

Supporting information

Covalent functionalization of single-walled carbon nanotubes by Bingel reaction for building charge-transfer complexes

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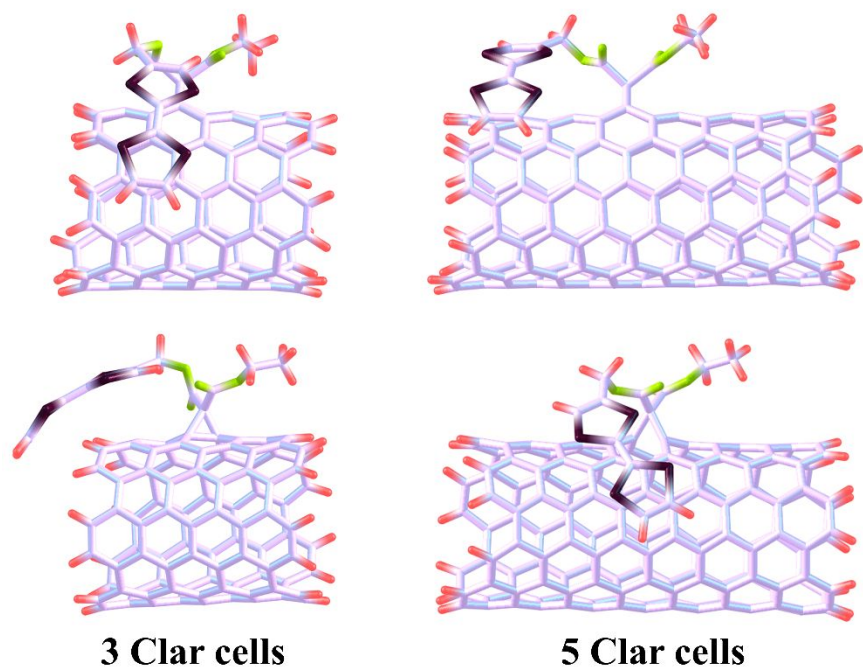


Figure S1. Optimized structures of (6,5)-SWCNT-TTF complex using 3 and 5 Clar cells models of nanotube.

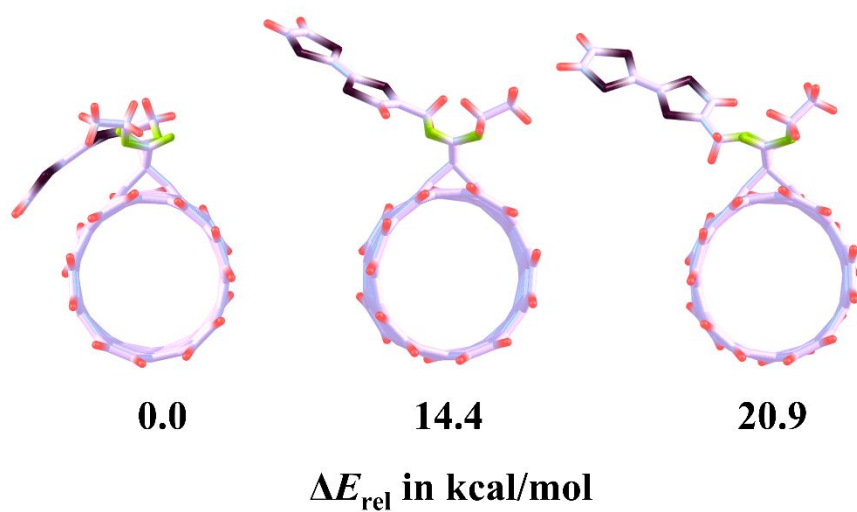


Figure S2. Different orientations of TTF molecule with respect to the nanotube.

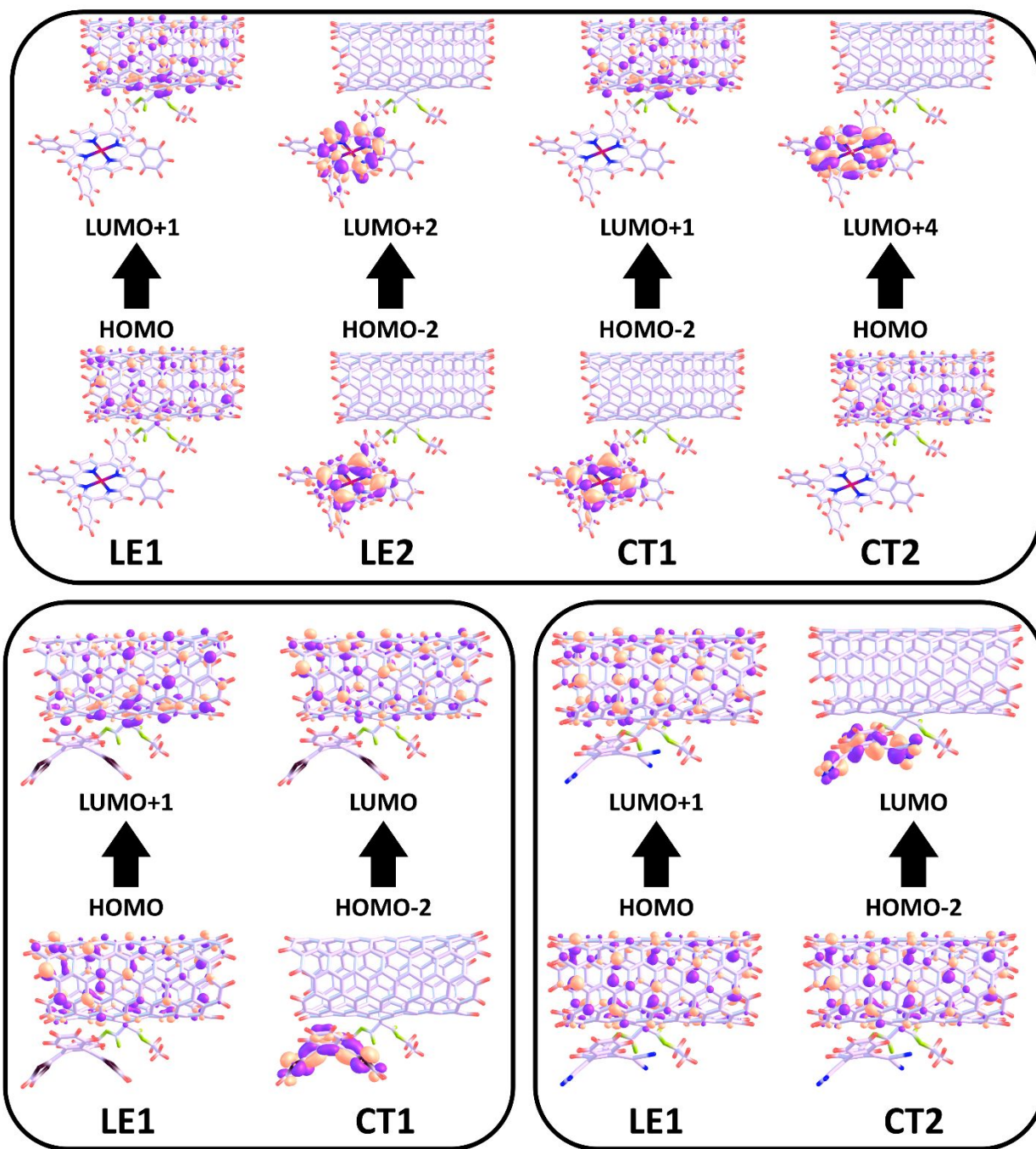


Figure S3. Frontier molecular orbitals representing lowest-lying singlet LE and CT excited states for (6,5)-SWCNT-ZnTPP (top), (6,5)-SWCNT-exTTF (bottom left) and (6,5)-SWCNT-TCAQ (bottom right) complexes.

Table S1. Characteristics of SWCNT-partner complexes.

(6,5)-SWCNT+partner	$d(C_\alpha-C_\beta)$, Å	$d(C_\alpha-C_\beta)$, Å	ΔE_{rel} , kcal/mol	ΔE_{rel} , kcal/mol
	<i>obl</i>	<i>per</i>	<i>obl</i>	<i>per</i>
-TTF	1.57	2.20	17.4	0.0
-exTTF	1.58	2.19	12.8	0.0
-TCAQ	1.57	2.22	11.3	0.0
-AQ	1.57	2.22	12.4	0.0
-ZnTPP	1.57	2.19	22.5	0.0

Table S2. Excitation energies (E_x , eV) and dipole moments in ground and selected excited states (μ_0 , D), change in dipole moments between ground state and state of interest ($\Delta\mu = \mu_i - \mu_0$, D) and solvation energies (E_{solv} , eV) calculated in DCM.

<i>(6,5)-SWCNT – Partner</i>					
	TTF	exTTF	ZnTPP	AQ	TCAQ
Ground state (GS)					
E_x	0.000	0.000	0.000	0.000	0.000
μ_0	4.913	4.229	1.584	0.583	4.225
E_{solv}	-0.455	-0.508	-0.487	-0.413	-0.474
LE_1 ((6,5)-SWCNT)					
E_x	1.747	1.751	1.746	1.759	1.922
$\Delta\mu$	0.63	0.90	0.65	0.86	2.96
E_{solv}	-0.464	-0.514	-0.501	-0.426	-0.484
Most absorptive transition ((6,5)-SWCNT)					
E_x	2.778	2.777	2.774	2.778	2.798
$\Delta\mu$	0.55	1.28	3.39	3.40	5.00
E_{solv}	-0.474	-0.525	-0.505	-0.445	-0.499
CT1 (Partner $\rightarrow$ (6,5)-SWCNT)					
E_x	2.228*	1.802	1.644		
$\Delta\mu$	13.60	33.85	59.31	n/a	n/a
E_{solv}	-0.769	-0.968	-1.269		
CT2 ((6,5)-SWCNT $\rightarrow$ Partner)					
E_x			1.937	2.094	0.963
$\Delta\mu$	n/a	n/a	62.34	13.82	26.01
E_{solv}			-1.010	-0.657	-1.109

Table S3. Energies of HOMO and LUMO for (6,5)-SWCNT–TCAQ complex at the CAM-B3LYP/def2SVP level of theory.

(6,5)-SWCNT – TCAQ	Empirical formula of SWCNT	HOMO, eV	LUMO, eV	Δ [HOMO-LUMO], eV
5 Clar cells	C ₁₆₀ H ₂₂	-5.63	-2.88	2.75
7 Clar cells	C ₂₂₄ H ₂₂	-5.59	-2.95	2.64
9 Clar cells	C ₂₈₈ H ₂₂	-5.57	-2.97	2.60
11 Clar cells	C ₃₅₂ H ₂₂	-5.54	-2.98	2.56

Methodology for investigation of charge-transfer complexes

The geometry optimization for all complexes was performed employing the DFT BLYP [S1,2] exchange-correlation functional. Vertical excitation energies were calculated using TDA formalism [S3] with the range-separated functional from Handy and coworkers' CAM-B3LYP [S4] and Ahlrichs' Def2-SVP basis set [S5,6], using Gaussian 16 (rev. A03) [S7]. The empirical dispersion D3 correction with Becke-Johnson damping [S8,9] was employed. All resulted structures were visualized with Chemcraft 1.8 [S10].

Analysis of excited states

The quantitative analysis of exciton delocalization and charge transfer in the donor-acceptor complexes was carried out using a tool suggested recently by Plasser *et al.* [S11,12]. A key quantity is the parameter Ω :

$$\Omega(A, B) = \frac{1}{2} \sum_{\alpha \in A, \beta \in B} \left[\left(SP^{0i} \right)_{\alpha\beta} \left(P^{0i} S \right)_{\alpha\beta} + P_{\alpha\beta}^{0i} \left(SP^{0i} S \right)_{\alpha\beta} \right] \quad (S1)$$

$$X(F_i) = \sum_{A \in F_i} \Omega(A, A) \quad (S2)$$

$$\Delta q(CT^{F_i \rightarrow F_j}) = \sum_{A \in F_i, B \in F_j} \Omega(A, B) + \Omega(B, A) \quad (S3)$$

$$\Delta q(CS^{F_i \rightarrow F_j}) = \sum_{A \in F_i, B \in F_j} \Omega(A, B) - \Omega(B, A) \quad (S4)$$

where A and B are atoms, F_i and F_j are fragments, α and β are atomic orbitals, $\mathbf{P}^{0i}$ is the transition density matrix for the $\psi_0 \rightarrow \psi_i$ excitation, and S is the overlap matrix. $X(F_i)$ is the extent of exciton localization on the fragment F_i . $\Delta q(CT^{F_i \rightarrow F_j})$ is the total amount of the electron density transferred between fragments F_i and F_j in the $\psi_0 \rightarrow \psi_i$ excitation. $\Delta q(CS^{F_i \rightarrow F_j})$ is a measure of the charge separation between fragments F_i and F_j . Note that in the situation when charge transfer ($F_i \rightarrow F_j$) is equal to the back transfer ($F_j \rightarrow F_i$) there is no charge separation between the fragments and $CS^{F_i \rightarrow F_j}$ is equal to zero.

Solvent Effects

The equilibrium solvation energy E_s^{eq} in a medium with dielectric constant ϵ was estimated using a COSMO-like polarizable continuum model (CPCM) in the monopole approximation [S13].

$$E_s^{\text{eq}}(\mathbf{Q}, \epsilon) = -\frac{1}{2} f(\epsilon) \mathbf{Q}^+ \mathbf{D} \mathbf{Q} \quad (\text{S5})$$

where $f(\epsilon)$ is the dielectric scaling factor, $f(\epsilon) = (\epsilon - 1)/\epsilon$, $\mathbf{Q}$ is the vector of n atomic charges in the molecular system, and $\mathbf{D}$ is the $n \times n$ symmetric matrix determined by the shape of the boundary surface between solute and solvent; $\mathbf{D} = \mathbf{B}^+ \mathbf{A}^{-1} \mathbf{B}$, where the $m \times m$ matrix $\mathbf{A}$ describes electrostatic interaction between m surface charges and the $m \times n$ $\mathbf{B}$ matrix describes the interaction of the surface charges with n atomic charges of the solute. Atomic charges in the excited state ψ_i , were calculated using Eqs. 1-4.

Electron transfer (ET) rates

The rate of the nonadiabatic ET, k_{ET} , can be expressed in terms of the electronic coupling squared, V^2 , and the Franck-Condon Weighted Density of states (FCWD):

$$k_{\text{ET}} = \frac{2\pi}{\hbar^2} V^2 (\text{FCWD}) \quad (\text{S6})$$

that accounts for the overlap of vibrational states of donor and acceptor and can be approximately estimated using the classical Marcus equation:[S14]

$$(\text{FCWD}) = (4\pi\lambda kT)^{-1/2} \cdot \exp\left[-(\Delta G^0 + \lambda)^2 / 4\lambda kT\right] \quad (\text{S7})$$

where λ is the reorganization energy and ΔG^0 is the standard Gibbs energy change of the process. The fragment charge difference (FCD) method [S15,16] was employed to calculate the electronic couplings in this work.

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Cartesian coordinates for stationary points (Int, TS, PC) at the BP86-D3(BJ)/DZP level

(6,5)-SWCNT pristine 3 cells				65 obl: Int_a			
118				134			
pristine65 -21559.7229				Int_alpha_obl -23816.4145			
C	5.364111	1.565460	2.898945	C	-2.655461	-5.194167	3.040988
C	4.310124	2.280389	2.252767	C	-1.644749	-4.198693	3.198250
C	2.984494	2.028783	2.711145	C	-2.078953	-2.843437	3.253017
C	2.712341	0.839534	3.448303	C	-3.378253	-2.498780	2.774316
C	3.765586	-0.087788	3.682280	C	-4.198752	-3.511188	2.204712
C	5.099551	0.409730	3.586830	C	-3.893209	-4.860828	2.550599
C	3.460875	-1.486766	3.605532	C	-4.989808	-3.170500	1.055173
C	2.115409	-1.875910	3.356098	C	-4.954154	-1.829077	0.582055
C	1.050583	-0.953194	3.594304	C	-4.511561	-0.778828	1.446302
C	1.353482	0.430030	3.616703	C	-3.686273	-1.120488	2.546324
C	4.471754	-2.466384	3.372756	C	-5.460758	-4.164257	0.146805
C	4.222149	-3.542561	2.559487	C	-5.465247	-3.926667	-1.205270
C	2.944595	-3.710079	1.948455	C	-5.010352	-2.678082	-1.723950
C	1.853252	-3.010372	2.533069	C	-4.983611	-1.577349	-0.822438
C	0.530197	-3.203090	2.028163	C	-4.622135	-0.276547	-1.295033
C	0.367854	-3.740356	0.728652	C	-3.901719	-0.171463	-2.509324
C	1.536851	-4.027046	-0.040652	C	-3.533928	-1.373040	-3.190340
C	2.789393	-4.207663	0.610682	C	-4.242782	-2.580649	-2.934032
C	-0.565858	-2.524117	2.632269	C	-4.629189	0.831516	-0.399750
C	-1.883268	-2.733907	2.136020	C	-4.276316	2.124731	-0.880424
C	-2.052055	-3.311634	0.853915	C	-3.589270	2.238548	-2.114733
C	-0.896667	-3.623454	0.083170	C	-3.229926	1.049412	-2.812265
C	-2.984494	-2.028783	2.711145	C	-4.235614	3.235452	0.018503
C	-4.310124	-2.280389	2.252767	C	-3.939778	4.540769	-0.473596
C	-4.487708	-2.903656	0.977230	C	-3.284491	4.663947	-1.739429
C	-3.324133	-3.206061	0.213625	C	-2.927849	3.466558	-2.424089
C	-3.363903	-3.050874	-1.198440	C	-1.697697	3.416010	-3.136816
C	-4.574543	-2.627671	-1.826762	C	-0.859131	4.572453	-3.182209
C	-5.788043	-2.759794	-1.076181	C	-1.459294	5.832800	-2.852870
C	-5.741444	-2.883021	0.285645	C	-2.628823	5.872071	-2.143446
C	-2.712341	-0.839534	3.448303	C	-4.104985	2.967843	1.413727
C	-3.765586	0.087788	3.682280	C	-3.652020	4.002830	2.278593
C	-5.099551	-0.409730	3.586830	C	-3.805810	5.343763	1.815412
C	-5.364111	-1.565460	2.898945	C	-3.956839	5.606788	0.477946
C	-0.935881	-3.419061	-1.321992	C	-1.984580	1.001169	-3.488098
C	-2.144048	-2.952434	-1.919928	C	-1.142522	2.152004	-3.474187
C	1.502568	-3.776201	-1.444320	C	-2.259095	-1.427805	-3.830537
C	0.290087	-3.296106	-2.028960	C	-1.421714	-0.268498	-3.796540
C	0.364231	-2.374390	-3.102208	C	-0.021904	-0.435938	-3.702977
C	-0.796602	-1.636457	-3.468689	C	0.800419	0.672218	-3.329426
C	-2.080457	-2.070825	-3.032822	C	0.269425	1.994126	-3.436878
C	3.909272	-4.516349	-0.214449	C	-3.842736	-3.735009	-3.669182
C	3.879762	-4.249471	-1.561359	C	-2.609432	-3.790236	-4.270777
C	2.724542	-3.674499	-2.163626	C	-1.705903	-2.690815	-4.179309
C	2.807933	-2.701636	-3.219705	C	-0.285686	-2.866365	-4.048846
C	1.653655	-1.925036	-3.519401	C	0.495250	-1.761441	-3.604620

C	-0.299554	-1.363928	3.409159	C	-4.541219	0.571778	0.996223
C	-1.353482	-0.430030	3.616703	C	-4.064782	1.606526	1.850468
C	-1.050583	0.953194	3.594304	C	-3.201320	1.261359	2.920258
C	0.299554	1.363928	3.409159	C	-2.883063	-0.107688	3.139646
C	0.565858	2.524117	2.632269	C	-1.564489	-0.447375	3.555310
C	1.883268	2.733907	2.136020	C	-1.123581	-1.794810	3.424699
C	-0.647482	-0.286931	-3.885631	C	1.959086	0.454692	-2.553543
C	0.647482	0.286931	-3.885631	C	2.215881	-0.864105	-2.074720
C	1.803265	-0.557273	-3.897560	C	1.618650	-1.984224	-2.756443
C	3.103036	0.012917	-3.935113	C	1.927257	-3.307858	-2.358198
C	4.196575	-0.888543	-4.045848	C	1.395191	-4.368862	-3.145615
C	4.053352	-2.212669	-3.702898	C	0.317387	-4.154460	-3.969726
C	0.796602	1.636457	-3.468689	C	2.800239	-1.065941	-0.824961
C	-0.364231	2.374390	-3.102208	C	3.411268	0.049973	-0.011597
C	-1.653655	1.925036	-3.519401	C	3.218954	1.408156	-0.651936
C	-1.803265	0.557273	-3.897560	C	2.575396	1.573525	-1.900392
C	-2.807933	2.701636	-3.219705	C	3.485585	2.551976	0.128997
C	-4.053352	2.212669	-3.702898	C	3.587712	3.793584	-0.549248
C	-4.196575	0.888543	-4.045848	C	3.035402	3.954461	-1.798477
C	-3.103036	-0.012917	-3.935113	C	2.317843	2.889534	-2.394150
C	-3.460875	1.486766	3.605532	C	-2.729370	3.652815	3.321468
C	-2.115409	1.875910	3.356098	C	-2.370729	2.284405	3.477236
C	-1.853252	3.010372	2.533069	C	-1.035539	1.943491	3.846870
C	-2.944595	3.710079	1.948455	C	-0.073474	2.974711	4.022727
C	-4.222149	3.542561	2.559487	C	-0.574724	4.287598	4.250776
C	-4.471754	2.466384	3.372756	C	-1.867883	4.617574	3.921735
C	-0.530197	3.203090	2.028163	C	-0.606892	0.589371	3.695564
C	-0.290087	3.296106	-2.028960	C	2.758017	0.074561	1.360680
C	-1.502568	3.776201	-1.444320	C	2.593903	1.315198	2.036034
C	-2.724542	3.674499	-2.163626	C	3.218977	2.501927	1.553498
C	0.935881	3.419061	-1.321992	C	2.118583	-1.073361	1.848450
C	2.144048	2.952434	-1.919928	C	2.245793	-2.340038	1.173797
C	2.080457	2.070825	-3.032822	C	2.595076	-2.325068	-0.203317
C	-1.536851	4.027046	-0.040652	C	1.594645	1.445329	3.048597
C	-2.789393	4.207663	0.610682	C	1.282266	2.727147	3.599009
C	-3.909272	4.516349	-0.214449	C	2.212742	3.770407	3.373251
C	-3.879762	4.249471	-1.561359	C	3.142459	3.658660	2.352910
C	0.896667	3.623454	0.083170	C	1.095081	-0.952245	2.833919
C	-0.367854	3.740356	0.728652	C	0.733051	0.339598	3.299661
C	2.052055	3.311634	0.853915	C	0.228490	-2.052633	3.091867
C	3.324133	3.206061	0.213625	C	0.599279	-3.368645	2.677994
C	3.363903	3.050874	-1.198440	C	1.638871	-3.497945	1.706684
C	4.487708	2.903656	0.977230	C	-0.262793	-4.468078	2.928330
C	5.741444	2.883021	0.285645	C	0.186752	-5.771227	2.526535
C	5.788043	2.759794	-1.076181	C	1.178930	-5.905203	1.596369
C	4.574543	2.627671	-1.826762	C	1.774661	-4.740766	1.006692
C	-4.502920	-1.832107	-2.977089	C	0.529602	4.405617	-3.241595
C	-3.261345	-1.367803	-3.445902	C	1.099954	3.121514	-3.146056
C	3.261345	1.367803	-3.445902	C	2.367470	-3.496161	-0.995862
C	4.502920	1.832107	-2.977089	C	2.178227	-4.721335	-0.330595
H	-5.489937	2.292200	3.718717	H	-2.174864	5.661448	3.979090

H	-5.932084	0.192005	3.950070	H	-3.670911	6.176282	2.505866
H	-6.400985	-1.854708	2.732212	H	-3.938623	6.641685	0.137454
H	-6.670293	-2.844584	0.853799	H	-2.996582	6.831831	-1.780721
H	-5.193812	0.510586	-4.269658	H	3.014060	4.949521	-2.242278
H	-5.426335	-1.378353	-3.334863	H	1.148476	5.290828	-3.100268
H	-4.940744	2.843400	-3.664710	H	3.973317	4.668302	-0.025880
H	-4.796628	4.360489	-2.139551	H	3.726286	4.540453	2.086448
H	-4.849052	4.830720	0.237834	H	2.098802	4.729435	3.876768
H	-5.047885	4.197173	2.282498	H	0.104180	5.080565	4.564091
H	-6.745173	-2.623012	-1.582588	H	-0.905659	6.753122	-3.049192
H	4.796628	-4.360489	-2.139551	H	-2.275958	-4.733782	-4.702146
H	4.849052	-4.830720	0.237834	H	-4.452805	-4.637376	-3.638997
H	5.047885	-4.197173	2.282498	H	-5.688256	-4.749134	-1.884449
H	4.940744	-2.843400	-3.664710	H	-0.155444	-5.009712	-4.451938
H	5.193812	-0.510586	-4.269658	H	1.750451	-5.388290	-2.995291
H	5.426335	1.378353	-3.334863	H	2.092875	-5.646599	-0.900312
H	6.745173	2.623012	-1.582588	H	1.428718	-6.890057	1.196270
H	6.670293	2.844584	0.853799	H	-0.345135	-6.657251	2.871858
H	6.400985	1.854708	2.732212	H	-2.408386	-6.246982	3.173119
H	5.932084	-0.192005	3.950070	H	-4.594735	-5.657408	2.303527
H	5.489937	-2.292200	3.718717	H	-5.678514	-5.170213	0.504754
				C	5.069892	-0.299976	0.021170
				C	5.269454	-1.620918	0.768627
				O	5.166230	-1.700234	1.978867
				O	5.503612	-2.667707	-0.042395
				C	5.508103	-3.943179	0.652073
				H	4.570833	-4.064625	1.207875
				H	5.596245	-4.692772	-0.138743
				H	6.357125	-3.990429	1.345476
				C	5.470021	-0.237135	-1.444392
				O	5.325637	-1.158668	-2.226567
				O	5.794096	1.022706	-1.810401
				C	5.760716	1.241770	-3.244063
				H	6.532203	0.641790	-3.741588
				H	4.769434	0.971664	-3.630568
				H	5.947787	2.311774	-3.368457
				Br	6.111283	1.030782	1.091898
65_obl: Int_β				65_obl: TS_α			
134				134			
Int_beta_obl -23817.7217				TS_alpha_obl -23801.8147			
C	1.410442	5.664676	2.825304	C	2.838122	5.248955	2.848867
C	0.818768	4.397469	3.122404	C	1.824672	4.262099	3.035743
C	1.676555	3.260071	3.075570	C	2.254661	2.908011	3.132981
C	2.914390	3.340184	2.370554	C	3.548115	2.544242	2.655158
C	3.248350	4.545876	1.692066	C	4.367268	3.536709	2.051701
C	2.584880	5.735135	2.121481	C	4.072021	4.896421	2.362475
C	3.880372	4.440594	0.409458	C	5.130922	3.163455	0.892211
C	4.191813	3.143943	-0.089904	C	5.077766	1.812041	0.453072
C	4.277855	2.035044	0.809091	C	4.650529	0.784695	1.352978
C	3.605038	2.129634	2.052217	C	3.844811	1.157967	2.457867
C	3.839181	5.505736	-0.540388	C	5.579030	4.132654	-0.051884

C	3.661526	5.237986	-1.874603	C	5.535223	3.863979	-1.398419
C	3.537588	3.894333	-2.336315	C	5.062232	2.606692	-1.871585
C	4.035415	2.871481	-1.482063	C	5.064364	1.528050	-0.944800
C	4.024254	1.509317	-1.917796	C	4.690755	0.216640	-1.375394
C	3.155686	1.140521	-2.974968	C	3.931627	0.083094	-2.564818
C	2.295072	2.139954	-3.528188	C	3.533946	1.269353	-3.257323
C	2.613444	3.518540	-3.370927	C	4.245972	2.483484	-3.050965
C	4.546861	0.488664	-1.072438	C	4.721781	-0.868836	-0.456352
C	4.546005	-0.863188	-1.520836	C	4.362760	-2.172278	-0.896475
C	3.712714	-1.227306	-2.607715	C	3.644745	-2.315403	-2.110480
C	2.874839	-0.237803	-3.193238	C	3.264169	-1.145286	-2.823273
C	5.032276	-1.901240	-0.665768	C	4.341229	-3.261540	0.030273
C	5.086331	-3.245552	-1.134811	C	4.044178	-4.578207	-0.424269
C	4.276698	-3.610641	-2.260224	C	3.364640	-4.734110	-1.677865
C	3.437194	-2.612296	-2.830508	C	2.982711	-3.554294	-2.375853
C	2.149848	-2.982071	-3.312057	C	1.732100	-3.523728	-3.050925
C	1.739524	-4.347019	-3.261476	C	0.900243	-4.683219	-3.048492
C	2.758539	-5.333966	-3.075349	C	1.515528	-5.931982	-2.715237
C	3.984900	-4.974673	-2.580327	C	2.706946	-5.952062	-2.039187
C	5.087945	-1.645663	0.736891	C	4.225925	-2.957617	1.418885
C	5.160143	-2.744444	1.639351	C	3.778966	-3.968271	2.314259
C	5.644795	-3.980309	1.113860	C	3.927707	-5.319150	1.885991
C	5.613256	-4.221815	-0.236064	C	4.067839	-5.617164	0.553217
C	1.567958	-0.612596	-3.613389	C	1.988904	-1.113312	-3.456828
C	1.163149	-1.974546	-3.493709	C	1.157244	-2.267979	-3.387469
C	0.973854	1.760827	-3.912037	C	2.241952	1.303699	-3.861991
C	0.584443	0.393721	-3.771279	C	1.415277	0.140356	-3.782416
C	-0.754777	0.098154	-3.404539	C	0.010614	0.303823	-3.654616
C	-1.089087	-1.205306	-2.954523	C	-0.784569	-0.793440	-3.224905
C	-0.192866	-2.283761	-3.202204	C	-0.251208	-2.113229	-3.294838
C	1.724346	4.457769	-3.968072	C	3.815033	3.618789	-3.792725
C	0.444718	4.090221	-4.313911	C	2.563238	3.653411	-4.362474
C	-0.017191	2.761389	-4.103453	C	1.672404	2.552323	-4.232750
C	-1.374231	2.466004	-3.711372	C	0.247140	2.719904	-4.094714
C	-1.652085	1.176319	-3.163216	C	-0.519814	1.624500	-3.598104
C	4.658117	0.752287	0.320786	C	4.668583	-0.575288	0.938784
C	4.699680	-0.355129	1.215831	C	4.197632	-1.585615	1.822127
C	3.989900	-0.271317	2.438636	C	3.350011	-1.210263	2.895348
C	3.285397	0.928050	2.748639	C	3.043613	0.164387	3.083951
C	2.037059	0.841021	3.414676	C	1.732187	0.522812	3.513960
C	1.162309	1.964694	3.392533	C	1.297579	1.868552	3.343693
C	-2.116230	-1.360196	-1.978841	C	-1.930828	-0.551385	-2.417420
C	-2.781674	-0.232550	-1.483063	C	-2.258640	0.771450	-2.067932
C	-2.651904	1.016361	-2.155753	C	-1.658461	1.865768	-2.772271
C	-3.313205	2.185542	-1.679553	C	-1.972623	3.210350	-2.423011
C	-3.283883	3.332045	-2.494981	C	-1.454718	4.232603	-3.252598
C	-2.348860	3.471684	-3.508078	C	-0.372255	3.994459	-4.075436
C	-3.407869	-0.266611	-0.094332	C	-2.882197	1.050529	-0.799129
C	-2.740001	-1.365588	0.706811	C	-3.331291	-0.089538	0.091054
C	-2.522674	-2.621606	0.080263	C	-3.136261	-1.469052	-0.476780
C	-2.208276	-2.638005	-1.315078	C	-2.497994	-1.674448	-1.704307

C	-2.235337	-3.772964	0.864723	C	-3.440440	-2.559904	0.351001
C	-2.084092	-5.008909	0.172913	C	-3.517847	-3.833704	-0.269155
C	-1.795454	-5.019386	-1.168406	C	-2.949839	-4.044604	-1.504612
C	-1.631016	-3.791790	-1.878334	C	-2.251179	-3.000367	-2.158304
C	4.399684	-2.671396	2.853066	C	2.867852	-3.587712	3.360314
C	3.655559	-1.486511	3.113747	C	2.519720	-2.214515	3.487247
C	2.374393	-1.583770	3.735085	C	1.194747	-1.856208	3.874014
C	1.853118	-2.867610	4.059452	C	0.228141	-2.874639	4.101393
C	2.791276	-3.939035	4.164055	C	0.723808	-4.185405	4.342143
C	4.029730	-3.842118	3.581700	C	2.007958	-4.531710	3.989572
C	1.503546	-0.450262	3.695775	C	0.773280	-0.502447	3.699796
C	-2.123991	-1.149822	1.940946	C	-2.669339	-0.033383	1.458993
C	-1.482197	-2.250484	2.607312	C	-2.502769	-1.242504	2.183153
C	-1.753383	-3.582772	2.199593	C	-3.179073	-2.431936	1.775357
C	-1.887606	0.178238	2.410525	C	-1.976047	1.109695	1.851975
C	-2.530377	1.274580	1.748377	C	-2.106865	2.354724	1.126915
C	-3.212045	1.100638	0.532742	C	-2.540079	2.320599	-0.205380
C	-0.365134	-2.001394	3.456358	C	-1.460963	-1.351934	3.153471
C	0.445193	-3.086737	3.898993	C	-1.143702	-2.618575	3.732889
C	-0.112284	-4.396118	3.797881	C	-2.106120	-3.644429	3.591347
C	-1.178981	-4.637805	2.970347	C	-3.096125	-3.550785	2.625079
C	-0.734450	0.424488	3.185762	C	-0.930688	1.018146	2.815569
C	0.112101	-0.662198	3.569584	C	-0.577050	-0.253699	3.332959
C	-0.233547	1.756704	3.308354	C	-0.053381	2.120345	3.013057
C	-1.075642	2.854672	2.966426	C	-0.424457	3.424622	2.556710
C	-2.247141	2.601712	2.203247	C	-1.482798	3.530750	1.610939
C	-0.596288	4.192178	3.094827	C	0.442841	4.528918	2.762873
C	-1.517891	5.252621	2.818389	C	-0.008240	5.818609	2.323922
C	-2.666460	5.013671	2.115273	C	-1.026412	5.929075	1.419056
C	-2.946713	3.697006	1.619799	C	-1.651260	4.751898	0.887702
C	0.377989	-4.644806	-3.080630	C	-0.493628	-4.522244	-3.054110
C	-0.552497	-3.624458	-2.841605	C	-1.063747	-3.244089	-2.950302
C	-3.538759	2.247986	-0.240881	C	-2.363152	3.457535	-1.044495
C	-3.604018	3.493236	0.401721	C	-2.122938	4.698271	-0.428449
H	4.670978	-4.722877	3.558236	H	2.304264	-5.578008	4.056504
H	5.913313	-4.791430	1.790398	H	3.793480	-6.133685	2.597460
H	5.859516	-5.219492	-0.598657	H	4.040796	-6.660680	0.241123
H	4.696623	-5.755240	-2.312411	H	3.087261	-6.902310	-1.664997
H	-1.548967	-5.965800	-1.648909	H	-2.920855	-5.058022	-1.903588
H	0.115432	-5.682376	-2.877221	H	-1.103014	-5.407406	-2.875741
H	-2.052648	-5.946318	0.728186	H	-3.914747	-4.683387	0.284952
H	-1.501243	-5.666188	2.807633	H	-3.716707	-4.424977	2.428559
H	0.388622	-5.239369	4.272817	H	-1.990240	-4.585170	4.128420
H	2.482304	-4.892752	4.591271	H	0.045764	-4.968455	4.680579
H	2.506172	-6.389176	-3.197888	H	0.960372	-6.858562	-2.873642
H	-0.255573	4.865121	-4.625359	H	2.211639	4.589530	-4.795369
H	1.996813	5.511758	-4.013775	H	4.413672	4.529070	-3.791047
H	3.481225	6.066799	-2.559068	H	5.735057	4.670968	-2.102906
H	-2.268866	4.430124	-4.019365	H	0.091018	4.837585	-4.586945
H	-3.903452	4.193029	-2.241457	H	-1.806156	5.257460	-3.133321
H	-3.937888	4.373184	-0.147606	H	-2.061126	5.605456	-1.028828

H	-3.305126	5.843829	1.806727	H	-1.284919	6.902807	0.998417
H	-1.251368	6.279103	3.069710	H	0.537051	6.712763	2.624133
H	0.861557	6.583574	3.029104	H	2.596003	6.305798	2.954287
H	2.939043	6.708071	1.780900	H	4.776373	5.682111	2.090097
H	3.792496	6.539361	-0.198691	H	5.809246	5.146282	0.274590
C	-5.036674	-0.618725	-0.069436	C	-4.652317	0.579836	-0.232017
C	-5.438677	-0.298750	1.367646	C	-5.158915	1.581103	0.750070
O	-5.159152	-1.022872	2.304471	O	-4.751480	1.658652	1.899354
O	-5.946420	0.944739	1.493440	O	-6.093346	2.415270	0.242681
C	-5.931822	1.440762	2.857712	C	-6.610776	3.347511	1.222642
H	-4.904307	1.406088	3.242598	H	-5.798098	3.973965	1.611189
H	-6.286780	2.472289	2.785986	H	-7.347127	3.947165	0.679892
H	-6.589782	0.835957	3.493263	H	-7.080550	2.801014	2.049932
C	-5.262565	-2.056874	-0.553571	C	-5.340942	0.398255	-1.548515
O	-5.152820	-2.376452	-1.722098	O	-6.057359	1.225927	-2.088676
O	-5.547714	-2.910051	0.444677	O	-5.018701	-0.781933	-2.117893
C	-5.624235	-4.296751	0.018699	C	-5.442216	-0.942667	-3.485789
H	-6.481290	-4.435179	-0.652110	H	-6.535399	-1.022884	-3.537504
H	-4.698992	-4.575588	-0.497970	H	-5.102069	-0.091435	-4.089059
H	-5.745672	-4.867641	0.943295	H	-4.966693	-1.871174	-3.817504
Br	-6.059391	0.498056	-1.380267	Br	-6.459777	-1.251871	0.932559
65_obl: TS_p				65_obl: PC			
134				134			
TS_beta_obl -23802.9896				PC_obl -23810.0840			
C	0.957722	5.832627	2.663442	C	-1.862444	5.723134	-2.649369
C	0.487180	4.523092	2.981948	C	-1.149989	4.526166	-2.957866
C	1.446285	3.470897	2.955083	C	-1.903777	3.319315	-2.994294
C	2.667968	3.652736	2.243270	C	-3.179223	3.266352	-2.360231
C	2.886470	4.870042	1.541914	C	-3.655393	4.410658	-1.664394
C	2.121061	6.000181	1.955368	C	-3.076625	5.666265	-2.012153
C	3.507790	4.796092	0.248438	C	-4.349870	4.201372	-0.423604
C	3.928426	3.524142	-0.228935	C	-4.577073	2.865718	0.009156
C	4.132469	2.448162	0.691806	C	-4.516973	1.790392	-0.932225
C	3.464471	2.503409	1.940743	C	-3.780398	1.989203	-2.126611
C	3.339399	5.826296	-0.722528	C	-4.445193	5.225146	0.563293
C	3.155978	5.509328	-2.046437	C	-4.322135	4.918851	1.896562
C	3.152977	4.150759	-2.473777	C	-4.117111	3.573219	2.315648
C	3.769064	3.203997	-1.609943	C	-4.478595	2.550219	1.396457
C	3.887874	1.838208	-2.016967	C	-4.383321	1.176721	1.783616
C	3.043546	1.360593	-3.050918	C	-3.551444	0.836220	2.879700
C	2.074042	2.253852	-3.606976	C	-2.810326	1.876630	3.522219
C	2.250554	3.659940	-3.482395	C	-3.231479	3.229697	3.396673
C	4.528426	0.896018	-1.164703	C	-4.773456	0.153752	0.875577
C	4.656399	-0.457050	-1.582756	C	-4.685246	-1.209057	1.271788
C	3.849945	-0.927429	-2.649558	C	-3.889171	-1.549145	2.394288
C	2.904137	-0.042300	-3.235475	C	-3.169907	-0.520982	3.061317
C	5.252959	-1.423154	-0.712662	C	-5.030223	-2.247458	0.351109
C	5.438961	-2.763681	-1.155798	C	-4.999875	-3.609160	0.767985
C	4.663960	-3.232253	-2.268609	C	-4.234900	-3.953897	1.931547
C	3.716559	-2.338397	-2.841116	C	-3.512780	-2.915495	2.583013
C	2.466354	-2.848395	-3.287189	C	-2.227829	-3.198613	3.120758

C	2.198709	-4.246449	-3.193602	C	-1.702572	-4.522288	3.039332
C	3.317276	-5.119898	-3.014106	C	-2.625708	-5.580847	2.766898
C	4.509743	-4.625246	-2.554483	C	-3.849524	-5.301381	2.217537
C	5.288605	-1.136687	0.684014	C	-5.018363	-1.941319	-1.041498
C	5.470954	-2.204142	1.606555	C	-4.942269	-3.003879	-1.983958
C	6.072150	-3.394465	1.103511	C	-5.350476	-4.293748	-1.536184
C	6.065367	-3.663190	-0.242662	C	-5.387547	-4.586789	-0.195734
C	1.636401	-0.559567	-3.631837	C	-1.861781	-0.807494	3.550091
C	1.378675	-1.952117	-3.469512	C	-1.339603	-2.123779	3.394295
C	0.795760	1.732491	-3.966687	C	-1.488829	1.589281	3.975233
C	0.553631	0.335259	-3.797344	C	-0.977773	0.265588	3.808365
C	-0.747492	-0.090563	-3.414886	C	0.403768	0.094374	3.520135
C	-0.929859	-1.401975	-2.908929	C	0.866909	-1.150302	3.021329
C	0.069738	-2.389251	-3.135704	C	0.049468	-2.306439	3.159281
C	1.258317	4.489463	-4.074941	C	-2.464269	4.211056	4.084320
C	0.020139	3.984831	-4.402460	C	-1.183137	3.934677	4.502947
C	-0.297657	2.619298	-4.169576	C	-0.600418	2.659079	4.270768
C	-1.618872	2.183317	-3.784551	C	0.797221	2.489367	3.959294
C	-1.758413	0.885591	-3.206423	C	1.216213	1.253275	3.383682
C	4.624611	1.198009	0.225914	C	-4.814990	0.463736	-0.516247
C	4.781067	0.119904	1.140479	C	-4.711513	-0.604950	-1.448552
C	4.071476	0.159622	2.367294	C	-3.936165	-0.413109	-2.620132
C	3.267474	1.293748	2.662718	C	-3.327086	0.850400	-2.845868
C	2.026623	1.099161	3.334034	C	-2.028954	0.892700	-3.433896
C	1.054226	2.138286	3.291897	C	-1.260405	2.085523	-3.319366
C	-1.923771	-1.629618	-1.915827	C	1.950303	-1.169217	2.090470
C	-2.730934	-0.579742	-1.479696	C	2.538053	0.032528	1.702293
C	-2.744554	0.644580	-2.201199	C	2.276158	1.228305	2.430702
C	-3.540163	1.744415	-1.760609	C	2.866415	2.467403	2.038326
C	-3.641513	2.855071	-2.619532	C	2.703393	3.565005	2.908722
C	-2.705870	3.072314	-3.618510	C	1.696079	3.577699	3.856773
C	-3.299308	-0.592958	-0.068841	C	3.158467	0.174070	0.363565
C	-2.641947	-1.658196	0.780714	C	2.982049	-1.037682	-0.612579
C	-2.209195	-2.888153	0.167025	C	2.591314	-2.325661	0.008773
C	-1.868187	-2.888972	-1.202809	C	2.160618	-2.395457	1.340474
C	-1.843244	-3.977290	0.989189	C	2.493820	-3.447554	-0.835690
C	-1.542478	-5.202444	0.334325	C	2.376398	-4.712814	-0.209157
C	-1.225380	-5.213381	-1.003834	C	1.981469	-4.801138	1.106968
C	-1.179109	-3.999595	-1.742969	C	1.658922	-3.632618	1.839280
C	4.703119	-2.183542	2.821668	C	-4.109802	-2.820459	-3.141518
C	3.852269	-1.069691	3.064682	C	-3.455876	-1.568827	-3.312260
C	2.591842	-1.271921	3.701180	C	-2.139903	-1.531473	-3.859594
C	2.194708	-2.587611	4.065854	C	-1.491010	-2.748984	-4.203277
C	3.224840	-3.564813	4.170952	C	-2.320375	-3.889313	-4.392491
C	4.445694	-3.367434	3.570773	C	-3.596593	-3.923076	-3.882272
C	1.621815	-0.222921	3.651702	C	-1.378564	-0.328206	-3.736384
C	-1.993924	-1.311404	2.018895	C	2.267142	-0.778388	-1.882553
C	-1.234011	-2.321978	2.689237	C	1.726207	-1.897977	-2.575355
C	-1.389886	-3.692496	2.331254	C	2.106108	-3.226968	-2.215759
C	-1.818340	0.042231	2.362564	C	1.880537	0.515420	-2.224895
C	-2.541258	1.078853	1.663144	C	2.372350	1.665992	-1.489485

C	-3.225909	0.805040	0.486013	C	2.931085	1.515654	-0.224085
C	-0.110765	-1.944910	3.483834	C	0.612671	-1.718213	-3.445648
C	0.803512	-2.938800	3.945801	C	-0.071761	-2.851573	-3.979141
C	0.360355	-4.285507	3.911415	C	0.602739	-4.094895	-3.918739
C	-0.706637	-4.652153	3.117878	C	1.660937	-4.276617	-3.047195
C	-0.686970	0.423720	3.138239	C	0.743633	0.707141	-3.071365
C	0.248515	-0.567745	3.544619	C	0.025317	-0.425606	-3.535599
C	-0.313973	1.796686	3.206653	C	0.140780	1.991811	-3.157502
C	-1.253610	2.810729	2.839953	C	0.866297	3.154446	-2.742838
C	-2.388624	2.432468	2.079545	C	2.008666	2.977691	-1.919338
C	-0.904186	4.184595	2.944907	C	0.277300	4.442645	-2.855359
C	-1.916875	5.148503	2.627441	C	1.079209	5.571194	-2.484142
C	-3.029862	4.786604	1.920494	C	2.189050	5.408154	-1.703856
C	-3.191364	3.436315	1.464260	C	2.554110	4.102633	-1.235198
C	0.880302	-4.676510	-2.970603	C	-0.315644	-4.699355	2.915080
C	-0.142134	-3.749001	-2.728464	C	0.534122	-3.595384	2.754069
C	-3.714439	1.863463	-0.317239	C	3.133396	2.642323	0.616720
C	-3.862284	3.127311	0.276845	C	3.138183	3.911931	0.023078
H	5.158033	-4.191597	3.548660	H	-4.151621	-4.859794	-3.920307
H	6.418304	-4.163616	1.793643	H	-5.503424	-5.097080	-2.256387
H	6.406686	-4.639100	-0.586292	H	-5.569326	-5.615469	0.113530
H	5.303900	-5.321936	-2.287303	H	-4.479968	-6.125048	1.883806
H	-0.866670	-6.139678	-1.450947	H	1.770207	-5.784386	1.525515
H	0.728129	-5.730205	-2.739862	H	0.043851	-5.702410	2.689243
H	-1.416549	-6.116419	0.914008	H	2.460039	-5.625849	-0.797833
H	-0.924907	-5.712173	2.989311	H	2.049967	-5.284415	-2.902611
H	0.948571	-5.067529	4.390365	H	0.199856	-4.963381	-4.438320
H	3.008389	-4.538366	4.609943	H	-1.903739	-4.799560	-4.822846
H	3.172354	-6.197630	-3.109885	H	-2.293901	-6.615950	2.866480
H	-0.760779	4.678581	-4.712893	H	-0.572097	4.749329	4.890574
H	1.415067	5.565932	-4.135793	H	-2.826519	5.236224	4.152295
H	2.875607	6.299391	-2.742708	H	-4.244829	5.731595	2.618210
H	-2.733598	4.016154	-4.162060	H	1.509664	4.498791	4.407773
H	-4.365612	3.640366	-2.402815	H	3.268443	4.481241	2.737164
H	-4.317352	3.942796	-0.283655	H	3.372642	4.795325	0.616086
H	-3.741998	5.545482	1.590464	H	2.728661	6.277967	-1.324709
H	-1.749938	6.201120	2.854501	H	0.740957	6.578054	-2.726529
H	0.325443	6.699649	2.851491	H	-1.384859	6.692552	-2.786130
H	2.381857	6.995277	1.595522	H	-3.529881	6.591341	-1.656925
H	3.195755	6.858217	-0.403862	H	-4.459350	6.272439	0.263366
C	-4.515187	-1.393685	0.354744	C	4.357210	-0.553026	-0.199433
C	-5.037121	-2.435516	-0.559697	C	5.127490	-1.478029	0.722050
O	-4.568693	-2.676061	-1.663434	O	5.276838	-1.281510	1.912599
O	-6.120428	-3.074425	-0.055885	O	5.520730	-2.555044	0.031345
C	-6.784366	-3.916666	-1.025124	C	6.317466	-3.498983	0.796355
H	-6.101317	-4.693191	-1.390988	H	5.775747	-3.784977	1.706104
H	-7.629208	-4.356968	-0.487502	H	6.458692	-4.353824	0.129583
H	-7.132613	-3.303826	-1.867067	H	7.276966	-3.017295	1.030808
C	-5.070217	-1.283417	1.741889	C	5.185664	0.188826	-1.229698
O	-5.463930	-2.230356	2.404704	O	5.264725	-0.138991	-2.398051
O	-5.012286	-0.020254	2.207456	O	5.740783	1.264997	-0.659269

C	-5.229497	0.124550	3.627413	C	6.610424	2.031146	-1.534639
H	-6.285530	-0.049451	3.869189	H	7.511389	1.430280	-1.721401
H	-4.598672	-0.584970	4.177497	H	6.082116	2.266877	-2.466167
H	-4.942675	1.157088	3.850568	H	6.850895	2.936745	-0.971231
Br	-6.487690	0.273534	-0.874043	Br	8.477432	-0.780804	-0.213570
65 obl2: Int_a				65 obl2: Int_a			
134				134			
Int_alpha_obl2	-23823.6124			Int_beta_obl2	-23823.6316		
C	2.586021	-5.906946	-1.768287	C	5.446616	4.063570	1.185728
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C	2.846783	-3.540491	-2.244696	C	4.592990	1.848157	1.715721
C	3.757824	-3.436566	-1.151537	C	5.132985	1.364975	0.486954
C	3.868205	-4.522221	-0.238085	C	5.599653	2.298908	-0.480547
C	3.444868	-5.802789	-0.702824	C	5.938908	3.602730	-0.008027
C	3.994163	-4.215953	1.158647	C	5.308777	2.035105	-1.860195
C	4.056927	-2.849026	1.546837	C	4.636969	0.825162	-2.193928
C	4.425634	-1.850459	0.590675	C	4.634627	-0.268274	-1.270719
C	4.247943	-2.143288	-0.784197	C	4.860479	0.015065	0.100009
C	3.637478	-5.160159	2.167570	C	5.293236	3.072618	-2.839888
C	2.978119	-4.753163	3.300207	C	4.342184	3.080119	-3.830880
C	2.651258	-3.377806	3.493604	C	3.369818	2.042266	-3.916368
C	3.393699	-2.427449	2.737900	C	3.667053	0.826691	-3.240402
C	3.182190	-1.029200	2.947881	C	2.773325	-0.284544	-3.346477
C	1.984504	-0.610246	3.571398	C	1.435470	-0.043743	-3.745365
C	1.015855	-1.596585	3.928498	C	1.025466	1.301800	-3.998157
C	1.413069	-2.954659	4.085243	C	2.001857	2.297013	-4.287498
C	3.949530	-0.076849	2.216016	C	3.086985	-1.514778	-2.703189
C	3.740835	1.313416	2.441901	C	2.195998	-2.616927	-2.827266
C	2.562861	1.736255	3.106866	C	0.868287	-2.383708	-3.262664
C	1.594998	0.758262	3.478624	C	0.456624	-1.051239	-3.533924
C	4.466314	2.279589	1.678481	C	2.478815	-3.847244	-2.155114
C	4.301966	3.671540	1.947647	C	1.618497	-4.968533	-2.327852
C	3.148336	4.100251	2.672999	C	0.284238	-4.745318	-2.812667
C	2.187741	3.111913	3.040312	C	-0.115474	-3.400624	-3.063150
C	0.805085	3.439026	3.003250	C	-1.454939	-3.009616	-2.793994
C	0.399271	4.763458	2.647158	C	-2.396068	-3.974573	-2.338613
C	1.395872	5.795561	2.712337	C	-2.051481	-5.350180	-2.473481
C	2.724356	5.469028	2.704323	C	-0.747071	-5.724103	-2.695050
C	5.030663	1.867591	0.434873	C	3.378630	-3.815304	-1.048309
C	5.389305	2.855274	-0.525311	C	3.369755	-4.892621	-0.118541
C	5.607593	4.179607	-0.038581	C	2.831539	-6.133237	-0.572697
C	5.091292	4.574652	1.168539	C	1.982494	-6.169782	-1.650369
C	0.220722	1.082210	3.386596	C	-0.870635	-0.660880	-3.194732
C	-0.154299	2.389657	2.966271	C	-1.763101	-1.625234	-2.657610
C	-0.368120	-1.276416	3.787758	C	-0.299657	1.690485	-3.640178
C	-0.738549	0.028525	3.326350	C	-1.175229	0.715789	-3.062865
C	-1.901067	0.190521	2.546051	C	-2.155821	1.116112	-2.114606
C	-2.088191	1.407700	1.812410	C	-2.865087	0.147100	-1.377460
C	-1.336878	2.567756	2.201688	C	-2.773989	-1.214673	-1.744397
C	0.405167	-3.882683	4.478459	C	1.521628	3.602981	-4.580339
C	-0.925107	-3.576179	4.329553	C	0.245265	3.978423	-4.221710

C	-1.328098	-2.320766	3.786338	C	-0.628775	3.069860	-3.569098
C	-2.481651	-2.177839	2.941505	C	-1.557487	3.481958	-2.540466
C	-2.638187	-0.980113	2.175609	C	-2.151287	2.501494	-1.721156
C	4.551964	-0.490991	0.997208	C	4.025185	-1.502447	-1.631991
C	4.883512	0.502991	0.031970	C	3.985742	-2.569892	-0.690586
C	4.662030	0.218014	-1.339136	C	4.168729	-2.274452	0.682990
C	4.168399	-1.064217	-1.709640	C	4.419377	-0.927486	1.073020
C	3.217382	-1.152677	-2.765944	C	3.840895	-0.438634	2.275574
C	2.435429	-2.334138	-2.893532	C	3.765026	0.968442	2.479383
C	-2.780107	1.419329	0.599935	C	-3.480745	0.516821	-0.027762
C	-3.471036	0.192253	0.036980	C	-2.684212	1.679776	0.531118
C	-3.279502	-1.035362	0.916671	C	-2.374488	2.768742	-0.331968
C	-3.601446	-2.293321	0.379275	C	-1.906513	3.999207	0.198410
C	-3.785791	-3.366347	1.292308	C	-1.717243	5.073074	-0.719143
C	-3.266985	-3.298289	2.561157	C	-1.562092	4.827130	-2.059361
C	-2.848432	-0.096115	-1.329781	C	-2.016686	1.620155	1.755621
C	-2.247673	0.947495	-2.062229	C	-1.960725	0.401867	2.509176
C	-2.370154	2.321117	-1.647492	C	-2.802859	-0.696836	2.142279
C	-2.593606	2.545436	-0.250644	C	-3.426183	-0.709063	0.873154
C	-1.887462	3.365918	-2.460269	C	-2.775996	-1.892222	2.927323
C	-2.013857	4.697506	-1.957956	C	-3.661202	-2.936419	2.549045
C	-2.168948	4.907884	-0.611777	C	-4.163191	-2.973565	1.272165
C	-2.237555	3.807797	0.291600	C	-3.859549	-1.938219	0.347766
C	5.101430	2.583405	-1.904111	C	3.502269	-4.578461	1.275915
C	4.543195	1.319069	-2.245533	C	3.690192	-3.218084	1.646380
C	3.559162	1.241213	-3.275792	C	3.051269	-2.716072	2.819428
C	3.134349	2.431662	-3.927890	C	2.207758	-3.578550	3.574461
C	4.003794	3.556974	-3.842427	C	2.402077	-4.981836	3.405129
C	4.968684	3.627966	-2.867423	C	3.038864	-5.468254	2.291037
C	2.775403	0.050217	-3.385052	C	2.973152	-1.301008	3.006879
C	-1.247529	0.657768	-3.030177	C	-0.831073	0.139068	3.310056
C	-0.479399	1.720713	-3.604878	C	-0.596482	-1.189106	3.794156
C	-0.939742	3.060484	-3.508652	C	-1.654084	-2.134554	3.791825
C	-0.812554	-0.680784	-3.187093	C	0.225720	1.094894	3.371293
C	-1.599088	-1.734629	-2.652620	C	-0.013429	2.426418	2.927481
C	-2.631529	-1.437272	-1.719463	C	-1.161258	2.707211	2.141000
C	0.871744	1.468259	-3.986845	C	0.747625	-1.640273	3.959821
C	1.742467	2.557631	-4.274811	C	1.008075	-3.028220	4.140140
C	1.133174	3.814437	-4.541184	C	-0.091060	-3.848052	4.529336
C	-0.168096	4.058673	-4.159317	C	-1.382956	-3.415686	4.356832
C	0.541122	-0.934930	-3.550317	C	1.560530	0.640263	3.489017
C	1.414291	0.165611	-3.760607	C	1.813102	-0.758246	3.605552
C	1.084511	-2.224685	-3.305910	C	2.624669	1.513806	3.120251
C	0.207345	-3.334929	-3.108016	C	2.386905	2.918454	3.029820
C	-1.159637	-3.080307	-2.814392	C	1.043368	3.377534	2.965634
C	0.739610	-4.637922	-2.884697	C	3.444840	3.803042	2.665356
C	-0.189856	-5.714021	-2.769227	C	3.155799	5.207117	2.671143
C	-1.521016	-5.472335	-2.523315	C	1.865378	5.660755	2.651961
C	-1.995276	-4.138806	-2.361213	C	0.774175	4.729639	2.584653
C	-0.822470	4.947304	1.995219	C	-3.443836	-3.547488	-1.492465
C	-1.578787	3.830966	1.575823	C	-3.510163	-2.235194	-1.037820

C	-3.251555	-2.534872	-1.016936	C	-1.268953	3.978170	1.493456
C	-3.066095	-3.827949	-1.493499	C	-0.413381	5.021632	1.909614
H	5.523006	4.557722	-2.742306	H	3.050450	-6.544252	2.118967
H	6.076234	4.924559	-0.681791	H	2.977469	-7.038397	0.016544
H	5.162083	5.623265	1.456123	H	1.478004	-7.105226	-1.890902
H	3.464672	6.263730	2.611078	H	-0.487036	-6.781267	-2.650367
H	-2.103935	5.925141	-0.225719	H	-4.691352	-3.865268	0.935229
H	-1.039953	5.935593	1.591700	H	-4.033412	-4.322252	-1.002507
H	-1.833669	5.551156	-2.610511	H	-3.814344	-3.793612	3.203516
H	-0.554718	5.074017	-4.246046	H	-2.199046	-4.114874	4.536378
H	1.733841	4.643681	-4.913591	H	0.081098	-4.878828	4.837919
H	3.823326	4.432034	-4.466730	H	1.927789	-5.683829	4.090599
H	1.086285	6.838927	2.625456	H	-2.805684	-6.110827	-2.260668
H	-1.666515	-4.353908	4.510218	H	-0.039442	5.025051	-4.328290
H	0.681651	-4.895692	4.769644	H	2.205424	4.364213	-4.954641
H	2.586993	-5.507163	3.982982	H	4.257364	3.958644	-4.470436
H	-3.324156	-4.175417	3.204517	H	-1.290164	5.648940	-2.720948
H	-4.230632	-4.300474	0.950067	H	-1.559999	6.085303	-0.346679
H	-3.568904	-4.663472	-1.006542	H	-0.526784	6.020028	1.488746
H	-2.194385	-6.305832	-2.312816	H	1.660082	6.727814	2.545398
H	0.172441	-6.741382	-2.746130	H	3.971239	5.924699	2.579522
H	2.170544	-6.883606	-2.015209	H	5.615149	5.104422	1.460603
H	3.686989	-6.697422	-0.129492	H	6.486990	4.289035	-0.653677
H	3.750005	-6.227488	1.978821	H	5.932982	3.946215	-2.717845
C	-5.083095	0.473466	0.032236	C	-5.057162	0.950791	-0.074354
C	-5.607200	0.204705	1.461412	C	-5.282714	2.390819	-0.549756
O	-6.397206	-0.661903	1.778848	O	-5.697699	3.285856	0.163608
O	-4.978339	1.025982	2.315927	O	-4.960414	2.523602	-1.844568
C	-5.149154	0.696291	3.717288	C	-5.013827	3.887061	-2.338375
H	-4.860638	-0.349353	3.882563	H	-4.408906	4.536922	-1.695459
H	-4.473454	1.374370	4.245877	H	-4.594184	3.836728	-3.346460
H	-6.191652	0.854713	4.018811	H	-6.054395	4.234467	-2.354947
C	-5.456230	1.887321	-0.428879	C	-5.640840	0.745836	1.342609
O	-5.945003	2.733610	0.296879	O	-6.525340	-0.030615	1.643412
O	-5.170288	2.057279	-1.727835	O	-4.949853	1.502379	2.208543
C	-5.364004	3.411096	-2.212946	C	-5.186081	1.202508	3.607195
H	-6.432534	3.659946	-2.202210	H	-6.212104	1.473618	3.884132
H	-4.807187	4.112773	-1.581021	H	-5.014960	0.133161	3.783571
H	-4.966056	3.403702	-3.231034	H	-4.453695	1.808068	4.148151
Br	-6.041154	-0.773849	-1.201065	Br	-6.092732	-0.210961	-1.328038
65_obl2: TS_α				65_obl2: TS_β			
134				134			
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C	2.220306	-4.774404	-2.318178	C	4.595524	-3.209521	-2.200914
C	2.957222	-3.562819	-2.194654	C	4.652343	-1.821284	-1.888150
C	3.902191	-3.418832	-1.136097	C	5.219563	-1.401903	-0.648755
C	4.067486	-4.480828	-0.205117	C	5.687133	-2.383904	0.267119
C	3.645070	-5.775402	-0.622228	C	5.991253	-3.669864	-0.265153
C	4.237842	-4.140176	1.182090	C	5.431553	-2.173276	1.666977
C	4.277154	-2.764918	1.538345	C	4.776538	-0.974413	2.061337

C	4.592084	-1.779363	0.548958	C	4.773852	0.159219	1.187083
C	4.379682	-2.108445	-0.813865	C	4.977442	-0.065470	-0.198338
C	3.941843	-5.067381	2.222851	C	5.418191	-3.252114	2.597081
C	3.306946	-4.649938	3.367472	C	4.479255	-3.295356	3.599818
C	2.947352	-3.282423	3.538205	C	3.516107	-2.256438	3.736903
C	3.640887	-2.332246	2.738753	C	3.818626	-1.012741	3.116771
C	3.397541	-0.935414	2.921590	C	2.936125	0.100562	3.282433
C	2.202040	-0.532106	3.565667	C	1.598590	-0.147058	3.680390
C	1.269473	-1.538140	3.965691	C	1.179618	-1.502013	3.864399
C	1.709417	-2.878961	4.149595	C	2.146825	-2.518188	4.101265
C	4.113737	0.018010	2.147325	C	3.255013	1.355542	2.695568
C	3.874097	1.404389	2.345373	C	2.374207	2.456713	2.870974
C	2.704787	1.812103	3.035677	C	1.047640	2.216628	3.309668
C	1.780104	0.821107	3.463929	C	0.628843	0.877610	3.524993
C	4.554021	2.371348	1.540545	C	2.661806	3.712802	2.249712
C	4.364480	3.761643	1.784522	C	1.811537	4.831513	2.477165
C	3.214318	4.179595	2.536582	C	0.477722	4.598528	2.966043
C	2.292622	3.176636	2.954260	C	0.069601	3.248477	3.162950
C	0.902716	3.472019	2.974585	C	-1.277408	2.881484	2.899565
C	0.453459	4.780174	2.631767	C	-2.220896	3.869986	2.505430
C	1.423044	5.829307	2.618553	C	-1.859541	5.234598	2.690095
C	2.761884	5.532991	2.555014	C	-0.545770	5.587053	2.898932
C	5.100703	1.943831	0.294697	C	3.556580	3.723690	1.139197
C	5.415513	2.915574	-0.694464	C	3.559737	4.843060	0.262386
C	5.605087	4.254575	-0.246581	C	3.031625	6.063045	0.773429
C	5.100746	4.664990	0.963210	C	2.183800	6.057410	1.854489
C	0.386337	1.110541	3.405605	C	-0.708420	0.515388	3.181166
C	-0.037169	2.402055	2.992875	C	-1.600150	1.508199	2.706166
C	-0.121724	-1.256942	3.848907	C	-0.145013	-1.861762	3.482779
C	-0.537484	0.033451	3.389893	C	-1.013792	-0.848765	2.966740
C	-1.734674	0.160249	2.642324	C	-1.991546	-1.184596	1.995963
C	-2.021849	1.380597	1.981617	C	-2.718994	-0.178936	1.342066
C	-1.268688	2.548629	2.295885	C	-2.632928	1.152352	1.790486
C	0.736125	-3.823479	4.578293	C	1.658695	-3.835055	4.317633
C	-0.606623	-3.556421	4.445067	C	0.380279	-4.182620	3.939217
C	-1.054371	-2.327827	3.885237	C	-0.484590	-3.233203	3.334754
C	-2.233353	-2.226975	3.071534	C	-1.423018	-3.584987	2.294748
C	-2.437711	-1.049110	2.297996	C	-1.999639	-2.549650	1.522060
C	4.702580	-0.411803	0.920573	C	4.181664	1.380152	1.609204
C	4.979460	0.566229	-0.073274	C	4.147891	2.489276	0.720455
C	4.731249	0.243874	-1.431799	C	4.316147	2.254316	-0.667847
C	4.251518	-1.053330	-1.758099	C	4.545452	0.926607	-1.120385
C	3.273992	-1.185433	-2.790977	C	3.936388	0.499204	-2.337996
C	2.507569	-2.379751	-2.861488	C	3.831446	-0.892868	-2.601719
C	-2.761885	1.372896	0.753311	C	-3.321914	-0.455558	-0.023377
C	-3.310506	0.080029	0.195965	C	-2.672745	-1.652184	-0.678566
C	-3.124446	-1.125258	1.078552	C	-2.272796	-2.764352	0.149538
C	-3.472042	-2.380900	0.559103	C	-1.874660	-3.975647	-0.452752
C	-3.597253	-3.449294	1.490781	C	-1.678415	-5.087872	0.409995
C	-3.011106	-3.366142	2.728302	C	-1.479075	-4.902664	1.756857
C	-2.751085	-0.206860	-1.185671	C	-2.004382	-1.518654	-1.940386

C	-2.170166	0.831621	-1.928847	C	-1.883787	-0.243066	-2.545701
C	-2.300213	2.212203	-1.523387	C	-2.690109	0.864566	-2.100150
C	-2.526377	2.473214	-0.150113	C	-3.313210	0.805179	-0.846073
C	-1.876539	3.257627	-2.377249	C	-2.654295	2.094546	-2.816581
C	-2.046236	4.590179	-1.903717	C	-3.528388	3.124061	-2.372933
C	-2.197870	4.828165	-0.558997	C	-4.049603	3.082141	-1.104697
C	-2.230524	3.750917	0.367588	C	-3.760258	1.988891	-0.240757
C	5.114402	2.600759	-2.065504	C	3.685039	4.593231	-1.148772
C	4.570300	1.320897	-2.361161	C	3.845503	3.249503	-1.583007
C	3.561233	1.201097	-3.361425	C	3.189658	2.812501	-2.771339
C	3.097721	2.370518	-4.024929	C	2.356549	3.722457	-3.479001
C	3.952296	3.508208	-3.996130	C	2.580683	5.110289	-3.250023
C	4.941010	3.618016	-3.047781	C	3.234090	5.535025	-2.118554
C	2.794644	-0.004795	-3.421203	C	3.082258	1.408784	-3.019707
C	-1.213128	0.546094	-2.935799	C	-0.750384	0.048963	-3.344427
C	-0.483765	1.613607	-3.548539	C	-0.497999	1.398231	-3.750374
C	-0.958984	2.948674	-3.448931	C	-1.538314	2.363137	-3.679504
C	-0.775745	-0.788953	-3.099539	C	0.278592	-0.920696	-3.467216
C	-1.531590	-1.841060	-2.526743	C	0.016020	-2.269201	-3.105937
C	-2.548399	-1.544488	-1.572829	C	-1.152008	-2.581671	-2.356496
C	0.851053	1.373032	-3.984377	C	0.847726	1.832448	-3.919233
C	1.691887	2.469253	-4.324261	C	1.134724	3.220380	-4.048515
C	1.056532	3.714764	-4.577325	C	0.045765	4.076176	-4.372343
C	-0.231060	3.947998	-4.145932	C	-1.252335	3.660277	-4.188484
C	0.574005	-1.028551	-3.497696	C	1.629075	-0.481166	-3.579086
C	1.420421	0.080873	-3.756943	C	1.901241	0.913061	-3.624809
C	1.143230	-2.302905	-3.239012	C	2.674657	-1.387875	-3.254906
C	0.288988	-3.420864	-2.988018	C	2.412202	-2.791279	-3.230195
C	-1.074893	-3.182120	-2.669822	C	1.061836	-3.231933	-3.195633
C	0.847622	-4.708353	-2.746644	C	3.455493	-3.709575	-2.916975
C	-0.060548	-5.792657	-2.577332	C	3.145916	-5.101063	-2.988736
C	-1.392627	-5.567900	-2.314234	C	1.843749	-5.534921	-3.000005
C	-1.886893	-4.239845	-2.175499	C	0.771115	-4.596209	-2.904005
C	-0.806149	4.928459	2.022963	C	-3.302356	3.490987	1.675866
C	-1.553772	3.805134	1.652134	C	-3.389168	2.205834	1.153794
C	-3.153824	-2.634188	-0.842506	C	-1.268205	-3.892433	-1.770518
C	-2.958879	-3.930025	-1.305757	C	-0.429724	-4.908999	-2.241171
H	5.482442	4.559403	-2.959857	H	3.263234	6.601689	-1.897827
H	6.029440	4.999031	-0.919906	H	3.179435	6.992984	0.224815
H	5.140822	5.723735	1.217211	H	1.685265	6.984627	2.135263
H	3.474197	6.342710	2.398755	H	-0.277734	6.643135	2.888505
H	-2.164394	5.856072	-0.198589	H	-4.595741	3.943358	-0.721715
H	-1.048963	5.904535	1.604006	H	-3.904498	4.290973	1.246564
H	-1.900949	5.434828	-2.575958	H	-3.674864	4.019025	-2.976224
H	-0.635057	4.956583	-4.228902	H	-2.057153	4.384253	-4.311081
H	1.630407	4.547096	-4.983342	H	0.229878	5.118484	-4.631062
H	3.740299	4.364774	-4.635545	H	2.112489	5.851705	-3.896974
H	1.087130	6.862599	2.513151	H	-2.609354	6.010387	2.523139
H	-1.322473	-4.351645	4.650519	H	0.087593	-5.231076	3.988159
H	1.043652	-4.824108	4.880539	H	2.337220	-4.620267	4.649298
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H	-3.027996	-4.237441	3.381515	H	-1.208903	-5.759446	2.372853
H	-4.065047	-4.383300	1.181979	H	-1.557057	-6.086926	-0.008057
H	-3.449878	-4.763498	-0.804462	H	-0.545734	-5.925404	-1.866187
H	-2.046720	-6.407125	-2.069879	H	1.623598	-6.602293	-2.936233
H	0.318440	-6.813234	-2.531879	H	3.946285	-5.836946	-2.915319
H	2.336253	-6.905639	-1.857461	H	5.603370	-5.103174	-1.785615
H	3.915376	-6.652411	-0.034606	H	6.527663	-4.397877	0.342945
H	4.073816	-6.135905	2.055351	H	6.046789	-4.125817	2.427940
C	-4.623719	0.805421	0.418960	C	-4.563354	-1.305117	-0.221456
C	-5.281498	0.752969	1.743680	C	-5.294225	-1.256573	-1.508259
O	-4.806498	0.243735	2.749667	O	-4.925556	-0.657133	-2.509042
O	-6.502717	1.342802	1.715571	O	-6.451112	-1.961648	-1.448944
C	-7.259709	1.147961	2.929364	C	-7.287248	-1.789485	-2.613134
H	-6.719754	1.557899	3.792030	H	-6.760483	-2.115202	-3.518864
H	-8.201240	1.680718	2.766281	H	-8.167236	-2.411837	-2.425828
H	-7.439904	0.075598	3.082018	H	-7.570192	-0.733087	-2.710380
C	-5.165864	1.736206	-0.620325	C	-4.945264	-2.346011	0.783817
O	-5.642329	2.837150	-0.391307	O	-5.321817	-3.475135	0.509877
O	-4.996384	1.235743	-1.861098	O	-4.751216	-1.904178	2.043047
C	-5.303590	2.156746	-2.929995	C	-4.890705	-2.913589	3.066520
H	-6.386173	2.330793	-2.976099	H	-5.948458	-3.180123	3.187551
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H	-4.946608	1.663788	-3.839168	H	-4.497040	-2.450070	3.976204
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65 obl2: PC				65 per: Int_α			
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C	-3.146440	-4.346064	2.487826	C	0.251662	-4.230370	-3.154784
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C	-4.502044	-2.854340	1.073695	C	2.083117	-2.602965	-3.406379
C	-4.738131	-3.946122	0.193737	C	3.017338	-3.653508	-3.177410
C	-4.548649	-5.254651	0.723565	C	2.552188	-4.988074	-3.379211
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C	-4.808131	-1.257442	-0.759507	C	3.701638	-0.942462	-2.613526
C	-4.756705	-1.516643	0.633684	C	2.508486	-1.242309	-3.316082
C	-4.486037	-4.712890	-2.173019	C	4.931954	-4.373328	-1.736688
C	-3.710384	-4.464721	-3.279719	C	5.456952	-4.143294	-0.490124
C	-3.158294	-3.171629	-3.502958	C	5.289471	-2.878396	0.148353
C	-3.771314	-2.084487	-2.820531	C	4.968531	-1.772833	-0.687594
C	-3.326260	-0.748532	-3.065005	C	4.871353	-0.460313	-0.127709
C	-2.041963	-0.553636	-3.631675	C	4.671275	-0.328407	1.268443
C	-1.230543	-1.698733	-3.898131	C	4.529546	-1.518138	2.049129
C	-1.836716	-2.978337	-4.038967	C	5.032592	-2.755867	1.555879
C	-3.959103	0.343410	-2.411450	C	4.578056	0.650465	-0.970548
C	-3.515256	1.667829	-2.669948	C	4.500429	1.957354	-0.409114
C	-2.252152	1.865466	-3.282132	C	4.343224	2.095494	0.992395
C	-1.446734	0.733186	-3.575989	C	4.228764	0.921627	1.790413
C	-4.112390	2.771587	-1.983811	C	4.166336	3.072507	-1.239663
C	-3.713157	4.102923	-2.292031	C	4.141322	4.387904	-0.691494

C	-2.459155	4.309127	-2.963731	C	4.026323	4.534924	0.727266
C	-1.659262	3.164131	-3.242110	C	3.905663	3.352749	1.513085
C	-0.245427	3.264870	-3.153843	C	3.032745	3.355550	2.635859
C	0.357248	4.517480	-2.848418	C	2.320268	4.547180	2.972407
C	-0.449658	5.686465	-2.973452	C	2.807962	5.780210	2.429007
C	-1.819057	5.582217	-3.015448	C	3.629117	5.770379	1.334055
C	-4.805358	2.509136	-0.765635	C	3.497346	2.816862	-2.472772
C	-5.052939	3.580979	0.135316	C	2.791331	3.874105	-3.113088
C	-5.020686	4.898562	-0.404641	C	3.166379	5.206002	-2.761803
C	-4.374481	5.151726	-1.589744	C	3.829883	5.455829	-1.588362
C	-0.032275	0.834338	-3.413564	C	3.316786	0.923883	2.881304
C	0.530886	2.077423	-3.028624	C	2.585844	2.115930	3.168264
C	0.175798	-1.598253	-3.693319	C	3.583631	-1.518816	3.117861
C	0.730704	-0.349511	-3.270495	C	2.855803	-0.319009	3.389556
C	1.879685	-0.334657	-2.429135	C	1.504159	-0.420735	3.806704
C	2.287998	0.868676	-1.828911	C	0.670721	0.727465	3.756868
C	1.712354	2.095875	-2.236483	C	1.249530	2.021629	3.643794
C	-0.977189	-4.066997	-4.350948	C	4.880587	-3.895801	2.397876
C	0.379521	-3.971735	-4.141421	C	3.948830	-3.898155	3.408586
C	0.954408	-2.783472	-3.614974	C	3.133087	-2.757462	3.651908
C	2.067522	-2.796887	-2.702662	C	1.748166	-2.866751	4.037726
C	2.367703	-1.615737	-1.966423	C	0.915951	-1.719492	3.897850
C	-4.696543	0.083229	-1.217272	C	3.961200	0.402911	-2.226497
C	-4.908902	1.156707	-0.309743	C	3.234546	1.461430	-2.843585
C	-4.816550	0.899215	1.081543	C	2.020785	1.160979	-3.504266
C	-4.555306	-0.425956	1.523168	C	1.578634	-0.191774	-3.564691
C	-3.697594	-0.619984	2.647585	C	0.193077	-0.473008	-3.476817
C	-3.122955	-1.901842	2.859642	C	-0.223848	-1.801840	-3.191234
C	3.023391	0.851838	-0.543275	C	-0.696249	0.569193	3.394447
C	3.139524	-0.532754	0.176285	C	-1.178056	-0.721248	3.079504
C	2.876507	-1.728362	-0.662837	C	-0.449892	-1.875979	3.516026
C	2.961138	-2.991465	-0.054029	C	-0.961526	-3.178210	3.275622
C	3.023460	-4.116623	-0.915101	C	-0.225534	-4.266826	3.807458
C	2.614628	-4.015990	-2.222544	C	1.092718	-4.117918	4.185887
C	2.493224	-0.613200	1.512352	C	-2.176947	-0.860061	2.076099
C	2.037078	0.548572	2.155450	C	-2.716779	0.283463	1.461546
C	2.374704	1.867578	1.664421	C	-2.475158	1.561584	2.024887
C	2.726676	2.021282	0.314315	C	-1.447372	1.716104	3.004771
C	2.046170	3.021152	2.432337	C	-3.052156	2.738210	1.455210
C	2.437533	4.280594	1.906520	C	-2.862503	3.957444	2.138578
C	2.716394	4.413058	0.566855	C	-1.862984	4.100960	3.085965
C	2.667127	3.285979	-0.292127	C	-1.002186	3.017496	3.378948
C	-4.905933	3.324445	1.542880	C	1.537494	3.568384	-3.737952
C	-4.576468	2.005449	1.958025	C	1.087236	2.218177	-3.729546
C	-3.678486	1.816808	3.048823	C	-0.303621	1.937877	-3.587465
C	-3.102577	2.953598	3.681068	C	-1.214487	3.014040	-3.428239
C	-3.777093	4.195529	3.510139	C	-0.774704	4.304716	-3.849805
C	-4.661919	4.374650	2.474269	C	0.561453	4.573963	-4.006828
C	-3.103942	0.523250	3.248577	C	-0.717954	0.605604	-3.261894
C	0.971834	0.469211	3.094465	C	-3.355347	0.181123	0.085694
C	0.355242	1.667654	3.575455	C	-3.136596	1.487194	-0.651493

C	1.022582	2.914073	3.440255	C	-3.370957	2.690823	0.044707
C	0.327926	-0.774567	3.298124	C	-2.734535	-0.994615	-0.629577
C	0.957906	-1.963724	2.854123	C	-2.568746	-2.205536	0.095616
C	2.062828	-1.882119	1.961380	C	-2.348193	-2.164122	1.502828
C	-1.031456	1.648625	3.902492	C	-2.524875	1.556698	-1.921504
C	-1.728436	2.872930	4.102055	C	-2.335295	2.827794	-2.552221
C	-0.940142	4.030579	4.346053	C	-3.039467	3.937038	-2.010658
C	0.396952	4.050386	4.020371	C	-3.510800	3.878500	-0.723682
C	-1.069801	-0.793898	3.586414	C	-2.079182	-0.875963	-1.861631
C	-1.763684	0.438376	3.700918	C	-1.859594	0.407595	-2.459632
C	-1.798457	-1.990844	3.356577	C	-1.378247	-2.007344	-2.400501
C	-1.102731	-3.234099	3.254784	C	-1.613495	-3.307884	-1.868053
C	0.300895	-3.213080	3.040684	C	-2.220503	-3.398746	-0.589120
C	-1.823190	-4.443734	3.041145	C	-0.941071	-4.448340	-2.401627
C	-1.074034	-5.656942	3.025343	C	-1.260982	-5.725246	-1.833992
C	0.290815	-5.642987	2.864553	C	-1.852374	-5.816004	-0.603793
C	0.980983	-4.409364	2.678034	C	-2.144943	-4.625168	0.141765
C	1.574382	4.529360	-2.135235	C	1.036797	4.441586	3.525465
C	2.123371	3.347258	-1.642333	C	0.413582	3.188758	3.653197
C	2.533748	-3.095121	1.333828	C	-1.911564	-3.331405	2.184921
C	2.132897	-4.318245	1.868318	C	-2.047971	-4.577600	1.535021
H	-5.052547	5.373816	2.284289	H	0.873921	5.599824	-4.199992
H	-5.386474	5.738239	0.185667	H	2.810041	6.046517	-3.357052
H	-4.247097	6.185854	-1.907853	H	3.986049	6.489126	-1.280017
H	-2.417959	6.490983	-2.963615	H	3.875223	6.713779	0.847205
H	2.857361	5.410620	0.152064	H	-1.652338	5.094659	3.479921
H	1.915659	5.488457	-1.746597	H	0.445874	5.353975	3.601438
H	2.363396	5.177507	2.519762	H	-3.394594	4.852123	1.814230
H	0.938850	4.992967	4.089566	H	-3.877113	4.790617	-0.252880
H	-1.416454	4.959005	4.659173	H	-3.061452	4.887716	-2.541537
H	-3.493506	5.057061	4.114041	H	-1.488826	5.123911	-3.928136
H	0.019447	6.668708	-2.891123	H	2.407331	6.723429	2.805685
H	0.991631	-4.865441	-4.258083	H	3.747692	-4.831892	3.933633
H	-1.398250	-5.034127	-4.623527	H	5.388897	-4.827187	2.150450
H	-3.408404	-5.301853	-3.908498	H	5.888235	-4.977957	0.062322
H	2.563075	-4.917866	-2.830447	H	1.664097	-5.006870	4.451456
H	3.283196	-5.096099	-0.514985	H	-0.651092	-5.270226	3.791924
H	2.526504	-5.245787	1.453687	H	-1.815289	-5.502530	2.061513
H	0.833311	-6.581388	2.734931	H	-1.975100	-6.788733	-0.123388
H	-1.594760	-6.613980	3.018025	H	-0.919569	-6.635396	-2.326776
H	-3.537132	-6.467753	2.145438	H	0.887442	-6.307276	-3.417084
H	-4.895228	-6.123935	0.165262	H	3.264124	-5.812796	-3.411241
H	-4.774565	-5.740372	-1.953786	H	4.957783	-5.384823	-2.141146
C	4.384435	0.234685	-0.216090	C	-5.020249	-0.058452	0.143474
C	5.179830	0.990249	0.839884	C	-5.355674	-1.472996	0.647730
O	5.611750	2.114090	0.678765	O	-5.719062	-2.391896	-0.062648
O	5.231383	0.270780	1.970783	O	-5.138872	-1.571794	1.968922
C	6.017544	0.890457	3.021195	C	-5.282418	-2.915960	2.495141
H	5.632658	1.897243	3.225711	H	-4.751174	-3.629068	1.855255
H	5.900728	0.234902	3.888336	H	-4.834514	-2.875904	3.492073
H	7.062352	0.927579	2.682532	H	-6.346764	-3.179403	2.547131

C	5.235172	-0.294080	-1.358932	C	-5.649105	1.028228	1.007959
O	5.371774	-1.467663	-1.641682	O	-5.577818	1.020717	2.223315
O	5.748844	0.747987	-2.028553	O	-6.211893	2.023610	0.289134
C	6.759207	0.373139	-3.005616	C	-6.618213	3.156057	1.096571
H	7.599181	-0.078482	-2.458584	H	-7.487780	2.887779	1.710234
H	6.335051	-0.330561	-3.731784	H	-5.790498	3.460935	1.748886
H	7.051895	1.311598	-3.484357	H	-6.871620	3.940333	0.377667
Br	8.182673	-0.353750	0.304393	Br	-5.636110	0.040296	-1.748319
65_per: Int_β				65_per: TS_α			
134				134			
Int_beta_per -23819.3320				TS_alpha_per -23795.2027			
C	-2.114151	5.155969	-3.294146	C	1.260024	-5.351493	-3.262720
C	-1.194484	4.067329	-3.378203	C	0.320057	-4.287865	-3.096865
C	-1.749631	2.755725	-3.400302	C	0.798621	-2.963147	-3.314405
C	-3.089926	2.549841	-2.956502	C	2.201530	-2.712068	-3.290799
C	-3.830433	3.654273	-2.451475	C	3.096907	-3.781542	-3.003299
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C	-4.681197	3.432371	-1.316594	C	4.241364	-3.499353	-2.189052
C	-4.781705	2.112948	-0.793208	C	4.463528	-2.158059	-1.766198
C	-4.414354	0.993664	-1.604211	C	3.826871	-1.079862	-2.454699
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C	-5.144496	4.317865	0.898835	C	5.400143	-4.288048	-0.204065
C	-4.817246	3.054965	1.476736	C	5.235399	-3.007923	0.405859
C	-4.869497	1.921281	0.618103	C	4.984991	-1.908396	-0.462023
C	-4.640370	0.613128	1.149154	C	4.897362	-0.584956	0.072133
C	-3.961536	0.491932	2.385403	C	4.636647	-0.425218	1.454392
C	-3.501950	1.681391	3.031087	C	4.430168	-1.595978	2.247293
C	-4.090994	2.937012	2.709689	C	4.921811	-2.854211	1.797227
C	-4.726279	-0.524675	0.295658	C	4.671241	0.519219	-0.800300
C	-4.506224	-1.824625	0.834571	C	4.600073	1.837585	-0.263938
C	-3.861887	-1.950768	2.090338	C	4.384107	2.002991	1.125778
C	-3.411583	-0.771921	2.752198	C	4.198797	0.844158	1.934104
C	-4.544735	-2.969131	-0.020923	C	4.331260	2.946674	-1.125141
C	-4.381585	-4.275470	0.527844	C	4.313973	4.271160	-0.598253
C	-3.769722	-4.406869	1.813612	C	4.144387	4.444565	0.811077
C	-3.322401	-3.219990	2.463170	C	3.957878	3.278482	1.608141
C	-2.110345	-3.252032	3.206955	C	3.037330	3.321892	2.690897
C	-1.382532	-4.476925	3.319246	C	2.345972	4.537974	2.980665
C	-2.086076	-5.690438	3.019611	C	2.893188	5.749345	2.443139
C	-3.236446	-5.652801	2.279989	C	3.756935	5.700003	1.383402
C	-4.353971	-2.770298	-1.420488	C	3.710005	2.686778	-2.381633
C	-3.973114	-3.875757	-2.231751	C	3.057414	3.749219	-3.068028
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C	-4.473109	-5.372796	-0.383790	C	4.068318	5.331438	-1.524811
C	-2.184118	-0.809274	3.459415	C	3.242254	0.888793	2.980900
C	-1.450779	-2.031187	3.513145	C	2.532712	2.103284	3.219380
C	-2.244461	1.645796	3.706131	C	3.437724	-1.554272	3.271813
C	-1.516116	0.415273	3.739143	C	2.725765	-0.334517	3.489079
C	-0.104861	0.451603	3.686605	C	1.359571	-0.395040	3.854027
C	0.623938	-0.740028	3.381374	C	0.553077	0.773948	3.743856

C	-0.030320	-2.002822	3.516797	C	1.175992	2.051863	3.638526
C	-3.605139	4.079176	3.411846	C	4.703808	-3.976322	2.650512
C	-2.388780	4.045965	4.048017	C	3.732549	-3.938024	3.620106
C	-1.588079	2.865994	4.026783	C	2.933424	-2.772208	3.805242
C	-0.154474	2.906926	3.940332	C	1.537340	-2.839161	4.140433
C	0.535877	1.719272	3.563815	C	0.738378	-1.675482	3.952159
C	-4.579635	-0.330082	-1.105279	C	4.100209	0.265505	-2.075310
C	-4.177069	-1.436867	-1.905961	C	3.430688	1.332124	-2.741648
C	-3.254273	-1.214114	-2.958464	C	2.236795	1.049471	-3.444805
C	-2.804791	0.111014	-3.216558	C	1.767577	-0.293035	-3.506934
C	-1.448144	0.312694	-3.595748	C	0.372298	-0.538573	-3.466291
C	-0.889586	1.619037	-3.498641	C	-0.090100	-1.850932	-3.186336
C	1.825636	-0.659568	2.646834	C	-0.802182	0.643179	3.350675
C	2.223499	0.611682	2.134337	C	-1.308382	-0.646302	3.047121
C	1.704794	1.806172	2.752905	C	-0.615430	-1.806860	3.522512
C	2.144223	3.081497	2.320163	C	-1.135160	-3.100984	3.262571
C	1.686683	4.215448	3.050583	C	-0.452424	-4.201464	3.850419
C	0.567047	4.131138	3.841653	C	0.846886	-4.075717	4.282305
C	2.868620	0.712753	0.901314	C	-2.269607	-0.792352	2.013402
C	3.389462	-0.485373	0.140035	C	-2.785267	0.373461	1.373030
C	3.066421	-1.794555	0.835189	C	-2.504023	1.675677	1.903364
C	2.362037	-1.853332	2.059833	C	-1.506381	1.809785	2.908949
C	3.241121	-2.988258	0.103358	C	-2.977650	2.843170	1.251344
C	3.209533	-4.208915	0.828609	C	-2.776606	4.081143	1.905881
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C	1.960843	-3.120543	2.584861	C	-1.025948	3.102628	3.265167
C	-2.990946	-3.652839	-3.253564	C	1.824721	3.462620	-3.741479
C	-2.503432	-2.329503	-3.447251	C	1.341110	2.124249	-3.729234
C	-1.130779	-2.126647	-3.778583	C	-0.060740	1.879453	-3.643586
C	-0.261548	-3.247675	-3.878529	C	-0.951704	2.978246	-3.551805
C	-0.873969	-4.518330	-4.077279	C	-0.461217	4.248959	-3.978107
C	-2.202221	-4.715546	-3.786291	C	0.886706	4.484371	-4.076266
C	-0.585241	-0.811908	-3.661503	C	-0.519723	0.564548	-3.311448
C	2.737524	-0.510089	-1.233195	C	-3.285884	0.266425	-0.100167
C	2.480705	-1.756194	-1.864636	C	-3.042761	1.552574	-0.844719
C	2.999153	-2.971258	-1.325821	C	-3.248815	2.773383	-0.173211
C	2.222097	0.671547	-1.784008	C	-2.725832	-0.953530	-0.769211
C	2.454595	1.947454	-1.158130	C	-2.578965	-2.135621	-0.002510
C	2.781332	1.958321	0.225794	C	-2.402722	-2.071952	1.413050
C	1.505214	-1.837388	-2.902436	C	-2.372543	1.582418	-2.084875
C	1.095167	-3.107146	-3.415405	C	-2.115915	2.835609	-2.726751
C	1.921966	-4.220154	-3.120578	C	-2.801701	3.976589	-2.230924
C	2.833549	-4.149364	-2.082024	C	-3.315289	3.955670	-0.960863
C	1.221257	0.603243	-2.796352	C	-1.979854	-0.862399	-1.959498
C	0.757520	-0.668613	-3.225894	C	-1.699142	0.405735	-2.553418
C	0.468593	1.766559	-3.125723	C	-1.283633	-2.013307	-2.445491
C	0.945832	3.058334	-2.747539	C	-1.574012	-3.297586	-1.904133
C	1.967362	3.132406	-1.751395	C	-2.229023	-3.347603	-0.649783
C	0.196019	4.220808	-3.067683	C	-0.908839	-4.462525	-2.389914
C	0.750927	5.492779	-2.700397	C	-1.285665	-5.719832	-1.817220
C	1.726210	5.574306	-1.746565	C	-1.928640	-5.771387	-0.609764

C	2.200002	4.386012	-1.097356	C	-2.221196	-4.562490	0.100569
C	0.013010	-4.433724	3.414894	C	1.040383	4.476280	3.482692
C	0.701521	-3.210811	3.294922	C	0.377841	3.240795	3.599560
C	2.636248	3.176595	0.965948	C	-2.024553	-3.249048	2.131553
C	2.569456	4.385729	0.249925	C	-2.181096	-4.495777	1.496070
H	-2.602882	-5.728365	-3.817715	H	1.232243	5.498028	-4.276998
H	-4.190090	-6.045953	-2.380117	H	3.138905	5.916137	-3.344359
H	-4.560975	-6.390480	-0.004566	H	4.236378	6.365612	-1.226076
H	-3.681215	-6.588968	1.942963	H	4.052337	6.628721	0.895869
H	2.474062	-5.240094	2.538993	H	-1.605980	5.202942	3.287230
H	0.552766	-5.375863	3.328063	H	0.473912	5.405667	3.528681
H	3.533145	-5.133884	0.352094	H	-3.267894	4.979998	1.535688
H	3.328812	-5.068855	-1.767725	H	-3.664893	4.886722	-0.516688
H	1.733651	-5.185375	-3.588869	H	-2.774730	4.917326	-2.778202
H	-0.260991	-5.381486	-4.336357	H	-1.151590	5.081058	-4.111427
H	-1.623407	-6.648001	3.266570	H	2.506774	6.708898	2.792034
H	-1.981870	4.971805	4.453981	H	3.489041	-4.854592	4.156844
H	-4.128283	5.031406	3.328970	H	5.202602	-4.922557	2.443468
H	-5.310048	5.183226	1.540168	H	5.785226	-5.123200	0.380497
H	0.159299	5.042925	4.277305	H	1.384517	-4.969245	4.598008
H	2.139283	5.191971	2.877966	H	-0.907242	-5.191713	3.838087
H	2.550168	5.336838	0.781807	H	-2.004273	-5.419322	2.045900
H	2.052829	6.548068	-1.375712	H	-2.098335	-6.731459	-0.118605
H	0.310695	6.408662	-3.093509	H	-0.947895	-6.647134	-2.278936
H	-1.767352	6.175896	-3.456671	H	0.911850	-6.383301	-3.296549
H	-4.025479	5.822134	-2.644008	H	3.298305	-5.949922	-3.194683
H	-5.201151	5.506025	-0.861908	H	4.943534	-5.543477	-1.856092
C	5.053439	-0.330753	0.075237	C	-4.647282	0.161691	0.532603
C	5.722528	-1.542119	-0.599310	C	-5.369186	-1.074903	0.874764
O	6.380758	-2.388387	-0.022256	O	-4.976082	-2.230763	0.911669
O	5.451506	-1.550213	-1.913594	O	-6.667472	-0.738867	1.171494
C	5.941746	-2.713252	-2.623014	C	-7.543882	-1.879622	1.283217
H	5.676050	-3.625548	-2.077642	H	-7.534193	-2.442486	0.340510
H	5.443095	-2.679334	-3.595637	H	-7.224366	-2.530849	2.106366
H	7.032067	-2.647416	-2.731015	H	-8.535806	-1.461195	1.478269
C	5.405402	0.971507	-0.647060	C	-5.439884	1.403088	0.876584
O	5.343300	1.084208	-1.857308	O	-5.610344	1.816603	2.011954
O	5.710009	1.981592	0.192043	O	-5.948052	1.983956	-0.225832
C	5.848736	3.261371	-0.478466	C	-6.663176	3.213775	0.035143
H	6.734549	3.250457	-1.125945	H	-7.573508	3.004696	0.611425
H	4.954258	3.464840	-1.078900	H	-6.026703	3.905312	0.601769
H	5.954909	3.992118	0.327707	H	-6.904900	3.616273	-0.952437
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C	-2.079664	5.250428	-3.274570	C	-1.737606	5.242599	-3.320102
C	-1.119126	4.192834	-3.305238	C	-0.822805	4.148908	-3.258122
C	-1.626998	2.864052	-3.390502	C	-1.375657	2.840333	-3.362391
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C	-3.377594	5.001797	-2.910744	C	-3.074950	5.051214	-3.082103
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C	-4.347161	0.987243	-1.810657	C	-4.328211	1.094857	-2.064554
C	-3.398366	1.256162	-2.826869	C	-3.256603	1.311014	-2.964133
C	-5.206747	4.450540	-0.660351	C	-5.164086	4.603672	-1.045435
C	-5.348243	4.242657	0.687599	C	-5.452214	4.419411	0.283123
C	-5.019171	2.979586	1.266064	C	-5.232102	3.153101	0.902169
C	-4.981516	1.859794	0.388737	C	-5.157901	2.021720	0.043859
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C	-4.369348	2.862946	2.539528	C	-4.688469	3.029844	2.225882
C	-4.732854	-0.574074	0.037892	C	-4.980962	-0.423959	-0.256230
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C	-3.948311	-2.005336	1.863188	C	-4.410436	-1.856975	1.643178
C	-3.581960	-0.824434	2.571598	C	-4.048456	-0.681973	2.359503
C	-4.457285	-3.007084	-0.303142	C	-4.775145	-2.868567	-0.546285
C	-4.287319	-4.316799	0.234599	C	-4.713154	-4.176454	0.017170
C	-3.758663	-4.451711	1.556033	C	-4.297485	-4.313191	1.377531
C	-3.395417	-3.263314	2.252977	C	-3.933009	-3.129806	2.082124
C	-2.237588	-3.271336	3.078072	C	-2.819923	-3.168104	2.964176
C	-1.481699	-4.474532	3.224679	C	-2.116499	-4.396722	3.157328
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C	-3.220462	-5.688630	2.040657	C	-3.841190	-5.563037	1.910373
C	-4.177602	-2.777153	-1.682710	C	-4.336510	-2.667996	-1.887470
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C	-4.278741	-5.400388	-0.697951	C	-4.659186	-5.271820	-0.900429
C	-2.400518	-0.835956	3.352825	C	-2.909238	-0.724080	3.208103
C	-1.637176	-2.036903	3.442318	C	-2.195703	-1.950773	3.346482
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C	-1.793454	0.402324	3.700197	C	-2.280550	0.495353	3.570731
C	-0.383713	0.480651	3.742997	C	-0.870169	0.523408	3.697462
C	0.398751	-0.682696	3.471725	C	-0.120116	-0.671341	3.505201
C	-0.222330	-1.965239	3.541208	C	-0.784744	-1.927853	3.516677
C	-3.967138	4.006862	3.291069	C	-4.295550	4.168171	2.987227
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C	-1.959003	2.842658	4.021036	C	-2.375222	2.948327	3.845809
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C	0.225895	1.767225	3.690160	C	-0.214922	1.790458	3.663651
C	-4.502735	-0.350494	-1.345015	C	-4.594916	-0.227945	-1.611209
C	-4.009325	-1.430581	-2.133246	C	-4.060385	-1.336642	-2.326117
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C	-2.597673	0.183872	-3.314616	C	-2.452970	0.200220	-3.347719
C	-1.230721	0.435902	-3.598591	C	-1.053805	0.393453	-3.501589
C	-0.725501	1.757640	-3.449184	C	-0.518116	1.699502	-3.327925
C	1.644447	-0.553799	2.815899	C	1.193837	-0.592095	2.957949
C	2.048684	0.738370	2.375250	C	1.685576	0.676937	2.570213
C	1.448414	1.901372	2.972670	C	1.067918	1.869211	3.057988
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C	1.337332	4.301656	3.310912	C	1.039751	4.269293	3.348770
C	0.166591	4.171295	4.016911	C	-0.200900	4.196885	3.943296
C	2.797934	0.885682	1.202607	C	2.649848	0.766328	1.535396
C	3.352200	-0.295924	0.461221	C	3.302239	-0.403225	1.099682
C	3.068430	-1.624623	1.106842	C	2.826753	-1.684443	1.466733
C	2.262058	-1.725440	2.264499	C	1.815919	-1.785586	2.475455
C	3.292390	-2.796746	0.359110	C	3.114533	-2.864911	0.688657
C	3.245824	-4.033945	1.055227	C	2.903695	-4.103010	1.364472
C	2.565829	-4.133838	2.242755	C	2.041240	-4.194005	2.428289
C	1.862120	-3.009002	2.741502	C	1.309738	-3.055381	2.860634
C	-2.666798	-3.582087	-3.432984	C	-2.662787	-3.557430	-3.434691
C	-2.208777	-2.241618	-3.570532	C	-2.135890	-2.238456	-3.532460
C	-0.823887	-1.991718	-3.803509	C	-0.726957	-2.045088	-3.633083
C	0.080314	-3.085326	-3.865646	C	0.133749	-3.178455	-3.599541
C	-0.477638	-4.370199	-4.132998	C	-0.448698	-4.446735	-3.891162
C	-1.813873	-4.611184	-3.933307	C	-1.805936	-4.629800	-3.823139
C	-0.324265	-0.663586	-3.621666	C	-0.189401	-0.734716	-3.449825
C	2.842764	-0.302446	-1.015240	C	3.255567	-0.372915	-1.082832
C	2.645516	-1.562990	-1.665486	C	2.821108	-1.654479	-1.495722
C	3.131348	-2.762669	-1.084491	C	3.144698	-2.846816	-0.755917
C	2.304045	0.890728	-1.566867	C	2.535830	0.786497	-1.431735
C	2.437508	2.134010	-0.878897	C	2.581732	2.001869	-0.643229
C	2.684343	2.126408	0.529692	C	2.678239	2.001626	0.785605
C	1.744133	-1.643635	-2.761622	C	1.827662	-1.760620	-2.514896
C	1.395747	-2.914613	-3.310534	C	1.420959	-3.037792	-2.993974
C	2.220399	-4.016670	-2.962540	C	2.207097	-4.155954	-2.590230
C	3.049100	-3.942352	-1.863843	C	3.016559	-4.068221	-1.487468
C	1.373360	0.798076	-2.629198	C	1.522639	0.690547	-2.425443
C	0.980234	-0.486772	-3.110376	C	1.113981	-0.587809	-2.901810
C	0.598715	1.941734	-2.983756	C	0.778368	1.843908	-2.790506
C	1.000822	3.235331	-2.539974	C	1.216816	3.130302	-2.358679
C	1.943367	3.320788	-1.476111	C	2.123608	3.199466	-1.265392
C	0.236426	4.385248	-2.891876	C	0.513889	4.298736	-2.766535
C	0.726834	5.660962	-2.462918	C	1.031067	5.563431	-2.337892
C	1.637113	5.750334	-1.445313	C	1.895370	5.636851	-1.281252
C	2.104143	4.565128	-0.790082	C	2.283382	4.444242	-0.587514
C	-0.098102	-4.390799	3.416774	C	-0.740267	-4.361212	3.404938
C	0.560417	-3.147388	3.357778	C	-0.036268	-3.143946	3.372828
C	2.449537	3.329083	1.275933	C	2.386696	3.217733	1.495047
C	2.393640	4.546967	0.577955	C	2.467065	4.433049	0.796967
H	-2.183519	-5.632678	-4.016684	H	-2.208162	-5.636692	-3.928894
H	-3.840488	-6.028297	-2.680759	H	-4.036562	-5.941803	-2.819071
H	-4.359224	-6.426742	-0.341351	H	-4.825502	-6.288831	-0.546785
H	-3.611440	-6.632098	1.660407	H	-4.250530	-6.495974	1.523658
H	2.443654	-5.112194	2.705267	H	1.824673	-5.176949	2.844612
H	0.475472	-5.315081	3.361932	H	-0.197948	-5.305654	3.384193
H	3.629314	-4.938295	0.584721	H	3.314368	-5.022244	0.949424
H	3.549626	-4.849401	-1.525286	H	3.468400	-4.979781	-1.097813
H	2.095275	-4.975712	-3.463357	H	2.065730	-5.126362	-3.063810
H	0.177338	-5.206702	-4.375158	H	0.192051	-5.312163	-4.056569
H	-1.650845	-6.650326	3.125076	H	-2.365240	-6.565989	3.085100

H	-2.444490	4.927891	4.452650	H	-2.810861	5.052964	4.224791
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H	-5.586614	5.089572	1.330506	H	-5.717290	5.284211	0.890798
H	-0.295272	5.061468	4.442736	H	-0.664930	5.117159	4.296248
H	1.776076	5.292475	3.193114	H	1.518004	5.243853	3.255061
H	2.316963	5.486569	1.124818	H	2.382737	5.379575	1.329410
H	1.908961	6.725263	-1.035953	H	2.185969	6.606282	-0.872581
H	0.283356	6.572731	-2.861799	H	0.644113	6.483638	-2.773987
H	-1.756802	6.282884	-3.403394	H	-1.362809	6.259995	-3.424603
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H	-5.333318	5.458221	-1.054978	H	-5.207244	5.610548	-1.459420
C	4.692094	-0.110748	-0.183052	C	4.304653	-0.283937	-0.011925
C	5.491220	-1.278680	-0.712557	C	5.404335	-1.377098	0.001406
O	6.010835	-2.137509	-0.025774	O	5.840282	-1.870841	1.020436
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H	7.328003	-2.385138	-2.223447	H	6.729179	-3.448128	-0.804190
H	5.792376	-3.292952	-2.408740	H	7.085095	-2.695254	-2.411290
H	6.322381	-2.160989	-3.709693	H	7.826467	-2.003021	-0.906093
C	5.235186	1.225799	-0.620706	C	5.139060	1.024791	-0.069975
O	5.575468	1.477271	-1.767494	O	5.409998	1.592941	-1.106920
O	5.330905	2.107315	0.390817	O	5.522914	1.372002	1.160266
C	5.702424	3.442799	-0.025764	C	6.376347	2.553942	1.203495
H	6.722767	3.442187	-0.429499	H	7.329026	2.299441	0.715134
H	5.003041	3.805300	-0.790233	H	5.867062	3.383306	0.696805
H	5.637905	4.046673	0.883686	H	6.513033	2.759367	2.268496
Br	5.556160	-0.151483	2.643289	Br	8.884298	0.274590	-0.079664
(5,5)-SWCNT pristine 3cells				55 obl: Int_a			
130				146			
pristine55 -24235.2413				Int_alpha_obl -26503.1702			
H	3.570369	-1.091105	-7.077984	H	-7.640478	0.929658	3.255988
H	2.140585	3.057867	-7.078047	H	-6.831780	-3.281879	2.358522
H	3.570010	1.090359	-7.078021	H	-7.239738	-1.191173	3.527952
H	0.066094	3.732123	-7.078084	H	-6.643201	-4.171196	0.368206
H	-2.246913	2.980998	-7.078116	H	-6.679440	-3.713141	-2.015851
H	-3.529369	-1.215668	-7.078100	H	-7.379098	0.218191	-3.803306
H	-3.529448	1.216298	-7.078095	H	-6.934239	-2.151763	-3.510747
H	-2.246918	-2.980194	-7.078169	H	-7.760713	2.072359	-2.731101
H	0.065872	-3.731959	-7.078116	H	-7.998526	3.090789	-0.538358
H	2.140744	-3.058459	-7.078021	H	-7.952953	2.686006	1.605769
C	2.383811	-2.577845	-6.131005	C	-6.941886	2.429155	1.921399
C	3.187965	1.470224	-6.131032	C	-6.224649	-1.432643	3.213331
C	3.188298	-1.470737	-6.131000	C	-6.766100	1.438827	2.851535
C	3.376738	-0.717078	-4.928402	C	-5.453377	0.947927	3.142939
C	2.383753	2.577157	-6.131053	C	-5.994501	-2.612334	2.554740
C	1.725271	2.989513	-4.928386	C	-4.717451	-2.874048	1.965448
C	3.376712	0.716522	-4.928376	C	-5.189903	-0.451705	3.320569
C	-0.413145	3.486289	-6.131037	C	-5.729405	-3.829612	-0.117987
C	0.361836	3.432709	-4.928429	C	-4.589257	-3.476369	0.666848
C	-3.443510	0.684459	-6.131090	C	-6.099558	-1.451226	-3.476934
C	-1.714698	3.063603	-6.131079	C	-5.749188	-3.572563	-1.465461

C	-2.310256	2.564837	-4.928466	C	-4.633176	-2.940234	-2.098845
C	-3.443467	-0.683835	-6.131095	C	-6.353173	-0.111657	-3.642722
C	-3.153002	-1.404436	-4.928487	C	-5.321238	0.846553	-3.402432
C	-3.153087	1.405056	-4.928466	C	-4.806106	-1.904508	-3.083692
C	-1.714735	-3.063058	-6.131148	C	-6.867698	2.409108	-2.204855
C	-2.310314	-2.564277	-4.928439	C	-5.572595	2.083987	-2.715917
C	-0.413377	-3.486040	-6.131138	C	-7.002913	2.984452	-0.968314
C	0.361698	-3.432688	-4.928461	C	-5.845717	3.257129	-0.171660
C	1.725187	-2.989973	-4.928450	C	-5.816239	2.988211	1.238580
C	2.285845	-2.546062	-3.701367	C	-4.548436	2.844647	1.864342
C	3.127707	1.386915	-3.701346	C	-3.852346	-0.907115	3.158257
C	3.127755	-1.387487	-3.701346	C	-4.363390	1.803505	2.831103
C	3.339341	-0.707002	-2.464871	C	-3.027901	1.392739	3.132022
C	2.285908	2.545612	-3.701373	C	-3.612669	-2.142911	2.477039
C	1.704141	2.957175	-2.464918	C	-2.299431	-2.389185	1.966300
C	3.339362	0.706473	-2.464913	C	-2.766917	0.010936	3.289968
C	-0.352665	3.403176	-3.701426	C	-3.363354	-3.301785	-0.030404
C	0.359941	3.394122	-2.464897	C	-2.173785	-2.988255	0.693727
C	-3.345728	0.716379	-3.701441	C	-3.713756	-1.019300	-3.306426
C	-1.714809	2.960831	-3.701436	C	-3.383287	-3.035760	-1.435359
C	-2.286077	2.534717	-2.464939	C	-2.205269	-2.467281	-2.025258
C	-3.345728	-0.715802	-3.701452	C	-3.978809	0.380339	-3.468196
C	-3.116923	-1.390747	-2.464982	C	-2.899599	1.301196	-3.301945
C	-3.116965	1.391323	-2.464971	C	-2.386595	-1.422305	-2.975740
C	-1.714942	-2.960313	-3.701515	C	-4.467598	2.775909	-2.151131
C	-2.286146	-2.534256	-2.464982	C	-3.149197	2.527736	-2.637700
C	-0.352877	-3.403070	-3.701399	C	-4.606998	3.375340	-0.857052
C	0.359634	-3.394159	-2.464982	C	-3.419474	3.694420	-0.128154
C	1.704014	-2.957582	-2.464913	C	-3.389795	3.419526	1.259935
C	2.292285	-2.543321	-1.228390	C	-2.120013	3.311829	1.909503
C	3.127014	1.393943	-1.228369	C	-1.418124	-0.452482	3.158431
C	3.127094	-1.394514	-1.228358	C	-1.935842	2.274101	2.864075
C	3.357630	-0.715247	0.000011	C	-0.609777	1.857171	3.170221
C	2.292364	2.542818	-1.228369	C	-1.178451	-1.675030	2.477921
C	1.717604	2.972039	0.000026	C	0.127019	-1.947004	1.955262
C	3.357651	0.714686	0.000079	C	-0.346499	0.463196	3.318726
C	-0.359571	3.404748	-1.228421	C	-0.924441	-2.900828	0.008609
C	0.357719	3.414103	0.000026	C	0.257120	-2.652857	0.741253
C	-3.349285	0.710320	-1.228443	C	-1.292585	-0.542563	-3.220570
C	-1.710169	2.966150	-1.228432	C	-0.950993	-2.625420	-1.393757
C	-2.296047	2.552190	-0.000021	C	0.221766	-2.022496	-1.950128
C	-3.349306	-0.709770	-1.228448	C	-1.552608	0.842888	-3.412411
C	-3.136598	-1.394827	-0.000064	C	-0.483572	1.770846	-3.267979
C	-3.136661	1.395419	-0.000058	C	0.030012	-0.949088	-2.877270
C	-1.710317	-2.965695	-1.228469	C	-2.043161	3.257613	-2.102413
C	-2.296158	-2.551703	-0.000026	C	-0.734208	3.009614	-2.601077
C	-0.359809	-3.404700	-1.228421	C	-2.182158	3.863149	-0.822187
C	0.357449	-3.414146	-0.000016	C	-1.004941	4.188091	-0.089976
C	1.717471	-2.972500	0.000016	C	-0.974454	3.905827	1.311054
C	2.292195	-2.543289	1.228421	C	0.293508	3.774528	1.949008
C	3.126972	1.393890	1.228448	C	0.993561	-0.003377	3.160122

C	3.127004	-1.394509	1.228448	C	0.477261	2.731200	2.890472
C	3.339278	-0.707076	2.465003	C	1.811955	2.306718	3.187318
C	2.292301	2.542813	1.228464	C	1.233822	-1.223917	2.492374
C	1.704078	2.957117	2.464971	C	2.552824	-1.470208	1.975400
C	3.339272	0.706457	2.464987	C	2.071848	0.926933	3.324108
C	-0.359549	3.404721	1.228395	C	1.590478	-2.844826	0.036602
C	0.359788	3.394116	2.465003	C	2.725101	-2.151371	0.772713
C	-3.349337	0.710309	1.228358	C	1.115722	-0.075634	-3.150929
C	-1.710237	2.966102	1.228379	C	1.486239	-2.207075	-1.354493
C	-2.286099	2.534796	2.464918	C	2.612098	-1.544950	-1.894339
C	-3.349332	-0.709727	1.228369	C	0.856678	1.309125	-3.357138
C	-3.116992	-1.390725	2.464876	C	1.934021	2.229934	-3.198696
C	-3.117055	1.391302	2.464902	C	2.437463	-0.486160	-2.822619
C	-1.710338	-2.965631	1.228374	C	0.371928	3.725866	-2.058870
C	-2.286231	-2.534251	2.464897	C	1.688286	3.462570	-2.547304
C	-0.359830	-3.404636	1.228395	C	0.233096	4.327702	-0.778439
C	0.359597	-3.394228	2.464918	C	1.421869	4.633273	-0.042787
C	1.703961	-2.957651	2.464955	C	1.452629	4.353980	1.342963
C	2.285728	-2.546152	3.701410	C	2.723117	4.241305	1.985755
C	3.127554	1.386889	3.701431	C	3.418925	0.473217	3.220768
C	3.127670	-1.387550	3.701378	C	2.908604	3.185772	2.936346
C	2.285797	2.545507	3.701441	C	3.666248	-0.756176	2.535709
C	-0.352760	3.403176	3.701367	C	3.963649	-1.990539	0.093909
C	-3.345818	0.716395	3.701325	C	3.539557	0.372385	-3.124593
C	-1.714952	2.960842	3.701378	C	3.918844	-1.692864	-1.309335
C	-3.345803	-0.715781	3.701378	C	3.281166	1.768452	-3.304468
C	-1.715016	-2.960366	3.701404	C	2.803595	4.181384	-2.020373
C	-0.352998	-3.403128	3.701404	C	2.665305	4.787471	-0.729606
C	-3.153177	1.405114	4.928408	C	4.867388	-0.060997	-2.875315
C	-3.443605	0.684501	6.131011	C	5.919657	0.835686	-3.216277
H	-3.529580	1.216314	7.078000	H	6.953124	0.489624	-3.209383
C	-3.153055	-1.404394	4.928392	C	4.355992	2.694599	-3.202707
C	-3.443563	-0.683872	6.131032	C	5.673588	2.178902	-3.379507
H	-3.529512	-1.215652	7.078021	H	6.516504	2.860014	-3.492015
C	0.361735	3.432625	4.928471	C	5.136154	-1.668482	0.820677
C	-0.413414	3.486278	6.131101	C	6.356296	-1.576108	0.074905
H	0.065872	3.732234	7.078053	H	7.315151	-1.569476	0.592729
C	-2.310451	2.564822	4.928381	C	5.053105	-1.131309	-1.924964
C	-1.714862	3.063682	6.131085	C	6.315514	-1.322526	-1.267918
H	-2.247220	2.981205	7.078021	H	7.244414	-1.123505	-1.801764
C	3.376495	0.716400	4.928566	C	4.491025	1.382547	3.432422
C	3.187838	1.469970	6.131132	C	5.816345	0.846673	3.375357
H	3.569734	1.090232	7.078169	H	6.660107	1.441250	3.724928
C	1.725033	2.989418	4.928545	C	4.983223	-1.047978	2.102401
C	2.383441	2.577146	6.131138	C	6.055250	-0.339326	2.734524
H	2.140310	3.057708	7.078158	H	7.084010	-0.667458	2.587364
C	1.725033	-2.989989	4.928413	C	3.866059	4.851039	1.404003
C	2.383663	-2.577871	6.131079	C	5.099819	4.733867	2.120497
H	2.140596	-3.058655	7.078037	H	5.952598	5.352135	1.841115
C	3.376537	-0.717141	4.928476	C	4.227944	2.783856	3.276256
C	3.188002	-1.470949	6.131106	C	5.276122	3.727933	3.032843

H	3.570232	-1.091275	7.078047	H	6.264943	3.567800	3.461870
C	-2.310393	-2.564245	4.928397	C	4.106015	3.944405	-2.534821
C	-1.714899	-3.063047	6.131069	C	5.168614	4.730785	-1.990881
H	-2.247130	-2.980263	7.078074	H	6.139695	4.750730	-2.485244
C	0.361502	-3.432709	4.928429	C	3.836184	5.134188	-0.003006
C	-0.413483	-3.486093	6.131085	C	5.037613	5.315666	-0.758514
H	0.065644	-3.732134	7.078090	H	5.906107	5.786548	-0.298677
				C	1.941849	-4.443591	0.056812
				C	2.597604	-4.749613	1.420976
				O	3.736264	-5.135177	1.594031
				O	1.736837	-4.420688	2.397838
				C	2.316534	-4.360385	3.725376
				H	2.620082	-5.362383	4.051521
				H	3.183436	-3.687574	3.713939
				H	1.520267	-3.959766	4.358753
				C	0.711001	-5.330725	-0.172129
				O	0.229767	-6.057950	0.677182
				O	0.243453	-5.183869	-1.419774
				C	-1.026107	-5.842643	-1.670600
				H	-0.891044	-6.931055	-1.653724
				H	-1.755561	-5.544946	-0.907640
				H	-1.333537	-5.493225	-2.659508
				Br	3.249703	-4.925495	-1.370863
55 obl: Int_β				55 obl: TS_α			
146				146			
Int_beta_obl	-26500.1185			TS_alpha_obl	-26484.5753		
H	-7.129649	1.272066	3.543713	H	7.047366	1.714540	-3.558290
H	-7.007107	-2.697794	1.745743	H	7.118188	-2.321384	-1.904557
H	-7.061621	-0.889702	3.376930	H	7.069894	-0.455910	-3.474035
H	-6.981293	-3.114563	-0.420033	H	7.148540	-2.779331	0.263777
H	-6.966159	-2.099824	-2.629666	H	7.118698	-1.792363	2.489444
H	-7.064988	2.214800	-3.449259	H	7.021104	2.511658	3.420917
H	-6.991951	-0.202443	-3.701681	H	7.069542	0.085787	3.596275
H	-7.136288	3.837521	-1.986020	H	6.996348	4.180874	2.010665
H	-7.184553	4.333180	0.394739	H	6.995161	4.734241	-0.359248
H	-7.183294	3.395503	2.363564	H	7.019353	3.817113	-2.340623
C	-6.221577	2.924699	2.565812	C	6.077369	3.308546	-2.543776
C	-6.106631	-1.199838	2.954210	C	6.138102	-0.814478	-3.037954
C	-6.191196	1.727638	3.229184	C	6.092983	2.123262	-3.227841
C	-4.966062	0.995927	3.348470	C	4.899076	1.341845	-3.352158
C	-6.073541	-2.217906	2.040604	C	6.163784	-1.861912	-2.161876
C	-4.860235	-2.535180	1.349217	C	4.974247	-2.247486	-1.458870
C	-4.921685	-0.430346	3.207473	C	4.916818	-0.086594	-3.248489
C	-6.032771	-2.795773	-0.852142	C	6.195076	-2.500393	0.711942
C	-4.842683	-2.808916	-0.053734	C	4.992749	-2.558331	-0.069290
C	-6.062455	0.343221	-3.540445	C	6.113748	0.591050	3.459979
C	-6.024092	-2.223181	-2.095664	C	6.178044	-1.945517	1.961152
C	-4.826756	-1.625518	-2.606955	C	4.958966	-1.408476	2.494660
C	-6.103839	1.703567	-3.399176	C	6.086791	1.953945	3.362854
C	-4.927653	2.425469	-3.014860	C	4.870065	2.628506	3.013490
C	-4.845122	-0.374533	-3.300133	C	4.927447	-0.177801	3.216010

C	-6.197671	3.893577	-1.435164	C	6.051492	4.200693	1.468294
C	-4.973096	3.494740	-2.063527	C	4.853458	3.725580	2.096539
C	-6.224882	4.172300	-0.095888	C	6.050775	4.511886	0.136859
C	-5.028619	4.068995	0.686011	C	4.851941	4.365939	-0.635606
C	-5.027374	3.458262	1.982599	C	4.865817	3.779566	-1.942051
C	-3.791000	2.986076	2.499698	C	3.646022	3.263156	-2.457560
C	-3.676638	-1.034652	2.893149	C	3.704123	-0.754257	-2.940162
C	-3.760787	1.730613	3.189144	C	3.664258	2.020651	-3.169427
C	-2.505049	1.067208	3.320903	C	2.438241	1.305962	-3.305446
C	-3.636258	-2.125686	1.958244	C	3.724267	-1.876406	-2.041828
C	-2.398021	-2.460369	1.356707	C	2.513347	-2.285866	-1.433598
C	-2.460948	-0.335130	3.152445	C	2.457428	-0.100952	-3.168531
C	-3.607227	-2.675222	-0.744616	C	3.762844	-2.499282	0.642164
C	-2.377348	-2.761926	-0.029484	C	2.532373	-2.635853	-0.061513
C	-3.634200	0.364740	-3.388467	C	3.682049	0.499892	3.346150
C	-3.596610	-2.055020	-2.031654	C	3.742388	-1.892660	1.933616
C	-2.360298	-1.518790	-2.492744	C	2.492366	-1.420091	2.423458
C	-3.677314	1.789177	-3.246330	C	3.654570	1.928412	3.243670
C	-2.465108	2.474826	-2.934719	C	2.408388	2.563398	2.962699
C	-2.381551	-0.292799	-3.193382	C	2.464031	-0.211645	3.147683
C	-3.765678	3.869952	-1.413766	C	3.621915	4.061129	1.469459
C	-2.509348	3.540180	-2.005479	C	2.390830	3.654169	2.063654
C	-3.794042	4.162410	-0.011617	C	3.621510	4.389751	0.075268
C	-2.564010	4.111397	0.712043	C	2.388333	4.298071	-0.637739
C	-2.563343	3.510494	1.991971	C	2.402040	3.724527	-1.930104
C	-1.318535	3.064493	2.538419	C	1.172937	3.234463	-2.474343
C	-1.203132	-0.954219	2.861834	C	1.231929	-0.779950	-2.879142
C	-1.290577	1.814928	3.210877	C	1.193854	1.998701	-3.170808
C	-0.045861	1.148221	3.366582	C	-0.022446	1.281730	-3.329377
C	-1.154573	-2.040976	1.948237	C	1.243198	-1.893422	-1.993319
C	0.085051	-2.445639	1.403463	C	0.035312	-2.354519	-1.436717
C	-0.002406	-0.269377	3.182836	C	0.001176	-0.138553	-3.168911
C	-1.140472	-2.687980	-0.725248	C	1.307437	-2.607604	0.662855
C	0.117436	-3.112743	0.017908	C	0.053001	-3.022234	-0.061320
C	-1.163369	0.440685	-3.328085	C	1.209063	0.460199	3.304434
C	-1.117986	-1.991721	-1.935999	C	1.271095	-1.934214	1.869996
C	0.108180	-1.486529	-2.475675	C	0.012795	-1.507033	2.433617
C	-1.205599	1.850259	-3.202357	C	1.182930	1.869966	3.220057
C	-0.002083	2.557672	-2.920800	C	-0.059730	2.522381	2.967467
C	0.080404	-0.236588	-3.146073	C	-0.005539	-0.268404	3.137774
C	-1.292510	3.951113	-1.372626	C	1.148048	4.020014	1.451775
C	-0.044796	3.626813	-1.978933	C	-0.077511	3.623362	2.060642
C	-1.319524	4.243590	0.015914	C	1.146855	4.352434	0.073738
C	-0.097536	4.210445	0.747668	C	-0.081764	4.280300	-0.647075
C	-0.097661	3.601573	2.040447	C	-0.066516	3.707060	-1.955315
C	1.137370	3.135186	2.572679	C	-1.285379	3.198321	-2.486686
C	1.242958	-0.885286	2.897265	C	-1.212018	-0.809800	-2.870650
C	1.162179	1.885299	3.245905	C	-1.261025	1.961834	-3.183399
C	2.413283	1.207988	3.389893	C	-2.483211	1.231435	-3.322721
C	1.282709	-1.974768	1.983574	C	-1.185620	-1.904696	-1.969235
C	2.561546	-2.311384	1.419381	C	-2.445920	-2.305303	-1.386409

C	2.454360	-0.194597	3.220537	C	-2.458335	-0.171305	-3.167568
C	1.372858	-2.634457	-0.698336	C	-1.225992	-2.752871	0.704488
C	2.591712	-2.612176	0.032013	C	-2.459927	-2.677727	-0.036608
C	1.287108	0.510224	-3.298684	C	-1.243070	0.408085	3.318589
C	1.342958	-1.929858	-1.909379	C	-1.199968	-2.049055	1.959710
C	2.568563	-1.380303	-2.430392	C	-2.438631	-1.551146	2.473598
C	1.245593	1.920742	-3.171402	C	-1.270955	1.827546	3.223349
C	2.460255	2.614435	-2.869773	C	-2.518629	2.465332	2.946119
C	2.539312	-0.153301	-3.130053	C	-2.460281	-0.314784	3.161754
C	1.166072	4.021059	-1.340127	C	-1.311973	3.975605	1.445629
C	2.419908	3.679110	-1.939513	C	-2.539803	3.555369	2.045251
C	1.139371	4.312921	0.049110	C	-1.313835	4.311822	0.064382
C	2.370161	4.249880	0.778425	C	-2.547632	4.211988	-0.653882
C	2.369097	3.650166	2.058955	C	-2.533021	3.647058	-1.949528
C	3.610548	3.196265	2.600702	C	-3.759696	3.151490	-2.489638
C	3.714963	-0.822482	2.994250	C	-3.687325	-0.857704	-2.933305
C	3.632849	1.941532	3.291968	C	-3.733987	1.908483	-3.201597
C	3.762815	-1.907684	2.052774	C	-3.676627	-1.955823	-2.011491
C	3.835854	-2.453743	-0.648468	C	-3.692830	-2.632613	0.667699
C	3.758270	0.574409	-3.293671	C	-3.710942	0.355686	3.345599
C	3.823741	-1.843192	-1.939312	C	-3.685512	-2.063788	1.984549
C	3.716859	1.998588	-3.149606	C	-3.740497	1.781370	3.222400
C	3.640093	4.077440	-1.314250	C	-3.785370	3.912548	1.443951
C	3.614422	4.369822	0.087875	C	-3.788838	4.253214	0.052582
C	5.006381	-0.094993	-3.178018	C	-4.924326	-0.371733	3.252605
C	6.186362	0.690978	-3.386217	C	-6.135239	0.351547	3.475056
H	7.149351	0.199595	-3.523421	H	-7.073344	-0.186226	3.608936
C	4.922915	2.704288	-2.886063	C	-4.981834	2.433330	2.990248
C	6.146738	2.051372	-3.240857	C	-6.164863	1.717044	3.343953
H	7.078701	2.615860	-3.264007	H	-7.125347	2.230670	3.374215
C	5.058323	-2.516019	0.074238	C	-4.915159	-2.713437	-0.046045
C	6.265381	-2.439253	-0.693110	C	-6.117064	-2.706580	0.732752
H	7.219696	-2.697543	-0.234044	H	-7.065341	-2.991041	0.277438
C	5.041269	-1.346858	-2.484994	C	-4.908570	-1.624138	2.542259
C	6.256500	-1.873026	-1.940278	C	-6.112093	-2.181015	1.996000
H	7.203877	-1.696290	-2.449304	H	-7.057527	-2.057127	2.523241
C	4.914676	-0.150152	3.345220	C	-4.920443	-0.236906	-3.262368
C	6.147162	-0.850024	3.123398	C	-6.113744	-0.994896	-3.032353
H	7.071558	-0.486992	3.571327	H	-7.061494	-0.663392	-3.455380
C	5.024113	-2.244724	1.478368	C	-4.907168	-2.378880	-1.439690
C	6.197165	-1.863204	2.203568	C	-6.105755	-2.035033	-2.141804
H	7.165493	-2.283491	1.930104	H	-7.048830	-2.509709	-1.870956
C	4.831489	3.737673	2.116403	C	-4.997691	3.628206	-1.983500
C	6.037433	3.273614	2.733433	C	-6.187579	3.124687	-2.598589
H	6.976266	3.797576	2.555793	H	-7.146460	3.604228	-2.403812
C	4.872984	1.276967	3.486889	C	-4.945515	1.193097	-3.391819
C	6.056814	2.077486	3.399362	C	-6.161729	1.938786	-3.283349
H	7.010993	1.676395	3.739923	H	-7.100845	1.501557	-3.621150
C	4.883097	3.772271	-1.932027	C	-5.004218	3.533079	2.065199
C	6.065955	4.237874	-1.271191	C	-6.213876	3.958341	1.431330
H	7.020871	4.233951	-1.796205	H	-7.162512	3.886603	1.962679

C	4.833124	4.346556	0.818365	C	-5.012893	4.197776	-0.665409
C	6.041646	4.516554	0.068553	C	-6.218382	4.283313	0.100629
H	6.977706	4.729263	0.584434	H	-7.170231	4.462318	-0.398656
C	0.128130	-4.743019	0.030750	C	-0.378831	-4.450705	0.186068
C	-0.454255	-5.204813	-1.323544	C	-0.010810	-5.113858	1.458678
O	-1.485976	-5.825920	-1.480339	O	0.539110	-4.562495	2.402283
O	0.314434	-4.721188	-2.312509	O	-0.354054	-6.424393	1.457624
C	-0.273585	-4.807456	-3.635225	C	0.157463	-7.150260	2.596721
H	-0.368392	-5.856580	-3.940043	H	1.255117	-7.121635	2.587242
H	-1.259397	-4.325359	-3.626050	H	-0.215723	-6.714431	3.531869
H	0.419387	-4.264252	-4.283520	H	-0.205972	-8.173945	2.468037
C	1.519118	-5.342390	0.266286	C	-1.345957	-5.122545	-0.736453
O	2.144396	-5.968365	-0.569914	O	-2.269407	-5.839347	-0.384394
O	1.950140	-5.071762	1.508112	O	-1.113600	-4.773562	-2.018830
C	3.330890	-5.441701	1.759862	C	-2.138315	-5.186329	-2.949944
H	3.426866	-6.534472	1.774035	H	-2.111849	-6.275632	-3.079393
H	3.975587	-5.018763	0.979995	H	-3.125873	-4.879467	-2.582144
H	3.564907	-5.007921	2.735559	H	-1.893224	-4.674106	-3.885158
Br	-1.041809	-5.478326	1.475610	Br	1.973486	-5.674293	-0.849878
55_obl: TS_β				55_per: Int_α			
146				146			
TS_beta_obl -26483.0168				Int_alpha_per -26500.6547			
H	-7.620666	-0.421765	-3.407663	H	-7.088475	0.015178	-3.615565
H	-6.568661	3.717057	-2.494975	H	-7.097298	2.958458	-0.368567
H	-7.074491	1.663352	-3.702473	H	-7.090883	1.926188	-2.570247
H	-6.383793	4.551745	-0.468825	H	-7.083388	2.552833	1.795655
H	-6.505520	4.052635	1.908488	H	-7.077107	0.760380	3.443136
H	-7.477910	0.152107	3.659303	H	-7.113301	-3.540189	2.494420
H	-6.884083	2.495954	3.389687	H	-7.093227	-1.401815	3.648940
H	-7.953232	-1.674878	2.561477	H	-7.120700	-4.490994	0.531629
H	-8.205237	-2.640182	0.343119	H	-7.117792	-4.009228	-1.852585
H	-8.083347	-2.174109	-1.788423	H	-7.103822	-2.399201	-3.328617
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C	-6.060889	1.835430	-3.341574	C	-6.144027	2.077785	-2.052276
C	-6.790810	-0.991758	-2.991021	C	-6.144631	-0.507284	-3.461092
C	-5.441858	-0.589144	-3.254789	C	-4.940979	0.240672	-3.249102
C	-5.776504	2.988412	-2.666201	C	-6.147709	2.661169	-0.813397
C	-4.497880	3.161300	-2.039449	C	-4.946733	2.706476	-0.033601
C	-5.082949	0.787791	-3.420242	C	-4.941185	1.503070	-2.574752
C	-5.510958	4.135372	0.033423	C	-6.134790	2.098587	2.083213
C	-4.371681	3.721857	-0.731953	C	-4.939479	2.434992	1.372006
C	-6.099360	1.740506	3.351295	C	-6.148745	-1.839299	3.326660
C	-5.578772	3.854670	1.370521	C	-6.133780	1.087855	3.007359
C	-4.514475	3.142958	2.016589	C	-4.930608	0.347541	3.254274
C	-6.434092	0.422876	3.503190	C	-6.160245	-3.044613	2.677607
C	-5.453780	-0.598605	3.279782	C	-4.962261	-3.555966	2.082438
C	-4.768702	2.111804	2.973537	C	-4.939779	-1.077751	3.418815
C	-7.072084	-2.049308	2.041121	C	-6.171985	-4.311909	0.026177
C	-5.765936	-1.806114	2.577823	C	-4.967659	-4.176457	0.790080
C	-7.214141	-2.592598	0.793517	C	-6.170306	-4.040832	-1.315168
C	-6.056614	-2.921016	0.015330	C	-4.964385	-3.618960	-1.963653

C	-5.978068	-2.622158	-1.383640	C	-4.956638	-2.556823	-2.924931
C	-4.690849	-2.557111	-1.983478	C	-3.724331	-1.894895	-3.179999
C	-3.725212	1.157395	-3.235247	C	-3.713559	1.968248	-2.023807
C	-4.417434	-1.517871	-2.930383	C	-3.715130	-0.471908	-3.340554
C	-3.053956	-1.191178	-3.197448	C	-2.474379	0.216597	-3.172631
C	-3.420268	2.377413	-2.543803	C	-3.719955	2.598308	-0.741862
C	-2.113222	2.543337	-2.006286	C	-2.478872	2.716333	-0.046943
C	-2.699465	0.170628	-3.338764	C	-2.470034	1.455403	-2.494529
C	-3.170825	3.473784	-0.012139	C	-3.699959	2.049365	1.960380
C	-1.987775	3.110419	-0.717840	C	-2.476378	2.404486	1.337829
C	-3.735838	1.164232	3.226902	C	-3.720060	-1.786786	3.252615
C	-3.241152	3.176847	1.384386	C	-3.703208	0.973203	2.911750
C	-2.124890	2.519783	1.985605	C	-2.469059	0.306039	3.168098
C	-4.088159	-0.216338	3.381607	C	-3.730272	-3.050411	2.577398
C	-3.064688	-1.198195	3.226410	C	-2.497492	-3.550227	2.056503
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C	-4.694061	-2.563144	2.029950	C	-3.741324	-4.245325	0.075619
C	-3.374061	-2.398464	2.544395	C	-2.502476	-4.160668	0.781143
C	-4.843501	-3.133581	0.724385	C	-3.739898	-3.961680	-1.328698
C	-3.663785	-3.512515	0.015224	C	-2.499827	-3.608408	-1.941030
C	-3.586896	-3.217541	-1.365928	C	-2.492951	-2.550499	-2.879482
C	-2.299640	-3.185351	-1.988939	C	-1.252044	-1.901415	-3.173089
C	-1.326631	0.544693	-3.178519	C	-1.230818	1.970248	-1.966629
C	-2.028130	-2.147396	-2.918349	C	-1.243465	-0.492554	-3.316775
C	-0.673621	-1.820634	-3.202581	C	-0.013034	0.213704	-3.161794
C	-1.016624	1.755276	-2.500654	C	-1.249907	2.685279	-0.762832
C	0.291259	1.951431	-1.982303	C	0.008245	3.105628	-0.028706
C	-0.316660	-0.442265	-3.322381	C	-0.004640	1.473524	-2.510015
C	-0.775440	2.901616	0.002990	C	-1.220439	2.019978	1.919945
C	0.437741	2.673351	-0.731667	C	0.000528	2.442251	1.352608
C	-1.343692	0.539110	3.184123	C	-1.247391	-1.813842	3.241062
C	-0.843551	2.585094	1.362510	C	-1.230616	0.949516	2.852147
C	0.291518	1.927311	1.968217	C	-0.009547	0.299866	3.168266
C	-1.691536	-0.820622	3.357995	C	-1.255531	-3.070503	2.580892
C	-0.675278	-1.814242	3.232537	C	-0.029712	-3.582364	2.068936
C	0.010150	0.870147	2.883312	C	-0.016612	-1.115731	3.369945
C	-2.300683	-3.187875	2.019711	C	-1.265396	-4.269501	0.067919
C	-0.987932	-3.026846	2.547904	C	-0.034215	-4.202182	0.781199
C	-2.450562	-3.761879	0.731466	C	-1.265309	-3.987427	-1.323291
C	-1.281233	-4.157497	0.017775	C	-0.034401	-3.640081	-1.950529
C	-1.206312	-3.861999	-1.377792	C	-0.029501	-2.578905	-2.902420
C	0.077170	-3.810039	-1.991913	C	1.200307	-1.917184	-3.177736
C	1.044368	-0.073646	-3.134978	C	1.228966	1.943296	-1.960437
C	0.347061	-2.767830	-2.915878	C	1.208265	-0.508360	-3.320993
C	1.711873	-2.430426	-3.181160	C	2.448780	0.184159	-3.178908
C	1.344952	1.122269	-2.436766	C	1.258026	2.652355	-0.755836
C	2.669191	1.247869	-1.875357	C	2.485849	2.672244	-0.041101
C	2.064125	-1.069414	-3.286207	C	2.460470	1.418191	-2.493152
C	1.750106	2.634832	0.026782	C	1.216659	2.019590	1.930481
C	2.856980	1.894894	-0.668055	C	2.478943	2.394395	1.350757
C	1.034346	-0.063988	3.185128	C	1.207260	-1.824399	3.237837

C	1.578419	2.072793	1.434801	C	1.216544	0.942781	2.857813
C	2.650416	1.340782	2.000512	C	2.449160	0.285955	3.170995
C	0.685565	-1.434838	3.358905	C	1.201955	-3.080951	2.577308
C	1.709549	-2.416821	3.206661	C	2.437891	-3.571831	2.049788
C	2.383562	0.273643	2.896002	C	2.444103	-1.115276	3.354891
C	0.081821	-3.803223	2.018642	C	1.194490	-4.281866	0.065076
C	1.403034	-3.621059	2.531102	C	2.434142	-4.184099	0.775380
C	-0.069492	-4.382376	0.728360	C	1.194194	-4.001445	-1.326492
C	1.111262	-4.755774	0.011684	C	2.431404	-3.637721	-1.947919
C	1.184748	-4.468685	-1.370215	C	2.434469	-2.581480	-2.888273
C	2.471475	-4.434495	-1.990151	C	3.673165	-1.941392	-3.193052
C	3.437684	-0.709008	-3.146684	C	3.709670	1.913968	-2.020541
C	2.743154	-3.384813	-2.925652	C	3.680983	-0.518036	-3.351284
C	3.746919	0.484705	-2.428320	C	3.724393	2.539707	-0.736675
C	4.066563	1.696627	0.037418	C	3.700292	2.022137	1.972125
C	3.424676	-0.657423	3.206221	C	3.679078	-1.820926	3.245654
C	3.974788	1.421412	1.445432	C	3.690997	0.942305	2.920388
C	3.078960	-2.037676	3.347438	C	3.676104	-3.083278	2.567978
C	2.482630	-4.401903	2.015663	C	3.670566	-4.282532	0.067667
C	2.329930	-4.991851	0.719766	C	3.669036	-4.003730	-1.337595
C	4.778830	-0.297212	2.994191	C	4.905813	-1.125690	3.415156
C	5.768688	-1.262818	3.337166	C	6.106942	-1.898859	3.317988
H	6.820015	-0.977845	3.362022	H	7.056213	-1.471908	3.640230
C	4.097441	-3.024841	3.248222	C	4.902211	-3.600944	2.070978
C	5.438889	-2.592101	3.457216	C	6.105884	-3.102081	2.664774
H	6.237597	-3.324567	3.569904	H	7.053967	-3.605956	2.478446
C	5.228319	1.291600	-0.664229	C	4.944124	2.382031	1.376272
C	6.427154	1.142367	0.107275	C	6.136538	2.033515	2.086628
H	7.396321	1.089756	-0.388099	H	7.090455	2.474325	1.795648
C	5.055966	0.784098	2.077693	C	4.911212	0.300618	3.259279
C	6.343523	0.902596	1.449178	C	6.123513	1.026548	3.014131
H	7.247649	0.664059	2.008402	H	7.062351	0.688720	3.451544
C	4.451995	-1.681731	-3.354021	C	4.931319	1.438401	-2.575814
C	5.807906	-1.237873	-3.243624	C	6.140465	1.998421	-2.052849
H	6.620812	-1.880744	-3.580154	H	7.085388	1.835974	-2.571209
C	5.066301	0.683215	-1.949669	C	4.953190	2.640652	-0.031800
C	6.105287	-0.086192	-2.564800	C	6.151950	2.581784	-0.813221
H	7.149079	0.165823	-2.377985	H	7.106031	2.866630	-0.369571
C	3.560855	-5.122404	-1.393646	C	4.898116	-2.617509	-2.940406
C	4.811142	-5.083266	-2.088742	C	6.102312	-1.941120	-3.318353
H	5.615481	-5.760428	-1.802616	H	7.045974	-2.485328	-3.350358
C	4.092255	-3.065630	-3.232987	C	4.915357	0.179856	-3.257900
C	5.069878	-4.080819	-2.985121	C	6.109613	-0.581478	-3.475192
H	6.074473	-3.982022	-3.395471	H	7.059352	-0.069946	-3.630330
C	3.786644	-4.247230	2.554773	C	4.898935	-4.223807	0.779635
C	4.809734	-5.092405	2.024018	C	6.100133	-4.374520	0.013953
H	5.769530	-5.172157	2.533769	H	7.048067	-4.561035	0.518188
C	3.488781	-5.407916	0.011869	C	4.895832	-3.677285	-1.976393
C	4.664480	-5.661604	0.785913	C	6.098458	-4.109467	-1.328653
H	5.511699	-6.179838	0.337716	H	7.045115	-4.089883	-1.868081
C	1.686604	4.097949	-0.342055	C	0.036687	4.764270	0.044563

C	2.058447	4.561688	-1.722218	C	-1.291966	5.318044	0.594403
O	1.366479	5.305637	-2.398686	O	-2.130353	5.898515	-0.068928
O	3.210926	4.012455	-2.150545	O	-1.422800	5.018964	1.895985
C	3.480214	4.175489	-3.561606	C	-2.721404	5.348255	2.454817
H	2.612516	3.848071	-4.148268	H	-3.517269	4.974535	1.800495
H	3.706103	5.225414	-3.785686	H	-2.744735	4.844777	3.425237
H	4.347366	3.537375	-3.755851	H	-2.809809	6.436142	2.567508
C	1.124248	5.069703	0.618830	C	1.235465	5.220413	0.879078
O	0.697895	4.772946	1.725721	O	1.225499	5.223086	2.096398
O	1.152506	6.337215	0.139025	O	2.309672	5.527562	0.126526
C	0.818642	7.329438	1.136323	C	3.519842	5.741342	0.899366
H	-0.195658	7.161694	1.518765	H	3.442558	6.679413	1.463615
H	1.540107	7.275505	1.962253	H	3.669847	4.904452	1.591605
H	0.889452	8.289837	0.617682	H	4.322028	5.787774	0.158002
Br	4.171896	4.804839	0.975628	Br	0.184435	5.368010	-1.846359
55_per: Int_β				55_per: TS_α			
146				146			
Int_beta_per -26500.6895				TS_alpha_per -26474.9003			
H	-7.002073	-1.602706	-3.685324	H	-7.039915	-0.132383	3.712129
H	-7.114073	2.333554	-1.823353	H	-7.050199	-3.027762	0.420286
H	-7.045530	0.556438	-3.487283	H	-7.027418	-2.029216	2.637244
H	-7.149710	2.715214	0.343615	H	-7.078165	-2.589033	-1.734103
H	-7.125354	1.674054	2.540258	H	-7.127094	-0.769454	-3.347789
H	-7.017963	-2.650191	3.298883	H	-7.216815	3.514420	-2.364925
H	-7.073994	-0.236709	3.589910	H	-7.179272	1.393787	-3.552647
H	-6.980745	-4.248664	1.809969	H	-7.213947	4.422938	-0.378439
H	-6.960812	-4.708318	-0.578681	H	-7.166449	3.909147	1.998403
H	-6.971013	-3.742444	-2.534560	H	-7.100240	2.284911	3.456212
C	-6.030419	-3.221724	-2.712315	C	-6.142168	1.768383	3.404844
C	-6.115294	0.908045	-3.042420	C	-6.086049	-2.158330	2.103833
C	-6.047686	-2.015382	-3.359551	C	-6.107889	0.407825	3.547767
C	-4.859197	-1.221582	-3.445480	C	-4.895494	-0.316277	3.308306
C	-6.151079	1.910247	-2.110377	C	-6.098548	-2.722333	0.854940
C	-4.969136	2.275325	-1.390866	C	-4.910801	-2.737544	0.058063
C	-4.889552	0.203610	-3.283116	C	-4.886173	-1.568442	2.613497
C	-6.193757	2.444179	0.791839	C	-6.141667	-2.117405	-2.031403
C	-4.991334	2.526928	0.018254	C	-4.929910	-2.441861	-1.344850
C	-6.114812	-0.731386	3.438396	C	-6.238064	1.838988	-3.231421
C	-6.180127	1.854867	2.028613	C	-6.170074	-1.090554	-2.937765
C	-4.965014	1.312474	2.556304	C	-4.986051	-0.329925	-3.198637
C	-6.083475	-2.089967	3.275508	C	-6.259349	3.033653	-2.563729
C	-4.865782	-2.744260	2.902079	C	-5.061861	3.552550	-1.974303
C	-4.932223	0.050996	3.232228	C	-5.019434	1.095883	-3.345868
C	-6.030645	-4.249185	1.276255	C	-6.254711	4.255251	0.110618
C	-4.839590	-3.799415	1.933433	C	-5.059194	4.152665	-0.672539
C	-6.019445	-4.507712	-0.067618	C	-6.227886	3.965908	1.447672
C	-4.816382	-4.332317	-0.825118	C	-5.004464	3.559740	2.072817
C	-4.822228	-3.703210	-2.113354	C	-4.962975	2.483248	3.017803
C	-3.601953	-3.162435	-2.600105	C	-3.716106	1.841108	3.246164
C	-3.682328	0.863992	-2.933551	C	-3.660289	-2.006463	2.038155
C	-3.621981	-1.897051	-3.271761	C	-3.680504	0.415728	3.386092

C	-2.398359	-1.170272	-3.369822	C	-2.433197	-0.249306	3.184983
C	-3.715681	1.939064	-1.980440	C	-3.676353	-2.612061	0.745869
C	-2.504646	2.328792	-1.349728	C	-2.444061	-2.699919	0.030690
C	-2.428166	0.229791	-3.179327	C	-2.419299	-1.478655	2.494360
C	-3.765343	2.443257	0.730403	C	-3.712011	-2.026468	-1.948270
C	-2.524884	2.600435	0.043373	C	-2.465964	-2.375510	-1.353432
C	-3.686853	-0.626495	3.330040	C	-3.807379	1.818337	-3.184005
C	-3.748105	1.811344	2.011197	C	-3.742793	-0.942734	-2.883746
C	-2.493616	1.334252	2.489029	C	-2.521900	-0.257539	-3.152344
C	-3.653956	-2.048768	3.165511	C	-3.828777	3.072172	-2.491418
C	-2.402820	-2.666524	2.865682	C	-2.597796	3.585162	-1.981662
C	-2.465532	0.097133	3.168829	C	-2.555763	1.145290	-3.316411
C	-3.603542	-4.101951	1.300740	C	-3.823911	4.236253	0.024249
C	-2.376027	-3.718182	1.920533	C	-2.594695	4.182422	-0.700275
C	-3.591595	-4.373947	-0.105793	C	-3.796091	3.932761	1.424554
C	-2.352673	-4.251192	-0.805240	C	-2.541232	3.593200	2.013242
C	-2.358894	-3.632829	-2.076731	C	-2.501617	2.522319	2.935063
C	-1.128169	-3.118654	-2.594101	C	-1.245545	1.890219	3.196785
C	-1.208674	0.905643	-2.855319	C	-1.183642	-1.970493	1.941860
C	-1.150560	-1.859133	-3.248628	C	-1.210832	0.478774	3.309759
C	0.062024	-1.129356	-3.369669	C	0.027520	-0.200423	3.131486
C	-1.232674	1.978038	-1.923081	C	-1.209710	-2.677611	0.736685
C	-0.027323	2.418373	-1.335739	C	0.047203	-3.053556	0.002257
C	0.029847	0.284912	-3.161341	C	0.050411	-1.451645	2.448177
C	-1.301304	2.598170	0.765851	C	-1.240285	-1.988295	-1.974107
C	-0.054300	3.075253	0.048447	C	0.010251	-2.414767	-1.437371
C	-1.214518	-0.575176	3.315569	C	-1.335799	1.881601	-3.202436
C	-1.267826	1.882963	1.966894	C	-1.269461	-0.893052	-2.870380
C	-0.030059	1.430805	2.521830	C	-0.058778	-0.213788	-3.184736
C	-1.181811	-1.983034	3.166047	C	-1.356090	3.130290	-2.528453
C	0.060583	-2.622732	2.895502	C	-0.132961	3.662843	-2.032741
C	-0.004584	0.168092	3.167603	C	-0.094249	1.203631	-3.353757
C	-1.129080	-4.058064	1.305215	C	-1.349374	4.305332	-0.004238
C	0.089391	-3.679164	1.938718	C	-0.128353	4.266505	-0.735998
C	-1.115957	-4.331672	-0.087676	C	-1.322255	4.002335	1.382325
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C	0.108626	-3.601820	-2.080476	C	-0.037869	2.587885	2.915272
C	1.328793	-3.066857	-2.582271	C	1.205050	1.947511	3.163918
C	1.237928	0.953362	-2.834605	C	1.280182	-1.919400	1.920319
C	1.303553	-1.807391	-3.236669	C	1.237442	0.532348	3.280364
C	2.522420	-1.066240	-3.343708	C	2.482197	-0.141433	3.119582
C	1.203973	2.018975	-1.897415	C	1.312340	-2.696043	0.732788
C	2.449789	2.421491	-1.305712	C	2.518133	-2.611606	-0.016533
C	2.488865	0.332367	-3.146144	C	2.501659	-1.377851	2.437098
C	1.205879	2.671515	0.788517	C	1.230871	-1.931902	-1.993309
C	2.438558	2.726634	0.080590	C	2.481207	-2.248431	-1.387033
C	1.236521	-0.518224	3.327126	C	1.117317	1.939296	-3.237493
C	1.191104	1.950534	1.988661	C	1.186835	-0.835879	-2.895369
C	2.435465	1.453925	2.521988	C	2.399609	-0.142377	-3.206510
C	1.269862	-1.926086	3.177100	C	1.098484	3.189890	-2.564341
C	2.523292	-2.552829	2.888325	C	2.332400	3.702019	-2.052727

C	2.456273	0.212156	3.194388	C	2.365145	1.259238	-3.379908
C	1.329806	-4.002558	1.317527	C	1.109132	4.362867	-0.039933
C	2.553940	-3.605891	1.944856	C	2.338214	4.297654	-0.770780
C	1.343370	-4.277794	-0.075006	C	1.136147	4.058925	1.348219
C	2.582832	-4.144471	-0.779868	C	2.388742	3.703125	1.941840
C	2.575401	-3.528153	-2.052416	C	2.423358	2.631553	2.863375
C	3.802767	-3.005131	-2.563201	C	3.674831	2.002502	3.137651
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C	3.775436	-1.738795	-3.232795	C	3.705526	0.578252	3.283530
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C	3.677102	2.625826	0.782673	C	3.694823	-1.843213	-2.016280
C	3.707283	-0.456335	3.366916	C	3.588221	1.989110	-3.284501
C	3.673193	1.989737	2.061633	C	3.655729	-0.767555	-2.957229
C	3.741601	-1.878162	3.199838	C	3.571317	3.245579	-2.597209
C	3.803561	-3.935023	1.338637	C	3.584035	4.407010	-0.080879
C	3.818576	-4.211599	-0.067009	C	3.610455	4.098538	1.318066
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C	6.136138	-0.451454	3.503352	C	6.011936	2.119211	-3.398148
H	7.069968	0.086094	3.666661	H	6.963755	1.714414	-3.741009
C	4.986473	-2.518094	2.949615	C	4.794360	3.784056	-2.116439
C	6.169114	-1.809554	3.336418	C	5.997216	3.318190	-2.737105
H	7.128098	-2.326276	3.368336	H	6.937271	3.841888	-2.565597
C	4.906269	2.757855	0.082645	C	4.945625	-2.217438	-1.456447
C	6.102975	2.728745	0.869841	C	6.121011	-1.838506	-2.172944
H	7.050184	3.044082	0.432452	H	7.084806	-2.268098	-1.900118
C	4.904925	1.542465	2.618204	C	4.862414	-0.104811	-3.313420
C	6.101291	2.139614	2.105996	C	6.083007	-0.810206	-3.079926
H	7.047251	2.001387	2.629302	H	7.015959	-0.446004	-3.508973
C	4.949878	0.415473	-3.217017	C	4.971729	-1.365772	2.497339
C	6.138934	1.174636	-2.958987	C	6.183370	-1.899923	1.956951
H	7.090307	0.864955	-3.390244	H	7.132039	-1.727644	2.464343
C	4.912216	2.493153	-1.324221	C	4.980038	-2.530813	-0.055726
C	6.117181	2.180585	-2.029847	C	6.186938	-2.462031	0.706534
H	7.056184	2.649357	-1.734281	H	7.138924	-2.723887	0.245223
C	5.040106	-3.492186	-2.062953	C	4.885255	2.698598	2.874977
C	6.232864	-2.958144	-2.648610	C	6.103331	2.035997	3.224727
H	7.192924	-3.438763	-2.462266	H	7.041031	2.590793	3.238960
C	4.984079	-1.008597	-3.388225	C	4.946560	-0.102372	3.179024
C	6.205106	-1.750108	-3.292159	C	6.131642	0.674422	3.374701
H	7.144023	-1.295210	-3.606458	H	7.091723	0.176533	3.507389
C	5.018178	-3.575004	1.983081	C	4.801006	4.382919	-0.812583
C	6.235032	-3.973033	1.340063	C	6.011698	4.536086	-0.063718
H	7.178500	-3.927814	1.883524	H	6.948677	4.745594	-0.578991
C	5.048016	-4.118461	-0.773423	C	4.851470	3.778598	1.930363
C	6.249713	-4.237179	-0.002598	C	6.036250	4.240312	1.272756
H	7.204460	-4.397421	-0.502958	H	6.992390	4.221173	1.794996
C	-0.108109	4.733465	-0.017420	C	0.001810	-4.372457	-0.723512
C	1.212712	5.311987	-0.561351	C	-1.326957	-5.018104	-1.009734
O	2.038805	5.905787	0.105677	O	-1.811712	-5.142684	-2.123138
O	1.352414	5.018963	-1.863043	O	-1.916067	-5.440098	0.127385
C	2.646468	5.371959	-2.417435	C	-3.252530	-5.970134	-0.058505

H	2.717115	6.461387	-2.527082	H	-3.204588	-6.921608	-0.602989
H	3.446584	5.009458	-1.761919	H	-3.644535	-6.111716	0.952362
H	2.680936	4.871413	-3.389020	H	-3.864480	-5.255007	-0.621509
C	-1.312039	5.173762	-0.852999	C	1.139031	-5.159109	-1.209298
O	-1.299109	5.181466	-2.070300	O	2.301437	-4.831225	-1.402294
O	-2.392615	5.461127	-0.101997	O	0.698047	-6.439840	-1.440587
C	-3.604696	5.657138	-0.876667	C	1.759935	-7.366481	-1.749276
H	-3.540856	6.597111	-1.439307	H	2.265840	-7.075702	-2.678630
H	-3.740736	4.818867	-1.570065	H	2.484791	-7.385336	-0.925145
H	-4.408853	5.689921	-0.136700	H	1.269020	-8.337921	-1.859879
Br	-0.270918	5.326970	1.875924	Br	1.164140	-5.284936	1.977342
55_per: TS_β				55_obl: PC			
146				146			
TS_beta_per -26474.7816				PC_obl -26487.8360			
H	7.113324	1.531418	-3.591755	H	-7.287617	-0.913302	-3.658081
H	7.083088	-2.463365	-1.797360	H	-6.814722	3.104445	-2.021185
H	7.094813	-0.633456	-3.399908	H	-7.012249	1.241207	-3.580145
H	7.076027	-2.919025	0.351872	H	-6.793604	3.600545	0.130085
H	7.054401	-1.936593	2.576021	H	-6.906786	2.690686	2.384680
H	7.069856	2.372137	3.423892	H	-7.413706	-1.548767	3.402553
H	7.047136	-0.047410	3.664226	H	-7.120938	0.862395	3.556827
H	7.101770	4.006066	1.976877	H	-7.618300	-3.202776	1.989652
H	7.125003	4.537268	-0.396382	H	-7.681121	-3.797318	-0.368136
H	7.127573	3.644112	-2.389521	H	-7.562175	-2.964140	-2.382523
C	6.175991	3.150590	-2.585271	C	-6.557276	-2.594802	-2.585083
C	6.145168	-0.971674	-2.986530	C	-6.041946	1.473054	-3.142239
C	6.167785	1.960337	-3.261175	C	-6.402601	-1.439380	-3.301723
C	4.959632	1.199985	-3.372761	C	-5.110601	-0.833537	-3.427364
C	6.137639	-2.004520	-2.086271	C	-5.930626	2.518134	-2.270794
C	4.935469	-2.351646	-1.394556	C	-4.702696	2.740375	-1.562690
C	4.948529	-0.227295	-3.234729	C	-4.931166	0.584839	-3.343227
C	6.123072	-2.630894	0.795339	C	-5.888775	3.208993	0.594037
C	4.930211	-2.657409	0.006850	C	-4.686706	3.076499	-0.176881
C	6.106036	0.480001	3.510405	C	-6.245998	0.226019	3.426658
C	6.111189	-2.075809	2.048415	C	-5.951594	2.698736	1.860667
C	4.906677	-1.507660	2.570826	C	-4.819792	2.020314	2.424079
C	6.119108	1.841882	3.376192	C	-6.410623	-1.127724	3.340658
C	4.926842	2.541647	3.002484	C	-5.299695	-1.968432	2.999750
C	4.902720	-0.260202	3.274697	C	-4.962826	0.816930	3.177798
C	6.158584	4.052992	1.433201	C	-6.682215	-3.371146	1.457971
C	4.945758	3.624584	2.063955	C	-5.433427	-3.064932	2.090863
C	6.171748	4.352157	0.098046	C	-6.717630	-3.705771	0.132364
C	4.972520	4.237671	-0.677524	C	-5.505735	-3.752490	-0.631300
C	4.975056	3.647204	-1.983867	C	-5.427962	-3.209905	-1.954651
C	3.745819	3.152206	-2.496056	C	-4.144365	-2.884080	-2.470671
C	3.716462	-0.860446	-2.915638	C	-3.639991	1.083412	-3.033634
C	3.738230	1.903103	-3.197434	C	-3.983300	-1.670913	-3.214711
C	2.495815	1.212477	-3.326154	C	-2.668281	-1.135783	-3.352508
C	3.707743	-1.950081	-1.986776	C	-3.515099	2.200546	-2.139226
C	2.470210	-2.321487	-1.386493	C	-2.259229	2.440560	-1.522280
C	2.483884	-0.191650	-3.171690	C	-2.492667	0.262098	-3.243596

C	3.699177	-2.554548	0.703609	C	-3.481615	2.863358	0.545564
C	2.462802	-2.654789	-0.003613	C	-2.246131	2.787900	-0.152746
C	3.677855	0.453119	3.366515	C	-3.824734	-0.025381	3.322784
C	3.683377	-1.958841	2.000426	C	-3.545155	2.317320	1.863970
C	2.438087	-1.453096	2.469871	C	-2.372986	1.697311	2.383415
C	3.691291	1.879677	3.235485	C	-3.998959	-1.444975	3.231963
C	2.464619	2.544544	2.936985	C	-2.853814	-2.251596	2.964340
C	2.438846	-0.228971	3.169861	C	-2.517928	0.507282	3.126063
C	3.727580	3.983724	1.426591	C	-4.258116	-3.580785	1.478960
C	2.481962	3.621540	2.021662	C	-2.985915	-3.345301	2.078444
C	3.741084	4.297391	0.028336	C	-4.295616	-3.933643	0.091160
C	2.507821	4.230398	-0.688151	C	-3.057523	-4.034974	-0.611910
C	2.510883	3.642804	-1.973934	C	-2.981123	-3.498941	-1.917965
C	1.272347	3.173495	-2.515619	C	-1.691508	-3.198804	-2.460666
C	1.242902	-0.848320	-2.887185	C	-1.185817	0.769582	-2.953448
C	1.265874	1.929432	-3.198529	C	-1.532958	-1.990327	-3.186551
C	0.033544	1.234330	-3.347232	C	-0.226641	-1.453111	-3.345583
C	1.235908	-1.950825	-1.999890	C	-1.050571	1.880370	-2.079139
C	-0.006127	-2.403910	-1.462783	C	0.206473	2.177247	-1.509360
C	0.020034	-0.184927	-3.189211	C	-0.051223	-0.039718	-3.216094
C	1.234189	-2.656220	0.710863	C	-1.036972	2.615975	0.577963
C	-0.021413	-3.039910	-0.018635	C	0.234460	2.814752	-0.157918
C	1.206884	0.479557	3.309149	C	-1.369776	-0.334805	3.291692
C	1.205913	-1.957925	1.922028	C	-1.087745	2.020498	1.826802
C	-0.030856	-1.463999	2.442853	C	0.103816	1.432427	2.401577
C	1.219878	1.892315	3.203778	C	-1.544233	-1.735711	3.223226
C	0.000438	2.573690	2.934891	C	-0.406553	-2.562744	2.989539
C	-0.022413	-0.217139	3.134373	C	-0.063172	0.208892	3.127057
C	1.252839	4.016819	1.402011	C	-1.804628	-3.895470	1.483878
C	0.015912	3.663872	2.011203	C	-0.539995	-3.670052	2.098450
C	1.265696	4.329618	0.017282	C	-1.841816	-4.251277	0.112236
C	0.040504	4.278103	-0.706281	C	-0.610961	-4.369547	-0.597739
C	0.045010	3.683725	-2.007435	C	-0.535686	-3.829200	-1.918074
C	-1.182861	3.196709	-2.534339	C	0.746187	-3.509133	-2.446959
C	-1.215012	-0.827642	-2.899315	C	1.240982	0.463457	-2.913079
C	-1.187959	1.951088	-3.217105	C	0.901488	-2.297262	-3.169315
C	-2.426725	1.254506	-3.357838	C	2.215031	-1.748390	-3.307526
C	-1.237834	-1.931817	-2.006243	C	1.362095	1.568464	-2.026933
C	-2.478247	-2.269282	-1.393946	C	2.656229	1.774751	-1.408486
C	-2.439671	-0.149127	-3.196414	C	2.386293	-0.354203	-3.178286
C	-1.285148	-2.695911	0.715415	C	1.532034	2.568642	0.688676
C	-2.497405	-2.635455	-0.021934	C	2.730115	2.160849	-0.078893
C	-1.241928	0.497318	3.296030	C	1.061991	-0.634257	3.319392
C	-1.257967	-1.944081	1.914693	C	1.377464	1.797601	1.950084
C	-2.484397	-1.423549	2.444685	C	2.523772	1.120000	2.450085
C	-1.231283	1.913123	3.187752	C	0.888492	-2.047008	3.248063
C	-2.461542	2.581584	2.900187	C	2.034151	-2.858822	2.989621
C	-2.478180	-0.193301	3.138084	C	2.369054	-0.097084	3.155373
C	-1.206097	4.036941	1.385019	C	0.635521	-4.204585	1.500862
C	-2.449227	3.659066	1.985083	C	1.906293	-3.954545	2.105014
C	-1.193397	4.350643	-0.001019	C	0.598711	-4.563372	0.125313

C	-2.426403	4.272484	-0.723935	C	1.838770	-4.653411	-0.582708
C	-2.420621	3.686618	-2.010424	C	1.913398	-4.119051	-1.888813
C	-3.656298	3.216463	-2.550289	C	3.201052	-3.813660	-2.426887
C	-3.685068	-0.794282	-2.944146	C	3.698668	0.152494	-2.936994
C	-3.659537	1.965592	-3.247999	C	3.356143	-2.594329	-3.162185
C	-3.701990	-1.877044	-2.010510	C	3.836865	1.247761	-2.028051
C	-3.738875	-2.514663	0.669849	C	3.936902	1.966946	0.634998
C	-3.710567	0.507399	3.315302	C	3.510932	-0.933730	3.364161
C	-3.732473	-1.917862	1.965843	C	3.839804	1.445054	1.968981
C	-3.701795	1.932978	3.179397	C	3.339186	-2.350557	3.265322
C	-3.680817	4.040480	1.372247	C	3.092505	-4.495437	1.520987
C	-3.668826	4.358369	-0.024790	C	3.056712	-4.857777	0.135759
C	-4.942533	-0.189935	3.212371	C	4.814627	-0.385965	3.275258
C	-6.137609	0.567859	3.423577	C	5.908778	-1.268285	3.516459
H	-7.089106	0.054759	3.560304	H	6.913165	-0.866973	3.647157
C	-4.923997	2.612962	2.929378	C	4.476979	-3.175190	3.054802
C	-6.130132	1.930493	3.283614	C	5.746279	-2.627222	3.406077
H	-7.075367	2.471920	3.309774	H	6.625473	-3.269304	3.448295
C	-4.961609	-2.592563	-0.043736	C	5.160252	1.858745	-0.068113
C	-6.163871	-2.548022	0.727522	C	6.344727	1.696349	0.718854
H	-7.114861	-2.821270	0.270793	H	7.326432	1.831745	0.266141
C	-4.953980	-1.446147	2.518564	C	4.980413	0.845930	2.542120
C	-6.160563	-1.994568	1.981832	C	6.255847	1.208999	1.993841
H	-7.108428	-1.840443	2.496554	H	7.169743	0.963450	2.533566
C	-4.903699	-0.145960	-3.286064	C	4.833796	-0.641578	-3.248175
C	-6.112625	-0.870330	-3.048715	C	6.119199	-0.056117	-3.019026
H	-7.053746	-0.516655	-3.468583	H	7.013552	-0.524425	-3.428783
C	-4.943140	-2.271473	-1.442771	C	5.108175	1.504549	-1.456388
C	-6.129208	-1.904500	-2.147811	C	6.251985	0.989563	-2.146273
H	-7.084771	-2.349267	-1.870386	H	7.249315	1.337086	-1.877901
C	-4.883811	3.732939	-2.056810	C	4.355418	-4.451007	-1.900812
C	-6.083915	3.255072	-2.673860	C	5.608084	-4.134019	-2.514777
H	-7.030109	3.764129	-2.492373	H	6.488125	-4.740476	-2.302602
C	-4.889396	1.281133	-3.435261	C	4.657694	-2.062594	-3.354777
C	-6.085756	2.061636	-3.344867	C	5.754933	-2.970978	-3.223227
H	-7.033741	1.646153	-3.685536	H	6.748463	-2.678383	-3.561454
C	-4.912801	3.698466	1.991021	C	4.348403	-4.283743	2.147348
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H	-7.061096	4.109509	1.872960	H	6.434851	-4.940878	2.070309
C	-4.890376	4.321458	-0.748398	C	4.280863	-4.989921	-0.571533
C	-6.098155	4.451034	0.009771	C	5.456371	-5.232768	0.206484
H	-7.041714	4.649819	-0.497694	H	6.376513	-5.553355	-0.281044
C	0.031040	-4.344234	-0.762940	C	1.067220	3.981218	0.325101
C	-1.108106	-5.163153	-1.197736	C	0.479328	4.864766	1.411544
O	-2.291911	-4.875265	-1.298515	O	-0.710913	5.047309	1.582364
O	-0.636480	-6.416314	-1.500511	O	1.471870	5.337007	2.177025
C	-1.682455	-7.381627	-1.739052	C	1.051711	6.373106	3.107514
H	-2.326442	-7.452779	-0.852838	H	0.706707	7.231577	2.513611
H	-2.283101	-7.090044	-2.609770	H	0.252921	5.994018	3.755864
H	-1.163087	-8.327038	-1.921575	H	1.949116	6.618874	3.681534
C	1.362219	-4.954057	-1.126062	C	2.010809	4.697648	-0.631296

O	1.792181	-5.038528	-2.265031	O	3.131858	5.050935	-0.323637
O	2.015563	-5.387639	-0.031651	O	1.465150	4.755451	-1.855369
C	3.356835	-5.871869	-0.293905	C	2.286769	5.448175	-2.828926
H	3.308940	-6.834632	-0.818401	H	2.359582	6.500963	-2.523497
H	3.905119	-5.146015	-0.906336	H	3.279113	4.982723	-2.874328
H	3.816052	-5.981271	0.692406	H	1.753527	5.343781	-3.777670
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55_per: PC				(9,0)-SWCNT_pristine 3 cells			
146				132			
PC_per -26514.0606				pristine90 -24185.1468			
H	-7.030058	1.142959	3.642395	C	4.592719	1.762875	-3.056253
H	-7.130875	-2.487307	1.199751	C	4.627692	-0.641998	-3.566136
H	-7.078417	-0.948413	3.086542	C	6.004796	-0.776488	-3.772886
H	-7.147407	-2.524456	-1.001854	C	6.667808	-1.926253	-3.339167
H	-7.120358	-1.046247	-2.936844	C	4.627756	-2.762014	-2.338440
H	-7.022194	3.367401	-2.905715	C	6.004759	-2.874835	-2.558138
H	-7.079793	1.027883	-3.553328	C	4.592962	-3.521606	-0.000153
H	-6.972648	4.765477	-1.230338	C	4.627713	-2.761903	2.338170
H	-6.955664	4.806450	1.203992	C	6.004992	-2.874702	2.557826
H	-6.981819	3.462388	2.924731	C	6.667924	-1.926121	3.338712
C	-6.044246	2.913105	3.004766	C	4.627724	-0.641913	3.565887
C	-6.143659	-1.235748	2.606565	C	6.005103	-0.776398	3.772515
C	-6.071497	1.603934	3.406622	C	4.592851	1.762954	3.056179
C	-4.887932	0.802712	3.350151	C	4.627364	3.403827	1.225035
C	-6.172958	-2.104161	1.550289	C	6.004400	3.651074	1.212229
C	-4.982623	-2.364005	0.797192	C	6.667236	3.851812	-0.000095
C	-4.921818	-0.578067	2.957591	C	4.627332	3.403737	-1.225119
C	-6.193983	-2.154495	-1.378065	C	6.004341	3.650979	-1.212382
C	-4.993345	-2.390902	-0.633382	C	3.912652	2.744673	-2.320633
C	-6.118078	1.495463	-3.344910	C	0.351104	1.773807	-3.075716
C	-6.179058	-1.319420	-2.461354	C	1.782068	1.779284	-3.085087
C	-4.962003	-0.672655	-2.848620	C	2.493430	0.631139	-3.531808
C	-6.085629	2.815961	-2.982474	C	3.912800	0.636145	-3.542228
C	-4.865891	3.413913	-2.532965	C	0.359195	-0.621423	-3.515478
C	-4.933618	0.696159	-3.281684	C	1.773077	-0.613592	-3.504196
C	-6.025159	4.664101	-0.701856	C	2.482027	-1.744512	-3.025290
C	-4.835330	4.319351	-1.420841	C	3.910726	-1.742787	-3.022486
C	-6.015600	4.687312	0.666002	C	0.359375	-2.728533	-2.294740
C	-4.815850	4.366054	1.379479	C	1.773072	-2.722416	-2.282341
C	-4.830974	3.496671	2.520433	C	2.493758	-3.367229	-1.217568
C	-3.616128	2.861501	2.891165	C	3.912948	-3.378495	-1.218547
C	-3.715130	-1.186233	2.523575	C	0.351448	-3.545133	-0.000058
C	-3.647237	1.491190	3.303125	C	1.782401	-3.555886	0.000000
C	-2.427908	0.752102	3.268846	C	2.493780	-3.367144	1.217393
C	-3.741714	-2.120932	1.437377	C	3.913012	-3.378384	1.218425
C	-2.512931	-2.452793	0.777668	C	0.359576	-2.728438	2.294608
C	-2.463667	-0.594382	2.859707	C	1.773030	-2.722305	2.282188
C	-3.761414	-2.169586	-1.298424	C	2.482217	-1.744401	3.025169
C	-2.523877	-2.478691	-0.643977	C	3.910869	-1.742660	3.022301
C	-3.692523	1.385875	-3.271657	C	0.359486	-0.621312	3.515457
C	-3.749364	-1.268186	-2.413535	C	1.773045	-0.613470	3.504132

C	-2.502642	-0.685667	-2.783373	C	2.493684	0.631197	3.531777
C	-3.656067	2.767860	-2.901035	C	3.912895	0.636246	3.542106
C	-2.401919	3.333758	-2.517160	C	0.351289	1.773913	3.075827
C	-2.472663	0.648297	-3.232300	C	1.782100	1.779443	3.085103
C	-3.599042	4.510115	-0.748550	C	2.493563	2.738048	2.311166
C	-2.372230	4.225835	-1.421696	C	3.912636	2.744842	2.320548
C	-3.589074	4.534466	0.684417	C	0.359158	3.348390	1.217679
C	-2.353019	4.272084	1.349755	C	1.772807	3.334727	1.218642
C	-2.367556	3.414903	2.472955	C	2.481783	3.486590	0.000053
C	-1.141884	2.797601	2.878276	C	3.910567	3.483706	-0.000032
C	-1.252342	-1.252300	2.490538	C	0.359094	3.348284	-1.217573
C	-1.173684	1.436463	3.277520	C	1.772776	3.334589	-1.218679
C	0.032354	0.685105	3.275284	C	2.493383	2.737921	-2.311118
C	-1.282752	-2.309306	1.544645	C	-0.359460	2.728374	-2.294634
C	-0.074331	-2.931912	1.168256	C	-3.910890	1.742671	-3.022269
C	-0.006970	-0.690879	2.878548	C	-2.482127	1.744338	-3.025174
C	-1.304729	-2.355979	-1.429768	C	-1.773130	0.613459	-3.504169
C	-0.095250	-2.968373	-1.048006	C	-0.359327	0.621296	-3.515457
C	-1.218536	1.331686	-3.277504	C	-3.912879	-0.636246	-3.542217
C	-1.286193	-1.330836	-2.409796	C	-2.493594	-0.631256	-3.531819
C	-0.045610	-0.782755	-2.829563	C	-1.782131	-1.779433	-3.085109
C	-1.181733	2.704308	-2.919932	C	-0.351199	-1.773940	-3.075737
C	0.063950	3.284345	-2.551862	C	-3.912673	-2.744805	-2.320601
C	-0.012223	0.580614	-3.268453	C	-2.493536	-2.738064	-2.311134
C	-1.123972	4.454393	-0.757986	C	-1.772807	-3.334743	-1.218690
C	0.094913	4.185638	-1.442704	C	-0.359158	-3.348422	-1.217600
C	-1.114095	4.478345	0.661992	C	-3.910609	-3.483643	0.000037
C	0.114186	4.231406	1.338406	C	-2.481810	-3.486659	0.000053
C	0.098594	3.365531	2.475823	C	-1.772828	-3.334626	1.218621
C	1.312357	2.732315	2.862799	C	-0.359131	-3.348295	1.217621
C	1.202672	-1.316507	2.477042	C	-3.912636	-2.744631	2.320596
C	1.276560	1.371284	3.262220	C	-2.493441	-2.737868	2.311123
C	2.492985	0.621501	3.238981	C	-1.782010	-1.779311	3.085087
C	1.166060	-2.372110	1.530738	C	-0.351178	-1.773792	3.075721
C	2.376321	-2.585092	0.750540	C	-3.912758	-0.636177	3.542323
C	2.451754	-0.725278	2.831231	C	-2.493494	-0.631134	3.531909
C	1.143980	-2.422747	-1.443450	C	-1.772945	0.613555	3.504296
C	2.365593	-2.606026	-0.671152	C	-0.359295	0.621408	3.515526
C	1.231641	1.266891	-3.292511	C	-3.910699	1.742692	3.022602
C	1.168756	-1.396724	-2.422966	C	-2.482101	1.744491	3.025380
C	2.412777	-0.815388	-2.811425	C	-1.772966	2.722363	2.282400
C	1.272480	2.639446	-2.935338	C	-0.359486	2.728528	2.294751
C	2.529304	3.203560	-2.548518	C	-3.912959	3.378421	1.218605
C	2.448164	0.517853	-3.261761	C	-2.493785	3.367128	1.217552
C	1.335138	4.389449	-0.773715	C	-1.782428	3.555695	0.000116
C	2.560837	4.095725	-1.453230	C	-0.351469	3.545011	0.000032
C	1.344997	4.412743	0.646271	C	-3.913043	3.378310	-1.218378
C	2.580034	4.140592	1.318210	C	-2.493790	3.367001	-1.217409
C	2.563704	3.283471	2.441494	C	-1.773151	2.722236	-2.282183
C	3.786673	2.664273	2.843668	C	-4.627666	2.761781	-2.338207
C	3.665565	-1.384396	2.481107	C	-6.667845	1.926094	-3.339008

C	3.750011	1.294366	3.256556	C	-6.005040	0.776494	-3.772790
C	3.628956	-2.320643	1.395645	C	-4.627687	0.641860	-3.566025
C	3.609671	-2.361378	-1.340264	C	-4.592825	-1.762991	-3.056237
C	3.704626	1.190154	-3.317814	C	-6.004437	-3.651000	-1.212213
C	3.631574	-1.461592	-2.455716	C	-4.627406	-3.403742	-1.225040
C	3.746675	2.572160	-2.948064	C	-6.667305	-3.851622	0.000058
C	3.809603	4.314259	-0.795818	C	-6.004400	-3.650841	1.212382
C	3.819579	4.337645	0.637171	C	-4.627338	-3.403589	1.225088
C	4.907207	0.435956	-3.342408	C	-4.592735	-1.762785	3.056316
C	6.131466	1.171051	-3.422238	C	-6.004754	0.776483	3.773113
H	7.064004	0.652726	-3.642879	C	-4.627697	0.642051	3.566263
C	4.993689	3.153363	-2.596135	C	-6.667813	1.926327	3.339278
C	6.174193	2.491517	-3.060629	C	-6.004759	2.874787	2.558292
H	7.139666	2.992269	-2.996318	C	-4.627819	2.762004	2.338482
C	4.836520	-2.648685	-0.691277	C	-4.592978	3.521500	0.000148
C	6.038357	-2.476289	-1.451208	C	-6.004945	2.874740	-2.557953
H	6.975098	-2.897537	-1.087453	H	5.674500	1.704263	-2.955106
C	4.868252	-0.931879	-2.907413	H	6.565015	0.029565	-4.247970
C	6.054019	-1.641557	-2.534571	H	7.733857	-2.042079	-3.539185
H	7.002275	-1.419238	-3.022537	H	6.564782	-3.688561	-2.096113
C	4.908330	-0.840704	2.898362	H	5.674701	-3.404308	-0.000127
C	6.088970	-1.563450	2.533395	H	6.564846	-3.688461	2.095743
H	7.043754	-1.325717	3.000946	H	7.734068	-2.041899	3.538587
C	4.846922	-2.628657	0.739448	H	6.565259	0.029676	4.247531
C	6.058883	-2.432309	1.477342	H	5.674606	1.704401	2.954936
H	6.990945	-2.864787	1.114519	H	6.564386	3.659541	2.147904
C	5.028600	3.233670	2.456504	H	7.733238	4.083608	-0.000127
C	6.215516	2.586182	2.925100	H	6.564296	3.659409	-2.148079
H	7.179925	3.084396	2.831731	H	-7.733973	2.041984	-3.538931
C	4.952992	0.540557	3.288538	H	-6.565142	-0.029576	-4.247954
C	6.178090	1.277439	3.327693	H	-5.674585	-1.704406	-2.955053
H	7.113880	0.766091	3.550829	H	-6.564391	-3.659583	-2.147925
C	5.025199	4.058513	-1.483847	H	-7.733349	-4.083285	0.000122
C	6.240691	4.340216	-0.780443	H	-6.564311	-3.659324	2.148073
H	7.185159	4.392262	-1.321360	H	-5.674511	-1.704199	2.955143
C	5.044661	4.104094	1.316416	H	-6.564999	-0.029470	4.248288
C	6.250259	4.362648	0.587455	H	-7.733878	2.042069	3.539291
H	7.202217	4.431897	1.113088	H	-6.564798	3.688577	2.096272
C	-0.111392	-3.967421	0.077190	H	-5.674727	3.404229	0.000159
C	1.075175	-4.965090	0.016506	H	-6.564814	3.688492	-2.095986
O	1.556581	-5.358582	-1.025188				
O	1.435384	-5.319507	1.251841				
C	2.502138	-6.312601	1.294847				
H	3.366794	-5.936441	0.733966				
H	2.733824	-6.427217	2.356924				
H	2.110813	-7.245075	0.861902				
C	-1.347217	-4.900702	0.170928				
O	-1.848637	-5.230606	1.225191				
O	-1.723873	-5.281455	-1.051503				
C	-2.838011	-6.222209	-1.060246				
H	-2.494564	-7.154895	-0.588993				

H	-3.684756	-5.781912	-0.519134				
H	-3.071736	-6.367452	-2.118110				
Br	-0.226952	-8.446840	0.163762				
90_obl: Int _α				90_obl: Int _β			
148				148			
Int_alpha_obl	-26448.0314			Int_beta_obl	-26447.9297		
C	-4.724193	1.230305	-2.299863	C	4.353979	3.040297	1.313665
C	-4.902610	2.203304	-0.056283	C	4.392085	3.126622	-1.136440
C	-6.300395	2.266381	0.041858	C	5.736277	3.474383	-1.303840
C	-6.924708	1.970852	1.253504	C	6.479184	2.920494	-2.349733
C	-4.791271	1.386825	2.245855	C	4.594944	1.540084	-2.993213
C	-6.186220	1.460572	2.327036	C	5.939037	1.904743	-3.140619
C	-4.479501	-0.763762	3.391465	C	4.853894	-0.882104	-3.377226
C	-4.214675	-3.193616	3.100312	C	5.134607	-3.075300	-2.298320
C	-5.561536	-3.556680	3.246481	C	6.531255	-3.146263	-2.360428
C	-6.098651	-4.587020	2.473957	C	7.251037	-3.696826	-1.298069
C	-4.006422	-4.824784	1.281524	C	5.212129	-3.968402	-0.019554
C	-5.353416	-5.166813	1.443812	C	6.607603	-4.031264	-0.104404
C	-3.967739	-4.765172	-1.172392	C	5.046419	-3.065536	2.257326
C	-4.179849	-3.270823	-3.113155	C	4.821478	-0.983493	3.551764
C	-5.541597	-3.474520	-3.366541	C	6.180948	-0.772932	3.809254
C	-6.339226	-2.405677	-3.780977	C	6.695662	0.525153	3.824326
C	-4.474008	-0.873206	-3.543847	C	4.542007	1.423624	3.162546
C	-5.832422	-1.104912	-3.800704	C	5.903621	1.606501	3.433111
C	-3.922156	0.408901	-3.107324	C	3.731386	2.335585	2.352469
C	-0.510979	1.777051	-2.230307	C	0.130540	2.628074	1.279556
C	-1.933227	1.622770	-2.291200	C	1.534830	2.755800	1.291941
C	-2.737609	2.204605	-1.264130	C	2.244409	3.105238	0.096063
C	-4.152528	2.015578	-1.291902	C	3.642497	3.264509	0.115551
C	-0.681776	3.107244	-0.050171	C	0.158314	2.634345	-1.162379
C	-2.087864	2.573400	-0.054278	C	1.558144	2.739871	-1.122769
C	-2.727390	2.178432	1.124369	C	2.356851	2.125414	-2.117528
C	-4.144971	1.965581	1.120575	C	3.774774	2.301955	-2.116266
C	-0.543042	1.867996	2.179157	C	0.366370	0.988387	-2.953042
C	-1.948870	1.701236	2.225328	C	1.768083	1.144038	-2.950372
C	-2.536860	0.659461	3.004933	C	2.624498	0.087506	-3.417739
C	-3.952478	0.482657	3.038583	C	4.034348	0.255859	-3.420288
C	-0.277141	-0.246411	3.391830	C	0.644096	-1.383316	-3.442561
C	-1.694034	-0.416436	3.415056	C	2.064635	-1.219350	-3.439871
C	-2.249697	-1.724282	3.471392	C	2.905729	-2.308983	-3.080945
C	-3.658049	-1.901662	3.489749	C	4.315152	-2.142791	-3.075299
C	0.017341	-2.640145	3.074308	C	0.889158	-3.529971	-2.323054
C	-1.388492	-2.800951	3.058877	C	2.292519	-3.352881	-2.302427
C	-1.973561	-3.815273	2.258730	C	3.052231	-3.859014	-1.217616
C	-3.391317	-3.987044	2.252152	C	4.470832	-3.687757	-1.199916
C	0.226694	-4.260030	1.268972	C	0.965163	-4.412782	-0.055254
C	-1.177663	-4.425351	1.252965	C	2.368696	-4.238280	-0.033119
C	-1.855041	-4.776470	0.033851	C	3.050228	-3.977618	1.207247
C	-3.263251	-4.958068	0.025697	C	4.461082	-3.820078	1.229806
C	0.247062	-4.276879	-1.166037	C	0.834664	-3.581508	2.227948
C	-1.172461	-4.462816	-1.175668	C	2.256356	-3.423621	2.251069

C	-1.947965	-3.958209	-2.257354	C	2.846030	-2.409962	3.059200
C	-3.356037	-4.140013	-2.268863	C	4.256629	-2.251440	3.084289
C	0.052018	-2.729184	-3.034498	C	0.584750	-1.479609	3.433844
C	-1.350444	-2.900590	-3.027079	C	1.989417	-1.320128	3.441673
C	-2.198096	-1.818549	-3.381871	C	2.550897	-0.021171	3.396910
C	-3.615350	-1.997983	-3.398805	C	3.967039	0.147392	3.422187
C	-0.245739	-0.344775	-3.422115	C	0.310803	0.903961	2.999923
C	-1.648308	-0.513524	-3.428867	C	1.715453	1.066863	3.026523
C	-2.510327	0.581169	-3.064799	C	2.320529	2.155075	2.322169
C	0.315686	0.902993	-2.998779	C	-0.506519	1.816212	2.245741
C	3.716131	2.267906	-2.212273	C	-4.102788	1.971255	1.174304
C	2.299820	2.078317	-2.202250	C	-2.683470	2.171209	1.189671
C	1.500075	2.711515	-1.221198	C	-2.036062	2.595203	0.026005
C	0.100607	2.595323	-1.252785	C	-0.626096	3.118918	0.051122
C	3.584297	3.292345	-0.008091	C	-4.099932	2.092122	-1.235783
C	2.187730	3.119812	-0.016950	C	-2.683551	2.267425	-1.196678
C	1.486274	2.797966	1.191136	C	-1.879171	1.707624	-2.235844
C	0.083261	2.655777	1.187098	C	-0.455931	1.847395	-2.163940
C	3.690001	2.429114	2.254602	C	-3.875012	0.536057	-3.095611
C	2.280759	2.235155	2.235557	C	-2.461896	0.694104	-3.041745
C	1.688060	1.162523	2.973860	C	-1.607949	-0.397307	-3.433188
C	0.284973	0.986101	2.957212	C	-0.204049	-0.241404	-3.415017
C	3.949350	0.275172	3.386597	C	-3.588250	-1.864091	-3.454714
C	2.534600	0.093283	3.372219	C	-2.169648	-1.698110	-3.426501
C	1.984923	-1.208815	3.456485	C	-1.333278	-2.797483	-3.099108
C	0.581661	-1.380989	3.458771	C	0.070680	-2.638539	-3.095465
C	4.259073	-2.129483	3.115790	C	-3.353389	-4.039370	-2.384736
C	2.849852	-2.301270	3.101100	C	-1.943735	-3.871099	-2.362406
C	2.266239	-3.342125	2.323818	C	-1.177599	-4.413175	-1.292141
C	0.845900	-3.513414	2.311081	C	0.243516	-4.240903	-1.271552
C	4.470352	-3.746866	1.304528	C	-3.278128	-4.922424	-0.113564
C	3.060968	-3.917706	1.292420	C	-1.868236	-4.754464	-0.094679
C	2.376932	-4.219379	0.062760	C	-1.192733	-4.444560	1.136531
C	0.975046	-4.407396	0.051589	C	0.213011	-4.292839	1.162781
C	4.469288	-3.683396	-1.128153	C	-3.406286	-4.014676	2.139509
C	3.052146	-3.867942	-1.134963	C	-1.987213	-3.856088	2.156312
C	2.283569	-3.400324	-2.230726	C	-1.396187	-2.870167	2.987035
C	0.881821	-3.590568	-2.240240	C	0.010880	-2.722362	3.012111
C	4.291966	-2.195265	-3.047262	C	-3.659232	-1.963589	3.435833
C	2.884127	-2.374164	-3.042034	C	-2.249318	-1.798179	3.427312
C	2.031654	-1.303147	-3.429180	C	-1.681968	-0.494150	3.410363
C	0.612533	-1.479516	-3.420438	C	-0.263652	-0.335825	3.396481
C	3.988038	0.189551	-3.461004	C	-3.930971	0.435000	3.051571
C	2.579776	0.008657	-3.447616	C	-2.513800	0.600337	3.028328
C	1.715857	1.070367	-3.006568	C	-1.913736	1.658727	2.280830
C	4.538944	1.490422	-3.072678	C	-4.758643	1.367801	2.280805
C	6.412845	2.905786	-2.477095	C	-6.882952	1.997683	1.296876
C	5.669954	3.481055	-1.442844	C	-6.251243	2.321949	0.096534
C	4.330030	3.125278	-1.258966	C	-4.853538	2.249789	0.002047
C	4.302100	3.108620	1.192914	C	-4.673575	1.341059	-2.268349
C	5.872809	1.751085	3.346930	C	-5.795561	-0.939647	-3.839942

C	4.511866	1.548309	3.087575	C	-4.436229	-0.727806	-3.571112
C	6.675894	0.688767	3.766525	C	-6.314179	-2.235702	-3.859258
C	6.172810	-0.613766	3.791095	C	-5.528001	-3.323259	-3.472284
C	4.814354	-0.843768	3.545117	C	-4.165554	-3.139334	-3.207585
C	5.052939	-2.958895	2.308266	C	-3.975575	-4.689119	-1.308581
C	6.613377	-3.976058	-0.032312	C	-5.375894	-5.152304	1.289895
C	5.217714	-3.923505	0.056527	C	-4.025137	-4.818403	1.142636
C	7.249019	-3.670193	-1.237724	C	-6.119946	-4.595675	2.333678
C	6.520056	-3.156839	-2.312346	C	-5.576543	-3.593332	3.137932
C	5.123034	-3.097052	-2.246527	C	-4.225839	-3.238582	3.007355
C	4.818021	-0.939136	-3.388174	C	-4.470277	-0.816031	3.367462
C	5.878662	1.863498	-3.237062	C	-6.153070	1.451825	2.358724
H	-5.786723	1.004431	-2.230461	H	5.440671	3.059792	1.278500
H	-6.898101	2.511126	-0.837428	H	6.214494	4.151675	-0.594727
H	-8.009256	2.057610	1.338586	H	7.516706	3.225002	-2.496265
H	-6.699987	1.083654	3.212445	H	6.570376	1.375623	-3.855609
H	-5.550900	-0.916112	3.273057	H	5.924317	-0.737432	-3.244656
H	-6.197354	-3.009913	3.943725	H	7.057979	-2.739624	-3.224529
H	-7.138247	-4.884645	2.620724	H	8.336335	-3.783704	-1.368983
H	-5.828723	-5.855791	0.744632	H	7.193350	-4.306148	0.773633
H	-5.055172	-4.779508	-1.132720	H	6.109618	-2.844526	2.187215
H	-5.983449	-4.459297	-3.210375	H	6.842375	-1.624828	3.971778
H	-7.391278	-2.577204	-4.014989	H	7.747292	0.686332	4.066901
H	-6.500921	-0.263075	-3.984641	H	6.352401	2.592707	3.308235
H	7.446445	3.216456	-2.637763	H	-7.967033	2.091141	1.380300
H	6.144833	4.182823	-0.755591	H	-6.842931	2.597242	-0.777734
H	5.388427	3.137460	1.152924	H	-5.738270	1.122283	-2.210005
H	6.312217	2.737148	3.191341	H	-6.455530	-0.086745	-4.002412
H	7.726882	0.866263	4.000395	H	-7.366749	-2.390838	-4.102150
H	6.842579	-1.454613	3.975508	H	-5.979415	-4.307963	-3.346007
H	6.113839	-2.730470	2.227969	H	-5.063289	-4.693118	-1.273984
H	7.205066	-4.220390	0.850748	H	-5.854785	-5.816066	0.569169
H	8.334801	-3.749316	-1.310687	H	-7.162903	-4.887562	2.467547
H	7.039587	-2.770449	-3.189997	H	-6.210012	-3.061194	3.848494
H	5.887600	-0.780812	-3.264727	H	-5.542474	-0.955458	3.240798
H	6.511600	1.320885	-3.940465	H	-6.673604	1.055539	3.231629
C	-0.836608	4.779143	-0.084446	C	-0.771793	4.787340	0.053487
C	0.502618	5.521838	-0.248570	C	0.578068	5.523736	-0.032217
O	1.100424	6.073256	0.657270	O	1.161658	6.002042	0.922817
O	0.933765	5.450875	-1.521226	O	1.038084	5.541748	-1.297008
C	2.269472	5.970151	-1.742755	C	2.373950	6.086851	-1.441866
H	2.911718	5.733075	-0.888150	H	2.335630	7.181947	-1.375900
H	2.620634	5.471465	-2.651406	H	3.026635	5.689809	-0.656785
H	2.219761	7.057558	-1.884861	H	2.705610	5.761449	-2.432179
C	-1.823614	5.059718	-1.217616	C	-1.711028	5.099566	-1.112109
O	-1.522379	4.930355	-2.389839	O	-1.368391	4.972780	-2.272877
O	-3.067789	5.332800	-0.779854	O	-2.964853	5.396606	-0.718982
C	-4.059731	5.390274	-1.839357	C	-3.915239	5.474381	-1.814027
H	-3.866841	6.255018	-2.486382	H	-3.682716	6.335818	-2.452355
H	-4.023663	4.466685	-2.429098	H	-3.874896	4.550790	-2.403623
H	-5.016791	5.487616	-1.319847	H	-4.889233	5.589246	-1.330793

Br	-1.564761	5.302890	1.690557	Br	-1.570440	5.274805	1.809851
90 obl: TS_α				90 obl: TS_β			
148				148			
TS_alpha_obl		-26421.0400		TS_beta_obl		-26421.0219	
C	4.773836	0.939938	2.271624	C	-4.144976	3.318409	-1.179091
C	4.993541	1.868066	0.007797	C	-4.173461	3.369104	1.269100
C	6.391403	1.844620	-0.098631	C	-5.494407	3.799970	1.447908
C	6.990133	1.521901	-1.315663	C	-6.263050	3.284594	2.492256
C	4.822272	1.076067	-2.299784	C	-4.466681	1.783471	3.112121
C	6.217080	1.063157	-2.388185	C	-5.783544	2.228133	3.271237
C	4.373133	-1.051120	-3.438804	C	-4.885845	-0.621000	3.424295
C	3.969675	-3.459387	-3.118900	C	-5.331595	-2.751500	2.275951
C	5.293085	-3.894871	-3.267014	C	-6.729409	-2.719462	2.345832
C	5.776207	-4.946366	-2.486897	C	-7.493885	-3.189705	1.276275
C	3.679309	-5.055997	-1.281670	C	-5.488302	-3.583516	-0.022630
C	5.004725	-5.472471	-1.447990	C	-6.884120	-3.543752	0.070889
C	3.653839	-4.991497	1.173156	C	-5.271933	-2.653149	-2.284777
C	3.960580	-3.510681	3.111286	C	-4.905401	-0.568771	-3.540512
C	5.307613	-3.793716	3.360579	C	-6.246116	-0.253160	-3.783301
C	6.170615	-2.773508	3.768663	C	-6.665438	1.079634	-3.757273
C	4.399661	-1.134732	3.533413	C	-4.450049	1.798811	-3.084794
C	5.743800	-1.445150	3.781279	C	-5.797639	2.088601	-3.339214
C	3.922128	0.173728	3.089271	C	-3.571316	2.620725	-2.255564
C	0.609715	1.777163	2.283104	C	0.048119	2.671853	-1.220919
C	2.002691	1.505084	2.285475	C	-1.349377	2.859174	-1.193464
C	2.839574	1.997646	1.230506	C	-2.032358	3.201805	0.023213
C	4.242787	1.729195	1.249909	C	-3.428151	3.456380	0.015789
C	0.849436	2.984240	0.012172	C	0.032060	2.651805	1.298242
C	2.211081	2.375203	0.021086	C	-1.381638	2.817041	1.234782
C	2.819558	1.971103	-1.163235	C	-2.200029	2.243198	2.234799
C	4.219592	1.680975	-1.166521	C	-3.604398	2.503946	2.241867
C	0.605707	1.817356	-2.206795	C	-0.276641	0.946970	3.024416
C	1.995563	1.552279	-2.249920	C	-1.668367	1.201983	3.039143
C	2.520790	0.481602	-3.044254	C	-2.592394	0.190319	3.473323
C	3.922072	0.225136	-3.084217	C	-3.988649	0.453948	3.498400
C	0.210191	-0.286732	-3.404385	C	-0.725167	-1.419872	3.428821
C	1.613190	-0.542418	-3.436836	C	-2.129394	-1.154217	3.445086
C	2.090256	-1.881672	-3.490709	C	-3.048060	-2.169726	3.060718
C	3.484835	-2.138056	-3.513989	C	-4.442018	-1.905631	3.073640
C	-0.220878	-2.659620	-3.074472	C	-1.131908	-3.513660	2.256288
C	1.171680	-2.903646	-3.066114	C	-2.517594	-3.233342	2.249984
C	1.701676	-3.941779	-2.258899	C	-3.318990	-3.657903	1.160139
C	3.107670	-4.193692	-2.257067	C	-4.721493	-3.383397	1.157503
C	-0.514552	-4.249642	-1.254980	C	-1.285126	-4.338615	-0.028620
C	0.877970	-4.495482	-1.244297	C	-2.672012	-4.061196	-0.036461
C	1.540220	-4.879464	-0.025739	C	-3.340924	-3.726427	-1.266343
C	2.935227	-5.142862	-0.022590	C	-4.736305	-3.466680	-1.274483
C	-0.524113	-4.251034	1.179468	C	-1.108712	-3.470795	-2.295161
C	0.881979	-4.521032	1.184263	C	-2.516080	-3.210799	-2.304988
C	1.689672	-4.061883	2.262462	C	-3.035417	-2.143390	-3.090593
C	3.083723	-4.329243	2.270117	C	-4.431184	-1.884120	-3.103083

C	-0.229011	-2.709814	3.040575	C	-0.716658	-1.368286	-3.459360
C	1.159516	-2.968921	3.032075	C	-2.105120	-1.110014	-3.455832
C	2.070987	-1.942340	3.388273	C	-2.570554	0.225970	-3.375361
C	3.473487	-2.205512	3.398255	C	-3.971298	0.493868	-3.386911
C	0.212333	-0.346452	3.430006	C	-0.269562	0.979908	-2.972257
C	1.601358	-0.604229	3.433962	C	-1.657705	1.242081	-2.985964
C	2.527307	0.428463	3.062073	C	-2.179933	2.342946	-2.236713
C	-0.272313	0.941224	3.023729	C	0.611543	1.814342	-2.205446
C	-3.607097	2.486022	2.246960	C	4.223697	1.665840	-1.160506
C	-2.201725	2.230730	2.237772	C	2.824852	1.961393	-1.159403
C	-1.386796	2.809041	1.237522	C	2.216407	2.368672	0.023789
C	0.027802	2.649811	1.299264	C	0.856686	2.982099	0.012638
C	-3.437324	3.441304	0.021763	C	4.244046	1.717044	1.256057
C	-2.040463	3.192286	0.027172	C	2.841905	1.990744	1.234583
C	-1.357862	2.853343	-1.190768	C	2.001460	1.501380	2.288269
C	0.040317	2.671552	-1.220426	C	0.609534	1.778682	2.283877
C	-3.580288	2.607379	-2.250217	C	3.914883	0.163756	3.095808
C	-2.187852	2.334952	-2.233445	C	2.520989	0.423676	3.066481
C	-1.662409	1.236929	-2.984596	C	1.590670	-0.605101	3.438457
C	-0.273271	0.980181	-2.973185	C	0.202631	-0.342045	3.432701
C	-3.973645	0.480203	-3.383278	C	3.456751	-2.213498	3.406686
C	-2.571884	0.217719	-3.373892	C	2.055251	-1.945007	3.394797
C	-2.101408	-1.116341	-3.456365	C	1.140290	-2.968496	3.038619
C	-0.711978	-1.369238	-3.462028	C	-0.247266	-2.704079	3.045141
C	-4.424015	-1.899805	-3.101439	C	3.060203	-4.337049	2.280546
C	-3.027247	-2.153664	-3.090992	C	1.667206	-4.064289	2.270822
C	-2.502763	-3.219876	-2.307174	C	0.859105	-4.521486	1.192109
C	-1.094381	-3.474400	-2.299421	C	-0.545916	-4.246019	1.185221
C	-4.720657	-3.485406	-1.274065	C	2.911445	-5.152649	-0.011431
C	-3.324253	-3.739738	-1.267986	C	1.517500	-4.883805	-0.016661
C	-2.652468	-4.073128	-0.039311	C	0.858307	-4.498506	-1.236482
C	-1.264499	-4.345182	-0.033541	C	-0.533221	-4.247237	-1.249195
C	-4.702999	-3.404514	1.157982	C	3.090500	-4.206305	-2.246590
C	-3.299446	-3.673574	1.158531	C	1.685482	-3.948967	-2.250530
C	-2.498300	-3.247054	2.247801	C	1.160551	-2.909584	-3.059433
C	-1.111550	-3.522014	2.252037	C	-0.231056	-2.660172	-3.069853
C	-4.426761	-1.927573	3.075233	C	3.477222	-2.153223	-3.504839
C	-3.031816	-2.186263	3.060247	C	2.083617	-1.891516	-3.483731
C	-2.116553	-1.167607	3.444411	C	1.611617	-0.550396	-3.431777
C	-0.711343	-1.427815	3.426092	C	0.209586	-0.289286	-3.401580
C	-3.981879	0.433305	3.501745	C	3.922970	0.208697	-3.076768
C	-2.584656	0.175102	3.474634	C	2.522591	0.470513	-3.038849
C	-1.665039	1.190758	3.040350	C	2.000426	1.543911	-2.246312
C	-4.465509	1.761397	3.117546	C	4.825442	1.057126	-2.292222
C	-6.268331	3.256411	2.501641	C	6.993743	1.495632	-1.305856
C	-5.502984	3.775775	1.456854	C	6.394733	1.822255	-0.090021
C	-4.180677	3.350033	1.275876	C	4.996838	1.851469	0.014603
C	-4.155177	3.301740	-1.172244	C	4.770655	0.926277	2.279004
C	-5.805984	2.067877	-3.331508	C	5.729479	-1.461386	3.791605
C	-4.456965	1.782989	-3.079122	C	4.386842	-1.146086	3.541736
C	-6.670448	1.056071	-3.749607	C	6.151237	-2.791368	3.780991

C	-6.246095	-0.275094	-3.777605	C	5.284827	-3.808758	3.373058
C	-4.903874	-0.585821	-3.536856	C	3.939189	-3.520849	3.121814
C	-5.260730	-2.672962	-2.282854	C	3.629120	-5.002787	1.185084
C	-6.866399	-3.572243	0.074013	C	4.981626	-5.491422	-1.433695
C	-5.470542	-3.606431	-0.021364	C	3.657525	-5.069899	-1.269627
C	-7.475970	-3.221804	1.280542	C	5.756554	-4.969113	-2.471955
C	-6.711940	-2.749599	2.349578	C	5.278459	-3.916553	-3.253715
C	-5.314110	-2.776115	2.277862	C	3.956487	-3.475995	-3.107826
C	-4.875047	-0.644993	3.427718	C	4.369586	-1.069569	-3.429598
C	-5.783859	2.200886	3.278817	C	6.220284	1.038571	-2.378801
H	5.822279	0.655532	2.210147	H	-5.227621	3.417910	-1.146569
H	7.007996	2.051756	0.776987	H	-5.929502	4.517547	0.751229
H	8.077083	1.546361	-1.406817	H	-7.278030	3.653141	2.648699
H	6.702796	0.665846	-3.280237	H	-6.444084	1.729842	3.981763
H	5.434982	-1.264278	-3.331988	H	-5.944230	-0.395695	3.309478
H	5.954799	-3.389873	-3.971475	H	-7.220147	-2.297114	3.223393
H	6.796950	-5.302428	-2.634397	H	-8.582247	-3.196706	1.352893
H	5.444742	-6.181328	-0.745557	H	-7.493968	-3.755737	-0.808080
H	4.738242	-5.071261	1.131458	H	-6.316366	-2.358700	-2.204383
H	5.689603	-4.803390	3.205572	H	-6.968973	-1.049585	-3.964009
H	7.211134	-3.007494	3.999316	H	-7.703782	1.322831	-3.988262
H	6.462477	-0.643880	3.956333	H	-6.172695	3.100780	-3.184345
H	-7.284475	3.620989	2.659799	H	8.080904	1.515692	-1.395610
H	-5.941652	4.492453	0.761496	H	7.011028	2.028295	0.786059
H	-5.238155	3.397034	-1.138204	H	5.818056	0.637740	2.219065
H	-6.184718	3.078453	-3.175094	H	6.450993	-0.662670	3.966673
H	-7.710000	1.295580	-3.979019	H	7.190580	-3.029040	4.013163
H	-6.966129	-1.074073	-3.958286	H	5.663145	-4.820054	3.219659
H	-6.306200	-2.382640	-2.200850	H	4.713256	-5.086775	1.144847
H	-7.476539	-3.785711	-0.804392	H	5.418034	-6.201250	-0.729985
H	-8.564191	-3.233162	1.358577	H	6.776184	-5.329089	-2.617657
H	-7.203189	-2.330032	3.228182	H	5.943033	-3.414663	-3.957705
H	-5.934443	-0.423635	3.314546	H	5.430472	-1.286713	-3.321284
H	-6.441606	1.699323	3.989625	H	6.705585	0.638260	-3.269733
C	0.895578	4.319407	0.689534	C	0.906753	4.317605	0.689641
C	1.996079	4.603269	1.695216	C	2.007333	4.596042	1.696587
O	1.829249	4.590435	2.903502	O	1.843545	4.570725	2.905069
O	3.167361	4.867397	1.090103	O	3.176135	4.871217	1.091440
C	4.279581	5.035392	2.002502	C	4.288429	5.039455	2.003804
H	4.131302	5.932139	2.617289	H	4.123664	5.915638	2.643311
H	4.367028	4.153444	2.650102	H	4.397392	4.142317	2.627082
H	5.156297	5.137372	1.356816	H	5.159960	5.176969	1.357802
C	-0.023430	5.437902	0.457332	C	-0.005975	5.439093	0.453503
O	-1.024840	5.458352	-0.241558	O	-1.000877	5.465107	-0.254584
O	0.421551	6.528524	1.155440	O	0.436354	6.526341	1.159445
C	-0.258505	7.752279	0.799131	C	-0.242048	7.752157	0.807278
H	0.221601	8.532166	1.397217	H	0.231739	8.527697	1.415943
H	-0.128355	7.943726	-0.274119	H	-0.103187	7.953080	-0.263142
H	-1.327148	7.678104	1.035492	H	-1.312632	7.674682	1.033554
Br	2.024498	5.246563	-1.937291	Br	2.053338	5.220571	-1.949541
90_obl: PC				90_par: Int_a			

148				148			
PC_obl	-26450.1677			Int_alpha_par	-26443.5016		
C	-1.500369	-4.802429	-1.731306	C	3.517503	-4.163389	-1.371365
C	-1.861677	-4.968393	0.666435	C	3.503605	-4.335851	1.084989
C	-1.870762	-6.360219	0.787274	C	4.703406	-5.042047	1.245598
C	-1.250957	-6.968214	1.883962	C	5.544745	-4.757820	2.322364
C	-0.475635	-4.823225	2.695374	C	4.092078	-2.948808	3.018610
C	-0.501252	-6.220047	2.793846	C	5.283254	-3.670779	3.160105
C	1.832987	-4.436483	3.445886	C	5.007320	-0.708665	3.440000
C	4.149013	-4.136699	2.691462	C	5.912774	1.310902	2.371163
C	4.560992	-5.470038	2.801777	C	7.270958	0.974608	2.442479
C	5.402886	-6.023356	1.835160	C	8.126444	1.297615	1.387262
C	5.315373	-3.976883	0.545574	C	6.266474	2.165582	0.100402
C	5.710518	-5.312670	0.672587	C	7.620435	1.818519	0.194487
C	4.668132	-4.021111	-1.822997	C	5.877111	1.409720	-2.205775
C	2.765698	-4.278486	-3.371498	C	5.088450	-0.467835	-3.582253
C	2.907939	-5.643240	-3.641995	C	6.333631	-1.048454	-3.851786
C	1.776271	-6.438043	-3.839730	C	6.462137	-2.438577	-3.895318
C	0.328324	-4.563029	-3.334918	C	4.141499	-2.702920	-3.248922
C	0.497948	-5.923814	-3.618006	C	5.397466	-3.260775	-3.522936
C	-0.847267	-3.997475	-2.668739	C	3.106983	-3.347126	-2.439949
C	-2.178771	-0.568680	-1.770972	C	-0.406260	-2.541466	-1.328814
C	-1.950143	-2.000021	-1.690353	C	0.919935	-3.084342	-1.346095
C	-2.280111	-2.814890	-0.542374	C	1.476980	-3.634398	-0.161480
C	-2.050652	-4.219017	-0.584391	C	2.780577	-4.203456	-0.179904
C	-2.856697	-0.930811	1.038691	C	-0.420744	-2.642286	1.065811
C	-2.320061	-2.199242	0.774920	C	0.896992	-3.171804	1.062285
C	-1.524824	-2.803368	1.764338	C	1.793986	-2.866657	2.112477
C	-1.301075	-4.207923	1.723790	C	3.110354	-3.424478	2.106064
C	-1.106735	-0.580454	2.685633	C	0.171264	-1.235098	2.958027
C	-0.868529	-1.978553	2.701584	C	1.480823	-1.782345	2.973263
C	0.318410	-2.536638	3.292720	C	2.591505	-1.010672	3.453666
C	0.529010	-3.945162	3.299767	C	3.900484	-1.568616	3.471197
C	1.205542	-0.243636	3.415598	C	1.111807	0.966133	3.458789
C	1.420215	-1.656616	3.457804	C	2.428138	0.403995	3.476502
C	2.731177	-2.183573	3.285392	C	3.548068	1.210400	3.131926
C	2.940602	-3.586368	3.309470	C	4.854959	0.653781	3.139657
C	3.490059	0.079114	2.638038	C	1.977628	2.966199	2.370239
C	3.683468	-1.320899	2.639858	C	3.269282	2.390294	2.357395
C	4.518485	-1.920115	1.663057	C	4.154783	2.668262	1.284669
C	4.712284	-3.335342	1.661721	C	5.464488	2.096225	1.273215
C	4.702993	0.249027	0.536440	C	2.333464	3.828799	0.121784
C	4.880534	-1.153680	0.525523	C	3.624159	3.249686	0.104025
C	4.955897	-1.870140	-0.721281	C	4.216293	2.828917	-1.138052
C	5.139185	-3.277588	-0.729448	C	5.522348	2.271544	-1.155165
C	4.187395	0.194595	-1.838701	C	1.995378	3.118817	-2.179912
C	4.365476	-1.225270	-1.843400	C	3.311146	2.558099	-2.202341
C	3.622481	-2.032790	-2.749868	C	3.592078	1.442756	-3.043950
C	3.798755	-3.440902	-2.758208	C	4.903064	0.891238	-3.069755
C	2.257193	-0.049115	-3.298710	C	1.163609	1.210546	-3.449666
C	2.419871	-1.450923	-3.279402	C	2.469062	0.661262	-3.471700

C	1.285688	-2.297047	-3.375450	C	2.632668	-0.749953	-3.459504
C	1.461411	-3.711837	-3.405993	C	3.948056	-1.312917	-3.484167
C	-0.158477	-0.337138	-3.178107	C	0.210363	-1.012586	-3.101646
C	-0.003894	-1.740090	-3.177951	C	1.521565	-1.564202	-3.132728
C	-1.018908	-2.587307	-2.608658	C	1.808117	-2.773408	-2.410992
C	-1.329090	0.236796	-2.600583	C	-0.827663	-1.663828	-2.376973
C	-2.421211	3.693537	-1.611178	C	-4.326292	-0.858089	-1.281952
C	-2.272720	2.279069	-1.650135	C	-3.048380	-1.465647	-1.313399
C	-2.840009	1.494139	-0.631217	C	-2.638748	-2.341944	-0.142582
C	-3.038196	0.128232	-0.878901	C	-1.154906	-2.584028	-0.138436
C	-3.049036	3.521838	0.726701	C	-4.380336	-1.026456	1.129382
C	-2.906291	2.106256	0.686597	C	-3.093966	-1.600045	1.114541
C	-2.326839	1.412123	1.814938	C	-2.157788	-1.238365	2.112235
C	-2.171205	-0.028891	1.897320	C	-0.842212	-1.805472	2.144857
C	-1.741703	3.633469	2.756584	C	-3.748793	0.437378	2.973016
C	-1.542797	2.226933	2.696249	C	-2.442809	-0.108277	2.936962
C	-0.318701	1.676640	3.216995	C	-1.324579	0.673998	3.383978
C	-0.102413	0.281896	3.215983	C	-0.027060	0.115102	3.409365
C	0.591120	3.963540	3.393404	C	-2.802797	2.645149	3.411300
C	0.788362	2.551531	3.362683	C	-1.490608	2.081528	3.403545
C	2.098724	2.029772	3.213625	C	-0.368914	2.898978	3.115151
C	2.307757	0.634134	3.232172	C	0.928111	2.337876	3.120715
C	2.888790	4.307095	2.645593	C	-1.932288	4.689971	2.414778
C	3.084870	2.901597	2.636857	C	-0.632535	4.118528	2.399218
C	3.973658	2.310335	1.695475	C	0.271511	4.434317	1.346159
C	4.171162	0.893083	1.690267	C	1.579607	3.853262	1.330369
C	4.138973	4.487127	0.561369	C	-1.572750	5.562874	0.168518
C	4.327725	3.080423	0.553023	C	-0.275105	4.987419	0.153611
C	4.388472	2.362020	-0.693457	C	0.295042	4.515979	-1.081310
C	4.581540	0.961349	-0.704783	C	1.595911	3.960138	-1.101635
C	3.609572	4.418242	-1.808810	C	-1.932671	4.773938	-2.104062
C	3.791041	3.001403	-1.810031	C	-0.620590	4.210032	-2.118528
C	3.099823	2.200009	-2.753639	C	-0.333849	3.109101	-2.969121
C	3.278251	0.797946	-2.752033	C	0.968499	2.556827	-2.990838
C	1.764479	4.190291	-3.377606	C	-2.760913	2.898908	-3.425426
C	1.929017	2.781470	-3.352707	C	-1.454482	2.338201	-3.425259
C	0.794919	1.929912	-3.472996	C	-1.287319	0.924725	-3.421517
C	0.957556	0.510097	-3.430165	C	0.025291	0.360443	-3.450625
C	-0.654464	3.907786	-3.264566	C	-3.704718	0.681192	-3.058211
C	-0.490268	2.493203	-3.256699	C	-2.399230	0.122908	-3.041830
C	-1.464591	1.648428	-2.618999	C	-2.124896	-1.085742	-2.301896
C	-1.826863	4.497155	-2.613501	C	-4.763290	-0.001945	-2.333148
C	-3.100582	6.369839	-1.758378	C	-7.000834	-0.035423	-1.394869
C	-3.493277	5.627442	-0.639759	C	-6.491332	-0.582698	-0.204891
C	-3.115540	4.287260	-0.526795	C	-5.153022	-0.938796	-0.117921
C	-2.621264	4.235108	1.852293	C	-4.727412	-0.115947	2.138380
C	-0.905142	5.849193	3.657812	C	-5.190861	2.380190	3.729228
C	-0.726595	4.489560	3.374873	C	-3.942448	1.798557	3.478707
C	0.203096	6.679971	3.828366	C	-5.317617	3.769419	3.790459
C	1.493508	6.206430	3.578873	C	-4.243649	4.595987	3.453112
C	1.700183	4.850175	3.306941	C	-2.985343	4.039178	3.198909

C	3.537627	5.088514	1.678313	C	-2.322334	5.520992	1.354546
C	4.101148	6.592809	-0.852425	C	-3.497198	6.418122	-1.244090
C	4.072876	5.200970	-0.716188	C	-2.302748	5.703426	-1.093697
C	3.568278	7.192642	-1.995986	C	-4.356449	6.125439	-2.304645
C	2.858087	6.433719	-2.928113	C	-4.118499	5.019518	-3.124712
C	2.812937	5.039641	-2.808419	C	-2.933203	4.288318	-2.991426
C	0.468724	4.721412	-3.463277	C	-3.865749	2.042694	-3.382004
C	-2.220566	5.838198	-2.703309	C	-6.126754	0.333968	-2.411896
H	-1.262210	-5.863079	-1.705313	H	4.558864	-4.479221	-1.341395
H	-2.339133	-6.973849	0.016834	H	4.993827	-5.792433	0.509086
H	-1.297158	-8.052900	1.991370	H	6.458147	-5.338652	2.461545
H	0.071891	-6.724887	3.572199	H	6.021755	-3.361916	3.900966
H	1.991874	-5.506582	3.329162	H	5.993688	-1.151504	3.315490
H	4.194246	-6.086080	3.623546	H	7.651215	0.429623	3.307181
H	5.748936	-7.051988	1.946332	H	9.189604	1.063857	1.464882
H	6.228609	-5.807214	-0.149959	H	8.270137	1.923899	-0.675095
H	4.700566	-5.106938	-1.755987	H	6.830738	0.889239	-2.139737
H	3.901872	-6.090546	-3.678567	H	7.208912	-0.413744	-3.995689
H	1.895746	-7.492067	-4.094598	H	7.427036	-2.883805	-4.143561
H	-0.367245	-6.587101	-3.640012	H	5.549047	-4.335255	-3.413218
H	-3.433085	7.404088	-1.857986	H	-8.064998	0.189606	-1.479421
H	-4.072753	6.101917	0.153119	H	-7.141543	-0.692664	0.664831
H	-2.668970	5.321000	1.821806	H	-5.685680	0.392412	2.058104
H	-1.911517	6.264473	3.720137	H	-6.071470	1.747537	3.846515
H	0.054306	7.730146	4.083733	H	-6.287301	4.212704	4.022449
H	2.337218	6.897318	3.575886	H	-4.392437	5.671963	3.354894
H	3.283664	6.145024	1.616332	H	-3.360441	5.844603	1.313741
H	4.507810	7.209613	-0.050197	H	-3.770694	7.179944	-0.512932
H	3.629250	8.275285	-2.115837	H	-5.266820	6.711651	-2.439876
H	2.307987	6.928464	-3.729390	H	-4.873488	4.702324	-3.845126
H	0.347671	5.796553	-3.347974	H	-4.853605	2.481599	-3.257271
H	-1.832668	6.470744	-3.502408	H	-6.491342	0.907323	-3.265793
C	-3.955549	-0.534751	0.101641	C	-3.267459	-3.898812	-0.195213
C	-4.772601	-1.705292	-0.505537	C	-2.422460	-4.669967	-1.224276
O	-5.063094	-1.768477	-1.681806	O	-2.547613	-4.490452	-2.420666
O	-5.104520	-2.571015	0.454874	O	-1.512646	-5.484554	-0.664635
C	-5.917230	-3.690726	-0.001929	C	-0.601715	-6.094245	-1.620728
H	-5.423127	-4.169522	-0.856563	H	-0.167224	-5.321132	-2.264662
H	-5.971567	-4.363796	0.857753	H	0.168160	-6.570180	-1.007500
H	-6.909108	-3.297912	-0.269349	H	-1.140610	-6.828893	-2.231949
C	-5.021752	0.387138	0.749493	C	-3.221060	-4.359927	1.257346
O	-5.268570	0.379377	1.937371	O	-2.220861	-4.782346	1.805396
O	-5.606014	1.132529	-0.191295	O	-4.367693	-4.056957	1.906334
C	-6.657387	2.010534	0.304543	C	-4.232293	-4.054806	3.350281
H	-7.503378	1.379437	0.614029	H	-3.944016	-5.048797	3.712023
H	-6.265524	2.606793	1.138009	H	-3.470845	-3.317553	3.638768
H	-6.919619	2.640390	-0.549632	H	-5.217537	-3.766413	3.726372
Br	-8.435675	-1.121711	0.196025	Br	-5.133515	-4.024842	-0.909245
90_par: Int_β				90_par: TS_α			
148				148			
Int_beta_par -26448.2121				TS_alpha_par -26443.5946			

C	4.396574	2.961609	1.165382	C	3.286184	4.412364	1.204104
C	4.360796	3.034217	-1.285218	C	3.254355	4.511634	-1.246084
C	5.709551	3.341052	-1.492662	C	4.408915	5.275618	-1.432350
C	6.410077	2.749689	-2.546980	C	5.291299	4.969681	-2.473065
C	4.473804	1.410429	-3.117764	C	3.969536	3.025358	-3.059116
C	5.823114	1.735873	-3.305719	C	5.116326	3.812781	-3.231445
C	4.665850	-1.022448	-3.471558	C	5.025635	0.828988	-3.420089
C	4.929373	-3.207975	-2.371867	C	6.057436	-1.118182	-2.326743
C	6.321664	-3.310920	-2.473841	C	7.392120	-0.704406	-2.411636
C	7.059978	-3.867672	-1.427624	C	8.271622	-0.961101	-1.358069
C	5.054145	-4.080266	-0.087237	C	6.469664	-1.904042	-0.044486
C	6.444505	-4.176374	-0.212399	C	7.799196	-1.482131	-0.151150
C	4.977822	-3.149011	2.182210	C	6.021626	-1.077928	2.223591
C	4.840117	-1.044633	3.451298	C	5.101546	0.822602	3.487786
C	6.211524	-0.862332	3.664539	C	6.307894	1.486946	3.739475
C	6.756355	0.422971	3.641605	C	6.351807	2.881753	3.736315
C	4.605282	1.361357	3.027957	C	4.023886	2.985601	3.070930
C	5.977960	1.516446	3.255599	C	5.240162	3.625215	3.333380
C	3.792164	2.279091	2.226658	C	2.949788	3.557779	2.256337
C	0.164086	2.645122	1.268868	C	-0.542998	2.605450	1.228812
C	1.573864	2.731402	1.227286	C	0.731990	3.223922	1.227262
C	2.253855	3.074962	0.011704	C	1.241591	3.814401	0.023788
C	3.652371	3.202157	-0.012446	C	2.514312	4.412777	0.019155
C	0.120314	2.629315	-1.168237	C	-0.562424	2.633619	-1.198791
C	1.520833	2.721420	-1.184288	C	0.706758	3.226020	-1.193339
C	2.275110	2.067113	-2.191194	C	1.667386	2.858921	-2.171687
C	3.696836	2.208790	-2.234238	C	2.946092	3.497293	-2.194481
C	0.236604	0.954203	-2.940858	C	0.174320	1.067016	-2.908179
C	1.640609	1.081170	-2.983883	C	1.440242	1.698590	-2.947507
C	2.459062	-0.001968	-3.460472	C	2.597723	0.983005	-3.412976
C	3.871349	0.133739	-3.507175	C	3.866977	1.619981	-3.453385
C	0.446808	-1.428754	-3.406888	C	1.238839	-1.079287	-3.374224
C	1.869848	-1.296023	-3.446203	C	2.516812	-0.437232	-3.407421
C	2.696094	-2.400036	-3.097511	C	3.686902	-1.170698	-3.067521
C	4.108351	-2.265912	-3.135607	C	4.954957	-0.533408	-3.093562
C	0.675739	-3.566256	-2.266689	C	2.231091	-3.011634	-2.276698
C	2.082709	-3.420834	-2.289191	C	3.485854	-2.358802	-2.280288
C	2.862577	-3.932567	-1.221583	C	4.391269	-2.564099	-1.209224
C	4.284622	-3.793939	-1.248006	C	5.661650	-1.910263	-1.214494
C	0.798688	-4.424393	0.008622	C	2.644642	-3.801963	-0.013396
C	2.205980	-4.283080	-0.013153	C	3.898292	-3.147839	-0.013448
C	2.930183	-4.025348	1.203431	C	4.456524	-2.642526	1.213362
C	4.344477	-3.901161	1.182134	C	5.725706	-2.005066	1.214133
C	0.756058	-3.564645	2.284326	C	2.245555	-3.013904	2.250866
C	2.181191	-3.440376	2.263190	C	3.525237	-2.372279	2.254069
C	2.818488	-2.431476	3.040592	C	3.732040	-1.199302	3.034022
C	4.232248	-2.305682	3.021209	C	5.003197	-0.568991	3.045382
C	0.591180	-1.442314	3.468500	C	1.285860	-1.090251	3.392813
C	1.999073	-1.315883	3.431675	C	2.553579	-0.457243	3.393983
C	2.588674	-0.032203	3.348515	C	2.638280	0.952768	3.327968
C	4.008758	0.103705	3.327292	C	3.914498	1.593712	3.345201

C	0.359000	0.940692	3.005458	C	0.216706	1.048985	2.927903
C	1.767060	1.068764	2.983691	C	1.478692	1.689369	2.956432
C	2.375651	2.127022	2.238740	C	1.678847	2.912718	2.243391
C	-0.460408	1.862972	2.262486	C	-0.854226	1.611829	2.157672
C	-4.083901	2.063335	1.291216	C	-4.355008	0.634533	1.202511
C	-2.659661	2.230788	1.258817	C	-3.102524	1.291701	1.204461
C	-2.043955	2.660204	0.077766	C	-2.759720	2.134501	0.013592
C	-0.618586	3.159630	0.064782	C	-1.398578	2.783386	0.024754
C	-4.152407	2.181723	-1.117274	C	-4.421689	0.748358	-1.202868
C	-2.733967	2.325156	-1.120352	C	-3.163831	1.369482	-1.206327
C	-1.971964	1.727526	-2.167006	C	-2.172424	0.975197	-2.116921
C	-0.542990	1.836940	-2.134767	C	-0.876604	1.618626	-2.124081
C	-4.016391	0.597491	-2.963714	C	-3.655265	-0.817094	-2.914010
C	-2.599212	0.722407	-2.948491	C	-2.376979	-0.199655	-2.888358
C	-1.781191	-0.392913	-3.349426	C	-1.211266	-0.931251	-3.294875
C	-0.374556	-0.268021	-3.371778	C	0.052604	-0.298832	-3.326020
C	-3.794163	-1.813803	-3.294626	C	-2.572180	-2.982186	-3.282131
C	-2.371832	-1.680153	-3.308986	C	-1.294010	-2.344310	-3.289880
C	-1.551152	-2.793366	-2.988556	C	-0.122373	-3.090644	-3.001457
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C	-3.577418	-3.977658	-2.197766	C	-1.573541	-4.957932	-2.265714
C	-2.164159	-3.842191	-2.219067	C	-0.308250	-4.314069	-2.268551
C	-1.379482	-4.387909	-1.164241	C	0.618934	-4.558488	-1.216438
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C	-3.455430	-4.832725	0.082279	C	-1.155352	-5.759752	-0.004621
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C	-1.322966	-4.391040	1.264250	C	0.640816	-4.558650	1.208960
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C	-1.652203	-0.405315	3.499739	C	-1.179249	-0.952233	3.330827
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C	-4.161806	-4.697206	1.358705	C	-1.885050	-5.891494	1.259598
C	-6.213743	-4.414266	2.609978	C	-3.924222	-6.371670	2.470659
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C	-4.269161	-3.095456	3.212765	C	-2.624372	-4.416561	3.069565
C	-4.447372	-0.664589	3.549737	C	-3.688206	-2.210299	3.351569
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H	-6.222272	-2.864418	4.111817	H	-4.547810	-4.902375	3.925065
H	-5.525903	-0.780298	3.457620	H	-4.651257	-2.708707	3.260240
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C	-0.741057	4.808405	0.014209	C	-2.701176	3.662856	0.058511
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C	-0.292909	0.264560	3.332440	C	0.036854	-0.517610	-3.392386
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C	0.113209	4.321298	1.283129	C	2.502328	-3.663390	-1.182967
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C	-1.314968	4.523512	-1.127262	C	1.389953	-4.514986	1.252677
C	0.093826	4.389684	-1.147876	C	2.514146	-3.655342	1.249760
C	-3.521208	4.047860	-2.125053	C	-0.726109	-5.260907	2.277264
C	-2.098191	3.912844	-2.138965	C	0.407572	-4.389893	2.266504
C	-1.492061	2.921612	-2.951884	C	0.401793	-3.211985	3.056460
C	-0.083860	2.793671	-2.974796	C	1.526568	-2.356161	3.053613
C	-3.745327	1.961579	-3.366174	C	-2.013262	-3.587074	3.493314
C	-2.328452	1.824790	-3.355484	C	-0.886675	-2.716859	3.457750
C	-1.741309	0.534758	-3.302173	C	-1.075458	-1.314629	3.367716
C	-0.316557	0.398402	-3.308163	C	0.060312	-0.439625	3.347531
C	-3.976162	-0.432308	-2.951941	C	-3.476739	-1.697828	3.007814
C	-2.560655	-0.560510	-2.911851	C	-2.348803	-0.836303	2.955485
C	-1.940230	-1.604369	-2.141526	C	-2.366844	0.341601	2.128318
C	-4.787447	-1.402270	-2.233759	C	-4.663240	-1.347794	2.243145
C	-6.906548	-2.144776	-1.316020	C	-6.842238	-1.866662	1.319944
C	-6.262504	-2.552900	-0.132815	C	-6.498572	-1.227759	0.113998
C	-4.880446	-2.476481	-0.033756	C	-5.280083	-0.575894	-0.001710
C	-4.724673	-1.433611	2.182666	C	-4.616129	-1.405580	-2.213579
C	-5.899335	0.865475	3.697816	C	-4.397504	-4.006656	-3.672767
C	-4.535610	0.683103	3.439300	C	-3.339461	-3.121928	-3.435215
C	-6.437515	2.152485	3.751307	C	-4.173523	-5.384645	-3.666543
C	-5.662805	3.261491	3.404841	C	-2.935569	-5.901511	-3.278746
C	-4.296901	3.107299	3.145437	C	-1.860771	-5.038533	-3.040649
C	-4.112716	4.719665	1.302322	C	-0.872336	-6.235983	-1.135026
C	-5.505268	5.176079	-1.302518	C	-1.816192	-7.285052	1.502922
C	-4.151324	4.859402	-1.143263	C	-0.836378	-6.302773	1.317320
C	-6.238989	4.597420	-2.339765	C	-2.735711	-7.163607	2.545959

C	-5.681755	3.582442	-3.121496	C	-2.794530	-5.993317	3.306981
C	-4.330455	3.248764	-2.979082	C	-1.827917	-4.997026	3.136467
C	-4.538696	0.812189	-3.301032	C	-3.294941	-3.037977	3.404578
C	-6.190620	-1.494125	-2.313440	C	-5.906728	-2.001233	2.337516
H	5.436162	-2.890000	-1.204888	H	3.222847	5.322788	1.062460
H	6.218597	-4.088259	0.662084	H	3.308715	6.639465	-0.842951
H	7.501412	-3.081947	2.540146	H	4.911434	6.437291	-2.731267
H	6.515067	-1.222203	3.853504	H	5.038588	4.322748	-4.022339
H	5.828435	0.854470	3.254325	H	5.552285	2.207712	-3.361716
H	6.933648	2.866432	3.251372	H	7.550756	1.083891	-3.295874
H	8.208323	3.956649	1.421425	H	9.190887	0.905041	-1.441312
H	7.072397	4.494643	-0.721484	H	8.493075	-0.070231	0.733540
H	6.011885	3.013243	-2.147899	H	6.815113	0.660037	2.141243
H	6.765510	1.799519	-3.927002	H	6.812964	2.130512	3.896070
H	7.711867	-0.495207	-4.001493	H	6.402663	4.578924	3.913109
H	6.350669	-2.425180	-3.245001	H	4.231495	5.475420	3.111263
H	-7.988741	-2.248874	-1.404877	H	-7.820615	-2.338784	1.418343
H	-6.855501	-2.863795	0.728898	H	-7.166637	-1.294632	-0.745779
H	-5.791965	-1.238237	2.100353	H	-5.416919	-2.135783	-2.116859
H	-6.546900	-0.001167	3.834462	H	-5.403413	-3.619060	-3.837126
H	-7.493791	2.285582	3.990008	H	-4.996531	-6.065405	-3.888798
H	-6.127459	4.243496	3.308134	H	-2.813491	-6.975515	-3.134140
H	-5.200070	4.711884	1.260351	H	-1.798063	-6.805371	-1.081005
H	-5.993744	5.846785	-0.594605	H	-1.879786	-8.127129	0.812837
H	-7.283826	4.876800	-2.483363	H	-3.472194	-7.951413	2.710898
H	-6.308320	3.026186	-3.819566	H	-3.614497	-5.840745	4.009603
H	-5.614867	0.933526	-3.196147	H	-4.141871	-3.715479	3.316498
H	-6.716461	-1.039740	-3.154074	H	-6.130938	-2.618510	3.208004
C	-1.464795	-4.377230	-0.077878	C	-3.378367	2.790696	0.007600
C	-1.584391	-5.094880	1.242143	C	-3.960753	3.365380	-1.263886
O	-1.036296	-4.727142	2.266277	O	-3.293664	3.832150	-2.168722
O	-2.448203	-6.125084	1.188243	O	-5.283214	3.150147	-1.278949
C	-2.589161	-6.826113	2.451042	C	-5.972418	3.769465	-2.397675
H	-2.983455	-6.146356	3.216187	H	-5.523469	3.440499	-3.342438
H	-3.290410	-7.639149	2.244091	H	-7.009965	3.436001	-2.310852
H	-1.615125	-7.216613	2.768796	H	-5.894413	4.858975	-2.276195
C	-1.625321	-5.182930	-1.339941	C	-3.869811	3.362322	1.319584
O	-2.152714	-6.276746	-1.422911	O	-4.885567	2.996011	1.879269
O	-1.158400	-4.495121	-2.397345	O	-2.977478	4.249875	1.785053
C	-1.253741	-5.168457	-3.668600	C	-3.386077	4.932717	2.996671
H	-2.297091	-5.432400	-3.879827	H	-4.224748	5.595271	2.741285
H	-0.874438	-4.446497	-4.397865	H	-3.677107	4.201454	3.759802
H	-0.632909	-6.072336	-3.651541	H	-2.509333	5.507202	3.308201
Br	1.438688	-5.960285	-0.159130	Br	-5.043817	6.295056	0.037690

Cartesian coordinates of donor-acceptor complexes of (6,5)-SWCNT in singlet ground state optimized at BP86-D3(BJ)/DZP level of theory

(6,5)-SWCNT – TTF				(6,5)-SWCNT – exTTF			
Atom	X	Y	Z	Atom	X	Y	Z
6	-9.920396	-2.262695	-1.909546	6	10.822413	1.340322	-1.064972
6	-9.930597	-2.928756	-0.698018	6	10.826902	1.719731	0.264645
6	-8.698594	-3.245135	-0.024027	6	9.601524	2.082165	0.928383
6	-7.509771	-3.260977	-0.824879	6	8.503454	2.467645	0.090600
6	-7.493067	-2.541866	-2.071260	6	8.487499	2.045093	-1.284920
6	-8.676445	-1.857186	-2.512211	6	9.587522	1.281464	-1.805115
6	-6.257313	-3.660982	-0.237409	6	7.279197	2.937059	0.686176
6	-5.071596	-3.710565	-1.045048	6	6.190442	3.356920	-0.150601
6	-5.045547	-2.950478	-2.260101	6	6.155940	2.888626	-1.505019
6	-6.217628	-2.217469	-2.650931	6	7.232768	2.068575	-1.987579
6	-3.832459	-4.138069	-0.460491	6	4.984051	3.852196	0.449329
6	-2.639154	-4.149000	-1.260328	6	3.880556	4.233688	-0.388598
6	-2.604750	-3.345458	-2.446643	6	3.827847	3.716916	-1.724659
6	-3.775604	-2.604326	-2.825680	6	4.901422	2.886859	-2.197771
6	-1.400354	-4.593140	-0.682761	6	2.677297	4.745491	0.208978
6	-0.204746	-4.576446	-1.477388	6	1.565405	5.097629	-0.629284
6	-0.164889	-3.735082	-2.638460	6	1.498420	4.537406	-1.948308
6	-1.330239	-2.978308	-2.993173	6	2.562773	3.688983	-2.401788
6	1.033768	-5.032670	-0.909143	6	0.365134	5.622720	-0.037643
6	2.232901	-4.985685	-1.696837	6	-0.757068	5.940770	-0.875289
6	2.277270	-4.112821	-2.831875	6	-0.836244	5.343031	-2.174786
6	1.110596	-3.350534	-3.170385	6	0.228035	4.487151	-2.613668
6	3.470856	-5.450392	-1.134986	6	-1.955074	6.474567	-0.287572
6	4.680672	-5.390864	-1.911373	6	-3.091991	6.776430	-1.116902
6	4.730234	-4.484666	-3.027991	6	-3.183288	6.142503	-2.405615
6	3.558309	-3.712192	-3.342253	6	-2.116744	5.271367	-2.822099
6	5.905402	-5.912195	-1.371299	6	-4.266117	7.367916	-0.537256
6	7.063830	-5.858358	-2.226926	6	-5.345235	7.681761	-1.439877
6	7.112713	-4.973064	-3.287580	6	-5.437543	7.056108	-2.669305
6	6.001997	-4.101247	-3.568655	6	-4.449315	6.092139	-3.079096
6	6.172803	-2.734747	-4.014935	6	-4.784518	4.894343	-3.820469
6	7.469925	-2.133020	-4.167083	6	-6.138836	4.555418	-4.168563
6	6.011219	-6.078571	0.058535	6	-4.463481	7.252629	0.888086
6	7.284824	-6.229143	0.726199	6	-5.749530	7.474077	1.511230
6	3.721741	-2.377965	-3.820639	6	-2.438167	4.108945	-3.584365
6	5.050349	-1.843093	-3.944033	6	-3.817552	3.835844	-3.885320
6	3.581281	-5.578375	0.282377	6	-2.164025	6.320408	1.116093
6	4.892407	-5.680677	0.865361	6	-3.488426	6.516776	1.642905
6	1.271856	-2.021025	-3.683745	6	-0.088318	3.335685	-3.408365
6	2.594905	-1.490226	-3.810795	6	-1.461225	3.065388	-3.709405
6	1.151949	-5.118396	0.518150	6	0.139044	5.422909	1.365092
6	2.463556	-5.194546	1.100523	6	-1.190327	5.593299	1.884004
6	-1.168895	-1.664259	-3.544551	6	2.251477	2.561674	-3.232340
6	0.149321	-1.127968	-3.701293	6	0.884203	2.292697	-3.563212

6	-1.274853	-4.635736	0.746290	6	2.436107	4.503799	1.603012
6	0.038908	-4.702953	1.326285	6	1.102778	4.666454	2.115935
6	-3.618939	-1.311274	-3.424898	6	4.601954	1.790166	-3.071634
6	-2.296812	-0.779702	-3.582378	6	3.231740	1.529270	-3.404567
6	-3.698837	-4.133875	0.968603	6	4.727008	3.566150	1.832216
6	-2.381837	-4.186696	1.544906	6	3.388646	3.717236	2.337585
6	-6.067351	-0.955533	-3.300935	6	6.949071	1.012294	-2.904954
6	-4.745924	-0.428454	-3.499919	6	5.584009	0.765921	-3.278480
6	-6.115522	-3.610570	1.182077	6	7.007865	2.610277	2.048876
6	-4.798707	-3.654440	1.755154	6	5.668539	2.754298	2.548724
6	-8.531289	-0.604645	-3.216273	6	9.314183	0.242234	-2.770107
6	-7.206499	-0.084502	-3.403670	6	7.946197	0.001250	-3.133289
6	-8.546735	-3.138537	1.411809	6	9.310144	1.698914	2.294052
6	-7.220687	-3.111424	1.957669	6	7.952739	1.781448	2.751213
6	-9.631990	0.311733	-3.406191	6	10.273609	-0.789731	-3.090453
6	-9.604702	-2.650039	2.255898	6	10.204011	0.875698	3.065157
6	5.134041	-5.030048	2.121263	6	-3.929383	5.672376	2.716074
6	6.488708	-4.822588	2.564893	6	-5.330997	5.610707	3.043198
6	7.516689	-5.630701	1.946847	6	-6.168512	6.688806	2.564872
6	2.719805	-4.503043	2.327861	6	-1.651306	4.714653	2.916345
6	4.085003	-4.263654	2.720380	6	-3.064249	4.632963	3.183217
6	0.303970	-3.970679	2.531757	6	0.627566	3.754094	3.116698
6	1.668248	-3.723971	2.911399	6	-0.784819	3.666621	3.367297
6	-2.108716	-3.413042	2.721267	6	2.901299	2.773865	3.301653
6	-0.742755	-3.159655	3.087078	6	1.486983	2.683281	3.535690
6	-4.517893	-2.839205	2.901935	6	5.169718	1.780039	3.476119
6	-3.151414	-2.576990	3.251673	6	3.754763	1.685121	3.692821
6	-6.931508	-2.253128	3.075919	6	7.441402	0.774114	3.642650
6	-5.555616	-1.979629	3.399429	6	6.017610	0.676707	3.831905
6	-9.323043	-1.804251	3.314452	6	9.706824	-0.107362	3.903430
6	-7.968758	-1.415478	3.602004	6	8.289754	-0.313358	4.034136
6	6.793958	-3.665519	3.314049	6	-5.871245	4.393114	3.511333
6	4.425296	-3.042386	3.387989	6	-3.642577	3.376051	3.555910
6	5.811649	-2.660697	3.521565	6	-5.077370	3.215230	3.537981
6	2.009496	-2.466765	3.513027	6	-1.364090	2.389074	3.670535
6	3.387266	-2.065690	3.569427	6	-2.786968	2.221638	3.574795
6	-0.396851	-1.880203	3.638063	6	0.904043	1.395801	3.786088
6	0.981236	-1.479468	3.665407	6	-0.516485	1.233100	3.662051
6	-2.801755	-1.280820	3.758946	6	3.169028	0.391145	3.898069
6	-1.420102	-0.884025	3.765604	6	1.747366	0.237231	3.752458
6	-5.205489	-0.675802	3.863597	6	5.433626	-0.615632	3.995389
6	-3.825737	-0.282652	3.864471	6	4.014861	-0.764929	3.843580
6	-7.613104	-0.073858	4.023205	6	7.697887	-1.632894	4.149981
6	-6.237470	0.325113	3.949382	6	6.288794	-1.771888	3.921880
6	-8.587794	0.974733	4.137226	6	8.483312	-2.835109	4.097525
6	6.141469	-1.238493	3.434568	6	-5.614631	1.919478	3.123973
6	7.480446	-0.765796	3.235619	6	-6.985861	1.739640	2.748249
6	3.718491	-0.686656	3.397231	6	-3.311759	0.980386	3.099788
6	5.085185	-0.322543	3.127302	6	-4.690229	0.917360	2.687478
6	1.313833	-0.101761	3.441731	6	-1.037750	0.001999	3.139960
6	2.668641	0.247010	3.127010	6	-2.398970	-0.044538	2.692744

6	-1.085975	0.484949	3.500847	6	1.229810	-0.975881	3.189660
6	0.265345	0.833424	3.166894	6	-0.126407	-1.020905	2.723372
6	-3.494488	1.079726	3.563092	6	3.505030	-1.963677	3.243682
6	-2.145670	1.404975	3.206121	6	2.157416	-1.979804	2.757000
6	-5.905821	1.684834	3.611777	6	5.782821	-2.959601	3.284578
6	-4.548849	1.996956	3.243142	6	4.431110	-2.958228	2.787594
6	-8.269876	2.278953	3.793583	6	8.000106	-3.969836	3.465024
6	-6.954945	2.619715	3.329572	6	6.697450	-3.978348	2.860845
6	7.733478	0.326544	2.420974	6	-7.332326	0.889600	1.710757
6	5.343858	0.803163	2.267664	6	-5.041017	0.052498	1.593722
6	6.662156	1.003042	1.750957	6	-6.325457	0.179500	0.978053
6	2.920653	1.338669	2.235236	6	-2.735586	-0.872359	1.573504
6	4.230415	1.499796	1.679826	6	-3.998720	-0.682902	0.929253
6	0.517550	1.918097	2.253818	6	-0.462419	-1.837237	1.584371
6	1.822667	2.059660	1.669403	6	-1.717978	-1.636075	0.917896
6	-1.905727	2.441951	2.252206	6	1.845748	-2.738867	1.586534
6	-0.604086	2.585587	1.667601	6	0.592241	-2.537584	0.916886
6	-4.310304	3.014246	2.268297	6	4.127358	-3.693120	1.600559
6	-3.016735	3.116526	1.658294	6	2.891663	-3.445216	0.916815
6	-6.721646	3.623667	2.305129	6	6.407968	-4.686396	1.624860
6	-5.443220	3.658246	1.657976	6	5.200205	-4.369408	0.920318
6	-7.793740	4.313234	1.646169	6	7.419103	-5.384698	0.883709
6	6.798536	1.551420	0.422523	6	-6.425368	-0.057889	-0.444997
6	8.022573	1.468613	-0.321279	6	-7.554567	0.365331	-1.223855
6	4.357902	2.035769	0.364663	6	-4.083801	-0.893497	-0.476141
6	5.608206	1.837531	-0.316793	6	-5.226430	-0.360367	-1.163475
6	1.974979	2.730610	0.403953	6	-1.858424	-1.985969	-0.476164
6	3.178199	2.430193	-0.368834	6	-2.919146	-1.315188	-1.215839
6	-0.464321	3.201344	0.383704	6	0.474666	-2.827162	-0.479479
6	0.836923	3.389831	-0.154760	6	-0.794513	-2.694191	-1.117884
6	-2.910752	3.525229	0.283479	6	2.849119	-3.519337	-0.517650
6	-1.668646	3.342192	-0.423391	6	1.716612	-2.981597	-1.226846
6	-5.356715	3.997043	0.261661	6	5.186548	-4.381576	-0.519063
6	-4.125167	3.730063	-0.442098	6	4.076339	-3.767722	-1.207057
6	-7.716381	4.607000	0.292623	6	7.415563	-5.367753	-0.503706
6	-6.559120	4.244298	-0.472637	6	6.396225	-4.666149	-1.228010
6	8.003708	1.219686	-1.681816	6	-7.379056	0.879711	-2.496860
6	5.581978	1.554075	-1.721625	6	-5.035294	0.194380	-2.469202
6	6.752827	1.030945	-2.364056	6	-6.058038	1.014396	-3.049759
6	3.138980	2.071712	-1.771169	6	-2.700451	-0.688941	-2.498821
6	4.293601	1.423972	-2.342287	6	-3.692064	0.239442	-2.977313
6	0.773989	2.809154	-2.270104	6	-0.443853	-1.707281	-3.040198
6	1.888856	1.954571	-2.506284	6	-1.392598	-0.644156	-3.134467
6	-1.719962	2.918979	-1.806562	6	1.954820	-2.298465	-2.477851
6	-0.561054	2.356935	-2.504091	6	0.957390	-1.431153	-3.101862
6	-4.190812	3.256939	-1.786123	6	4.330433	-3.042969	-2.408733
6	-3.025136	2.643150	-2.356126	6	3.326732	-2.139135	-2.889930
6	-6.651313	3.693444	-1.824954	6	6.686720	-3.871498	-2.422154
6	-5.491625	3.012475	-2.351105	6	5.694889	-2.911279	-2.844733
6	-7.908355	3.414967	-2.423543	6	8.016598	-3.693635	-2.886451
6	6.586599	0.020816	-3.389060	6	-5.657204	2.173210	-3.821922

6	7.671233	-0.799407	-3.855180	6	-6.562800	3.237209	-4.160511
6	4.128797	0.365845	-3.288044	6	-3.294269	1.421894	-3.669403
6	5.258502	-0.448916	-3.650017	6	-4.256313	2.464736	-3.906725
6	1.690911	0.749927	-3.261551	6	-0.953525	0.641061	-3.605031
6	2.803537	-0.100139	-3.558581	6	-1.895891	1.706533	-3.769202
6	-0.761303	1.125383	-3.213050	6	1.399259	-0.131354	-3.520876
6	0.360047	0.283310	-3.514000	6	0.447699	0.926786	-3.690391
6	-3.210761	1.481814	-3.180033	6	3.754415	-0.885910	-3.443308
6	-2.087927	0.625445	-3.425614	6	2.799157	0.175701	-3.558559
6	-5.668190	1.836980	-3.148069	6	6.115458	-1.646515	-3.366221
6	-4.536400	0.985361	-3.400979	6	5.153509	-0.583927	-3.490469
6	-8.111477	2.213644	-3.137797	6	8.461624	-2.423319	-3.315235
6	-6.992313	1.333308	-3.351714	6	7.513530	-1.342095	-3.393489
6	-9.431474	1.676420	-3.379739	6	9.864404	-2.078069	-3.366469
1	-10.871819	-1.916897	-2.334218	1	11.745205	0.944057	-1.508959
1	-10.889103	-3.092641	-0.187764	1	11.752456	1.612919	0.846417
1	8.341056	-2.762884	-4.390067	1	-6.883951	5.350645	-4.303371
1	8.057448	-4.846505	-3.832842	1	-6.342438	7.202682	-3.274367
1	8.118411	-6.712581	0.199565	1	-6.454762	8.185305	1.060446
1	7.971098	-6.413151	-1.954069	1	-6.179366	8.308306	-1.096995
1	-10.657729	-0.077396	-3.452218	1	11.347118	-0.579261	-2.993741
1	-10.652201	-2.815649	1.971750	1	11.285234	0.915759	2.877577
1	-10.154619	-1.321087	3.844515	1	10.406190	-0.819324	4.361896
1	7.853545	-3.441628	3.494690	1	-6.963667	4.319907	3.594854
1	8.526490	-5.638637	2.383058	1	-7.196777	6.778929	2.945709
1	-9.634767	0.724955	4.353084	1	9.530422	-2.818717	4.427588
1	8.328764	-1.351439	3.614574	1	-7.761581	2.379684	3.189174
1	-9.074480	3.024751	3.748310	1	8.677878	-4.820430	3.312225
1	8.772865	0.584347	2.182477	1	-8.373195	0.872317	1.363456
1	-8.746632	4.472140	2.167805	1	8.290637	-5.802551	1.404679
1	8.981361	1.467371	0.212008	1	-8.549593	0.406888	-0.761698
1	-8.612563	4.984913	-0.217470	1	8.286136	-5.770017	-1.039002
1	8.949193	1.010780	-2.199005	1	-8.237982	1.328285	-3.013240
1	-8.797580	3.982070	-2.118254	1	8.778255	-4.454396	-2.669788
1	8.697068	-0.408077	-3.836653	1	-7.632475	3.022235	-4.286117
1	-10.291963	2.361353	-3.400397	1	10.608477	-2.879556	-3.485374
6	0.959649	4.090471	-1.492627	6	-0.879556	-3.089394	-2.590576
6	2.242259	4.956790	-1.573718	6	-2.230534	-3.748343	-3.030616
8	2.387723	5.888727	-0.798101	8	-2.422642	-4.931588	-2.800918
8	3.108420	4.676991	-2.567609	8	-3.113761	-2.967260	-3.679937
6	4.305422	5.534158	-2.586006	6	-4.445409	-3.553317	-3.911648
1	3.962069	6.585451	-2.525048	1	-4.296484	-4.611977	-4.199013
1	4.759775	5.341331	-3.572428	1	-4.852223	-2.982634	-4.764219
6	-0.096095	5.182474	-1.870549	6	0.084051	-4.234655	-3.056157
8	-0.401213	5.418166	-3.023809	8	0.519748	-4.314353	-4.187975
8	-0.509157	5.877605	-0.797942	8	0.262886	-5.145580	-2.083924
6	-1.475447	6.942590	-1.038015	6	1.122760	-6.278340	-2.375827
1	-1.028695	7.671812	-1.743453	1	0.645731	-6.884327	-3.172893
1	-2.362077	6.499067	-1.534642	1	2.086811	-5.897583	-2.770093
6	5.893121	3.314496	4.404317	6	1.289409	-7.045487	-1.070967
6	7.215773	3.078451	4.249960	1	0.306655	-7.391053	-0.693570

16	8.032759	3.849492	2.874978	1	1.940751	-7.928316	-1.225108
1	7.823560	2.452246	4.913405	1	1.750750	-6.400789	-0.297275
16	5.093837	4.372354	3.230232	16	-10.141869	-4.063759	-0.619721
1	5.275047	2.909624	5.215263	6	-11.548557	-4.651794	0.272649
6	6.515508	4.434791	2.133313	6	-11.584797	-4.424995	1.605776
6	6.413013	4.878062	0.847163	1	-12.334906	-5.155240	-0.304222
16	4.875084	5.527614	0.220135	6	-9.231580	-3.504003	0.827264
16	7.722185	4.807868	-0.366723	6	-3.058319	-7.413885	1.112460
6	5.303489	5.237574	-1.497177	6	-3.114524	-7.159994	2.440467
6	6.600295	4.900444	-1.733466	16	-3.814995	-5.620196	2.945294
1	7.020980	4.738747	-2.734043	1	-2.737582	-7.823326	3.229217
6	-1.807160	7.552134	0.316906	16	-10.222850	-3.562805	2.327468
1	-0.877096	7.847700	0.842067	6	-7.889376	-3.176810	0.809084
1	-2.439390	8.453127	0.185316	1	-12.405449	-4.716169	2.273982
1	-2.353029	6.825419	0.950553	16	-3.683979	-6.181929	0.016922
				1	-2.629232	-8.314956	0.655996
				6	-6.668727	-2.957504	-2.822263
				6	-4.902923	-3.814223	-1.417248
				6	-5.350112	-3.438963	-2.697359
				6	-5.718628	-3.731048	-0.276213
				1	-3.868712	-4.127311	-1.284994
				6	-7.063231	-3.264046	-0.413883
				6	-5.213837	-4.069255	1.068411
				6	-7.508143	-2.882737	-1.699003
				1	-8.507407	-2.447717	-1.819166
				6	-7.678054	-1.986054	3.046211
				6	-7.136398	-2.801865	2.028661
				6	-6.916825	-1.601948	4.160066
				1	-8.693767	-1.587454	2.935537
				6	-5.779577	-3.241562	2.150966
				6	-5.020795	-2.826026	3.267319
				6	-5.579149	-2.018112	4.268022
				1	-3.956602	-3.084906	3.321369
				1	-7.357111	-0.941527	4.919517
				6	-4.332696	-5.110607	1.302164
				1	-4.957847	-1.687896	5.111690
				1	-7.039756	-2.611208	-3.797646
(6,5)-SWCNT – ZnTPP				(6,5)-SWCNT – AQ			
Atom	X	Y	Z	Atom	X	Y	Z
6	12.420143	-2.275354	-0.687387	6	-9.821208	-2.600371	-1.593347
6	12.462335	-2.183901	0.691635	6	-9.777906	-3.175543	-0.348839
6	11.423918	-1.498188	1.414490	6	-8.524532	-3.405666	0.305699
6	10.623207	-0.568823	0.672043	6	-7.363529	-3.447040	-0.522131
6	10.557357	-0.685982	-0.760789	6	-7.402850	-2.822671	-1.809100
6	11.325329	-1.701314	-1.426567	6	-8.612522	-2.204771	-2.255341
6	9.624251	0.216278	1.350532	6	-6.089788	-3.766671	0.052986
6	8.842499	1.171306	0.616471	6	-4.929665	-3.836453	-0.779730
6	8.739052	1.014053	-0.804560	6	-4.960246	-3.170916	-2.039910
6	9.462761	-0.049746	-1.443767	6	-6.160757	-2.505964	-2.446188

6	7.868321	1.970608	1.304169	6	-3.668052	-4.182768	-0.204351
6	7.057436	2.895203	0.560902	6	-2.500540	-4.212133	-1.030720
6	6.917010	2.696668	-0.851373	6	-2.523209	-3.502272	-2.266312
6	7.633162	1.622815	-1.482745	6	-3.723082	-2.831062	-2.663706
6	6.093664	3.709739	1.249518	6	-1.238956	-4.575353	-0.460189
6	5.266145	4.612617	0.499687	6	-0.069236	-4.576077	-1.282280
6	5.094260	4.376923	-0.904678	6	-0.086710	-3.826388	-2.496106
6	5.791017	3.283997	-1.519382	6	-1.280921	-3.139164	-2.871957
6	4.311887	5.440389	1.185453	6	1.191529	-4.951911	-0.719816
6	3.463778	6.318417	0.429144	6	2.364751	-4.919604	-1.536273
6	3.262362	6.048319	-0.963610	6	2.351759	-4.135763	-2.725515
6	3.953306	4.944293	-1.565056	6	1.155945	-3.444011	-3.087728
6	2.515183	7.153443	1.112917	6	3.624754	-5.306093	-0.979211
6	1.644341	8.019620	0.362318	6	4.808790	-5.257441	-1.783934
6	1.412190	7.714915	-1.024818	6	4.801160	-4.436792	-2.956401
6	2.099512	6.593668	-1.607856	6	3.600418	-3.734647	-3.297098
6	0.740851	8.898344	1.051006	6	6.057254	-5.697150	-1.243548
6	-0.078159	9.757301	0.233868	6	7.190971	-5.656876	-2.120797
6	-0.314120	9.447424	-1.092457	6	7.184915	-4.854497	-3.233300
6	0.270065	8.275084	-1.688584	6	6.040780	-4.053145	-3.551567
6	-0.436736	7.455124	-2.650553	6	6.150643	-2.733588	-4.110657
6	-1.787602	7.733108	-3.058991	6	7.415568	-2.106783	-4.349746
6	0.404576	8.602303	2.422988	6	6.197091	-5.784293	0.179569
6	-0.748984	9.180480	3.075026	6	7.482352	-5.870027	0.822186
6	1.419080	5.803755	-2.581807	6	3.704296	-2.446260	-3.881527
6	0.064044	6.139619	-2.927435	6	5.004453	-1.882321	-4.083871
6	2.150908	6.828037	2.454245	6	3.769578	-5.349534	0.431878
6	0.960048	7.415403	3.007154	6	5.088794	-5.385679	0.987865
6	3.286571	4.171296	-2.572530	6	1.257673	-2.161034	-3.704017
6	1.939182	4.510200	-2.918051	6	2.552227	-1.600695	-3.907060
6	3.915898	5.082623	2.517521	6	1.344315	-4.947540	0.698694
6	2.710687	5.649696	3.057018	6	2.664236	-4.956026	1.251768
6	5.143288	2.539269	-2.559575	6	-1.178373	-1.873126	-3.520937
6	3.805170	2.883658	-2.935660	6	0.110997	-1.311256	-3.753410
6	5.670380	3.323565	2.565272	6	-1.078984	-4.523801	0.956828
6	4.459850	3.886838	3.099263	6	0.243089	-4.521484	1.505798
6	7.012076	0.910456	-2.560795	6	-3.624981	-1.587465	-3.354856
6	5.674581	1.262217	-2.938485	6	-2.330297	-1.031471	-3.584908
6	7.415957	1.553725	2.600865	6	-3.500399	-4.081519	1.209657
6	6.197197	2.110021	3.125912	6	-2.174969	-4.062445	1.752283
6	8.874826	-0.722007	-2.557247	6	-6.069065	-1.295837	-3.182062
6	7.550698	-0.352248	-2.973558	6	-4.775936	-0.748299	-3.454452
6	9.144970	-0.228131	2.619458	6	-5.915095	-3.618419	1.453650
6	7.924265	0.324400	3.138378	6	-4.589524	-3.588892	1.991259
6	10.762544	-2.344950	-2.590648	6	-8.526698	-1.007327	-3.038978
6	9.436605	-1.971404	-2.992758	6	-7.231016	-0.468377	-3.304332
6	10.907647	-1.982678	2.677816	6	-8.340918	-3.199577	1.716460
6	9.651071	-1.470670	3.142206	6	-7.009882	-3.104870	2.222686
6	11.291001	-3.576775	-3.129910	6	-9.655369	-0.140080	-3.247131
6	11.363750	-3.213212	3.268210	6	-9.387292	-2.689435	2.550274
6	0.139356	6.614249	3.869402	6	5.336640	-4.675358	2.200090

6	-1.208184	7.033593	4.157122	6	6.688265	-4.408777	2.596207
6	-1.529907	8.424327	3.923325	6	7.721242	-5.214479	1.998727
6	1.867559	4.836908	3.881176	6	2.925130	-4.202985	2.431568
6	0.507741	5.253883	4.111772	6	4.285682	-3.910968	2.781723
6	3.596915	3.056695	3.890424	6	0.511743	-3.725382	2.659853
6	2.237912	3.472106	4.109556	6	1.870170	-3.425576	2.995938
6	5.315773	1.263779	3.876837	6	-1.899506	-3.223706	2.872249
6	3.955898	1.679930	4.082486	6	-0.539787	-2.916959	3.192753
6	7.024619	-0.537917	3.848949	6	-4.307799	-2.708180	3.077780
6	5.664758	-0.121541	4.037941	6	-2.948219	-2.391742	3.379511
6	8.731361	-2.350808	3.813229	6	-6.721335	-2.180405	3.276304
6	7.364945	-1.927719	3.973763	6	-5.353094	-1.853925	3.550523
6	10.469990	-4.067931	3.889861	6	-9.107388	-1.782113	3.542597
6	9.074405	-3.733407	3.975491	6	-7.764677	-1.344704	3.773461
6	-2.205681	6.051579	4.341927	6	6.978490	-3.209861	3.260063
6	-0.529297	4.269417	4.202093	6	4.605459	-2.653052	3.370188
6	-1.913684	4.676834	4.136177	6	5.977831	-2.228415	3.435786
6	1.199128	2.482139	4.132586	6	2.187939	-2.136134	3.519316
6	-0.169163	2.895026	3.989047	6	3.549674	-1.698066	3.517353
6	2.914795	0.692156	4.055095	6	-0.219122	-1.608006	3.663519
6	1.552761	1.114296	3.888783	6	1.141339	-1.172199	3.635377
6	4.622437	-1.105225	3.965891	6	-2.625257	-1.068140	3.805359
6	3.264452	-0.671349	3.783697	6	-1.261311	-0.636737	3.754925
6	6.328172	-2.902337	3.861954	6	-5.031201	-0.525575	3.932734
6	4.975764	-2.463399	3.673855	6	-3.669290	-0.097405	3.877603
6	8.023539	-4.720499	3.814930	6	-7.439741	0.018158	4.109704
6	6.690243	-4.261621	3.554931	6	-6.084288	0.446081	3.984193
6	8.302970	-6.098351	3.519010	6	-8.435717	1.040773	4.186330
6	-2.862181	3.779275	3.475580	6	6.263573	-0.817864	3.229719
6	-4.178399	4.190631	3.087083	6	7.574972	-0.334206	2.941062
6	-1.076685	2.061484	3.266129	6	3.834614	-0.334849	3.237008
6	-2.346747	2.598637	2.850073	6	5.175935	0.035705	2.891662
6	0.657729	0.300992	3.117183	6	1.427402	0.189146	3.312247
6	-0.581459	0.861872	2.665073	6	2.755440	0.543035	2.927580
6	2.381988	-1.462031	2.975958	6	-0.973756	0.713325	3.396925
6	1.152423	-0.894664	2.504260	6	0.352264	1.071108	3.001048
6	4.107918	-3.236835	2.834348	6	-3.385557	1.244212	3.485789
6	2.897804	-2.643820	2.349429	6	-2.061846	1.578230	3.071152
6	5.832650	-5.019491	2.681738	6	-5.801125	1.783028	3.556644
6	4.627577	-4.405434	2.187940	6	-4.469254	2.105036	3.135107
6	7.484530	-6.819009	2.663578	6	-8.164964	2.319236	3.757368
6	6.329923	-6.212430	2.063275	6	-6.878764	2.661041	3.238348
6	-4.753513	3.729943	1.910894	6	7.768239	0.680154	2.033148
6	-2.927003	2.132889	1.616457	6	5.369945	1.071216	1.924447
6	-4.035163	2.839820	1.044680	6	6.659201	1.263211	1.352478
6	-1.121657	0.440505	1.408049	6	2.942890	1.551616	1.940442
6	-2.185599	1.192202	0.816008	6	4.222257	1.684261	1.327680
6	0.626382	-1.295651	1.224881	6	0.546515	2.087398	2.007820
6	-0.409947	-0.512581	0.613214	6	1.818885	2.209911	1.367569
6	2.415501	-2.998263	1.051218	6	-1.879468	2.541020	2.041584
6	1.382373	-2.217599	0.434303	6	-0.605027	2.675134	1.410680

6	4.164427	-4.735938	0.877509	6	-4.288374	3.048046	2.087772
6	3.166331	-3.916277	0.254856	6	-3.021976	3.132517	1.435379
6	5.897462	-6.511984	0.708342	6	-6.702961	3.589526	2.146615
6	4.954651	-5.634466	0.078878	6	-5.449502	3.612372	1.466803
6	6.632072	-7.390864	-0.155676	6	-7.806279	4.198883	1.475631
6	-4.108349	2.930474	-0.401799	6	6.738073	1.729951	-0.003406
6	-4.927185	3.897585	-1.079555	6	7.940741	1.673614	-0.771118
6	-2.247950	1.285936	-0.607764	6	4.291207	2.125795	-0.017227
6	-3.048497	2.342274	-1.165213	6	5.524763	1.940898	-0.718140
6	-0.572070	-0.526962	-0.816382	6	1.912528	2.798905	0.057780
6	-1.266431	0.607012	-1.419499	6	3.088242	2.460548	-0.730471
6	1.260253	-2.189756	-0.992766	6	-0.520538	3.197472	0.088737
6	0.194029	-1.454652	-1.583481	6	0.752520	3.414191	-0.493138
6	3.201582	-3.710139	-1.167682	6	-2.970120	3.425210	0.038090
6	2.402228	-2.668100	-1.762256	6	-1.748138	3.228655	-0.685681
6	5.047869	-5.375165	-1.333952	6	-5.411889	3.848413	0.054670
6	4.301605	-4.270690	-1.887991	6	-4.200523	3.558602	-0.660886
6	6.745121	-7.115828	-1.510774	6	-7.773615	4.399001	0.113512
6	6.117947	-5.959766	-2.081646	6	-6.634102	4.014956	-0.654368
6	-4.456655	4.553125	-2.206458	6	7.895335	1.384342	-2.113576
6	-2.543776	3.040285	-2.311052	6	5.474920	1.621624	-2.104667
6	-3.133588	4.286930	-2.702602	6	6.641976	1.117024	-2.752895
6	-0.723147	1.345572	-2.543213	6	3.026899	2.055015	-2.108013
6	-1.246242	2.663604	-2.800946	6	4.181753	1.424509	-2.682352
6	1.047019	-0.310027	-3.248335	6	0.644636	2.715844	-2.597386
6	0.570567	1.025942	-3.128897	6	1.770762	1.881364	-2.809936
6	2.981352	-1.894465	-2.840382	6	-1.824085	2.739041	-2.033898
6	2.442523	-0.598853	-3.256040	6	-0.671586	2.194626	-2.745709
6	4.900326	-3.484422	-2.915951	6	-4.288836	3.015124	-1.967154
6	4.345354	-2.192154	-3.202968	6	-3.128407	2.405221	-2.533636
6	6.774668	-5.127466	-3.089847	6	-6.749030	3.381788	-1.959426
6	6.246839	-3.801687	-3.310851	6	-5.590397	2.709411	-2.481522
6	8.106476	-5.385158	-3.508688	6	-8.008126	3.032555	-2.493846
6	-2.264851	5.330829	-3.208248	6	6.484741	0.053217	-3.709297
6	-2.675808	6.702887	-3.320217	6	7.578746	-0.757843	-4.148763
6	-0.375776	3.716515	-3.216931	6	4.029777	0.323876	-3.565781
6	-0.854872	5.072839	-3.227243	6	5.172281	-0.471475	-3.903690
6	1.492387	2.107538	-3.315778	6	1.593324	0.632089	-3.487631
6	1.031518	3.460516	-3.254151	6	2.718715	-0.197828	-3.763593
6	3.370568	0.486808	-3.392726	6	-0.852622	0.927620	-3.379439
6	2.900287	1.840508	-3.338217	6	0.279847	0.109206	-3.669340
6	5.254663	-1.114838	-3.477646	6	-3.299291	1.209245	-3.293725
6	4.780379	0.233361	-3.367374	6	-2.162363	0.377836	-3.521052
6	7.147839	-2.718477	-3.561294	6	-5.752566	1.496522	-3.208389
6	6.664544	-1.367145	-3.461113	6	-4.608545	0.666505	-3.447182
6	9.023198	-4.323825	-3.674625	6	-8.191862	1.801422	-3.138675
6	8.555810	-2.970262	-3.526640	6	-7.059437	0.947681	-3.342818
6	10.453207	-4.533239	-3.664995	6	-9.496519	1.217893	-3.306758
1	13.145725	-2.920314	-1.199917	1	-10.785023	-2.323144	-2.013815
1	13.218367	-2.759986	1.241624	1	-10.707946	-3.339641	0.191189
1	-2.165229	8.763420	-3.028369	1	8.291238	-2.716774	-4.559244

1	-1.062027	10.026489	-1.650021	1	8.102661	-4.738310	-3.805657
1	-1.081730	10.187831	2.791568	1	8.306756	-6.360802	0.309523
1	-0.645644	10.574031	0.698712	1	8.113720	-6.156610	-1.835490
1	12.356964	-3.808304	-3.005363	1	-10.659893	-0.557217	-3.243606
1	12.391488	-3.557095	3.092639	1	-10.425983	-2.902923	2.308538
1	10.811282	-5.068198	4.188317	1	-9.931145	-1.300396	4.064910
1	-3.248833	6.391118	4.389564	1	8.025554	-2.946852	3.390360
1	-2.478249	8.827477	4.307813	1	8.727457	-5.183090	2.416759
1	9.248921	-6.546843	3.849897	1	-9.458382	0.781836	4.450781
1	-4.689502	4.982959	3.650244	1	8.443727	-0.848930	3.346388
1	7.802140	-7.820381	2.344005	1	-8.980573	3.036451	3.697073
1	-5.699854	4.175625	1.577158	1	8.780825	0.959009	1.752813
1	7.242496	-8.197027	0.271827	1	-8.737676	4.374751	2.009039
1	-5.869594	4.229080	-0.623551	1	8.903478	1.742645	-0.270176
1	7.446126	-7.709491	-2.112554	1	-8.681104	4.725487	-0.390029
1	-5.039545	5.387586	-2.618045	1	8.826546	1.208162	-2.648122
1	8.511929	-6.403869	-3.450448	1	-8.897523	3.579929	-2.190511
1	-3.735290	6.940583	-3.484673	1	8.579519	-0.334037	-4.199323
1	10.851046	-5.516536	-3.955614	1	-10.367838	1.871470	-3.348864
6	0.068845	-1.445722	-3.088665	6	0.790560	4.049964	-1.881963
6	-1.398371	-1.284509	-3.606681	6	1.995739	5.036679	-2.056744
8	-2.307896	-1.935341	-3.132147	8	1.920143	6.137533	-1.544650
8	-1.449983	-0.468180	-4.679110	8	3.053495	4.604527	-2.774536
6	-2.673807	-0.310001	-5.495744	6	4.232038	5.511851	-2.734254
1	-2.606461	-1.067229	-6.301621	1	3.865379	6.542545	-2.807883
1	-2.529564	0.692829	-5.939405	1	4.795701	5.237120	-3.630364
6	0.490164	-2.719202	-3.882352	6	-0.374672	5.038499	-2.276871
8	0.919996	-2.668189	-5.019312	8	-0.715914	5.174479	-3.435143
8	0.232253	-3.852675	-3.199867	8	-0.854670	5.713861	-1.221185
6	0.639144	-5.101898	-3.838922	6	-2.050182	6.535378	-1.492803
1	-0.143778	-5.378481	-4.574871	1	-1.747977	7.370491	-2.138057
1	1.576778	-4.918913	-4.398788	1	-2.766091	5.907838	-2.039472
6	0.806145	-6.152999	-2.751168	6	-2.583592	6.987081	-0.146439
1	-0.123050	-6.260877	-2.158444	1	-1.834002	7.584363	0.389450
1	1.042254	-7.132039	-3.214596	1	-3.482945	7.600878	-0.296033
1	1.633337	-5.883848	-2.066782	1	-2.853886	6.123277	0.473519
6	-7.378209	-1.099678	-2.149267	8	8.613783	4.096239	1.915261
6	-8.056791	-4.879445	0.939220	6	7.387012	4.240259	1.979045
6	-12.585088	-3.248664	1.969324	6	6.446121	5.089935	-1.579863
6	-11.844964	0.619247	-0.992129	6	4.469424	5.292718	-0.215869
7	-10.280017	-3.776653	1.179631	6	5.056773	5.301106	-1.482878
7	-8.070874	-2.837177	-0.491464	6	5.212670	4.953182	0.915694
7	-9.655762	-0.529725	-1.311228	1	3.413650	5.475686	-0.069179
7	-11.832215	-1.426009	0.440771	6	6.598801	4.730828	0.812596
6	-10.553383	0.494144	-1.561839	6	4.465164	4.703401	2.183398
6	-8.542627	-0.291951	-2.100275	6	7.213552	4.856244	-0.442130
6	-7.156257	-2.253537	-1.350481	1	8.284432	4.681535	-0.512983
6	-7.459523	-3.959013	0.042895	6	7.259632	3.076116	4.180170
6	-12.438753	-0.303768	-0.093491	6	6.607203	3.809011	3.178462
6	-12.778795	-2.053613	1.233532	6	6.528724	2.491493	5.210373
6	-11.397787	-4.022451	1.956944	1	8.334832	2.936194	4.097402

6	-9.359862	-4.763758	1.481768	6	5.210914	4.001065	3.261332
6	-9.979604	1.419522	-2.526329	6	4.486101	3.435358	4.319249
6	-8.747374	0.919279	-2.878164	6	5.137517	2.662048	5.275239
6	-5.909715	-3.008595	-1.324763	1	3.407662	3.577605	4.337626
6	-6.106381	-4.071661	-0.477934	1	7.035695	1.880887	5.956633
6	-9.907378	-5.653222	2.493669	8	3.267191	4.979713	2.291578
6	-11.167006	-5.191388	2.791550	1	4.565218	2.179020	6.066363
6	-13.818783	-0.229886	0.362873	1	6.923699	5.083810	-2.559740
6	-14.028740	-1.313461	1.181504				
1	-10.463260	2.328182	-2.893298				
1	-8.037847	1.332993	-3.598663				
1	-4.995602	-2.752948	-1.866329				
1	-5.392698	-4.857427	-0.222113				
1	-9.381440	-6.502233	2.936970				
1	-11.869317	-5.587117	3.528700				
1	-14.539675	0.536666	0.070265				
1	-14.953388	-1.602266	1.686896				
6	-6.288362	-0.771354	-3.123644				
6	-5.923816	-1.739197	-4.091997				
6	-5.539881	0.426197	-3.064395				
1	-6.517945	-2.659253	-4.171589				
1	-5.812633	1.201472	-2.336868				
6	-4.788503	-1.566528	-4.890601				
6	-4.412795	0.605722	-3.883547				
1	-4.483443	-2.362884	-5.585012				
1	-3.825983	1.528283	-3.800737				
6	-3.990317	-0.412115	-4.761808				
6	-7.252691	-6.082020	1.329447				
6	-6.070042	-5.954830	2.092367				
6	-7.655430	-7.371921	0.912359				
1	-5.761288	-4.957705	2.434769				
1	-8.576933	-7.479041	0.323329				
6	-5.296362	-7.084429	2.409399				
6	-6.882661	-8.502130	1.229177				
1	-4.376499	-6.966750	3.000241				
1	-7.203833	-9.496660	0.886456				
6	-5.696288	-8.360810	1.972436				
1	-5.084450	-9.242897	2.209788				
6	-13.711115	-3.736494	2.828403				
6	-14.168914	-2.975902	3.929463				
6	-14.323680	-4.985158	2.569996				
1	-13.696694	-2.007030	4.142129				
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6	-15.198868	-3.456711	4.756424				
6	-15.354737	-5.465891	3.394754				
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1	-15.817405	-6.439715	3.177630				
6	-15.793130	-4.705049	4.494286				
1	-16.593369	-5.084798	5.145871				
6	-12.690470	1.791851	-1.386358				
6	-13.173327	1.932938	-2.707158				

6	-13.078838	2.746656	-0.418049				
1	-12.888023	1.186691	-3.461335				
1	-12.708140	2.640181	0.610721				
6	-14.032961	2.992063	-3.046951				
6	-13.938315	3.805480	-0.756101				
1	-14.413915	3.076347	-4.075086				
1	-14.237840	4.532191	0.013245				
6	-14.422225	3.928965	-2.071713				
1	-15.105516	4.749364	-2.334376				
30	-9.958916	-2.141821	-0.048471				
(6,5)-SWCNT – TCAQ							
Atom	X	Y	Z				
6	10.236353	2.270268	-1.014926				
6	10.186017	2.651016	0.301973				
6	8.928356	2.878797	0.948515				
6	7.807395	3.136782	0.104752				
6	7.851565	2.713033	-1.261391				
6	9.029128	2.076642	-1.763668				
6	6.539089	3.466183	0.686410				
6	5.420846	3.751721	-0.157647				
6	5.451836	3.282492	-1.503458				
6	6.615272	2.594442	-1.973494				
6	4.166677	4.106547	0.428608				
6	3.037592	4.350847	-0.415440				
6	3.056237	3.833587	-1.743299				
6	4.218282	3.137957	-2.205385				
6	1.784974	4.723794	0.168301				
6	0.651804	4.939157	-0.676142				
6	0.661354	4.378804	-1.988184				
6	1.815398	3.664072	-2.431133				
6	-0.598714	5.326870	-0.098814				
6	-1.737323	5.510056	-0.943535				
6	-1.735797	4.912232	-2.236529				
6	-0.581731	4.189037	-2.665752				
6	-2.985833	5.910461	-0.370658				
6	-4.136479	6.077843	-1.207312				
6	-4.143982	5.441036	-2.488694				
6	-2.987011	4.702205	-2.897212				
6	-5.368950	6.532304	-0.643228				
6	-6.466097	6.714607	-1.548097				
6	-6.475950	6.087196	-2.767766				
6	-5.384340	5.251309	-3.168853				
6	-5.572164	4.039941	-3.920635				
6	-6.871221	3.558154	-4.279814				
6	-5.560452	6.413137	0.771909				
6	-6.862187	6.499537	1.380244				
6	-3.163857	3.527972	-3.673034				
6	-4.494477	3.106611	-3.993141				
6	-3.183820	5.753947	1.025924				

6	-4.519046	5.809723	1.540977
6	-0.753501	3.026297	-3.474840
6	-2.077069	2.607902	-3.798186
6	-0.807368	5.124606	1.298204
6	-2.144620	5.155305	1.807774
6	1.645901	2.523109	-3.270315
6	0.329252	2.106687	-3.624275
6	1.566417	4.475955	1.556687
6	0.227075	4.497132	2.061952
6	4.056515	2.025015	-3.082184
6	2.734811	1.613441	-3.431714
6	3.936876	3.809477	1.805735
6	2.593408	3.815338	2.302503
6	6.463987	1.520430	-2.889114
6	5.146186	1.123370	-3.278282
6	6.298791	3.123546	2.042479
6	4.954759	3.119920	2.532617
6	8.886381	1.021835	-2.724434
6	7.566208	0.632437	-3.105085
6	8.674241	2.477926	2.305614
6	7.321012	2.414532	2.754078
6	9.956067	0.110614	-3.032571
6	9.645805	1.766489	3.080510
6	-4.869710	4.941298	2.617656
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6	-2.508535	4.255510	2.849625
6	-3.901631	4.019216	3.105917
6	-0.145331	3.561171	3.073408
6	-1.535550	3.322645	3.318921
6	2.212491	2.841994	3.272587
6	0.822083	2.599936	3.504195
6	4.565503	2.110167	3.462539
6	3.175331	1.860768	3.673271
6	6.922848	1.367530	3.644701
6	5.524405	1.113447	3.826671
6	9.259834	0.745118	3.913535
6	7.880305	0.385795	4.036557
6	-6.657549	3.455267	3.371402
6	-4.336044	2.713860	3.477253
6	-5.736712	2.386620	3.428204
6	-1.966659	1.997089	3.623987
6	-3.355664	1.672685	3.506152
6	0.388450	1.263286	3.756367
6	-0.997751	0.947898	3.619728
6	2.739325	0.517153	3.878302
6	1.350645	0.208133	3.723021
6	5.090387	-0.228130	3.988604
6	3.704193	-0.533645	3.828255
6	7.442399	-0.981840	4.150133
6	6.065494	-1.276863	3.920346

6	8.355589	-2.080576	4.100033
6	-6.110914	1.044835	3.005933
6	-7.440593	0.685970	2.633048
6	-3.722004	0.400444	2.997152
6	-5.071106	0.179074	2.567506
6	-1.365635	-0.318377	3.072553
6	-2.693650	-0.493591	2.587659
6	0.980128	-1.045821	3.152735
6	-0.349616	-1.230357	2.666125
6	3.338410	-1.774311	3.226797
6	2.011815	-1.936806	2.728456
6	5.702317	-2.507262	3.284576
6	4.368770	-2.655712	2.780131
6	8.009227	-3.254307	3.472583
6	6.724319	-3.409981	2.867706
6	-7.674700	-0.187422	1.593025
6	-5.306024	-0.705271	1.468008
6	-6.589653	-0.743967	0.851906
6	-2.913327	-1.324841	1.458027
6	-4.178808	-1.288688	0.809407
6	-0.575878	-2.065790	1.523330
6	-1.821313	-1.982967	0.830983
6	1.800371	-2.718723	1.560190
6	0.547182	-2.655091	0.878292
6	4.161040	-3.414712	1.597386
6	2.919028	-3.301412	0.904036
6	6.525180	-4.146680	1.641972
6	5.301741	-3.968864	0.931258
6	7.607235	-4.732687	0.917616
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6	-7.811046	-0.704390	-1.350865
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6	-5.426235	-1.152076	-1.277221
6	-1.911125	-2.368444	-0.551773
6	-3.027189	-1.819902	-1.305539
6	0.475125	-2.966808	-0.509481
6	-0.787646	-2.994488	-1.157211
6	2.901630	-3.377740	-0.522549
6	1.727858	-2.978854	-1.243280
6	5.303680	-3.987104	-0.500792
6	4.146101	-3.499813	-1.198381
6	7.614944	-4.722764	-0.459375
6	6.538173	-4.139084	-1.191503
6	-7.690624	-0.196611	-2.624820
6	-5.296607	-0.614713	-2.590388
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6	-3.970813	-0.426615	-3.096354
6	-0.540280	-1.999325	-3.126691
6	-1.593946	-1.052739	-3.238115
6	1.893940	-2.297960	-2.497150

6	0.813907	-1.564365	-3.151776
6	4.326522	-2.772842	-2.401887
6	3.237631	-1.995126	-2.901053
6	6.751017	-3.327174	-2.380181
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6	-7.142629	2.210970	-4.286669
6	-3.705662	0.778675	-3.795304
6	-4.774380	1.702611	-4.032637
6	-1.300461	0.268121	-3.708436
6	-2.351900	1.216873	-3.879594
6	1.111168	-0.232168	-3.575431
6	0.054197	0.707545	-3.768549
6	3.525399	-0.714536	-3.462523
6	2.461984	0.228258	-3.591677
6	5.945472	-1.202687	-3.352530
6	4.875503	-0.259160	-3.493261
6	8.351268	-1.704585	-3.261685
6	7.293001	-0.744005	-3.364447
6	9.700669	-1.206665	-3.302649
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1	10.987328	0.442963	-2.938818
1	10.706246	1.930558	2.903770
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1	8.500656	-5.059685	1.444525
1	-8.798575	-0.755873	-0.897010
1	8.515226	-5.040916	-0.980748
1	-8.585334	0.143997	-3.141531
1	8.886279	-3.656442	-2.579548
1	-8.170209	1.880805	-4.422762
1	10.522686	-1.912658	-3.420245
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6	-2.069281	-4.267558	-3.028491
8	-2.046067	-5.470725	-2.864808
8	-3.144095	-3.601482	-3.509560
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1	-4.138714	-5.417134	-3.860235
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6	0.305434	-4.434532	-3.088293

8	0.734157	-4.445902	-4.224607
8	0.623086	-5.275632	-2.097419
6	1.715583	-6.224655	-2.370907
1	1.351845	-6.947846	-3.112520
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6	2.063737	-6.863408	-1.039703
1	1.181560	-7.355153	-0.609377
1	2.855947	-7.611230	-1.184410
1	2.425564	-6.108051	-0.330348
6	-8.331752	-4.772888	1.817505
6	-7.075589	-4.236198	1.592754
6	-6.462790	-4.149413	-2.138167
6	-4.386691	-4.591033	-1.005603
6	-5.085279	-4.392665	-2.200044
6	-5.010153	-4.505077	0.248676
1	-3.322456	-4.745226	-1.047413
6	-6.419636	-4.309979	0.286836
6	-4.235107	-4.485885	1.506256
6	-7.121731	-4.138111	-0.914468
1	-8.183765	-3.919423	-0.893264
6	-6.885257	-2.822460	3.642662
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6	-6.123894	-2.189302	4.616519
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7	-9.737481	-5.999264	0.015131
6	-2.089096	-4.947394	2.703881
7	-1.266513	-4.845257	3.526732
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