.75397000	-4.02657000 L
B-B_2	0	-5.13078400	1.91690400	-5.12076200 L
N-N_3	0	-5.12882300	3.40948900	-4.78205800 L
N-N_3	0	-6.41352600	1.31199900	-5.69304900 L
B-B_2	0	-7.70356900	1.92971200	-5.14960900 L
B-B_2	0	-8.98670300	-0.19371200	-5.48207000 L
N-N_3	0	-8.97824200	1.32779700	-5.74179000 L
N-N_3	0	-10.28933900	-0.96113400	-5.74632700 L
B-B_2	0	-11.48648200	-0.14121600	-5.25080600 L
B-	0	-12.84305600	-2.20088200	-5.00273300 L
N-N_3	0	-12.59979500	-0.79422500	-4.43262600 L
B-	0	12.78042800	4.79518400	1.74991600 L
B-B_2	0	11.56901300	5.57264900	-0.23895600 L
N-N_3	0	11.61859500	5.70321300	1.28195100 L
N-N_3	0	10.28670300	5.86941000	-1.01774700 L
B-B_2	0	9.01287900	5.55817400	-0.23690300 L
B-B_2	0	7.72941700	5.03147300	-2.32290000 L
N-N_3	0	7.72497500	5.83395200	-1.01532300 L
N-N_3	0	6.44030500	4.99318400	-3.14632200 L
B-B_2	0	5.15611700	5.02171300	-2.31510900 L
B-B_2	0	3.86823700	3.74607400	-4.02846800 L
N-N_3	0	3.87005400	4.99384000	-3.14267300 L
N-N_3	0	2.58229900	3.40258600	-4.78179900 L
B-B_2	0	1.29765600	3.75003000	-4.02757800 L
B-B_2	0	0.01026700	1.91319000	-5.11824100 L
N-N_3	0	0.01174700	3.40548300	-4.78062300 L
N-N_3	0	-1.27547000	1.30682200	-5.68213900 L
B-B_2	0	-2.55989700	1.91485200	-5.11727600 L
B-B_2	0	-3.84660200	-0.20072200	-5.43034700 L
N-N_3	0	-3.84517600	1.30841100	-5.68255300 L
N-N_3	0	-5.13045600	-0.97655100	-5.72880400 L
B-B_2	0	-6.41908600	-0.20146500	-5.44787500 L
B-B_2	0	-7.70487800	-2.29160700	-4.96043000 L

N-N_3	0	-7.70107300	-0.97961900	-5.75839100 L
N-N_3	0	-8.97877900	-3.13681600	-4.96505300 L
B-B_2	0	-10.26674100	-2.30684100	-5.01732800 L
B-B_2	0	-11.49079900	-3.84548000	-3.59294300 L
N-N_3	0	-11.57524200	-3.09048200	-4.91084000 L
N-N_3	0	-12.60974400	-3.74083200	-2.55739100 L
B-	0	12.78108100	4.63926200	-2.11562900 L
N-N_3	0	12.86991700	5.69596700	-1.01331000 L
N-N_3	0	11.61783200	4.94190100	-3.08974700 L
B-B_2	0	10.29345400	5.03765300	-2.31352500 L
B-B_2	0	9.01019000	3.76052700	-4.05032900 L
N-N_3	0	9.01459800	5.00948100	-3.15829700 L
N-N_3	0	7.72091200	3.40185200	-4.79201300 L
B-B_2	0	6.43922900	3.74427700	-4.03175200 L
B-B_2	0	5.15132100	1.90738700	-5.12610700 L
N-N_3	0	5.15272000	3.39897900	-4.78323400 L
N-N_3	0	3.86401900	1.30204100	-5.68782500 L
B-B_2	0	2.58044800	1.91052100	-5.12076100 L
B-B_2	0	1.29311800	-0.20397000	-5.42976400 L
N-N_3	0	1.29421100	1.30471200	-5.68401600 L
N-N_3	0	0.00731200	-0.97822400	-5.72171700 L
B-B_2	0	-1.27655100	-0.20166000	-5.42747500 L
B-B_2	0	-2.56243600	-2.27885100	-4.91966900 L
N-N_3	0	-2.56144300	-0.97642500	-5.72212400 L
N-N_3	0	-3.84697800	-3.10781400	-4.90271900 L
B-B_2	0	-5.13264700	-2.27987900	-4.92647500 L
B-B_2	0	-6.42079900	-4.02490100	-3.68372900 L
N-N_3	0	-6.41465600	-3.11294400	-4.91599600 L
N-N_3	0	-7.70343800	-4.79665000	-3.36072100 L
B-B_2	0	-8.98869200	-4.04207000	-3.71511500 L
N-N_3	0	-10.29181500	-4.77445500	-3.36588800 L
N-N_3	0	12.86670500	3.29938400	-4.69406900 L
B-B_2	0	11.56607300	3.76556600	-4.06251300 L
B-B_2	0	10.28793400	1.91916800	-5.14875300 L
N-N_3	0	10.28315600	3.42408600	-4.82238100 L
N-N_3	0	9.00790800	1.30304800	-5.72485700 L
B-B_2	0	7.72437000	1.90877800	-5.14552400 L
B-B_2	0	6.43340300	-0.21071100	-5.44617100 L
N-N_3	0	6.43380700	1.29959400	-5.69751200 L
N-N_3	0	5.14591500	-0.98443400	-5.73438800 L
B-B_2	0	3.86293000	-0.20727600	-5.43582200 L
B-B_2	0	2.57604000	-2.28402400	-4.92482000 L
N-N_3	0	2.57626800	-0.98100000	-5.72667700 L
N-N_3	0	1.29011200	-3.11154900	-4.90399800 L

B-B_2	0	0.00686700	-2.28045200	-4.91894200 L
B-B_2	0	-1.27853300	-4.01565300	-3.66864600 L
N-N_3	0	-1.27820500	-3.10863400	-4.90048800 L
N-N_3	0	-2.56370400	-4.77586300	-3.33970700 L
B-B_2	0	-3.84827400	-4.01420000	-3.67019600 L
N-N_3	0	-5.13266200	-4.77671800	-3.34246600 L
B-	0	12.77314500	1.77305700	-4.72563700 L
B-B_2	0	11.55943200	-0.21742900	-5.49601900 L
N-N_3	0	11.61135200	1.30273300	-5.63212500 L
N-N_3	0	10.27607100	-0.99399700	-5.79544900 L
B-B_2	0	9.00397000	-0.21210300	-5.47889600 L
B-B_2	0	7.71932600	-2.30141400	-4.95730200 L
N-N_3	0	7.71389300	-0.98845900	-5.75136300 L
N-N_3	0	6.42893900	-3.12331200	-4.92190600 L
B-B_2	0	5.14651100	-2.28949800	-4.93486700 L
B-B_2	0	3.86037100	-4.02077400	-3.67674600 L
N-N_3	0	3.85924200	-3.11547600	-4.91021700 L
N-N_3	0	2.57519900	-4.78048300	-3.34346000 L
B-B_2	0	1.29054300	-4.01932400	-3.67258000 L
N-N_3	0	0.00527700	-4.77887300	-3.34077600 L
B-	0	12.76861100	-2.10283200	-4.57373400 L
N-N_3	0	12.85990300	-0.99252200	-5.62159300 L
N-N_3	0	11.60650200	-3.07402600	-4.88806400 L
B-B_2	0	10.28275300	-2.29575300	-4.97286400 L
B-B_2	0	9.00159600	-4.04621400	-3.71093400 L
N-N_3	0	9.00301100	-3.13925800	-4.94913400 L
N-N_3	0	7.71304500	-4.79173800	-3.35786200 L
B-B_2	0	6.43102500	-4.02593200	-3.68538200 L
N-N_3	0	5.14509200	-4.78215800	-3.34736200 L
N-N_3	0	12.85827900	-4.70174700	-3.27132400 L
B-B_2	0	11.55734400	-4.06198300	-3.72466800 L
N-N_3	0	10.27472000	-4.82328200	-3.38712900 L
H-H_	0	-12.27226100	-3.48157400	0.92173100 L
H-H_	0	-12.25030000	-1.78976500	3.09518800 L
H-H_	0	-12.25378600	0.97360700	3.46475700 L
H-H_	0	-12.27607800	3.19950100	1.80857900 L
H-H_	0	12.88137000	-6.58729300	1.46698400 L
H-H_	0	12.88399400	-3.60132700	5.68789200 L
H-H_	0	-12.26821900	3.57100200	-0.90479700 L
H-H_	0	-12.24588700	1.87867800	-3.07568300 L
H-H_	0	12.88708000	1.48234200	6.57531200 L
H-H_	0	12.88836500	5.73138000	3.63542700 L
H-H_	0	-12.26061700	-0.88771300	-3.44844700 L
H-H_	0	-12.27900500	-3.11002300	-1.79254600 L

H-H_	0	12.88935900	6.64016400	-1.46136600 L
H-H_	0	12.88983500	3.64964000	-5.67866300 L
H-H_	0	12.88151100	-1.43316700	-6.56922500 L
H-H_	0	12.87617000	-5.68342300	-3.62997900 L
C-C_3	0	-0.11369900	-1.73807500	0.00301400 H
H-H_	0	-0.16087200	0.12874700	1.13184400 H
H-H_	0	0.83756600	-1.14877200	1.86256600 H
C-C_3	0	-0.09557200	-0.94790200	1.32624900 H
H-H_	0	-0.93197100	-1.23250900	1.96934000 H
N-N_3	0	0.94308400	-1.33114300	-0.90719500 H
H-H_	0	1.51474800	-2.09832300	-1.23433100 H
H-H_	0	1.53183900	-0.59486400	-0.54043600 H
C-C_R	0	-1.49504500	-1.59970900	-0.65901100 H
O-O_R	0	-1.77401400	-0.98125200	-1.65815700 H
O-O_R	0	-2.43197900	-2.28891300	0.05592400 H
H-H_	0	-3.28276500	-2.16834600	-0.39806300 H
H-H_	0	-0.02032200	-2.79939500	0.25526100 H

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B-B_2	0	-10.27213000	-5.41818800	-1.24966100 L
N-N_3	0	-11.57926100	-5.81741900	-0.56518200 L
B-	0	-12.84795000	-5.35435100	-1.32817900 L
B-B_2	0	-5.13646300	-5.34269700	-1.21638600 L
N-N_3	0	-6.42069800	-5.84042700	-0.55241400 L
B-B_2	0	-7.70941800	-5.36618900	-1.22666300 L
B-B_2	0	-8.99361900	-5.44521500	0.91728800 L
N-N_3	0	-8.98435900	-5.88495100	-0.56185300 L
N-N_3	0	-10.29653100	-5.61000000	1.71242300 L
B-B_2	0	-11.49761000	-5.23142400	0.83651500 L
B-	0	-12.84890600	-4.70603200	2.84707900 L
N-N_3	0	-12.60936700	-4.33223100	1.37558600 L
B-B_2	0	0.00425200	-5.35459000	-1.21601300 L
N-N_3	0	-1.28115500	-5.85162400	-0.55190300 L
B-B_2	0	-2.56530200	-5.35092000	-1.21560300 L
B-B_2	0	-3.85174500	-5.41461000	0.91822500 L
N-N_3	0	-3.85256200	-5.84085000	-0.55095600 L
N-N_3	0	-5.13749000	-5.60485700	1.72498300 L
B-B_2	0	-6.42506000	-5.41809500	0.92082500 L
B-B_2	0	-7.70940500	-4.65766400	2.92521900 L
N-N_3	0	-7.70826800	-5.62276900	1.73137000 L
N-N_3	0	-8.98303700	-4.54338200	3.76294500 L
B-B_2	0	-10.27221600	-4.70776600	2.94913600 L
B-B_2	0	-11.49159700	-3.08255200	4.27673900 L

N-N_3	0	-11.57926600	-4.49253900	3.71236800 L
N-N_3	0	-12.59707100	-2.06152900	4.01162200 L
B-B_2	0	5.14595400	-5.34284100	-1.21854600 L
N-N_3	0	3.86123400	-5.83810000	-0.55224800 L
B-B_2	0	2.57446300	-5.34539300	-1.21587600 L
B-B_2	0	1.29058800	-5.42494100	0.91866300 L
N-N_3	0	1.29106200	-5.84752500	-0.55193300 L
N-N_3	0	0.00541700	-5.61863500	1.72565100 L
B-B_2	0	-1.28066300	-5.42883500	0.91892800 L
B-B_2	0	-2.56520000	-4.63728900	2.90404800 L
N-N_3	0	-2.56757300	-5.61228900	1.72484500 L
N-N_3	0	-3.84989400	-4.49891000	3.72310300 L
B-B_2	0	-5.13655400	-4.63458100	2.90816900 L
B-B_2	0	-6.42183700	-3.15561800	4.46101000 L
N-N_3	0	-6.41852800	-4.50422100	3.73199100 L
N-N_3	0	-7.70296500	-2.72587900	5.18220500 L
B-B_2	0	-8.98995300	-3.17974900	4.48594200 L
B-B_2	0	-10.26724600	-1.21863500	5.40088100 L
N-N_3	0	-10.29159600	-2.73086200	5.16449600 L
N-N_3	0	-11.57575800	-0.52893600	5.78898100 L
B-	0	-12.84451200	-1.28589800	5.31528600 L
B-B_2	0	10.28294100	-5.35715200	-1.23973000 L
N-N_3	0	9.00509500	-5.85945600	-0.55844100 L
B-B_2	0	7.71907800	-5.35652200	-1.22405200 L
B-B_2	0	6.43246900	-5.40999900	0.91576800 L
N-N_3	0	6.43115100	-5.83898500	-0.55353400 L
N-N_3	0	5.14771300	-5.60451900	1.72207200 L
B-B_2	0	3.86138000	-5.41247400	0.91703500 L
B-B_2	0	2.57620300	-4.63963000	2.90553600 L
N-N_3	0	2.57759600	-5.61139800	1.72391100 L
N-N_3	0	1.29074500	-4.50411000	3.72260300 L
B-B_2	0	0.00543600	-4.64316700	2.90511300 L
B-B_2	0	-1.27871000	-3.15042900	4.43788300 L
N-N_3	0	-1.28002700	-4.50242400	3.72165400 L
N-N_3	0	-2.56247300	-2.71355000	5.14506200 L
B-B_2	0	-3.84906200	-3.14901300	4.44313400 L
B-B_2	0	-5.13240300	-1.19162300	5.31215900 L
N-N_3	0	-5.13183800	-2.71399100	5.15439300 L
N-N_3	0	-6.41359700	-0.52250200	5.81179600 L
B-B_2	0	-7.70499600	-1.19918900	5.34736700 L
B-B_2	0	-8.98575600	0.95024700	5.42727900 L
N-N_3	0	-8.97832500	-0.52977300	5.86545300 L
N-N_3	0	-10.28772400	1.74475700	5.59877200 L
B-B_2	0	-11.48575600	0.87268100	5.20502400 L

B-	0	-12.84052700	2.88935700	4.71380300 L
N-N_3	0	-12.59917100	1.42444200	4.31557100 L
B-	0	12.77103000	-4.92423800	-1.15123400 L
B-B_2	0	11.55923500	-5.44818600	0.91889100 L
N-N_3	0	11.60810200	-5.76576100	-0.57429000 L
N-N_3	0	10.27711900	-5.64642700	1.72875300 L
B-B_2	0	9.00319300	-5.43325000	0.91583700 L
B-B_2	0	7.72072300	-4.65137200	2.92020400 L
N-N_3	0	7.71552200	-5.61027300	1.72262400 L
N-N_3	0	6.43132100	-4.50870300	3.73159800 L
B-B_2	0	5.14761700	-4.63922100	2.90937300 L
B-B_2	0	3.86128400	-3.15459500	4.44550500 L
N-N_3	0	3.86097100	-4.50429700	3.72500200 L
N-N_3	0	2.57513400	-2.71769400	5.14762400 L
B-B_2	0	1.29106700	-3.15233800	4.43921600 L
B-B_2	0	0.00735200	-1.19363300	5.30103900 L
N-N_3	0	0.00619500	-2.71524000	5.14317300 L
N-N_3	0	-1.27656600	-0.52450600	5.79263900 L
B-B_2	0	-2.56195000	-1.19191600	5.30278900 L
B-B_2	0	-3.84571700	0.94758000	5.37381500 L
N-N_3	0	-3.84541800	-0.52282700	5.79682700 L
N-N_3	0	-5.12890300	1.75376300	5.58091500 L
B-B_2	0	-6.41812200	0.95210100	5.39179800 L
B-B_2	0	-7.70226900	2.97057700	4.66116900 L
N-N_3	0	-7.69952300	1.76227400	5.60877300 L
N-N_3	0	-8.97584400	3.81059400	4.56313000 L
B-B_2	0	-10.26429200	2.99390700	4.71450800 L
B-B_2	0	-11.48763800	4.35024100	3.11491300 L
N-N_3	0	-11.57209100	3.76026900	4.51459000 L
N-N_3	0	-12.60893000	4.12470100	2.10131700 L
B-	0	12.77199900	-4.29173100	2.66688000 L
N-N_3	0	12.86043700	-5.47545400	1.70213800 L
N-N_3	0	11.60909800	-4.47287700	3.67108700 L
B-B_2	0	10.28461200	-4.66155300	2.91240100 L
B-B_2	0	9.00299800	-3.17868000	4.47860800 L
N-N_3	0	9.00569100	-4.52795400	3.74701200 L
N-N_3	0	7.71368700	-2.72908400	5.16916400 L
B-B_2	0	6.43213100	-3.15920200	4.45449600 L
B-B_2	0	5.14727700	-1.19886400	5.31555400 L
N-N_3	0	5.14524700	-2.72089600	5.15516900 L
N-N_3	0	3.86083000	-0.52847200	5.79996900 L
B-B_2	0	2.57671100	-1.19600300	5.30545200 L
B-B_2	0	1.29353200	0.94349200	5.37012800 L
N-N_3	0	1.29184100	-0.52641900	5.79383900 L

N-N_3	0	0.00940600	1.74843200	5.57345600 L
B-B_2	0	-1.27577300	0.94540700	5.36926100 L
B-B_2	0	-2.55933400	2.95173100	4.62742500 L
N-N_3	0	-2.55959800	1.75038000	5.57462700 L
N-N_3	0	-3.84370700	3.77364500	4.51118800 L
B-B_2	0	-5.12986600	2.95471200	4.63207100 L
B-B_2	0	-6.41676800	4.53558400	3.18591000 L
N-N_3	0	-6.41185100	3.78051500	4.52013900 L
N-N_3	0	-7.69895300	5.26156900	2.76855400 L
B-B_2	0	-8.98486300	4.55729900	3.21252200 L
B-B_2	0	-10.26466900	5.50112400	1.26725800 L
N-N_3	0	-10.28722800	5.24272300	2.77593900 L
N-N_3	0	-11.57092400	5.90376200	0.58329000 L
B-	0	-12.84042100	5.44381200	1.34686600 L
N-N_3	0	12.85999800	-2.65022400	5.06522100 L
B-B_2	0	11.55885700	-3.18701500	4.49372100 L
B-B_2	0	10.28379200	-1.21963100	5.34614600 L
N-N_3	0	10.27606100	-2.75304800	5.20514800 L
N-N_3	0	9.00473900	-0.53571600	5.84244300 L
B-B_2	0	7.72023500	-1.20412500	5.33900200 L
B-B_2	0	6.43355300	0.93960300	5.38422000 L
N-N_3	0	6.43054900	-0.53033300	5.81254200 L
N-N_3	0	5.14814900	1.74503700	5.58001200 L
B-B_2	0	3.86313300	0.94145200	5.37500500 L
B-B_2	0	2.58018000	2.94765100	4.62787600 L
N-N_3	0	2.57851300	1.74667300	5.57567600 L
N-N_3	0	1.29599400	3.76997400	4.50989700 L
B-B_2	0	0.01042400	2.94990300	4.62654000 L
B-B_2	0	-1.27345600	4.52073300	3.17579900 L
N-N_3	0	-1.27383400	3.77205600	4.50998900 L
N-N_3	0	-2.55819600	5.23449900	2.75260300 L
B-B_2	0	-3.84408000	4.52309500	3.17720500 L
B-B_2	0	-5.12947900	5.41394800	1.23435700 L
N-N_3	0	-5.12817100	5.23869300	2.75475100 L
N-N_3	0	-6.41222400	5.91385300	0.56892800 L
B-B_2	0	-7.70211700	5.44374300	1.24417300 L
B-B_2	0	-8.98649400	5.52540800	-0.90016700 L
N-N_3	0	-8.97591000	5.96489400	0.57911000 L
N-N_3	0	-10.28939600	5.69350400	-1.69472700 L
B-B_2	0	-11.49111400	5.31769700	-0.81843900 L
B-	0	-12.84434900	4.79382300	-2.82785800 L
N-N_3	0	-12.60434800	4.41980600	-1.35653700 L
B-	0	12.76968900	-1.13124800	4.91070800 L
B-B_2	0	11.55958100	0.94060400	5.43199400 L

N-N_3	0	11.60828600	-0.55174800	5.75213600 L
N-N_3	0	10.27811500	1.75046200	5.63573400 L
B-B_2	0	9.00412700	0.93888100	5.41612700 L
B-B_2	0	7.72360000	2.95347600	4.64851500 L
N-N_3	0	7.71599100	1.74516200	5.59414700 L
N-N_3	0	6.43542900	3.76872900	4.51618600 L
B-B_2	0	5.15075300	2.94645000	4.63189500 L
B-B_2	0	3.86700000	4.51492300	3.17570600 L
N-N_3	0	3.86581900	3.76747100	4.51087500 L
N-N_3	0	2.58278400	5.22956700	2.75159000 L
B-B_2	0	1.29674900	4.51840300	3.17547700 L
B-B_2	0	0.01211300	5.40882800	1.23205600 L
N-N_3	0	0.01224800	5.23272400	2.75195300 L
N-N_3	0	-1.27300800	5.90324000	0.56584500 L
B-B_2	0	-2.55845200	5.41049300	1.23273300 L
B-B_2	0	-3.84482500	5.47825600	-0.90296200 L
N-N_3	0	-3.84370600	5.90436900	0.56665800 L
N-N_3	0	-5.12976800	5.67624500	-1.70921000 L
B-B_2	0	-6.41787500	5.49169800	-0.90475600 L
B-B_2	0	-7.70466100	4.73788100	-2.91046900 L
N-N_3	0	-7.70090700	5.70063200	-1.71463700 L
N-N_3	0	-8.97946900	4.62616900	-3.74682900 L
B-B_2	0	-10.26757600	4.79163100	-2.93167500 L
B-B_2	0	-11.49035400	3.16837200	-4.25830600 L
N-N_3	0	-11.57556800	4.57845300	-3.69387700 L
N-N_3	0	-12.59528800	2.14774800	-3.98949400 L
B-	0	12.77203800	2.69763100	4.28723500 L
N-N_3	0	12.86177000	1.72242600	5.46198900 L
N-N_3	0	11.61234600	3.70240300	4.48215200 L
B-B_2	0	10.28698300	2.94322900	4.66184800 L
B-B_2	0	9.00823400	4.53033600	3.19812700 L
N-N_3	0	9.00927200	3.78079000	4.53747900 L
N-N_3	0	7.72092700	5.23008400	2.75777700 L
B-B_2	0	6.43764600	4.51375400	3.17876000 L
B-B_2	0	5.15384500	5.40304400	1.23159900 L
N-N_3	0	5.15306800	5.22582100	2.75171500 L
N-N_3	0	3.86862100	5.89652900	0.56477200 L
B-B_2	0	2.58269700	5.40542700	1.23164600 L
B-B_2	0	1.29707500	5.47391200	-0.90423900 L
N-N_3	0	1.29792500	5.90061700	0.56523100 L
N-N_3	0	0.01165300	5.67150100	-1.70961400 L
B-B_2	0	-1.27370200	5.47642100	-0.90351600 L
B-B_2	0	-2.56037300	4.70926900	-2.89724500 L
N-N_3	0	-2.55933300	5.67295000	-1.70878500 L

N-N_3	0	-3.84628200	4.57814600	-3.71536500 L
B-B_2	0	-5.13165500	4.71157900	-2.89739100 L
B-B_2	0	-6.42055000	3.23782200	-4.45126300 L
N-N_3	0	-6.41507000	4.58497200	-3.71945800 L
N-N_3	0	-7.70346800	2.80862300	-5.16952900 L
B-B_2	0	-8.98879900	3.26311800	-4.47084900 L
B-B_2	0	-10.26903000	1.30269800	-5.38289900 L
N-N_3	0	-10.29184400	2.81514800	-5.14738400 L
N-N_3	0	-11.57873800	0.61357000	-5.76830400 L
B-	0	-12.84605400	1.37140700	-5.29208500 L
N-N_3	0	12.86568900	5.11902300	2.67849300 L
B-B_2	0	11.56398800	4.54189200	3.20738000 L
B-B_2	0	10.29089100	5.41341100	1.24864300 L
N-N_3	0	10.28254400	5.25914300	2.78063600 L
N-N_3	0	9.01292100	5.91664000	0.56803900 L
B-B_2	0	7.72700400	5.41493300	1.23476700 L
B-B_2	0	6.43887500	5.46798100	-0.90496200 L
N-N_3	0	6.43876600	5.89727200	0.56446800 L
N-N_3	0	5.15347300	5.66351700	-1.71048800 L
B-B_2	0	3.86783900	5.46949500	-0.90463200 L
B-B_2	0	2.58115400	4.70508300	-2.89930300 L
N-N_3	0	2.58273600	5.66802400	-1.71015300 L
N-N_3	0	1.29540800	4.57590400	-3.71771200 L
B-B_2	0	0.01039000	4.70820100	-2.89848100 L
B-B_2	0	-1.27664100	3.22996400	-4.44068000 L
N-N_3	0	-1.27552200	4.57781500	-3.71662900 L
N-N_3	0	-2.56239500	2.79452400	-5.14550300 L
B-B_2	0	-3.84756000	3.23077200	-4.44055500 L
B-B_2	0	-5.13401100	1.27324400	-5.30251000 L
N-N_3	0	-5.13242100	2.79597700	-5.14806900 L
N-N_3	0	-6.41643700	0.60330700	-5.79785300 L
B-B_2	0	-7.70673100	1.28179900	-5.33315400 L
B-B_2	0	-8.98915900	-0.86697500	-5.40845200 L
N-N_3	0	-8.98119800	0.61248200	-5.84856000 L
N-N_3	0	-10.29154700	-1.66078200	-5.57936400 L
B-B_2	0	-11.48872900	-0.78810000	-5.18428000 L
B-	0	-12.84485500	-2.80597500	-4.69882100 L
N-N_3	0	-12.60450800	-1.34137100	-4.29863000 L
B-	0	12.77817700	4.97736500	1.15805500 L
B-B_2	0	11.56599700	5.50459600	-0.91083400 L
N-N_3	0	11.61600300	5.82093300	0.58253300 L
N-N_3	0	10.28343200	5.70337700	-1.71983500 L
B-B_2	0	9.00981600	5.49054600	-0.90629500 L
B-B_2	0	7.72580100	4.71111100	-2.91117600 L

N-N_3	0	7.72165600	5.66845700	-1.71233100 L
N-N_3	0	6.43640900	4.57167300	-3.72313500 L
B-B_2	0	5.15248000	4.70210800	-2.90125600 L
B-B_2	0	3.86438600	3.22504900	-4.44412800 L
N-N_3	0	3.86614500	4.57230100	-3.71857200 L
N-N_3	0	2.57824200	2.79140900	-5.14894900 L
B-B_2	0	1.29386300	3.22827500	-4.44236600 L
B-B_2	0	0.00674000	1.27120900	-5.29940400 L
N-N_3	0	0.00785500	2.79351700	-5.14688700 L
N-N_3	0	-1.27874600	0.60065900	-5.78561500 L
B-B_2	0	-2.56321900	1.27226200	-5.29844400 L
B-B_2	0	-3.84928200	-0.86625100	-5.35434800 L
N-N_3	0	-3.84819300	0.60154100	-5.78631600 L
N-N_3	0	-5.13269400	-1.67258300	-5.55858100 L
B-B_2	0	-6.42165900	-0.86982700	-5.37283000 L
B-B_2	0	-7.70689600	-2.88738300	-4.64005500 L
N-N_3	0	-7.70325900	-1.67990200	-5.58873900 L
N-N_3	0	-8.98055900	-3.72740100	-4.54382800 L
B-B_2	0	-10.26875000	-2.91040100	-4.69581000 L
B-B_2	0	-11.49379600	-4.26713500	-3.09837000 L
N-N_3	0	-11.57667200	-3.67686100	-4.49794100 L
N-N_3	0	-12.61311800	-4.03657900	-2.08381600 L
B-	0	12.77747100	4.34754200	-2.65893300 L
N-N_3	0	12.86669500	5.53168800	-1.69484000 L
N-N_3	0	11.61399800	4.52839700	-3.66254200 L
B-B_2	0	10.28984300	4.71864100	-2.90354700 L
B-B_2	0	9.00627200	3.23793600	-4.47029100 L
N-N_3	0	9.01071000	4.58681000	-3.73802500 L
N-N_3	0	7.71676200	2.79101500	-5.16196400 L
B-B_2	0	6.43534000	3.22351400	-4.44857500 L
B-B_2	0	5.14755600	1.26623200	-5.30982300 L
N-N_3	0	5.14859100	2.78851000	-5.15144900 L
N-N_3	0	3.86014700	0.59679100	-5.79299200 L
B-B_2	0	2.57680100	1.26914800	-5.30295900 L
B-B_2	0	1.29004300	-0.86776000	-5.35301600 L
N-N_3	0	1.29056600	0.59903100	-5.78770800 L
N-N_3	0	0.00461900	-1.67187500	-5.55004700 L
B-B_2	0	-1.27937900	-0.86607700	-5.35108500 L
B-B_2	0	-2.56461100	-2.86842100	-4.59886400 L
N-N_3	0	-2.56389000	-1.67095200	-5.55085700 L
N-N_3	0	-3.84879400	-3.69006300	-4.48434500 L
B-B_2	0	-5.13473100	-2.87113400	-4.60681800 L
B-B_2	0	-6.42274700	-4.45493100	-3.16498100 L
N-N_3	0	-6.41653300	-3.69731300	-4.49762000 L

N-N_3	0	-7.70564600	-5.18127300	-2.75050700 L
B-B_2	0	-8.99084600	-4.47535800	-3.19395800 L
N-N_3	0	-10.29401500	-5.16007800	-2.75837600 L
N-N_3	0	12.86268100	2.70204500	-5.05399000 L
B-B_2	0	11.56209600	3.24170300	-4.48377000 L
B-B_2	0	10.28400900	1.27653500	-5.33694600 L
N-N_3	0	10.27903200	2.80999100	-5.19603900 L
N-N_3	0	9.00390900	0.59476300	-5.83341600 L
B-B_2	0	7.72052400	1.26598100	-5.33102700 L
B-B_2	0	6.43008200	-0.87490600	-5.37214700 L
N-N_3	0	6.42985200	0.59395800	-5.80419600 L
N-N_3	0	5.14269400	-1.67806500	-5.56431100 L
B-B_2	0	3.85972700	-0.87095800	-5.36041200 L
B-B_2	0	2.57363600	-2.87187400	-4.60322200 L
N-N_3	0	2.57318400	-1.67437200	-5.55531900 L
N-N_3	0	1.28808200	-3.69153900	-4.48347600 L
B-B_2	0	0.00449500	-2.86890100	-4.59761400 L
B-B_2	0	-1.28030000	-4.44480600	-3.15081700 L
N-N_3	0	-1.28013700	-3.68972000	-4.48125700 L
N-N_3	0	-2.56546700	-5.16050600	-2.73352700 L
B-B_2	0	-3.85005400	-4.44358400	-3.15290100 L
N-N_3	0	-5.13477300	-5.16042500	-2.73550800 L
B-	0	12.76912400	1.18320700	-4.89980100 L
B-B_2	0	11.55599500	-0.88621200	-5.42350300 L
N-N_3	0	11.60739400	0.60631600	-5.74251100 L
N-N_3	0	10.27278100	-1.69361500	-5.62627300 L
B-B_2	0	9.00057300	-0.87951900	-5.40594400 L
B-B_2	0	7.71678400	-2.89114500	-4.63558400 L
N-N_3	0	7.71063700	-1.68345500	-5.58207800 L
N-N_3	0	6.42676600	-3.70335200	-4.50116000 L
B-B_2	0	5.14402300	-2.87763300	-4.61385300 L
B-B_2	0	3.85867400	-4.44573200	-3.15669600 L
N-N_3	0	3.85706900	-3.69516700	-4.48987100 L
N-N_3	0	2.57394300	-5.16067700	-2.73437800 L
B-B_2	0	1.28863500	-4.44584200	-3.15258700 L
N-N_3	0	0.00404600	-5.16273100	-2.73394600 L
B-	0	12.76625200	-2.64577100	-4.28050800 L
N-N_3	0	12.85664400	-1.67045400	-5.45510900 L
N-N_3	0	11.60429000	-3.64819000	-4.47426600 L
B-B_2	0	10.28021000	-2.88637200	-4.65235700 L
B-B_2	0	8.99991300	-4.47162200	-3.18763000 L
N-N_3	0	9.00084100	-3.72132600	-4.52654300 L
N-N_3	0	7.71184400	-5.16962900	-2.74671800 L
B-B_2	0	6.42933600	-4.45015900	-3.16479700 L

N-N_3	0	5.14389200	-5.16082000	-2.73778200 L
N-N_3	0	12.85692500	-5.06678700	-2.67166300 L
B-B_2	0	11.55570700	-4.48761200	-3.19950900 L
N-N_3	0	10.27347900	-5.20271900	-2.77166700 L
H-H_	0	-12.27037200	-3.34447700	1.33345400 L
H-H_	0	-12.24885400	-1.39328300	3.28730300 L
H-H_	0	-12.26078600	1.39927700	3.32701400 L
H-H_	0	-12.28228200	3.40333200	1.41926300 L
H-H_	0	12.88023400	-6.35768300	2.26242000 L
H-H_	0	12.88155900	-2.87810400	6.08514700 L
H-H_	0	-12.26655700	3.43163700	-1.31450700 L
H-H_	0	-12.24531300	1.47987300	-3.26567000 L
H-H_	0	12.88502600	2.27469100	6.34918000 L
H-H_	0	12.88587400	6.13700800	2.91500700 L
H-H_	0	-12.26883000	-1.31715500	-3.30913600 L
H-H_	0	-12.28321500	-3.31576900	-1.40272800 L
H-H_	0	12.88606700	6.41366500	-2.25553500 L
H-H_	0	12.88582700	2.93003100	-6.07385600 L
H-H_	0	12.87788000	-2.22256000	-6.34244800 L
H-H_	0	12.87510900	-6.08491600	-2.90772200 L
C-C_3	0	-0.04409300	-1.79711000	0.05624500 H
H-H_	0	-0.00647100	0.21620500	0.92881900 H
H-H_	0	0.96673600	-0.98768400	1.79978200 H
C-C_3	0	0.02659400	-0.82698500	1.26097700 H
H-H_	0	-0.79598300	-1.00328600	1.96227700 H
N-N_3	0	1.03082300	-1.68162600	-0.92226400 H
H-H_	0	1.93268700	-1.57154700	-0.47030100 H
H-H_	0	0.87029500	-0.89473100	-1.54587900 H
C-C_R	0	-1.36639300	-1.60773600	-0.67143000 H
O-O_R	0	-1.51987100	-0.96623700	-1.68931700 H
O-O_R	0	-2.39279000	-2.21199500	-0.02606300 H
H-H_	0	-3.20261100	-2.02583700	-0.53135500 H
H-H_	0	-0.04442400	-2.81410700	0.45589800 H

bTS2@D

B-B_2	0	-10.29299100	5.23411300	-2.01747500 L
N-N_3	0	-11.60065700	5.17046300	-2.80692600 L
B-	0	-12.86952700	5.21517400	-1.91561400 L
B-B_2	0	-5.15749300	5.15187100	-1.99649400 L
N-N_3	0	-6.44037100	5.18413700	-2.82824800 L
B-B_2	0	-7.73032700	5.17905100	-2.00549400 L
B-B_2	0	-9.01290900	4.02921300	-3.81989900 L
N-N_3	0	-9.00462000	5.22859600	-2.84858300 L

N-N_3	0	-10.31540200	3.71803200	-4.57029500 L
B-B_2	0	-11.51497600	3.89476100	-3.63124400 L
B-	0	-12.86834900	2.33256100	-4.99835500 L
N-N_3	0	-12.62473000	2.84605900	-3.57026500 L
B-B_2	0	-0.01590600	5.15242000	-1.99579300 L
N-N_3	0	-1.30125700	5.17962400	-2.82460400 L
B-B_2	0	-2.58641700	5.15112900	-1.99571500 L
B-B_2	0	-3.87172000	3.99443700	-3.79440500 L
N-N_3	0	-3.87179600	5.17794600	-2.82445500 L
N-N_3	0	-5.15604000	3.70200100	-4.57238200 L
B-B_2	0	-6.44464500	4.00195800	-3.80437900 L
B-B_2	0	-7.72913300	2.24891400	-5.04180800 L
N-N_3	0	-7.72703000	3.71694400	-4.59178800 L
N-N_3	0	-9.00296000	1.68758900	-5.67401300 L
B-B_2	0	-10.29159500	2.27807200	-5.08935800 L
B-B_2	0	-11.51186000	0.18845900	-5.28605500 L
N-N_3	0	-11.59962700	1.67405400	-5.60128100 L
N-N_3	0	-12.62470100	-0.51530900	-4.51048500 L
B-B_2	0	5.12575100	5.15292800	-1.99629800 L
N-N_3	0	3.83992000	5.17963500	-2.82427800 L
B-B_2	0	2.55461800	5.15217000	-1.99552500 L
B-B_2	0	1.26954100	3.99601800	-3.79362600 L
N-N_3	0	1.26944000	5.18015900	-2.82449400 L
N-N_3	0	-0.01563300	3.70283000	-4.56935000 L
B-B_2	0	-1.30088300	3.99540100	-3.79354600 L
B-B_2	0	-2.58549900	2.23656000	-5.01003100 L
N-N_3	0	-2.58599000	3.70180200	-4.56935100 L
N-N_3	0	-3.87011700	1.66901800	-5.61584000 L
B-B_2	0	-5.15638200	2.23643300	-5.01370300 L
B-B_2	0	-6.44268800	0.14434300	-5.48286900 L
N-N_3	0	-6.43852800	1.67082400	-5.62596000 L
N-N_3	0	-7.72432700	-0.61297100	-5.84265500 L
B-B_2	0	-9.01062600	0.15226300	-5.51599000 L
B-B_2	0	-10.28905700	-1.98617700	-5.18625200 L
N-N_3	0	-10.31268400	-0.59754400	-5.82991600 L
N-N_3	0	-11.59667200	-2.77626800	-5.12763000 L
B-	0	-12.86553300	-1.88444000	-5.16634600 L
B-B_2	0	10.26270900	5.17664100	-1.99264600 L
N-N_3	0	8.98406700	5.20476200	-2.83765900 L
B-B_2	0	7.69891700	5.16740200	-2.00283300 L
B-B_2	0	6.41084500	3.99843500	-3.79662900 L
N-N_3	0	6.40995100	5.18337100	-2.82725000 L
N-N_3	0	5.12498300	3.70370400	-4.57048800 L
B-B_2	0	3.84000100	3.99579200	-3.79384700 L

B-B_2	0	2.55491700	2.23809200	-5.01077200 L
N-N_3	0	2.55474200	3.70320500	-4.56955900 L
N-N_3	0	1.26971000	1.67064700	-5.61507300 L
B-B_2	0	-0.01529000	2.23747400	-5.00973000 L
B-B_2	0	-1.29958600	0.14736500	-5.46353100 L
N-N_3	0	-1.30013200	1.66987900	-5.61473400 L
N-N_3	0	-2.58396600	-0.60753000	-5.80862500 L
B-B_2	0	-3.87003600	0.14615600	-5.46646900 L
B-B_2	0	-5.15431600	-1.96156800	-5.09714100 L
N-N_3	0	-5.15351100	-0.60959700	-5.81458400 L
N-N_3	0	-6.43612000	-2.79436800	-5.13655400 L
B-B_2	0	-7.72681600	-1.97265000	-5.12920700 L
B-B_2	0	-9.00910900	-3.79549200	-3.99156300 L
N-N_3	0	-9.00032900	-2.81664400	-5.18475400 L
N-N_3	0	-10.31147000	-4.54860400	-3.68631900 L
B-B_2	0	-11.51142000	-3.60897400	-3.85740300 L
B-	0	-12.86485800	-4.99648400	-2.31158900 L
N-N_3	0	-12.62745300	-3.56350800	-2.81446800 L
B-	0	12.74956700	4.76630400	-1.82149400 L
B-B_2	0	11.53745200	4.03083200	-3.82606700 L
N-N_3	0	11.58732400	5.13602500	-2.77317800 L
N-N_3	0	10.25496000	3.73983200	-4.60706100 L
B-B_2	0	8.98162000	4.02025400	-3.81366300 L
B-B_2	0	7.69880600	2.24604000	-5.03331500 L
N-N_3	0	7.69300800	3.71138000	-4.57849400 L
N-N_3	0	6.40936300	1.67362700	-5.62591300 L
B-B_2	0	5.12579200	2.23925700	-5.01518800 L
B-B_2	0	3.84021600	0.14876800	-5.46792400 L
N-N_3	0	3.83951900	1.67165000	-5.61747200 L
N-N_3	0	2.55490200	-0.60584100	-5.81120000 L
B-B_2	0	1.27030600	0.14800400	-5.46441700 L
B-B_2	0	-0.01382900	-1.95890500	-5.09263100 L
N-N_3	0	-0.01456000	-0.60663300	-5.80834900 L
N-N_3	0	-1.29862400	-2.78766100	-5.12523400 L
B-B_2	0	-2.58362000	-1.95912200	-5.09172700 L
B-B_2	0	-3.86826900	-3.76769300	-3.94988200 L
N-N_3	0	-3.86798600	-2.78847400	-5.12553900 L
N-N_3	0	-5.15233600	-4.54844000	-3.66559100 L
B-B_2	0	-6.44101700	-3.77865400	-3.96121400 L
B-B_2	0	-7.72620100	-5.02713100	-2.21799700 L
N-N_3	0	-7.72314000	-4.56875400	-3.68323100 L
N-N_3	0	-9.00010000	-5.66175400	-1.66005500 L
B-B_2	0	-10.28864100	-5.07703900	-2.24981100 L
B-B_2	0	-11.51262500	-5.28154000	-0.16382300 L

N-N_3	0	-11.59585100	-5.59532100	-1.65012100 L
N-N_3	0	-12.62675500	-4.50469600	0.53647200 L
B-	0	12.74904600	2.09164800	-4.62407000 L
N-N_3	0	12.83855600	3.61257700	-4.48918800 L
N-N_3	0	11.58692300	1.68004500	-5.55847000 L
B-B_2	0	10.26248500	2.26062200	-5.03488200 L
B-B_2	0	8.98161700	0.15459300	-5.50510000 L
N-N_3	0	8.98352500	1.68248000	-5.65127000 L
N-N_3	0	7.69301400	-0.60448400	-5.82820400 L
B-B_2	0	6.41088700	0.15006200	-5.47539400 L
B-B_2	0	5.12641200	-1.95805200	-5.09965400 L
N-N_3	0	5.12486800	-0.60516200	-5.81499500 L
N-N_3	0	3.84076600	-2.78635500	-5.12854700 L
B-B_2	0	2.55554000	-1.95835400	-5.09587400 L
B-B_2	0	1.27132800	-3.76734800	-3.95307000 L
N-N_3	0	1.27078000	-2.78780300	-5.12845300 L
N-N_3	0	-0.01325300	-4.54518200	-3.66404800 L
B-B_2	0	-1.29821400	-3.76695200	-3.94986200 L
B-B_2	0	-2.58284400	-5.00060200	-2.20340700 L
N-N_3	0	-2.58294800	-4.54598200	-3.66432700 L
N-N_3	0	-3.86805300	-5.60671500	-1.63840600 L
B-B_2	0	-5.15342000	-5.00020700	-2.20345200 L
B-B_2	0	-6.44129300	-5.47246900	-0.11515500 L
N-N_3	0	-6.43622600	-5.61389100	-1.64147900 L
N-N_3	0	-7.72361400	-5.83071000	0.64174300 L
B-B_2	0	-9.00952300	-5.50554600	-0.12471600 L
B-B_2	0	-10.28954500	-5.17005400	2.01067400 L
N-N_3	0	-10.31203600	-5.81958900	0.62460400 L
N-N_3	0	-11.59721300	-5.10773700	2.80020300 L
B-	0	-12.86609800	-5.15390000	1.90897900 L
N-N_3	0	12.83874800	-0.60993400	-5.69593200 L
B-B_2	0	11.53737900	0.15409800	-5.52190600 L
B-B_2	0	10.26317300	-1.95364200	-5.12850800 L
N-N_3	0	10.25510600	-0.60380700	-5.86943500 L
N-N_3	0	8.98469400	-2.79882900	-5.15768100 L
B-B_2	0	7.69952300	-1.96414600	-5.11738500 L
B-B_2	0	6.41236800	-3.76252500	-3.95337400 L
N-N_3	0	6.41060200	-2.78867100	-5.13446200 L
N-N_3	0	5.12711500	-4.53851300	-3.66195100 L
B-B_2	0	3.84149700	-3.76186600	-3.94996500 L
B-B_2	0	2.55701500	-4.98825800	-2.19958900 L
N-N_3	0	2.55754300	-4.54167900	-3.66281000 L
N-N_3	0	1.27304300	-5.59854900	-1.63611800 L
B-B_2	0	-0.01289300	-4.99452400	-2.20147900 L

B-B_2	0	-1.29748200	-5.45856700	-0.11506200 L
N-N_3	0	-1.29678000	-5.60576000	-1.63810500 L
N-N_3	0	-2.58299400	-5.80005400	0.63949800 L
B-B_2	0	-3.86821800	-5.45780000	-0.11565800 L
B-B_2	0	-5.15431700	-5.08006400	1.98839200 L
N-N_3	0	-5.15263700	-5.80335800	0.63987600 L
N-N_3	0	-6.43682000	-5.11454600	2.82058800 L
B-B_2	0	-7.72702600	-5.11179000	1.99827600 L
B-B_2	0	-9.01066400	-3.96361100	3.81306500 L
N-N_3	0	-9.00106700	-5.16290800	2.84165800 L
N-N_3	0	-10.31348300	-3.65404000	4.56356100 L
B-B_2	0	-11.51281600	-3.83192100	3.62444700 L
B-	0	-12.86788100	-2.27066500	4.99074800 L
N-N_3	0	-12.62314500	-2.78389400	3.56275800 L
B-	0	12.74946900	-1.78228100	-4.71770200 L
B-B_2	0	11.53867400	-3.78912500	-3.98648200 L
N-N_3	0	11.58795600	-2.73391700	-5.08938800 L
N-N_3	0	10.25675800	-4.57182600	-3.69795300 L
B-B_2	0	8.98297900	-3.77825500	-3.97598700 L
B-B_2	0	7.70083200	-5.00483800	-2.20610800 L
N-N_3	0	7.69488900	-4.54491700	-3.66976500 L
N-N_3	0	6.41185700	-5.60039400	-1.63584000 L
B-B_2	0	5.12793600	-4.98894400	-2.19958400 L
B-B_2	0	3.84191200	-5.44869900	-0.11197200 L
N-N_3	0	3.84222400	-5.59478500	-1.63477900 L
N-N_3	0	2.55721500	-5.79568500	0.64153000 L
B-B_2	0	1.27190900	-5.45309100	-0.11316700 L
B-B_2	0	-0.01373600	-5.07891500	1.99015500 L
N-N_3	0	-0.01254400	-5.79991900	0.64063800 L
N-N_3	0	-1.29929100	-5.10441400	2.81741500 L
B-B_2	0	-2.58344600	-5.07670400	1.98763200 L
B-B_2	0	-3.86976100	-3.92101000	3.78601700 L
N-N_3	0	-3.86866900	-5.10405800	2.81602900 L
N-N_3	0	-5.15417700	-3.63213700	4.56498100 L
B-B_2	0	-6.44256100	-3.93276800	3.79699600 L
B-B_2	0	-7.72876200	-2.18272700	5.03641000 L
N-N_3	0	-7.72509900	-3.65028500	4.58503200 L
N-N_3	0	-9.00331500	-1.62294500	5.66849700 L
B-B_2	0	-10.29116400	-2.21418900	5.08294700 L
B-B_2	0	-11.51319400	-0.12561400	5.27966600 L
N-N_3	0	-11.59992400	-1.61136700	5.59443000 L
N-N_3	0	-12.62627300	0.57746700	4.50380500 L
B-	0	12.75070600	-4.59186200	-2.04944600 L
N-N_3	0	12.84017200	-4.45258300	-3.56997200 L

N-N_3	0	11.58914600	-5.52810800	-1.64048100 L
B-B_2	0	10.26442900	-5.00404200	-2.22003900 L
B-B_2	0	8.98335900	-5.47948000	-0.11583900 L
N-N_3	0	8.98593400	-5.62309100	-1.64388900 L
N-N_3	0	7.69488000	-5.80429200	0.64257000 L
B-B_2	0	6.41269300	-5.45255000	-0.11222300 L
B-B_2	0	5.12707400	-5.07701800	1.99394300 L
N-N_3	0	5.12686700	-5.79410400	0.64219800 L
N-N_3	0	3.84099600	-5.10472100	2.82132000 L
B-B_2	0	2.55620900	-5.07719200	1.99213700 L
B-B_2	0	1.26997500	-3.92258000	3.79040100 L
N-N_3	0	1.27074300	-5.10572700	2.82002600 L
N-N_3	0	-0.01531200	-3.63273000	4.56675000 L
B-B_2	0	-1.29914300	-3.92073200	3.78685900 L
B-B_2	0	-2.58506000	-2.16635500	5.00820200 L
N-N_3	0	-2.58472700	-3.62959400	4.56221100 L
N-N_3	0	-3.87079600	-1.60091900	5.61349500 L
B-B_2	0	-5.15609700	-2.16771600	5.00913700 L
B-B_2	0	-6.44411700	-0.07776700	5.48013000 L
N-N_3	0	-6.43894300	-1.60428100	5.62180900 L
N-N_3	0	-7.72660300	0.67854600	5.83895600 L
B-B_2	0	-9.01208000	-0.08757000	5.51117800 L
B-B_2	0	-10.29186300	2.04986800	5.18060400 L
N-N_3	0	-10.31490900	0.66122400	5.82430900 L
N-N_3	0	-11.59994500	2.83912300	5.12116700 L
B-	0	-12.86820300	1.94643300	5.15960800 L
N-N_3	0	12.84020700	-5.66972100	0.64998500 L
B-B_2	0	11.53920600	-5.49512500	-0.11442400 L
B-B_2	0	10.26397500	-5.10147500	1.99218600 L
N-N_3	0	10.25678100	-5.84319200	0.64280900 L
N-N_3	0	8.98504700	-5.12996300	2.83677600 L
B-B_2	0	7.70020200	-5.09225100	2.00150400 L
B-B_2	0	6.41133100	-3.92428700	3.79530800 L
N-N_3	0	6.41088200	-5.10857000	2.82536100 L
N-N_3	0	5.12505600	-3.63034200	4.56876200 L
B-B_2	0	3.84035200	-3.92146100	3.79117800 L
B-B_2	0	2.55439500	-2.16679700	5.01146500 L
N-N_3	0	2.55485500	-3.63073800	4.56707400 L
N-N_3	0	1.26999500	-1.60180200	5.61939200 L
B-B_2	0	-0.01518000	-2.17007800	5.01628600 L
B-B_2	0	-1.30091800	-0.07945900	5.46648900 L
N-N_3	0	-1.30134800	-1.60201900	5.61825300 L
N-N_3	0	-2.58596200	0.67583700	5.80948400 L
B-B_2	0	-3.87140500	-0.07812600	5.46605000 L

B-B_2	0	-5.15690700	2.02829400	5.09487200 L
N-N_3	0	-5.15571400	0.67685300	5.81318500 L
N-N_3	0	-6.43933200	2.86044100	5.13240400 L
B-B_2	0	-7.72953000	2.03794300	5.12502500 L
B-B_2	0	-9.01252700	3.85919900	3.98543600 L
N-N_3	0	-9.00363200	2.88113200	5.17929000 L
N-N_3	0	-10.31514000	4.61163100	3.67965000 L
B-B_2	0	-11.51468200	3.67144600	3.85067000 L
B-	0	-12.86856700	5.05832900	2.30464000 L
N-N_3	0	-12.63063000	3.62548900	2.80766100 L
B-	0	12.75090200	-4.69090800	1.82191000 L
B-B_2	0	11.53795900	-3.95566100	3.82604700 L
N-N_3	0	11.58834200	-5.06081300	2.77314900 L
N-N_3	0	10.25523100	-3.66499400	4.60674600 L
B-B_2	0	8.98210500	-3.94575300	3.81310100 L
B-B_2	0	7.69854200	-2.17220700	5.03265400 L
N-N_3	0	7.69323300	-3.63744600	4.57772000 L
N-N_3	0	6.40892800	-1.60044900	5.62528300 L
B-B_2	0	5.12551900	-2.16644900	5.01447200 L
B-B_2	0	3.83922500	-0.07744100	5.46786900 L
N-N_3	0	3.83928800	-1.60014100	5.61752900 L
N-N_3	0	2.55360000	0.67646600	5.81062900 L
B-B_2	0	1.26909500	-0.07925800	5.46643000 L
B-B_2	0	-0.01618300	2.02586700	5.08994600 L
N-N_3	0	-0.01603100	0.67545700	5.80937800 L
N-N_3	0	-1.30107600	2.85473500	5.12129700 L
B-B_2	0	-2.58609900	2.02627300	5.09044700 L
B-B_2	0	-3.87166900	3.83264500	3.94504600 L
N-N_3	0	-3.87086400	2.85561800	5.12262400 L
N-N_3	0	-5.15590300	4.61299700	3.65940400 L
B-B_2	0	-6.44440500	3.84329400	3.95579300 L
B-B_2	0	-7.72985700	5.09081600	2.21134800 L
N-N_3	0	-7.72677900	4.63274300	3.67678900 L
N-N_3	0	-9.00395500	5.72515800	1.65346500 L
B-B_2	0	-10.29233100	5.13984400	2.24306500 L
B-B_2	0	-11.51621800	5.34415300	0.15706500 L
N-N_3	0	-11.59970100	5.65768600	1.64336400 L
N-N_3	0	-12.62940200	4.56599600	-0.54324500 L
B-	0	12.74882600	-2.01596300	4.62383900 L
N-N_3	0	12.83880100	-3.53690400	4.48937000 L
N-N_3	0	11.58637500	-1.60444900	5.55787000 L
B-B_2	0	10.26221100	-2.18572500	5.03433700 L
B-B_2	0	8.98047400	-0.08015800	5.50394800 L
N-N_3	0	8.98301300	-1.60800600	5.65054500 L

N-N_3	0	7.69156400	0.67843100	5.82678500 L
B-B_2	0	6.40982300	-0.07695600	5.47443700 L
B-B_2	0	5.12446900	2.02994300	5.09716300 L
N-N_3	0	5.12358100	0.67769800	5.81387000 L
N-N_3	0	3.83811200	2.85700700	5.12464400 L
B-B_2	0	2.55369300	2.02723100	5.09205400 L
B-B_2	0	1.26870600	3.83181100	3.94413600 L
N-N_3	0	1.26833900	2.85528200	5.12204800 L
N-N_3	0	-0.01634100	4.60975400	3.65691100 L
B-B_2	0	-1.30119900	3.83124200	3.94346200 L
B-B_2	0	-2.58637000	5.06170000	2.19517600 L
N-N_3	0	-2.58614700	4.60960900	3.65689700 L
N-N_3	0	-3.87161400	5.67008800	1.63190700 L
B-B_2	0	-5.15721000	5.06391600	2.19680100 L
B-B_2	0	-6.44493200	5.53905300	0.10829100 L
N-N_3	0	-6.43996300	5.67812000	1.63503200 L
N-N_3	0	-7.72765600	5.89669200	-0.64821000 L
B-B_2	0	-9.01324900	5.56977600	0.11801400 L
N-N_3	0	-10.31599400	5.88318200	-0.63119900 L
N-N_3	0	12.83722200	0.68610900	5.69464800 L
B-B_2	0	11.53617500	-0.07851700	5.52073400 L
B-B_2	0	10.26104900	2.02876200	5.12728600 L
N-N_3	0	10.25357400	0.67889100	5.86820800 L
N-N_3	0	8.98209600	2.87331500	5.15610800 L
B-B_2	0	7.69744200	2.03789700	5.11546300 L
B-B_2	0	6.40951600	3.83592200	3.95090400 L
N-N_3	0	6.40799600	2.86167400	5.13188300 L
N-N_3	0	5.12378200	4.61135800	3.65934000 L
B-B_2	0	3.83881900	3.83282800	3.94597900 L
B-B_2	0	2.55403400	5.06244400	2.19598800 L
N-N_3	0	2.55364600	4.61041200	3.65780400 L
N-N_3	0	1.26899200	5.67111600	1.63225700 L
B-B_2	0	-0.01618500	5.06227000	2.19529400 L
B-B_2	0	-1.30124800	5.52688500	0.10864100 L
N-N_3	0	-1.30138300	5.67080800	1.63193700 L
N-N_3	0	-2.58662400	5.87112700	-0.64560100 L
B-B_2	0	-3.87206300	5.52668800	0.10846600 L
N-N_3	0	-5.15672500	5.87282100	-0.64640500 L
B-	0	12.74731900	1.85861400	4.71665000 L
B-B_2	0	11.53596200	3.86537000	3.98626800 L
N-N_3	0	11.58543800	2.80966800	5.08867100 L
N-N_3	0	10.25367900	4.64730300	3.69726800 L
B-B_2	0	8.98021400	3.85297900	3.97457400 L
B-B_2	0	7.69806400	5.07987600	2.20457600 L

N-N_3	0	7.69177700	4.61906300	3.66800600 L
N-N_3	0	6.40922600	5.67577500	1.63423500 L
B-B_2	0	5.12498000	5.06431200	2.19743400 L
B-B_2	0	3.83964500	5.52632800	0.10933200 L
N-N_3	0	3.83928300	5.67083600	1.63271500 L
N-N_3	0	2.55466100	5.87172800	-0.64512100 L
B-B_2	0	1.26917200	5.52724200	0.10887700 L
N-N_3	0	-0.01603700	5.87215000	-0.64546300 L
B-	0	12.74853000	4.66895700	2.05007500 L
N-N_3	0	12.83722000	4.52979600	3.57063900 L
N-N_3	0	11.58652800	5.60434900	1.64037900 L
B-B_2	0	10.26178800	5.07972200	2.21943600 L
B-B_2	0	8.98129700	5.55498200	0.11484000 L
N-N_3	0	8.98329800	5.69842200	1.64290900 L
N-N_3	0	7.69313800	5.87984300	-0.64404600 L
B-B_2	0	6.41051100	5.52877500	0.11038100 L
N-N_3	0	5.12509800	5.87082400	-0.64467000 L
N-N_3	0	12.83842800	5.74533500	-0.64970800 L
B-B_2	0	11.53717200	5.57085200	0.11432100 L
N-N_3	0	10.25498300	5.91863200	-0.64341800 L
H-H_	0	-12.28209200	2.05134000	-2.98424500 L
H-H_	0	-12.28604200	-0.66865300	-3.53366700 L
H-H_	0	-12.29328100	-2.98039000	-2.01406900 L
H-H_	0	-12.29001800	-3.52642200	0.68459100 L
H-H_	0	12.85935500	4.02881600	-5.44780800 L
H-H_	0	12.85991100	-0.99191000	-6.66870500 L
H-H_	0	-12.28061200	-1.98894000	2.97699400 L
H-H_	0	-12.28744100	0.73103300	3.52708200 L
H-H_	0	12.86167000	-5.40999400	-3.98895200 L
H-H_	0	12.86058400	-6.64232300	1.03243500 L
H-H_	0	-12.29618200	3.04243900	2.00732800 L
H-H_	0	-12.29145400	3.58816400	-0.69153300 L
H-H_	0	12.85948600	-3.95289700	5.44809900 L
H-H_	0	12.85837900	1.06791100	6.66749000 L
H-H_	0	12.85771100	5.48723300	3.98960900 L
H-H_	0	12.85890600	6.71787000	-1.03232500 L
C-C_R	0	-0.24913800	-1.59886000	0.50945700 H
H-H_	0	-2.01551200	-0.84888900	-0.53469700 H
H-H_	0	-2.29609500	-2.27064900	0.48177200 H
C-C_3	0	-1.57459300	-1.80158100	-0.19718700 H
H-H_	0	-1.47838000	-2.44766100	-1.07487600 H
N-N_R	0	-0.21680700	-0.61721100	1.58837700 H
H-H_	0	-0.67267400	0.25723600	1.32474500 H
H-H_	0	-0.67545900	-0.96492000	2.42180600 H

C-C_R	0	0.95866300	-1.57985300	-0.27742500 H
O-O_R	0	1.97542300	-2.02285200	0.37838500 H
O-O_R	0	1.05880600	-1.30228600	-1.56908900 H
H-H_	0	1.93306700	-1.58284200	-1.89025800 H
H-H_	0	0.99685100	-2.34454300	1.08525700 H

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B-B_2	0	10.29193100	5.61064900	-0.20420600 L
N-N_3	0	11.59934100	5.86897700	0.54487800 L
B-	0	12.86808600	5.55393700	-0.29034400 L
B-B_2	0	5.15653400	5.52886700	-0.19211600 L
N-N_3	0	6.43935800	5.89007200	0.55779500 L
B-B_2	0	7.72934100	5.55626100	-0.19417100 L
B-B_2	0	9.01152600	5.22654500	1.92862800 L
N-N_3	0	9.00350000	5.93825100	0.55923100 L
N-N_3	0	10.31372500	5.24079800	2.74146300 L
B-B_2	0	11.51430200	5.02936700	1.81068900 L
B-	0	12.86632000	4.14803500	3.69242300 L
N-N_3	0	12.62818700	4.04943700	2.17711500 L
B-B_2	0	0.01487900	5.53096100	-0.19394700 L
N-N_3	0	1.30016000	5.88581400	0.55566700 L
B-B_2	0	2.58543500	5.52888800	-0.19295500 L
B-B_2	0	3.87025100	5.18466900	1.91771800 L
N-N_3	0	3.87077900	5.88359800	0.55649900 L
N-N_3	0	5.15438600	5.22579700	2.74804100 L
B-B_2	0	6.44319400	5.19537000	1.92440500 L
B-B_2	0	7.72727500	4.07891400	3.75643900 L
N-N_3	0	7.72533900	5.24742600	2.76050200 L
N-N_3	0	9.00064200	3.81456500	4.55998100 L
B-B_2	0	10.28979200	4.12656100	3.79096700 L
B-B_2	0	11.51153500	2.28768200	4.79959200 L
N-N_3	0	11.59672700	3.77734800	4.50312200 L
N-N_3	0	12.62258700	1.33589100	4.35836400 L
B-B_2	0	-5.12684400	5.53251400	-0.19555000 L
N-N_3	0	-3.84126600	5.88604600	0.55413400 L
B-B_2	0	-2.55568100	5.53118800	-0.19489800 L
B-B_2	0	-1.27120500	5.18588900	1.91518600 L
N-N_3	0	-1.27066600	5.88664500	0.55485900 L
N-N_3	0	0.01376400	5.22518400	2.74396400 L
B-B_2	0	1.29932500	5.18541100	1.91607700 L
B-B_2	0	2.58365200	4.05422500	3.73077800 L
N-N_3	0	2.58430000	5.22432800	2.74488200 L
N-N_3	0	3.86818000	3.77287700	4.51195700 L

B-B_2	0	5.15458200	4.05578900	3.73474900 L
B-B_2	0	6.44101000	2.32024600	4.99268700 L
N-N_3	0	6.43652600	3.77909400	4.52125500 L
N-N_3	0	7.72271700	1.76642100	5.62208600 L
B-B_2	0	9.00910300	2.34167500	5.02109600 L
B-B_2	0	10.28818600	0.24693200	5.55825900 L
N-N_3	0	10.31115000	1.77682700	5.60593900 L
N-N_3	0	11.59626800	-0.50255300	5.81298700 L
B-	0	12.86502700	0.33244100	5.49712800 L
B-B_2	0	-10.26390000	5.55355800	-0.21082100 L
N-N_3	0	-8.98553300	5.91379000	0.55455300 L
B-B_2	0	-7.70002500	5.54863000	-0.19650700 L
B-B_2	0	-6.41272300	5.18697300	1.91423200 L
N-N_3	0	-6.41137500	5.89037700	0.55447100 L
N-N_3	0	-5.12735200	5.22377500	2.74228800 L
B-B_2	0	-3.84176900	5.18483400	1.91425300 L
B-B_2	0	-2.55703600	4.05452300	3.72896000 L
N-N_3	0	-2.55689900	5.22473300	2.74305700 L
N-N_3	0	-1.27206500	3.77304100	4.50919200 L
B-B_2	0	0.01331100	4.05476900	3.72960900 L
B-B_2	0	1.29785300	2.31432200	4.97211500 L
N-N_3	0	1.29810700	3.77293100	4.51006700 L
N-N_3	0	2.58220200	1.75669100	5.58714500 L
B-B_2	0	3.86835200	2.31480300	4.97612600 L
B-B_2	0	5.15311200	0.23257100	5.46723100 L
N-N_3	0	5.15182600	1.75781600	5.59438700 L
N-N_3	0	6.43526700	-0.51718000	5.83110200 L
B-B_2	0	7.72575900	0.23575500	5.50100200 L
B-B_2	0	9.00853900	-1.88725800	5.17138200 L
N-N_3	0	8.99972600	-0.51797400	5.88348600 L
N-N_3	0	10.31121200	-2.69910600	5.18652600 L
B-B_2	0	11.50997700	-1.76716200	4.97198400 L
B-	0	12.86458200	-3.64637000	4.09132000 L
N-N_3	0	12.62140300	-2.13212600	3.98880200 L
B-	0	-12.75154100	5.11107500	-0.20711800 L
B-B_2	0	-11.53949800	5.22572000	1.92524700 L
N-N_3	0	-11.58877200	5.82550800	0.52153300 L
N-N_3	0	-10.25753500	5.26777000	2.75849800 L
B-B_2	0	-8.98360500	5.21237000	1.91968000 L
B-B_2	0	-7.70118400	4.06600400	3.74221900 L
N-N_3	0	-7.69548500	5.23206100	2.74505200 L
N-N_3	0	-6.41212500	3.77546800	4.51374200 L
B-B_2	0	-5.12805100	4.05497000	3.73034800 L
B-B_2	0	-3.84233400	2.31445800	4.97248700 L

N-N_3	0	-3.84220500	3.77282800	4.50903100 L
N-N_3	0	-2.55703400	1.75677400	5.58567200 L
B-B_2	0	-1.27219600	2.31440800	4.97148100 L
B-B_2	0	0.01277900	0.23167400	5.45823300 L
N-N_3	0	0.01266300	1.75645800	5.58513700 L
N-N_3	0	1.29725000	-0.51675500	5.81668100 L
B-B_2	0	2.58236600	0.23194200	5.46033300 L
B-B_2	0	3.86762200	-1.87970800	5.12371400 L
N-N_3	0	3.86683700	-0.51666000	5.81865100 L
N-N_3	0	5.15207600	-2.70882200	5.17022300 L
B-B_2	0	6.44049700	-1.88458000	5.13796700 L
B-B_2	0	7.72584000	-3.72043900	4.02886600 L
N-N_3	0	7.72293000	-2.71996300	5.19353100 L
N-N_3	0	8.99996900	-4.52395000	3.76770000 L
B-B_2	0	10.28812800	-3.75155700	4.07517800 L
B-B_2	0	11.51004700	-4.76747500	2.23959300 L
N-N_3	0	11.59633700	-4.46249800	3.72748800 L
N-N_3	0	12.62626600	-4.34167100	1.28664100 L
B-	0	-12.75080100	3.75841100	3.42366800 L
N-N_3	0	-12.84104200	5.10223200	2.69878900 L
N-N_3	0	-11.58955100	3.75078200	4.44562600 L
B-B_2	0	-10.26487700	4.07807300	3.73611300 L
B-B_2	0	-8.98371700	2.33046600	5.00175600 L
N-N_3	0	-8.98626200	3.79162200	4.53170400 L
N-N_3	0	-7.69498500	1.76191500	5.59925900 L
B-B_2	0	-6.41301500	2.31630800	4.97725200 L
B-B_2	0	-5.12779200	0.23183400	5.46499200 L
N-N_3	0	-5.12697300	1.75738600	5.58794200 L
N-N_3	0	-3.84145100	-0.51675200	5.81799000 L
B-B_2	0	-2.55711700	0.23190300	5.45936000 L
B-B_2	0	-1.27214300	-1.88088500	5.12205100 L
N-N_3	0	-1.27200100	-0.51689500	5.81528500 L
N-N_3	0	0.01246900	-2.70926200	5.16981400 L
B-B_2	0	1.29732500	-1.88076300	5.12373600 L
B-B_2	0	2.58222900	-3.70216500	4.00572900 L
N-N_3	0	2.58256300	-2.70801800	5.16840000 L
N-N_3	0	3.86787500	-4.48208400	3.72781900 L
B-B_2	0	5.15320400	-3.70138400	4.00554900 L
B-B_2	0	6.44028800	-4.96613700	2.27655300 L
N-N_3	0	6.43583700	-4.48795900	3.73299900 L
N-N_3	0	7.72216000	-5.59710000	1.72521500 L
B-B_2	0	9.00819500	-4.99228200	2.29712200 L
B-B_2	0	10.28699300	-5.54041900	0.20463700 L
N-N_3	0	10.31049200	-5.57882500	1.73476900 L

N-N_3	0	11.59396200	-5.80146800	-0.54414100 L
B-	0	12.86319100	-5.48872900	0.29121700 L
N-N_3	0	-12.84072100	1.70164000	5.47748400 L
B-B_2	0	-11.53937000	2.33488800	5.01575900 L
B-B_2	0	-10.26425200	0.24465400	5.49216300 L
N-N_3	0	-10.25712200	1.77775500	5.63630200 L
N-N_3	0	-8.98530800	-0.51883500	5.85443700 L
B-B_2	0	-7.70071500	0.23180300	5.48527600 L
B-B_2	0	-6.41266000	-1.88109200	5.13070900 L
N-N_3	0	-6.41117600	-0.51776800	5.82721300 L
N-N_3	0	-5.12682800	-2.70851600	5.17131000 L
B-B_2	0	-3.84195200	-1.88045300	5.12394100 L
B-B_2	0	-2.55714100	-3.70720500	4.01051400 L
N-N_3	0	-2.55699100	-2.70891200	5.16996900 L
N-N_3	0	-1.27239800	-4.49050900	3.73554300 L
B-B_2	0	0.01216500	-3.70722700	4.00997100 L
B-B_2	0	1.29692000	-4.95604900	2.27566100 L
N-N_3	0	1.29814300	-4.48651100	3.73170600 L
N-N_3	0	2.58240800	-5.56772500	1.71734100 L
B-B_2	0	3.86761400	-4.95230600	2.27216100 L
B-B_2	0	5.15206200	-5.44766600	0.19170800 L
N-N_3	0	5.15145800	-5.57105700	1.71699800 L
N-N_3	0	6.43391200	-5.81314600	-0.55762900 L
B-B_2	0	7.72459600	-5.48150000	0.19423900 L
B-B_2	0	9.00738500	-5.15564200	-1.92865700 L
N-N_3	0	8.99809000	-5.86632900	-0.55877800 L
N-N_3	0	10.30984200	-5.17173200	-2.74113000 L
B-B_2	0	11.51055300	-4.96203300	-1.81012500 L
B-	0	12.86388900	-4.07962400	-3.69004300 L
N-N_3	0	12.62452400	-3.98164500	-2.17492300 L
B-	0	-12.74987000	0.23715100	5.04585800 L
B-B_2	0	-11.53905900	-1.89459100	5.17556900 L
N-N_3	0	-11.58868500	-0.48734300	5.76660100 L
N-N_3	0	-10.25669100	-2.72674600	5.22143800 L
B-B_2	0	-8.98332900	-1.88749800	5.15980300 L
B-B_2	0	-7.70122400	-3.71678600	4.02352500 L
N-N_3	0	-7.69481700	-2.71219900	5.18304700 L
N-N_3	0	-6.41242600	-4.49007000	3.73666700 L
B-B_2	0	-5.12807100	-3.70554600	4.01043700 L
B-B_2	0	-3.84289900	-4.95704200	2.27761800 L
N-N_3	0	-3.84285900	-4.48740600	3.73375900 L
N-N_3	0	-2.55838400	-5.57325500	1.72127700 L
B-B_2	0	-1.27259300	-4.96197800	2.27966100 L
B-B_2	0	0.01173100	-5.44273400	0.19538900 L

N-N_3	0	0.01280600	-5.57273200	1.72006300 L
N-N_3	0	1.29606400	-5.79926400	-0.55464400 L
B-B_2	0	2.58126200	-5.44170500	0.19278300 L
B-B_2	0	3.86598200	-5.10604600	-1.91959700 L
N-N_3	0	3.86552200	-5.80027200	-0.55633100 L
N-N_3	0	5.15038500	-5.15181500	-2.74918700 L
B-B_2	0	6.43904200	-5.12082600	-1.92528200 L
B-B_2	0	7.72481500	-4.00840300	-3.75782100 L
N-N_3	0	7.72139800	-5.17589100	-2.76086600 L
N-N_3	0	8.99893200	-3.74472400	-4.56039600 L
B-B_2	0	10.28736400	-4.05736700	-3.79051600 L
B-B_2	0	11.51058000	-2.21866100	-4.79782200 L
N-N_3	0	11.59500200	-3.70844300	-4.50160100 L
N-N_3	0	12.62220100	-1.26753000	-4.35653900 L
B-	0	-12.75187000	-3.40246100	3.71939800 L
N-N_3	0	-12.84022200	-2.66974300	5.05905500 L
N-N_3	0	-11.58952700	-4.42326300	3.71515300 L
B-B_2	0	-10.26490000	-3.71125800	4.03752900 L
B-B_2	0	-8.98449000	-4.98270600	2.29473200 L
N-N_3	0	-8.98633200	-4.50781700	3.75415000 L
N-N_3	0	-7.69623400	-5.58128000	1.72657500 L
B-B_2	0	-6.41384400	-4.95917600	2.27958300 L
B-B_2	0	-5.12920300	-5.44695100	0.19651300 L
N-N_3	0	-5.12831700	-5.57166500	1.72161100 L
N-N_3	0	-3.84307900	-5.79880400	-0.55281300 L
B-B_2	0	-2.55808600	-5.44348000	0.19670700 L
B-B_2	0	-1.27349000	-5.10341800	-1.91590700 L
N-N_3	0	-1.27330900	-5.79882900	-0.55307700 L
N-N_3	0	0.01040800	-5.14846200	-2.74559700 L
B-B_2	0	1.29581100	-5.10606900	-1.91845800 L
B-B_2	0	2.58123100	-3.98565700	-3.73956400 L
N-N_3	0	2.58070900	-5.15032100	-2.74729200 L
N-N_3	0	3.86679900	-3.70334400	-4.51857200 L
B-B_2	0	5.15194100	-3.98470200	-3.73894800 L
B-B_2	0	6.44023600	-2.24955900	-4.99427100 L
N-N_3	0	6.43494100	-3.70862500	-4.52390700 L
N-N_3	0	7.72253200	-1.69549500	-5.62231800 L
B-B_2	0	9.00833000	-2.27170600	-5.02102700 L
B-B_2	0	10.28866700	-0.17725400	-5.55674800 L
N-N_3	0	10.31093800	-1.70716500	-5.60486100 L
N-N_3	0	11.59716100	0.57156400	-5.81133800 L
B-	0	12.86538900	-0.26418100	-5.49525300 L
N-N_3	0	-12.84144900	-5.46349500	1.66991500 L
B-B_2	0	-11.54037700	-4.99919400	2.30151400 L

B-B_2	0	-10.26621600	-5.47077800	0.21049500 L
N-N_3	0	-10.25796900	-5.61784600	1.74322400 L
N-N_3	0	-8.98761100	-5.83079700	-0.55466100 L
B-B_2	0	-7.70235600	-5.46540500	0.19680200 L
B-B_2	0	-6.41465300	-5.10295500	-1.91361100 L
N-N_3	0	-6.41320900	-5.80603100	-0.55389500 L
N-N_3	0	-5.12914200	-5.14043600	-2.74117200 L
B-B_2	0	-3.84363300	-5.09916500	-1.91328200 L
B-B_2	0	-2.55898200	-3.97652900	-3.73193400 L
N-N_3	0	-2.55954900	-5.14330700	-2.74254200 L
N-N_3	0	-1.27477200	-3.69862600	-4.51407000 L
B-B_2	0	0.01105000	-3.98268700	-3.73655800 L
B-B_2	0	1.29673600	-2.24323000	-4.97705100 L
N-N_3	0	1.29565500	-3.70295700	-4.51813000 L
N-N_3	0	2.58177600	-1.68434600	-5.58975400 L
B-B_2	0	3.86738100	-2.24425100	-4.97949900 L
B-B_2	0	5.15360700	-0.16100500	-5.46556700 L
N-N_3	0	5.15153600	-1.68598000	-5.59572900 L
N-N_3	0	6.43607800	0.58885600	-5.82852500 L
B-B_2	0	7.72627700	-0.16497300	-5.49946800 L
B-B_2	0	9.01015400	1.95759400	-5.16920700 L
N-N_3	0	9.00054100	0.58843500	-5.88161300 L
N-N_3	0	10.31319800	2.76878900	-5.18502100 L
B-B_2	0	11.51150800	1.83626200	-4.97039800 L
B-	0	12.86745900	3.71565700	-4.09191800 L
N-N_3	0	12.62395900	2.20152300	-3.98848500 L
B-	0	-12.75383400	-5.02801300	0.20629900 L
B-B_2	0	-11.54137700	-5.14258300	-1.92578900 L
N-N_3	0	-11.59097300	-5.74252300	-0.52216600 L
N-N_3	0	-10.25928900	-5.18482800	-2.75881100 L
B-B_2	0	-8.98548800	-5.12933700	-1.91973600 L
B-B_2	0	-7.70273800	-3.98400400	-3.74277300 L
N-N_3	0	-7.69718500	-5.14925300	-2.74476400 L
N-N_3	0	-6.41378500	-3.69482600	-4.51473000 L
B-B_2	0	-5.12976100	-3.97371800	-3.73121200 L
B-B_2	0	-3.84332600	-2.23629400	-4.97475800 L
N-N_3	0	-3.84437700	-3.69430800	-4.51109700 L
N-N_3	0	-2.55776000	-1.68005500	-5.58821800 L
B-B_2	0	-1.27325600	-2.23970800	-4.97489800 L
B-B_2	0	0.01311600	-0.15801800	-5.45779800 L
N-N_3	0	0.01190100	-1.68242800	-5.58811800 L
N-N_3	0	1.29840900	0.59027800	-5.81347000 L
B-B_2	0	2.58291800	-0.15990500	-5.45881300 L
B-B_2	0	3.86955000	1.95177100	-5.11961600 L

N-N_3	0	3.86776700	0.58913900	-5.81574200 L
N-N_3	0	5.15412600	2.78084000	-5.16661700 L
B-B_2	0	6.44217200	1.95603200	-5.13469300 L
B-B_2	0	7.72867400	3.79248900	-4.02709100 L
N-N_3	0	7.72489700	2.79092300	-5.19094200 L
N-N_3	0	9.00348200	4.59523700	-3.76686600 L
B-B_2	0	10.29103700	3.82179900	-4.07422800 L
B-B_2	0	11.51421100	4.83735900	-2.23958100 L
N-N_3	0	11.59970600	4.53223700	-3.72744500 L
N-N_3	0	12.62889200	4.40799600	-1.28646200 L
B-	0	-12.75220200	-3.67494600	-3.42425700 L
N-N_3	0	-12.84278500	-5.01881900	-2.69953100 L
N-N_3	0	-11.59089600	-3.66752400	-4.44613100 L
B-B_2	0	-10.26633300	-3.99528500	-3.73660700 L
B-B_2	0	-8.98451700	-2.24863800	-5.00293100 L
N-N_3	0	-8.98771700	-3.70962400	-4.53236900 L
N-N_3	0	-7.69565600	-1.68098800	-5.60094800 L
B-B_2	0	-6.41391900	-2.23606700	-4.97914200 L
B-B_2	0	-5.12742300	-0.15289000	-5.46664400 L
N-N_3	0	-5.12763600	-1.67828200	-5.59019800 L
N-N_3	0	-3.84047200	0.59480300	-5.81895600 L
B-B_2	0	-2.55671900	-0.15546100	-5.46057200 L
B-B_2	0	-1.27043400	1.95520300	-5.11958400 L
N-N_3	0	-1.27077500	0.59236500	-5.81497700 L
N-N_3	0	0.01520000	2.78220500	-5.16386100 L
B-B_2	0	1.29930100	1.95281700	-5.11759800 L
B-B_2	0	2.58530300	3.77570200	-4.00111500 L
N-N_3	0	2.58466100	2.78016400	-5.16293300 L
N-N_3	0	3.87095500	4.55714500	-3.72631900 L
B-B_2	0	5.15604200	3.77530500	-4.00314900 L
B-B_2	0	6.44418400	5.04256400	-2.27629700 L
N-N_3	0	6.43925800	4.56149400	-3.73196000 L
N-N_3	0	7.72717800	5.67161100	-1.72517600 L
B-B_2	0	9.01237800	5.06462700	-2.29663900 L
N-N_3	0	10.31546400	5.64962800	-1.73434100 L
N-N_3	0	-12.84125500	-1.61754200	-5.47743500 L
B-B_2	0	-11.54012600	-2.25157400	-5.01611800 L
B-B_2	0	-10.26393700	-0.16211900	-5.49303100 L
N-N_3	0	-10.25777000	-1.69523600	-5.63714100 L
N-N_3	0	-8.98455500	0.60067500	-5.85525400 L
B-B_2	0	-7.70039400	-0.15093100	-5.48657000 L
B-B_2	0	-6.41109200	1.96068900	-5.13040900 L
N-N_3	0	-6.41038600	0.59796400	-5.82815100 L
N-N_3	0	-5.12464400	2.78709000	-5.16986200 L

B-B_2	0	-3.84043500	1.95763100	-5.12320600 L
B-B_2	0	-2.55481600	3.78021200	-4.00451900 L
N-N_3	0	-2.55458500	2.78464300	-5.16642100 L
N-N_3	0	-1.26935000	4.56190900	-3.72880000 L
B-B_2	0	0.01527100	3.77820900	-4.00241200 L
B-B_2	0	1.30054600	5.03472600	-2.27287200 L
N-N_3	0	1.30087600	4.55972800	-3.72732800 L
N-N_3	0	2.58611500	5.65043500	-1.71820200 L
B-B_2	0	3.87132500	5.03291100	-2.27200800 L
N-N_3	0	5.15622500	5.65072300	-1.71776700 L
B-	0	-12.74936600	-0.15300300	-5.04612900 L
B-B_2	0	-11.53747600	1.97804000	-5.17669200 L
N-N_3	0	-11.58794900	0.57064700	-5.76735100 L
N-N_3	0	-10.25445300	2.80924300	-5.22190400 L
B-B_2	0	-8.98174800	1.96905600	-5.16003400 L
B-B_2	0	-7.69869900	3.79726700	-4.02265300 L
N-N_3	0	-7.69262100	2.79283800	-5.18244300 L
N-N_3	0	-6.40936600	4.56963900	-3.73533800 L
B-B_2	0	-5.12567800	3.78354400	-4.00822500 L
B-B_2	0	-3.84024000	5.03710200	-2.27534200 L
N-N_3	0	-3.83951600	4.56353900	-3.73044400 L
N-N_3	0	-2.55515900	5.65357400	-1.72016300 L
B-B_2	0	-1.26982200	5.03657300	-2.27413100 L
N-N_3	0	0.01552500	5.65277900	-1.71926200 L
B-	0	-12.74986900	3.48662100	-3.72104000 L
N-N_3	0	-12.83808600	2.75417500	-5.06085300 L
N-N_3	0	-11.58668800	4.50649100	-3.71594500 L
B-B_2	0	-10.26241500	3.79359300	-4.03784100 L
B-B_2	0	-8.98178600	5.06463800	-2.29459700 L
N-N_3	0	-8.98336900	4.58926000	-3.75388500 L
N-N_3	0	-7.69353300	5.66325200	-1.72643400 L
B-B_2	0	-6.41105300	5.04055400	-2.27864000 L
N-N_3	0	-5.12555600	5.65385600	-1.72118700 L
N-N_3	0	-12.83879300	5.54655100	-1.67075200 L
B-B_2	0	-11.53770200	5.08196600	-2.30213000 L
N-N_3	0	-10.25525100	5.70028700	-1.74357900 L
H-H_	0	12.29169300	3.08526800	1.95462800 L
H-H_	0	12.28162900	0.81285300	3.52017300 L
H-H_	0	12.28049000	-1.91378600	3.02521700 L
H-H_	0	12.29246600	-3.50457100	0.75732700 L
H-H_	0	-12.86306900	5.86333900	3.41493900 L
H-H_	0	-12.86319600	1.73771600	6.52191500 L
H-H_	0	12.28761000	-3.01765200	-1.95229900 L
H-H_	0	12.28151600	-0.74427600	-3.51837000 L

H-H_	0	-12.86035800	-3.38141700	5.82440200 L
H-H_	0	-12.86053600	-6.50807800	1.70340400 L
H-H_	0	12.28391600	1.98369300	-3.02448200 L
H-H_	0	12.29273300	3.57143900	-0.75777200 L
H-H_	0	-12.86482400	-5.77985500	-3.41575700 L
H-H_	0	-12.86416800	-1.65379900	-6.52185000 L
H-H_	0	-12.85719700	3.46597900	-5.82610600 L
H-H_	0	-12.85767000	6.59113700	-1.70428200 L
C-C_R	0	0.44456800	-1.52789300	-0.05013500 H
H-H_	0	1.93362700	-0.44477500	1.08651100 H
H-H_	0	2.20908000	-2.18865500	1.00913100 H
C-C_3	0	1.42572800	-1.41998300	1.08093000 H
H-H_	0	0.92702100	-1.53946300	2.04550300 H
N-N_R	0	0.86787600	-1.39912600	-1.42795500 H
H-H_	0	1.23348000	-0.47055500	-1.63333400 H
H-H_	0	1.60109700	-2.06437600	-1.66182300 H
C-C_R	0	-0.87735100	-1.73452100	0.09828400 H
O-O_R	0	-1.73504600	-1.84459000	-0.94978300 H
O-O_R	0	-1.50214200	-1.83692100	1.29641600 H
H-H_	0	-2.42128700	-2.09214100	1.13442700 H
H-H_	0	-1.16126000	-1.75983000	-1.73975600 H

bTS3@D

B-B_2	0	10.29074600	5.45732300	-1.30822800 L
N-N_3	0	11.59864000	5.85788000	-0.62543000 L
B-	0	12.86699500	5.38314100	-1.38204700 L
B-B_2	0	5.15533000	5.38052600	-1.27770700 L
N-N_3	0	6.43853400	5.88314200	-0.61494400 L
B-B_2	0	7.72814300	5.40660500	-1.28636600 L
B-B_2	0	9.01117100	5.50357300	0.85914600 L
N-N_3	0	9.00274000	5.92992200	-0.62410000 L
N-N_3	0	10.31381500	5.67786100	1.65244800 L
B-B_2	0	11.51364100	5.28530900	0.78144800 L
B-	0	12.86644400	4.79265500	2.79933900 L
N-N_3	0	12.62662200	4.39575700	1.33390000 L
B-B_2	0	0.01370600	5.38279800	-1.27776900 L
N-N_3	0	1.29929100	5.87968700	-0.61431200 L
B-B_2	0	2.58424000	5.38068900	-1.27739200 L
B-B_2	0	3.86983000	5.46277200	0.85902500 L
N-N_3	0	3.86992600	5.87715200	-0.61396000 L
N-N_3	0	5.15441900	5.66742900	1.66408900 L
B-B_2	0	6.44281800	5.47344900	0.86234500 L
B-B_2	0	7.72738900	4.74206600	2.87895600 L

N-N_3	0	7.72543800	5.68970300	1.67093500 L
N-N_3	0	9.00111400	4.64166100	3.71839200 L
B-B_2	0	10.28995200	4.79387200	2.90205800 L
B-B_2	0	11.51125800	3.19092800	4.25523300 L
N-N_3	0	11.59727300	4.59186100	3.66850600 L
N-N_3	0	12.62285500	2.17052600	4.01390000 L
B-B_2	0	-5.12793700	5.38459800	-1.27810800 L
N-N_3	0	-3.84210100	5.88054000	-0.61444700 L
B-B_2	0	-2.55681900	5.38310400	-1.27791200 L
B-B_2	0	-1.27169900	5.46532700	0.85822700 L
N-N_3	0	-1.27153300	5.88080800	-0.61449200 L
N-N_3	0	0.01363500	5.66840100	1.66216300 L
B-B_2	0	1.29886200	5.46416400	0.85830000 L
B-B_2	0	2.58362200	4.71578700	2.86105600 L
N-N_3	0	2.58425300	5.66663100	1.66230700 L
N-N_3	0	3.86849700	4.59431100	3.68192200 L
B-B_2	0	5.15462500	4.71664100	2.86346000 L
B-B_2	0	6.44098900	3.26440400	4.44007300 L
N-N_3	0	6.43690700	4.60074600	3.68863500 L
N-N_3	0	7.72271500	2.84583100	5.16644600 L
B-B_2	0	9.00909200	3.28966400	4.46279800 L
B-B_2	0	10.28757800	1.34291400	5.40568500 L
N-N_3	0	10.31113700	2.85165000	5.14778300 L
N-N_3	0	11.59529700	0.65874100	5.80492000 L
B-	0	12.86432000	1.41427000	5.33006900 L
B-B_2	0	-10.26488100	5.40304300	-1.29571000 L
N-N_3	0	-8.98624000	5.90905800	-0.61841900 L
B-B_2	0	-7.70107500	5.40065200	-1.28157300 L
B-B_2	0	-6.41318900	5.46785500	0.85844400 L
N-N_3	0	-6.41214900	5.88540400	-0.61442500 L
N-N_3	0	-5.12755000	5.66861900	1.66222700 L
B-B_2	0	-3.84226800	5.46492000	0.85826100 L
B-B_2	0	-2.55721400	4.71820100	2.86124400 L
N-N_3	0	-2.55708600	5.66877000	1.66214600 L
N-N_3	0	-1.27197700	4.59670300	3.68140600 L
B-B_2	0	0.01319800	4.71742800	2.86091900 L
B-B_2	0	1.29770000	3.25733900	4.42315800 L
N-N_3	0	1.29832800	4.59544900	3.68122800 L
N-N_3	0	2.58219400	2.83163900	5.13569200 L
B-B_2	0	3.86828900	3.25717400	4.42586000 L
B-B_2	0	5.15254600	1.31275800	5.31900300 L
N-N_3	0	5.15182700	2.83299400	5.14169700 L
N-N_3	0	6.43441600	0.64947400	5.82425400 L
B-B_2	0	7.72516400	1.32157100	5.35150900 L

B-B_2	0	9.00730600	-0.82503500	5.44990000 L
N-N_3	0	8.99882400	0.65831600	5.87612700 L
N-N_3	0	10.30968600	-1.61818500	5.62620700 L
B-B_2	0	11.50904000	-0.74771800	5.23181100 L
B-	0	12.86299500	-2.76517100	4.74250400 L
N-N_3	0	12.62122100	-1.30106200	4.34186000 L
B-	0	-12.75218900	4.96996300	-1.20213600 L
B-B_2	0	-11.53994600	5.51121100	0.86323200 L
N-N_3	0	-11.58947700	5.81657100	-0.63238300 L
N-N_3	0	-10.25747900	5.71729900	1.67071200 L
B-B_2	0	-8.98401100	5.49486000	0.85939400 L
B-B_2	0	-7.70141400	4.73394000	2.87308500 L
N-N_3	0	-7.69562100	5.67826700	1.66387900 L
N-N_3	0	-6.41224500	4.60177800	3.68666400 L
B-B_2	0	-5.12827100	4.71987300	2.86315800 L
B-B_2	0	-3.84267500	3.25978700	4.42520800 L
N-N_3	0	-3.84224900	4.59747000	3.68205800 L
N-N_3	0	-2.55733900	2.83382700	5.13626300 L
B-B_2	0	-1.27245100	3.25863800	4.42366000 L
B-B_2	0	0.01210100	1.31248000	5.31116600 L
N-N_3	0	0.01256700	2.83234700	5.13492500 L
N-N_3	0	1.29650300	0.64862900	5.80937100 L
B-B_2	0	2.58182000	1.31188200	5.31242900 L
B-B_2	0	3.86637400	-0.82528000	5.39989400 L
N-N_3	0	3.86602300	0.64830000	5.81159100 L
N-N_3	0	5.15043100	-1.62927300	5.61023500 L
B-B_2	0	6.43923000	-0.82817700	5.41583100 L
B-B_2	0	7.72419200	-2.84767000	4.69273500 L
N-N_3	0	7.72134500	-1.63640100	5.63621700 L
N-N_3	0	8.99810100	-3.68734800	4.59614400 L
B-B_2	0	10.28651100	-2.86994200	4.74538500 L
B-B_2	0	11.50870900	-4.22911300	3.14761100 L
N-N_3	0	11.59440200	-3.63630100	4.54601300 L
N-N_3	0	12.62435900	-3.99827400	2.12910600 L
B-	0	-12.75225700	4.37347400	2.62394500 L
N-N_3	0	-12.84101100	5.54655100	1.64644000 L
N-N_3	0	-11.58974000	4.56648700	3.62621200 L
B-B_2	0	-10.26521400	4.74575400	2.86532500 L
B-B_2	0	-8.98420200	3.28238000	4.45073100 L
N-N_3	0	-8.98640400	4.62193500	3.70149500 L
N-N_3	0	-7.69557000	2.84228200	5.14841300 L
B-B_2	0	-6.41342600	3.26309800	4.42953100 L
B-B_2	0	-5.12863900	1.31544000	5.31801900 L
N-N_3	0	-5.12747500	2.83536900	5.13848600 L

N-N_3	0	-3.84250500	0.65055600	5.81136300 L
B-B_2	0	-2.55787600	1.31394900	5.31289700 L
B-B_2	0	-1.27320900	-0.82421100	5.39665300 L
N-N_3	0	-1.27281800	0.64928300	5.80880300 L
N-N_3	0	0.01089400	-1.62766200	5.60755200 L
B-B_2	0	1.29607600	-0.82516200	5.39859500 L
B-B_2	0	2.58046000	-2.83291100	4.66454900 L
N-N_3	0	2.58083000	-1.62783400	5.60689000 L
N-N_3	0	3.86595500	-3.65280400	4.54721100 L
B-B_2	0	5.15151000	-2.83290800	4.66527600 L
B-B_2	0	6.43871100	-4.41498600	3.22110700 L
N-N_3	0	6.43400100	-3.65818500	4.55419300 L
N-N_3	0	7.72058100	-5.14270100	2.80566800 L
B-B_2	0	9.00663600	-4.43711000	3.24715700 L
B-B_2	0	10.28576000	-5.38763700	1.30447000 L
N-N_3	0	10.30889700	-5.12354200	2.81214700 L
N-N_3	0	11.59297300	-5.79099200	0.62216000 L
B-	0	12.86207200	-5.31876600	1.37910700 L
N-N_3	0	-12.84132500	2.76088200	5.04176500 L
B-B_2	0	-11.53998600	3.29072900	4.46432600 L
B-B_2	0	-10.26525500	1.33398100	5.34063200 L
N-N_3	0	-10.25767600	2.86560000	5.18163600 L
N-N_3	0	-8.98652700	0.65600600	5.84567100 L
B-B_2	0	-7.70164000	1.31958900	5.33701000 L
B-B_2	0	-6.41402000	-0.82185400	5.40384300 L
N-N_3	0	-6.41236700	0.65153100	5.81971600 L
N-N_3	0	-5.12833700	-1.62524400	5.60619300 L
B-B_2	0	-3.84333600	-0.82258400	5.39768100 L
B-B_2	0	-2.55862900	-2.83179300	4.66294400 L
N-N_3	0	-2.55852800	-1.62616500	5.60478200 L
N-N_3	0	-1.27486500	-3.65551700	4.55099800 L
B-B_2	0	0.01059100	-2.83550700	4.66817300 L
B-B_2	0	1.29527300	-4.40419900	3.21651500 L
N-N_3	0	1.29603700	-3.65556800	4.55082300 L
N-N_3	0	2.58073500	-5.11464900	2.79086500 L
B-B_2	0	3.86598500	-4.40193200	3.21346000 L
B-B_2	0	5.15092800	-5.29896800	1.27234200 L
N-N_3	0	5.14990000	-5.11839500	2.79192400 L
N-N_3	0	6.43281100	-5.80584500	0.61043700 L
B-B_2	0	7.72338600	-5.33203000	1.28203600 L
B-B_2	0	9.00648300	-5.43288100	-0.86323500 L
N-N_3	0	8.99702800	-5.85822700	0.62027600 L
N-N_3	0	10.30915500	-5.60923400	-1.65612100 L
B-B_2	0	11.50938300	-5.21857000	-0.78482400 L

B-	0	12.86317500	-4.72460200	-2.80138800 L
N-N_3	0	12.62240000	-4.32831500	-1.33597000 L
B-	0	-12.75123300	1.24020000	4.90483400 L
B-B_2	0	-11.54032300	-0.82553400	5.44772900 L
N-N_3	0	-11.58987700	0.67002900	5.75276000 L
N-N_3	0	-10.25832400	-1.63285100	5.65767900 L
B-B_2	0	-8.98467900	-0.82230700	5.43281500 L
B-B_2	0	-7.70256000	-2.84004500	4.67932200 L
N-N_3	0	-7.69629900	-1.62649000	5.61805000 L
N-N_3	0	-6.41364100	-3.65465600	4.55123500 L
B-B_2	0	-5.12961800	-2.83093300	4.66382500 L
B-B_2	0	-3.84423600	-4.40245300	3.21386200 L
N-N_3	0	-3.84424400	-3.65155900	4.54682000 L
N-N_3	0	-2.55968000	-5.11779200	2.79293100 L
B-B_2	0	-1.27426000	-4.40614100	3.21761900 L
B-B_2	0	0.01037500	-5.29391800	1.27285500 L
N-N_3	0	0.01083600	-5.11751700	2.79280100 L
N-N_3	0	1.29536600	-5.79038700	0.60899800 L
B-B_2	0	2.58020700	-5.29212100	1.27148100 L
B-B_2	0	3.86528900	-5.38232600	-0.86519700 L
N-N_3	0	3.86447800	-5.79234600	0.60864700 L
N-N_3	0	5.14967500	-5.59268700	-1.66891200 L
B-B_2	0	6.43819300	-5.39847700	-0.86737500 L
B-B_2	0	7.72410600	-4.67210300	-2.88426700 L
N-N_3	0	7.72072100	-5.61818700	-1.67516800 L
N-N_3	0	8.99844600	-4.57254700	-3.72285600 L
B-B_2	0	10.28665500	-4.72517600	-2.90570000 L
B-B_2	0	11.50937100	-3.12245500	-4.25801000 L
N-N_3	0	11.59456800	-4.52346900	-3.67128600 L
N-N_3	0	12.62162700	-2.10273200	-4.01673300 L
B-	0	-12.75195500	-2.59115400	4.31590100 L
N-N_3	0	-12.84185200	-1.60807400	5.48414700 L
N-N_3	0	-11.59074400	-3.59331000	4.51610600 L
B-B_2	0	-10.26607300	-2.83186900	4.69153400 L
B-B_2	0	-8.98553300	-4.42513500	3.23652200 L
N-N_3	0	-8.98754200	-3.66895800	4.57211900 L
N-N_3	0	-7.69720200	-5.12518200	2.79954800 L
B-B_2	0	-6.41497300	-4.40477000	3.21680500 L
B-B_2	0	-5.13007900	-5.30066200	1.27351000 L
N-N_3	0	-5.12937000	-5.11644700	2.79258700 L
N-N_3	0	-3.84400500	-5.79600600	0.60992200 L
B-B_2	0	-2.55917300	-5.29814200	1.27351200 L
B-B_2	0	-1.27422500	-5.38430800	-0.86410800 L
N-N_3	0	-1.27373500	-5.79434700	0.61001500 L

N-N_3	0	0.01062500	-5.59127600	-1.66747700 L
B-B_2	0	1.29511300	-5.38081900	-0.86490800 L
B-B_2	0	2.58051100	-4.64804500	-2.87276700 L
N-N_3	0	2.58007500	-5.59027700	-1.66762000 L
N-N_3	0	3.86634800	-4.52632000	-3.69176700 L
B-B_2	0	5.15125400	-4.64611900	-2.87126800 L
B-B_2	0	6.43926800	-3.19483900	-4.44605000 L
N-N_3	0	6.43442300	-4.53127800	-3.69507200 L
N-N_3	0	7.72151900	-2.77588100	-5.17125600 L
B-B_2	0	9.00734100	-3.22050100	-4.46713300 L
B-B_2	0	10.28699300	-1.27383400	-5.40873100 L
N-N_3	0	10.30988600	-2.78268200	-5.15122900 L
N-N_3	0	11.59506300	-0.59024700	-5.80781600 L
B-	0	12.86360600	-1.34656200	-5.33287800 L
N-N_3	0	-12.84239200	-5.02075500	2.71977800 L
B-B_2	0	-11.54129800	-4.43954600	3.24576600 L
B-B_2	0	-10.26702400	-5.32129400	1.29201100 L
N-N_3	0	-10.25894800	-5.15782100	2.82308200 L
N-N_3	0	-8.98835400	-5.82733500	0.61468900 L
B-B_2	0	-7.70322600	-5.31849200	1.27760600 L
B-B_2	0	-6.41538000	-5.38592000	-0.86250600 L
N-N_3	0	-6.41406100	-5.80269700	0.61037700 L
N-N_3	0	-5.12974700	-5.58749300	-1.66601500 L
B-B_2	0	-3.84425000	-5.38188900	-0.86291400 L
B-B_2	0	-2.55965000	-4.64397600	-2.86919300 L
N-N_3	0	-2.55982200	-5.58987700	-1.66667300 L
N-N_3	0	-1.27531300	-4.52583900	-3.69092800 L
B-B_2	0	0.01050400	-4.64824100	-2.87220000 L
B-B_2	0	1.29567500	-3.18886700	-4.43264900 L
N-N_3	0	1.29542500	-4.52830500	-3.69308300 L
N-N_3	0	2.58077200	-2.76089700	-5.14294700 L
B-B_2	0	3.86640900	-3.18810500	-4.43351400 L
B-B_2	0	5.15196700	-1.24183900	-5.32155800 L
N-N_3	0	5.15055700	-2.76240000	-5.14770700 L
N-N_3	0	6.43406500	-0.57810000	-5.82595600 L
B-B_2	0	7.72461400	-1.25141200	-5.35444800 L
B-B_2	0	9.00785500	0.89486300	-5.45174100 L
N-N_3	0	8.99850200	-0.58831100	-5.87868400 L
N-N_3	0	10.31053500	1.68729300	-5.62877600 L
B-B_2	0	11.50954700	0.81622700	-5.23458900 L
B-	0	12.86495800	2.83343000	-4.74766500 L
N-N_3	0	12.62300600	1.36955900	-4.34622800 L
B-	0	-12.75439800	-4.88819700	1.19855400 L
B-B_2	0	-11.54219900	-5.42945300	-0.86679400 L

N-N_3	0	-11.59168100	-5.73483900	0.62880100 L
N-N_3	0	-10.25983100	-5.63572900	-1.67435400 L
B-B_2	0	-8.98622800	-5.41342200	-0.86316100 L
B-B_2	0	-7.70369500	-4.65351400	-2.87717800 L
N-N_3	0	-7.69788800	-5.59724000	-1.66763000 L
N-N_3	0	-6.41483900	-4.52261700	-3.69118800 L
B-B_2	0	-5.13056800	-4.64095400	-2.86829400 L
B-B_2	0	-3.84460100	-3.18343000	-4.43042600 L
N-N_3	0	-3.84535100	-4.52149000	-3.68839100 L
N-N_3	0	-2.55936600	-2.75843700	-5.14174200 L
B-B_2	0	-1.27443100	-3.18678000	-4.43128600 L
B-B_2	0	0.01132500	-1.23963900	-5.31257100 L
N-N_3	0	0.01059000	-2.76007000	-5.14199700 L
N-N_3	0	1.29623900	-0.57529500	-5.80877200 L
B-B_2	0	2.58122700	-1.24056000	-5.31424200 L
B-B_2	0	3.86724100	0.89703300	-5.39848700 L
N-N_3	0	3.86565800	-0.57603800	-5.81233500 L
N-N_3	0	5.15136000	1.70096800	-5.60938800 L
B-B_2	0	6.43986100	0.89922700	-5.41604600 L
B-B_2	0	7.72615900	2.91891400	-4.69439600 L
N-N_3	0	7.72216800	1.70695000	-5.63714900 L
N-N_3	0	9.00070300	3.75775100	-4.59907700 L
B-B_2	0	10.28849500	2.93937400	-4.74843800 L
B-B_2	0	11.51236600	4.29808700	-3.15193400 L
N-N_3	0	11.59688000	3.70509200	-4.55026900 L
N-N_3	0	12.62660900	4.06359000	-2.13277400 L
B-	0	-12.75437800	-4.29095500	-2.62704700 L
N-N_3	0	-12.84332400	-5.46433600	-1.64992800 L
N-N_3	0	-11.59200900	-4.48394700	-3.62948100 L
B-B_2	0	-10.26743700	-4.66407800	-2.86885800 L
B-B_2	0	-8.98596200	-3.20135000	-4.45443400 L
N-N_3	0	-8.98880300	-4.54095200	-3.70529300 L
N-N_3	0	-7.69725300	-2.76204500	-5.15240900 L
B-B_2	0	-6.41530200	-3.18400100	-4.43392800 L
B-B_2	0	-5.12927600	-1.23708000	-5.32093300 L
N-N_3	0	-5.12924800	-2.75710100	-5.14294000 L
N-N_3	0	-3.84251400	-0.57296200	-5.81333900 L
B-B_2	0	-2.55855300	-1.23828700	-5.31508100 L
B-B_2	0	-1.27265400	0.89870900	-5.39562900 L
N-N_3	0	-1.27286600	-0.57423600	-5.80953800 L
N-N_3	0	0.01263500	1.70100800	-5.60292300 L
B-B_2	0	1.29700600	0.89747000	-5.39458500 L
B-B_2	0	2.58288900	2.90570800	-4.66156700 L
N-N_3	0	2.58191000	1.70003700	-5.60346000 L

N-N_3	0	3.86830800	3.72657500	-4.54809200 L
B-B_2	0	5.15357000	2.90585100	-4.66554500 L
B-B_2	0	6.44213300	4.49046900	-3.22476000 L
N-N_3	0	6.43655500	3.73063900	-4.55631700 L
N-N_3	0	7.72522600	5.21644400	-2.80989200 L
B-B_2	0	9.01030500	4.50865300	-3.25073300 L
N-N_3	0	10.31349900	5.19358700	-2.81598100 L
N-N_3	0	-12.84287800	-2.67691700	-5.04387900 L
B-B_2	0	-11.54167900	-3.20783400	-4.46705900 L
B-B_2	0	-10.26585800	-1.25197300	-5.34394800 L
N-N_3	0	-10.25934600	-2.78361000	-5.18490500 L
N-N_3	0	-8.98667200	-0.57475700	-5.84894600 L
B-B_2	0	-7.70227000	-1.23927600	-5.34032400 L
B-B_2	0	-6.41325300	0.90145300	-5.40613500 L
N-N_3	0	-6.41244700	-0.57184000	-5.82247200 L
N-N_3	0	-5.12692200	1.70395300	-5.60801400 L
B-B_2	0	-3.84259200	0.90004900	-5.39901600 L
B-B_2	0	-2.55700700	2.90823300	-4.66294800 L
N-N_3	0	-2.55693600	1.70242500	-5.60484600 L
N-N_3	0	-1.27168100	3.72934400	-4.54845100 L
B-B_2	0	0.01296200	2.90715200	-4.66160700 L
B-B_2	0	1.29861600	4.48255400	-3.21682600 L
N-N_3	0	1.29836100	3.72808500	-4.54789000 L
N-N_3	0	2.58426700	5.19645600	-2.79632700 L
B-B_2	0	3.86932400	4.48136600	-3.21706600 L
N-N_3	0	5.15431800	5.19710500	-2.79718500 L
B-	0	-12.75146000	-1.15625900	-4.90743400 L
B-B_2	0	-11.53963500	0.90839900	-5.45202200 L
N-N_3	0	-11.59007100	-0.58731300	-5.75612600 L
N-N_3	0	-10.25699900	1.71484700	-5.66144000 L
B-B_2	0	-8.98395600	0.90354200	-5.43600500 L
B-B_2	0	-7.70081400	2.92087600	-4.68242100 L
N-N_3	0	-7.69496400	1.70694000	-5.62075000 L
N-N_3	0	-6.41150300	3.73502200	-4.55453100 L
B-B_2	0	-5.12780000	2.91048700	-4.66640000 L
B-B_2	0	-3.84200300	4.48390500	-3.21764500 L
N-N_3	0	-3.84171000	3.73025200	-4.54940100 L
N-N_3	0	-2.55683400	5.19877300	-2.79692100 L
B-B_2	0	-1.27166400	4.48381700	-3.21726900 L
N-N_3	0	0.01376100	5.19832400	-2.79675600 L
B-	0	-12.75083500	2.67464600	-4.32103900 L
N-N_3	0	-12.84061500	1.69174200	-5.48942000 L
N-N_3	0	-11.58878800	3.67604600	-4.52030700 L
B-B_2	0	-10.26443900	2.91390700	-4.69536400 L

B-B_2	0	-8.98345800	4.50687300	-3.24025800 L
N-N_3	0	-8.98550400	3.75037400	-4.57567800 L
N-N_3	0	-7.69508700	5.20696300	-2.80352300 L
B-B_2	0	-6.41276700	4.48654200	-3.22073400 L
N-N_3	0	-5.12715400	5.19877300	-2.79723500 L
N-N_3	0	-12.84030000	5.10283700	-2.72332500 L
B-B_2	0	-11.53926700	4.52168100	-3.24958800 L
N-N_3	0	-10.25682600	5.23970200	-2.82679700 L
H-H_	0	12.28860000	3.40712300	1.30736000 L
H-H_	0	12.28280700	1.49078000	3.29647800 L
H-H_	0	12.28158500	-1.27764400	3.35369000 L
H-H_	0	12.28969800	-3.28214500	1.44536600 L
H-H_	0	-12.86102000	6.43485100	2.19704300 L
H-H_	0	-12.86302600	3.00053000	6.05898700 L
H-H_	0	12.28400900	-3.33981100	-1.30922800 L
H-H_	0	12.28202500	-1.42277500	-3.29930000 L
H-H_	0	-12.86389300	-2.15440500	6.37503400 L
H-H_	0	-12.86196900	-6.03730800	2.96242600 L
H-H_	0	12.28453300	1.34661800	-3.35765300 L
H-H_	0	12.28955900	3.34799000	-1.44964500 L
H-H_	0	-12.86352000	-6.35245800	-2.20081100 L
H-H_	0	-12.86539800	-2.91683100	-6.06102000 L
H-H_	0	-12.86160700	2.23816200	-6.38027700 L
H-H_	0	-12.85987600	6.11943800	-2.96577000 L
C-C_R	0	0.46476100	-1.48572900	0.19705600 H
H-H_	0	1.79563500	-0.17810500	1.31241800 H
H-H_	0	2.15424700	-1.90243600	1.50294000 H
C-C_3	0	1.33609100	-1.17811200	1.36416800 H
H-H_	0	0.72715800	-1.20046100	2.27131500 H
N-N_R	0	0.97112600	-1.49229200	-1.19018400 H
H-H_	0	1.31699400	-0.59182900	-1.53014300 H
H-H_	0	1.67933900	-2.20205600	-1.38458000 H
C-C_R	0	-0.87435800	-1.76489500	0.08664400 H
O-O_R	0	-1.37977600	-1.96927500	-1.09395900 H
O-O_R	0	-1.68476000	-1.83024300	1.17428000 H
H-H_	0	-2.56325900	-2.06813600	0.84275000 H
H-H_	0	-0.10865900	-1.76130300	-1.61296600 H

bINT3@SWBNNT(8.8)

B-B_2	0	-10.29107900	5.49646200	1.13603100 L
N-N_3	0	-11.59896000	5.87515900	0.44085900 L
B-	0	-12.86733400	5.42476100	1.21217400 L
B-B_2	0	-5.15564900	5.41884800	1.10794400 L
N-N_3	0	-6.43886900	5.90016200	0.42958300 L
B-B_2	0	-7.72846400	5.44510200	1.11576600 L
B-B_2	0	-9.01148900	5.47390000	-1.03171900 L
N-N_3	0	-9.00307400	5.94712000	0.43724600 L
N-N_3	0	-10.31413900	5.62285100	-1.83015600 L
B-B_2	0	-11.51395600	5.25816600	-0.94711200 L
B-	0	-12.86674700	4.70109900	-2.94812400 L
N-N_3	0	-12.62666700	4.35107700	-1.47083100 L
B-B_2	0	-0.01402300	5.42129600	1.10798100 L
N-N_3	0	-1.29962100	5.89689400	0.42911600 L
B-B_2	0	-2.58455900	5.41909000	1.10764500 L
B-B_2	0	-3.87013600	5.43337400	-1.03029400 L
N-N_3	0	-3.87025900	5.89425000	0.42881300 L
N-N_3	0	-5.15473600	5.61230800	-1.84145400 L
B-B_2	0	-6.44313000	5.44380600	-1.03396400 L
B-B_2	0	-7.72766600	4.64872300	-3.02635700 L

N-N_3	0	-7.72576100	5.63421600	-1.84901000 L
N-N_3	0	-9.00139500	4.52169700	-3.86218300 L
B-B_2	0	-10.29023500	4.69958700	-3.05103600 L
B-B_2	0	-11.51137500	3.05444100	-4.35277900 L
N-N_3	0	-11.59758900	4.47319500	-3.81060500 L
N-N_3	0	-12.62297200	2.04209800	-4.07959300 L
B-B_2	0	5.12762500	5.42323500	1.10829800 L
N-N_3	0	3.84178200	5.89790500	0.42927400 L
B-B_2	0	2.55650500	5.42168000	1.10813700 L
B-B_2	0	1.27140000	5.43616200	-1.02952300 L
N-N_3	0	1.27120900	5.89810700	0.42929100 L
N-N_3	0	-0.01393500	5.61357900	-1.83951200 L
B-B_2	0	-1.29916400	5.43490900	-1.02958900 L
B-B_2	0	-2.58388300	4.62327900	-3.00758600 L
N-N_3	0	-2.58456100	5.61170200	-1.83962800 L
N-N_3	0	-3.86874600	4.47575800	-3.82420100 L
B-B_2	0	-5.15489100	4.62393400	-3.01004700 L
B-B_2	0	-6.44118500	3.12240400	-4.53990600 L
N-N_3	0	-6.43716700	4.48186600	-3.83114200 L
N-N_3	0	-7.72287300	2.68107600	-5.25275300 L
B-B_2	0	-9.00928100	3.14683700	-4.56347600 L
B-B_2	0	-10.28768100	1.17130300	-5.44471200 L
N-N_3	0	-10.31129600	2.68738600	-5.23431000 L
N-N_3	0	-11.59537900	0.47494000	-5.82236400 L
B-	0	-12.86441900	1.24495600	-5.37141500 L
B-B_2	0	10.26458100	5.44232100	1.12532900 L
N-N_3	0	8.98592800	5.92661300	0.43236100 L
B-B_2	0	7.70076400	5.43942500	1.11125900 L
B-B_2	0	6.41289300	5.43877200	-1.02977800 L
N-N_3	0	6.41183500	5.90281200	0.42910900 L
N-N_3	0	5.12725900	5.61389200	-1.83953700 L
B-B_2	0	3.84197100	5.43581000	-1.02951800 L
B-B_2	0	2.55695600	4.62580300	-3.00775200 L
N-N_3	0	2.55679300	5.61401000	-1.83948000 L
N-N_3	0	1.27174000	4.47827500	-3.82365600 L
B-B_2	0	-0.01345600	4.62500300	-3.00745200 L
B-B_2	0	-1.29789500	3.11600000	-4.52255800 L
N-N_3	0	-1.29856700	4.47699600	-3.82349700 L
N-N_3	0	-2.58234500	2.66792600	-5.22131400 L
B-B_2	0	-3.86848300	3.11570600	-4.52537800 L
B-B_2	0	-5.15266900	1.14399400	-5.35679200 L
N-N_3	0	-5.15198200	2.66907000	-5.22749900 L
N-N_3	0	-6.43448400	0.46514600	-5.84107700 L
B-B_2	0	-7.72528100	1.15174000	-5.38976700 L

B-B_2	0	-9.00738200	-0.99694900	-5.42092400 L
N-N_3	0	-8.99889400	0.47232300	-5.89340500 L
N-N_3	0	-10.30974500	-1.79524900	-5.57239900 L
B-B_2	0	-11.50913400	-0.91288500	-5.20550400 L
B-	0	-12.86308700	-2.91419800	-4.65371800 L
N-N_3	0	-12.62154500	-1.43824300	-4.29902800 L
B-	0	12.75199600	5.00676200	1.04557100 L
B-B_2	0	11.53966100	5.48209200	-1.03591500 L
N-N_3	0	11.58916900	5.83474100	0.44926800 L
N-N_3	0	10.25718500	5.66236400	-1.84953700 L
B-B_2	0	8.98371800	5.46577100	-1.03157300 L
B-B_2	0	7.70114900	4.64122100	-3.02005300 L
N-N_3	0	7.69532900	5.62351400	-1.84148100 L
N-N_3	0	6.41199000	4.48324200	-3.82902200 L
B-B_2	0	5.12801000	4.62743900	-3.00969200 L
B-B_2	0	3.84246400	3.11840500	-4.52453100 L
N-N_3	0	3.84200300	4.47904000	-3.82429200 L
N-N_3	0	2.55715200	2.67007900	-5.22171500 L
B-B_2	0	1.27225100	3.11728700	-4.52298500 L
B-B_2	0	-0.01222800	1.14395600	-5.34841200 L
N-N_3	0	-0.01272500	2.66863900	-5.22041300 L
N-N_3	0	-1.29657900	0.46472500	-5.82548900 L
B-B_2	0	-2.58195700	1.14334000	-5.34990000 L
B-B_2	0	-3.86646800	-0.99556600	-5.37039700 L
N-N_3	0	-3.86608700	0.46437800	-5.82810300 L
N-N_3	0	-5.15047800	-1.80576300	-5.55570200 L
B-B_2	0	-6.43931100	-0.99899100	-5.38657000 L
B-B_2	0	-7.72429900	-2.99487800	-4.60074200 L
N-N_3	0	-7.72140000	-1.81373300	-5.58166800 L
N-N_3	0	-8.99821500	-3.83110600	-4.47791600 L
B-B_2	0	-10.28661700	-3.01882100	-4.65283200 L
B-B_2	0	-11.50896600	-4.32710300	-3.01327700 L
N-N_3	0	-11.59448000	-3.77862300	-4.42966900 L
N-N_3	0	-12.62460500	-4.06404500	-2.00260300 L
B-	0	12.75200400	4.28899300	-2.75956700 L
N-N_3	0	12.84072400	5.49256400	-1.81985500 L
N-N_3	0	11.58947900	4.45000200	-3.76746300 L
B-B_2	0	10.26494700	4.65333500	-3.01266500 L
B-B_2	0	8.98397300	3.14032100	-4.55084200 L
N-N_3	0	8.98614300	4.50297900	-3.84448400 L
N-N_3	0	7.69534200	2.67831300	-5.23422600 L
B-B_2	0	6.41320400	3.12164100	-4.52899700 L
B-B_2	0	5.12846100	1.14676800	-5.35542300 L
N-N_3	0	5.12725800	2.67161600	-5.22401300 L

N-N_3	0	3.84233000	0.46664700	-5.82754900 L
B-B_2	0	2.55772000	1.14537000	-5.35015200 L
B-B_2	0	1.27309800	-0.99447800	-5.36682100 L
N-N_3	0	1.27269100	0.46540500	-5.82488700 L
N-N_3	0	-0.01100500	-1.80408000	-5.55263300 L
B-B_2	0	-1.29615200	-0.99542500	-5.36860100 L
B-B_2	0	-2.58056200	-2.97935000	-4.57265400 L
N-N_3	0	-2.58086500	-1.80417700	-5.55199400 L
N-N_3	0	-3.86609100	-3.79513200	-4.42993500 L
B-B_2	0	-5.15162700	-2.97930000	-4.57362400 L
B-B_2	0	-6.43889700	-4.51525400	-3.08066200 L
N-N_3	0	-6.43413300	-3.80067800	-4.43684200 L
N-N_3	0	-7.72081300	-5.22941400	-2.64247100 L
B-B_2	0	-9.00682900	-4.53805600	-3.10601500 L
B-B_2	0	-10.28600900	-5.42657300	-1.13428500 L
N-N_3	0	-10.30911900	-5.21039500	-2.64958300 L
N-N_3	0	-11.59323000	-5.80801300	-0.43950400 L
B-	0	-12.86232200	-5.36006400	-1.21107000 L
N-N_3	0	12.84111600	2.60037500	-5.12490500 L
B-B_2	0	11.53974300	3.14825000	-4.56460900 L
B-B_2	0	10.26504700	1.16477800	-5.37880800 L
N-N_3	0	10.25746000	2.70065500	-5.26819100 L
N-N_3	0	8.98633400	0.47121500	-5.86227000 L
B-B_2	0	7.70144800	1.15042000	-5.37467300 L
B-B_2	0	6.41387000	-0.99218400	-5.37426800 L
N-N_3	0	6.41217400	0.46745900	-5.83607600 L
N-N_3	0	5.12820200	-1.80155800	-5.55142300 L
B-B_2	0	3.84318900	-0.99283900	-5.36798200 L
B-B_2	0	2.55849200	-2.97848900	-4.57134000 L
N-N_3	0	2.55839800	-1.80252500	-5.54999000 L
N-N_3	0	1.27475400	-3.79846500	-4.43401300 L
B-B_2	0	-0.01067700	-2.98237800	-4.57644900 L
B-B_2	0	-1.29543100	-4.50481800	-3.07649100 L
N-N_3	0	-1.29621100	-3.79822100	-4.43351200 L
N-N_3	0	-2.58097800	-5.20132900	-2.62864300 L
B-B_2	0	-3.86617500	-4.50214700	-3.07341700 L
B-B_2	0	-5.15117000	-5.33720700	-1.10501200 L
N-N_3	0	-5.15014000	-5.20488200	-2.62953900 L
N-N_3	0	-6.43307900	-5.82268800	-0.42730600 L
B-B_2	0	-7.72362700	-5.37038400	-1.11361300 L
B-B_2	0	-9.00672700	-5.40292400	1.03375900 L
N-N_3	0	-8.99729300	-5.87522900	-0.43547800 L
N-N_3	0	-10.30939600	-5.55396800	1.83185200 L
B-B_2	0	-11.50961600	-5.19116300	0.94857900 L

B-	0	-12.86341600	-4.63312600	2.94832500 L
N-N_3	0	-12.62248600	-4.28362100	1.47107700 L
B-	0	12.75094400	1.08477200	-4.94011300 L
B-B_2	0	11.54016900	-0.99702600	-5.41802400 L
N-N_3	0	11.58968700	0.48822600	-5.76982000 L
N-N_3	0	10.25820800	-1.81057000	-5.60262600 L
B-B_2	0	8.98453000	-0.99342900	-5.40326300 L
B-B_2	0	7.70246800	-2.98670000	-4.58707200 L
N-N_3	0	7.69617500	-1.80306700	-5.56324900 L
N-N_3	0	6.41359900	-3.79700700	-4.43365500 L
B-B_2	0	5.12950200	-2.97733800	-4.57200000 L
B-B_2	0	3.84413300	-4.50291800	-3.07381900 L
N-N_3	0	3.84419400	-3.79407800	-4.42960700 L
N-N_3	0	2.55964300	-5.20484800	-2.63065900 L
B-B_2	0	1.27410900	-4.50736300	-3.07794400 L
B-B_2	0	-0.01055200	-5.33275000	-1.10589700 L
N-N_3	0	-0.01107300	-5.20475100	-2.63071100 L
N-N_3	0	-1.29560700	-5.80754300	-0.42643500 L
B-B_2	0	-2.58042500	-5.33053600	-1.10442300 L
B-B_2	0	-3.86553800	-5.35227800	1.03397700 L
N-N_3	0	-3.86474200	-5.80926300	-0.42596800 L
N-N_3	0	-5.14989200	-5.53692600	1.84404400 L
B-B_2	0	-6.43843900	-5.36841000	1.03676400 L
B-B_2	0	-7.72432900	-4.57828800	3.02960100 L
N-N_3	0	-7.72095000	-5.56231100	1.85116700 L
N-N_3	0	-8.99866100	-4.45225200	3.86464500 L
B-B_2	0	-10.28687800	-4.63066200	3.05271800 L
B-B_2	0	-11.50952600	-2.98589600	4.35365300 L
N-N_3	0	-11.59481600	-4.40473400	3.81148100 L
N-N_3	0	-12.62173300	-1.97423400	4.08034300 L
B-	0	12.75184700	-2.72628500	-4.23144000 L
N-N_3	0	12.84173000	-1.78026800	-5.42989200 L
N-N_3	0	11.59068700	-3.73426900	-4.40019600 L
B-B_2	0	10.26598600	-2.97875700	-4.59942800 L
B-B_2	0	8.98546800	-4.52566600	-3.09526100 L
N-N_3	0	8.98749800	-3.81176300	-4.45391600 L
N-N_3	0	7.69716700	-5.21171000	-2.63655800 L
B-B_2	0	6.41490300	-4.50491700	-3.07637800 L
B-B_2	0	5.12996200	-5.33900900	-1.10592300 L
N-N_3	0	5.12934900	-5.20302700	-2.63007100 L
N-N_3	0	3.84384800	-5.81302500	-0.42702600 L
B-B_2	0	2.55901400	-5.33658200	-1.10622900 L
B-B_2	0	1.27404100	-5.35476200	1.03297000 L
N-N_3	0	1.27359900	-5.81162200	-0.42735200 L

N-N_3	0	-0.01090600	-5.53547100	1.84244800 L
B-B_2	0	-1.29534700	-5.35081800	1.03353600 L
B-B_2	0	-2.58073400	-4.55421400	3.01701800 L
N-N_3	0	-2.58030500	-5.53442700	1.84257300 L
N-N_3	0	-3.86651600	-4.40676900	3.83187900 L
B-B_2	0	-5.15146900	-4.55257200	3.01566500 L
B-B_2	0	-6.43949100	-3.05231500	4.54392000 L
N-N_3	0	-6.43461200	-4.41178600	3.83548800 L
N-N_3	0	-7.72173600	-2.61079000	5.25562300 L
B-B_2	0	-9.00755300	-3.07737400	4.56585500 L
B-B_2	0	-10.28722700	-1.10204500	5.44579800 L
N-N_3	0	-10.31009900	-2.61823200	5.23581600 L
N-N_3	0	-11.59533000	-0.40630100	5.82320200 L
B-	0	-12.86383800	-1.17712600	5.37208200 L
N-N_3	0	12.84232300	-5.10466400	-2.55994400 L
B-B_2	0	11.54124000	-4.54028500	-3.10396500 L
B-B_2	0	10.26692800	-5.36000100	-1.12345400 L
N-N_3	0	10.25889700	-5.24491400	-2.65891700 L
N-N_3	0	8.98823800	-5.84439000	-0.43051700 L
B-B_2	0	7.70311700	-5.35685200	-1.10927400 L
B-B_2	0	6.41517600	-5.35634200	1.03178800 L
N-N_3	0	6.41392800	-5.81970800	-0.42710700 L
N-N_3	0	5.12950600	-5.53225800	1.84123500 L
B-B_2	0	3.84403200	-5.35235600	1.03192800 L
B-B_2	0	2.55940400	-4.55086500	3.01357400 L
N-N_3	0	2.55957200	-5.53467300	1.84182900 L
N-N_3	0	1.27492900	-4.40616200	3.83079400 L
B-B_2	0	-0.01074700	-4.55411900	3.01614300 L
B-B_2	0	-1.29596300	-3.04670400	4.53045500 L
N-N_3	0	-1.29561600	-4.40853300	3.83301000 L
N-N_3	0	-2.58104400	-2.59666300	5.22695600 L
B-B_2	0	-3.86662500	-3.04589000	4.53116900 L
B-B_2	0	-5.15222200	-1.07273800	5.35771200 L
N-N_3	0	-5.15079000	-2.59799900	5.23162000 L
N-N_3	0	-6.43432500	-0.39354300	5.84107100 L
B-B_2	0	-7.72486100	-1.08131800	5.39088600 L
B-B_2	0	-9.00812300	1.06695100	5.42088500 L
N-N_3	0	-8.99876000	-0.40212100	5.89407500 L
N-N_3	0	-10.31081300	1.86452600	5.57300000 L
B-B_2	0	-11.50980900	0.98154100	5.20623500 L
B-	0	-12.86522000	2.98269500	4.65684500 L
N-N_3	0	-12.62349000	1.50695400	4.30134800 L
B-	0	12.75434400	-4.92419500	-1.04365500 L
B-B_2	0	11.54202400	-5.39976600	1.03772400 L

N-N_3	0	11.59156900	-5.75235900	-0.44745200 L
N-N_3	0	10.25960200	-5.58024400	1.85135700 L
B-B_2	0	8.98603900	-5.38379800	1.03345200 L
B-B_2	0	7.70342300	-4.56023000	3.02221400 L
N-N_3	0	7.69765500	-5.54194300	1.84328600 L
N-N_3	0	6.41452700	-4.40350700	3.83158000 L
B-B_2	0	5.13028800	-4.54793500	3.01279500 L
B-B_2	0	3.84430300	-3.04143500	4.52776300 L
N-N_3	0	3.84502800	-4.40241200	3.82860300 L
N-N_3	0	2.55904300	-2.59411900	5.22520000 L
B-B_2	0	1.27412900	-3.04438500	4.52843700 L
B-B_2	0	-0.01159000	-1.07075100	5.34871900 L
N-N_3	0	-0.01079200	-2.59576200	5.22575200 L
N-N_3	0	-1.29651000	-0.39122500	5.82387800 L
B-B_2	0	-2.58148600	-1.07168900	5.35042400 L
B-B_2	0	-3.86751500	1.06750100	5.36761500 L
N-N_3	0	-3.86592700	-0.39187800	5.82740900 L
N-N_3	0	-5.15164200	1.87763700	5.55321500 L
B-B_2	0	-6.44013400	1.07021800	5.38509100 L
B-B_2	0	-7.72644400	3.06624800	4.60046300 L
N-N_3	0	-7.72244700	1.88445900	5.58077100 L
N-N_3	0	-9.00098300	3.90167500	4.47884500 L
B-B_2	0	-10.28878000	3.08843500	4.65389800 L
B-B_2	0	-11.51275000	4.39629500	3.01557800 L
N-N_3	0	-11.59712700	3.84763300	4.43191000 L
N-N_3	0	-12.62702400	4.12967700	2.00438100 L
B-	0	12.75414700	-4.20594800	2.76096100 L
N-N_3	0	12.84310600	-5.40980000	1.82164000 L
N-N_3	0	11.59171200	-4.36693700	3.76895600 L
B-B_2	0	10.26717200	-4.57111800	3.01437500 L
B-B_2	0	8.98565500	-3.05877000	4.55270300 L
N-N_3	0	8.98849500	-4.42145300	3.84640800 L
N-N_3	0	7.69691800	-2.59758900	5.23637500 L
B-B_2	0	6.41499300	-3.04200600	4.53150100 L
B-B_2	0	5.12897400	-1.06800700	5.35672200 L
N-N_3	0	5.12890700	-2.59287800	5.22658400 L
N-N_3	0	3.84224900	-0.38875800	5.82812600 L
B-B_2	0	2.55827400	-1.06930000	5.35096300 L
B-B_2	0	1.27238100	1.06915000	5.36471600 L
N-N_3	0	1.27262200	-0.39010900	5.82453400 L
N-N_3	0	-0.01291600	1.87753700	5.54677900 L
B-B_2	0	-1.29728400	1.06784100	5.36373700 L
B-B_2	0	-2.58318200	3.05207300	4.56807100 L
N-N_3	0	-2.58219600	1.87654900	5.54733000 L

N-N_3	0	-3.86861000	3.86895200	4.42885100 L
B-B_2	0	-5.15386100	3.05231100	4.57203600 L
B-B_2	0	-6.44244200	4.59075900	3.08212100 L
N-N_3	0	-6.43685100	3.87324300	4.43694400 L
N-N_3	0	-7.72554600	5.30325100	2.64454100 L
B-B_2	0	-9.01062100	4.60973500	3.10752300 L
N-N_3	0	-10.31382000	5.28062100	2.65138700 L
N-N_3	0	12.84257200	-2.51590100	5.12523300 L
B-B_2	0	11.54136400	-3.06484900	4.56555000 L
B-B_2	0	10.26553500	-1.08225800	5.38029700 L
N-N_3	0	10.25902800	-2.61815200	5.26964100 L
N-N_3	0	8.98635700	-0.38948900	5.86374600 L
B-B_2	0	7.70196100	-1.06965100	5.37622400 L
B-B_2	0	6.41296500	1.07215200	5.37490500 L
N-N_3	0	6.41214700	-0.38738800	5.83716200 L
N-N_3	0	5.12665900	1.88060400	5.55162100 L
B-B_2	0	3.84231700	1.07057300	5.36793600 L
B-B_2	0	2.55672000	3.05470100	4.56936200 L
N-N_3	0	2.55667400	1.87902000	5.54860300 L
N-N_3	0	1.27138200	3.87180000	4.42914000 L
B-B_2	0	-0.01325500	3.05355500	4.56808200 L
B-B_2	0	-1.29892700	4.58269100	3.07446100 L
N-N_3	0	-1.29866600	3.87049000	4.42861300 L
N-N_3	0	-2.58459100	5.28294700	2.63164300 L
B-B_2	0	-3.86963400	4.58146300	3.07472300 L
N-N_3	0	-5.15463900	5.28357100	2.63246200 L
B-	0	12.75107000	-1.00031400	4.94087200 L
B-B_2	0	11.53932300	1.08046200	5.42040200 L
N-N_3	0	11.58975100	-0.40495700	5.77133000 L
N-N_3	0	10.25671400	1.89309400	5.60452600 L
B-B_2	0	8.98365700	1.07513700	5.40464500 L
B-B_2	0	7.70052400	3.06791500	4.58830700 L
N-N_3	0	7.69468600	1.88394600	5.56417500 L
N-N_3	0	6.41121600	3.87766400	4.43498500 L
B-B_2	0	5.12751400	3.05705200	4.57268000 L
B-B_2	0	3.84169800	4.58416200	3.07525100 L
N-N_3	0	3.84142100	3.87274900	4.43004200 L
N-N_3	0	2.55651600	5.28539600	2.63220900 L
B-B_2	0	1.27135600	4.58402100	3.07487900 L
N-N_3	0	-0.01408400	5.28488600	2.63203800 L
B-	0	12.75050900	2.81045700	4.23465900 L
N-N_3	0	12.84031900	1.86457000	5.43320200 L
N-N_3	0	11.58849000	3.81762100	4.40256100 L
B-B_2	0	10.26414200	3.06133800	4.60140200 L

B-B_2	0	8.98315000	4.60787000	3.09710400 L
N-N_3	0	8.98521200	3.89365300	4.45560200 L
N-N_3	0	7.69477200	5.29385500	2.63856000 L
B-B_2	0	6.41246100	4.58691500	3.07824200 L
N-N_3	0	5.12684000	5.28544800	2.63253200 L
N-N_3	0	12.83996400	5.18756800	2.56182300 L
B-B_2	0	11.53896700	4.62310600	3.10601800 L
N-N_3	0	10.25649400	5.32736500	2.66080400 L
H-H_	0	-12.28828400	3.36390700	-1.41290600 L
H-H_	0	-12.28292700	1.38517200	-3.34121700 L
H-H_	0	-12.28221900	-1.38387100	-3.31197200 L
H-H_	0	-12.28993500	-3.32657500	-1.34194300 L
H-H_	0	12.86069300	6.36290900	-2.39842400 L
H-H_	0	12.86295000	2.80783900	-6.14917300 L
H-H_	0	-12.28389500	-3.29653100	1.41298300 L
H-H_	0	-12.28202900	-1.31713200	3.34196500 L
H-H_	0	12.86381600	-2.35422400	-6.30323600 L
H-H_	0	12.86185900	-6.12836400	-2.77041000 L
H-H_	0	-12.28531900	1.45305600	3.31387400 L
H-H_	0	-12.29003900	3.39273800	1.34429700 L
H-H_	0	12.86323100	-6.27996100	2.40047800 L
H-H_	0	12.86518400	-2.72359700	6.14943600 L
H-H_	0	12.86137300	2.43858400	6.30653300 L
H-H_	0	12.85936100	6.21131500	2.77207600 L
C-C_R	0	-0.44871600	-1.53759700	-0.14056300 H
H-H_	0	-1.74694400	-0.21543000	-1.28946100 H
H-H_	0	-2.15445100	-1.93459200	-1.43984900 H
C-C_3	0	-1.31542000	-1.23129600	-1.31091700 H
H-H_	0	-0.70440900	-1.29301900	-2.21419000 H
N-N_R	0	-1.00491200	-1.45621900	1.22938900 H
H-H_	0	-1.35902400	-0.53143400	1.50129400 H
H-H_	0	-1.73425000	-2.14387400	1.43880300 H
C-C_R	0	0.90751100	-1.77975500	-0.01436500 H
O-O_R	0	1.47537500	-1.93460000	1.11657000 H
O-O_R	0	1.65634700	-1.85546900	-1.15874100 H
H-H_	0	2.55446500	-2.06640400	-0.86207000 H
H-H_	0	-0.11247300	-1.67422200	1.77245200 H