

Supporting Information for
Automatic Reaction Pathway Search via Combined
Molecular Dynamics and Coordinate Driving Method

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I. Scheme of renumbering atomic labels

Here we define an intrinsic set of coordinates for a structure using properties of the *center-of-mass system* (COM) and the *inertia principal axis system* (IPAS).^{1,2,3} The resulting RMSD using this type of coordinates is independent of original atomic tags or coordinates of molecules.

In this scheme, a structure in its initial coordinate system is translated into its COM system, followed by a projection to its IPAS system. Assuming the original position of the i -th atom within the molecule is $\mathbf{x}_i' = (x_i', y_i', z_i')$, the coordinates $\mathbf{x}_i = (x_i, y_i, z_i)$ in the COM can be written as follows.

$$x_i = x_i' - \frac{\sum_{i=1}^N m_i x_i'}{\sum_{i=1}^N m_i} \quad \text{etc.} \quad (1-1)$$

The corresponding moments of inertia and products of inertia are defined as

$$I_{xx} \equiv \sum_{i=1}^N m_i (y_i^2 + z_i^2) \quad \text{etc.}, \quad I_{xy} \equiv -\sum_{i=1}^N m_i x_i y_i \quad \text{etc.} \quad (1-2)$$

and the inertia tensor $\mathbf{I}_{xyz}$ is

$$\mathbf{I}_{xyz} = \begin{pmatrix} I_{xx} & I_{xy} & I_{xz} \\ I_{xy} & I_{yy} & I_{yz} \\ I_{xz} & I_{yz} & I_{zz} \end{pmatrix} \quad (1-3)$$

Diagonalizing the above symmetric matrix leads to three diagonal elements I_a, I_b, I_c and a orthogonal square matrix of eigenvectors $\mathbf{L}$, which gives

$$\mathbf{L}^{-1} \mathbf{I}_{xyz} \mathbf{L} = \mathbf{I}_{abc} \quad (1-4)$$

Here we always sort three diagonal elements I_a, I_b, I_c by size ($I_a > I_b > I_c$).

Assume further the coordinates in IPAS system are $\mathbf{a}_i = (a_i, b_i, c_i)$, then

$$\mathbf{a}_i = \mathbf{L}^{-1} \mathbf{x}_i \quad (1-5)$$

which means that by left multiplying $\mathbf{L}^{-1}$, the molecule is projected into the IPAS system in which three coordinate axes are inertia principal axes. Since $\mathbf{L}$ is an orthogonal matrix and three eigenvectors in it are all unity (so is $\mathbf{L}^{-1}$), this projection in fact equals to rotating the coordinate axes of the structure to coincide with their inertia principal axes. Once $\mathbf{a}_i$ is obtained, we can get a set of new atomic tags via sorting $\mathbf{a}_i$ by size. Because the COM and IPAS are intrinsic properties of a molecule, the new coordinates and atomic tags now are independent of original ones.

However, we should note that: this method sometimes fails when dealing with some spherical tops ($I_a = I_b = I_c$) molecules like fullerene (C60). Because for such special molecules any randomly chosen three directions (perpendicular to each other) could be their inertia principals, in other words, such structures have infinite sets of coordinates in IPAS system. The correspondence of atomic tags may not be the best in such cases.

II. Scheme of selecting active hydrogen atoms

In the MD/CD method, we will calculate C–H bond dissociation energy (BDE) $E_{BDE}(\text{C–H})$, according to equation (1), to judge the activity of carbon-bonded hydrogen atoms. In order to find a suitable value to define a “chemically active” hydrogen atom, we have calculated BDE values for a variety of organic molecules. The latter two quantities in equation (1) are calculated together by constrained optimization with the distance of C–H bond fixed at 4.0 Å. Calculated and experimental BDEs are listed in Table 1.

$$E_{BDE}(\text{C–H}) = E_{\text{elec}}(\text{C–H}) - E_{\text{elec}}(\text{C}\cdot) - E_{\text{elec}}(\text{H}\cdot) \quad (1)$$

Table S1. Calculated (6-31G(d)) and experimental bond dissociation energies $E_{BDE}(\text{C–H})$

(kcal/mol)

Species	UHF		UB3LYP		UMP2		Experimental
	BDE	$\Delta\text{BDE}^{\text{a}}$	BDE	$\Delta\text{BDE}^{\text{a}}$	BDE	$\Delta\text{BDE}^{\text{a}}$	BDE
methane	87.2	-17.7	112.8	7.9	102.9	-2	104.9±0.1 ^b
ethane	84.7	-16.7	108.0	6.9	100.0	-1.4	101.1±0.4 ^b
propane(CH ₂)	82.1	-16.5	103.9	5.3	97.3	-1.3	98.6±0.4 ^b
t-butane(CH)	79.9	-16.6	100.4	3.9	95.3	-1.2	96.5±0.4 ^b
toluene(CH ₃)	65.4	-23.1	94.9	6.4	96.0	7.5	88.5±1.5 ^b
propene(CH ₃)	85.4	-2.8	92.1	3.9	102.4	14.2	88.2±2.1 ^b
cyclopropane	91.0	-15.3	113.7	7.4	103.6	-2.7	106.3±0.3 ^c
cyclobutane	82.5	-14	103.3	6.8	93.6	-2.9	96.5±1.0 ^c
cyclopentane	78.8	-15.7	101.5	7.0	/	/	94.5±1.0 ^c
ethene	90.5	-20.7	116.5	5.3	90.0	-21.2	111.2±0.8 ^b
ethyne	106.0	-26.8	138.6	5.8	91.4	-41.4	132.8±0.7 ^b
benzene	/	/	117.2	6.0	/	/	111.2±0.8 ^b

^a ΔBDE =calculated BDE-experimental BDE. ^b Values taken from Ref⁴. ^c Values taken from Ref⁵.

In Figure S1, we plotted the UB3LYP/6-31G(d)-calculated BDE values and experimental data taken from the Refs^{4,5} for a variety of molecules. One can see that although the calculated values are always overestimated, the solid and dashed lines are approximately parallel. Thus, calculated BDE values at the UB3LYP/6-31G(d) level can provide a good qualitative judgment for measuring the activity of C-H bonds. In this work, we adopted the $E_{BDE}(C-H)$ for toluene ($C_6H_5CH_2-H$) to be the critical value: $E_{BDE,c}(C-H) = 95 \text{ kcal/mol}$. Carbon-bonded hydrogen atoms are regarded as active ones when calculated values are less than $E_{BDE,c}(C-H)$.

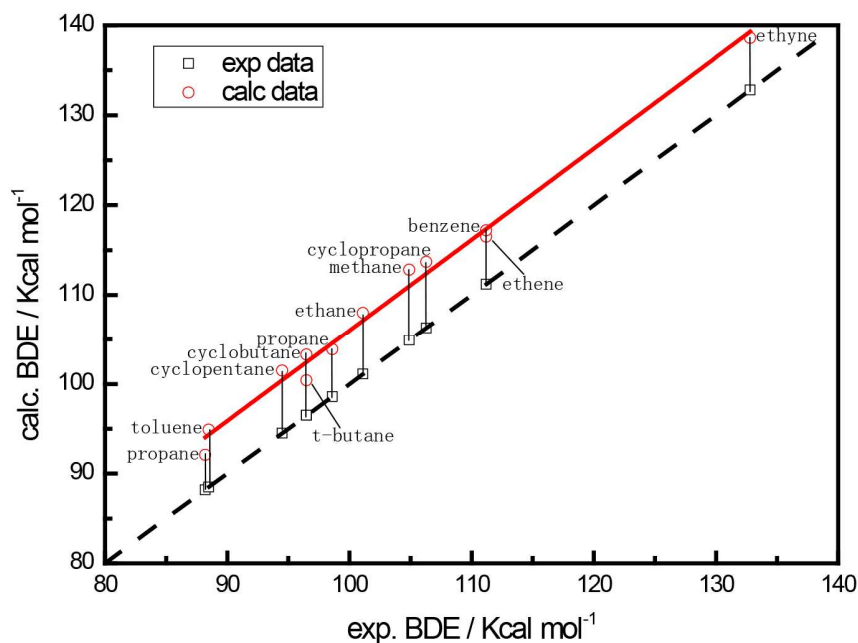


Figure S1. UB3LYP/6-31G(d)-calculated versus averaged experimental bond dissociation energies. Ethene and benzene, and t-butane and cyclopentane have the same experimental BDEs. Solid line: fitting line through all calculated data point; Dashed line: unity slope. The vertical bars just serve as a guide to the eye.

III. Local minima and TSs structures for the electrocyclic reaction

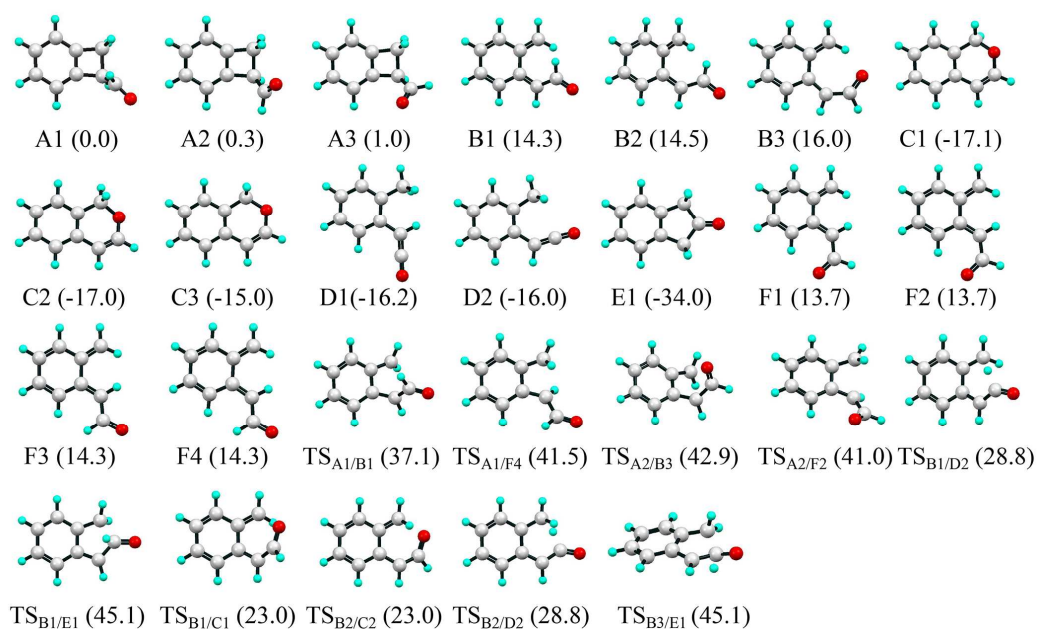


Figure S2. All local minima and TSs located for the electrocyclic reaction of benzocyclobutene-7-carboxaldehyde by the MD/CD method with $E_{\text{cut}} = 50$ kcal/mol. Relative free energies (kcal/mol) of all species calculated at the M06-2X/6-31G* level, relative to the reactant **A1**, are given in parentheses. Different conformers of one structure are labeled with the same capital. Cartesian coordinates for all these structures are available in SI.

IV. Local minima and TSs structures of the intramolecular Diels-Alder reaction

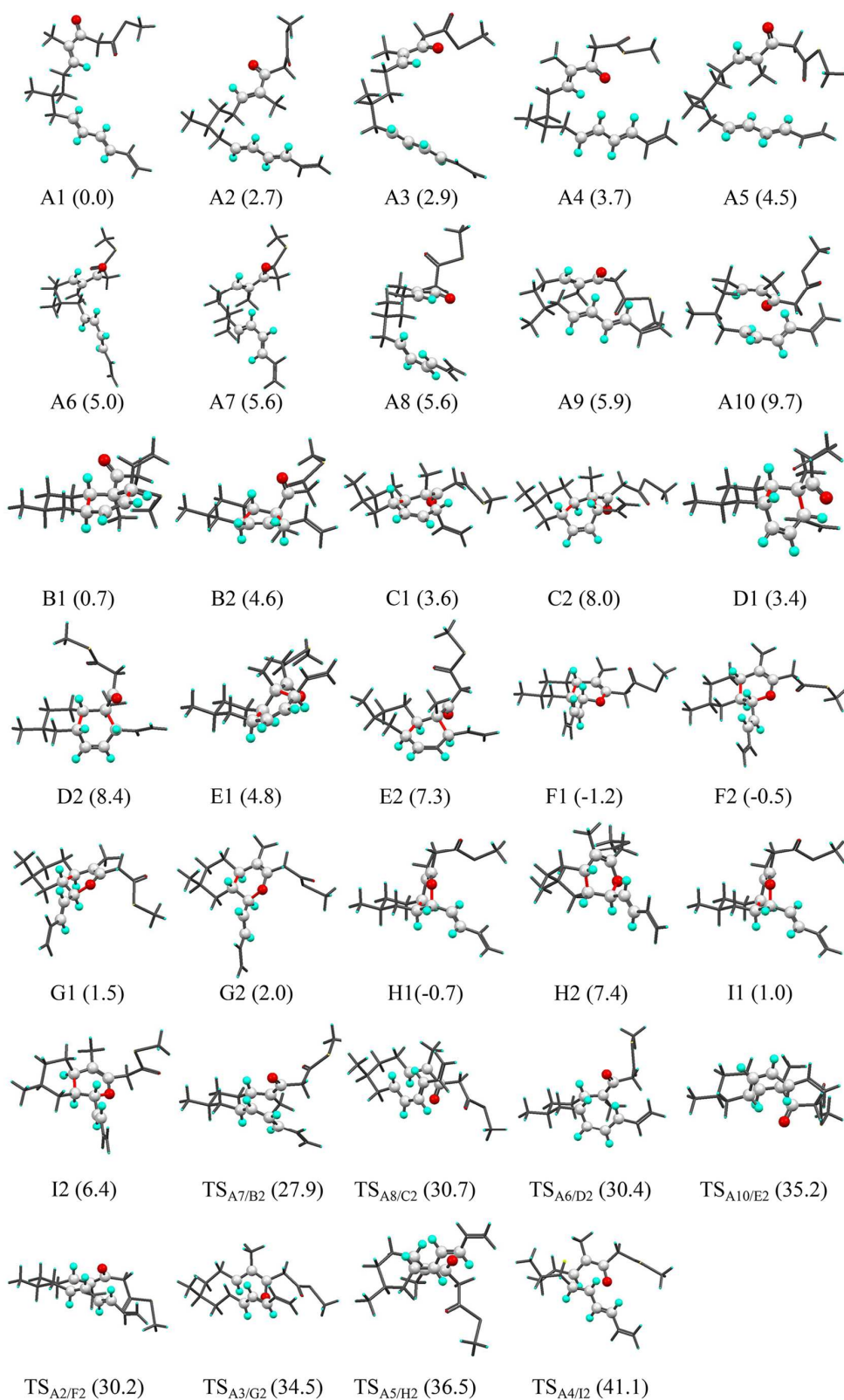


Figure S3. Optimized structures of stationary points along eight low-energy reaction pathways in the intramolecular D-A reaction of ketothioester obtained by the MD/CD method ($E_{cut} = 40$ kcal/mol). Target atoms are denoted by a ball-and-stick model. In MD/CD calculations, all target hydrogen atoms are automatically selected as “inactive” for the reactant (**A**). While for products (**B-I**), only those target hydrogen atoms bonded to the α -carbon of C=C double bonds were automatically selected as “active”. Relative free energies (kcal/mol) of all species calculated at the B3LYP/6-31G level, relative to **A1**, are given in parentheses. Different conformers of each structural isomer are labeled with the same capital. For each structural isomer, a few low-energy conformers are shown above. Cartesian coordinates for all listed structures are available in SI.

V. Reaction pathways for the aldol reaction of vinyl alcohol and formaldehyde

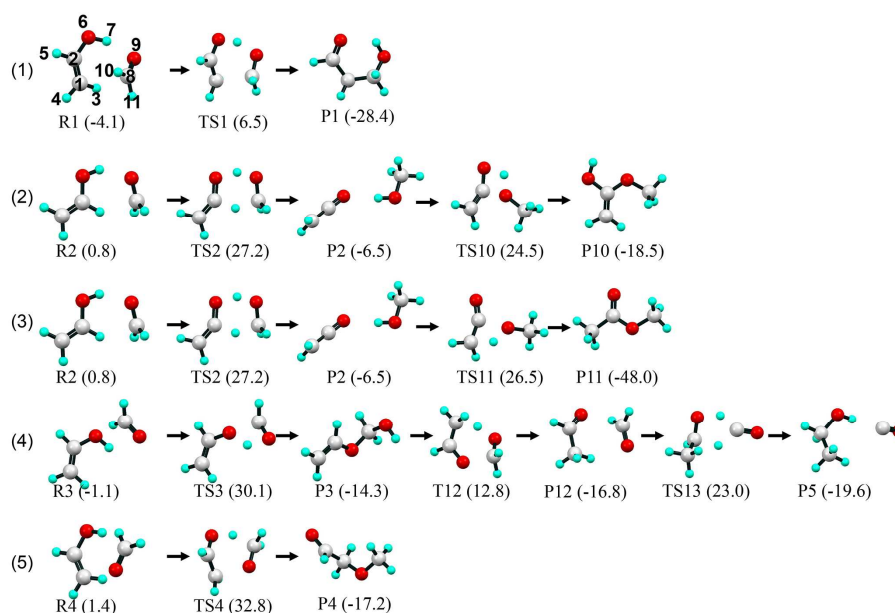


Figure S4. Structures of all stationary points involved in the five low-energy pathways leading to five different final products obtained by the MD/CD method with $E_{cut} = 40$ kcal/mol. Encounter complexes **R1-R4** were obtained by IRC calculations. Relative electronic energies (kcal/mol) of all species calculated at the B3LYP/6-31G level, relative to the isolated reactants, are given in parentheses.

The corresponding reaction variables used to locate intermediate or each product in Figure S4 are shown as follows:

Starting structure	Reaction variable	Intermediate or product
R1	C1-C8 or H7-O9	P1
R2	H5-C8	P2
P2	C2-O9 and O6-H7	P10
P2	C2-O9 and C1-H10	P11
R3	O6-C8 and O9-H7	P3
P3	H5-C1	P12
P12	C2-H10 and O6-H11	P5
R4	C1-C9 and H7-O8	P4

VI. Cartesian coordinates for structures of the Claisen rearrangement

A1.gif

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0  1
C  -0.5451694114  -1.9556286325  0.6025379136
O   0.0894727466  -0.7242408422  0.5831361003
C   0.0058479921  0.0664638271  -0.6483398142
C   0.8074490941  1.3131972088  -0.439184512

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C	0.3560133359	2.5456903887	-0.6923787889
C	-1.2606284664	-2.5280574008	-0.3739836744
H	-0.3807652666	-2.4243682814	1.5662272466
H	-1.6992083525	-3.5046412484	-0.2095744363
H	-1.4370254407	-2.0701725486	-1.3397424248
H	0.4123808892	-0.537783491	-1.4737284576
H	-1.0444511113	0.2925482693	-0.8738160175
H	1.8208020805	1.1557523598	-0.0753669723
H	-0.6569924668	2.7256217	-1.0445827169
H	0.9812743772	3.4226186912	-0.5582034455

A2.gif

0	1		
C	-1.0307103727	-1.5974811278	-0.4644127638
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C	-0.1361056328	0.4958697806	0.41592575
C	0.8872919895	0.9264961637	1.4199367793
C	1.8281783459	1.8462472915	1.1837900461
C	-1.9413469441	-1.0298853536	-1.2655091226
H	-0.9064293596	-2.6711938431	-0.3800172627
H	-2.5921597858	-1.6590024697	-1.8602834265
H	-2.0743434323	0.0406763342	-1.3638184891
H	0.0772585206	0.9035988287	-0.5808221361
H	-1.1466552936	0.8181574638	0.7101416215
H	0.8100348347	0.4472926553	2.3938188117
H	1.9304729498	2.3280406076	0.2142405119
H	2.5321933438	2.1540318144	1.9503352896

A3.gif

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C	-0.3019195609	-1.7229073226	1.1461529679
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C	1.0522226242	0.1151878757	0.3005291207
C	1.3318212766	0.8332677764	-0.9868206602
C	0.7808253483	0.5455953476	-2.1688355321
C	0.1070003283	-1.6260685407	2.4172687436
H	-1.0202049904	-2.4622555901	0.8111787663
H	-0.289454695	-2.3111428217	3.156468092
H	0.8235691746	-0.892513255	2.7659919519
H	0.6535221542	0.8097250507	1.0566797142
H	1.9757948899	-0.319758836	0.7140617905
H	2.0504588046	1.6471994398	-0.8933605023
H	0.0651212089	-0.2615461445	-2.2737724935
H	1.0325892038	1.1108170506	-3.0605615525

A4.gif

0 1

C	-0.387335464	-1.339856795	-1.2206648619
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C	2.0002843472	0.1732979379	0.2326243016
C	1.9634036607	0.6787720722	1.4700657026
C	-1.1279681942	-0.9884121743	-0.1632797224
H	-0.8175630188	-1.5772744262	-2.1873797029
H	-2.205742765	-0.944117676	-0.2641561762
H	-0.7133961675	-0.7205636509	0.7997735479
H	1.3640952302	-1.8305587151	0.74629419
H	2.7544176777	-1.7509168451	-0.362476106
H	2.2253200494	0.8107200954	-0.6207917932
H	1.7378115954	0.0618470761	2.3374753402
H	2.162180138	1.7275166311	1.6665605223

A5.gif

0 1

C	0.1713448682	-1.9311138164	-0.0137787682
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C	0.5434318004	0.1745511891	1.194088528
C	0.2654549507	1.3192875314	0.2549208738
C	0.5826230408	1.3531180225	-1.0418702423
C	-1.1523207961	-1.8083340995	-0.1598251413
H	0.7216058984	-2.8110671105	-0.3274574755
H	-1.7162017687	-2.623378328	-0.5970321419
H	-1.7067749822	-0.9194668908	0.1153285362
H	-0.3559084309	-0.0873588743	1.7702051331
H	1.3261669695	0.4510593434	1.9096975728
H	-0.2146697032	2.1766478342	0.728038884
H	1.0654328023	0.5120084957	-1.5282789652
H	0.3656294433	2.2210287507	-1.6561463831

A6.gif

0 1

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C	0.9866383296	-0.5300222074	0.4952556434
C	1.8566270458	-0.4658314121	1.5091574159
C	-1.3406900412	-0.7532680813	-2.0071475932
H	-1.8662366305	1.3022694874	-1.8276751617

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H	-0.6270869941	-1.5519528692	-1.8438931873
H	1.3127538799	-0.4392122277	-1.6447610484
H	1.9931327225	0.9248561188	-0.7281698119
H	0.1037183523	-1.1614256046	0.5697453088
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H	1.720935499	-1.0417866886	2.4192674032

A7.gif

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C	-0.8312448412	-0.9273084488	0.8902614392
C	0.2649825059	-1.6421561781	0.6244660827
C	0.2930989137	1.618984463	-1.1571545511
H	1.7803311227	2.2850160507	0.2174590939
H	0.7391208841	2.1239822369	-2.0053476144
H	-0.5959123415	1.0305324426	-1.3476513667
H	-1.144482322	0.600736865	2.3681445781
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H	-1.8176184929	-1.3891558866	0.8337165712
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H	0.2044823193	-2.6873439759	0.3386459818

A8.gif

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C	-0.5779819052	-1.0885600747	0.7341372749
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H	0.8612774153	0.856487585	-0.8553811018
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H	3.6817269066	1.1201086504	0.3952060615
H	0.3783089391	-1.5552104975	-1.1421328257
H	0.9320223305	-2.5441178796	0.229295507
H	-0.4002480747	-0.9756583275	1.8022700296
H	-1.9831035153	-0.9420713579	-0.8508415531
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A9.gif

0	1
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C	-1.3498759297	-0.3540148474	0.8586405053
C	-1.1236808202	-0.4493119112	2.1738536393
C	1.6561875611	1.1008434162	-1.8333233933
H	1.3970078917	0.2206787118	0.0921130476
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A10.gif

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C	0.0071910145	1.4521038264	-1.5945363364
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A11.gif

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C	1.6995557941	1.2416683203	1.6847895949
H	-0.3895015916	0.8306287962	1.8384241379
H	1.6362456078	2.2293162981	2.124489181
H	2.673006571	0.8806474804	1.3738310528
H	-0.3609192737	-2.5399463806	0.8258065406

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H	-2.2798464514	-1.5564633136	-0.6198392486
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H	-1.3120880651	-0.1266690232	-2.3642817179

A12.gif

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C	-1.1720779575	1.9401741336	0.0500510577
C	-1.2910877368	1.7912017465	-1.2717437888
C	2.2263997156	-1.4466224241	0.2331309868
H	0.8399842705	-0.993276964	1.7903254265
H	2.6973144263	-2.2674033371	0.7599422797
H	2.5858502091	-1.2013850521	-0.7594197495
H	-0.8068274585	0.5863022284	1.6791135298
H	0.4354084277	1.8358295933	1.473675637
H	-1.774241071	2.6752263081	0.5836641873
H	-0.6917308665	1.0662747094	-1.8102397327
H	-1.9880297354	2.3926843027	-1.8467222954

A13.gif

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C	-0.5196518942	0.9714893575	-1.1142512783
C	-0.7061140164	1.9932215934	-0.0312572505
C	-0.0886408624	1.9788039603	1.1528310863
C	1.585685797	-2.0008738588	-1.389457324
H	-0.3534504866	-1.4015532883	-2.0476445297
H	1.5905466883	-2.9329012234	-1.9410430853
H	2.4519942213	-1.7586764096	-0.7849855575
H	-0.183572036	1.4534149962	-2.045573216
H	-1.4752185277	0.4669421946	-1.3348866105
H	-1.4079722414	2.7878002832	-0.2835366636
H	0.6144534111	1.1944716505	1.4083683821
H	-0.269381993	2.7519897301	1.8928340532

A14.gif

O	1		
C	0.4041975575	0.3662102758	1.9539015325
O	0.4037248017	0.2539137378	0.5663328921
C	-0.8307195412	-0.2457858693	-0.0475471832

C	-0.8005768946	0.1087405294	-1.5018642129
C	-1.0095365005	-0.7669548611	-2.4899725087
C	1.5363446707	0.4792237667	2.6511874799
H	-0.582244503	0.3868620789	2.4175384946
H	1.508256553	0.617643128	3.7250966617
H	2.5037010157	0.4500164206	2.163453977
H	-0.9064274772	-1.3310120843	0.0979395952
H	-1.6886573238	0.2299019471	0.4548481112
H	-0.6071833788	1.1576089255	-1.7175998638
H	-1.1886584152	-1.8215283148	-2.2939334414
H	-1.0092205645	-0.4648396803	-3.5323815343

A15.gif

0	1		
C	-0.798048039	1.0057221038	-1.1234330668
O	-0.5048265826	0.1928665789	-0.0319595065
C	-0.2303203587	-1.2177702501	-0.32497924
C	-0.3566657217	-1.988480335	0.9522245163
C	0.5749711978	-2.8277312702	1.4154504498
C	-0.7367210303	2.3365805801	-1.0473399401
H	-1.1087413098	0.4771127662	-2.0247757316
H	-1.0194337379	2.9486200565	-1.8951099061
H	-0.4188909094	2.8348396633	-0.1389154003
H	-0.9628179219	-1.5689910488	-1.0698116336
H	0.7737559612	-1.3199668294	-0.7562767546
H	-1.2873522602	-1.8341450251	1.4945377684
H	1.5175155701	-2.9829428528	0.8956762604
H	0.4325751424	-3.3917141375	2.3317121847

A16.gif

0	1		
C	0.9953747226	-1.1650512697	0.8503552107
O	1.4287200665	-0.1578607433	-0.0077619237
C	1.0794436905	1.220205408	0.3620229798
C	-0.2944505116	1.5951972355	-0.1126020458
C	-0.5505684138	2.6338903637	-0.9149268332
C	0.9511968714	-2.4443912028	0.4726595506
H	0.734632491	-0.8344861594	1.8561986906
H	0.6650892491	-3.2151529088	1.1778170967
H	1.2127809877	-2.7434493147	-0.5355689895
H	1.1639454753	1.3208821041	1.4554578085
H	1.8456196148	1.8428767459	-0.1042698902
H	-1.1069440355	0.961507402	0.2413510849
H	0.2429303766	3.2755359471	-1.2911828673

H -1.5597705845 2.8842963924 -1.2265498721

A17.gif

O 1

C	0.4077743633	1.7737568345	1.1688429914
O	-0.8890672644	1.493823598	0.7558246224
C	-1.1084874495	0.9586703779	-0.5910350204
C	-0.7875603932	-0.50752212	-0.6919204412
C	-0.1629366311	-1.0743539856	-1.7295166225
C	1.5534070136	1.5837752036	0.5044101496
H	0.3688873896	2.2063521723	2.1625062091
H	2.4877276325	1.8788479292	0.9667355609
H	1.6129795536	1.1271849433	-0.4749349018
H	-2.1771733081	1.1329328163	-0.7511595723
H	-0.5442487868	1.5476298977	-1.3258484561
H	-1.1425839793	-1.1130069775	0.1403101562
H	0.2031010109	-0.4894708617	-2.5708275966
H	0.0031808489	-2.1456198281	-1.7823870787

A18.gif

O 1

C	-0.7128185161	0.8110741876	1.2406116445
O	-0.8634300529	-0.5027249475	0.8234082991
C	-0.8436589984	-0.797181474	-0.6179685253
C	0.5549279075	-0.8907457522	-1.1576537103
C	1.0329944813	-1.9689157839	-1.7884625713
C	-0.5233685531	1.9091798519	0.4977092832
H	-0.7797159068	0.842586072	2.3225156466
H	-0.4441749016	2.8721907226	0.9869975174
H	-0.4407479289	1.9043197074	-0.5825220046
H	-1.3626264791	-1.7538190587	-0.7048139449
H	-1.4334068437	-0.0302328631	-1.1392741224
H	1.1851523073	-0.015385012	-1.0144629324
H	0.4293522398	-2.8617924486	-1.9353510414
H	2.0435212446	-2.0015532015	-2.1837335382

B1.gif

O 1

C	-1.7741111219	0.7591983562	-1.7303114567
O	-1.8508181002	-0.0036429945	-2.7005966537
C	1.2894842825	-1.671036824	1.2520142048
C	0.013631243	-1.360032858	0.9954255663
C	-0.5371798488	-1.0142855601	-0.3645699972
C	-1.1350280263	0.4046703405	-0.4116618476

H	-2.1923868885	1.7821577897	-1.7936786409
H	-1.8968190673	0.5381703556	0.3746345798
H	-0.3641612374	1.1601376147	-0.191679042
H	1.631482101	-1.9150972186	2.2533071941
H	2.0403616463	-1.6994924783	0.4656530822
H	-0.7066089028	-1.3456549608	1.8159190738
H	-1.3218304813	-1.7295649594	-0.6490326422
H	0.2459844016	-1.1045266028	-1.1264234206

B2.gif

0	1		
C	1.6162621052	0.7014766261	-0.9423535949
O	2.4562491815	-0.1918909101	-1.1025548888
C	-2.4892490501	-1.8764510691	-0.1204650935
C	-1.49853666	-1.1717429623	0.4383684571
C	-0.1206730498	-0.9992510077	-0.148415408
C	0.2144096687	0.4767454709	-0.4350994749
H	1.8725764538	1.7529308678	-1.1750494517
H	-0.4872355401	0.9002105287	-1.1713113011
H	0.0842246883	1.0939427014	0.4695889952
H	-3.4640216836	-1.9697306053	0.3487718411
H	-2.3588193674	-2.3933674791	-1.0685040024
H	-1.6738305231	-0.6706706774	1.392488003
H	-0.0261107216	-1.5800259252	-1.0733907354
H	0.6377544982	-1.3981755586	0.5399266543

B3.gif

0	1		
C	1.4363579098	-0.571599847	-1.2083466072
O	0.738814604	-1.3697673651	-1.8464303219
C	-2.3466354776	0.8072392133	0.6075627191
C	-1.439691607	0.0029137189	0.0406517609
C	-0.2292998712	-0.5551933067	0.7504407028
C	1.1085841098	-0.0508953746	0.1687421767
H	2.3834016796	-0.1959560616	-1.6410256162
H	1.1266608437	1.0493685202	0.1294665515
H	1.9467373581	-0.3330285084	0.8272687656
H	-3.2027487236	1.1849567152	0.0564426381
H	-2.2716701933	1.1143146564	1.6488619524
H	-1.5488205667	-0.2911919278	-1.0017991562
H	-0.2403856708	-1.6519103251	0.6846361953
H	-0.272304395	-0.2922501077	1.8145282392

B4.gif

0	1		
C	1.447006935	0.7468192462	-0.3648732069
O	1.6486222407	0.8189005091	0.8537092548
C	-2.3875178025	-1.1629177123	0.7014972035
C	-1.1054838007	-0.7849635276	0.7669584253
C	0.0011419575	-1.3605804655	-0.0843193149
C	0.6361148051	-0.3297922178	-1.0418411514
H	1.8850223844	1.5035106904	-1.0436494405
H	1.3041385206	-0.8315653904	-1.7613350538
H	-0.136026406	0.1607973928	-1.6547607613
H	-3.149355188	-0.7193266376	1.3356838162
H	-2.7245051415	-1.9370290319	0.0149428967
H	-0.801028256	-0.0124899646	1.4710710048
H	-0.3861295397	-2.1993256991	-0.6756869234
H	0.7929992912	-1.7580371916	0.5656032511

B5.gif

0	1		
C	-1.4422001097	1.0668204158	1.4120403595
O	-2.58681714	0.7413768975	1.7494128508
C	0.9446427152	-1.6378244919	-1.2563660685
C	-0.2957756006	-1.91806085	-0.8379932858
C	-1.1688226977	-1.0711131544	0.0555201472
C	-0.5426318728	0.2447862451	0.5247877988
H	-1.0107832575	2.0228058171	1.7656687516
H	0.3946400675	0.0635497733	1.0753050906
H	-0.2533158486	0.8742844254	-0.3322652396
H	1.4898942471	-2.3191965964	-1.9020834138
H	1.4684452228	-0.7277394829	-0.9787238264
H	-0.7563111157	-2.8529183505	-1.1595969098
H	-1.467194083	-1.6602281733	0.9351526761
H	-2.1147705272	-0.8535424748	-0.4618589308

B6.gif

0	1		
C	-2.0127340867	0.5204661968	0.3216585926
O	-2.0661679378	0.988595301	-0.8210316291
C	1.4177832729	1.0364071296	-1.1925784103
C	1.164986696	0.1481232652	-0.2250722759
C	0.0549087459	-0.876400446	-0.2561193064
C	-1.0655769105	-0.5719684572	0.7609422286
H	-2.7089265391	0.8834191179	1.1020641708
H	-1.6798097933	-1.4697291226	0.9445309284
H	-0.6523079684	-0.2969019557	1.7429233265

H	2.2289256174	1.7544818737	-1.1136209741
H	0.8122984174	1.083307015	-2.0935066474
H	1.783331414	0.1446482662	0.6749994373
H	0.4671359748	-1.8700923973	-0.0329190032
H	-0.3828469026	-0.9213557865	-1.2592704376

B7.gif

0	1		
C	1.3600297552	-0.6641068963	-1.2357150746
O	0.913484099	-1.800873392	-1.0462549747
C	-1.9116785712	-0.6204034815	0.7150014975
C	-0.9960730228	0.3538451154	0.7529637034
C	0.4760817196	0.1521482573	1.0256119073
C	1.3563565716	0.4438863421	-0.2080946257
H	1.8271156653	-0.4068547776	-2.2058166336
H	1.0525249999	1.3768361879	-0.7061590017
H	2.4062743788	0.6023008587	0.0912318068
H	-2.9585263762	-0.4153408437	0.5104739757
H	-1.6423960797	-1.660652612	0.8763118082
H	-1.302539454	1.3854518656	0.5672721383
H	0.6571531697	-0.8775277959	1.3527494651
H	0.7911931446	0.816291172	1.842424008

B8.gif

0	1		
C	-2.8961351089	0.0307530961	-0.5422656718
O	-3.6702461646	0.9733656808	-0.7408419534
C	1.8862796972	0.121212966	0.5901650052
C	0.8945778026	-0.5596382344	0.0051129577
C	-0.5662395319	-0.4306104066	0.3553135835
C	-1.4201506643	0.050891676	-0.8483095039
H	-3.2732677342	-0.9179580217	-0.1103393592
H	-1.1315080031	1.0594158149	-1.1598291024
H	-1.2432274055	-0.6254618574	-1.7008273316
H	2.9233463409	-0.0100787841	0.2970176894
H	1.6971287185	0.8357861847	1.3878547917
H	1.1265893757	-1.2652401994	-0.7946195255
H	-0.6892629892	0.2654674773	1.1944296206
H	-0.9528843332	-1.4059053923	0.6921387996

B9.gif

0	1		
C	0.7258125813	-1.2627654308	1.8048498758
O	0.6302509687	-1.0887625269	3.0245807928

C	-2.0514964202	0.5615932368	-1.8180104204
C	-0.8454256268	0.1052715887	-1.4624368843
C	-0.5839172972	-0.8578765743	-0.3322301331
C	0.3380578717	-0.2492263038	0.758345406
H	1.1216597994	-2.2191904384	1.4081365055
H	1.2630011328	0.1112106863	0.2787194809
H	-0.1380403668	0.6067511678	1.246312527
H	-2.1818477735	1.2569106485	-2.6415619954
H	-2.9560557196	0.2542300895	-1.2984095731
H	0.0380635119	0.441693621	-2.0079521384
H	-0.1067273632	-1.7692556622	-0.7267296771
H	-1.5333352984	-1.1685841021	0.1213862338

B10.gif

0	1		
C	-1.6281236907	-2.0315116401	0.7751620432
O	-2.142628966	-3.1552838853	0.7562436863
C	1.1702200703	1.2550192184	-1.487249654
C	0.5563289065	0.0758228851	-1.637092248
C	-0.6725634267	-0.3606044612	-0.8799495515
C	-0.4129584577	-1.6298205113	-0.0210630079
H	-2.0613899523	-1.2319321943	1.4081415483
H	-0.1050989621	-2.4754060156	-0.6452731174
H	0.4055447677	-1.4127646896	0.6822633236
H	2.0559220835	1.5172354887	-2.0577830515
H	0.8065713618	2.0062632507	-0.789742594
H	0.9536349189	-0.6495952732	-2.3484381744
H	-1.48663855	-0.5790006786	-1.5867811927
H	-1.0218201033	0.4565785063	-0.2344380101

B11.gif

0	1		
C	-0.1417288125	-2.118027056	-1.1860579618
O	-0.7971489423	-3.1277486086	-1.466811234
C	0.0486724275	2.1547564243	1.1514589669
C	-0.7689435078	1.1608118482	0.7861895327
C	-0.5579561916	0.262191571	-0.4062485026
C	-0.4017063778	-1.2287995917	0.0029540405
H	0.7054918165	-1.8082835966	-1.8295946114
H	0.4533396668	-1.3131079232	0.6912424624
H	-1.2920573641	-1.5926061371	0.5268274864
H	-0.1504586206	2.7699238859	2.0236271797
H	0.9479336821	2.3942473095	0.5883212626
H	-1.6610156758	0.9544125018	1.3792437954

H	0.3306501986	0.586648382	-0.9643913697
H	-1.4140722989	0.3475809904	-1.0917610471

B12.gif

O	1		
C	-1.7139996092	-1.3543053522	-0.0853224572
O	-1.4819939244	-2.5567735349	0.0779628442
C	0.9916589147	1.0413573662	-1.2207546952
C	0.5230678856	0.7948625068	0.0080257941
C	-0.9062388001	0.9998655579	0.4474774358
C	-1.5615487951	-0.2983590672	0.9833244736
H	-2.0772219881	-0.9834779529	-1.0639244369
H	-0.9917633028	-0.7234918701	1.8171481938
H	-2.5681325587	-0.0597298408	1.3631947406
H	2.0314138926	0.8720369052	-1.4829990543
H	0.3515146657	1.4242358489	-2.0124474895
H	1.1992487989	0.4078665456	0.7718224086
H	-1.4997731871	1.3947039718	-0.388604435
H	-0.9472319919	1.7552089159	1.2450966774

B13.gif

O	1		
C	-0.386387404	-0.781020708	1.3380528394
O	0.3275448691	-1.5603869106	1.9777901866
C	0.7884073565	0.7543846983	-1.9221224797
C	-0.0073463804	-0.2988998796	-1.7039279277
C	-1.3244175032	-0.2526799838	-0.9683166808
C	-1.3590491515	-1.1965762529	0.260375237
H	-0.3549694494	0.3060625796	1.5489003314
H	-2.3704179688	-1.1765060672	0.6973756395
H	-1.1470848039	-2.2338758546	-0.0216982344
H	1.7286292998	0.6618128458	-2.4568322638
H	0.5279367309	1.7518194851	-1.5750530021
H	0.2942085699	-1.282556559	-2.0671568214
H	-2.1403232788	-0.5456470065	-1.6442919074
H	-1.5367308863	0.7770696135	-0.6490949166

B14.gif

O	1		
C	0.5688939529	-0.673762559	1.1336276578
O	1.5094793862	-1.0048590919	1.8662607167
C	-1.0368621555	1.1041490963	-1.8761500875
C	-1.4154761728	0.0032586504	-1.2158199352
C	-0.5900799395	-1.2521016255	-1.0689745594

C	-0.3230860085	-1.6513583196	0.4088595084
H	0.3330186225	0.3944726616	0.9768587471
H	-1.2857639139	-1.6935924359	0.9444570065
H	0.1295500025	-2.6462466498	0.4738151139
H	-1.6813206731	1.9740225267	-1.9585096329
H	-0.0677113889	1.1742507905	-2.3646971965
H	-2.3981860442	-0.022984529	-0.7407605229
H	0.3636681379	-1.1399713488	-1.6003022692
H	-1.1171238054	-2.0912771659	-1.5456645469

B15.gif

0 1

C	0.0441615758	0.2468953113	-1.6493371999
O	1.1975235044	0.2659833948	-2.0932969486
C	0.7187849075	-0.0019117531	1.5402872266
C	-0.6143598426	-0.0915381746	1.4571106183
C	-1.4183483502	-0.5676837726	0.2688191008
C	-0.6001586768	-0.9450150625	-0.9818414545
H	-0.605870747	1.1393971067	-1.7444333647
H	0.1710596361	-1.6888386612	-0.7568722441
H	-1.2825994936	-1.3975440522	-1.7192293378
H	1.2011509501	0.3504444552	2.4468550877
H	1.3816740403	-0.2654788354	0.7220221276
H	-1.2156901643	0.1946080836	2.3209846624
H	-2.1511779158	0.2103822101	-0.0011719945
H	-2.022149424	-1.4357002501	0.5721037207

B16.gif

0 1

C	0.0980715774	1.3490805424	-0.133461368
O	-0.2320905031	2.0763510287	0.8096977415
C	-0.6596600714	-1.5551182236	1.1562010868
C	-0.2905918847	-1.819348814	-0.1032809835
C	-0.3542336307	-0.877009921	-1.2835282568
C	-0.8635817232	0.5447069078	-0.975973151
H	1.162829141	1.2672089217	-0.4298049289
H	-0.9847482084	1.0834876804	-1.9295719644
H	-1.8427643172	0.5316256467	-0.4862737505
H	-0.5766849208	-2.3081170673	1.9339095256
H	-1.0497802269	-0.5915689346	1.4689428932
H	0.0960299701	-2.8112359555	-0.3408521106
H	-0.9936108455	-1.3217232848	-2.0603224194
H	0.6468156433	-0.8103385269	-1.7406823141

B17.gif

0 1

C	0.9268849998	-1.544427002	1.1751168498
O	2.0504167839	-1.092346201	1.4211245228
C	-1.3475436855	1.0006000859	-1.6109307349
C	-0.721594859	-0.0251540979	-1.0232024312
C	-1.2792107781	-0.8277697326	0.1261901209
C	-0.3690599658	-0.8018661712	1.3853887924
H	0.8158374296	-2.5718267926	0.7725367101
H	-0.1473249251	0.2246473314	1.6925719548
H	-0.9032515022	-1.29786988	2.2114275958
H	-0.9018834049	1.5486823112	-2.4353281665
H	-2.3327003386	1.3310111281	-1.2889677607
H	0.2681671509	-0.3188985358	-1.3764829696
H	-1.4170096203	-1.8767117341	-0.1822113328
H	-2.2717272846	-0.4490707093	0.3967668492

B18.gif

0 1

C	-1.053443508	0.2826122651	-1.8246957992
O	-1.3895609143	1.4471130739	-2.065941137
C	0.9514004468	-0.1549382038	2.0740301898
C	0.6586111955	-0.1761194705	0.7689572115
C	-0.2653133333	-1.1713096524	0.1112829741
C	-1.4703187951	-0.5027800662	-0.6064795998
H	-0.4012490912	-0.2670531521	-2.5335187818
H	-2.1571656618	-1.2951559724	-0.9444454723
H	-2.0204778757	0.1553987328	0.0727988522
H	1.6218615772	0.5851765199	2.4998980205
H	0.5307478458	-0.8799588021	2.7673474792
H	1.1010173632	0.574110923	0.1115254498
H	-0.6441513378	-1.8773138135	0.8595059129
H	0.2930420887	-1.7677823817	-0.6282652999

B19.gif

0 1

C	0.4644726982	1.9237500004	0.9302819504
O	0.4835028511	2.3763572796	2.0801251599
C	-0.9817601558	-2.0124923203	-0.639409536
C	-1.3819700308	-0.8294917347	-1.1193425136
C	-0.9777697455	0.5355690331	-0.6141832143
C	0.0188516392	0.531301955	0.5625160145
H	0.7980219397	2.5516463127	0.0799718961
H	-0.4052691672	0.0516437423	1.4503441501

H	0.913987702	-0.0406189577	0.268821955
H	-1.3305605959	-2.9440710281	-1.0739623347
H	-0.3000741391	-2.1056962566	0.2007134863
H	-2.0746818649	-0.8100805785	-1.9614098317
H	-1.8841669857	1.087131089	-0.3195768129
H	-0.5485841453	1.1090514637	-1.4518903693

B20.gif

0	1		
C	-0.3931233663	-1.8472919619	0.811059457
O	-1.5547574074	-2.0884421679	0.4655480868
C	-0.0179889958	0.5058876477	-1.673650727
C	-0.7485648965	1.0680606518	-0.7045246441
C	-0.7849181553	0.6842172236	0.7576697126
C	0.1324958742	-0.4751841652	1.166297453
H	0.3385111541	-2.6722220117	0.9109087168
H	1.1407730833	-0.3622766087	0.7441263737
H	0.2767541406	-0.4738875054	2.2599263621
H	-0.068788386	0.8617667571	-2.697834524
H	0.6497341438	-0.3331311098	-1.4992890103
H	-1.4051057183	1.8999661403	-0.9624280694
H	-1.818650826	0.4231506547	1.0252180558
H	-0.5323706441	1.5713864556	1.3569727572

B21.gif

0	1		
C	-2.5598082548	0.6727971699	0.1385815894
O	-3.51094968	0.8321608884	-0.6342983436
C	1.7015911917	-0.4354999539	-0.6710763199
C	0.9193553095	-1.0834246522	0.1998230509
C	-0.5358179973	-0.8016734728	0.4922435391
C	-1.1446937625	0.3791344492	-0.2902597719
H	-2.714011073	0.7505944238	1.2333959711
H	-0.5420453506	1.2815891374	-0.0979771365
H	-1.1349322794	0.1970395854	-1.3695788314
H	2.7413332724	-0.714394691	-0.8103594073
H	1.345048624	0.3895781809	-1.2803461039
H	1.3417464758	-1.9086514082	0.7740803144
H	-0.6498921153	-0.6192242299	1.5732166214
H	-1.1209243605	-1.7120254269	0.2885548282

B22.gif

0	1		
C	-0.8869645003	-1.8897690946	-0.5219492708

O	-0.7595535224	-1.3848760343	-1.6426762973
C	-1.4962404851	1.1793290298	0.9190007791
C	-0.1797849293	1.1018702308	0.6956576861
C	0.6548917722	-0.151500879	0.5580173044
C	-0.1039992677	-1.4766462613	0.7034367361
H	-1.5925731862	-2.7290578593	-0.3690221318
H	0.6045437227	-2.2966993978	0.9085387483
H	-0.7828030518	-1.4614007789	1.5675936793
H	-1.9999313288	2.1372580599	1.0015634529
H	-2.1309809014	0.303275474	1.0187999191
H	0.3877422907	2.027862627	0.595489734
H	1.4629120533	-0.1155544678	1.3034798005
H	1.148741334	-0.1370906487	-0.4239301398

B23.gif

O	1		
C	1.5577228253	-0.7040453362	-0.2508523579
O	2.6715080604	-0.1762600189	-0.1405476654
C	-2.7369913235	-1.0981901894	-0.6251268815
C	-1.53781696	-0.5114834532	-0.7194420808
C	-0.7806062911	0.0773450399	0.4468137562
C	0.5125743938	-0.7078822121	0.8346071418
H	1.2778999512	-1.209584754	-1.1939555292
H	0.9558167525	-0.2721837228	1.7360707051
H	0.2329025512	-1.7493440224	1.0492383162
H	-3.2457816522	-1.5092325869	-1.4917494481
H	-3.2583774997	-1.184520481	0.3257394115
H	-1.0592167548	-0.4402572253	-1.6965948175
H	-1.431464516	0.103282299	1.3291844926
H	-0.5001695373	1.1173566632	0.227614957

B24.gif

O	1		
C	0.5045772505	-0.9528988769	-2.0008447589
O	1.2142774794	-0.7521590355	-2.9944582169
C	-0.9843142198	-0.6707561122	2.0554826559
C	-0.0955886803	-0.606704546	1.056889548
C	-0.0347637092	0.5041606333	0.0361480125
C	-0.4323114868	0.0689132524	-1.4102739111
H	0.538885492	-1.9318911982	-1.4872420402
H	-1.4439751178	-0.3604133339	-1.3762789435
H	-0.4452526378	0.9419709164	-2.0709728568
H	-0.9904688995	-1.4903229634	2.7676374928
H	-1.73797731	0.1000755642	2.2015616246

H	0.6469203371	-1.399193004	0.9584710847
H	0.9782790821	0.9295967709	0.0021436772
H	-0.7092875798	1.3146219331	0.3377366317

C.gif

0 1

C	0.404644	-1.907645	-2.031301
O	-0.415073	-1.546471	-2.819581
C	-1.547430	-0.706967	0.877001
C	-1.126880	0.390556	0.233650
C	-0.304013	1.491962	0.845628
C	1.307245	-2.303759	-1.162150
H	0.646020	1.623022	0.310120
H	1.181369	-2.060665	-0.115237
H	2.172340	-2.869840	-1.481774
H	-2.150702	-1.464144	0.384964
H	-1.315295	-0.879762	1.925794
H	-1.392468	0.522453	-0.815958
H	-0.077271	1.288675	1.897844
H	-0.830486	2.454585	0.790996

D.gif

0 1

C	-0.827150	1.080483	1.478617
O	-1.986414	0.656491	1.394465
C	-0.945574	-1.397424	-1.141609
C	0.144671	-1.925198	-1.643715
C	1.232638	-2.456460	-2.146831
C	-0.169852	1.963700	0.456871
H	-0.194213	0.793156	2.339612
H	0.376528	2.781909	0.940360
H	-0.910760	2.363081	-0.239456
H	-1.306693	-1.645697	-0.147188
H	-1.549935	-0.686522	-1.700174
H	0.561690	1.369970	-0.109718
H	1.206751	-3.382033	-2.716682
H	2.210310	-1.998455	-2.017553

E1.gif

0 1

C	-0.676206	0.180285	1.928126
O	0.249560	0.635103	1.083824
C	0.587656	0.174909	-0.137144
C	1.620543	0.856271	-0.831229

C	2.087918	0.531570	-2.064413
C	-1.508421	-0.988297	1.575735
H	-0.729401	0.747143	2.843237
H	-2.210733	-1.211483	2.382316
H	-2.092024	-0.821595	0.650801
H	-0.901234	-1.894287	1.390216
H	0.056593	-0.685702	-0.522214
H	2.052027	1.705077	-0.302215
H	1.688635	-0.306050	-2.629657
H	2.882080	1.100060	-2.533385

E2.gif

0 1

C	0.111776	2.060347	0.959080
O	-0.978175	1.613439	0.339816
C	-1.292774	0.649518	-0.543104
C	-0.414505	-0.295124	-1.144771
C	-0.822365	-1.241994	-2.032164
C	1.474592	1.499592	0.789710
H	-0.114072	2.891230	1.609886
H	2.169031	2.062714	1.419927
H	1.544816	0.438933	1.084494
H	-2.350662	0.667571	-0.762958
H	1.842131	1.564308	-0.248301
H	0.638335	-0.260553	-0.883747
H	-1.860950	-1.332956	-2.337693
H	-0.122178	-1.944029	-2.469178

TSA9/B13.gif

0 1

C	-0.021977	-1.762758	0.182376
O	0.004413	-1.332413	1.423596
C	0.885706	0.420053	1.445043
C	0.128918	1.109755	0.487117
C	0.213527	0.778261	-0.858279
C	-0.901879	-1.264662	-0.763328
H	0.805303	-2.401158	-0.157847
H	-0.888783	-1.655547	-1.777362
H	-1.802637	-0.751085	-0.450196
H	0.744358	0.614521	2.501432
H	1.856242	0.011029	1.181886
H	-0.735264	1.674168	0.829653
H	1.114412	0.327440	-1.262266
H	-0.441337	1.238396	-1.591825

TSA8/B12.gif

O 1
C 0.554477 1.690294 -0.006937
O -0.558657 1.958788 0.637421
C -0.995346 0.418881 1.773334
C -0.970610 -0.620307 0.832629
C 0.225091 -1.034275 0.261721
C 0.603283 0.826940 -1.088191
H 1.501545 2.015949 0.445512
H 1.547826 0.639689 -1.592142
H -0.298928 0.598987 -1.642439
H -0.147075 0.578876 2.431529
H -1.938251 0.803737 2.142822
H -1.901446 -0.878181 0.332851
H 1.164642 -0.908658 0.790489
H 0.240448 -1.767719 -0.538597

TSA16/B14.gif

O 1
C 1.043042 -0.941611 0.871386
O 1.904707 -0.002483 1.162976
C 1.205535 1.847563 0.688329
C -0.141149 1.580321 0.437814
C -0.531975 0.883801 -0.697907
C 0.613043 -1.213909 -0.416645
H 0.516080 -1.425601 1.705372
H -0.110337 -2.003873 -0.593815
H 1.210555 -0.898156 -1.263305
H 1.519025 2.314508 1.613988
H 1.915262 1.905302 -0.128697
H -0.835968 1.638840 1.273135
H 0.055596 0.943968 -1.607089
H -1.555415 0.545329 -0.822543

TSA4/B16.gif

O 1
C -0.224149 -1.124152 -0.992046
O 0.725022 -2.022962 -0.990879
C 2.376981 -1.386489 0.009944
C 2.103096 -0.026608 0.161967
C 1.117484 0.409771 1.037337
C -0.846510 -0.665186 0.156950
H -0.420861 -0.593068 -1.933699

H	-1.625740	0.087892	0.090834
H	-0.816656	-1.260616	1.061445
H	2.160135	-2.083017	0.811478
H	3.084322	-1.733965	-0.733047
H	2.434728	0.650508	-0.622583
H	0.883801	-0.161994	1.928374
H	0.798346	1.446883	1.048928

TSA9/C.gjf

0 1

C	0.456075	-1.214955	-0.793740
O	-0.711038	-1.734515	-0.756040
C	-2.005313	-0.679419	0.592241
C	-1.501665	0.588216	0.379985
C	-0.163883	0.851105	0.734288
C	1.666163	-1.503663	-1.308218
H	0.460882	-0.114151	-0.191109
H	2.506813	-0.838020	-1.167885
H	1.813576	-2.405713	-1.892024
H	-2.941675	-0.997615	0.148366
H	-1.605847	-1.322501	1.367889
H	-1.986705	1.235748	-0.345456
H	0.259155	0.376967	1.619369
H	0.305465	1.790515	0.452334

TSA8/D.gjf

0 1

C	-0.80934800	0.86548100	1.07728000
O	-1.86344000	0.33769100	0.55124100
C	-1.23796600	-1.25846800	-0.72799500
C	0.07594600	-0.96156500	-1.04698000
C	1.11770500	-1.39490600	-1.75719800
C	0.19131300	1.43595900	0.26768600
H	-0.58346200	0.65773100	2.13341400
H	1.09585200	1.81933500	0.73196400
H	-0.10908600	1.92707300	-0.65609000
H	-1.49482000	-1.94141000	0.07557500
H	-2.06020400	-0.96546600	-1.37169800
H	0.38513900	0.15536500	-0.40613200
H	1.07483900	-2.30587400	-2.34935300
H	2.05953300	-0.85394600	-1.77471500

TSA1/E1.gjf

0 1

C	-0.92680500	0.37944900	1.88225200
O	-0.09670000	0.99286900	1.01655800
C	0.30411300	0.18179400	-0.09323400
C	1.56947100	0.60320300	-0.66053500
C	1.98621400	0.32112300	-1.91192900
C	-1.25352800	-0.95221800	1.54304300
H	-0.98713700	0.86446100	2.84623800
H	-1.55918700	-1.59248900	2.37051000
H	-1.87010400	-1.14940900	0.65772500
H	-0.12040500	-1.09264600	0.82439100
H	-0.50665300	-0.04914100	-0.78541900
H	2.23429500	1.12932900	0.02310900
H	1.35596100	-0.20790700	-2.62254800
H	2.97746200	0.59458500	-2.25616100

TSA2/E1.gjf

0 1

C	0.17854200	1.12407000	1.85576600
O	-0.68989700	0.67074200	0.93103400
C	-0.10313900	-0.16951400	-0.06891300
C	-1.06480500	-1.07350200	-0.66761400
C	-0.92081800	-1.66916600	-1.86912300
C	1.51098300	0.69073000	1.67630600
H	-0.29514400	1.49521000	2.75355400
H	2.13192200	0.67956400	2.57210900
H	2.08694200	1.05211700	0.81575700
H	0.58186600	0.35413800	-0.73692300
H	1.10940200	-0.39926300	0.99046800
H	-1.92468500	-1.31699600	-0.04506500
H	-0.07353500	-1.45929500	-2.51727300
H	-1.63663500	-2.39883600	-2.23108900

TSA6/E2.gjf

0 1

C	0.70580000	1.90208800	0.08570700
O	0.00975400	1.26504600	-0.87291400
C	-0.39947900	-0.07294600	-0.52473000
C	0.60195700	-1.12564200	-0.62743200
C	0.33198700	-2.43964900	-0.77002200
C	0.87458600	1.19285900	1.30133500
H	0.78118900	2.96887500	-0.07533700
H	0.99828700	1.82418500	2.18276300
H	1.54444200	0.32942000	1.36406500
H	-0.16483200	0.42118800	1.04483300

H	-1.35909100	-0.26167500	-0.99843900
H	1.64404500	-0.81221500	-0.56504000
H	-0.68555100	-2.81286600	-0.85040900
H	1.12390300	-3.17966300	-0.80138300

TSA17/E2.gif

0 1

C	0.11240100	1.77770700	1.28725900
O	-1.02579300	1.45827100	0.64602000
C	-0.83714600	0.94139300	-0.68708200
C	-0.44236200	-0.45470100	-0.81532300
C	-0.64948600	-1.21891300	-1.90755600
C	1.30727000	1.61562000	0.54242900
H	-0.04549900	2.39527400	2.16096000
H	2.12428700	2.27305300	0.84408600
H	1.69684400	0.61973100	0.30895200
H	-1.67824800	1.26892500	-1.29229200
H	0.65248400	1.67500000	-0.60216400
H	0.07524900	-0.89463800	0.03702900
H	-1.17101900	-0.84167300	-2.78324700
H	-0.29398000	-2.24205200	-1.95807300

VII. Cartesian coordinates for structures of the Electrocyclic reaction

A1.gif

0 1

C	-1.700590	-0.219206	0.842562
C	-2.557500	0.725153	1.775840
H	-1.588864	-1.251688	1.182272
H	-2.903355	0.230922	2.687184
H	-3.412844	1.201339	1.284360
C	-2.162318	-0.198096	-0.591462
H	-2.330125	0.823492	-1.000107
O	-2.342832	-1.177876	-1.268110
C	-1.311369	1.576779	1.918234
C	-0.545868	0.735543	1.122409
C	-0.792361	2.725737	2.492057
C	0.787641	0.979973	0.837692
C	0.555678	2.984237	2.219923
H	-1.376622	3.394589	3.116586
C	1.325112	2.135220	1.415489
H	1.392006	0.330028	0.212410

H 1.022692 3.868819 2.642842
H 2.366520 2.385036 1.235820

A2.gif

O 1
C -0.272961 -0.323291 1.730825
C 0.291753 1.056365 2.202838
H 0.476168 -1.080645 1.468027
H 1.382970 1.114389 2.227890
H -0.116751 1.376592 3.164350
C -1.317147 -0.940992 2.628328
H -1.841265 -1.819064 2.194886
O -1.610296 -0.528256 3.721437
C -0.368953 1.646303 0.968507
C -0.868497 0.422949 0.537363
C -0.581870 2.814793 0.258060
C -1.618451 0.279108 -0.616533
C -1.340180 2.689795 -0.912669
H -0.196086 3.779085 0.574449
C -1.845690 1.457364 -1.338218
H -2.011318 -0.672974 -0.960491
H -1.546373 3.573200 -1.509822
H -2.429054 1.417279 -2.253227

A3.gif

O 1
C 0.548870 2.343705 0.881986
C 0.455671 0.975480 1.669769
H 0.622693 3.209446 1.553055
H 0.504483 1.070124 2.757613
H 1.179088 0.220844 1.343281
C 1.664996 2.420807 -0.126519
H 2.688185 2.348434 0.301999
O 1.499509 2.545980 -1.312892
C -0.930034 0.846628 1.062116
C -0.835869 2.036675 0.353573
C -2.050604 0.035000 0.999358
C -1.840436 2.493348 -0.481389
C -3.081390 0.488552 0.168882
H -2.141683 -0.898071 1.547094
C -2.977967 1.682130 -0.554829
H -1.762262 3.411601 -1.054260
H -3.988148 -0.102177 0.076256
H -3.805103 1.980495 -1.192093

B1.gif

0 1

C 0.873421 0.435558 -0.510529
C 0.446545 0.553888 2.470403
H 1.200240 0.696262 -1.515368
H 1.472936 0.296353 2.232691
H 0.127090 0.422892 3.500511
C 1.300631 -0.895646 -0.061258
H 0.714772 -1.341260 0.766390
O 2.191003 -1.521909 -0.598702
C -0.385904 1.088318 1.554077
C 0.009596 1.261929 0.138114
C -1.667760 1.659180 1.964875
C -0.620490 2.363961 -0.575884
C -2.292333 2.567977 1.191832
H -2.052663 1.390375 2.944657
C -1.722917 2.966966 -0.083999
H -0.230295 2.622895 -1.556150
H -3.214960 3.033548 1.523373
H -2.219914 3.743712 -0.657034

B2.gif

0 1

C 0.009405 -0.387644 1.796428
C 0.506424 2.547198 2.275038
H -0.455156 -1.371521 1.825762
H 0.697731 1.968746 3.172372
H 0.848245 3.578390 2.267341
C 1.399327 -0.359530 2.268558
H 2.009316 0.500537 1.930146
O 1.895070 -1.250460 2.927452
C -0.191370 2.045635 1.235695
C -0.655497 0.640493 1.204379
C -0.649041 2.924327 0.160590
C -1.871357 0.380650 0.446129
C -1.687461 2.569193 -0.620115
H -0.181909 3.900926 0.068838
C -2.345665 1.287415 -0.433183
H -2.329891 -0.599366 0.542899
H -2.062950 3.247002 -1.379926
H -3.215221 1.053008 -1.039403

B3.gif


```

0    1
C    1.182255 0.815109 1.693248
C    -1.498978 1.972966 2.841675
H    2.049725 0.573554 1.081988
H    -0.971172 1.401579 3.592297
H    -2.458208 2.411876 3.106216
C    1.254099 0.141826 2.986091
H    2.150412 -0.505732 3.063399
O    0.494512 0.198217 3.937768
C    -1.021827 2.167219 1.591901
C    0.268760 1.638226 1.080799
C    -1.834808 2.978910 0.683481
C    0.620756 2.039051 -0.279146
C    -1.446390 3.290850 -0.565511
H    -2.783390 3.336635 1.074337
C    -0.173629 2.807276 -1.052390
H    1.569505 1.680723 -0.667480
H    -2.070719 3.901535 -1.208989
H    0.141097 3.067181 -2.058683

```

C1.gif

```

0    1
C    0.756097 0.778107 -0.128015
C    -0.187934 2.596060 1.698931
H    1.159084 0.227979 -0.970291
H    -0.441901 2.959474 2.696738
H    -0.213938 3.445083 0.997173
C    1.580322 1.446394 0.690775
H    2.660995 1.457100 0.593058
O    1.162219 2.140447 1.777323
C    -1.134414 1.521128 1.232797
C    -0.658159 0.665342 0.227065
C    -2.437846 1.405270 1.694832
C    -1.517785 -0.290868 -0.316432
C    -3.293093 0.451530 1.142967
H    -2.793176 2.068774 2.479781
C    -2.831162 -0.390665 0.134744
H    -1.150463 -0.962584 -1.087875
H    -4.315230 0.368332 1.498380
H    -3.494617 -1.133903 -0.296949

```

C2.gif

```

0    1
C    -2.262934 1.635086 -0.013157

```

C -1.442504 -0.682821 1.203977
 H -2.753138 2.532930 -0.370804
 H -2.220745 -0.665660 1.983721
 H -0.880442 -1.614834 1.290857
 C -2.672036 0.432928 -0.441315
 H -3.463231 0.280893 -1.168134
 O -2.099824 -0.735682 -0.061929
 C -0.556207 0.527201 1.343079
 C -1.048439 1.722825 0.796366
 C 0.647806 0.513567 2.033192
 C -0.323320 2.902057 0.974447
 C 1.364702 1.696803 2.211690
 H 1.023830 -0.420499 2.444020
 C 0.873460 2.888954 1.685711
 H -0.696184 3.828854 0.546222
 H 2.300398 1.687039 2.761518
 H 1.427809 3.812359 1.823538

C3.gif

0 1
 C 1.101597 1.200997 1.567966
 C -0.254726 0.726376 -0.895876
 H 1.660890 1.364490 2.481101
 H -0.320156 1.421265 -1.742376
 H -0.716395 -0.217189 -1.212323
 C 1.715431 0.701761 0.491435
 H 2.767733 0.439057 0.465854
 O 1.135835 0.452372 -0.702155
 C -0.993550 1.291833 0.298679
 C -0.321622 1.522830 1.505357
 C -2.348510 1.581148 0.190533
 C -1.031190 2.045101 2.589447
 C -3.050612 2.101943 1.275850
 H -2.863001 1.398391 -0.750896
 C -2.387254 2.333544 2.477698
 H -0.508931 2.224283 3.525686
 H -4.108735 2.324367 1.181394
 H -2.925806 2.739433 3.328626

D1.gif

0 1
 C 0.467409 -0.565425 0.713854
 C -2.042557 0.638615 -0.134534
 H -0.245048 -1.165437 0.161140

H -1.640885 0.265875 -1.084018
 H -2.388505 -0.228976 0.439321
 C 1.577994 -1.189204 1.064772
 H -2.915144 1.254766 -0.363188
 O 2.556671 -1.736520 1.374842
 C -1.013313 1.431866 0.628694
 C 0.198728 0.844552 1.037809
 C -1.248551 2.770549 0.942690
 C 1.129392 1.615406 1.745604
 C -0.320930 3.532062 1.645087
 H -2.185492 3.221484 0.625060
 C 0.875563 2.946024 2.047898
 H 2.067355 1.164604 2.063671
 H -0.530964 4.571556 1.875561
 H 1.613277 3.522202 2.597737

D2.gif

O 1
 C 1.640974 0.619979 1.025222
 C 0.046824 2.499829 -0.679852
 H 2.153139 -0.087515 1.671654
 H 0.588170 1.924517 -1.440934
 H -0.706437 3.099901 -1.195865
 C 2.473511 1.277939 0.235932
 H 0.762123 3.192566 -0.219747
 O 3.265781 1.816989 -0.425847
 C -0.593887 1.602286 0.342830
 C 0.180872 0.727647 1.130551
 C -1.975533 1.623350 0.527210
 C -0.458759 -0.091155 2.069964
 C -2.604328 0.807936 1.462619
 H -2.569917 2.299057 -0.082642
 C -1.836665 -0.055098 2.237784
 H 0.141439 -0.764271 2.676457
 H -3.682147 0.846976 1.583308
 H -2.306159 -0.700933 2.973355

E1.gif

O 1
 C -0.854575 -0.342315 1.778560
 C 0.082598 1.914020 2.320080
 H -0.288011 -1.276658 1.867423
 H 1.106455 2.081995 2.674213
 H -0.521484 2.753996 2.682845

C -0.454205 0.606243 2.914804
 H -1.914999 -0.602304 1.878515
 O -0.546999 0.363043 4.089499
 C -0.014913 1.699923 0.833019
 C -0.539667 0.437946 0.529862
 C 0.340616 2.576173 -0.186556
 C -0.711093 0.047865 -0.793844
 C 0.168387 2.184039 -1.512105
 H 0.748058 3.556224 0.046866
 C -0.354672 0.926810 -1.814168
 H -1.118835 -0.931438 -1.029970
 H 0.442579 2.861088 -2.315327
 H -0.485239 0.631348 -2.850717

F1.gjf

0 1
 C -1.268236 -0.888198 1.448353
 C 1.146776 0.793868 1.301430
 H -0.358395 -1.297023 1.879043
 H 2.002810 1.449103 1.432431
 H 1.353891 -0.257533 1.135358
 C -2.349066 -1.866988 1.282056
 H -2.069418 -2.891780 1.601311
 O -3.465596 -1.662282 0.846351
 C -0.103605 1.294133 1.303896
 C -1.312681 0.439122 1.143919
 C -0.297530 2.742384 1.368680
 C -2.531651 1.109077 0.707127
 C -1.483975 3.297305 1.063635
 H 0.566812 3.353845 1.612550
 C -2.607190 2.456973 0.686570
 H -3.385822 0.491838 0.463280
 H -1.611113 4.375042 1.074411
 H -3.539009 2.936114 0.400599

F2.gjf

0 1
 C 0.712610 0.607512 2.437365
 C 0.811929 2.109531 -0.095919
 H 1.635342 1.136934 2.216586
 H 0.953584 2.517924 -1.092043
 H 1.306950 2.624071 0.720260
 C 0.608517 0.130625 3.821445
 H 1.479562 0.407208 4.449770

O -0.302552 -0.507027 4.313202
 C 0.018041 1.039190 0.098209
 C -0.199108 0.431120 1.440356
 C -0.744154 0.496775 -1.026115
 C -1.391542 -0.392739 1.597838
 C -1.765119 -0.355212 -0.825281
 H -0.493724 0.854305 -2.021082
 C -2.114299 -0.770923 0.522152
 H -1.635235 -0.739355 2.593140
 H -2.352141 -0.723254 -1.660662
 H -2.972661 -1.422684 0.656778

F3.gif

O 1
 C 0.451832 -0.194555 2.549498
 C 0.426718 2.747505 2.413665
 H 0.825580 0.317884 3.431638
 H 0.259167 3.818356 2.478441
 H 1.300516 2.354641 2.921787
 C 0.743405 -1.630118 2.537188
 H 0.382422 -2.222017 1.675052
 O 1.362013 -2.176011 3.427831
 C -0.405500 1.967944 1.698171
 C -0.235419 0.491371 1.598126
 C -1.475469 2.584507 0.913754
 C -0.894196 -0.155968 0.466531
 C -2.128910 1.895518 -0.037974
 H -1.683005 3.636264 1.090464
 C -1.793981 0.504023 -0.290309
 H -0.694708 -1.202289 0.267958
 H -2.895165 2.371276 -0.641248
 H -2.299300 -0.014333 -1.099574

F4.gif

O 1
 C -0.073122 -0.671972 0.658675
 C -2.580890 0.692270 -0.064915
 H -0.850903 -1.307292 0.244238
 H -3.571584 1.123902 -0.170325
 H -2.316753 -0.104563 -0.751440
 C 1.235185 -1.326200 0.740120
 H 2.074623 -0.750772 1.173958
 O 1.419918 -2.460059 0.347710
 C -1.724356 1.165187 0.859608

C	-0.363078	0.593504	1.061654
C	-2.094826	2.337947	1.651760
C	0.596461	1.448255	1.756772
C	-1.179965	3.016432	2.365865
H	-3.127130	2.672490	1.597164
C	0.205358	2.577956	2.379779
H	1.632938	1.138226	1.815206
H	-1.456906	3.906304	2.921482
H	0.934030	3.172384	2.922689

TSA1/B1.gif

0 1

C	-1.29452500	-0.39151400	0.51457300
C	-2.59434300	0.84125100	1.93944300
H	-0.99657200	-1.43979100	0.44081600
H	-2.59618600	-0.10261100	2.46868000
H	-3.55614900	1.35428100	1.90230500
C	-2.33662600	-0.00534100	-0.45231000
H	-2.44461600	1.08908500	-0.59828600
O	-2.98944300	-0.80358500	-1.09150600
C	-1.35449800	1.51559600	1.75841000
C	-0.47855100	0.59122900	1.15254400
C	-0.91163300	2.81377000	2.09344800
C	0.91598500	0.80372400	1.17588300
C	0.44430000	3.04536500	2.02644100
H	-1.59844900	3.56807400	2.46543700
C	1.35309800	2.03712200	1.60693700
H	1.60881900	0.05811200	0.79760100
H	0.83993900	4.00982200	2.32985100
H	2.41445300	2.26541400	1.59573100

TSA1/F4.gif

0 1

C	-1.57634300	-0.21840000	0.63587400
C	-2.74251600	1.17907300	1.99890200
H	-1.82281000	-0.93123600	1.41502200
H	-3.35917800	1.07451200	2.89284600
H	-3.28773100	1.33109200	1.07728000
C	-1.77658200	-0.68281800	-0.74270300
H	-1.27693800	-0.06734200	-1.52256400
O	-2.45417100	-1.64128300	-1.04903500
C	-1.37267600	1.54968500	2.04578400
C	-0.74700200	0.90227500	0.95889700
C	-0.63885400	2.41140600	2.89094700

C	0.49475500	1.36150100	0.47338000
C	0.61299500	2.78782300	2.45656900
H	-1.07210100	2.82329500	3.79757900
C	1.15619200	2.29874500	1.23855600
H	0.95343600	0.93436100	-0.41374800
H	1.19517200	3.49440500	3.04010400
H	2.13935700	2.64290800	0.93230800

TSA2/B3.gjf

0 1

C	-0.61211000	-0.73174500	1.42725600
C	0.47799700	1.21557400	2.11205000
H	-0.26815600	-1.73239000	1.15199900
H	1.32220400	0.57237800	1.90516800
H	0.56002100	1.83706800	3.00443400
C	-1.32285000	-0.68742200	2.72703400
H	-1.00122400	-1.49374400	3.42001100
O	-2.22070200	0.06580200	3.03659300
C	-0.42845400	1.50803900	1.06789600
C	-0.78984700	0.28732300	0.45053300
C	-0.90650100	2.73876700	0.56079500
C	-1.30121600	0.27996300	-0.86379700
C	-1.49634900	2.71154100	-0.68111000
H	-0.73910200	3.67153400	1.09075500
C	-1.65489300	1.49670100	-1.40375200
H	-1.49478300	-0.64992100	-1.39018400
H	-1.82836000	3.63746900	-1.14058000
H	-2.10967800	1.53506600	-2.38909600

TSA2/F2.gjf

0 1

C	-0.49145400	-0.47917900	1.65106800
C	0.35047700	1.53907300	2.27804400
H	0.56505700	-0.71389300	1.58479800
H	1.33033900	1.94150700	2.54131200
H	-0.31670200	1.36401900	3.11104000
C	-1.35083700	-1.49234500	2.27798600
H	-0.83709600	-2.25209300	2.90060200
O	-2.55837800	-1.51829600	2.14371700
C	-0.21079700	1.66823200	0.97998500
C	-1.01183500	0.52516900	0.77351600
C	-0.14125700	2.68721800	0.00451000
C	-2.02449800	0.52640000	-0.20685500
C	-1.06948300	2.63279500	-1.01155500

H	0.55196600	3.51805100	0.09734200
C	-2.02550400	1.58461200	-1.09135100
H	-2.72244900	-0.29875600	-0.29350700
H	-1.09934100	3.42227300	-1.75655900
H	-2.75221100	1.60721500	-1.89809000

TSB1/C1.gjf

0 1

C	1.14274600	0.67939900	-0.35284700
C	0.42244600	0.39730400	2.36840700
H	1.47225700	0.94073600	-1.35462200
H	1.49307100	0.54182900	2.32326300
H	0.03104800	-0.06837100	3.26949200
C	1.35602900	-0.68608400	0.02421700
H	1.63263300	-1.33810600	-0.82264500
O	1.17581900	-1.23538200	1.12067500
C	-0.40254200	1.08901200	1.51029900
C	0.12309800	1.44434800	0.21459700
C	-1.73703400	1.48172300	1.86303200
C	-0.57570200	2.46175000	-0.51842300
C	-2.40269700	2.39003500	1.09962600
H	-2.16114500	1.10707100	2.79103300
C	-1.78642600	2.91285100	-0.08378600
H	-0.15070800	2.82015300	-1.45191500
H	-3.38684500	2.74238400	1.38922600
H	-2.31705000	3.66434500	-0.66162600

TSB1/D2.gjf

0 1

C	0.95909000	0.51027500	-0.49903500
C	0.44033300	0.22833100	2.17991800
H	1.18934000	0.60618500	-1.55691200
H	1.52027800	0.35329500	2.17917800
H	0.03894400	-0.26236900	3.06499600
C	1.34444300	-0.71394500	0.10738700
H	0.55064900	-0.88701400	1.04774300
O	2.22101100	-1.52142800	-0.04135100
C	-0.35693200	1.12851000	1.45106100
C	0.01904200	1.36645300	0.08882300
C	-1.56176500	1.69576000	1.95223400
C	-0.69635800	2.36346600	-0.64264300
C	-2.24066100	2.62581100	1.21425200
H	-1.88390600	1.43717400	2.95722300
C	-1.78145900	2.98025000	-0.08582600

H	-0.38342900	2.59704600	-1.65616300
H	-3.12451900	3.10707100	1.61971000
H	-2.32510200	3.73012900	-0.65259600

TSB1/E1.gif

0 1

C	0.91500100	0.47216100	-0.43282800
C	0.59857400	0.16033500	1.94510000
H	1.37676300	0.50071900	-1.41790800
H	1.54077000	0.60015300	2.27390900
H	0.21178300	-0.51896800	2.70499000
C	1.21152700	-0.60229900	0.53494700
H	0.21005900	-1.14625000	0.32360200
O	2.25015600	-1.29808200	0.61878600
C	-0.33893500	1.13683200	1.39253800
C	-0.03908600	1.40005400	0.02660200
C	-1.47750100	1.70925800	1.96717700
C	-0.77580500	2.36188500	-0.70315200
C	-2.19265500	2.64722700	1.23931900
H	-1.75593300	1.47205400	2.98950500
C	-1.83581000	2.98560100	-0.08436000
H	-0.51579200	2.58349000	-1.73398300
H	-3.03705700	3.14998700	1.70138200
H	-2.41705600	3.73084500	-0.61763000

TSB2/C2.gif

0 1

C	0.02893100	-0.39572900	1.80322700
C	0.48540600	2.32490600	2.42644600
H	-0.29329100	-1.42061400	1.64082800
H	0.38521200	1.78335200	3.35701800
H	1.00158400	3.28057600	2.47265500
C	1.42684700	-0.22924100	2.06578400
H	2.02280300	-1.13614000	1.86260200
O	2.05065900	0.79469800	2.38000800
C	-0.30645000	1.99472700	1.34936900
C	-0.73397700	0.62188200	1.22925100
C	-0.73272700	2.95542800	0.37189400
C	-1.83065600	0.35240600	0.34337800
C	-1.72333500	2.63918400	-0.50530000
H	-0.31105600	3.95661600	0.40897400
C	-2.30187000	1.32831200	-0.48327600
H	-2.23535800	-0.65503900	0.30243200
H	-2.09830000	3.37581900	-1.20773900

H	-3.11442000	1.10386000	-1.16855100
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TSB2/D2.gif

0 1

C	-0.06102900	-0.38647100	1.88423200
C	0.76828400	2.21240700	2.16574000
H	-0.37504900	-1.42337500	1.79683700
H	0.62981400	1.91279500	3.20168900
H	1.43643600	3.05971400	2.02181700
C	1.25542800	-0.17950100	2.37243200
H	1.62706500	0.90043500	1.88296600
O	2.00318100	-0.74035800	3.12644400
C	-0.25121100	1.95031600	1.23294500
C	-0.76587700	0.61335700	1.20153300
C	-0.69117400	2.89047200	0.25936900
C	-1.88087500	0.34009100	0.35160900
C	-1.74333400	2.58751200	-0.56014100
H	-0.23059300	3.87439700	0.23519100
C	-2.35901400	1.30582700	-0.48874900
H	-2.31828400	-0.65403200	0.36302700
H	-2.12280700	3.32509900	-1.25955800
H	-3.20096300	1.08631600	-1.13838400

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C	-0.58679800	0.17386900	-0.85071400
C	-0.71842900	-0.30557600	1.51534900
H	-0.60238400	0.04799300	-1.93150400
H	-1.61243400	-0.92914000	1.48435800
H	-0.13330700	-0.52667700	2.40824000
C	-0.03271500	-0.86008700	0.04502500
H	0.95046600	-0.26925500	0.21133000
O	0.05219800	-2.09313700	-0.16177100
C	-0.98227900	1.10394000	1.22881300
C	-1.03382200	1.32599900	-0.17597500
C	-1.06483400	2.19496500	2.09895200
C	-1.33779100	2.60613300	-0.69495900
C	-1.35902700	3.44439200	1.57623700
H	-0.96510800	2.05269500	3.17079800
C	-1.51153300	3.64857600	0.18739100
H	-1.41217300	2.75787400	-1.76771200
H	-1.49378200	4.28571700	2.24963900
H	-1.74908500	4.64148700	-0.18047800

VIII. Cartesian coordinates for structures of the Diels-Alder reaction

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C	-0.28513400	-2.03017900	-3.77116000
C	-0.80891800	-0.91081600	-3.21373800
H	-0.26181000	-0.42654400	-2.40768600
C	-2.06602100	-0.18408100	-3.60227100
H	-1.77306800	0.77562400	-4.05792200
H	-2.62824600	-0.72572700	-4.36794200
C	-2.97451500	0.13578900	-2.38722200
H	-3.80511400	0.77072900	-2.72932000
H	-2.40129900	0.73562400	-1.66750000
C	-3.55732300	-1.09769600	-1.65915800
H	-2.71975700	-1.76017900	-1.38565600
C	-4.26927300	-0.67590000	-0.33941900
H	-4.76058600	-1.57169300	0.07350000
H	-5.07158100	0.03825400	-0.57550200
C	-3.35179800	-0.09355200	0.69985700
H	-2.52965100	-0.73569300	1.02401400
C	-3.47577400	1.13230200	1.25412900
H	-4.29762700	1.77434800	0.93376000
C	-2.58988900	1.67266800	2.26712000
H	-1.76614300	1.03377100	2.58848100
C	-2.72234300	2.90104700	2.82827400
H	-3.54517000	3.54241200	2.51047600
C	-1.83272800	3.43780800	3.84202500
H	-1.01149300	2.79163600	4.15337800
C	-1.95942500	4.65553900	4.40518000
H	-2.76253500	5.33287600	4.12553000
C	-0.89171700	-2.79435900	-4.92613200
H	-1.02533500	-3.84928700	-4.66302100
H	-1.85548100	-2.38561900	-5.23341500
H	-0.21931000	-2.77904400	-5.79185200
C	0.99247900	-2.60087600	-3.27840600
C	1.74126500	-1.98497500	-2.07298800
H	2.44375900	-2.75081600	-1.73983400
H	1.04557800	-1.75616100	-1.26029000
C	2.49068900	-0.70978700	-2.41297100
S	4.23716100	-1.01730000	-2.95557700
C	4.76335100	0.75887200	-3.32041200
H	3.91303800	1.39772600	-3.07235400
H	5.62445000	0.99787800	-2.69749400

H	5.01365700	0.83692300	-4.37776400
O	1.48869200	-3.61135100	-3.81564800
O	2.00220600	0.42127700	-2.34948400
C	-4.52739200	-1.89757700	-2.54964100
H	-5.37896600	-1.27458200	-2.85453200
H	-4.03873600	-2.26593000	-3.45787200
H	-4.92396900	-2.76756800	-2.01281100
H	-1.26719800	5.01218800	5.16027100

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C	-0.81446200	0.08341800	1.81057900
C	0.49145200	-0.16320900	1.54397100
H	1.21470900	0.36604600	2.16499400
C	1.07541700	-1.05043100	0.48488000
H	1.75022400	-1.77492900	0.96891700
H	0.30843200	-1.62944900	-0.03278900
C	1.90755700	-0.23831500	-0.54385500
H	2.64980500	0.35409400	0.01042600
H	1.25233600	0.48595300	-1.04877300
C	2.64795000	-1.08910800	-1.60868400
H	3.03574100	-1.99512300	-1.11450200
C	1.73269100	-1.54016100	-2.78644500
H	2.38821000	-2.00242500	-3.54330400
H	1.29978000	-0.64620100	-3.25811000
C	0.64113800	-2.51620100	-2.44511600
H	0.96070900	-3.44356300	-1.96450300
C	-0.67185800	-2.34388500	-2.71657000
H	-0.99359800	-1.42061300	-3.20051400
C	-1.70977000	-3.30845300	-2.40601700
H	-1.38835000	-4.23837600	-1.93448500
C	-3.03067700	-3.12756100	-2.66141200
H	-3.35683600	-2.20029900	-3.13366300
C	-4.06418400	-4.09709600	-2.34648800
H	-3.72947500	-5.02303400	-1.87787300
C	-5.37765800	-3.92338400	-2.59300400
H	-5.75583000	-3.01644500	-3.05809600
C	-1.98006400	-0.53137900	1.06835500
H	-2.65012000	0.24127800	0.67672000
H	-1.64788600	-1.14198300	0.22677300
H	-2.57518600	-1.18317100	1.72362100
C	-1.08854600	1.03511500	2.92799800
C	-2.54243300	1.48191700	3.20253600
H	-2.58687200	1.78819600	4.24850200

H	-3.24292600	0.65971300	3.03036200
C	-2.95146200	2.63519900	2.30361800
S	-2.93124600	4.27172600	3.17592700
C	-3.42995800	5.39421900	1.74282800
H	-4.34678300	5.91611000	2.01450800
H	-2.62068500	6.09933500	1.55664500
H	-3.59073100	4.74792400	0.87715300
O	-0.19189400	1.50079100	3.65849200
O	-3.25022400	2.51975400	1.11203300
C	3.85101300	-0.30338300	-2.17149600
H	4.39815300	-0.89241200	-2.91714400
H	3.51841000	0.62441000	-2.65535900
H	4.55193200	-0.03147300	-1.37409400
H	-6.11294700	-4.67913700	-2.33854000

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C	-4.90514900	-0.99317600	0.06636300
C	-4.35757100	-0.28756500	-0.95154400
H	-3.41750400	-0.67543100	-1.34480000
C	-4.85863400	0.96569300	-1.60529500
H	-5.05083300	0.74539100	-2.66628900
H	-5.81108100	1.30034900	-1.17784300
C	-3.82148400	2.11536400	-1.51302300
H	-2.88001600	1.79804200	-1.98183200
H	-3.59267000	2.29395900	-0.45297100
C	-4.29199000	3.44211900	-2.15245600
H	-5.25469700	3.71336600	-1.68928500
C	-3.30705700	4.60386100	-1.80746100
H	-3.25710800	4.70625600	-0.71481700
H	-3.74982100	5.53636700	-2.19218600
C	-1.91520300	4.45014800	-2.35894100
H	-1.81553400	4.45968400	-3.44524500
C	-0.79830300	4.31675700	-1.60999100
H	-0.88932000	4.31369000	-0.52269800
C	0.54198800	4.18109500	-2.14674700
H	0.63711000	4.18773600	-3.23346700
C	1.66240600	4.04926300	-1.39264600
H	1.57143300	4.04121000	-0.30591800
C	3.00214500	3.91415800	-1.93490400
H	3.08499100	3.92304800	-3.02208300
C	4.11891400	3.78154600	-1.19245500
H	4.08335500	3.76650100	-0.10599000
C	-6.20132400	-0.64247500	0.76219600

H	-6.65576700	0.25404900	0.33648000
H	-6.93992200	-1.45021800	0.67924100
H	-6.05181200	-0.45271700	1.83310500
C	-4.15462800	-2.20862600	0.51168700
C	-4.76191800	-3.03317500	1.65818300
H	-5.73780200	-3.42054000	1.33786700
H	-4.93316700	-2.38649800	2.52596100
C	-3.89809900	-4.21413800	2.03535100
S	-2.72961900	-3.84092300	3.43538900
C	-1.79968300	-5.48047900	3.49532700
H	-2.26333700	-6.12754400	2.74715100
H	-0.75373800	-5.29605900	3.25356700
H	-1.90276700	-5.90301900	4.49409800
O	-3.08050000	-2.56436500	-0.00991200
O	-3.95516700	-5.31173900	1.48665100
C	-4.52049500	3.32167500	-3.67247400
H	-4.79707100	4.29169200	-4.10337900
H	-3.61624400	2.97011800	-4.18419600
H	-5.32780600	2.61875400	-3.90526300
H	5.09949700	3.68279400	-1.64550400

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C	-1.45560300	0.92057800	1.37388900
C	-1.43453800	1.50410900	0.15037600
H	-0.61601900	1.21065400	-0.50521000
C	-2.37269900	2.52813000	-0.41909400
H	-3.29415000	2.60862300	0.16744000
H	-1.87845400	3.51140100	-0.33869800
C	-2.71057800	2.32268000	-1.92094600
H	-1.77318000	2.23643400	-2.48659900
H	-3.20303800	3.24079500	-2.27037600
C	-3.62790600	1.12621000	-2.28873000
H	-3.87982800	1.26459100	-3.35323100
C	-2.93470700	-0.26374100	-2.17618500
H	-3.69994300	-1.02358600	-2.40685300
H	-2.62536000	-0.44504800	-1.13936900
C	-1.76343900	-0.44984100	-3.10274600
H	-1.97226900	-0.31829700	-4.16737200
C	-0.50898500	-0.77434800	-2.71745300
H	-0.29164000	-0.90407200	-1.65675800
C	0.60347800	-0.97048400	-3.62772000
H	0.39674800	-0.86000800	-4.69364500
C	1.86386800	-1.27992000	-3.23030000

H	2.06841100	-1.38557000	-2.16469100
C	2.97889400	-1.48110600	-4.13777900
H	2.76086600	-1.37329800	-5.20103400
C	4.23405000	-1.78631700	-3.75311000
H	4.49572600	-1.90290900	-2.70448200
C	-2.47805700	1.21542900	2.44929500
H	-3.00730700	0.30940900	2.77185700
H	-2.01436300	1.65248400	3.34340500
H	-3.23087000	1.92503400	2.10073800
C	-0.37518300	-0.06935700	1.65810100
C	-0.24980800	-0.58442800	3.09953700
H	-1.19621900	-1.04303400	3.40779300
H	-0.06499500	0.26805200	3.76582700
C	0.89362500	-1.55892600	3.26662000
S	0.36767200	-3.33409900	3.09128300
C	2.05144800	-4.16646600	3.26418700
H	2.28439200	-4.67797700	2.33115100
H	2.77293600	-3.37039000	3.46208800
H	2.00746400	-4.86875500	4.09573100
O	0.41223400	-0.48006900	0.78070200
O	2.05218400	-1.22351400	3.50092000
C	-4.95175100	1.13655900	-1.49961600
H	-5.64541300	0.38578300	-1.89616700
H	-4.78991800	0.90471500	-0.43961200
H	-5.44478400	2.11470500	-1.56011200
H	5.03500900	-1.92781800	-4.47105300

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C	0.06258600	0.79004500	1.76435500
C	1.31959300	0.47527300	1.36708600
H	1.88734800	1.27516100	0.89150800
C	2.01036200	-0.85422100	1.43962600
H	2.90684100	-0.76599600	2.07375800
H	1.37078800	-1.60612000	1.91056700
C	2.45181500	-1.33859000	0.03087900
H	3.26347400	-0.68846500	-0.32463700
H	1.61871600	-1.21229000	-0.67237200
C	2.92251200	-2.81108400	-0.01648000
H	3.62189300	-2.97503700	0.81940400
C	1.74217500	-3.81899000	0.19183600
H	1.28912500	-3.64078900	1.17551500
H	2.17453300	-4.82960400	0.22884100
C	0.67270800	-3.76422600	-0.86820600

H	0.90573500	-4.22999400	-1.82656200
C	-0.52582500	-3.15762300	-0.71597800
H	-0.75985800	-2.68832100	0.24089600
C	-1.55074900	-3.06311800	-1.73779400
H	-1.35708800	-3.57843700	-2.67973000
C	-2.70865600	-2.37068300	-1.58875800
H	-2.89280100	-1.83465200	-0.65789300
C	-3.73739600	-2.26803600	-2.60775900
H	-3.54618000	-2.79136700	-3.54535300
C	-4.88882500	-1.58191600	-2.45842900
H	-5.11637600	-1.05251500	-1.53671400
C	-0.89170700	-0.15507500	2.46047700
H	-0.44669400	-1.14120200	2.60677700
H	-1.16594400	0.22233400	3.45552300
H	-1.81858900	-0.28260200	1.89147700
C	-0.39340300	2.18069700	1.47327200
C	-1.90300800	2.50640500	1.55462600
H	-1.98674600	3.59217700	1.61795200
H	-2.35491300	2.04965100	2.43973600
C	-2.65017700	1.99437500	0.33396000
S	-2.83183700	3.28198600	-0.98360100
C	-3.68263200	2.26074300	-2.32429900
H	-3.73082900	1.22931500	-1.97025700
H	-4.68298300	2.66080100	-2.48609100
H	-3.08398000	2.32971800	-3.23175600
O	0.38439500	3.09326600	1.13517100
O	-3.07385400	0.84100200	0.20804400
C	3.67989600	-3.09653500	-1.32839800
H	4.57477400	-2.46807600	-1.40686300
H	3.99851400	-4.14475100	-1.38269700
H	3.05052600	-2.88882100	-2.20217200
H	-5.63425800	-1.53581100	-3.24548600

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C	-0.80327600	-3.29927800	-1.24288800
C	-0.53512500	-3.79678300	-0.01013600
H	-1.29851700	-3.62638800	0.74940500
C	0.65235400	-4.60054000	0.43671400
H	0.34978200	-5.66164100	0.42573200
H	1.48715000	-4.52029900	-0.26981200
C	1.15824900	-4.28392300	1.86875600
H	1.75809800	-5.14103000	2.20340700
H	0.30019600	-4.22401300	2.55565000

C	2.02735100	-3.01120900	2.02404600
H	2.79591200	-3.03513500	1.23294500
C	1.20587000	-1.70248000	1.84510700
H	0.46720600	-1.62903200	2.65654300
H	0.63246900	-1.77460000	0.90919800
C	2.04943200	-0.45717700	1.80488100
H	2.82393700	-0.43607300	1.03572500
C	1.90883900	0.59851200	2.63501400
H	1.15358200	0.53001400	3.41821100
C	2.67353500	1.84344300	2.61437500
H	2.58504500	2.45915300	3.50984700
C	3.45531500	2.30854700	1.60787000
H	3.53726200	1.74325100	0.67979200
C	4.20288000	3.55162800	1.67492700
H	4.10954000	4.11859200	2.60171800
C	4.98389100	4.03173600	0.68706900
H	5.10700200	3.49953500	-0.25295300
C	0.10381400	-3.43787700	-2.44485700
H	0.99251100	-4.02767100	-2.21150300
H	-0.41520000	-3.92832300	-3.27551000
H	0.44904200	-2.45846600	-2.80481800
C	-2.09785100	-2.57116100	-1.39039100
C	-2.55159300	-2.11077000	-2.79326000
H	-1.69797400	-1.77591100	-3.38980600
H	-3.24283600	-1.28008700	-2.64548300
C	-3.23624800	-3.23272300	-3.55475300
S	-5.08194100	-3.06747400	-3.57789400
C	-5.52310200	-4.63257200	-4.53621300
H	-6.12684500	-5.27321600	-3.89452700
H	-6.07431300	-4.34602000	-5.43104300
H	-4.58090400	-5.11937200	-4.79718900
O	-2.84584700	-2.31853800	-0.42530200
O	-2.64421700	-4.17371400	-4.09050000
C	2.74645000	-3.02489700	3.38770300
H	3.38974700	-3.90732100	3.48704900
H	3.36621900	-2.13177900	3.51692600
H	2.01672900	-3.04638700	4.20837700
H	5.52337800	4.96746900	0.78685100

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C	-2.32914800	-2.70602900	0.30116300
C	-1.64588500	-2.43506600	1.43983700
H	-2.11155400	-1.71773800	2.11663100

C	-0.33325900	-2.99401500	1.90570300
H	-0.52359700	-3.62708200	2.78763200
H	0.12310900	-3.64659100	1.15540900
C	0.66688200	-1.88805100	2.33446300
H	1.54520400	-2.36795000	2.79046000
H	0.19697100	-1.28296800	3.12357300
C	1.13793200	-0.94780800	1.19889900
H	0.24621600	-0.52905000	0.70861200
C	1.93058400	0.24574200	1.81333400
H	2.82244900	-0.16476500	2.31594300
H	1.31291700	0.70647800	2.59628400
C	2.34827300	1.30119100	0.82527100
H	3.08971400	1.00610900	0.08332300
C	1.85476600	2.55797300	0.80336200
H	1.08973000	2.81561500	1.53648700
C	2.22233100	3.63306900	-0.11545900
H	1.54167100	4.48459500	-0.13140300
C	3.31132700	3.68426400	-0.92284900
H	4.03699200	2.87135100	-0.90645800
C	3.59701300	4.78540900	-1.82536000
H	2.87338700	5.60111900	-1.83271200
C	4.67406300	4.85513100	-2.63249500
H	5.41995800	4.06453200	-2.65816900
C	-1.87591100	-3.67204200	-0.77065600
H	-0.95764100	-4.18798900	-0.48336300
H	-2.63963800	-4.43250600	-0.96543600
H	-1.67426600	-3.15542200	-1.71956100
C	-3.62361900	-1.98215200	0.12250800
C	-4.51460500	-2.31220700	-1.09518100
H	-3.90558000	-2.53181300	-1.97697000
H	-5.12882700	-1.43121000	-1.28606800
C	-5.39915100	-3.51892100	-0.83211200
S	-7.16383900	-3.06162600	-0.49969500
C	-7.87871700	-4.78022800	-0.18647500
H	-8.27783500	-4.80892500	0.82670800
H	-8.66180200	-4.96863600	-0.91993800
H	-7.05708100	-5.49044400	-0.30217000
O	-4.02929400	-1.11391400	0.91971200
O	-4.99913700	-4.68626900	-0.81921500
C	1.96714500	-1.69732500	0.13821500
H	2.88479300	-2.10825600	0.58126100
H	1.40485300	-2.52941800	-0.29903100
H	2.25608200	-1.03470500	-0.68426800
H	4.84302100	5.70054700	-3.29074900

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C	-3.16390000	-0.23490000	-2.71840000
C	-2.76930000	-0.43930000	-1.43810000
H	-1.76810000	-0.08970000	-1.18490000
C	-3.52520000	-1.08550000	-0.31560000
H	-3.72920000	-0.31790000	0.44690000
H	-4.49920000	-1.46490000	-0.64460000
C	-2.71760000	-2.23560000	0.33920000
H	-1.76300000	-1.84400000	0.71720000
H	-2.46350000	-2.97130000	-0.43680000
C	-3.46440000	-2.95850000	1.48340000
H	-4.41890000	-3.33020000	1.07630000
C	-2.67380000	-4.22160000	1.94900000
H	-2.54790000	-4.89460000	1.08990000
H	-3.30500000	-4.75550000	2.67760000
C	-1.33010000	-3.94270000	2.56830000
H	-1.33340000	-3.34340000	3.47890000
C	-0.15340000	-4.38150000	2.07140000
H	-0.17470000	-4.94750000	1.13950000
C	1.17580000	-4.17040000	2.64080000
H	2.00880000	-4.35920000	1.96320000
C	1.47030000	-3.78510000	3.90760000
H	0.66640000	-3.62900000	4.62680000
C	2.82210000	-3.57380000	4.39430000
H	3.62380000	-3.73900000	3.67390000
C	3.13400000	-3.19410000	5.64910000
H	2.36700000	-3.01680000	6.39900000
C	-4.50890000	-0.63230000	-3.28440000
H	-5.15240000	-1.07180000	-2.51990000
H	-5.03180000	0.23300000	-3.70570000
H	-4.40370000	-1.37700000	-4.08590000
C	-2.17600000	0.44130000	-3.61080000
C	-2.60520000	0.86200000	-5.03460000
H	-3.27440000	0.11820000	-5.47690000
H	-1.69450000	0.93490000	-5.63040000
C	-3.33390000	2.19450000	-5.02870000
S	-2.27110000	3.60090000	-5.60200000
C	-3.49690000	5.02140000	-5.39550000
H	-3.65380000	5.48810000	-6.36730000
H	-4.42440000	4.58560000	-5.01790000
H	-3.08330000	5.73400000	-4.68280000
O	-1.00730000	0.69510000	-3.25930000

O	-4.50350000	2.34820000	-4.66630000
C	-3.79320000	-2.02430000	2.66560000
H	-2.88950000	-1.54120000	3.05660000
H	-4.49160000	-1.23300000	2.37250000
H	-4.25870000	-2.58410000	3.48620000
H	4.16140000	-3.04760000	5.96460000

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C	-1.27993400	2.94529900	0.50460400
C	-0.43164100	3.01087300	1.56085900
H	0.62975500	3.04467500	1.31888200
C	-0.77125800	3.02132100	3.02253900
H	-0.53531800	4.01414000	3.43885300
H	-1.84551200	2.87090500	3.17487700
C	0.00380800	1.95813600	3.85455300
H	-0.39321200	1.99503200	4.87775400
H	1.06277900	2.24464300	3.92644400
C	-0.10285900	0.50932100	3.29577800
H	-0.98431400	0.46144900	2.63996900
C	1.14836400	0.16117100	2.42558800
H	1.96427600	-0.11435500	3.11450300
H	1.48405700	1.05761600	1.89294200
C	0.92312100	-0.92906700	1.41485900
H	0.65244100	-1.91648900	1.79262800
C	1.02295300	-0.73236800	0.08140200
H	1.28801100	0.26099100	-0.28265900
C	0.78783000	-1.74106500	-0.93085800
H	0.50812000	-2.73847100	-0.58841900
C	0.88820300	-1.50119500	-2.26397000
H	1.16558700	-0.50145500	-2.59741700
C	0.62879300	-2.48466700	-3.29366600
H	0.33081500	-3.47938600	-2.95774400
C	0.72835500	-2.24506000	-4.62023500
H	1.01991900	-1.25716000	-4.97243100
C	-2.78892200	2.94507600	0.60567300
H	-3.21420700	3.90115500	0.26773900
H	-3.22435200	2.15119300	-0.00848200
H	-3.12290000	2.79718300	1.63464900
C	-0.65200300	2.87620500	-0.84710100
C	-1.52493900	3.03711400	-2.10523600
H	-0.89737900	3.49081700	-2.87434400
H	-2.37583600	3.69884800	-1.90754200
C	-2.08968500	1.71771800	-2.61422100

S	-1.65210000	1.37646300	-4.38130600
C	-2.55706334	-0.13617057	-4.62905796
H	-2.87704034	-0.47530857	-3.64195996
H	-3.41920834	0.07558243	-5.26131496
H	-1.89029834	-0.85957457	-5.09699096
O	0.57387600	2.69728900	-1.01196600
O	-2.78299800	0.95129400	-1.94116800
C	-0.29252800	-0.52039500	4.42644800
H	-1.21401800	-0.32541600	4.98824000
H	-0.35182300	-1.54225600	4.03362300
H	0.54701200	-0.48164700	5.13336200
H	0.53475515	-2.97979275	-5.37361862

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C	-0.65408800	2.70015900	-0.22509800
C	0.54871100	3.23413500	-0.54682800
H	1.18272300	3.52521000	0.28864400
C	1.12003500	3.41130800	-1.93103400
H	0.35976400	3.81057800	-2.61531600
H	1.92392300	4.15571800	-1.89329100
C	1.66331500	2.08452900	-2.53867900
H	2.05767500	2.29403800	-3.54420100
H	0.82027100	1.39552000	-2.66930800
C	2.75692400	1.37836100	-1.70290900
H	2.42233400	1.35943300	-0.65368400
C	2.92617800	-0.10543700	-2.14494800
H	3.76768000	-0.52852100	-1.57301100
H	3.21561600	-0.14355400	-3.20512000
C	1.68914200	-0.93248100	-1.91299300
H	1.28716200	-0.90394600	-0.89840300
C	1.06186900	-1.68331400	-2.84222900
H	1.51149100	-1.76004800	-3.83352200
C	-0.18098300	-2.43130400	-2.64868500
H	-0.31030700	-3.31608400	-3.27311700
C	-1.18605100	-2.09302300	-1.80360000
H	-1.10362200	-1.17340400	-1.22399400
C	-2.41036800	-2.85741200	-1.63230300
H	-2.47128600	-3.79704500	-2.18230200
C	-3.44790300	-2.47618900	-0.86122600
H	-3.44873600	-1.54000000	-0.30747800
C	-1.67778500	2.24300700	-1.23961100
H	-1.32281500	2.40047500	-2.25979600
H	-1.92211500	1.17882300	-1.14107100

H	-2.61947700	2.79484600	-1.13110900
C	-0.94241000	2.53651800	1.23041100
C	-1.98847300	1.49833500	1.67587900
H	-1.90914800	1.44527700	2.76647700
H	-1.73937400	0.51694700	1.25641300
C	-3.43312100	1.77695500	1.31142100
S	-4.04331000	3.42735000	1.91054900
C	-5.82700300	3.33248100	1.29691300
H	-5.99679700	4.15084800	0.59828500
H	-5.94261600	2.36566800	0.80255700
H	-6.49048700	3.41089900	2.15722100
O	-0.30192300	3.14136400	2.11311700
O	-4.15281100	0.98258000	0.70261600
C	4.10415000	2.12152500	-1.76416400
H	4.85450500	1.63072900	-1.13296100
H	4.49008600	2.14125800	-2.79205300
H	4.01144400	3.15873300	-1.42219100
H	-4.34199100	-3.08484300	-0.77326700

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C	1.13107200	-0.05284400	-0.37272200
C	-0.43211800	-0.01602000	-0.39781100
H	-0.77228300	-0.86565700	0.21228100
C	-1.07269400	1.25430300	0.21124600
H	-0.68854000	1.43025200	1.21907900
H	-0.80786000	2.13218600	-0.39606700
C	-2.60888100	1.11572700	0.25958800
H	-3.05361600	2.03282900	0.66946700
H	-2.87279500	0.30264300	0.95378700
C	-3.22817200	0.81224300	-1.12356900
H	-3.03770700	1.68432900	-1.77207700
C	-2.52877200	-0.40374600	-1.77036900
H	-2.92147900	-0.56261100	-2.78530400
H	-2.76308200	-1.31250600	-1.19460700
C	-0.99260600	-0.22014000	-1.82919000
H	-0.81493700	0.70988300	-2.40035700
C	-0.30493300	-1.34540900	-2.55829400
H	-0.79443600	-1.71835400	-3.45759400
C	0.86228600	-1.87597900	-2.17247300
H	1.30823100	-2.69206900	-2.73773200
C	1.63974100	-1.45449900	-0.93583800
H	2.69194100	-1.31937500	-1.23015600
C	1.60038300	-2.58405600	0.08235400

H	0.63511400	-2.76507500	0.55212600
C	2.64570600	-3.36298000	0.38680900
H	3.62284600	-3.21934800	-0.07045100
C	1.74406800	1.07151600	-1.24324500
H	1.41708100	2.06043600	-0.91188300
H	2.83919700	1.05277200	-1.21586900
H	1.44921700	0.93778600	-2.28775500
C	1.63603300	0.02453800	1.07863200
C	3.12048700	0.30918600	1.33875700
H	3.76741400	-0.18203700	0.60580600
H	3.35463700	-0.10936300	2.32519800
C	3.43594100	1.79271600	1.38941800
S	5.25659000	2.14101200	1.17342000
C	5.23817100	4.01632900	1.39299300
H	4.19577200	4.30462400	1.54592200
H	5.84358700	4.27060700	2.26201700
H	5.63950000	4.47351000	0.48942600
O	0.89931800	-0.20114600	2.04971100
O	2.60923500	2.68385700	1.57431000
C	-4.74991500	0.60763100	-1.03204800
H	-5.24279900	1.49002400	-0.60616600
H	-5.18739800	0.42082500	-2.02057100
H	-4.98915800	-0.25118200	-0.39104600
H	2.56461900	-4.17836600	1.09884400

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C	-0.56459800	-0.21431600	-0.64768300
C	0.16814800	-0.75402700	0.64003400
H	-0.29060000	-0.22311900	1.48382100
C	-0.04839700	-2.26892100	0.86605800
H	-1.12083300	-2.49769400	0.86992800
H	0.38956600	-2.83993000	0.03551900
C	0.60194500	-2.74529600	2.17755800
H	0.43848100	-3.82433700	2.30318200
H	0.11760500	-2.25054400	3.03391700
C	2.11339000	-2.43611400	2.20880300
H	2.58272900	-2.97593000	1.36861200
C	2.33562300	-0.92663500	1.98754900
H	3.41186900	-0.70133200	1.96905800
H	1.91560200	-0.38045400	2.84731500
C	1.68129700	-0.38360700	0.69513900
H	2.19057400	-0.85041500	-0.16826300
C	1.80512700	1.12084000	0.61989500

H	2.49711700	1.61689100	1.29795600
C	1.02554800	1.82921900	-0.20522200
H	1.06656700	2.91532200	-0.23194400
C	0.12583500	1.14135800	-1.21030900
H	0.77198100	0.78233600	-2.02661900
C	-0.86635600	2.10858000	-1.82366800
H	-1.48480300	2.66153500	-1.11579600
C	-1.00211200	2.33600400	-3.13629700
H	-0.38805900	1.82372600	-3.87377400
C	-0.53484800	-1.23157300	-1.81005100
H	0.49145200	-1.58018600	-1.96992000
H	-1.16381300	-2.10273800	-1.61395100
H	-0.86497800	-0.76765600	-2.74701700
C	-2.00939900	0.14670600	-0.23376600
C	-3.19898600	-0.11987700	-1.17529500
H	-2.87786900	-0.18658200	-2.21878000
H	-3.88782000	0.72321800	-1.08352000
C	-3.92514100	-1.40621000	-0.82698800
S	-5.77064900	-1.24943200	-0.95916400
C	-6.26571700	-3.02298500	-0.54285400
H	-6.90528500	-3.00322800	0.33863700
H	-6.79059800	-3.44828200	-1.39738900
H	-5.34131500	-3.56827600	-0.34025800
O	-2.25167400	0.69313000	0.85361200
O	-3.37235500	-2.46226300	-0.51054800
C	2.77109200	-2.91578900	3.51381800
H	2.33308300	-2.40405000	4.38099200
H	2.62927700	-3.99419200	3.65499100
H	3.84937000	-2.71388100	3.51500700
H	-1.72008000	3.05300000	-3.52332100

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C	1.06702100	-0.56795700	2.36230500
C	-0.40062700	-0.98058900	2.00809600
H	-0.49016900	-0.88746200	0.91594900
C	-1.50912000	-0.09144300	2.62165600
H	-1.50281100	-0.18783000	3.71671600
H	-1.32914500	0.96107700	2.38707000
C	-2.89271300	-0.49881100	2.06779100
H	-2.90769500	-0.28472200	0.98922600
H	-3.67478500	0.12506500	2.52105300
C	-3.22863900	-1.99632500	2.28652100
H	-4.11032800	-2.23276400	1.67185300

C	-2.06150500	-2.88222900	1.78152100
H	-2.00185200	-2.81881700	0.68525800
H	-2.25973900	-3.93544800	2.02710300
C	-0.69328800	-2.45906700	2.37350200
H	-0.78659000	-2.52885300	3.47143100
C	0.42060900	-3.38356700	1.95424800
H	0.19582100	-4.44979400	1.94683200
C	1.64842700	-2.96419400	1.62352900
H	2.41074600	-3.68028100	1.32301500
C	2.08557400	-1.50855600	1.58004700
H	3.05435500	-1.43263500	2.09750500
C	2.31776500	-1.10550000	0.13198300
H	1.42532400	-1.01302100	-0.48439500
C	3.52578600	-0.90741800	-0.40933500
H	4.44006900	-0.99894800	0.17369600
C	1.34737400	-0.69823500	3.88037400
H	0.69426400	-0.04609500	4.46972000
H	1.18449100	-1.72892300	4.20649600
H	2.38545100	-0.44673400	4.12032400
C	1.33239800	0.87071100	1.86966300
C	2.56212000	1.60445300	2.42891700
H	3.45136200	0.98266000	2.27613300
H	2.43088600	1.74222600	3.50852700
C	2.74424000	2.97609000	1.81948400
S	3.91815400	3.00260500	0.37802400
C	3.79628100	4.83094400	-0.07042400
H	3.10417400	5.28144700	0.64470200
H	4.78669100	5.27737400	0.01115800
H	3.41214100	4.91400400	-1.08634700
O	0.61384800	1.41897300	1.02212300
O	2.17718600	3.98424200	2.23632900
C	-3.60712500	-2.30287000	3.75086900
H	-3.86693900	-3.36156800	3.87399800
H	-2.79163100	-2.07843800	4.44798100
H	-4.47489800	-1.70640600	4.05758800
H	3.64904100	-0.64437400	-1.45481500

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C	-2.07909100	-0.68404200	-0.00796800
C	-2.51572700	-2.19906900	0.03997000
H	-1.69800400	-2.75453400	-0.43592700
C	-3.80270800	-2.49231200	-0.76686800
H	-4.64987500	-1.92798700	-0.35762700

H	-3.67521100	-2.15405300	-1.80479600
C	-4.14863600	-3.99483100	-0.76359100
H	-3.35209600	-4.54633700	-1.28393400
H	-5.07337100	-4.16400100	-1.33179900
C	-4.29653300	-4.56550500	0.66739600
H	-4.38362700	-5.65922400	0.58189100
C	-3.01051200	-4.26607000	1.46993600
H	-2.17989200	-4.83455200	1.02492400
H	-3.11762600	-4.62459400	2.50370600
C	-2.60513100	-2.77258700	1.48988600
H	-3.37030800	-2.20505900	2.04921200
C	-1.25441400	-2.59272800	2.14566300
H	-0.81490500	-3.43710700	2.67274600
C	-0.58893700	-1.44106500	2.00090400
H	0.40760400	-1.29668600	2.40875500
C	-1.25965100	-0.26204400	1.32680200
H	-2.05045400	0.09239800	2.00753900
C	-0.29973000	0.89001300	1.11785700
H	0.57500500	0.68595700	0.49932300
C	-0.44935700	2.10670300	1.65715100
H	-1.29847200	2.35415200	2.29095500
C	-3.28648400	0.27966600	-0.09052800
H	-4.00179400	0.04318500	0.70439900
H	-2.97403000	1.31876400	0.05535300
H	-3.81749200	0.21112700	-1.04451300
C	-1.12419100	-0.50895900	-1.20978900
C	-1.12499500	0.82674400	-1.97195000
H	-1.24681600	1.65481600	-1.26739600
H	-1.98395900	0.83934400	-2.65340400
C	0.16833500	1.04396100	-2.72418600
S	-0.01855200	0.95589300	-4.56829600
C	1.77895800	1.22664900	-5.07236800
H	1.83680400	2.11795500	-5.69597000
H	2.34418800	1.35895600	-4.14693200
H	2.12254000	0.34647500	-5.61429300
O	-0.35099400	-1.41166700	-1.56305100
O	1.24502000	1.26655500	-2.17036000
C	-5.57175400	-4.06658300	1.37825500
H	-5.57408900	-2.97952800	1.51744300
H	-6.46609100	-4.32768500	0.79921800
H	-5.66760700	-4.52589100	2.36971300
H	0.27966500	2.89538800	1.49754400

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C	-1.58938900	-0.37470000	-1.10223600
C	-0.95160600	0.84318800	-1.87092800
H	-1.71269400	1.24182100	-2.55930300
C	-0.53923200	2.02234000	-0.95646900
H	-1.40763500	2.39184200	-0.39791500
H	0.19898600	1.68242600	-0.22186400
C	0.08318200	3.17590700	-1.76774000
H	0.35753500	3.99714700	-1.09137900
H	-0.66175600	3.58281200	-2.47060300
C	1.32140600	2.71038200	-2.56206300
H	2.06705800	2.34783200	-1.83565600
C	0.92994800	1.53206500	-3.47697600
H	1.81667800	1.15481800	-4.00572300
H	0.24040800	1.90210400	-4.25107100
C	0.24888800	0.35796800	-2.73097800
H	-0.14355400	-0.31075600	-3.51555500
C	1.21172500	-0.44018800	-1.87816900
H	2.23674900	-0.51869700	-2.23891900
C	0.85838500	-1.07042300	-0.75006200
H	1.59563200	-1.64578000	-0.19375600
C	-0.54326200	-1.08389000	-0.15890200
H	-0.85036200	-2.13783500	-0.11241000
C	-0.51137100	-0.58056500	1.27584300
H	-0.17611100	0.44296800	1.43371500
C	-0.81357300	-1.33686600	2.33832200
H	-1.13982400	-2.36915500	2.23209100
C	-2.85817300	0.05464800	-0.31461300
H	-3.33704500	-0.81160700	0.15578500
H	-2.60106200	0.75277500	0.48404600
H	-3.58973700	0.54458700	-0.96712500
C	-2.05887600	-1.41673900	-2.14837400
C	-3.14556700	-1.00241200	-3.16474500
H	-3.22854700	0.08464200	-3.24370900
H	-4.10511100	-1.38417300	-2.79855600
C	-2.85197300	-1.54630000	-4.54760700
S	-4.13210900	-2.73063500	-5.16741500
C	-3.38701100	-3.14483100	-6.85055700
H	-2.46269400	-2.56878600	-6.93367800
H	-3.18164300	-4.21405700	-6.88241100
H	-4.09637700	-2.85872400	-7.62613200
O	-1.65209100	-2.58608400	-2.16723300
O	-1.86201600	-1.22319000	-5.20681800
C	1.95215500	3.86124000	-3.36392200

H	1.24126600	4.25969200	-4.10026200
H	2.25077800	4.68673400	-2.70614000
H	2.84289300	3.52450100	-3.90823000
H	-0.74226900	-0.95704500	3.35340000

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C	0.80759800	-0.69299500	-0.70980600
C	0.57878500	-1.93704800	0.29119800
H	-0.50384300	-2.13153800	0.34316100
C	1.24105300	-3.26062800	-0.16113200
H	0.86817100	-3.54766100	-1.14848400
H	2.32645900	-3.12143500	-0.24571100
C	0.95651200	-4.40565500	0.83131700
H	1.43787000	-5.32677600	0.47501400
H	-0.12648400	-4.60810500	0.85674500
C	1.43571900	-4.07881800	2.25979400
H	2.52803100	-3.93466800	2.22109400
C	0.78978100	-2.75716400	2.72400700
H	1.16553900	-2.48269900	3.71996600
H	-0.29376900	-2.91719200	2.83256400
C	1.02768300	-1.58034500	1.75383200
H	0.38811800	-0.74675600	2.08618400
C	2.45851000	-1.09197900	1.71788500
H	3.20312200	-1.54036700	2.37131000
C	2.76266100	-0.12008100	0.84691300
H	3.76619100	0.28591100	0.74894400
C	1.64720500	0.46619800	0.00851100
H	0.92720000	0.94443100	0.68658000
C	2.13725800	1.52776400	-0.95237100
H	3.03352000	1.28281800	-1.52359400
C	1.56019900	2.72378300	-1.12241300
H	0.66988000	3.01158400	-0.56936600
C	1.50834100	-1.10404300	-2.02387900
H	2.53086100	-1.43218600	-1.81573700
H	0.98832600	-1.91564200	-2.53547600
H	1.56853700	-0.25135400	-2.70814900
C	-0.60125600	-0.12502800	-0.96983700
C	-1.40325600	-0.54399800	-2.22623400
H	-0.77790800	-0.43458500	-3.11715600
H	-2.24967800	0.14185000	-2.28608100
C	-1.89890000	-1.97637600	-2.18620300
S	-3.64268200	-2.11880800	-1.56558500
C	-3.84510300	-3.99450900	-1.63573100

H	-4.04429800	-4.36056400	-0.62920900
H	-4.67231400	-4.22698600	-2.30525500
H	-2.90685900	-4.39980400	-2.02066500
O	-1.14644600	0.65701900	-0.17613400
O	-1.22912900	-2.95934300	-2.51550800
C	1.14119300	-5.22567900	3.24126700
H	1.61880600	-6.15802500	2.91621200
H	1.50766300	-4.99184300	4.24841500
H	0.06083300	-5.40948200	3.31252200
H	1.95729400	3.45681400	-1.81873000

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C	-1.53271000	2.07228000	-1.73019100
C	-2.81025200	1.22670400	-1.32928100
H	-3.11632600	1.69167300	-0.38226400
C	-2.57248400	-0.27568300	-0.99722300
H	-1.63197100	-0.40818300	-0.44760200
H	-3.36385400	-0.56971500	-0.29145600
C	-2.63713300	-1.25168500	-2.18850300
H	-2.57638300	-2.28074400	-1.80818500
H	-1.77460400	-1.12244300	-2.85751500
C	-3.93156400	-1.07539100	-3.01000800
H	-4.78349400	-1.28301200	-2.34011000
C	-4.04929200	0.38776300	-3.48302900
H	-4.99226900	0.52727400	-4.03136800
H	-3.24328500	0.59897500	-4.19755700
C	-4.00929000	1.40358200	-2.30678800
H	-4.90973500	1.18740900	-1.70375200
C	-4.13216200	2.82489700	-2.80068100
H	-5.01402400	3.05115800	-3.39917200
C	-3.24049100	3.79143500	-2.54342400
H	-3.40868500	4.79747100	-2.92365800
C	-1.97778100	3.59543900	-1.72469100
H	-2.19347700	3.83275000	-0.67331400
C	-0.87175300	4.52798700	-2.18267000
H	-0.70439900	4.58299600	-3.25862900
C	-0.11896900	5.27166700	-1.36178900
H	-0.25948600	5.25347300	-0.28398100
C	-0.91543600	1.70245300	-3.09454800
H	-1.58869500	1.99700600	-3.90301100
H	0.03345800	2.22534100	-3.25544700
H	-0.72949400	0.63057400	-3.19360000
C	-0.53702600	1.90898300	-0.56220900

C	0.83066500	1.25428900	-0.80124800
H	1.50985400	2.02662000	-1.18402300
H	0.75480500	0.47525000	-1.56488700
C	1.37432600	0.61711000	0.45757500
S	2.82563800	1.50860400	1.18487000
C	3.12604500	0.42504800	2.69984100
H	2.38765200	-0.37896200	2.65936400
H	4.13911600	0.02788100	2.64879000
H	2.98828300	1.03308900	3.59302800
O	-0.83194900	2.31427600	0.57314900
O	0.89766800	-0.40651900	0.94961400
C	-3.99853500	-2.05859900	-4.19061500
H	-3.16718200	-1.88846700	-4.88770400
H	-3.93773400	-3.09750300	-3.84447000
H	-4.93417400	-1.94330500	-4.75126500
H	0.66258900	5.92575600	-1.73736400

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C	-0.93399800	0.05749900	-0.79266100
C	0.62127200	0.23428300	-0.61266800
H	0.88800800	-0.48743800	0.16956200
C	1.02385800	1.63760100	-0.08164600
H	0.47453000	2.42912800	-0.60438200
H	0.74164900	1.72388300	0.97252000
C	2.53340800	1.88118200	-0.26097000
H	3.08735200	1.06916100	0.23082700
H	2.82874700	2.80639400	0.25008500
C	2.93318300	1.96247600	-1.76697200
H	3.93531100	1.51990900	-1.87379300
C	1.95430700	1.12856700	-2.63771700
H	2.44932500	0.83585600	-3.57379000
H	1.09332400	1.74616200	-2.92643000
C	1.46130800	-0.13251200	-1.88432200
H	2.37566300	-0.62758400	-1.51105400
C	0.79064100	-1.13388800	-2.78967600
H	1.32685800	-1.38740600	-3.70372200
C	-0.37253700	-1.73673400	-2.51429100
H	-0.78192600	-2.47756700	-3.19811100
C	-1.18369000	-1.44762300	-1.26482200
H	-0.81399500	-2.07429800	-0.43920900
C	-2.64679400	-1.78246100	-1.47513300
H	-3.11330600	-1.35639700	-2.36376800
C	-3.36840100	-2.57352600	-0.67047000

H	-2.93772500	-3.03227500	0.21654000
C	-1.54433500	1.04825700	-1.80491200
H	-1.12011500	0.87925800	-2.79748200
H	-2.62890800	0.92814200	-1.89244600
H	-1.34823400	2.08657300	-1.52821600
C	-1.58294600	0.14712600	0.60443700
C	-2.92236500	0.86034900	0.82036400
H	-3.25619400	0.58366300	1.82836200
H	-3.67075100	0.49353000	0.11122900
C	-2.84988800	2.37199100	0.77137900
S	-4.48875600	3.15394200	0.34834100
C	-4.01553400	4.97357200	0.51851200
H	-4.61823500	5.41774500	1.30967200
H	-2.95415100	4.99977000	0.77535500
H	-4.19701900	5.46805800	-0.43496200
O	-1.07409500	-0.44666600	1.56957400
O	-1.84456700	3.03755100	1.01887600
C	3.00609300	3.41711100	-2.26656200
H	3.25082100	3.45879100	-3.33550300
H	2.04435000	3.92799200	-2.12491300
H	3.77056400	3.98494800	-1.72288400
H	-4.41210300	-2.79709300	-0.87114900

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C	0.64882200	0.51494900	2.67521900
C	-0.03691800	1.85451500	2.42794200
H	-0.96023900	1.87804900	3.03725200
C	0.80173000	3.08549600	2.85497400
H	1.09824300	3.00062500	3.90694800
H	1.72943700	3.11003400	2.26386900
C	0.00905900	4.39196800	2.64912600
H	0.63382400	5.25516800	2.91619400
H	-0.85029800	4.40318500	3.33843700
C	-0.51318200	4.55681300	1.20399900
H	0.36382600	4.64717800	0.54122100
C	-1.29459400	3.29756200	0.76202400
H	-1.60330400	3.40164000	-0.28557200
H	-2.21928300	3.21653200	1.35634700
C	-0.45125900	2.02220300	0.94481000
H	0.46848200	2.12940300	0.34681000
C	-1.14081400	0.73661700	0.44984400
H	-2.00072400	0.50467700	1.09494200
C	-1.54976000	0.76167600	-0.98922800

H	-0.73540600	0.88029900	-1.70337500
C	-2.82043200	0.64896900	-1.42112300
H	-3.62065300	0.51165800	-0.69301300
C	-3.21924400	0.69421700	-2.82268100
H	-2.41609300	0.82084700	-3.54851600
C	-4.48896200	0.58756400	-3.25373900
H	-5.31784200	0.45950400	-2.56192900
C	1.34115100	0.33227300	4.00655500
H	2.25949300	0.92978000	4.08454100
H	0.68162200	0.65559600	4.82389100
H	1.59954700	-0.71006200	4.20625800
C	0.56512500	-0.46971500	1.75933200
C	1.21108100	-1.82681800	1.80598200
H	2.09789300	-1.82730900	2.45015700
H	1.54699100	-2.09094200	0.79769400
C	0.28429000	-2.92136200	2.31705000
S	0.74758800	-4.60893400	1.65679500
C	-0.50122300	-5.65958500	2.60375200
H	-1.10767000	-4.96901100	3.19443700
H	-1.11730100	-6.19675700	1.88359100
H	0.03885200	-6.35255900	3.24805500
O	-0.17703900	-0.38132100	0.56816800
O	-0.64022400	-2.75574900	3.10847900
C	-1.36135700	5.83065700	1.05062300
H	-2.25245200	5.78529900	1.69069400
H	-0.79076300	6.72342200	1.33412200
H	-1.69909000	5.96049600	0.01531400
H	-4.74092400	0.62225400	-4.30827600

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C	-0.06557400	0.63783100	1.29737900
C	0.74118000	0.01735700	0.15818900
H	1.29162900	0.82666600	-0.35854600
C	1.80632800	-1.00752600	0.62240700
H	2.48390900	-0.55086400	1.35298900
H	1.30416600	-1.84261500	1.13259800
C	2.62398000	-1.53404700	-0.57336000
H	3.35222100	-2.28097700	-0.22923300
H	3.20622800	-0.70390300	-1.00442800
C	1.73682700	-2.14406800	-1.68099900
H	1.23842800	-3.03179300	-1.25706700
C	0.62994500	-1.14852200	-2.09751500
H	-0.03332600	-1.62033300	-2.83297100

H	1.09161400	-0.28274400	-2.60058000
C	-0.18379900	-0.66014100	-0.88455300
H	-0.64976700	-1.53334200	-0.40082900
C	-1.32953400	0.29548200	-1.26584700
H	-0.90899800	1.22886100	-1.66958800
C	-2.33076700	-0.28413800	-2.21575800
H	-2.87448300	-1.15193900	-1.84404400
C	-2.57701000	0.19525700	-3.44998500
H	-2.03608300	1.07593500	-3.79845500
C	-3.53707100	-0.38592900	-4.38069200
H	-4.08432800	-1.25892100	-4.02548400
C	-3.77668000	0.08684100	-5.61703200
H	-3.25165200	0.95501500	-6.00791700
C	0.67758100	0.96203400	2.57248500
H	0.95854400	0.05356900	3.12082700
H	1.60766500	1.50507500	2.35393600
H	0.09380500	1.58139700	3.25797700
C	-1.38226200	0.87934400	1.13859700
C	-2.35295400	1.40141900	2.16189600
H	-3.08529300	2.04579100	1.66562100
H	-1.84927200	2.00955700	2.92207400
C	-3.09474100	0.29650000	2.90371200
S	-4.74225000	0.88183200	3.57260600
C	-5.26396000	-0.67650300	4.49971600
H	-5.34491300	-0.44466400	5.56117000
H	-6.22046800	-1.01144100	4.10011400
H	-4.48600000	-1.42253300	4.32150200
O	-2.09595900	0.63864400	-0.04848800
O	-2.67446900	-0.84064500	3.09675100
C	2.57196100	-2.59678900	-2.89062500
H	1.94036300	-3.05758200	-3.65981100
H	3.08940700	-1.74320400	-3.34837900
H	3.33230100	-3.32987400	-2.59492100
H	-4.50347400	-0.37536500	-6.27644400

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C	-2.74334600	1.71395100	0.75044100
C	-1.48758600	1.45168300	1.57514100
H	-1.59315300	0.45178900	2.03856300
C	-1.26594400	2.44926200	2.74003700
H	-1.13646100	3.46115200	2.33049000
H	-2.15013000	2.48398400	3.38712600
C	-0.03866000	2.03915000	3.58121500

H	-0.26065600	1.07905700	4.07111000
H	0.12578600	2.76910200	4.38528700
C	1.25747900	1.88254000	2.74536700
H	2.00246900	1.37985700	3.38018000
C	1.00121200	0.96545700	1.52016300
H	0.82397500	-0.06341300	1.87065700
H	1.89816200	0.93069100	0.88955000
C	-0.21522300	1.42359500	0.69227500
H	-0.03351800	2.44545300	0.32604800
C	-0.46873200	0.56022300	-0.55830200
H	-0.78098700	-0.44991000	-0.25642300
C	0.67862300	0.49398600	-1.51603100
H	0.99329500	1.44929000	-1.93508200
C	1.30930100	-0.64253700	-1.86877600
H	0.96815200	-1.59196800	-1.45472100
C	2.43912900	-0.70476100	-2.78793300
H	2.77053400	0.24395200	-3.20982000
C	3.07283700	-1.83957900	-3.13439600
H	2.77212000	-2.80566800	-2.73652300
C	-4.01158900	2.06199500	1.49753800
H	-3.97086900	3.07172400	1.92871500
H	-4.90198000	1.99780200	0.86877700
H	-4.16290900	1.36757600	2.33585900
C	-2.71116900	1.58584800	-0.59161000
C	-3.84695300	1.84636600	-1.55890400
H	-3.40269600	2.04654300	-2.53839600
H	-4.44014200	2.71280500	-1.25651900
C	-4.80133600	0.66708600	-1.66213600
S	-4.12474600	-0.77161800	-2.63467000
C	-5.59124500	-1.95064400	-2.47828000
H	-5.96396600	-2.17559000	-3.47708900
H	-5.25774900	-2.85788400	-1.97538800
H	-6.35083500	-1.43484300	-1.88670800
O	-1.58719600	1.16442300	-1.32141800
O	-5.91890800	0.64537600	-1.14185100
C	1.85803700	3.24476300	2.33953500
H	2.78715300	3.10727200	1.77310400
H	1.17400300	3.83223500	1.71689700
H	2.09124200	3.84347800	3.22833000
H	3.90817500	-1.84105000	-3.82642500

G2.gif

0 1

C	-4.30850000	0.00080000	0.09750000
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C	-4.17370000	1.46060000	-0.32730000
H	-3.93200000	2.05040000	0.57770000
C	-5.46800000	2.07680000	-0.91570000
H	-5.74760000	1.53030000	-1.82760000
H	-6.30150000	1.96110000	-0.21310000
C	-5.27030000	3.57760000	-1.21710000
H	-5.11840000	4.10470000	-0.26320000
H	-6.18430000	3.99350000	-1.66210000
C	-4.06090000	3.86710000	-2.14220000
H	-3.87520000	4.95130000	-2.11490000
C	-2.78890000	3.16620000	-1.59730000
H	-2.48770000	3.64770000	-0.65390000
H	-1.95800000	3.30670000	-2.29940000
C	-3.01700000	1.66410000	-1.33750000
H	-3.30150000	1.17800000	-2.28310000
C	-1.76100000	0.92440000	-0.83880000
H	-1.49910000	1.27380000	0.17040000
C	-0.57920000	1.01170000	-1.75200000
H	-0.72450000	0.59050000	-2.74620000
C	0.60250000	1.56240000	-1.41360000
H	0.73560000	1.96120000	-0.40730000
C	1.74810000	1.66660000	-2.30900000
H	1.61620000	1.25790000	-3.31070000
C	2.92600000	2.22170000	-1.97130000
H	3.09750000	2.63920000	-0.98210000
C	-5.56800000	-0.37600000	0.84410000
H	-5.75400000	0.33620000	1.66010000
H	-6.45380000	-0.35380000	0.19550000
H	-5.51330000	-1.36790000	1.29800000
C	-3.30350000	-0.86830000	-0.13790000
C	-3.26400000	-2.34300000	0.14370000
H	-2.96010000	-2.87440000	-0.76560000
H	-4.24960000	-2.72190000	0.43300000
C	-2.27590000	-2.76680000	1.22220000
S	-2.19010000	-1.60580000	2.68810000
C	-0.99040000	-2.59220000	3.76090000
H	-0.70300000	-3.47480000	3.18500000
H	-0.12290000	-1.96800000	3.97230000
H	-1.49720000	-2.87820000	4.68220000
O	-2.08400000	-0.51750000	-0.74350000
O	-1.63040000	-3.81140000	1.17550000
C	-4.34850000	3.49640000	-3.61210000
H	-3.48960000	3.73780000	-4.25000000
H	-4.56490000	2.42940000	-3.73760000

H	-5.21400000	4.05500000	-3.98860000
H	3.75540000	2.27460000	-2.66830000

H1.gif

0 1

C	2.38264500	0.01223300	0.02384200
C	2.54977500	0.61250200	-1.36525400
H	3.38067300	1.33665400	-1.31788800
C	2.94751700	-0.46018300	-2.41963600
H	3.89243200	-0.93039000	-2.12053800
H	2.19449700	-1.26031600	-2.42151800
C	3.07918600	0.13238500	-3.83355500
H	3.33930300	-0.65948900	-4.54922900
H	3.90694200	0.85951500	-3.85450000
C	1.78389000	0.84240700	-4.28086500
H	0.98043300	0.08866800	-4.31339600
C	1.39991700	1.92410900	-3.24635000
H	0.45958500	2.40631300	-3.54178100
H	2.17447500	2.70622600	-3.26898200
C	1.28571200	1.40665000	-1.79397500
H	1.19887100	2.28065200	-1.13114200
C	0.02087900	0.55662600	-1.52923000
H	0.07101900	-0.39427300	-2.07466700
C	-1.26521300	1.26260700	-1.82700000
H	-1.43707900	2.17718100	-1.25994200
C	-2.18024200	0.83618200	-2.71857500
H	-2.00192900	-0.09144800	-3.26362400
C	-3.42528100	1.53397600	-3.01616100
H	-3.60583500	2.45499500	-2.46204300
C	-4.33739700	1.11057300	-3.90955800
H	-4.19508300	0.19697400	-4.48152800
C	3.64897400	-0.42889600	0.71894300
H	3.48596100	-0.74040000	1.75388300
H	4.11166600	-1.28057300	0.20198000
H	4.39119000	0.38156100	0.72667600
C	1.15655200	-0.12349100	0.56455600
C	0.80384000	-0.66447600	1.92153100
H	-0.05712000	-0.10996700	2.31001400
H	1.62289700	-0.52859500	2.63711500
C	0.46041700	-2.14809800	1.90927800
S	-0.54225600	-2.65170400	3.40844500
C	-0.64561000	-4.50944200	3.09333100
H	-0.15789200	-5.03274100	3.91505400
H	-1.69579600	-4.78979300	3.02118200

H	-0.12837600	-4.69648700	2.14943300
O	-0.03840100	0.23044900	-0.08562600
O	0.81611800	-2.95629100	1.05630300
C	1.92159100	1.44781600	-5.68825700
H	2.71181100	2.21030100	-5.70719100
H	2.18006900	0.67902700	-6.42656100
H	0.98779400	1.92491700	-6.00951400
H	-5.25411900	1.65955400	-4.09648200

H2.gif

0 1

C	0.25839800	0.35654000	-0.00722000
C	1.11077300	-0.67947100	-0.74851000
H	1.44126200	-0.21048800	-1.69033400
C	2.41744900	-1.12512000	-0.02430500
H	3.13511000	-1.42412300	-0.79920800
H	2.86623200	-0.26327500	0.47964100
C	2.23556700	-2.29828600	0.97931000
H	2.85089800	-2.12638800	1.87237300
H	2.60380600	-3.23346400	0.53033100
C	0.76586600	-2.50946200	1.38785600
H	0.38826700	-1.58318100	1.84079000
C	-0.08602200	-2.80550300	0.13034100
H	-1.14362300	-2.67621600	0.39019800
H	0.04873100	-3.86172600	-0.14622000
C	0.25589600	-1.92049500	-1.11113300
H	0.82573900	-2.51693700	-1.83567700
C	-1.04467200	-1.47238900	-1.81179000
H	-1.70344100	-2.33608400	-1.94642500
C	-0.85623900	-0.76752900	-3.12391000
H	-0.39341100	0.21750500	-3.08395300
C	-1.22660600	-1.28519100	-4.31149000
H	-1.70658300	-2.26464400	-4.33891900
C	-1.03200600	-0.62481500	-5.59626600
H	-0.56135800	0.35793900	-5.56688100
C	-1.39402900	-1.14790400	-6.78165800
H	-1.86588300	-2.12468700	-6.85472800
C	0.97802400	1.40608100	0.80798600
H	1.82123700	1.82745100	0.24391900
H	0.32996400	2.23889400	1.09253400
H	1.38975200	0.99045800	1.73720900
C	-1.08629600	0.33268900	-0.12127600
C	-2.08046600	1.21110200	0.58734800
H	-2.96535000	1.33228100	-0.04495100

H	-1.67761300	2.21367000	0.77312400
C	-2.51432500	0.65319400	1.93714000
S	-4.17006700	1.33074400	2.48082200
C	-4.28374100	0.52860400	4.18532900
H	-3.39364500	-0.09438800	4.29853200
H	-4.30947200	1.31216300	4.94181500
H	-5.18813100	-0.07755800	4.22131000
O	-1.80883900	-0.59957800	-0.89069500
O	-1.86256600	-0.12123300	2.63414000
C	0.61756000	-3.63214100	2.42830800
H	1.17441200	-3.39835400	3.34394100
H	-0.43400500	-3.77716100	2.70339300
H	0.99905200	-4.58476900	2.03559900
H	-1.23261100	-0.61876200	-7.71473800

II.gjf

0 1

C	-0.10592400	-1.29836900	1.26796900
C	0.62888000	-1.56855700	-0.04800400
H	0.40966000	-2.61164500	-0.33380900
C	2.17339000	-1.46255400	0.05178700
H	2.54489200	-2.08853900	0.87083300
H	2.59651600	-1.88329900	-0.87241200
C	2.66948400	-0.01506500	0.20924000
H	3.76686700	0.00048600	0.25937600
H	2.30306200	0.40775300	1.15737200
C	2.18456800	0.87284600	-0.95627400
H	2.61044600	0.46084700	-1.88712900
C	0.64691200	0.80050700	-1.06245200
H	0.30776900	1.38027200	-1.93329200
H	0.20494000	1.27858300	-0.17796300
C	0.10962700	-0.64536700	-1.18355300
H	0.44774500	-1.06280400	-2.14277200
C	-1.43431400	-0.64802100	-1.19683000
H	-1.79643300	0.10946200	-1.89901500
C	-2.06131200	-1.97678700	-1.50681200
H	-1.99894500	-2.73452400	-0.72806000
C	-2.68440100	-2.25517600	-2.66858800
H	-2.76444000	-1.47982100	-3.43233600
C	-3.27556200	-3.54712900	-2.99469800
H	-3.20625700	-4.31542300	-2.22476300
C	-3.88517300	-3.83143400	-4.15979700
H	-3.97497000	-3.09263700	-4.95243200
C	0.50772600	-1.88213700	2.52109200

H	1.43840200	-1.37034000	2.80014500
H	-0.16380400	-1.84490500	3.38138300
H	0.76173100	-2.93964600	2.36446500
C	-1.28849500	-0.64594400	1.26869100
C	-2.13326500	-0.25567900	2.45000000
H	-2.39652500	0.80448200	2.36412600
H	-1.58866100	-0.38869600	3.39012900
C	-3.45427800	-1.00328200	2.57265100
S	-3.31385200	-2.85280600	2.30935500
C	-5.10349800	-3.33003300	2.67157500
H	-5.63898100	-2.40277400	2.88752900
H	-5.51641200	-3.81910800	1.79002800
H	-5.12053500	-3.99847000	3.53187000
O	-1.92733500	-0.16156500	0.11323300
O	-4.51514400	-0.46602900	2.88020600
C	2.66841100	2.32549400	-0.81006000
H	2.27127800	2.77672700	0.10873500
H	3.76306400	2.37585500	-0.76272200
H	2.33836400	2.94192900	-1.65515800
H	-4.31421700	-4.80767800	-4.35885900

I2.gjf

0 1

C	-1.13290000	0.89870000	1.39430000
C	-1.83920000	1.14430000	0.06660000
H	-2.16120000	2.19920000	0.08910000
C	-3.12350000	0.29590000	-0.12870000
H	-2.82990000	-0.75120000	-0.28380000
H	-3.73590000	0.30790000	0.77950000
C	-3.95540000	0.80900000	-1.33250000
H	-4.70060000	1.54130000	-0.99280000
H	-4.51990000	-0.02950000	-1.76420000
C	-3.07750000	1.45440000	-2.44140000
H	-2.91230000	2.51180000	-2.18070000
C	-1.69990000	0.76340000	-2.47920000
H	-1.11280000	1.12280000	-3.33260000
H	-1.85490000	-0.31330000	-2.65120000
C	-0.89770000	0.97830000	-1.16620000
H	-0.29730000	1.89440000	-1.25960000
C	0.09300000	-0.18150000	-0.93220000
H	-0.46930000	-1.11460000	-0.77930000
C	1.10550000	-0.34680000	-2.02230000
H	1.76150000	0.50820000	-2.18310000
C	1.23810000	-1.45460000	-2.77630000

H	0.58680000	-2.30870000	-2.58810000
C	2.21330000	-1.60700000	-3.84930000
H	2.86960000	-0.75570000	-4.02890000
C	2.34380000	-2.71310000	-4.60360000
H	1.70930000	-3.58350000	-4.45490000
C	-1.92880000	1.25350000	2.63050000
H	-2.71400000	0.51290000	2.83180000
H	-1.31630000	1.31870000	3.53320000
H	-2.42820000	2.22320000	2.50000000
C	0.13280000	0.43470000	1.43830000
C	1.01700000	0.24440000	2.63650000
H	0.60190000	0.73100000	3.52540000
H	1.99420000	0.69880000	2.43640000
C	1.30260000	-1.20420000	3.01100000
S	-0.13650000	-2.37240000	2.75410000
C	0.64280000	-3.93920000	3.46240000
H	0.64990000	-4.70380000	2.68640000
H	1.66100000	-3.67930000	3.76060000
H	0.05690000	-4.26360000	4.32200000
O	0.86650000	0.07140000	0.29770000
O	2.36750000	-1.57500000	3.49970000
C	-3.78110000	1.41670000	-3.80820000
H	-3.19540000	1.93990000	-4.57370000
H	-3.92420000	0.38080000	-4.14320000
H	-4.76930000	1.89050000	-3.75740000
H	3.08770000	-2.78640000	-5.38970000

TSA7/B2.gjf

0 1

C	-0.99050700	-1.20170900	-0.25688700
C	-0.05003500	-1.56669200	0.75455700
H	-0.46736800	-1.44675100	1.75478300
C	0.80416400	-2.82129500	0.58299600
H	0.13430600	-3.66986800	0.38097100
H	1.45298600	-2.73341400	-0.30038600
C	1.66291400	-3.13916100	1.81863400
H	2.17512800	-4.09935100	1.66873600
H	1.00573900	-3.26857600	2.69243900
C	2.70730700	-2.04948400	2.13437300
H	3.39646100	-1.98781000	1.27465300
C	2.04487000	-0.66578200	2.29754500
H	2.82596300	0.06823900	2.54601700
H	1.35735600	-0.68633800	3.15659000
C	1.29232600	-0.17563700	1.05809300

H	1.83307700	-0.36434400	0.12798600
C	0.64904200	1.08557600	1.13573700
H	0.45637600	1.50440300	2.11899400
C	0.16093700	1.79078400	0.01875000
H	-0.37377200	2.71883700	0.21021200
C	0.17781800	1.30814600	-1.27534200
H	0.76135000	0.42520100	-1.51736200
C	-0.47943900	1.96650800	-2.38236500
H	-1.03662900	2.87315600	-2.14500200
C	-0.45862300	1.52516900	-3.66055400
H	0.08934300	0.63110700	-3.94646700
C	-0.97971200	-1.82609000	-1.62922600
H	0.03161000	-2.12245900	-1.92785300
H	-1.61063600	-2.72446100	-1.65624100
H	-1.36462300	-1.14939200	-2.40020600
C	-2.00808200	-0.27920600	0.17628900
C	-3.17313000	0.12502400	-0.73694500
H	-2.82369100	0.31052500	-1.76145800
H	-3.58796200	1.05577700	-0.34458900
C	-4.25839700	-0.92852000	-0.81228500
S	-5.97514500	-0.20475000	-0.68847600
C	-6.99024200	-1.78353100	-0.87699000
H	-7.60949300	-1.90429900	0.01118300
H	-7.60528300	-1.70206400	-1.77261100
H	-6.27627100	-2.60555700	-0.96725500
O	-1.95227500	0.24635900	1.33473500
O	-4.06687500	-2.13718700	-0.95501000
C	3.53384100	-2.41431100	3.38051100
H	2.89086700	-2.48595200	4.26752400
H	4.03596500	-3.38054200	3.25223700
H	4.30244000	-1.65880500	3.58332400
H	-0.97700500	2.05052700	-4.45535100

TSA8/C2.gjf

0 1

C	-2.79862900	-0.72274300	-0.96139800
C	-3.18358500	-2.06683700	-0.66392800
H	-2.70872200	-2.77982500	-1.33868300
C	-4.64086400	-2.39570100	-0.34353600
H	-4.97131500	-1.87017500	0.56267000
H	-5.27174800	-2.00968300	-1.15806600
C	-4.89239300	-3.90877000	-0.19918100
H	-4.59620400	-4.40045900	-1.13729300
H	-5.96893900	-4.08987300	-0.07743000

C	-4.12786900	-4.56741200	0.97299000
H	-4.24448100	-5.65623800	0.86390200
C	-2.61076000	-4.27412300	0.88847700
H	-2.19980100	-4.73741300	-0.01998000
H	-2.11354200	-4.76748000	1.73693000
C	-2.23497000	-2.79076700	0.89435700
H	-2.79233100	-2.19935000	1.62164400
C	-0.86107800	-2.45973500	0.77875100
H	-0.17958100	-3.21801100	0.40392600
C	-0.34260100	-1.17000500	1.00169300
H	0.70320900	-0.99909800	0.76158900
C	-1.11986400	-0.07428000	1.32747500
H	-2.14834900	-0.21642500	1.64806900
C	-0.61860800	1.28180600	1.36385900
H	0.40308800	1.42889500	1.01876800
C	-1.35190300	2.35010400	1.75229100
H	-2.37750900	2.24564500	2.09816000
C	-3.70537600	0.45709600	-0.70866600
H	-4.41124700	0.25310800	0.10293400
H	-3.15429300	1.36479700	-0.43821700
H	-4.31082000	0.70135900	-1.59611900
C	-1.53532700	-0.60025100	-1.64453300
C	-1.04560800	0.77447300	-2.13141600
H	-1.27556200	1.54951400	-1.39274900
H	-1.56661500	1.03259600	-3.06153500
C	0.45019900	0.78139800	-2.34563700
S	0.94221400	0.75491100	-4.13647900
C	2.81687700	0.70078800	-3.94260800
H	3.24737500	1.55965300	-4.45646000
H	3.01926800	0.74484500	-2.86998600
H	3.18384200	-0.23284500	-4.36745100
O	-0.80868800	-1.62411100	-1.84927000
O	1.27717100	0.81103900	-1.43216500
C	-4.72247800	-4.19161200	2.34708200
H	-4.67291800	-3.11473700	2.54527300
H	-5.77676400	-4.48780600	2.40516700
H	-4.18494100	-4.70076000	3.15612100
H	-0.94196000	3.35449900	1.75165500

TSA6/D2.gjf

0 1

C	0.19948100	-1.85301300	-0.62654900
C	0.46199100	-2.64266000	0.54446700
H	-0.43506400	-2.74311200	1.16155300

C	1.23849900	-3.95287600	0.39909700
H	0.72307500	-4.58149700	-0.34207200
H	2.24019600	-3.76020100	-0.00644600
C	1.35238800	-4.73215200	1.72209400
H	1.87254200	-5.68255500	1.54066300
H	0.34205700	-4.99140600	2.07611400
C	2.08174600	-3.95333600	2.83657600
H	3.11443600	-3.76791200	2.49887200
C	1.39493500	-2.59058000	3.08358000
H	1.89497900	-2.07448100	3.91572400
H	0.36269300	-2.77573000	3.41255400
C	1.36256000	-1.65362500	1.87026100
H	0.57450000	-0.90115600	1.94922900
C	2.59768200	-1.18628200	1.33999000
H	3.50704100	-1.73353800	1.57924600
C	2.69769700	-0.13966500	0.41216600
H	3.66893000	0.03401400	-0.05045900
C	1.63510300	0.65576600	-0.00233200
H	0.69813100	0.63780400	0.54375800
C	1.77105500	1.65155200	-1.04036500
H	2.71850600	1.66626000	-1.57972200
C	0.81523800	2.55028300	-1.37187000
H	-0.13812300	2.58579000	-0.85159900
C	1.00722300	-2.08233000	-1.87516200
H	2.08070200	-2.06182500	-1.64018600
H	0.79943000	-3.06927100	-2.31410700
H	0.81258400	-1.34599300	-2.65461700
C	-0.91532800	-0.93472000	-0.54090400
C	-1.44931300	-0.21672200	-1.79963700
H	-0.63823800	0.30365500	-2.32118800
H	-2.17230400	0.51798100	-1.44021400
C	-2.11432200	-1.15776300	-2.78015700
S	-3.93306500	-1.38980900	-2.43760100
C	-4.34278000	-2.63046800	-3.79888500
H	-4.69585400	-3.55216200	-3.33740000
H	-5.10947200	-2.19993600	-4.44221700
H	-3.41895600	-2.80247600	-4.35600800
O	-1.48448400	-0.67604300	0.56436400
O	-1.54084000	-1.73663600	-3.70544500
C	2.15179200	-4.77389300	4.13696400
H	2.65058200	-5.73609400	3.97079600
H	2.70428500	-4.23663100	4.91710900
H	1.14421100	-4.98019600	4.52118400
H	0.96887000	3.28364500	-2.15622800

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C	-1.13627700	1.19652900	-0.91926600
C	0.25211800	1.52045900	-1.14341200
H	0.74610300	1.71910900	-0.19004100
C	0.60425200	2.55227100	-2.21878100
H	-0.00514400	2.39861800	-3.11468800
H	0.31483300	3.53553000	-1.81776800
C	2.10420200	2.58533800	-2.61441900
H	2.39964400	3.61815600	-2.83878800
H	2.26091100	2.01435700	-3.54211500
C	3.02361000	1.99432900	-1.52949600
H	2.77704400	2.46711100	-0.56692600
C	2.77085600	0.46690700	-1.42204200
H	3.24824200	0.08794100	-0.50942800
H	3.29272700	-0.00786200	-2.26559200
C	1.29682200	0.00764800	-1.44363300
H	0.99202100	-0.46872800	-0.50874500
C	0.82189200	-0.62629400	-2.63043800
H	1.37823000	-0.46897600	-3.55312100
C	-0.39363500	-1.31501500	-2.70774600
H	-0.75368600	-1.60285200	-3.69503300
C	-1.20061300	-1.61016700	-1.61207600
H	-0.79938000	-1.52604800	-0.60798900
C	-2.50061600	-2.22606400	-1.75345100
H	-2.89002500	-2.31051800	-2.76826100
C	-3.24386100	-2.69858400	-0.72644100
H	-2.89154400	-2.65374600	0.30053600
C	-2.17829900	1.55328900	-1.94764000
H	-1.87510400	1.19857700	-2.94141700
H	-3.15884000	1.13359700	-1.72254000
H	-2.31396900	2.64200500	-2.02567100
C	-1.45286400	0.65860700	0.38489900
C	-2.91786000	0.51088400	0.84981600
H	-2.88087300	-0.06620400	1.77585700
H	-3.50907400	-0.03620200	0.10709700
C	-3.59421900	1.84166100	1.09920500
S	-3.32331900	2.47724500	2.83184400
C	-4.25391200	4.11374000	2.70396100
H	-3.55211000	4.92979100	2.87329900
H	-4.67029100	4.16092300	1.69511200
H	-5.04624200	4.12155200	3.45176300
O	-0.54521700	0.27393800	1.18684500

O	-4.24760900	2.46963900	0.26328900
C	4.50834100	2.27321400	-1.81942100
H	5.15415700	1.81708300	-1.05935800
H	4.79897800	1.86337600	-2.79590000
H	4.71199600	3.35043700	-1.83281100
H	-4.21239400	-3.15959800	-0.88806900

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C	-0.10822500	0.28641100	1.07096200
C	0.95118600	-0.06167100	0.18286900
H	1.28599600	0.77696900	-0.42786000
C	2.05925500	-0.98964300	0.65808700
H	2.50278000	-0.55853400	1.56918400
H	1.63860300	-1.95943600	0.96019600
C	3.16976800	-1.20740700	-0.38119900
H	3.96757700	-1.82049800	0.05976400
H	3.62421800	-0.23698700	-0.63532400
C	2.66654500	-1.87619900	-1.67490900
H	2.27233600	-2.87137700	-1.40736600
C	1.51299700	-1.07437300	-2.31160500
H	1.24676800	-1.55419900	-3.26535600
H	1.86715600	-0.06371600	-2.56752600
C	0.24577200	-0.96433300	-1.45262500
H	-0.04375900	-1.90002600	-0.96774100
C	-0.83203100	-0.22625700	-2.00247700
H	-0.61734900	0.50493900	-2.77661800
C	-2.20407200	-0.57329200	-1.78097000
H	-2.41319600	-1.28408800	-0.98430900
C	-3.25073700	-0.07302400	-2.49962900
H	-3.05274200	0.64606500	-3.29477400
C	-4.63097900	-0.44080000	-2.27251600
H	-4.81576700	-1.12795000	-1.44755600
C	-5.67243400	0.01930200	-2.99828000
H	-5.53044400	0.70926600	-3.82634300
C	-0.33175200	-0.44216200	2.37267600
H	-0.82557200	-1.41462300	2.22576400
H	0.61212200	-0.63417700	2.89585400
H	-0.96818800	0.13136100	3.05434700
C	-1.01437500	1.24690400	0.56306000
C	-2.22292500	1.74954600	1.35275200
H	-2.71823400	2.49642500	0.71959300
H	-1.90621900	2.26841700	2.26670900
C	-3.26023300	0.71054100	1.72492200

S	-4.42483500	1.32680900	3.05952900
C	-5.58526000	-0.15694600	3.17071300
H	-5.59140300	-0.51323200	4.20023200
H	-6.58250200	0.15236800	2.85965500
H	-5.18720800	-0.91935800	2.49724200
O	-0.85815300	1.69954100	-0.63672800
O	-3.38091600	-0.40948700	1.22975800
C	3.81485100	-2.07402900	-2.68123700
H	3.46715500	-2.58986400	-3.58433800
H	4.23530200	-1.10719600	-2.98793000
H	4.62598100	-2.66830600	-2.24401400
H	-6.69386000	-0.27767300	-2.78564300

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C	-4.04927300	0.09042900	-0.42829200
C	-4.33431500	1.49302000	-0.48721700
H	-4.09830600	1.99468100	0.45277700
C	-5.62601700	1.97253500	-1.13934100
H	-5.64818200	1.69172300	-2.20131400
H	-6.46789600	1.43821600	-0.67309100
C	-5.85007200	3.48657800	-0.97446800
H	-5.90087600	3.71343300	0.10053100
H	-6.82413300	3.76409300	-1.39954900
C	-4.74325800	4.35571800	-1.61526900
H	-4.90054800	5.38850700	-1.26885200
C	-3.33856200	3.93478700	-1.11977300
H	-3.26873600	4.09891800	-0.03459200
H	-2.59635900	4.60342900	-1.57993200
C	-2.94839400	2.48064900	-1.42345100
H	-3.19260400	2.16150200	-2.43989300
C	-1.66715500	2.04168300	-0.99113900
H	-1.17225300	2.55445700	-0.17411600
C	-0.92309000	1.07030800	-1.73696000
H	-1.36576700	0.72927100	-2.67401600
C	0.28274200	0.54785000	-1.36434900
H	0.70546000	0.83148700	-0.40263400
C	1.02995800	-0.39952600	-2.15966800
H	0.60966600	-0.66136000	-3.13100700
C	2.18941300	-0.96712400	-1.76513600
H	2.62864900	-0.74358600	-0.79723300
C	-4.78749000	-0.90553800	-1.28642300
H	-4.50292800	-1.93651900	-1.05907200
H	-5.87543900	-0.83067300	-1.15503100

H	-4.59361800	-0.74902100	-2.36006700
C	-2.91776600	-0.23512500	0.35199000
C	-2.41777300	-1.68399700	0.49767200
H	-2.02123900	-2.03803600	-0.46241800
H	-3.24263900	-2.34325400	0.78726000
C	-1.29885800	-1.78123600	1.50733400
S	-1.90324100	-2.22831500	3.21868300
C	-0.26621800	-2.13782400	4.14892300
H	0.50064900	-1.91250400	3.40393700
H	-0.32859000	-1.34406500	4.89258300
H	-0.07822100	-3.10142600	4.62147000
O	-2.21992800	0.71408400	0.88223700
O	-0.10987700	-1.59661400	1.25751900
C	-4.83924500	4.38323800	-3.15575300
H	-4.05669800	5.02119900	-3.58417000
H	-4.73340600	3.38679900	-3.59979000
H	-5.80989200	4.78270300	-3.47345600
H	2.71931800	-1.67955700	-2.38844300

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C	0.54150800	0.60332900	0.42605300
C	1.37257000	-0.19705300	-0.42003900
H	1.34436100	0.14183900	-1.45339500
C	2.73673900	-0.72401400	0.04140000
H	3.44053700	-0.65221600	-0.79726400
H	3.12629800	-0.05646500	0.82020500
C	2.76106900	-2.17996200	0.58870700
H	3.63408700	-2.29355300	1.24463400
H	2.90790500	-2.89279900	-0.23549900
C	1.48139000	-2.56324800	1.36078700
H	1.31738100	-1.79390900	2.12630100
C	0.23449800	-2.59652700	0.42369100
H	-0.64148800	-2.20156600	0.95167000
H	0.00883500	-3.64881700	0.18716600
C	0.39577600	-1.85807300	-0.90456700
H	1.21400000	-2.24035300	-1.51964800
C	-0.75079200	-1.52457000	-1.66564400
H	-1.71407400	-1.46559400	-1.16875200
C	-0.73774600	-1.49858000	-3.09977600
H	0.22646500	-1.64799700	-3.58770300
C	-1.83881300	-1.30641900	-3.87867300
H	-2.80146000	-1.13917400	-3.39670800
C	-1.81934000	-1.30510300	-5.32534800

H	-0.84881800	-1.46160900	-5.79674900
C	-2.90636500	-1.12223400	-6.10398200
H	-3.89260300	-0.96078300	-5.67646100
C	0.76475800	0.79571600	1.90882200
H	1.79264500	0.57042200	2.20371100
H	0.57330200	1.83478300	2.20635100
H	0.10418100	0.16307300	2.51843200
C	-0.64286200	1.07444900	-0.19175900
C	-1.73123100	1.81121100	0.58395800
H	-2.29244300	2.43367800	-0.12051200
H	-1.31528300	2.47783400	1.34966400
C	-2.70139200	0.86949800	1.27396500
S	-4.27282400	1.72652500	1.81102100
C	-5.14906500	0.27843400	2.64740000
H	-4.49691700	-0.59070000	2.53655000
H	-5.29958900	0.52033500	3.69889700
H	-6.10183600	0.11489500	2.14517100
O	-0.90416500	0.77887800	-1.42045500
O	-2.50856500	-0.32884500	1.48668000
C	1.64976600	-3.90859100	2.09195700
H	2.46257500	-3.86441700	2.82703100
H	0.73074700	-4.18688700	2.62203400
H	1.88135500	-4.71247200	1.38043900
H	-2.84207700	-1.12437200	-7.18676200

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C	-1.50874700	0.84149800	1.09736500
C	-1.45191000	1.61600400	-0.10631400
H	-0.45565500	1.99515400	-0.32891800
C	-2.60161200	2.58194300	-0.41312200
H	-3.48248600	2.31699500	0.18022500
H	-2.29796300	3.58343300	-0.07289600
C	-3.02703000	2.66383000	-1.89187500
H	-2.16969300	2.97564900	-2.50204600
H	-3.78018100	3.45457400	-2.00553600
C	-3.60800200	1.32653500	-2.43189700
H	-3.48471200	1.34023700	-3.52565900
C	-2.82251100	0.09779500	-1.88961200
H	-2.95876400	-0.74070700	-2.58683500
H	-3.24814300	-0.23178800	-0.93167600
C	-1.33577800	0.42145000	-1.71743400
H	-0.99084500	1.18048400	-2.42279800
C	-0.36822900	-0.59484200	-1.52279000

H	-0.66395700	-1.52280700	-1.03875200
C	0.89651600	-0.59572900	-2.20177700
H	1.17059700	0.31517900	-2.73433900
C	1.74923200	-1.65758100	-2.22887000
H	1.47947000	-2.56133800	-1.68321300
C	3.00933400	-1.66948600	-2.93964700
H	3.27942500	-0.75311700	-3.46462200
C	3.84998100	-2.72436700	-2.98308700
H	3.61969200	-3.65733700	-2.47469700
C	-2.74422100	0.78177200	1.97057500
H	-3.60820700	0.33767700	1.45419400
H	-2.57299900	0.18447800	2.86929600
H	-3.05614500	1.77898700	2.30670400
C	-0.38579500	0.02015600	1.34375900
C	-0.32742200	-0.93051400	2.55415000
H	-1.16948700	-1.63230000	2.53691400
H	-0.39370600	-0.34960000	3.48232100
C	0.97541000	-1.69499700	2.59638800
S	0.86901800	-3.36974800	1.76756300
C	2.66786800	-3.90489500	1.94922700
H	3.11357700	-3.98830200	0.95855900
H	3.16474300	-3.12419300	2.53031200
H	2.69689300	-4.85951400	2.47342000
O	0.57436600	-0.02918400	0.48373000
O	2.00500200	-1.29084400	3.12775900
C	-5.11269400	1.18389000	-2.13516700
H	-5.49660900	0.22375400	-2.50150900
H	-5.31005900	1.22873900	-1.05609800
H	-5.68949300	1.98247200	-2.61633600
H	4.78994500	-2.68648900	-3.52294000

IX. References

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