

Supporting Information

DFT Study on the Mechanism and Stereochemistry of the Petasis-Ferrier Rearrangements

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1. Computational Methods

All DFT calculations were carried out with the Gaussian 03 program package.¹ The geometry optimizations of all the minima and transition states were performed at the B3LYP² level of theory with the 6-31G(d)³ basis set. The vibrational frequencies were computed at the same level of theory to check whether every optimized structure is an energy minimum or a transition state and to evaluate its zero-point vibration energy (ZPE). IRC calculations⁴ were carried out to confirm that each transition state is connected with its corresponding reactant and product. Solvent effects were computed with the CPCM⁵ model and UAHF radii in toluene for five-membered substrates and in dichloromethane (DCM) for six-membered ones using the gas phase optimized structures. ΔG_{sol} and ΔG_{gas} reported in this paper are relative Gibbs free energies calculated at 298K in solution and in the gas phase, respectively. ΔE_0 is the zero-point vibration energy (ZPE)-corrected electronic energy in the gas phase. All discussed energies in the paper and the Supporting Information are Gibbs free energies in solution (ΔG_{sol}) unless specified. Computed structures are illustrated using CYLVIEW drawings.⁶ We point out here that, using bigger basis set of 6-311+G(d,p) at the B3LYP level gave very close activation energies as those from B3LYP/6-31G(d), suggesting that the present system is not sensitive to the basis set used in DFT calculations (see Page S6).

2. Computational Results

2.1 Computed Energies for the Model Substrate 4-Methylene-1,3-Dioxolane with Me₃Al as the Active Promoting Species

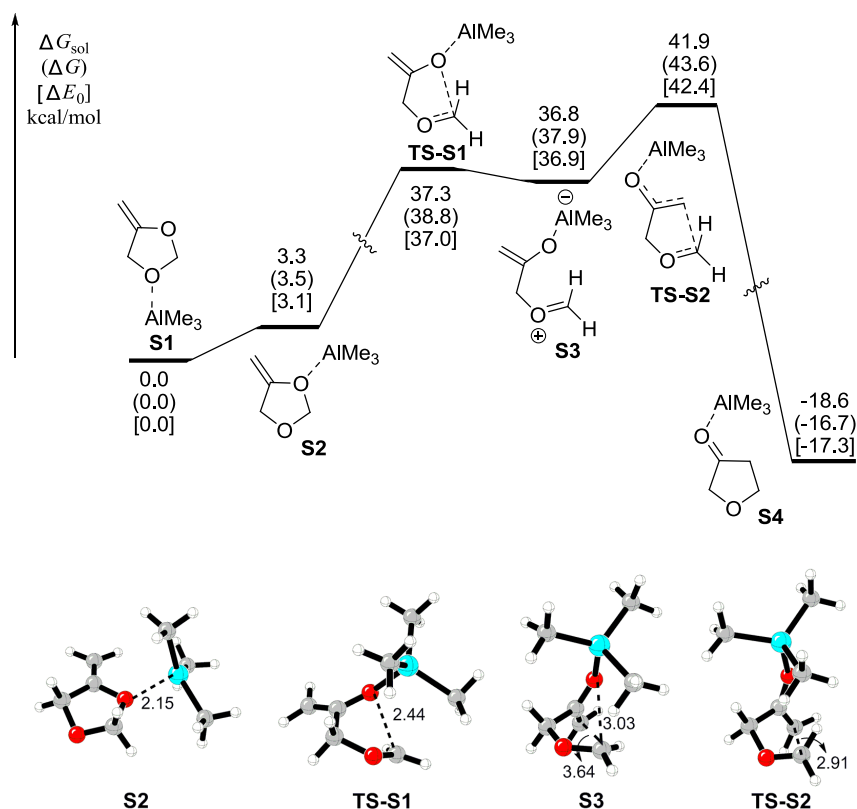


Figure S1. Energy surface for the model substrate 4-methylene-1,3-dioxolane with Me₃Al as the active promoting species in the gas phase and toluene solution by the B3LYP method together with the DFT computed structures of the key stationary points (distances in Å).

Table S1. Single Point Energies Calculated with Various Computational Methods⁷⁻⁹

	S1	S2	TS-S1	S3	TS-S2	S4
ΔE_{MP2}^a (kcal/mol)	0.0	1.7	42.3	44.8	48.8	-16.7
$\Delta E_{\text{CCSD(T)}}^b$ (kcal/mol)	0.0	2.1	43.0	47.5	50.4	-16.7
ΔE_{M06}^b (kcal/mol)	0.0	2.1	39.6	41.6	45.8	-18.6

^a 6-311+G(d,p) basis set was used. ^b 6-31G(d) basis set was used.

2.2 Computed Energies for the Model Substrate 4-Methylene-1,3-Dioxane with Me₂AlCl as the Active Promoting Species

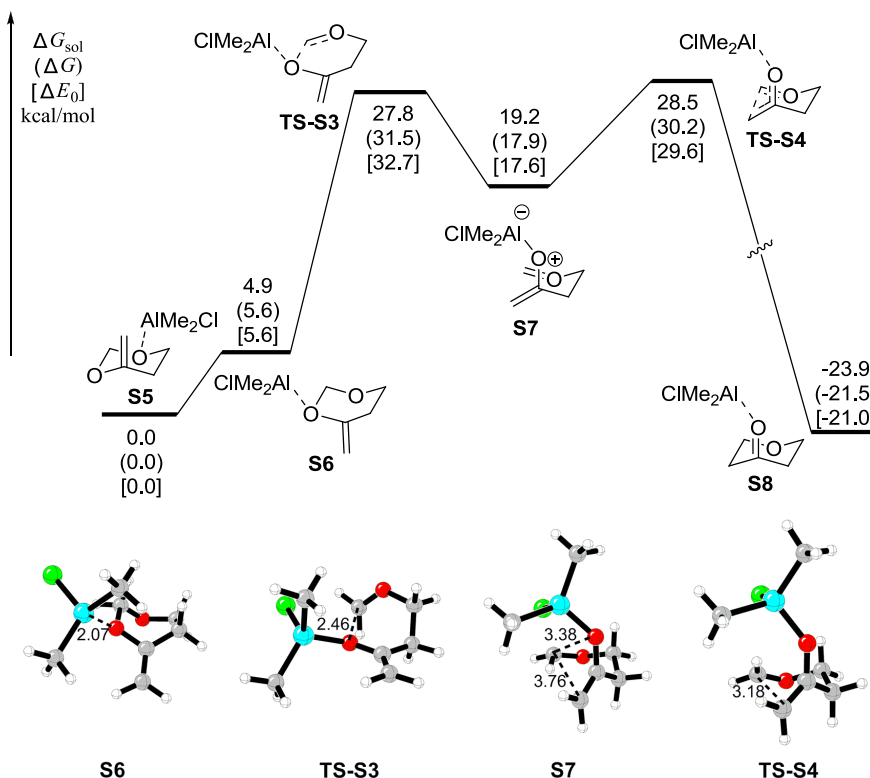


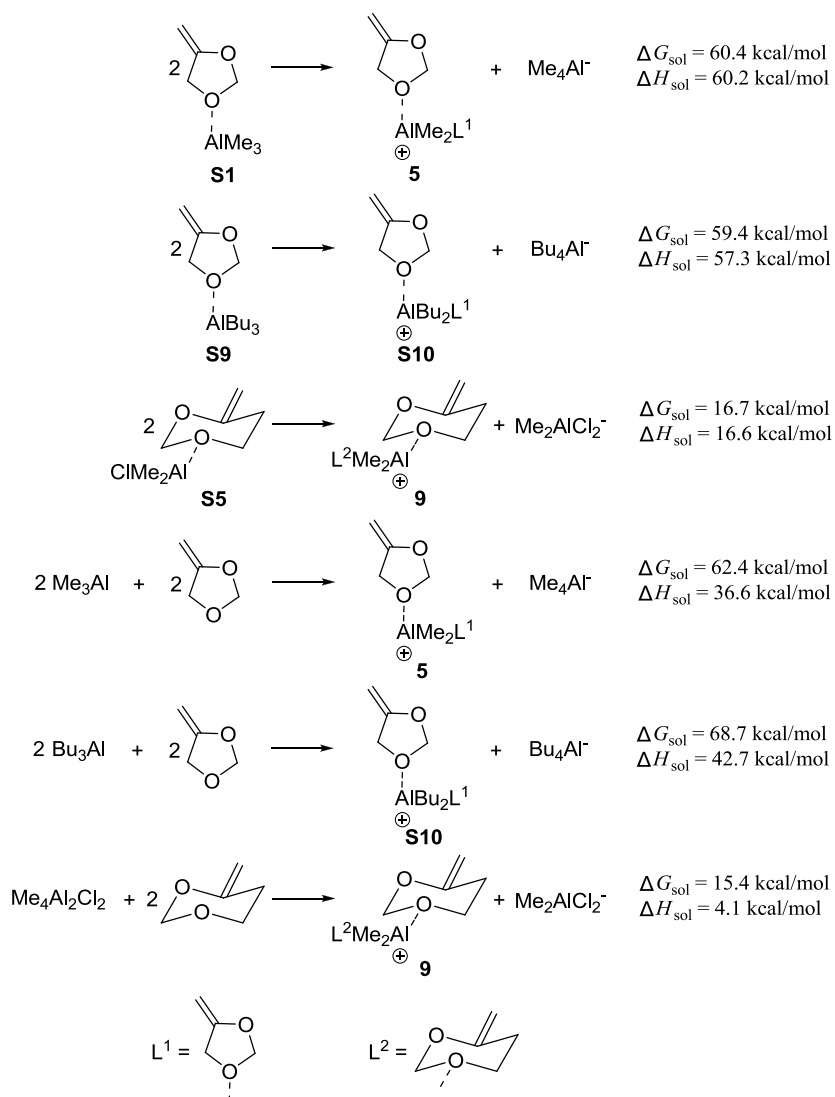
Figure S2. Energy surface for the model substrate 4-methylene-1,3-dioxane with Me₂AlCl as the active promoting species in the gas phase and DCM solution by the B3LYP method together with the DFT computed structures of the key stationary points (distances in Å).

Table S2. Single Point Energies Calculated with Various Computational Methods⁷⁻⁹

	S5	S6	TS-S3	S7	TS-S4	S8
ΔE_{MP2}^a (kcal/mol)	0.0	5.4	40.7	19.8	36.8	-18.7
$\Delta E_{\text{CCSD(T)}}^b$ (kcal/mol)	0.0	4.9	40.3	23.1	38.2	-19.3
ΔE_{M06}^b (kcal/mol)	0.0	4.7	37.7	17.7	32.5	-21.9

^a 6-311+G(d,p) basis set was used. ^b 6-31G(d) basis set was used.

2.3 Computed Energies of the Dissociation Reactions



2.4 Computed Single Point Energies Using B3LYP/6-311+G(d,p) Method with Me_2Al^+ as the Active Promoting Species

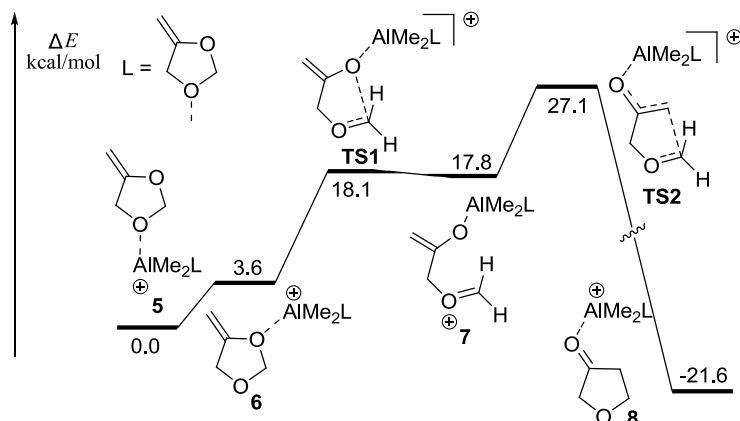


Figure S3. Single point energies (without ZPE corrections) using B3LYP/6-311+G(d,p) method for the model substrate 4-methylene-1,3-dioxolane with Me_2Al^+ as the active promoting species.

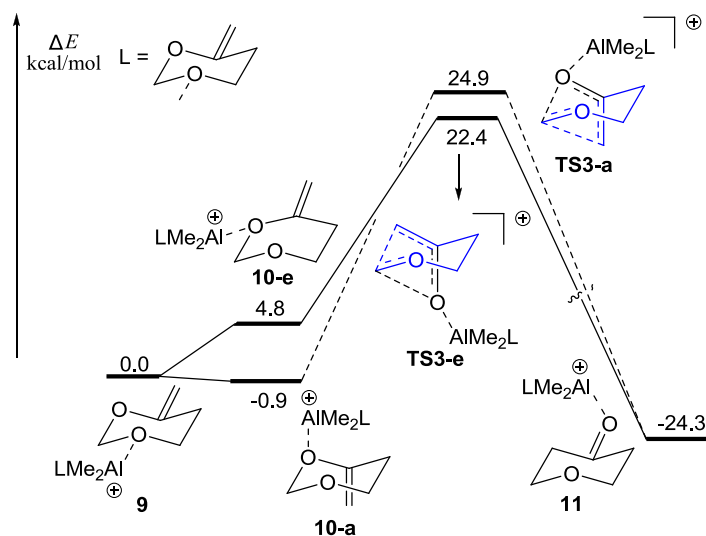


Figure S4. Single point energies (without ZPE corrections) using B3LYP/6-311+G(d,p) method for the model substrate 4-methylene-1,3-dioxane with Me_2Al^+ as the active promoting species.

2.5 Computed Activation Free Energies with Two Lewis Acids as the Possible Active Promoting Species

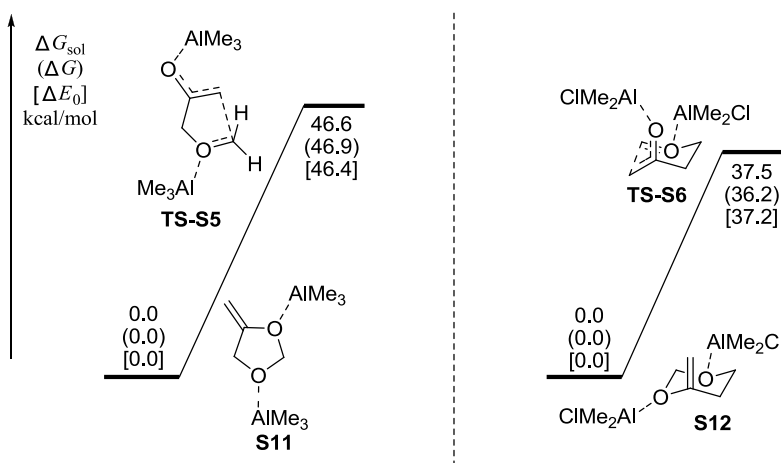


Figure S5. Activation free energies with two neutral Lewis acids as the possible active promoting species.

We have also tried to compute the activation free energies with two cationic Lewis acids as the possible active promoting species. However, one cationic Lewis acid (red part in Figure S6) always departs away in the key transition states, indicating that it is disfavored to have two cationic Lewis acids as the active promoting species in these reaction systems (Figure S6). Such two-Lewis acids systems will generate oxocarbenium enolates with two positive charges in the transition states and are disfavored.

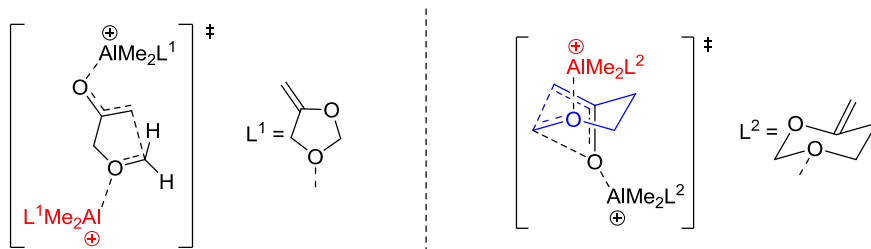


Figure S6. Expected but not located key transition states with two cationic Lewis acids as the possible active promoting species.

2.6 Computed Energies of All Stationary Points

Sum of electronic and zero-point energies (E_0 , in Hartree)

Sum of electronic and thermal free energies (G , in Hartree)

Thermal correction to Gibbs free energy ($TCGFE$, in Hartree)

Total free energy in solution (E_{sol} , in hartree)

Sum of electronic and thermal free energies in solution (G_{sol} , which equals to $E_{\text{sol}} + TCGFE$, in Hartree).

Structure	$TCGFE$	E_0	G	G_{sol}	E_{sol}
5	0.220335	-934.716525	-934.768235	-934.798536	-935.018871
6	0.223301	-934.712166	-934.761213	-934.79056	-935.013861
TS1	0.21685	-934.687752	-934.740073	-934.767883	-934.984733
7	0.217875	-934.687938	-934.739306	-934.767096	-934.984971
TS2	0.217685	-934.674865	-934.725911	-934.754194	-934.971879
8	0.220802	-934.752783	-934.803648	-934.835563	-935.056365
9	0.280873	-1013.302601	-1013.353838	-1013.404101	-1013.684974
10-a	0.282863	-1013.304847	-1013.354216	-1013.401365	-1013.684228
10-e	0.280499	-1013.296267	-1013.347256	-1013.39626	-1013.676759
TS3-a	0.276577	-1013.263603	-1013.314709	-1013.362049	-1013.638626
TS3-e	0.275941	-1013.267511	-1013.319214	-1013.365195	-1013.641136
11	0.279938	-1013.342989	-1013.395085	-1013.446314	-1013.726252
4-methylene-1,3-dioxolane	0.068916	-306.337565	-306.366423	-306.368314	-306.43723
dihydrofuran-3(2H)-one	0.068869	-306.361977	-306.390841	-306.394566	-306.463435
4-methylene-1,3-dioxane	0.097695	-345.625542	-345.655442	-345.660414	-345.758109
dihydro-2H-pyran-4(3H)-one	0.097536	-345.652809	-345.682979	-345.690553	-345.788089
anti-12	0.422581	-1475.268325	-1475.333963	-1475.345758	-1475.768339
syn-12	0.421045	-1475.270098	-1475.337253	-1475.350158	-1475.771203
anti-TS4	0.422784	-1475.259094	-1475.324129	-1475.336779	-1475.759563
syn-TS4	0.421965	-1475.260145	-1475.325908	-1475.339669	-1475.761634
anti-14	0.421287	-1475.26899	-1475.335975	-1475.347378	-1475.768665
syn-14	0.42275	-1475.271081	-1475.336809	-1475.345394	-1475.768144
anti-TS5	0.420499	-1475.258565	-1475.325505	-1475.338321	-1475.75882
syn-TS5	0.422162	-1475.262523	-1475.328038	-1475.340098	-1475.76226
TS6-a	0.490012	-1327.590845	-1327.653774	-1327.692047	-1328.182059
TS6-e	0.489185	-1327.596535	-1327.66024	-1327.69429	-1328.183475
TS7-a	0.491425	-1327.590252	-1327.652015	-1327.688074	-1328.179499
TS7-e	0.490784	-1327.586868	-1327.649832	-1327.683267	-1328.174051
S1	0.163676	-668.439883	-668.483031	-668.479596	-668.643272
S2	0.164356	-668.434882	-668.477436	-668.474327	-668.638683
TS-S1	0.163554	-668.380987	-668.421217	-668.420221	-668.583775
S3	0.161167	-668.381037	-668.42267	-668.420904	-668.582071
TS-S2	0.161964	-668.37235	-668.413506	-668.412906	-668.57487
S4	0.164523	-668.467373	-668.509715	-668.509296	-668.673819
S5	0.160529	-1128.125585	-1128.168361	-1128.169344	-1128.329873
S6	0.160026	-1128.116648	-1128.159417	-1128.161547	-1128.321573
TS-S3	0.153893	-1128.073421	-1128.118225	-1128.125051	-1128.278944
S7	0.159222	-1128.097621	-1128.139905	-1128.13874	-1128.297962
TS-S4	0.157626	-1128.078403	-1128.120164	-1128.123872	-1128.281498

S8	0.159721	-1128.159025	-1128.202589	-1128.207441	-1128.367162
S9	0.404997	-1021.987065	-1022.046766	-1022.036556	-1022.441553
S10	0.3836	-1170.415773	-1170.476389	-1170.499037	-1170.882637
Me ₄ Al ⁻	0.105952	-401.995897	-402.030486	-402.064415	-402.170367
Bu ₄ Al ⁻	0.428585	-873.406924	-873.463034	-873.479393	-873.907978
Me ₂ AlCl ₂ ⁻	0.03975	-1242.817381	-1242.851715	-1242.90804	-1242.94779
Me ₃ Al	0.072001	-362.082455	-362.117254	-362.112864	-362.184865
Bu ₃ Al	0.314529	-715.633088	-715.683527	-715.675653	-715.990182
Me ₄ Al ₂ Cl ₂	0.104495	-1564.980027	-1565.023984	-1565.015869	-1565.120364
S11	0.259268	-1030.532443	-1030.588969	-1030.578445	-1030.837713
TS-S5	0.255561	-1030.458435	-1030.514251	-1030.50424	-1030.759801
S12	0.223388	-1910.61484	-1910.669884	-1910.665827	-1910.889215
TS-S6	0.217322	-1910.555576	-1910.612171	-1910.606093	-1910.823415

3. References

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4. Coordinates of All Stationary Points

5

C	2.01757800	-1.17919900	0.37510400
O	1.34793000	-0.02148100	-0.23533200
C	2.20547500	0.34005200	-1.38461100
O	3.49060000	0.07383900	-0.94899500
C	3.44303700	-1.04580100	-0.12844500
C	4.50085300	-1.79500100	0.14606100
H	1.92359200	-1.08401500	1.45711800
H	1.51983000	-2.08905300	0.02660100
H	2.08280600	1.40015900	-1.59495900
H	1.89763000	-0.29747900	-2.22193400
H	4.42673400	-2.62569000	0.83859600
H	5.46439100	-1.58365100	-0.30261700
Al	0.07601500	1.16390500	0.66262600
C	0.20494100	0.78198900	2.57317000
C	0.17489300	2.85841700	-0.30413600
H	0.01738100	-0.25936500	2.86373300
H	1.19409300	1.04995000	2.96710700
H	-0.51562900	1.39619900	3.12969600
H	1.15748900	3.33055500	-0.17089800
H	-0.55321300	3.57027700	0.10717700
H	-0.01024100	2.81368000	-1.38504600
H	-1.73253400	0.93364400	-1.92395600
C	-2.40154500	0.70158000	-1.09727100
O	-1.58896600	0.33495600	0.08634000
O	-3.13436500	-0.43714000	-1.37240600
H	-3.02509400	1.55542200	-0.80956300
C	-2.36665300	-0.67188600	0.82307300
C	-3.46477600	-1.02642100	-0.15878300
H	-1.69576200	-1.50576600	1.04074200
H	-2.73485800	-0.23220500	1.75261300
C	-4.54000100	-1.77964900	0.02058200
H	-4.72687700	-2.26143000	0.97366000
H	-5.24232500	-1.94787200	-0.78752100

6

C	-3.73502200	-1.03674600	-0.19506800
O	-3.87773200	0.37471900	0.00788600
C	-2.88244300	0.95687100	-0.73459100
O	-1.68601800	0.08708700	-0.46929300
C	-2.23932200	-1.22519000	-0.37763200

C	-1.50098900	-2.31683100	-0.49606700
H	-4.13276600	-1.54554400	0.68470800
H	-4.28868100	-1.36029900	-1.08688500
H	-2.66878800	1.96506600	-0.38726500
H	-3.03737000	0.90449800	-1.81931000
H	-1.96396100	-3.29308200	-0.40370200
H	-0.43683400	-2.27927500	-0.69402900
Al	-0.21637300	0.76095600	0.68899100
C	-0.11104100	2.65918500	0.23366600
C	-0.35515700	-0.09542700	2.43436100
H	-0.28954400	2.91138400	-0.81950100
H	-0.82478700	3.24691600	0.82621100
H	0.88051200	3.05683500	0.48960500
H	-1.28125200	0.22700200	2.92902900
H	0.46265200	0.20830100	3.10119600
H	-0.37575000	-1.19094600	2.41381000
H	1.55835100	1.45320300	-1.61540200
C	1.99785900	0.48527700	-1.38354700
O	1.26036800	-0.11401900	-0.25211700
O	3.28950100	0.63534500	-0.91191600
H	1.92548100	-0.22288500	-2.21736400
C	2.23831300	-1.01265300	0.38384700
C	3.56593400	-0.43361300	-0.06803900
H	2.07864200	-0.97236900	1.46121600
H	2.06073700	-2.02729400	0.01521400
C	4.79490800	-0.80286300	0.26223500
H	4.96004500	-1.60704200	0.97016800
H	5.65895400	-0.30000400	-0.15604700

TS1

C	-3.22394200	-0.83005600	-1.39873700
O	-3.44929200	-1.79551000	-0.26655600
C	-3.41829300	-1.35018900	0.90865700
O	-1.54849200	-0.02338800	0.03671000
C	-2.45594000	0.35625700	-0.87555800
C	-2.74301000	1.59561300	-1.30313700
H	-2.66066600	-1.45728500	-2.09186700
H	-4.20601300	-0.59096300	-1.80843000
H	-3.36719600	-2.10108500	1.69620800
H	-3.56364400	-0.29710500	1.13562700
H	-3.54146400	1.76038400	-2.01838300
H	-2.16242500	2.45560700	-0.99082200
Al	-0.11819900	0.71620400	0.92874100

C	-0.01101800	2.67507700	0.83174800
C	0.08372100	-0.34023000	2.57149900
H	0.00706800	3.10339500	-0.17899200
H	-0.86931300	3.13031100	1.34500700
H	0.87944100	3.05056300	1.35417600
H	-0.62898200	0.00209100	3.33508700
H	1.07746100	-0.22098800	3.02310500
H	-0.08389800	-1.41896700	2.44934600
H	2.14108600	2.01703400	-0.66822100
C	2.29443400	0.98770200	-0.98366700
O	1.36477900	0.12400000	-0.25151700
O	3.55658500	0.54501200	-0.60845700
H	2.10329000	0.84420300	-2.05436900
C	2.02866400	-1.17670900	-0.17760900
C	3.48816500	-0.82175700	-0.39053800
H	1.82003100	-1.59995100	0.80539500
H	1.62350500	-1.82283900	-0.96269800
C	4.55380500	-1.61010100	-0.35824400
H	4.45460800	-2.66457500	-0.12760600
H	5.54554600	-1.21504500	-0.54412400

7

C	-3.17031900	-0.76373800	-1.42584200
O	-3.68477400	-1.72922000	-0.34920500
C	-3.73064600	-1.37755800	0.84660300
O	-1.51298700	-0.02202600	0.05464500
C	-2.45914800	0.39022500	-0.79695600
C	-2.83968600	1.64840200	-1.08647600
H	-2.52179200	-1.43907400	-1.98584500
H	-4.06351700	-0.51217900	-1.99704600
H	-4.00767400	-2.15488300	1.55935900
H	-3.54289100	-0.35048000	1.15429900
H	-3.66084400	1.83430100	-1.76971300
H	-2.31465000	2.50877200	-0.68789800
Al	-0.06656900	0.69761400	0.91421000
C	0.08064600	2.65389100	0.78577100
C	0.17285300	-0.32976300	2.57048300
H	0.02306000	3.07098800	-0.22830400
H	-0.71999800	3.13535600	1.36452300
H	1.01991400	3.01397700	1.22750200
H	-0.52150300	0.03173000	3.34212400
H	1.17693700	-0.20901100	2.99829000
H	-0.00803700	-1.40858100	2.47198900

H	2.10719000	1.94966600	-0.82638600
C	2.29163900	0.90760100	-1.07648400
O	1.39708900	0.06536800	-0.28395100
O	3.57214000	0.53096500	-0.68656900
H	2.09946000	0.69083400	-2.13481700
C	2.09996900	-1.20883600	-0.14828100
C	3.54880100	-0.81707700	-0.36737400
H	1.89610100	-1.59710200	0.84965500
H	1.72187700	-1.90003600	-0.90852800
C	4.64139100	-1.56137300	-0.26317300
H	4.57586700	-2.59876900	0.04405600
H	5.62115100	-1.14583200	-0.46699100

TS2

C	-3.14707200	-0.98529200	-1.23803100
O	-3.61767900	-1.93731400	-0.22128600
C	-4.47555100	-1.43323600	0.58703900
O	-1.21693300	0.03073700	-0.31053200
C	-2.50209500	0.14161700	-0.41017500
C	-3.33331200	0.98110200	0.28656300
H	-2.42980400	-1.53487100	-1.84200600
H	-3.99559800	-0.64140400	-1.83629900
H	-4.61737400	-1.97229200	1.52120500
H	-5.18719100	-0.68027200	0.27221300
H	-4.33260600	1.20676700	-0.06481100
H	-2.94225500	1.61522600	1.07532000
Al	0.08087500	1.20892900	0.33546500
C	0.22075600	2.75275700	-0.86422200
C	0.06526300	1.22809400	2.29768100
H	0.18898000	2.49890600	-1.93180700
H	-0.60991000	3.44967800	-0.68998500
H	1.13896400	3.32995500	-0.69209300
H	-0.73220000	1.88144800	2.67713700
H	1.00060600	1.63301400	2.70693100
H	-0.09270700	0.24452100	2.75867300
H	2.40390000	1.21052000	-1.70578000
C	2.45755200	0.18940100	-1.33386200
O	1.61725800	0.08193800	-0.13927600
O	3.73904700	-0.10194900	-0.88671100
H	2.09360100	-0.54295000	-2.06533800
C	2.23257300	-0.94687000	0.69643700
C	3.64159000	-1.02646000	0.14099700
H	2.18648200	-0.60081100	1.72974400

H	1.67062100	-1.87916500	0.58463700
C	4.65277600	-1.78811000	0.53538900
H	4.54413300	-2.45581300	1.38235700
H	5.61256600	-1.74385500	0.03440900

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C	-3.11211400	-1.68455200	-0.54745900
O	-4.43136700	-1.49953000	-0.09121100
C	-4.70056700	-0.09229500	-0.11715700
O	-1.13915100	-0.31327700	-0.17929600
C	-2.37212100	-0.44312800	-0.11183000
C	-3.38600800	0.54974900	0.37503000
H	-2.68706700	-2.60154500	-0.12539400
H	-3.04062700	-1.75205300	-1.65063600
H	-5.55395700	0.09429800	0.53431300
H	-4.94225000	0.24199200	-1.13613000
H	-3.18317700	1.56644500	0.02376600
H	-3.34334200	0.55397600	1.47485700
Al	0.12925700	1.08363900	0.27715500
C	-0.01118200	2.44704400	-1.11700200
C	0.09144100	1.26092900	2.22302600
H	-0.11796600	2.04804500	-2.13374500
H	-0.87609000	3.10130900	-0.94470600
H	0.86375900	3.11093300	-1.11878900
H	-0.76982400	1.86051500	2.54644900
H	0.97828100	1.79268100	2.59285100
H	0.03568300	0.30939200	2.76659400
H	2.32344800	1.10523200	-1.85153800
C	2.51745400	0.14046300	-1.38758100
O	1.69581500	0.03161500	-0.16431300
O	3.82046400	0.06907400	-0.92997000
H	2.24528900	-0.70279700	-2.03325500
C	2.46148700	-0.81518900	0.75985200
C	3.84710700	-0.81174500	0.14269700
H	2.41932600	-0.34453400	1.74324400
H	2.00254500	-1.80694500	0.79258000
C	4.93379700	-1.46789800	0.52290400
H	4.91916700	-2.10122900	1.40265900
H	5.86460000	-1.36635400	-0.02269500

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C	4.25812400	-0.00083400	-0.25310100
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C	3.57569100	-1.24485300	0.25404800
C	2.22801800	-1.45173600	-0.43790100
O	1.44953700	-0.19761700	-0.37717300
C	2.23578500	0.89770100	-0.97749100
O	3.39733600	1.11210200	-0.27044500
C	5.53248000	0.15263900	-0.59271100
H	3.40781200	-1.15427300	1.33586200
H	4.20156300	-2.12714700	0.08911200
H	2.34010800	-1.69008700	-1.50025300
H	2.41943300	0.59391500	-2.01511800
H	5.91393800	1.11626700	-0.91211200
H	6.22596400	-0.67853600	-0.52969300
H	1.61940200	-2.21330800	0.04687400
H	1.61956500	1.79134500	-0.91480100
Al	-0.00369900	0.13661800	0.89016100
C	-0.23041600	-1.50947900	1.91837300
H	-1.11042100	-1.41100600	2.56759600
H	-0.37453400	-2.43675000	1.35055300
H	0.62353300	-1.67576300	2.58853100
C	0.21971700	1.95471600	1.57472400
H	-0.59283000	2.21345100	2.26679000
H	1.14680900	2.01683300	2.15974000
H	0.27088800	2.76140300	0.83297200
O	-1.45730800	0.22317700	-0.42167300
C	-2.32883700	1.40049100	-0.61344000
C	-2.15848500	-0.98553800	-0.89259400
C	-3.65531600	1.17010100	0.11127500
H	-1.77731700	2.25446100	-0.22439300
H	-2.46088600	1.50915000	-1.69449400
O	-3.29918900	-1.21122800	-0.15557900
H	-1.47605800	-1.81908800	-0.74256700
H	-2.36613800	-0.81046400	-1.95510800
C	-4.24222900	-0.17077200	-0.24793400
H	-3.47950400	1.21322400	1.19480000
H	-4.34722800	1.97862700	-0.14345000
C	-5.50289500	-0.45669600	-0.55100800
H	-6.25775600	0.32147800	-0.56955400
H	-5.81108200	-1.47568800	-0.75784900

10-a

C	-1.62534200	-1.40812500	0.23898700
C	-3.07490100	-1.44571000	0.63323300
C	-3.96863800	-1.06092500	-0.55575900

O	-3.49759900	0.17856100	-1.12371500
C	-2.21665900	0.07473800	-1.57227400
O	-1.27957100	-0.17070300	-0.41741700
C	-0.68027300	-2.32653300	0.39255400
H	-3.24734200	-0.73254500	1.44967200
H	-3.33478300	-2.44385300	0.99786400
H	-3.95616700	-1.83936700	-1.33039900
H	-2.04549400	-0.77946300	-2.23864700
H	0.33940000	-2.17611500	0.05395100
H	-0.91664000	-3.25983300	0.89274600
H	-4.99820700	-0.87870600	-0.24724100
H	-1.90207600	1.01887100	-2.00890500
Al	-0.48408300	1.32208200	0.58080600
C	-0.75585500	2.92064100	-0.51319100
H	-0.19778100	3.76460800	-0.08543500
H	-0.46853500	2.86018300	-1.57054700
H	-1.81232200	3.21962500	-0.49228800
C	-0.91040100	1.08863700	2.47344500
H	-0.24510900	1.69107800	3.10612200
H	-1.92611700	1.45772600	2.66974800
H	-0.87147600	0.06025300	2.85120800
H	1.41243300	-0.39240500	2.03460900
C	2.12511000	-0.06387100	1.28184200
O	1.41126700	0.87596500	0.40624300
O	2.55607700	-1.16410100	0.56311900
H	2.95725300	0.49822900	1.72164800
C	2.32083600	1.37999800	-0.63912900
C	3.46018000	-0.83883300	-0.46697400
C	2.90265200	0.19470000	-1.41026700
H	1.72756900	2.04506200	-1.26436300
H	3.09486800	1.95897300	-0.12527900
C	4.61932600	-1.48136700	-0.54642500
H	2.10732100	-0.25729800	-2.01827700
H	3.67755100	0.55633800	-2.09286400
H	5.30527100	-1.28560200	-1.36311000
H	4.89584800	-2.23071400	0.18720800

10-e

C	4.57901900	-0.00515100	-0.52125700
O	3.70817600	1.02688600	-1.04156000
C	2.71082200	1.36507100	-0.19426400
O	1.71148900	0.20458000	-0.10697300
C	2.33033000	-1.05150700	-0.40087200

C	3.73164900	-1.12545000	0.13065400
C	1.65483300	-1.95932600	-1.09426900
H	5.12386700	-0.36700400	-1.39321200
H	5.28722100	0.43869800	0.18763000
H	2.13896300	2.19508700	-0.60143400
H	3.03236300	1.54556100	0.83840400
H	4.15941800	-2.10807300	-0.08201100
H	3.71353600	-1.00805900	1.22167000
H	2.09696600	-2.92993000	-1.28774300
H	0.66217200	-1.76673600	-1.48313200
Al	0.09788700	0.37886500	0.99873600
C	-0.12307300	2.31503100	1.19348900
C	0.19051700	-0.95323100	2.42327200
H	0.65889400	2.74212000	1.83577900
H	-0.12542500	2.90402800	0.26752100
H	-1.07136300	2.52973700	1.70424700
H	0.46218700	-1.96391800	2.09623900
H	-0.75508100	-1.02858700	2.97552800
H	0.94496500	-0.64875700	3.16154300
O	-1.23280700	-0.24224800	-0.28505800
C	-1.82907700	0.63423000	-1.31353300
C	-2.17147600	-1.33927900	0.03475000
C	-3.18898000	1.13860100	-0.82759800
H	-1.11548600	1.44062000	-1.47972800
H	-1.91077200	0.02777200	-2.22074200
O	-3.33925600	-0.83849800	0.56406900
H	-1.68038500	-1.95729900	0.78188600
H	-2.32825400	-1.87366600	-0.90990900
C	-4.03965500	0.00239700	-0.32151800
H	-3.02792800	1.86237300	-0.01795300
H	-3.68903200	1.66363500	-1.64721700
C	-5.32671700	-0.22333700	-0.55650300
H	-5.89922300	0.44488200	-1.19013100
H	-5.84010500	-1.06178800	-0.09872600

TS3-a

O	1.14025100	0.16138500	0.18021000
C	2.89148500	-1.43772500	1.79068000
C	1.18488300	-1.86193300	-1.06892200
C	1.72386000	-0.68463400	-0.68458700
C	3.14135000	-0.29246000	-1.07819800
C	4.17339400	-0.93242600	-0.13749300
H	4.23651400	-2.01574300	-0.25942500

H	5.16074000	-0.47493200	-0.18356400
O	3.73448000	-0.67834800	1.26405800
H	2.57261500	-2.35831400	1.30060100
H	2.50161200	-1.12304000	2.75718100
H	0.18111600	-2.14269800	-0.76600100
H	1.71449500	-2.52136200	-1.74964600
H	3.25005000	0.79453000	-1.06476700
H	3.39860200	-0.64934000	-2.08220900
Al	0.16941700	1.67096500	-0.05056600
C	0.50607900	2.49115200	-1.80829600
H	-0.25439100	3.24423200	-2.05343200
H	0.53354200	1.78583600	-2.65010800
H	1.46894800	3.02108000	-1.81629100
C	0.08480200	2.64685300	1.65242300
H	-0.63023800	3.47986100	1.64211800
H	1.06342900	3.09873000	1.86681400
H	-0.15983500	2.01885800	2.51990000
O	-1.68326600	0.93291500	-0.26275900
C	-2.77276500	1.05050200	0.70801100
C	-2.02529400	-0.02466900	-1.29539700
C	-3.07112100	-0.33103600	1.29375600
H	-2.43723100	1.76455100	1.45815400
H	-3.63441700	1.46187800	0.17091100
O	-2.21690900	-1.29587900	-0.76001700
H	-1.18191200	-0.06862200	-1.98132300
H	-2.93166100	0.34592400	-1.79003100
C	-3.24096000	-1.35116100	0.19675300
H	-2.23132700	-0.62509600	1.93777300
H	-3.96874700	-0.27843500	1.91721200
C	-4.18112600	-2.28506700	0.09614500
H	-4.94849400	-2.38215100	0.85603800
H	-4.18980700	-2.98325000	-0.73373400

TS3-e

C	-3.37789500	-1.06431300	1.66299800
C	-0.65196900	-1.95927500	-0.85930800
O	-1.30961800	0.08135200	0.19127400
C	-1.48767000	-0.92465700	-0.71152400
C	-2.79819800	-0.82413400	-1.47257100
C	-3.94947100	-0.41190700	-0.56651500
O	-3.97407400	-1.36209500	0.61015000
H	0.27122600	-2.01924600	-0.29220200
H	-0.87242500	-2.75739400	-1.55993000

H	-2.74903500	-0.03046900	-2.23421600
H	-3.02690800	-1.76013800	-1.98892000
H	-3.82887400	0.58735100	-0.14893000
H	-4.93462600	-0.54814000	-1.01018600
H	-2.88361300	-0.09878700	1.77791000
H	-3.36817400	-1.83232600	2.43754500
Al	-0.32396500	1.59632700	0.06319900
C	-0.61087600	2.60116700	1.73166300
H	0.09866700	3.43329700	1.83000700
H	-1.61048300	3.05746400	1.76246100
H	-0.51418600	2.00030600	2.64694400
C	-0.35626500	2.39276600	-1.73724200
H	0.34159000	3.23347100	-1.84688900
H	-0.14158000	1.68569700	-2.54978900
H	-1.35179900	2.81100800	-1.94385200
H	2.22966900	1.67291300	-1.53172700
C	2.63492400	1.08666700	-0.70888800
O	1.53439800	0.90230000	0.24230800
C	3.14385100	-0.28528800	-1.15423800
H	3.40926000	1.66485800	-0.19269200
C	1.96164300	0.08958600	1.36677800
C	3.40867400	-1.17061400	0.03643300
H	2.38094400	-0.75171900	-1.79151500
H	4.05070800	-0.15922500	-1.75329400
O	2.34228500	-1.18019700	0.95086300
H	1.10311300	-0.01064100	2.02726900
H	2.78801600	0.62278900	1.85332500
C	4.46285300	-1.94921500	0.25466000
H	5.27056100	-2.00192100	-0.46681100
H	4.52797300	-2.56697300	1.14367300

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C	-4.41991500	-0.38140100	0.13449000
C	-3.78351700	0.04110100	-1.16467000
C	-2.40029300	-0.58962000	-1.32947600
O	-1.61738500	-0.36708900	-0.09971200
C	-2.34862500	-0.90386400	1.06119600
O	-3.54754300	-0.24472700	1.22906000
C	-5.67145800	-0.77425500	0.34112200
H	-3.67450900	1.13383600	-1.17783100
H	-4.41125900	-0.24075800	-2.01541800
H	-2.45044700	-1.67386500	-1.46993000
H	-2.47866700	-1.97388400	0.85940300

H	-6.02294100	-1.01948100	1.33733600
H	-6.37716200	-0.83015500	-0.48023000
H	-1.82842200	-0.14178300	-2.14121800
H	-1.72377800	-0.72268300	1.93192300
Al	-0.20998000	0.96575900	0.05414100
C	-0.37951100	2.18076700	-1.47132900
H	0.36411600	2.98623900	-1.40397800
H	-0.23869300	1.70993000	-2.45254700
H	-1.35775500	2.67873100	-1.48964600
C	-0.05479900	1.40686300	1.95488100
H	0.66934400	2.21929200	2.10363400
H	-1.00425900	1.77347300	2.36631100
H	0.27294200	0.57553400	2.59251600
O	1.21435400	-0.25834600	-0.37438400
C	2.45924800	-0.22683700	-0.49577000
C	3.20792400	-1.46329500	-0.86500000
C	3.28638800	0.98454900	-0.21129500
C	4.38137500	-1.67243900	0.14375900
H	3.65368200	-1.31304100	-1.85722600
H	2.53699400	-2.32536200	-0.90108400
C	4.45595800	0.58959800	0.74747100
H	3.73576000	1.32120600	-1.15472200
H	2.68706300	1.79913000	0.20472000
O	5.17066600	-0.50734500	0.22944100
H	5.02870900	-2.47654800	-0.21003800
H	3.98048300	-1.95203500	1.12965600
H	5.15509300	1.42357600	0.82887600
H	4.05604400	0.36685100	1.74814700

4-methylene-1,3-dioxolane

C	-0.10094000	1.18329000	0.12710400
O	-1.37300700	0.66349600	-0.25793500
C	-1.33926900	-0.68785900	0.11729500
O	0.00866500	-1.13014100	-0.04488900
C	0.81467100	-0.01947900	0.00849400
C	2.14416700	-0.07106200	-0.03693300
H	0.15955400	2.00318000	-0.54607700
H	-0.12937600	1.56448600	1.16094800
H	-1.99053500	-1.26415400	-0.54404100
H	-1.63435100	-0.82531500	1.17116300
H	2.72741600	0.84225700	-0.01637800
H	2.67025400	-1.01663500	-0.09878200

dihydrofuran-3(2H)-one

O	1.30682800	-0.76331700	-0.21901700
C	-0.01065000	-1.20977400	0.05154700
C	-0.90178900	0.03719200	-0.01007000
C	0.04883900	1.22940600	-0.14161700
C	1.40000200	0.60146100	0.21390700
O	-2.10875700	0.05665300	0.04939100
H	-0.09980100	-1.66337400	1.05440000
H	-0.30396900	-1.95848100	-0.69100000
H	-0.26441600	2.06024600	0.49592200
H	0.02983200	1.57056800	-1.18480000
H	2.25476800	1.04625700	-0.30007500
H	1.58059900	0.64838200	1.29996100

4-methylene-1,3-dioxane

C	-1.15207500	1.10006400	0.30855900
O	-1.73294300	-0.12322500	-0.14442900
C	-0.92400800	-1.20768400	0.20599000
O	0.38015100	-1.14940200	-0.36549700
C	1.05794100	0.02680000	-0.09928400
C	0.23400400	1.27170800	-0.32562400
C	2.34179000	-0.01389500	0.25919600
H	-1.83721300	1.89850100	0.01311800
H	-1.07514900	1.09115300	1.40831000
H	-1.39119700	-2.10902400	-0.19190700
H	-0.82428400	-1.27142400	1.30387400
H	0.09752300	1.41653600	-1.40573900
H	0.74415200	2.15327600	0.07577000
H	2.90641900	0.90104600	0.40116200
H	2.85617000	-0.96099800	0.38179500

dihydro-2H-pyran-4(3H)-one

C	0.17045100	-1.07656200	1.17445200
O	0.83232200	-1.51936800	0.00000000
C	0.17045100	-1.07656200	-1.17445200
C	0.17045100	0.46222200	-1.27514800
C	-0.38663000	1.08004300	0.00000000
C	0.17045100	0.46222200	1.27514800
O	-1.21303300	1.97137100	0.00000000
H	0.70503300	-1.52219600	2.01783800
H	-0.86630600	-1.45250700	1.19013100

H	0.70503300	-1.52219600	-2.01783800
H	-0.86630600	-1.45250700	-1.19013100
H	1.20904600	0.80019100	-1.39613200
H	-0.41044600	0.81240800	-2.13385400
H	-0.41044600	0.81240800	2.13385400
H	1.20904600	0.80019100	1.39613200

anti-12

C	-1.45706100	-2.47911900	-0.60925100
O	-2.83673400	-1.85780200	-0.45516200
C	-3.03949200	-0.63127500	-0.74984100
O	-0.38085900	-0.53731500	0.21007200
C	-0.58118400	-1.84181900	0.44288100
C	-0.12111000	-2.58331100	1.46267400
H	-1.67798800	-3.51487100	-0.35859700
H	-2.24944100	-0.07546500	-1.24895300
H	-0.38957700	-3.62984300	1.54876900
H	0.54596200	-2.17532900	2.21183000
C	-4.27842500	0.00011900	-0.44465500
C	-4.45153900	1.34759400	-0.84162700
C	-5.32300200	-0.68540900	0.22383100
C	-5.64958800	1.99589600	-0.57687500
H	-3.64232500	1.86941500	-1.34425100
C	-6.51332800	-0.02702400	0.48194700
H	-5.17898200	-1.71722500	0.52593000
C	-6.67607000	1.30893400	0.08182700
H	-5.78967700	3.02899700	-0.87727000
H	-7.32047400	-0.54155700	0.99316500
H	-7.61330500	1.81758400	0.28853000
C	-0.98051500	-2.34833300	-2.04496200
H	-0.07212100	-2.94952100	-2.14749700
H	-1.72767400	-2.73027300	-2.74743800
H	-0.71774700	-1.31890600	-2.30017500
Al	0.25454700	0.88531700	1.12624300
C	0.77833400	0.57285900	2.99590500
H	1.07142200	1.50877800	3.49068600
H	-0.06048400	0.16688300	3.57753700
H	1.61348200	-0.12736500	3.12294900
C	-0.91918200	2.37851400	0.57095100
H	-1.01738200	2.46774600	-0.52126300
H	-1.93036400	2.19404300	0.96194600
H	-0.63303800	3.36802100	0.94675100
H	4.92296000	3.07088600	-2.56064000

C	4.02361200	3.34144600	-2.01999900
C	3.46373500	2.50426500	-1.15425600
H	3.58554300	4.31516400	-2.20606200
C	2.24604800	2.72126900	-0.28036100
O	3.94429400	1.23284100	-0.92183500
O	1.97031500	1.34401700	0.17235900
H	1.37312400	3.02377100	-0.85942800
C	2.49462600	3.67276400	0.88634600
C	3.29096100	0.66585100	0.18505600
H	2.72217400	4.66632300	0.48676200
H	1.61390800	3.75382700	1.52844700
H	3.35031700	3.35608400	1.49046900
C	3.21077100	-0.82309500	0.05592000
H	3.77896100	0.96417600	1.12038300
C	2.88959800	-1.41335000	-1.17371100
C	3.55786200	-1.62749000	1.14608400
C	2.91194100	-2.79998600	-1.30264100
H	2.66041400	-0.78378400	-2.02766900
C	3.57437100	-3.01738400	1.01546000
H	3.83749400	-1.16849800	2.09126900
C	3.25338300	-3.60276500	-0.20912700
H	2.69115900	-3.25686200	-2.26358900
H	3.85531500	-3.63702300	1.86171000
H	3.28463500	-4.68315000	-0.31839200

syn-12

C	3.48287600	-0.88452600	0.27428900
C	2.25426000	-1.73628900	2.14196000
H	3.03242900	-1.69766800	-0.29207900
O	3.32155100	-0.86561600	1.54495400
O	0.83042600	-0.91094100	0.46579800
C	0.95300800	-1.03613200	1.79361700
C	0.07573200	-0.64517800	2.73121800
H	-0.86383800	-0.17668000	2.46068000
H	0.26887300	-0.78956100	3.78602200
H	2.31264400	-2.68204000	1.58986300
C	2.62587500	-1.92105400	3.59650100
H	1.90384800	-2.59058800	4.07191000
H	3.61646400	-2.37598300	3.68062600
H	2.62729600	-0.96746500	4.13052900
C	4.28391100	0.08855900	-0.38470100
C	4.86535500	1.17565700	0.31374700
C	4.49619500	-0.05943100	-1.77651800

C	5.64635100	2.08765500	-0.37591500
H	4.69130600	1.28210000	1.37911000
C	5.28076900	0.86185500	-2.45548800
H	4.04053600	-0.89126400	-2.30641500
C	5.85384100	1.93039400	-1.75556000
H	6.09702900	2.92435300	0.14786900
H	5.44851700	0.75554800	-3.52212200
H	6.46730900	2.65101700	-2.28864000
Al	-0.14245600	0.18591500	-0.62278000
C	-0.24490500	2.01907600	0.06581700
H	0.76904100	2.44607400	0.07382400
H	-0.85283700	2.66967500	-0.57330600
H	-0.63611600	2.11545400	1.08362000
C	0.45143800	-0.20192900	-2.46487800
H	1.36415300	0.36921500	-2.68799400
H	0.68475000	-1.25726600	-2.66158300
H	-0.28351600	0.10919800	-3.21942300
H	-5.45163400	-2.99771800	-1.92401200
C	-4.36919900	-3.03379000	-1.96042000
C	-3.63236000	-2.11137500	-1.35196400
H	-3.90105000	-3.83201000	-2.52467500
C	-2.12153400	-2.00898000	-1.27325100
O	-4.17907400	-1.03633200	-0.68667100
O	-1.94034100	-0.71995700	-0.57797400
H	-1.67761500	-1.87271200	-2.26087700
C	-1.46046000	-3.16056600	-0.52568700
C	-3.21584700	-0.45307100	0.14772600
H	-1.67299700	-4.09454000	-1.05604000
H	-0.37805800	-3.02225500	-0.47405600
H	-1.85743200	-3.25344400	0.48991600
C	-3.49196900	1.00004400	0.35520300
H	-3.13923200	-0.99815800	1.09679900
C	-3.77022000	1.83165200	-0.73765400
C	-3.53421000	1.51523200	1.65430300
C	-4.06679000	3.17546300	-0.52680200
H	-3.76840800	1.42049800	-1.74259200
C	-3.83379400	2.86220400	1.86349100
H	-3.34971100	0.86186600	2.50436200
C	-4.09646900	3.69164700	0.77289600
H	-4.28560200	3.81985800	-1.37306000
H	-3.87104100	3.25861600	2.87367300
H	-4.33480800	4.73904400	0.93378200

anti-TS4

C	3.49202700	-0.19733200	-0.82309000
C	1.95573900	-0.31731300	0.93738900
C	1.53040400	0.98535100	-1.15848500
O	-0.11442400	-0.48612800	-0.25181900
C	1.05651900	0.02225300	-0.05908300
O	2.98825000	1.00765900	-1.03273700
H	1.22322600	2.01134100	-0.93881700
H	3.04463200	-1.04498600	-1.33519600
H	2.70085900	0.38615400	1.27988500
H	1.72015600	-1.12992200	1.61812200
C	4.84789600	-0.31997900	-0.36374100
C	5.47066400	-1.58476600	-0.42930800
C	5.56281600	0.79214900	0.13292100
C	6.78560400	-1.73375400	-0.00758500
H	4.91800500	-2.43933100	-0.81109800
C	6.87829900	0.63422700	0.54549800
H	5.08090300	1.76324000	0.17633700
C	7.48831800	-0.62571700	0.47837800
H	7.26672100	-2.70520200	-0.05873900
H	7.43508900	1.48714000	0.92056800
H	8.51710100	-0.74289700	0.80611000
C	1.08852300	0.59821400	-2.56447600
H	0.00182900	0.68230900	-2.63396000
H	1.54224500	1.27744400	-3.29150200
H	1.35850000	-0.43065600	-2.82215500
Al	-1.24186700	-1.58472200	0.71981100
C	-1.17481500	-3.34493500	-0.15425900
H	-0.17417500	-3.77778100	-0.01147400
H	-1.87833400	-4.08217200	0.25149900
H	-1.33490500	-3.30198800	-1.23974900
C	-1.12256700	-1.29619100	2.66022100
H	-0.79219600	-0.28814100	2.93747900
H	-2.08438000	-1.46951200	3.16178900
H	-0.41424000	-2.00043700	3.11756900
H	-0.28933000	4.70796200	0.59171000
C	-0.94019000	3.83839800	0.56450400
C	-1.33153600	3.22378900	1.75521900
C	-1.40898400	3.35439300	-0.66222800
C	-2.19562400	2.12817600	1.72006800
H	-0.98525700	3.60896900	2.70953000
C	-2.26073000	2.25189200	-0.70037700
H	-1.12979800	3.85311700	-1.58633600
C	-2.65343800	1.63374200	0.49408100

H	-2.52332500	1.66663600	2.64792700
H	-2.65176900	1.88974200	-1.64563100
C	-3.61295300	0.48410600	0.47498100
O	-2.97041900	-0.81487900	0.12542700
O	-4.57471700	0.63572700	-0.53009100
H	-4.08349000	0.33065000	1.45342600
C	-4.05167600	-1.65559700	-0.42880800
C	-4.98590900	-0.60122500	-0.98683600
H	-3.58861800	-2.25224300	-1.21558600
C	-4.69142000	-2.53895600	0.63735500
C	-6.03243100	-0.76060000	-1.78790400
H	-5.50652400	-3.10844900	0.17942300
H	-3.97056800	-3.24816300	1.05268700
H	-5.11949600	-1.94280000	1.44903400
H	-6.29305100	-1.74281300	-2.16460700
H	-6.64227100	0.08320600	-2.08865500

syn-TS4

C	-3.80900200	-0.35325200	-0.68550600
C	-2.22393600	0.57846800	0.75784000
H	-3.35043100	-1.33955800	-0.64104800
O	-3.34623700	0.50671100	-1.58071300
O	-0.19731600	-0.26973100	-0.20858300
C	-1.36787800	0.27339600	-0.28533200
C	-1.89959100	0.40462200	-1.71473100
H	-1.95923100	0.30022900	1.77369000
H	-2.96886700	1.35536100	0.65863700
H	-1.66782000	-0.53497900	-2.23529300
C	-1.39583800	1.59900600	-2.50643800
H	-0.30784400	1.53490500	-2.59911500
H	-1.82889300	1.60375000	-3.51044700
H	-1.65134200	2.53523200	-2.00207800
C	-5.14389400	-0.19498900	-0.18058500
C	-5.87698000	0.99351500	-0.39302300
C	-5.72715100	-1.26427100	0.53284200
C	-7.17166400	1.09755900	0.09512800
H	-5.42590900	1.81030300	-0.94663200
C	-7.02117100	-1.14714200	1.02340400
H	-5.15994200	-2.17704900	0.69611800
C	-7.74229900	0.03178600	0.80420800
H	-7.74279300	2.00529400	-0.07203200
H	-7.47182400	-1.96845800	1.57122100
H	-8.75481400	0.12180800	1.18658900

Al	0.94638500	-0.52692400	1.24747900
C	1.23483400	1.14097700	2.23177400
H	1.32896400	2.03175000	1.60165100
H	0.39465700	1.31571700	2.91846100
H	2.13687200	1.09281200	2.85370600
C	0.46424400	-2.19311300	2.18080100
H	-0.42300500	-2.01524200	2.80526900
H	0.22448600	-3.05168900	1.54169900
H	1.25100800	-2.51594000	2.87649500
H	4.33199100	4.76658500	0.96871400
C	4.14220000	3.75065100	0.63474300
C	3.30901800	3.52261500	-0.46172600
C	4.74479400	2.67595100	1.29586300
C	3.07509300	2.21700400	-0.89430600
H	2.85476400	4.35803800	-0.98604200
C	4.51126000	1.37185300	0.86745700
H	5.40300700	2.85721800	2.14020600
C	3.66657800	1.13983900	-0.22602400
H	2.44377400	2.03575100	-1.76154600
H	4.99329600	0.53510000	1.36295400
C	3.42775400	-0.24851900	-0.71970500
O	2.51365000	-1.04245600	0.15940700
O	4.59951300	-1.01275600	-0.71239000
H	2.95757500	-0.25714900	-1.71048600
C	2.84771700	-2.45744500	-0.09635700
C	4.29200400	-2.34759100	-0.54466800
H	2.75818400	-2.96337900	0.86586400
C	1.92269300	-3.07784400	-1.13693500
C	5.17283300	-3.32051200	-0.74554000
H	2.22819000	-4.11518300	-1.30774200
H	0.88565900	-3.07350500	-0.79167100
H	1.98547800	-2.54985700	-2.09338900
H	4.90940500	-4.35302600	-0.54756500
H	6.17581800	-3.10435400	-1.09428200

anti-14

C	1.87480900	-0.72493800	2.56812500
O	3.16674300	-0.77708200	1.78281100
C	3.42026800	0.09834600	0.88510500
O	0.67255900	-0.18507000	0.60374600
C	0.78125200	-1.08729600	1.58637300
C	0.06409000	-2.20874700	1.76815500
H	2.03917900	-1.52647600	3.28600800

H	2.78973200	0.98109100	0.81966000
H	0.27759300	-2.87272700	2.59783600
H	-0.74009600	-2.48983600	1.09809900
C	4.52133100	-0.05926500	-0.00157700
C	4.77099600	0.97374500	-0.93702600
C	5.35760000	-1.20285200	0.03758200
C	5.83991300	0.86531200	-1.81495400
H	4.11943200	1.84248100	-0.96763300
C	6.42165500	-1.29775800	-0.84300600
H	5.15484200	-1.99081000	0.75496500
C	6.66217700	-0.26667100	-1.76538100
H	6.03710200	1.65197700	-2.53563400
H	7.06933900	-2.16817600	-0.82265600
H	7.49896600	-0.35028800	-2.45287100
C	1.72208400	0.61583900	3.26679400
H	0.88194900	0.53643100	3.96401000
H	2.61757600	0.86586900	3.84414600
H	1.49156600	1.42372800	2.56806600
Al	-0.16030400	-0.08479300	-1.01467000
C	-0.74436900	-1.78346400	-1.80258400
H	-1.19286100	-1.60955800	-2.78996400
H	0.12008800	-2.44215900	-1.96737100
H	-1.47674100	-2.35486300	-1.22314800
C	0.88313900	1.21762100	-2.07050600
H	1.14510700	2.14895400	-1.54917700
H	1.83154400	0.74755000	-2.37009600
H	0.38993200	1.50541300	-3.00750900
H	-1.55185700	2.76319700	-2.39228000
C	-2.17506700	3.07605800	-1.55065800
C	-1.73329200	2.38978400	-0.26487600
H	-2.07871900	4.16025200	-1.43272400
H	-3.22171400	2.84795000	-1.77155600
O	-1.79417500	0.92227100	-0.43344900
C	-2.66909100	2.60923200	0.90084800
H	-0.70269700	2.64737800	-0.01052700
C	-2.76310200	0.37039700	0.56285400
O	-3.48168200	1.49970200	0.98703500
C	-2.78994900	3.66805200	1.69303200
C	-3.66521600	-0.66685500	-0.02710700
H	-2.15698800	-0.02736800	1.38520800
H	-3.53650300	3.69600000	2.47820700
H	-2.16796800	4.54351500	1.54377200
C	-3.80296200	-1.89722400	0.62326000
C	-4.41207900	-0.40050500	-1.18159000

C	-4.67527700	-2.86309000	0.11876700
H	-3.23669600	-2.09659000	1.52989200
C	-5.27756700	-1.36705600	-1.68655000
H	-4.31401700	0.55765100	-1.68268100
H	-4.78193700	-3.81592400	0.62847800
C	-5.40937200	-2.59878000	-1.03767500
H	-5.85350300	-1.16073800	-2.58375500
H	-6.08707600	-3.34949000	-1.43363200

syn-14

C	2.34333400	0.32459900	0.38915500
C	1.89568700	2.48636900	-0.52893100
H	1.43814800	0.47286500	0.97720600
O	2.79567300	1.30579900	-0.29597000
O	0.25198800	0.93053000	-1.16822800
C	0.91723900	2.01932800	-1.58924300
C	0.76916100	2.66018500	-2.75932200
H	0.02490500	2.35025500	-3.48400700
H	1.36618100	3.52816300	-3.00649000
H	1.36018600	2.62904900	0.41651300
C	2.80713400	3.65391800	-0.83575200
H	2.20544600	4.55705500	-0.96927500
H	3.49729700	3.82553500	-0.00520000
H	3.38581600	3.47955200	-1.74641100
C	3.04190000	-0.91517700	0.44622400
C	4.19768000	-1.16036500	-0.33418000
C	2.55245000	-1.90960900	1.32519600
C	4.84526900	-2.38012600	-0.22707100
H	4.56061200	-0.39283000	-1.00928600
C	3.21124900	-3.12687000	1.42479300
H	1.66514600	-1.70934500	1.91944200
C	4.35421600	-3.35931400	0.65025200
H	5.73086000	-2.58020700	-0.82143600
H	2.84487200	-3.89410700	2.09898800
H	4.86860500	-4.31279000	0.72837400
Al	-0.86284700	-0.22230300	-2.01211800
C	-2.18219600	0.62037100	-3.21128900
H	-1.78424200	0.71639500	-4.23095300
H	-3.10374700	0.02984700	-3.30898400
H	-2.48720600	1.62875100	-2.90127700
C	0.05015300	-1.91194700	-2.43812300
H	0.82074100	-1.73222800	-3.20124800
H	0.56304300	-2.36365100	-1.57882400

H	-0.61602400	-2.67583200	-2.85980200
H	-1.45172900	-3.31549500	-0.44070300
C	-2.40100500	-3.05015300	0.03165200
C	-2.95670600	-1.76250500	-0.56052400
H	-3.11311100	-3.86293600	-0.14356600
H	-2.25694500	-2.95008100	1.11166000
O	-1.97595400	-0.66592000	-0.38193700
C	-4.17029300	-1.21996000	0.15890700
H	-3.14144600	-1.86783400	-1.63337400
C	-2.62673500	0.41743100	0.40205900
O	-3.73307300	-0.20824900	0.99248900
C	-5.43273800	-1.62460700	0.10400900
C	-1.71561300	0.98905100	1.44879500
H	-2.94753600	1.17420400	-0.32314700
H	-6.19946600	-1.14665100	0.70253000
H	-5.71839400	-2.45993600	-0.52521900
C	-1.47615500	2.36492100	1.47487100
C	-1.16128000	0.16729500	2.43913600
C	-0.67883000	2.92141200	2.47912400
H	-1.92151900	3.00509500	0.71754900
C	-0.35866400	0.72079600	3.43647100
H	-1.37798900	-0.89692800	2.43926400
H	-0.51391000	3.99472600	2.50650000
C	-0.11535100	2.09925500	3.45679000
H	0.05514200	0.08540000	4.21470300
H	0.49476100	2.53082500	4.24518300

anti-TS5

C	-3.74659300	-0.28895600	0.69523900
C	-2.16666900	0.60348700	-0.76885400
C	-1.80039400	0.45815800	1.70206400
O	-0.13179000	-0.26338000	0.14676700
C	-1.29532900	0.28877500	0.25941700
O	-3.25324800	0.56592500	1.57872600
H	-1.49631800	1.42302500	2.11939600
H	-3.31368700	-1.28401300	0.63628800
H	-2.89694800	1.39262900	-0.66106400
H	-1.91796000	0.32429100	-1.78848000
C	-5.08775700	-0.10350200	0.21647900
C	-5.70826500	-1.16346200	-0.47937100
C	-5.79121600	1.10123400	0.43817600
C	-7.00937700	-1.02145900	-0.94369700
H	-5.16404400	-2.08888900	-0.64957700

C	-7.09324500	1.23028700	-0.02366100
H	-5.31180200	1.91096000	0.97814900
C	-7.70076400	0.17347500	-0.71536500
H	-7.48856100	-1.83558700	-1.47784800
H	-7.64162900	2.15062200	0.15059300
H	-8.71893400	0.28313900	-1.07706800
C	-1.39879100	-0.66830900	2.64735700
H	-0.31500000	-0.66180000	2.78492100
H	-1.87455200	-0.51679700	3.62002900
H	-1.67797800	-1.65464000	2.26423700
Al	0.91147100	-0.66929600	-1.35356400
C	0.36236700	-2.45244200	-1.98329700
H	-0.61830500	-2.37974100	-2.47522600
H	1.03910700	-2.87666700	-2.73582100
H	0.25225200	-3.20089600	-1.18745200
C	1.16456000	0.87245500	-2.53565900
H	1.26342900	1.82690500	-2.00615100
H	2.06927100	0.75509200	-3.14668600
H	0.32879200	0.97597700	-3.24085200
C	4.73528200	2.84542000	-0.88143400
C	4.43931400	1.54802500	-0.47319100
C	3.93705600	3.91325400	-0.45870500
H	5.59090700	3.02760200	-1.52467400
C	3.33745200	1.31269700	0.35956600
H	5.06606800	0.71907900	-0.78714200
C	2.84370900	3.68334600	0.37711300
H	4.17320700	4.92452200	-0.77675500
C	3.01120300	-0.07131500	0.81870700
C	2.54519900	2.38290300	0.78627000
H	2.23056000	4.51327200	0.71542900
H	2.18613000	-0.08714000	1.53890300
O	2.56085600	-0.95384800	-0.31314000
O	4.13106000	-0.74021800	1.32050500
H	1.70055900	2.20025800	1.44636000
C	3.18551200	-2.28457400	-0.15084300
C	3.96841200	-2.09884400	1.12926800
H	2.37977000	-3.01223700	-0.03457700
C	4.04818100	-2.60028600	-1.36584000
C	4.48895200	-3.01494700	1.93610200
H	4.48273700	-3.59823700	-1.24972900
H	3.45187600	-2.59268200	-2.28269200
H	4.86378500	-1.87793900	-1.46147100
H	5.05658400	-2.72882100	2.81392800
H	4.38374200	-4.07079100	1.71345400

syn-TS5

C	-3.62784700	-0.02826900	-0.78095600
C	-2.22960000	-0.09244300	1.08946400
H	-3.11887300	-0.86482900	-1.25676000
O	-3.14158400	1.18758000	-0.97627000
O	-0.09040600	-0.25500300	0.01727500
C	-1.27324300	0.24725600	0.14886000
C	-1.68341300	1.17996200	-0.99288500
H	-2.04026500	-0.90763700	1.78194800
H	-3.00112500	0.60745500	1.37785100
H	-1.35269400	0.71205000	-1.93026900
C	-1.18325900	2.61022700	-0.89465300
H	-0.08944200	2.61171700	-0.89551100
H	-1.53362400	3.19528900	-1.74970100
H	-1.53535900	3.08098200	0.02777900
C	-5.00838200	-0.18574900	-0.41638900
C	-5.79085300	0.91297000	0.00214500
C	-5.58474900	-1.47181300	-0.49390100
C	-7.12641800	0.72064800	0.32610000
H	-5.34440300	1.90039500	0.05462800
C	-6.92036600	-1.65492300	-0.15988600
H	-4.97977700	-2.31596900	-0.81473400
C	-7.68999400	-0.56015800	0.24882000
H	-7.73477100	1.56289900	0.64018600
H	-7.36562000	-2.64284500	-0.21959000
H	-8.73482700	-0.70412900	0.50787800
Al	0.97282000	-1.26353900	1.15833600
C	1.24417900	-0.36585400	2.88303000
H	1.27651200	0.72745100	2.81559300
H	0.42384700	-0.61801900	3.56890200
H	2.16437300	-0.69023500	3.38806500
C	0.46110200	-3.15826600	1.00852600
H	-0.51863500	-3.31874400	1.48052400
H	0.37294700	-3.53294300	-0.01914600
H	1.15612000	-3.82391900	1.53822700
H	3.10062100	4.19384700	1.99274700
C	3.10435700	3.51309100	1.14688800
C	3.38724100	2.16032100	1.34473500
C	2.84356200	3.98743000	-0.13879700
C	3.40437200	1.27961200	0.25851200
H	3.60664000	1.79282700	2.34350800
C	2.86589100	3.10970900	-1.22893400

H	2.63574900	5.04194400	-0.29660700
C	3.76852400	-0.15532700	0.47915100
C	3.14658200	1.75961100	-1.03279600
H	2.68313400	3.48379000	-2.23231000
H	4.01343500	-0.36664800	1.52542300
O	2.64697200	-1.09898400	0.13419600
O	4.80148100	-0.55900300	-0.37222600
H	3.18799800	1.08193100	-1.87987900
C	3.20487700	-2.23420500	-0.63491600
C	4.68062500	-1.91241000	-0.62369000
H	2.98244100	-3.14550900	-0.07690000
C	2.58351300	-2.27099200	-2.02493200
C	5.71753600	-2.70553000	-0.86107400
H	2.96999100	-3.13869500	-2.56895700
H	1.49505900	-2.36080200	-1.96249200
H	2.83722600	-1.36936900	-2.58966700
H	6.73081900	-2.32153500	-0.84035100
H	5.56873800	-3.75085200	-1.10709500

TS6-a

C	1.89305000	-0.09783400	2.25092100
C	4.01636800	1.73040400	0.23248600
O	1.46416100	0.16535000	-0.07235300
C	2.12144300	-0.39376000	0.94767600
H	2.50634100	-0.60805200	2.99215800
C	0.83681300	0.83061700	2.77321100
H	1.26438400	1.59762200	3.43282700
H	0.09542500	0.29016200	3.37781900
H	0.30893600	1.33225500	1.95853600
Al	0.08968400	0.21925900	-1.22875600
C	0.23607900	1.97024200	-2.13896500
H	1.11939200	1.89478900	-2.79263800
H	0.37015400	2.86422200	-1.51769600
H	-0.60312700	2.17801600	-2.81490000
C	-0.02612000	-1.25315900	-2.53712600
H	-0.95551700	-1.19420300	-3.11821800
H	0.78586000	-1.08679000	-3.26103800
H	0.07265100	-2.28955000	-2.19852500
C	3.28304500	-1.32961100	0.57372300
H	3.38716600	-2.06109000	1.38643700
H	3.07568800	-1.41849900	-1.60543000
H	2.09863800	-2.59030800	-0.72558400
H	3.83532800	-2.85310400	-0.88611800

C	3.06804900	-2.08727300	-0.74115300
H	3.88084400	1.79549100	1.31493200
O	4.46694900	0.65671100	-0.24987400
C	4.62534300	-0.55673900	0.63348900
H	4.76616500	-0.15655500	1.64182100
H	5.99754900	-2.18984400	0.72099500
H	6.75871400	-0.64985900	0.28909600
C	5.86868400	-1.26876500	0.14333100
H	5.79062600	-1.53346100	-0.91363800
C	3.63500200	2.82887400	-0.65802600
H	3.84599000	3.80067100	-0.20218000
H	4.09314900	2.73211700	-1.64458900
H	2.53958300	2.74806800	-0.77957700
H	-0.06114600	-1.90326500	1.17119300
C	-0.98565500	-2.22573700	0.68415600
C	-2.02553200	-1.12298100	0.70554800
H	-1.38526500	-3.06845700	1.25987500
H	-0.76326200	-2.58147800	-0.32066400
O	-1.54015300	0.12440600	0.03296000
C	-3.41116500	-1.50175400	0.13526500
H	-2.16525200	-0.81722000	1.74979000
C	-2.53089200	1.18727500	0.35509100
C	-4.32867500	-0.30561300	0.25109900
H	-3.79700700	-2.28879200	0.79573700
C	-3.38736600	-2.03904000	-1.30852700
O	-3.74997600	0.87554000	-0.23626100
H	-2.61365300	1.14156200	1.44889900
C	-2.11418600	2.56342400	-0.09305600
C	-5.59184900	-0.30585800	0.68031700
H	-2.72980600	-2.90752800	-1.41210300
H	-4.39685600	-2.34609500	-1.59600400
H	-3.05866400	-1.27111500	-2.01310300
H	-2.85487200	3.26662100	0.29924300
H	-1.13489200	2.83262900	0.30726500
H	-2.10596600	2.64343200	-1.17955500
H	-5.99736400	-1.26614700	0.99452800
C	-6.51124200	0.87725000	0.73671300
H	-6.88704000	1.03092100	1.75625300
H	-6.01423200	1.79179000	0.40591400
H	-7.38958700	0.71484500	0.09926100

TS6-e

C	-2.10655000	-1.27746500	1.95264900
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C	-3.92496900	1.53221300	0.29488100
O	-1.40163600	0.18413700	0.22473900
Al	-0.01428400	0.65758000	-0.81530400
C	0.27787300	-0.40581900	-2.46046600
H	-0.04002300	0.19214900	-3.32665400
H	-0.27268200	-1.35463000	-2.51965600
H	1.33335100	-0.65259900	-2.63210500
C	-0.33956600	2.58533400	-1.12957800
H	-0.58000500	3.18602500	-0.24396000
H	-1.20745800	2.65319600	-1.80752100
H	0.46904400	3.10142200	-1.66139900
C	-2.11356800	-0.88308000	0.66650500
H	-2.74739700	-2.10363300	2.24186100
C	-1.26497300	-0.66867400	3.03771800
H	-0.63483000	0.13656000	2.65184700
H	-0.61483700	-1.42018200	3.50515500
H	-1.88870900	-0.26244000	3.84590800
C	-3.00660800	-1.50880100	-0.40930600
H	-2.33874900	-1.91232100	-1.18830500
C	-3.91570600	-2.64567500	0.07277900
H	-4.44700400	-3.10887100	-0.76306100
H	-4.65595800	-2.29965300	0.80148500
H	-3.31670700	-3.42753400	0.54603900
C	-4.53377300	2.28754100	1.39829700
H	-4.71172900	3.32208500	1.07436000
H	-3.79277400	2.35024900	2.20918500
H	-5.45360000	1.82545900	1.75908300
H	-3.00621300	1.87618200	-0.18611500
C	-3.75221500	-0.38958300	-1.16533400
H	-3.03100200	0.28894000	-1.62168600
C	-4.83696700	-0.78804900	-2.14174500
H	-4.39930200	-1.45109300	-2.89559900
H	-5.24179800	0.08695600	-2.65855000
H	-5.65532400	-1.31955200	-1.65072500
O	-4.44905100	0.46201300	-0.09934900
H	1.72439200	3.16732600	0.24640300
C	1.96052800	2.63817200	1.16767400
C	2.56545300	1.26791800	0.94120100
H	1.05449800	2.56451600	1.77678000
H	2.69053700	3.23503100	1.72605700
O	1.56365500	0.29381100	0.40859200
C	3.82572000	1.21149800	0.05108700
H	2.82613900	0.85457700	1.92260400
C	2.17986900	-1.05662800	0.52650800

C	4.29808700	-0.22584700	-0.02717800
H	4.59514500	1.78865600	0.57922300
C	3.63894000	1.81949900	-1.35346600
O	3.27309700	-1.13627800	-0.33009100
H	2.50762300	-1.09663000	1.57295800
C	1.21739100	-2.17902300	0.22888000
C	5.55638000	-0.65377400	0.09058200
H	3.33680300	2.87036800	-1.30507300
H	4.58559600	1.77007800	-1.89861900
H	2.89535900	1.26917600	-1.93786600
H	1.71104100	-3.11388800	0.51149900
H	0.30184800	-2.08189700	0.81730000
H	0.98109400	-2.23002100	-0.83349000
H	6.31338300	0.10753200	0.27109800
C	6.02718400	-2.07170800	-0.03459200
H	6.56501600	-2.38434400	0.86936900
H	5.19602200	-2.75998500	-0.20234100
H	6.73120000	-2.17349400	-0.87023000

TS7-a

C	1.14306600	-1.83212400	-0.95170700
C	2.53517600	-0.97337000	2.09683700
O	1.04486300	0.35788600	-0.07885200
C	4.04271300	-1.02006000	0.22544300
C	5.53750800	-0.77739800	0.24081400
H	5.77317500	0.28345800	0.35153900
H	6.01728000	-1.33296100	1.05179400
H	3.81334900	-2.08802300	0.27986100
H	4.60865600	1.22250500	-1.44679500
O	3.52130300	-0.44213500	1.52207500
H	3.38736500	1.71432400	-0.25784100
C	3.56269500	1.10579300	-1.14907100
H	2.94631300	1.50971600	-1.95526500
C	3.21879900	-0.37042600	-0.91390000
H	3.53112900	-0.93805600	-1.79930600
C	1.72416100	-0.63796900	-0.68423100
H	0.08169600	-1.90866600	-0.72347200
H	1.72996000	-3.91635800	-0.92611300
H	1.19800800	-3.33140800	-2.49040700
H	2.80289700	-2.90308000	-1.90148400
H	0.94505200	0.10135800	2.84505000
C	1.89631600	-0.30118400	3.23167000
H	2.50061800	0.52392200	3.61219800

H	1.64600700	-1.02145000	4.01800100
H	2.15240900	-1.91882100	1.70426700
Al	0.10663300	1.87108800	-0.32123000
C	0.44380300	2.92739800	-1.95300000
H	-0.45826600	3.45570600	-2.29031600
H	1.18534000	3.70658100	-1.72814700
H	0.82473700	2.36824500	-2.81587700
C	0.27185700	2.80926100	1.40909400
H	-0.25961700	3.76673300	1.45367400
H	-0.00933700	2.24300400	2.30643900
H	1.33964600	3.05382700	1.52089800
H	5.96043600	-1.12754900	-0.70641700
C	1.76208900	-3.04363400	-1.59375600
H	-5.09595600	-3.54285700	1.17453800
C	-5.25606400	-2.53870000	0.76111300
C	-4.15596500	-2.17877400	-0.19360000
H	-6.22278300	-2.56566200	0.24301700
H	-5.34525500	-1.84383300	1.60104700
C	-3.29844700	-1.16079000	-0.09287800
H	-4.02783800	-2.83102500	-1.05596100
O	-2.28361600	-1.05983700	-1.06094700
C	-3.19966300	-0.09969100	0.98340400
C	-2.19365400	0.20553300	-1.65156100
C	-3.01440500	1.27636700	0.30508400
H	-4.15695900	-0.04875400	1.51376600
C	-2.09339500	-0.45007100	1.99873200
O	-1.84497100	1.19657200	-0.61531800
H	-3.18258200	0.51972700	-2.00873400
C	-1.21482800	0.16937700	-2.79770600
H	-3.86458900	1.43430800	-0.36894300
C	-2.94550500	2.47681300	1.22784900
H	-2.03118300	0.29382600	2.79986900
H	-2.30928400	-1.41984500	2.45722100
H	-1.12104400	-0.51734800	1.50044500
H	-1.58360200	-0.57005800	-3.51493400
H	-1.16787300	1.14105900	-3.29112400
H	-0.21698500	-0.13656800	-2.47980300
H	-2.76342800	3.39223700	0.65753200
H	-3.92313600	2.57772300	1.71285100
H	-2.18877000	2.39192400	2.00547900

TS7-e

C	-0.77427800	-1.82891800	-0.37537300
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C	-3.43170700	-0.32695100	1.82415500
O	-1.18819500	0.39271600	0.25695500
Al	-0.17733300	1.85341300	-0.06794400
C	-0.27709800	2.31320700	-1.98675000
H	0.06228800	1.53538600	-2.68205000
H	0.24156600	3.24158100	-2.25040300
H	-1.33825500	2.49454000	-2.21874600
C	-0.62972700	3.23370800	1.26966200
H	-1.40837300	3.90011600	0.87176500
H	-1.00592600	2.84485500	2.22547100
H	0.22362700	3.88125800	1.51144000
C	-1.50430900	-0.70664500	-0.51259300
H	0.07756500	-1.70799000	0.29291600
C	-0.87096100	-3.20561000	-0.97842400
H	-1.82706700	-3.44317400	-1.44040100
H	-0.08874300	-3.35597000	-1.73550200
H	-0.68758500	-3.95686100	-0.20041000
C	-2.74629200	-0.42898200	-1.36920100
H	-2.46017100	0.39334200	-2.04487500
C	-3.29018100	-1.56473800	-2.24361300
H	-4.07621900	-1.19318200	-2.90742000
H	-3.70731200	-2.38667000	-1.65404500
H	-2.49895500	-1.96438800	-2.88041300
C	-3.82681400	0.23874600	-0.49005500
H	-3.44621200	1.17915600	-0.09261600
C	-5.21891200	0.39566400	-1.06170900
H	-5.15194700	0.98330900	-1.98353000
H	-5.86989600	0.93476500	-0.36714800
H	-5.67563500	-0.56715600	-1.30168200
H	-2.90974600	0.63068400	1.87481700
C	-3.47236800	-1.23752300	2.97726600
H	-2.43553700	-1.51547700	3.21950000
H	-3.85458800	-0.69963800	3.85501500
H	-4.06346200	-2.13189100	2.77579400
O	-3.98348000	-0.65346900	0.74579300
H	6.44224800	-2.20551200	0.53900900
C	5.54597600	-2.28474200	-0.08879600
C	4.31969400	-1.91144700	0.69106300
H	5.48837500	-3.32933600	-0.42093800
H	5.69979800	-1.66296400	-0.97504600
C	3.42499700	-0.96905600	0.38596800
H	4.12180000	-2.48857400	1.59288500
O	2.29502200	-0.85293600	1.21899700
C	3.40468800	-0.02830500	-0.80223100

C	2.04377400	0.45184800	1.64353800
C	3.00609500	1.38506700	-0.32219100
H	4.43107200	0.06989700	-1.17447200
C	2.52959500	-0.58126200	-1.94535300
O	1.74175700	1.28932100	0.46653400
H	2.95591500	0.89189900	2.06667300
C	0.93761400	0.45003600	2.66990400
H	3.74603900	1.71139800	0.41819400
C	2.92899200	2.45417800	-1.39261600
H	2.57250600	0.06094200	-2.83044100
H	2.89215200	-1.57162800	-2.23622500
H	1.48383900	-0.68572800	-1.64160000
H	1.26565000	-0.17914200	3.50252200
H	0.76121200	1.46116600	3.04249600
H	0.01693600	0.04377800	2.24999800
H	2.62303000	3.41310200	-0.96310600
H	3.93544100	2.58392500	-1.80649100
H	2.25639100	2.20109900	-2.20979500

S1

C	-1.18578800	-0.91094200	0.13487800
O	-0.24355000	0.13203100	-0.21138400
C	-0.89786700	1.36774500	0.11704500
O	-2.26495800	1.14219900	-0.13002000
C	-2.51583100	-0.20950000	-0.02588700
C	-3.73719900	-0.73106400	-0.07430500
H	-1.03177000	-1.74128400	-0.55452900
H	-1.00392600	-1.24192000	1.16484000
H	-0.51714200	2.14624100	-0.54256500
H	-0.72587600	1.60898400	1.17461800
H	-3.87637100	-1.80464600	-0.02669700
H	-4.61307400	-0.10017700	-0.16864100
Al	1.82101200	-0.12880600	-0.00264600
C	2.02767100	-1.77091200	-1.10283700
C	2.40210100	1.60368300	-0.78906500
H	1.65079400	-1.64647500	-2.12767300
H	3.09114300	-2.03460300	-1.19940900
H	1.53651200	-2.65927500	-0.68055400
H	3.49884800	1.63153300	-0.86786700
H	2.12450200	2.48673500	-0.19559800
H	2.02269100	1.76253500	-1.80850700
C	1.94729000	-0.32147800	1.97628800
H	1.41340800	-1.19653700	2.37431100

H	2.99776500	-0.45176200	2.27585500
H	1.58513500	0.55610000	2.53134500

S2

C	-2.73000600	0.13339000	0.26986000
O	-2.51959900	-1.16465800	-0.28971700
C	-1.16663400	-1.42178700	-0.11457900
O	-0.49704300	-0.13198400	-0.30140100
C	-1.45742600	0.86470500	-0.08465200
C	-1.21227100	2.16224900	-0.20476600
H	-3.62362400	0.56577200	-0.18270500
H	-2.86691000	0.06911700	1.36105900
H	-0.80946000	-2.11195000	-0.87675700
H	-0.92452900	-1.77038000	0.89882600
H	-2.01309400	2.87304600	-0.03490400
H	-0.23286900	2.54290600	-0.46518200
Al	1.61620800	-0.04262600	0.08590600
C	1.54800600	0.26561300	2.04827200
C	2.21145600	1.43815100	-1.09809300
H	1.02896800	1.19524400	2.31898200
H	1.06211200	-0.54922200	2.60389900
H	2.56422700	0.35015700	2.46066300
H	1.69761700	1.44565800	-2.06945300
H	3.28176900	1.31966500	-1.32329000
H	2.10120100	2.44046600	-0.66227000
C	2.03658400	-1.88405100	-0.54569600
H	3.12570900	-2.03517400	-0.50331800
H	1.60110600	-2.69360800	0.05692600
H	1.75195400	-2.06403000	-1.59239000

TS-S1

C	-1.03976000	-1.61692000	-0.90481900
O	-0.32375900	0.69211000	-0.58129600
C	-1.55304000	0.88166800	-0.14377800
C	-2.07711900	-0.23597600	0.73358700
O	-1.52589300	-1.53737600	0.26607400
C	-2.36153600	1.91205500	-0.45912100
Al	1.36625600	0.14765900	0.10556200
C	1.10761700	-0.24042500	2.05658600
C	2.59539200	1.64201400	-0.34653100
H	-0.49633400	-2.53207000	-1.11174500
H	-1.30470300	-0.92362600	-1.69476100

H	-3.38596400	1.94831500	-0.10414200
H	-1.98331900	2.75678700	-1.02383900
H	-1.70525800	-0.20107500	1.75856200
H	-3.16378200	-0.33462600	0.71880700
H	0.50396200	-1.13219500	2.28368100
H	0.65521600	0.60417400	2.59943700
H	2.08348500	-0.41199200	2.53448500
H	2.28510300	2.58913700	0.11773900
H	3.62480100	1.45181100	-0.00900800
H	2.64955400	1.82642700	-1.42900400
C	1.84824600	-1.54565000	-0.94606500
H	1.60977200	-2.52154100	-0.50038800
H	1.59625800	-1.58334300	-2.01532200
H	2.94829400	-1.47421500	-0.91418800

S3

O	-1.93005700	-1.32709000	0.29885900
C	-1.87941400	0.02740900	0.95026600
C	-1.30993100	1.11439700	0.07468000
C	-2.14017700	2.08940500	-0.35637400
C	-1.59776200	-1.46515900	-0.94485900
O	-0.02910300	1.03050800	-0.23694400
H	-1.26504600	-0.15913700	1.83254500
H	-2.91453100	0.20972900	1.24025200
H	-1.76201800	2.91268400	-0.95293600
H	-3.18973500	2.09568700	-0.08495800
H	-1.80436600	-2.45381000	-1.34819300
H	-1.62180800	-0.59674600	-1.60409800
Al	1.47803300	0.02726600	0.07283300
C	3.04244000	1.04079700	-0.61628300
C	1.54723700	-0.64025000	1.95374600
H	3.23688100	1.93071600	-0.00121300
H	3.96393800	0.44234400	-0.60878000
H	2.89241800	1.39086400	-1.64619900
H	0.76917900	-1.37158500	2.22041000
H	1.48226200	0.17377100	2.69037100
H	2.50802400	-1.14192000	2.14183300
C	0.99822000	-1.51211500	-1.22758300
H	-0.12029900	-1.54907100	-0.90040300
H	0.97471300	-1.24424800	-2.29141800
H	1.34556500	-2.54798800	-1.13091800

TS-S2

O	-2.44332500	-1.01710800	0.26502900
C	-1.58415500	-0.11235400	1.10447800
C	-1.13583700	1.06309900	0.23200800
C	-2.12040300	1.87410800	-0.26309600
C	-2.27020000	-0.94406000	-0.99176400
O	0.10546200	1.09860100	-0.12599700
H	-0.74985200	-0.71950300	1.45562600
H	-2.25079300	0.14745700	1.92623600
H	-1.88220300	2.63522700	-0.99748600
H	-3.12724500	1.84409700	0.13992900
H	-2.96771100	-1.53203100	-1.58477700
H	-1.42594100	-0.43936700	-1.44495800
Al	1.59309200	-0.10462000	-0.03420700
C	3.05718100	0.89254000	-0.93044200
C	1.87347900	-0.51129100	1.91622400
H	3.30791000	1.82512100	-0.40556400
H	3.98503800	0.30438200	-0.98267300
H	2.80473300	1.17070100	-1.96356000
H	1.18364800	-1.23249900	2.38123300
H	1.85550800	0.39425500	2.53990600
H	2.87694200	-0.94572200	2.03927700
C	0.87590000	-1.70066200	-1.06042000
H	0.01972500	-2.18139100	-0.55344200
H	0.55942500	-1.43682100	-2.08217000
H	1.62774800	-2.49406700	-1.17706600

S4

O	-2.92306300	0.94593900	-0.17019800
C	-1.51965100	0.99095700	0.01536700
C	-1.04752400	-0.44296100	-0.14156700
C	-2.27844100	-1.31458100	-0.23070000
C	-3.37489900	-0.34888400	0.24402500
O	0.11044400	-0.84478500	-0.16700300
H	-1.23555900	1.34204400	1.02365000
H	-1.06336800	1.66155800	-0.71803400
H	-2.16463700	-2.23471800	0.34835000
H	-2.42100400	-1.58878400	-1.28506700
H	-4.34965300	-0.51960600	-0.21580800
H	-3.48585300	-0.39010100	1.33861800
Al	1.94371500	0.08085100	0.04407400
C	3.10976500	-1.36463000	-0.65165800
C	1.73349800	1.69389800	-1.11533300

H	2.90870100	-1.60342200	-1.70539600
H	4.17181000	-1.08452500	-0.59624900
H	3.00530700	-2.30008100	-0.08484200
H	1.16735100	2.52170300	-0.66517800
H	1.27788700	1.47808200	-2.09314800
H	2.73016800	2.10261700	-1.33982100
C	1.88139700	0.36454000	2.01704300
H	1.06674500	1.02313300	2.35280400
H	1.78797400	-0.57577600	2.57777300
H	2.81191700	0.83754700	2.36393700

S5

C	0.82308500	1.24584100	0.22208800
O	0.17219900	0.04663300	-0.29889000
C	0.90513200	-1.13855200	0.09716900
O	2.19808700	-1.12909600	-0.42705700
C	2.95791200	-0.02378300	-0.04920800
C	2.25792800	1.28596900	-0.30466300
C	4.19551100	-0.19812600	0.40693400
H	0.22748800	2.08670000	-0.13139000
H	0.77929900	1.20256600	1.31623100
H	0.37542200	-1.98571200	-0.33114400
H	0.91410700	-1.17395500	1.19424600
H	2.22378600	1.46918700	-1.38671000
H	2.79892200	2.11440300	0.16274700
H	4.82415600	0.65422100	0.63953900
H	4.61116400	-1.19258500	0.52686600
Cl	-2.20343200	-0.06590600	1.78270600
Al	-1.85675400	-0.01512000	-0.37912700
C	-2.18295100	-1.73314800	-1.28855300
C	-2.29819300	1.70837400	-1.22745500
H	-1.63334700	-1.82090700	-2.23614500
H	-1.94538400	-2.61631400	-0.68189000
H	-3.24916500	-1.81571500	-1.54111400
H	-2.12378200	2.58267400	-0.58768900
H	-3.36673100	1.72550600	-1.48315500
H	-1.75261400	1.86714100	-2.16803800

S6

C	-3.09283100	-0.74428100	0.27194300
O	-2.26328300	-1.37014100	-0.72170600
C	-0.93723200	-1.38744100	-0.37315600

O	-0.38776500	0.00134000	-0.41415100
C	-1.36933300	0.98858300	-0.16896300
C	-2.40713200	0.53220200	0.81541300
C	-1.28639800	2.15987600	-0.79070500
H	-4.02239600	-0.50752500	-0.24890600
H	-3.30911300	-1.45855400	1.07750600
H	-0.36918700	-1.94270300	-1.11412800
H	-0.75665900	-1.77046100	0.63861000
H	-3.13880500	1.32525000	0.98995300
H	-1.91527800	0.32157800	1.77356600
H	-2.00373900	2.94113800	-0.56648700
H	-0.50307400	2.37117400	-1.50846300
Cl	2.30851900	-1.64904600	-0.12678600
Al	1.55266300	0.38137000	0.19157800
C	1.30209200	0.81694200	2.09912000
C	2.24877100	1.67128600	-1.12234500
H	0.71666500	1.73340100	2.25380400
H	0.81713700	0.01198100	2.66748800
H	2.27713800	0.98462900	2.57682400
H	1.97736000	1.40988500	-2.15342300
H	3.34655500	1.68282700	-1.08354500
H	1.91471900	2.70075200	-0.93893700

TS-S3

C	-1.23816400	-1.84465100	-0.51480200
O	-0.24998500	0.40085500	-0.39421200
C	-1.21699400	1.32978500	-0.30484900
C	-2.59065400	0.71584600	-0.49572000
C	-2.89544000	-0.38664600	0.50880400
O	-2.05058100	-1.61437100	0.42442100
C	-1.05090800	2.64163700	-0.07754200
Al	1.53288800	0.35682300	0.12857100
Cl	1.70452800	-1.89296200	-0.18542600
C	1.67652400	0.75039500	2.06265200
C	2.67537600	1.28778600	-1.18804700
H	-0.65301700	-2.75021600	-0.40245000
H	-1.20505700	-1.25923300	-1.42393600
H	-1.90407200	3.30919500	-0.02771600
H	-0.06552200	3.07756500	0.04660800
H	-3.37373700	1.46855100	-0.34945200
H	-2.72162800	0.34148300	-1.52221500
H	-2.71663500	-0.05815000	1.53387500
H	-3.91163900	-0.77965800	0.42378600

H	2.70004700	0.58522600	2.42595900
H	1.02066100	0.11519600	2.67379700
H	1.42224600	1.79359100	2.29737100
H	2.47498400	0.95947900	-2.21651100
H	3.74143300	1.10405700	-0.99740700
H	2.53351100	2.37778200	-1.16553900

S7

C	-0.88170500	1.61272800	0.11693400
C	-2.18330600	1.08925900	0.70510700
C	-2.19926300	-0.40500100	1.02525200
O	-2.29281000	-1.30092000	-0.11295400
C	-1.36085200	-1.23394700	-1.07156100
O	0.20763400	1.13598600	0.75293300
C	-0.85659800	2.49147800	-0.89867100
H	-3.03285600	1.35426700	0.06650200
H	-2.34230900	1.58862100	1.67289400
H	-1.30930300	-0.68076300	1.59835400
H	-1.09660800	-0.23758800	-1.42326000
H	0.07616300	2.90131300	-1.27130000
H	-1.77857500	2.84060800	-1.35112000
H	-3.08646300	-0.65832700	1.60826600
H	-1.59658400	-1.94117200	-1.86369000
Al	1.67090100	0.29426500	0.22307500
Cl	0.38577500	-1.89753400	-0.46618800
C	2.41906800	0.77017000	-1.53327200
H	2.99728400	1.70293300	-1.47080900
H	3.10487500	-0.00375100	-1.90150100
H	1.65297400	0.92362000	-2.30307900
C	2.72428200	-0.39780800	1.72702800
H	2.09125600	-0.79834100	2.52796900
H	3.41153900	-1.19604400	1.41856200
H	3.34036400	0.39544800	2.17270200

TS-S4

C	-1.07837000	-1.42231900	-0.23105100
C	-2.22989200	-0.86012000	-1.04298400
C	-2.18442200	0.66827000	-1.04302700
O	-2.42790600	1.21627200	0.31322700
C	-1.60008700	0.98508800	1.24643500
O	0.09956100	-1.02214900	-0.67347500
C	-1.31512600	-2.16480400	0.88026800

H	-3.20091200	-1.21962700	-0.68865500
H	-2.11889300	-1.15657400	-2.09428900
H	-1.20269800	1.03986600	-1.34318700
H	-0.72971200	0.36930600	1.13166600
H	-0.49915700	-2.56128100	1.47484300
H	-2.32575500	-2.45622000	1.14446500
H	-2.98065600	1.12246800	-1.63061600
H	-1.85286000	1.44199800	2.20114000
Al	1.66010000	-0.25974100	-0.08247100
Cl	0.92700500	1.94475100	0.16663600
C	2.08681400	-0.87130100	1.75316800
H	2.39051400	-1.92797300	1.76527400
H	2.92394000	-0.29616600	2.17141200
H	1.25665700	-0.77539500	2.46781200
C	2.97036300	-0.31002800	-1.54948000
H	2.56249000	0.10235600	-2.48129000
H	3.87235800	0.26845100	-1.31055600
H	3.29537700	-1.33704600	-1.76670100

S8

C	-3.17234300	-0.72103100	-0.75471600
O	-3.52127200	0.43577400	-0.02312600
C	-2.42003200	1.31246700	0.14027300
O	0.21150600	-1.02005400	0.01900200
C	-0.93605700	-0.67145300	0.32944300
C	-2.10521900	-1.55664500	0.00476300
C	-1.28477600	0.64393300	0.96202800
H	-4.08539200	-1.30758400	-0.88012900
H	-2.79137200	-0.45241800	-1.75246800
H	-2.79178200	2.19178600	0.67019300
H	-2.02591700	1.63321000	-0.83523600
H	-2.55477800	-1.90314300	0.94430800
H	-1.77463700	-2.42197900	-0.57585200
H	-1.67115900	0.43859200	1.96923300
H	-0.41339000	1.29700100	1.02917800
Cl	1.61624700	1.73848400	-0.78833300
Al	2.05153600	-0.24323300	0.06920700
C	3.00285500	-1.43127900	-1.17474900
C	2.44645500	-0.18487100	2.00232800
H	3.05413800	-2.46339800	-0.80168700
H	2.52725000	-1.46387800	-2.16331600
H	4.03697800	-1.09736300	-1.33298000
H	1.74803400	0.43853800	2.57624200

H	3.44800000	0.23173600	2.17548400
H	2.44069300	-1.18579600	2.45576000

S9

C	-2.73949800	0.40014100	-0.43609000
O	-1.67260600	0.04109700	0.47176800
C	-2.30499100	-0.63808700	1.56611200
O	-3.56639100	-0.02894500	1.70465900
C	-3.93083000	0.51077400	0.48963400
C	-5.13229400	1.02579800	0.25037900
H	-2.46709900	1.33806900	-0.92125900
H	-2.85797200	-0.38837100	-1.18853400
H	-1.71160500	-0.48474800	2.46563100
H	-2.41217400	-1.70424500	1.32598800
H	-5.35463800	1.47442000	-0.71065400
H	-5.90713800	1.01657500	1.00775600
Al	0.38532300	0.17643900	-0.00407700
C	0.44103500	-0.73586200	-1.78915800
C	1.03613700	-0.71465300	1.67258900
H	-0.37647600	-0.34673800	-2.42439400
H	1.35128800	-0.34454500	-2.27653400
H	0.58498400	-0.17145600	2.52216500
H	0.64996600	-1.74641200	1.75236600
C	0.49873100	2.17807200	-0.09715900
H	0.68310800	2.57569600	0.91596300
H	-0.49657500	2.57341900	-0.36708500
C	2.56499800	-0.76102600	1.91579700
C	3.28628900	-1.61964700	0.86556000
C	2.90210300	-1.26248300	3.33037800
H	2.95917200	0.26379900	1.83227200
H	3.12389000	-1.24385500	-0.15218200
H	4.36875700	-1.64422200	1.04206300
H	2.92201400	-2.65541400	0.89411800
H	2.43357200	-0.63233200	4.09611100
H	2.53671800	-2.28822700	3.47598300
H	3.98457000	-1.26534100	3.51433000
C	1.53287400	2.80682400	-1.06081500
C	2.97110700	2.41766900	-0.68506300
C	1.40099400	4.33827300	-1.12437000
H	1.34157300	2.42036100	-2.07428400
H	3.12157100	1.33082200	-0.71641900
H	3.70285900	2.86973100	-1.36625800
H	3.21198800	2.75490100	0.33196500

H	0.39071300	4.63701500	-1.42989700
H	1.59380800	4.78488000	-0.13968500
H	2.11140000	4.78003800	-1.83582400
C	0.46032100	-2.27637000	-1.91373900
C	0.72928500	-2.73066700	-3.35903700
C	-0.83755600	-2.91540700	-1.39732900
H	1.28228600	-2.66275400	-1.29257600
H	1.67651400	-2.32235200	-3.73091000
H	0.77950600	-3.82465200	-3.44119400
H	-0.06650200	-2.38196400	-4.03145200
H	-1.00734400	-2.68167500	-0.33929800
H	-1.70477100	-2.55352000	-1.96856800
H	-0.81742500	-4.00791600	-1.49425400

S10

C	-2.84691900	0.29912700	0.65212900
O	-1.81485400	0.00386700	-0.34966500
C	-2.56472800	-0.15700900	-1.60988200
O	-3.75313400	-0.75824900	-1.23086900
C	-4.09901100	-0.28392900	0.02616300
C	-5.31833000	-0.38607200	0.53545400
H	-2.55751400	-0.18357200	1.58490200
H	-2.90087100	1.38460200	0.78520400
H	-2.00341200	-0.80919500	-2.27435700
H	-2.71199900	0.84648200	-2.02789100
H	-5.52587200	-0.05237700	1.54569100
H	-6.12856900	-0.81730500	-0.04061200
Al	0.06532100	-0.52148600	0.00131300
C	0.01073800	-0.96558300	1.92131400
C	0.56856700	-1.40961800	-1.68570300
H	-0.30081600	-0.07832200	2.49985700
H	-0.81724100	-1.68352200	2.04652500
H	-0.05422200	-2.31571900	-1.77808000
H	0.24474200	-0.76980600	-2.52467900
H	1.28284100	1.32550900	-2.21072600
C	1.60922400	1.82465800	-1.30142200
O	0.86765200	1.26388700	-0.15534100
O	1.24639600	3.16086300	-1.31887200
H	2.67631100	1.67574300	-1.10062500
C	0.81342200	2.34563800	0.83416500
C	1.10499000	3.57736400	-0.00221700
H	-0.18673000	2.34473700	1.27135000
H	1.56047100	2.15399000	1.60824100

C	1.19103400	4.84460700	0.37623100
H	1.02068600	5.12767100	1.40878700
H	1.41916000	5.62528600	-0.33999000
C	1.26617600	-1.56609300	2.60869400
H	1.53539700	-2.49033200	2.07870800
C	0.96108200	-1.94716700	4.06600900
H	1.83125400	-2.41032300	4.54480600
H	0.68920600	-1.06089600	4.65426100
H	0.12890700	-2.65747000	4.12666000
C	2.47395400	-0.61963200	2.54519500
H	2.76412800	-0.38237900	1.51200600
H	2.25878000	0.32381000	3.06572000
H	3.34989400	-1.06232900	3.03107300
C	2.04430200	-1.82379200	-1.93917000
H	2.69129700	-0.94190000	-1.79992700
C	2.23397500	-2.30327100	-3.38724600
H	3.27730500	-2.57686300	-3.58050800
H	1.61468700	-3.18646100	-3.58767500
H	1.95230600	-1.52790800	-4.10967100
C	2.51259500	-2.90106100	-0.95147900
H	3.55229600	-3.18605200	-1.14436800
H	2.45416200	-2.56135300	0.08946700
H	1.89933800	-3.80636500	-1.04264700

Me₄Al⁻

C	-1.06018000	-1.56154200	-0.78655800
C	0.02358400	-0.15307400	2.03577000
H	-0.59809200	-2.53978800	-0.57017600
H	-2.08883500	-1.61667400	-0.39202100
H	-1.15725800	-1.50686400	-1.88419100
H	0.63115600	0.63096300	2.51864400
H	0.43328100	-1.11517200	2.38774300
H	-0.98432000	-0.07236900	2.47739500
C	-0.88376800	1.76354100	-0.53900300
H	-1.90161600	1.86866400	-0.12682900
H	-0.32210700	2.64751900	-0.19182600
H	-0.98437900	1.87720800	-1.63177700
C	1.91886200	-0.04870000	-0.70782500
H	2.54666700	0.74978500	-0.27757500
H	2.43190700	-0.99787300	-0.47874200
H	1.97732100	0.07380400	-1.80259700
Al	0.00194500	-0.00004300	-0.00325800

Bu₄Al⁻

C	1.14116000	1.67466100	-0.60857400
C	-1.37785000	-0.28538100	-1.57277200
H	0.43273700	2.43507300	-0.98326400
H	1.75287300	1.41861700	-1.49537200
H	-0.89162900	-0.10112200	-2.55077100
H	-1.59471100	-1.36935300	-1.58004100
C	1.12996100	-1.64878500	0.20278600
H	0.45221000	-2.51465400	0.33376700
H	1.61785400	-1.53955300	1.18946900
C	2.06350500	2.36751200	0.41715700
C	2.64676500	3.69327600	-0.11163300
C	3.20539600	1.45070400	0.88210900
H	1.46452600	2.61543900	1.30872100
H	1.84670800	4.38292600	-0.41051100
H	3.27193700	4.20648400	0.63619100
H	3.27108700	3.51306100	-0.99885300
H	2.81729000	0.53360100	1.33592500
H	3.83288100	1.15481700	0.02909800
H	3.85734400	1.94849200	1.61532700
C	2.21780400	-2.05763900	-0.81251800
C	1.61737300	-2.43818100	-2.17501300
C	3.10576700	-3.20909700	-0.29977300
H	2.88061900	-1.19292100	-0.97895000
H	1.02605800	-1.61767800	-2.59379300
H	2.39611400	-2.70881600	-2.90358900
H	0.94671400	-3.30338300	-2.07108000
H	3.58657900	-2.94166300	0.64996000
H	2.50192600	-4.11013500	-0.11873600
H	3.89930000	-3.47842000	-1.01478000
C	-2.73088300	0.45850500	-1.58342600
C	-3.67676800	-0.05268000	-2.68817100
C	-2.55474800	1.97901500	-1.71468300
H	-3.23444000	0.27382400	-0.62121900
H	-3.85082900	-1.13174600	-2.58700900
H	-4.65692500	0.44974100	-2.66886900
H	-3.23701200	0.11568100	-3.68195400
H	-1.95482000	2.37915000	-0.89108400
H	-2.03531300	2.22957100	-2.65066500
H	-3.52178100	2.50376800	-1.72070500
C	-0.89259300	0.45054900	1.73893000
H	-1.71110300	1.18503800	1.61522700
H	-0.13617400	0.98772000	2.34086800

C	-1.42631300	-0.71399100	2.60030400
H	-0.61764600	-1.45325100	2.72024400
C	-2.60269700	-1.43644700	1.92532800
H	-2.32486700	-1.80313000	0.93158400
H	-2.95535000	-2.29105800	2.52168200
H	-3.45245400	-0.75083500	1.79605800
C	-1.83738600	-0.26659800	4.01718900
H	-2.64400800	0.47920300	3.96718900
H	-2.19711600	-1.10439100	4.63549600
H	-0.99381200	0.19963500	4.54249500
Al	-0.00120900	0.04674800	-0.07319200

Me₂AlCl₂⁻

C	0.00035600	1.43539100	-1.69580200
Cl	1.81094800	-0.94558400	-0.00036600
C	0.00073400	1.43416200	1.69664500
H	-0.88418800	2.08500200	-1.77616700
H	0.88577600	2.08390500	-1.77564800
H	0.00023800	0.78293100	-2.57967100
H	0.00148900	0.78076000	2.57982800
H	-0.88434300	2.08293100	1.77809600
H	0.88563600	2.08331300	1.77677500
Cl	-1.81161400	-0.94471200	-0.00017600
Al	0.00001200	0.38606700	0.00007400

Me₃Al

Al	-0.00032400	-0.00012400	-0.00106500
C	0.71476600	1.84065100	-0.00053100
C	-1.95202100	-0.30160200	-0.00098700
H	-0.06218900	2.61163300	-0.06556600
H	1.29471800	2.03896500	0.91246700
H	1.40894100	2.00161200	-0.83740800
H	-2.23120600	-1.35867100	-0.08449800
H	-2.44277800	0.23568500	-0.82456400
H	-2.40920800	0.08273700	0.92250300
C	1.23734100	-1.53902100	0.00211500
H	0.99324300	-2.25259000	0.80135400
H	1.16314900	-2.10437900	-0.93841200
H	2.28902400	-1.25355200	0.12438400

Bu₃Al

Al	0.18105400	-0.23814800	-0.32430300
C	-0.11812400	1.48079400	0.63594500
C	2.01240100	-0.84459800	-0.80212700
H	0.83128400	2.03716400	0.69456400
H	-0.37065600	1.24523500	1.68409400
H	2.04409000	-1.94650000	-0.76512000
H	2.14728900	-0.60731300	-1.87315900
C	-1.36573700	-1.34740900	-0.90705400
H	-0.99798500	-2.33632000	-1.22573900
H	-1.77668300	-0.89233600	-1.82506100
C	-1.21016700	2.41422900	0.06172400
C	-0.88393200	2.83732300	-1.37930900
C	-1.42404700	3.65327500	0.94677900
H	-2.16099000	1.86010100	0.03644700
H	-0.81436200	1.97113700	-2.05330800
H	-1.65138400	3.50455900	-1.78984500
H	0.07619000	3.36842000	-1.42286900
H	-1.69483000	3.36620600	1.96968900
H	-0.50626800	4.25365700	1.00307100
H	-2.22166900	4.29837400	0.55599200
C	-2.51988900	-1.54642900	0.10408900
C	-2.02501900	-2.22373300	1.39177700
C	-3.68113400	-2.34697400	-0.50833600
H	-2.91345300	-0.55642200	0.38123100
H	-1.25672100	-1.62240900	1.89912100
H	-2.84046200	-2.37759800	2.10886600
H	-1.58611500	-3.20611300	1.17225100
H	-4.07020800	-1.85431300	-1.40723700
H	-3.34865600	-3.35234800	-0.79886300
H	-4.51242500	-2.46144300	0.19942300
C	3.21024200	-0.27781700	-0.00796900
C	4.55407800	-0.72695400	-0.60606000
C	3.12976400	-0.66596400	1.47650300
H	3.17634900	0.82113500	-0.06484000
H	4.64264500	-0.42213100	-1.65566200
H	5.40435100	-0.29964200	-0.05880300
H	4.64915600	-1.82040400	-0.56962300
H	2.21365200	-0.28302600	1.94621000
H	3.13432000	-1.75789800	1.59435800
H	3.97922800	-0.26830400	2.04497200
Me ₄ Al ₂ Cl ₂			
C	-2.53492300	-1.75725000	-0.00021600

Cl	-0.00026800	-0.00004800	-1.65529200
C	-2.53538200	1.75703700	0.00021200
H	-3.17610300	-1.88461200	0.88194100
H	-3.17451800	-1.88464200	-0.88353400
H	-1.81079200	-2.58014400	0.00041300
H	-1.81180600	2.58040000	-0.00109800
H	-3.17490100	1.88449200	0.88357600
H	-3.17689800	1.88345100	-0.88185900
Cl	0.00002400	-0.00000500	1.65539600
Al	-1.67504800	0.00001500	0.00012100
Al	1.67491700	0.00006000	-0.00002200
C	2.53531100	1.75706700	-0.00038300
H	3.17478200	1.88423800	-0.88382300
H	1.81174600	2.58045000	0.00072700
H	3.17684100	1.88367900	0.88164700
C	2.53553900	-1.75682800	0.00012000
H	3.17575800	-1.88363400	0.88307900
H	1.81210000	-2.58031900	-0.00012900
H	3.17637400	-1.88360400	-0.88238700

S11

C	-0.77912400	1.60689500	0.29636100
O	-1.20473300	0.32311300	-0.21890000
C	-0.09212000	-0.54441100	-0.07048300
O	1.05450600	0.29851500	-0.29046800
C	0.67084500	1.63567500	-0.10294700
C	1.48777800	2.66320800	-0.28215800
H	-1.38945400	2.37475800	-0.17711900
H	-0.91971600	1.62864200	1.38471100
H	-0.13360700	-1.31547200	-0.83493800
H	-0.04588000	-0.95993900	0.94178100
H	1.11611000	3.67116000	-0.13780000
H	2.52398200	2.53119000	-0.56628400
Al	3.03896700	-0.60184400	0.07557000
C	3.15825300	-0.19717400	2.01502200
C	4.17636200	0.40935500	-1.19819200
H	3.13973500	0.87912600	2.23349900
H	2.36284200	-0.66387300	2.61299700
H	4.10623600	-0.57606900	2.42438700
H	3.67779700	0.60965500	-2.15657300
H	5.06946400	-0.18492900	-1.44175000
H	4.54596400	1.36915100	-0.81276600
C	2.50317000	-2.43680700	-0.47225100

H	3.38574100	-3.09189100	-0.42227800
H	1.74589700	-2.91373800	0.16545900
H	2.14711300	-2.49785000	-1.51037300
Al	-3.21813800	-0.35544700	-0.01256300
C	-3.28812100	-0.51636500	1.96928000
H	-2.57416700	-1.24462100	2.37996700
H	-3.12222100	0.43263100	2.49923100
H	-4.28330100	-0.86322900	2.28433500
C	-3.03126600	-2.02323200	-1.07492200
H	-4.01141100	-2.50942000	-1.18680700
H	-2.66491900	-1.84550100	-2.09579000
H	-2.37590600	-2.77808900	-0.61756700
C	-4.10897200	1.20945400	-0.85025700
H	-3.74194000	1.41713800	-1.86499700
H	-5.18829100	1.02312700	-0.95017100
H	-4.01987000	2.14020800	-0.27202700

TS-S5

O	1.01895000	0.32790200	0.27794900
C	0.09570400	0.58479500	-0.90228200
C	-0.93950900	1.60447100	-0.44232500
C	-0.48420500	2.86866200	-0.17842700
C	0.56916300	0.66055400	1.43393400
O	-2.10938900	1.15860400	-0.12029500
H	-0.33374100	-0.38256800	-1.16087600
H	0.79155800	0.93380100	-1.66325600
H	-1.13446900	3.59458800	0.29674900
H	0.48716500	3.19831300	-0.53092800
H	1.29034700	0.57537400	2.24157100
H	-0.47860900	0.86792900	1.60513500
Al	-2.96759000	-0.55121100	0.02067900
C	-4.86324300	-0.09592100	0.39038400
C	-2.60979200	-1.52010500	-1.70499300
H	-5.32950000	0.45196100	-0.44047400
H	-5.47564100	-0.99429700	0.55514200
H	-4.97801000	0.53031700	1.28622400
H	-1.63183900	-2.01527200	-1.80535900
H	-2.73964300	-0.88033800	-2.59014600
H	-3.35461900	-2.32410200	-1.80153100
C	-1.93540200	-1.33193000	1.58365300
H	-0.87040100	-1.47879900	1.32514600
H	-1.98694300	-0.68266100	2.47161800
H	-2.30097700	-2.31653900	1.90561700

H	3.28710800	1.00330300	-2.26457500
C	3.78541500	1.02696100	-1.28630700
Al	3.29847100	-0.48047100	-0.09859200
H	3.59912300	2.01345400	-0.84064200
H	4.86435700	0.99276900	-1.49911400
C	2.75932000	-2.21750300	-0.86669800
C	3.78140900	-0.36761000	1.82185100
H	2.21341200	-2.12503500	-1.81462700
H	3.64980500	-2.82497000	-1.08623300
H	2.14030600	-2.81647400	-0.18635000
H	4.82118900	-0.70625900	1.94418500
H	3.75473100	0.64977200	2.23657300
H	3.18419600	-1.01869800	2.47505000

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C	1.27885400	1.81883100	0.45237800
O	1.19321900	0.36309100	0.30441800
C	0.18818700	-0.00589000	-0.63982600
O	-1.09061800	0.43757100	-0.18433600
C	-1.15743400	1.85813500	-0.05373400
C	-0.08954300	2.35832000	0.87348800
C	-2.09284400	2.52846700	-0.71254100
H	2.04187800	1.98772300	1.21071900
H	1.61360600	2.23255200	-0.50465000
H	0.16338600	-1.08983600	-0.68736800
H	0.40126000	0.45591000	-1.60857500
H	-0.30883100	2.02252200	1.89507400
H	-0.06423600	3.45222700	0.87184600
H	-2.16945500	3.60374800	-0.59132100
H	-2.81173100	2.02404500	-1.34856600
Cl	3.63888500	0.20039400	-1.67158600
Al	3.00664900	-0.66403100	0.23485400
C	2.42289800	-2.53811400	0.12202300
C	3.91821300	0.06980600	1.81783200
H	1.73982800	-2.82434300	0.93288000
H	1.94498700	-2.80844700	-0.82764900
H	3.30286400	-3.18999900	0.21483000
H	4.25475900	1.10773200	1.70434600
H	4.82032900	-0.52316700	2.02253100
H	3.30043600	0.01235900	2.72470800
Al	-2.65795200	-0.84097100	0.42509100
Cl	-3.97418600	-0.59836200	-1.29368000
C	-3.25775000	0.07445300	2.05833400

C	-1.71779200	-2.57010200	0.45430200
H	-2.49064200	0.07280000	2.84497500
H	-3.55860900	1.11463400	1.88619000
H	-4.13430900	-0.43990400	2.47486200
H	-1.36189800	-2.90878600	-0.52705800
H	-2.42487200	-3.33866000	0.79740500
H	-0.86925700	-2.60136200	1.15084400

TS-S6

C	-1.18816300	1.91037000	-0.02711300
C	-0.00773700	1.94961200	-0.97667200
C	0.49489000	0.53329500	-1.24187100
O	1.00956300	-0.09075200	0.02349800
C	0.19136400	-0.30035700	0.99365900
O	-2.17941200	1.16186400	-0.46912300
C	-1.10602100	2.49086400	1.20068700
H	0.80544000	2.58289400	-0.61190000
H	-0.32951300	2.32967800	-1.95537100
H	-0.30049800	-0.13301300	-1.57746800
H	-0.84010700	-0.03094400	0.94253000
H	-1.93663000	2.44534300	1.89717100
H	-0.24920200	3.09993600	1.46567300
H	1.36224600	0.50001300	-1.89659800
H	0.63558200	-0.75176700	1.87533600
Al	-3.31294100	-0.21816600	-0.02807800
Cl	-1.77752400	-1.99912100	-0.14547000
C	-3.82185400	-0.11617900	1.88141000
H	-4.48371800	0.74010400	2.07446300
H	-4.37229200	-1.01695400	2.18458200
H	-2.97533300	-0.02267700	2.57669500
C	-4.61189100	-0.45105800	-1.48412900
H	-4.12437000	-0.53156300	-2.46397100
H	-5.21337400	-1.35933300	-1.34909600
H	-5.31241000	0.39343400	-1.54022600
H	2.56167600	-2.82564400	-1.08278400
C	3.30032400	-2.03580400	-1.26835600
Al	3.32540100	-0.69349700	0.15595200
H	4.28073200	-2.52776000	-1.33193400
H	3.09900700	-1.61278400	-2.25942200
Cl	3.95467500	1.29134000	-0.41107900
C	3.32895900	-1.06672100	2.08297600
H	2.98465300	-0.22422700	2.69559800
H	4.36289700	-1.26511400	2.39837800

H	2.75124200	-1.95875200	2.35877700
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