Supporting Information

Why [4+2+1] but Not [2+2+1]? Why Allenes? A Mechanistic Study of the Rhodium-Catalyzed [4+2+1] Cycloaddition of *In Situ* Generated Ene−Ene−Allenes and Carbon Monoxide

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S1. Visual kinetic analysis of [4+2+1] reaction.

A solution of substrate **1b**, 1,3,5-trimethoxybenzene (internal standard), and $[Rh(CO)_2Cl]_2$ in anhydrous 1,2-dichloroethane was split into a reaction tube. The reaction mixture was stirred at 40 °C for an indicated time under a balloon of CO. After cooling, the 1,2-dichloroethane was removed through the rotary evaporator, and $CDCl_3$ was added. Nuclear magnetic resonance (NMR) spectra were measured on Bruker AVANCE III 400 (^{1}H at 400 MHz).

Since the substrate and product are stable, the conclusions obtained using the substrate concentration and the product concentration are consistent. In the determination of orders of the reaction, we used the concentration of the substrate as the vertical axis when making visual kinetic graphs. When the concentration of the product is chosen as the vertical axis, the conclusion obtained remains the same.

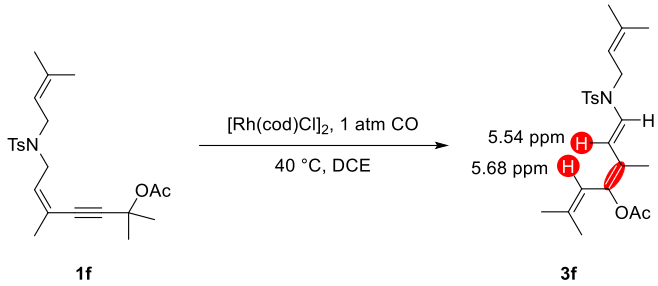
Table S1. Kinetic data for substrate **1b**.

[**1b**]$_0$	[cat]	[CO]/atm	time/min	[**1b**]/M	[**2b**]/M
0.050 M	5.0 mol%	1.0	0	0.05000	0.00000
0.050 M	5.0 mol%	1.0	30	0.04492	0.00458
0.050 M	5.0 mol%	1.0	60	0.03962	0.01024
0.050 M	5.0 mol%	1.0	90	0.03495	0.01375
0.050 M	5.0 mol%	1.0	120	0.03091	0.01914
0.050 M	5.0 mol%	1.0	150	0.02704	0.02165
0.050 M	5.0 mol%	1.0	180	0.02273	0.02615
0.050 M	5.0 mol%	1.0	210	0.01923	0.02866
0.050 M	5.0 mol%	1.0	240	0.01626	0.03288
0.050 M	5.0 mol%	0.2	0	0.05000	0.00000
0.050 M	5.0 mol%	0.2	45	0.04207	0.00537
0.050 M	5.0 mol%	0.2	105	0.03402	0.01320
0.050 M	5.0 mol%	0.2	150	0.02822	0.02032
0.050 M	5.0 mol%	0.2	195	0.02350	0.02549
0.050 M	5.0 mol%	0.2	240	0.01929	0.02898
0.050 M	2.5 mol%	1.0	0	0.05000	0.00000
0.050 M	2.5 mol%	1.0	50	0.04247	0.00463
0.050 M	2.5 mol%	1.0	100	0.03694	0.01289
0.050 M	2.5 mol%	1.0	150	0.03200	0.01620
0.050 M	2.5 mol%	1.0	200	0.02639	0.02289
0.050 M	2.5 mol%	1.0	250	0.02182	0.02778
0.030 M	5.0 mol%	1.0	0	0.03000	0.00000
0.030 M	5.0 mol%	1.0	50	0.01893	0.00609
0.030 M	5.0 mol%	1.0	100	0.01320	0.01219
0.030 M	5.0 mol%	1.0	150	0.00885	0.01589
0.030 M	5.0 mol%	1.0	200	0.00486	0.01966
0.030 M	5.0 mol%	1.0	250	0.00239	0.02183

0.070 M	5.0 mol%	1.0	0	0.07000	0.00000
0.070 M	5.0 mol%	1.0	50	0.05137	0.00848
0.070 M	5.0 mol%	1.0	100	0.04572	0.01689
0.070 M	5.0 mol%	1.0	150	0.03801	0.02479
0.070 M	5.0 mol%	1.0	200	0.03121	0.03095
0.070 M	5.0 mol%	1.0	250	0.02472	0.04039

S2. NOESY determination of triene structure.

In our original reports,[1] we proposed that the middle alkene of trienes (as side products) was in a *trans* configuration with respect to the connected two vinyl groups. Two triene products (**3a** shown in the main text of the present paper and **3f** shown below) were characterized by NMR. Based on DFT calculation results, we then decided to determine the stereochemistry of triene **3f** by NOESY. To our delight, the synthesized compound **3f**, in its NOESY spectrum, demonstrated a strong correlation between hydrogens in red color (Scheme S1). We excluded the interference of COSY signal and proved the reliability of NOESY signal (Figures S1 and S2). As a result, the middle double bond in this triene product should adopt a *cis* configuration. Therefore, we corrected the original stereochemistry of triene **3a** shown in Scheme 2a of the main text by analog to **3f** (NMR peaks of hydrogens in alkene moieties of **3a** are overlapped and its structure cannot be determined by NOESY).



Scheme S1. Preparation of **3f**.

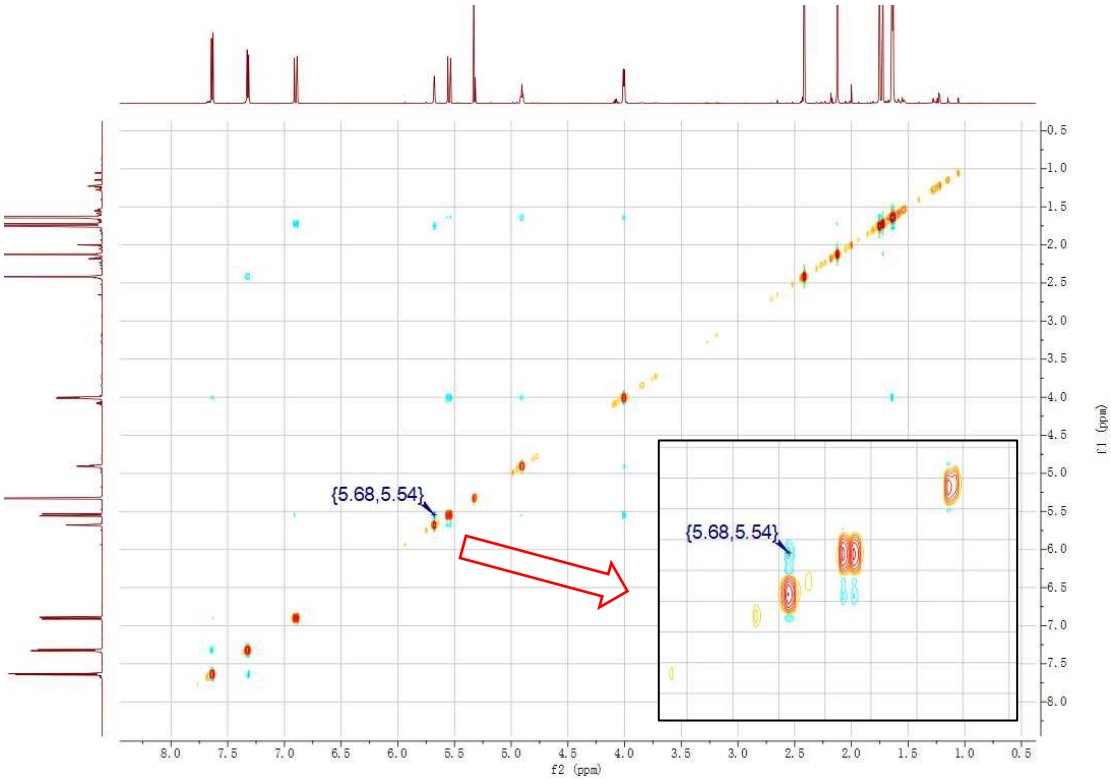


Figure S1. 2D NMR spectra of **3f** (NOSEY, 600 MHz, CD_2Cl_2).

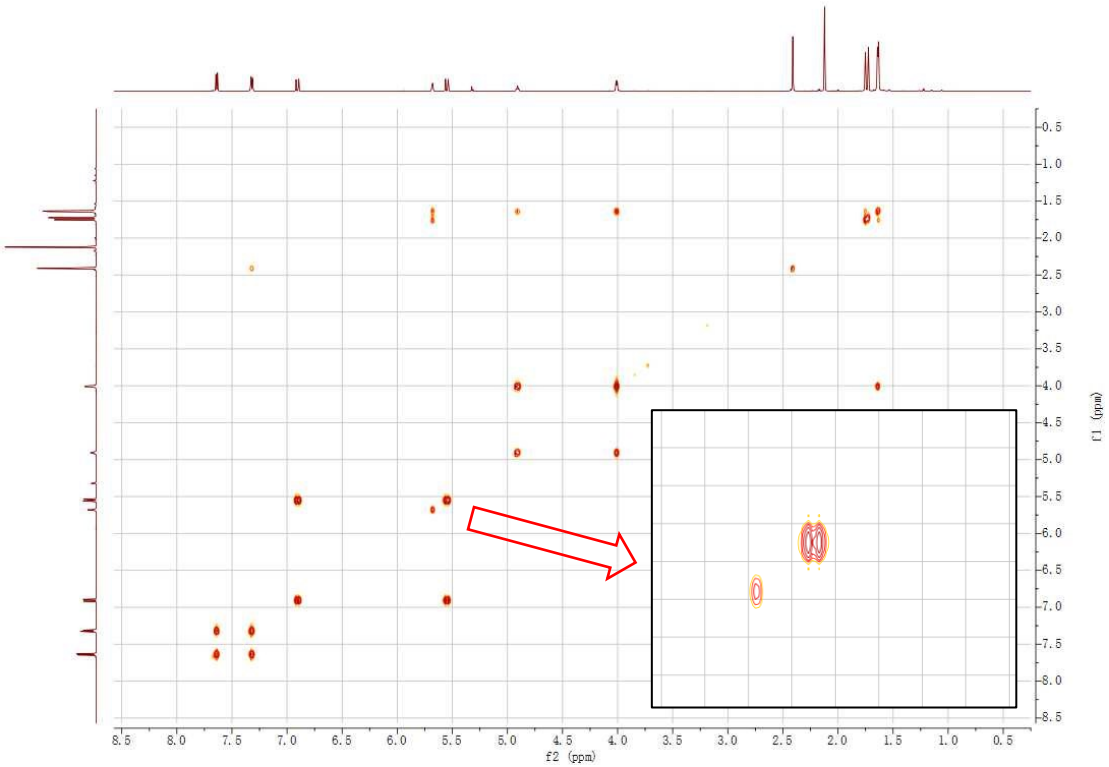


Figure S2. 2D NMR spectra of **3f** (^{1}H-^{1}H COSY, 600 MHz, CD_2Cl_2).

S3. Pathway starting from ene−alkyne oxidative cyclization.

The ene−ene moiety may undergo oxidative cyclization with rhodium, whereas the allene moiety could not participate in this (Figure S3). Intermediate **IN4** could undergo ene−ene oxidative cyclization via **TSS1** with an activation Gibbs free energy of 39.4 kcal/mol. The barrier of this process is very high, indicating that it is not favored compared to the concerted cycloaddition discussed in the main text. In addition, intermediate **IN6** could also undergo ene−ene oxidative cyclization via **TSS2** with an activation of Gibbs free energy of 63.2 kcal/mol, which is even higher. Therefore, ene−ene oxidative cyclization can be excluded for further study.

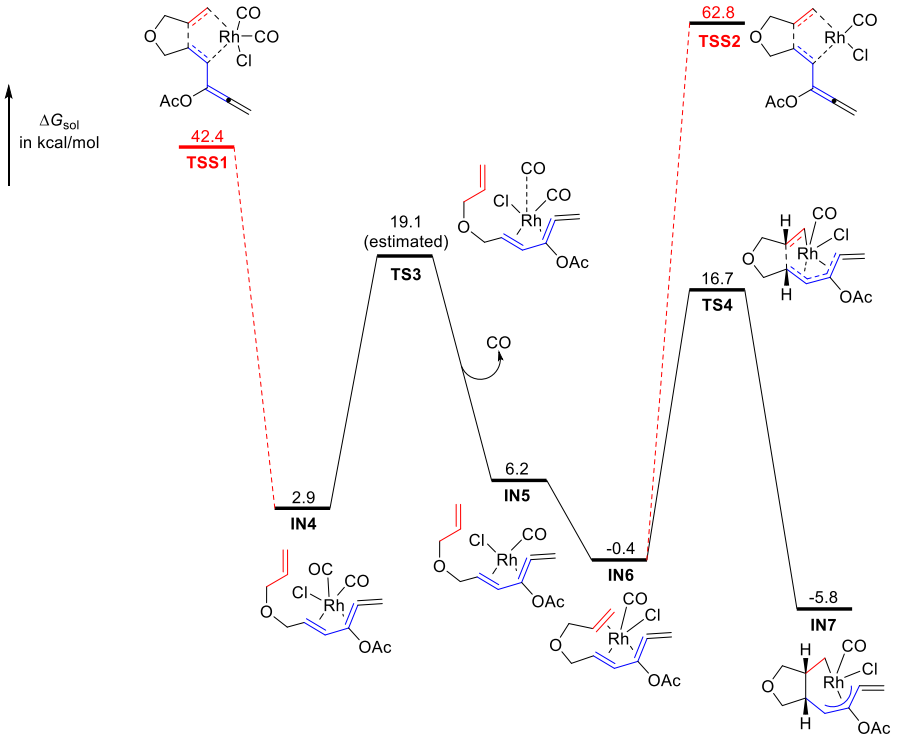


Figure S3. Potential energy surface for discussing the ene−ene oxidative cyclization pathway, which is not favored kinetically.

S4. Quantum chemical calculations for substrate 1d.

In our main text, we used simplified substrate *Z*-**1c** with an ether tether for calculations. However, experimentally we used substrate with a TsN tether and substituents (*Z*-**1a**, Scheme 2).[1] To support those calculations in the main text can reflect the experimental results, we performed calculations using substrate **1d** with an NMs tether, which is close to the real substrate *Z*-**1a** (Figure S4). Here our main concerns were about the processes of CO dissociation, C−H activation, and triene formation. Therefore, we searched for all conformations for these processes. However, we did not search conformations for 1,3-acyloxy migration process (we estimated that the conformation of 2π component had little influence on the relative energies of this process. Calculations found that introducing the methyl substituents in the substrate helped this process).

The results of these calculations also demonstrated that triene formation through C−H activation is disfavored than the [4+2+1] reaction by 15 kcal/mol, suggesting no triene will be generated, in contrast to the experimental observation. Therefore, triene was generated by [1,5]-H shift from *Z*-**5d**, which was generated from **INS3** or **INS4** by loss of Rh catalyst. The [1,5]-H shift of *Z*-**5d** giving the final triene product is easy, with a computed activation free energy of 23.3 kcal/mol (Scheme 6). Here we show the one possible way of catalyst loss from **INS4** through ligand exchange with **1d**.

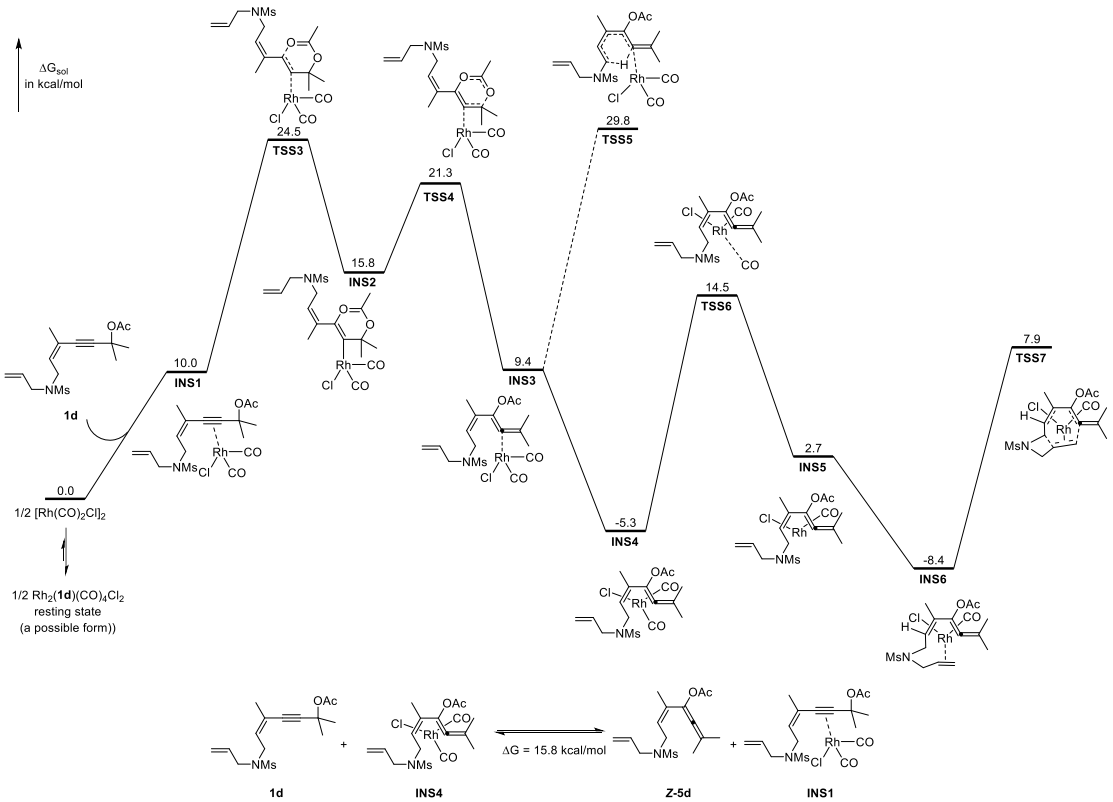
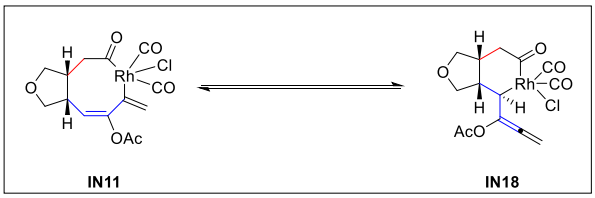
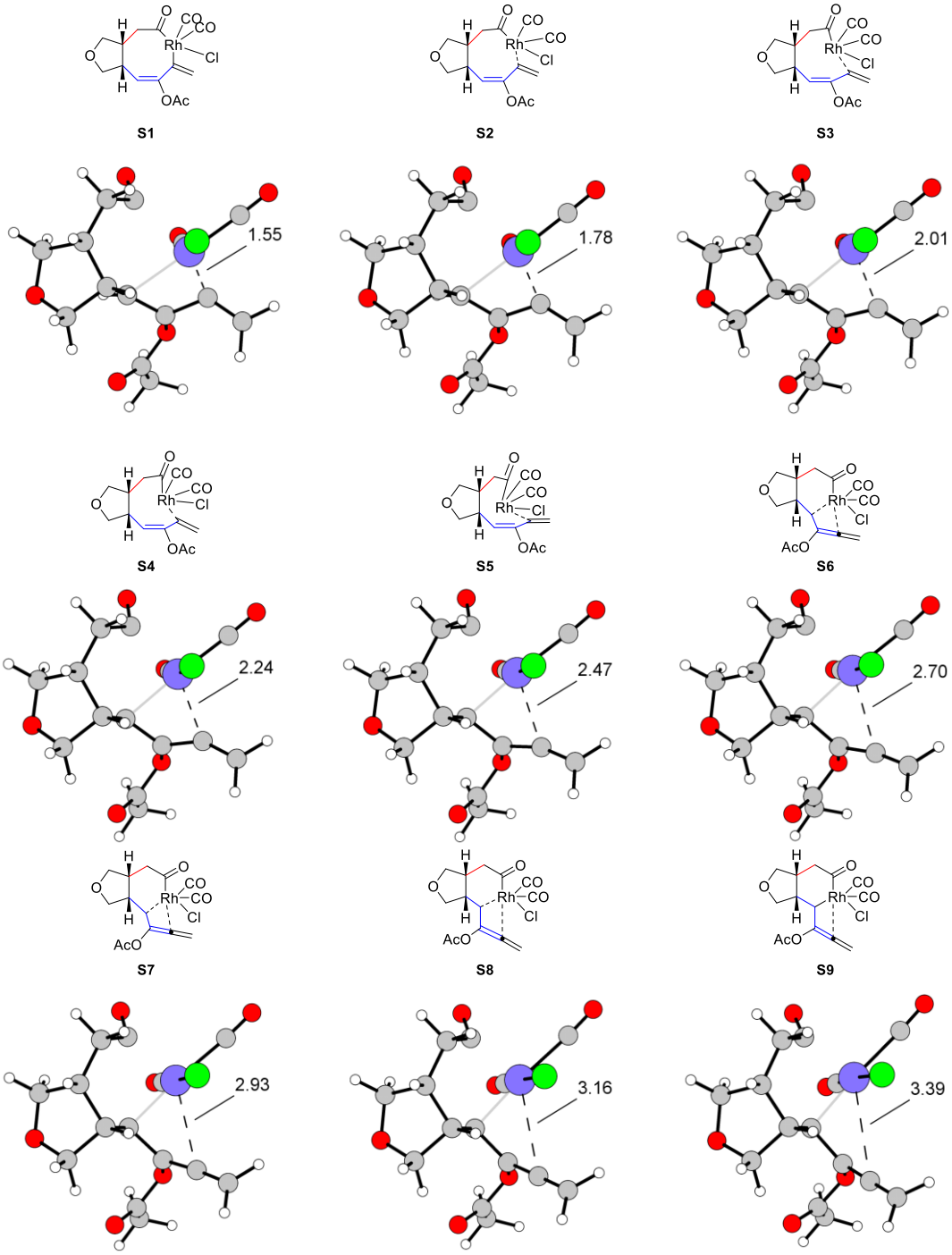


Figure S4. Computed free energy profiles of substrate **1d**.

S5. Intermediate IN11 to intermediate IN18.

Intermediate **IN11** can isomerize to **IN18**, which is a barrierless process indicated by quantum chemical calculations.





Entry	Single point energy	Bond distance
S1	-1561.739006	1.55
S2	-1561.865390	1.78
S3	-1561.906543	2.01
S4	-1561.916598	2.24
S5	-1561.919132	2.47
S6	-1561.920813	2.70
S7	-1561.922152	2.93
S8	-1561.923150	3.16
S9	-1561.923553	3.39

Figure S5. Scanning potential surface from **IN11** to **IN18**. The unit of bond distance is Å. The unit of single-point energy is Hartree.

S6. The [4+1] cycloaddition pathway.

The [4+1] cycloaddition pathway contains two elementary stages: CO migratory insertion and reductive elimination (Figure S6). Intermediate **IN15** is formed via an oxidative cyclization. Then, the CO ligand is inserted into the Rh−Csp^2 bond via **TSS8**, requiring 19.2 kcal/mol of Gibbs free energy. Intermediate **INS7** has a coordination by the terminal alkene, leading to ring distortion and loss of diene conjugation. As a result, intermediate **INS7** isomerizes to a more stable allylic coordinated intermediate **INS8**. Then, the reductive elimination step via **TSS9** achieves the [4+1] product-catalyst complex **INS9**, requiring 30.3 kcal/mol. Finally, the CO molecule coordinates to rhodium to form product complex **INS10** to accomplish [4+1] cycloaddition. The rate-determining step of [4+1] is reductive elimination, which is higher than the rate-determining step of [4+2+1] cycloadditions in terms of Gibbs free energy. Therefore, [4+1] reaction is not favored. This agrees with experimental results.

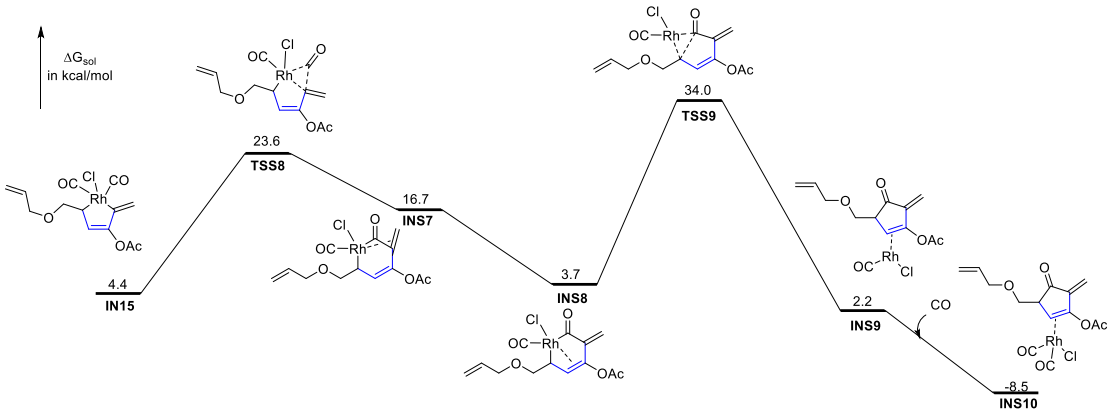
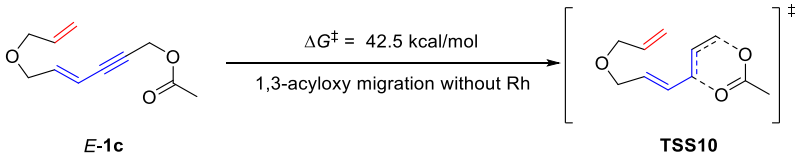


Figure S6. Potential energy profile of [4+1] cycloaddition.

S7. 1,3-Acyloxy migration without rhodium catalyst.

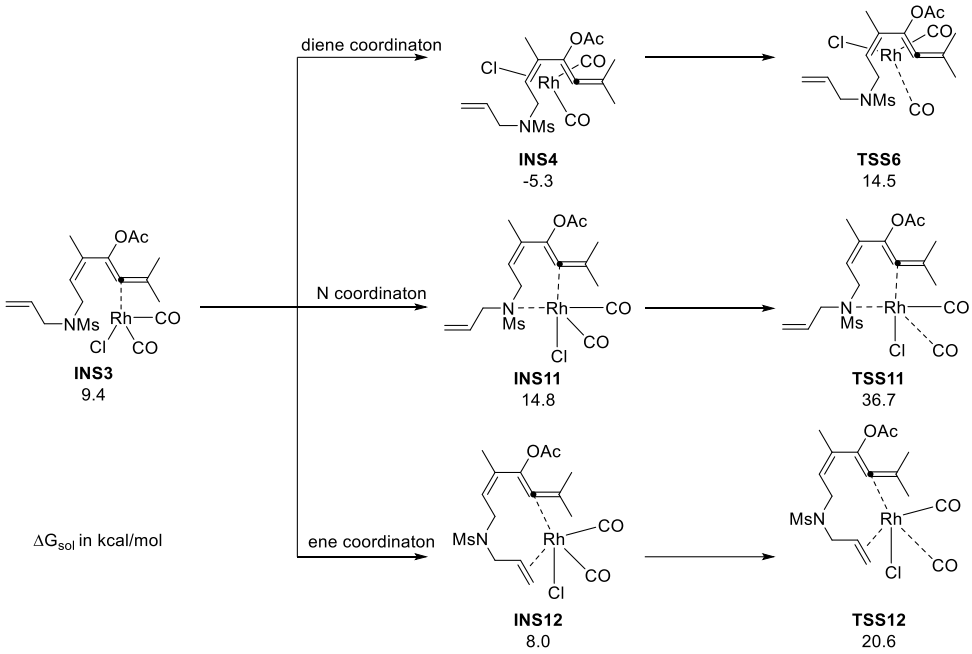
We considered the possibility of a direct 1,3-acyloxy migration, finding that an activation of Gibbs free energy is 42.5 kcal/mol. Rhodium catalysts are necessary for the 1,3-acyloxy migration.



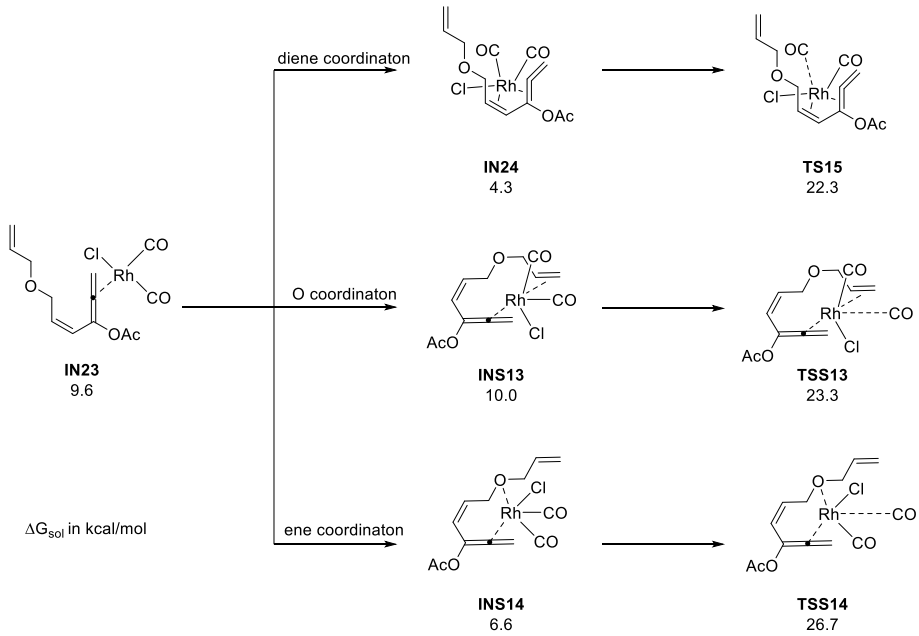
Scheme S2. 1,3-Acyloxy migration without rhodium catalysts. Computed at the SMD(DCE)-DLPNO-CCSD(T)/def2-TZVPP//BMK-def2-SVP level.

S8. Different ways of dissociation of carbon monoxide.

We have considered other scenarios of dissociation of CO, indicating that diene coordination is most favored for this process (all were estimated computationally by elongating the CO−Rh bonds).



Scheme S3. Different ways of dissociation of carbon monoxide for NMs-tether substrate. Computed at the SMD(DCE)-DLPNO-CCSD(T)/def2-TZVPP//BMK-def2-SVP level.



Scheme S4. Different ways of dissociation of carbon monoxide for O-tether substrate. Computed at the SMD(DCE)-DLPNO-CCSD(T)/def2-TZVPP//BMK-def2-SVP level.

S9. CO insertion and reductive elimination for reaction of ene−dienes and CO.

In ene−ene−allene system, we found that UP CO insertion is favored compared to DOWN CO insertion. For ene−diene system, we also found that UP CO insertion is favored compared to DOWN CO insertion, by 12.1 kcal/mol (Figure S7).

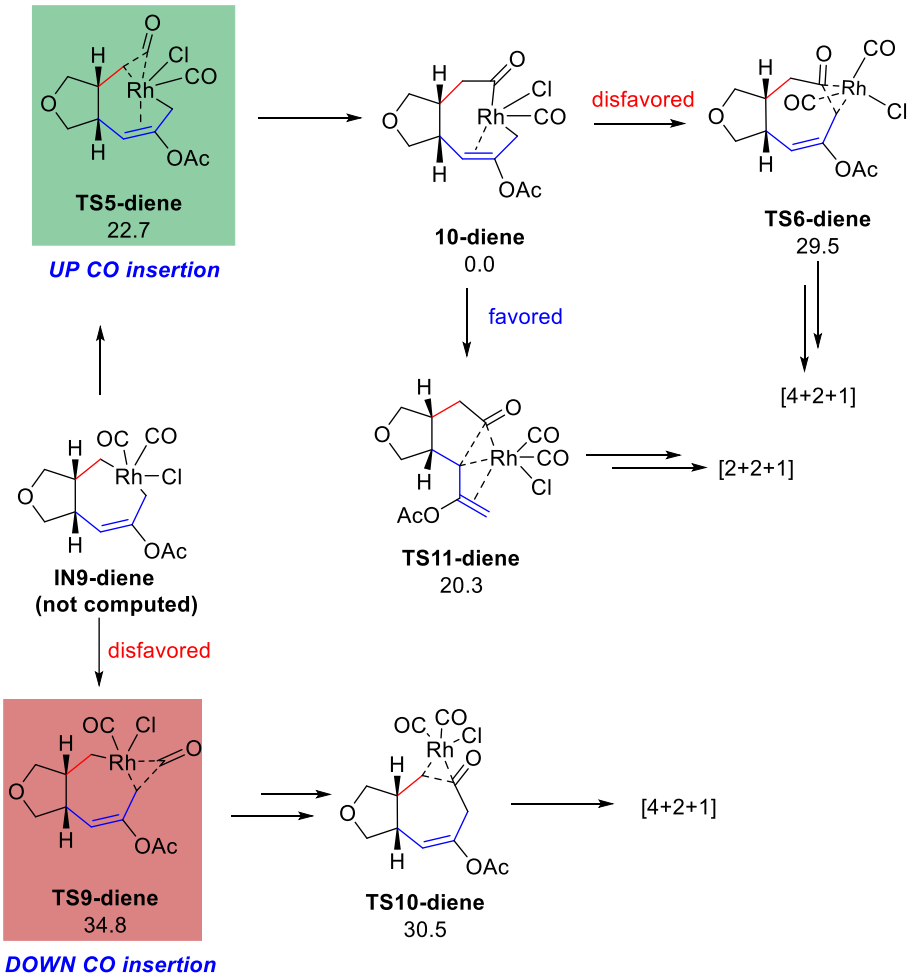


Figure S7. The competition of [4+2+1] and [2+2+1] cycloadditions for ene−diene system (all are relative free energies with respect to **10-diene**).

S10. Coordination modes of [4+2+1] reductive elimination.

In the reductive elimination of the [4+2+1] reaction, carbon monoxide may have other coordination modes. The favored reaction path is reported in the main text. Intermediate **IN10** coordinates a CO molecule to form intermediate **IN11**, which then undergoes reductive elimination via **TS6**. Intermediate **IN10** may undergo reductive elimination directly, which is not favored (Figure S8).

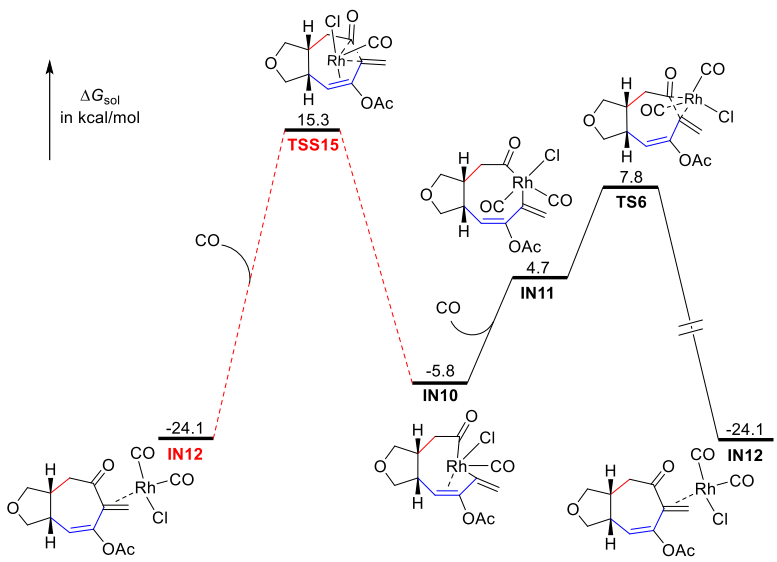


Figure S8. Coordination modes of [4+2+1] reductive elimination.

S11. DOWN CO insertion pathway.

In the DOWN CO insertion pathway (Figure S9), intermediate **IN17** tends to be coordinated by a CO molecule to form intermediate **IN17CO**, which then undergoes reductive elimination to give the [4+2+1] product. Intermediate **IN17** does not undergo reductive elimination directly via **TSS16** since **TSS16** lacks a coordination group. An extra double bond coordination exists in **TSS15** (Figure S8), which does not exist in **TSS16**. As a result, **TSS16** is of high Gibbs free energy, indicating this process is not favored.

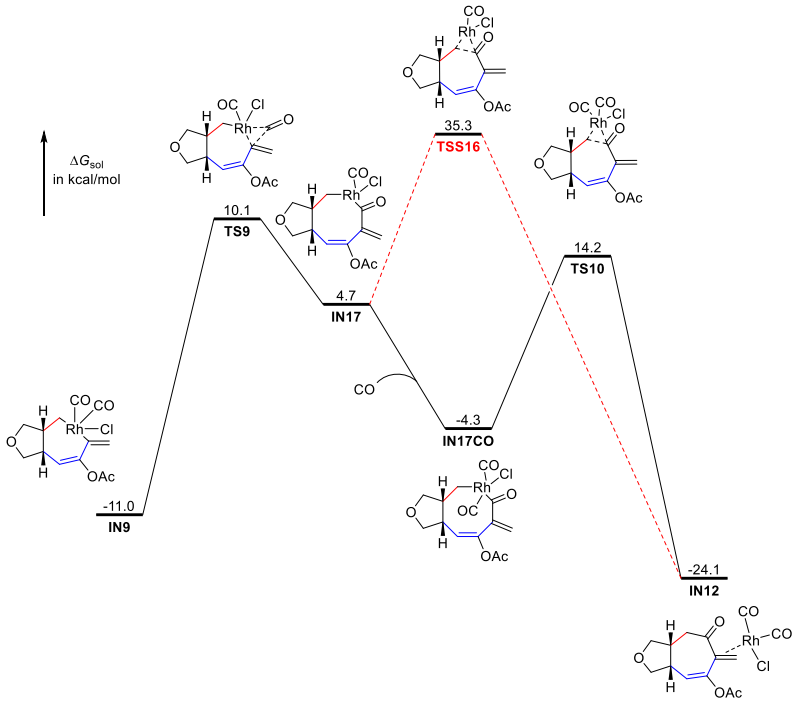


Figure S9. CO insertion and reductive elimination in DOWN CO insertion pathway.

S12. Coordination modes of [2+2+1] reductive elimination.

In the reductive elimination of the [2+2+1] reaction, carbon monoxide may have other coordination modes. The favored reaction path is reported in the main text. Intermediate **IN18** undergoes reductive elimination via **TS11**. Intermediate **INS15** may undergo reductive elimination via **TSS17**, which is not favored (Figure S10).

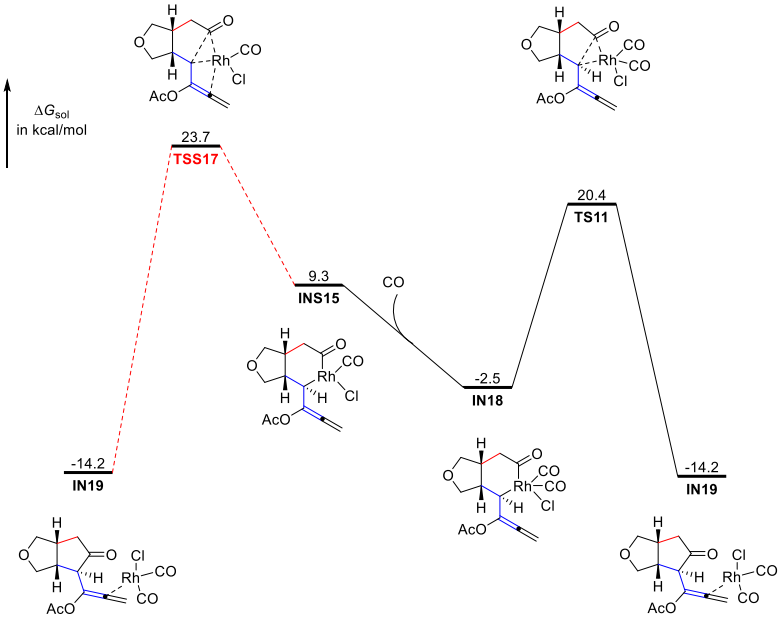


Figure S10. Coordination modes of [2+2+1] reductive elimination.

S13. Computed energies of the stationary points.

Table S2. Computed Energies of the Stationary Points.

Entry	SPE[a]	TCG[a]	G[a]	SPE[b]	SPE[c]	G[c]
$[Rh(CO)_2Cl]_2$	-1592.916752	-0.008305	-1592.92506	-1592.91839	-1593.12214	-1593.13208
CO	-113.1727454	-0.01386	-113.186605	-113.167302	-113.158173	-113.16659
2c	-765.534132	0.205165	-765.328967	-765.550844	-765.326714	-765.138261
E-1c	-652.2460091	0.18056	-652.065449	-652.264575	-652.077808	-651.915814
Z-1c	-652.2466381	0.180759	-652.065879	-652.264444	-652.078293	-651.91534
3c	-652.2779428	0.18167	-652.096273	-652.294786	-652.103756	-651.93893
3d	-1337.6163	0.308292	-1337.30801	-1337.6415	-1337.20841	-1336.92532
1d	-1337.59265	0.309922	-1337.28273	-1337.61469	-1337.19268	-1336.9048
Z-5c	-652.2429714	0.180692	-652.06228	-652.258096	-652.070927	-651.905359
Z-5d	-1337.589781	0.305124	-1337.28466	-1337.61334	-1337.18546	-1336.90389
3e	-390.0553098	0.193309	-389.862001	-390.065066	-389.924404	-389.740851
5e	-390.0332045	0.190007	-389.843197	-390.043275	-389.901206	-389.72127
IN1	-1448.694569	0.186234	-1448.50834	-1448.71624	-1448.63656	-1448.472
IN2	-1448.683341	0.191978	-1448.49136	-1448.71181	-1448.61984	-1448.45633
IN3	-1448.694934	0.18811	-1448.50682	-1448.71684	-1448.63358	-1448.46737
IN4	-1448.713806	0.191874	-1448.52193	-1448.73123	-1448.65016	-1448.47571
IN5	-1335.510127	0.185918	-1335.32421	-1335.53199	-1335.46611	-1335.30206
IN6	-1335.536596	0.195466	-1335.34113	-1335.55538	-1335.48923	-1335.31255
IN7	-1335.553849	0.196535	-1335.35731	-1335.57511	-1335.49637	-1335.3211
IN8	-1448.737625	0.201595	-1448.53603	-1448.75537	-1448.66165	-1448.4778
IN9	-1448.726765	0.199601	-1448.52716	-1448.75286	-1448.67138	-1448.49787
IN10	-1448.74096	0.202581	-1448.53838	-1448.76654	-1448.66662	-1448.48962
IN11	-1561.922253	0.21006	-1561.71219	-1561.94731	-1561.82627	-1561.64127
IN12	-1561.967254	0.208483	-1561.75877	-1561.98963	-1561.8733	-1561.68719
IN13	-1335.523089	0.192578	-1335.33051	-1335.54286	-1335.47661	-1335.30381
IN14	-1335.537158	0.195089	-1335.34207	-1335.56265	-1335.48414	-1335.31454
IN15	-1448.699784	0.192834	-1448.50695	-1448.72737	-1448.63861	-1448.47336
IN16	-1335.502857	0.193289	-1335.30957	-1335.53158	-1335.45307	-1335.2885
IN17	-1448.719602	0.204147	-1448.51546	-1448.7487	-1448.64793	-1448.47288
IN17CO	-1561.92986	0.209264	-1561.72059	-1561.95418	-1561.84058	-1561.65564
IN18	-1561.923553	0.206704	-1561.71685	-1561.94735	-1561.83577	-1561.65287
IN19	-1561.955557	0.20887	-1561.74669	-1561.97484	-1561.861	-1561.67141
IN20	-1335.583804	0.198087	-1335.38572	-1335.61348	-1335.52784	-1335.35944
IN21	-1448.698795	0.189542	-1448.50925	-1448.71717	-1448.64072	-1448.46955
IN22	-1448.683923	0.197007	-1448.48692	-1448.70984	-1448.62185	-1448.45076
IN23	-1448.693552	0.18949	-1448.50406	-1448.71524	-1448.63234	-1448.46454
IN24	-1448.7132	0.194814	-1448.51839	-1448.73163	-1448.64936	-1448.47298
IN25	-1335.506299	0.189871	-1335.31643	-1335.52688	-1335.46248	-1335.29318

IN26	-1335.534192	0.195126	-1335.33907	-1335.55404	-1335.48783	-1335.31254
IN27	-1448.674925	0.189236	-1448.48569	-1448.70069	-1448.61292	-1448.44945
IN28	-1448.73742	0.190707	-1448.54671	-1448.75516	-1448.67209	-1448.49912
TS1	-1448.666765	0.187088	-1448.47968	-1448.68893	-1448.60619	-1448.44126
TS2	-1448.66969	0.188857	-1448.48083	-1448.69186	-1448.60935	-1448.44267
TS4	-1335.513547	0.196962	-1335.31659	-1335.53487	-1335.46094	-1335.28531
TS5	-1448.708543	0.199897	-1448.50865	-1448.73403	-1448.63989	-1448.46548
TS6	-1561.916513	0.209557	-1561.70696	-1561.93813	-1561.8243	-1561.63636
TS7	-1335.502105	0.195333	-1335.30677	-1335.52358	-1335.45215	-1335.27829
TS8	-1335.447233	0.194174	-1335.25306	-1335.47897	-1335.39521	-1335.23277
TS9	-1448.71073	0.202062	-1448.50867	-1448.73667	-1448.64034	-1448.46422
TS10	-1561.901872	0.209519	-1561.69235	-1561.92711	-1561.81043	-1561.62614
TS11	-1561.898544	0.208971	-1561.68957	-1561.91734	-1561.80648	-1561.6163
TS12	-1335.512829	0.194323	-1335.31851	-1335.53626	-1335.46431	-1335.29342
TS13	-1448.665249	0.191473	-1448.47378	-1448.68729	-1448.60662	-1448.43719
TS14	-1448.671067	0.19381	-1448.47726	-1448.69025	-1448.61156	-1448.43693
TS16	-1335.513792	0.196536	-1335.31726	-1335.53577	-1335.46269	-1335.28813
TS17	-1448.660684	0.186875	-1448.47381	-1448.68013	-1448.60255	-1448.43513
TS18	-1448.66125	0.187183	-1448.47407	-1448.68249	-1448.60383	-1448.43789
TS19	-652.2107449	0.179731	-652.031014	-652.225318	-652.035319	-651.870161
TS20	-1337.550788	0.302736	-1337.24805	-1337.57484	-1337.14549	-1336.86681
TS21	-389.9909934	0.188784	-389.80221	-390.000559	-389.856415	-389.677197
INS1	-2134.049209	0.319061	-2133.73015	-2134.06798	-2133.75371	-2133.45342
INS2	-2134.038206	0.324262	-2133.71394	-2134.06327	-2133.74337	-2133.44417
INS3	-2134.051974	0.321528	-2133.73045	-2134.07326	-2133.75457	-2133.45433
INS4	-2134.067276	0.322983	-2133.74429	-2134.09366	-2133.77447	-2133.47788
INS5	-2020.860752	0.316122	-2020.54463	-2020.88862	-2020.58476	-2020.2965
INS6	-2020.88173	0.318827	-2020.5629	-2020.9117	-2020.60314	-2020.31428
INS7	-1448.688445	0.195201	-1448.49324	-1448.71596	-1448.62138	-1448.4537
INS8	-1448.705323	0.19476	-1448.51056	-1448.74025	-1448.63428	-1448.47446
INS9	-1448.714255	0.195972	-1448.51828	-1448.7446	-1448.64252	-1448.4769
INS10	-1561.931748	0.203619	-1561.72813	-1561.95538	-1561.84229	-1561.6623
INS11	-2134.034598	0.324	-2133.7106	-2134.0592	-2133.74523	-2133.44583
INS12	-2134.038738	0.321807	-2133.71693	-2134.06701	-2133.75012	-2133.45659
INS13	-1448.699179	0.196968	-1448.50221	-1448.71981	-1448.64031	-1448.46397
INS14	-1448.710716	0.196077	-1448.51464	-1448.72897	-1448.64722	-1448.4694
INS15	-1448.71716	0.202847	-1448.51431	-1448.74439	-1448.64114	-1448.46552
TSS1	-1448.659751	0.198834	-1448.46092	-1448.67742	-1448.59397	-1448.41281
TSS2	-1335.437286	0.193701	-1335.24359	-1335.458	-1335.38482	-1335.21183
TSS3	-2134.01914	0.321659	-2133.69748	-2134.04078	-2133.73041	-2133.43039
TSS4	-2134.027747	0.322675	-2133.70507	-2134.051	-2133.73476	-2133.43534
TSS5	-2134.002503	0.316693	-2133.68581	-2134.0298	-2133.71127	-2133.42187
TSS7	-2020.859878	0.31953	-2020.54035	-2020.89082	-2020.57689	-2020.2883

TSS8	-1448.675159	0.193022	-1448.48214	-1448.70433	-1448.60661	-1448.44275
TSS9	-1448.666858	0.194778	-1448.47208	-1448.69959	-1448.58828	-1448.42623
TSS10	-652.1778828	0.181803	-651.996079	-652.202545	-652.005249	-651.848108
TSS15	-1448.714	0.202944	-1448.51106	-1448.73901	-1448.63389	-1448.45596
TSS16	-1448.67313	0.201583	-1448.47155	-1448.71157	-1448.58726	-1448.42411
TSS17	-1448.69334	0.202685	-1448.49066	-1448.71822	-1448.62031	-1448.4425
IN10-diene	-1410.727278	0.199646	-1410.52763	-1410.75351	-1410.66638	-1410.49296
TS5-diene	-1410.68858	0.198196	-1410.49039	-1410.7121	-1410.63143	-1410.45675
TS6-diene	-1523.880697	0.207094	-1523.6736	-1523.90506	-1523.79714	-1523.61441
TS9-diene	-1410.664809	0.196976	-1410.46783	-1410.69158	-1410.60778	-1410.43757
TS10-diene	-1523.869641	0.206428	-1523.66321	-1523.89489	-1523.79406	-1523.61288
TS11-diene	-1523.896409	0.207141	-1523.68927	-1523.91371	-1523.81889	-1523.62905

[a]Computed at the BMK/def2-SVP level.

[b]Computed at the SMD(DCE)/BMK/def2-SVP//BMK/def2-SVP level.

[c]Computed at the DLPNO-CCSD(T)/def2-TZVPP//BMK/def2-SVP level. We used 5.5 mM as the concentration of CO and 1.0 M for other species.

$$\Delta G_{\text{std}} = -RT\ln\left(\frac{V_1}{V_2}\right) = -RT\ln\left(\frac{\frac{1}{24.46}}{1}\right) = 1.89\ \text{kcal/mol}$$

$$\Delta G_{\text{CO}} = -RT\ln\left(\frac{V_1}{V_2}\right) - RT\ln\left(\frac{c_1}{c_2}\right) = -RT\ln\left(\frac{\frac{1}{24.46}}{1}\right) - RT\ln\left(\frac{1}{0.0055}\right)$$

$$= -1.19\ \text{kcal/mol}$$

Table S3. Imaginary frequencies of transition states.

Entry	Imaginary frequency/cm^{-1}	**Entry**	Imaginary frequency/cm^{-1}
TS1	-356.3593	**TS21**	-1335.1021
TS2	-447.0594	**TSS1**	-261.0721
TS4	-143.6943	**TSS2**	-314.3725
TS5	-244.1988	**TSS3**	-260.8249
TS6	-257.8754	**TSS4**	-273.8351
TS7	-220.5741	**TSS5**	-1336.0629
TS8	-288.2987	**TSS7**	-64.2367
TS9	-256.5804	**TSS8**	-96.0086
TS10	-325.0564	**TSS9**	-84.0406
TS11	-246.5176	**TSS10**	-267.9261
TS12	-396.3887	**TSS15**	-226.0715
TS13	-325.2014	**TSS16**	-468.1105
TS14	-419.8845	**TSS17**	-194.4324
TS16	-77.6100	**TS5-diene**	-188.9420
TS17	-854.0273	**TS6-diene**	-290.7938

TS18	-751.4606	**TS9-diene**	-284.4574
TS19	-1352.5882	**TS10-diene**	-313.6033
TS20	-1314.7212	**TS11-diene**	-249.8685

S14. Cartesian coordinates of the stationary points

1d

C	3.539281	-0.668131	0.704000
C	4.416999	0.553317	0.553193
C	5.075598	1.136567	1.559648
C	1.274160	0.420913	0.930247
C	1.311981	1.856872	0.461937
C	0.251325	2.539717	-0.021843
H	3.985189	-1.493327	0.125973
H	3.502971	-0.972498	1.768519
H	4.501373	0.941876	-0.470327
H	5.723398	2.003124	1.394512
H	4.996549	0.760035	2.586753
H	0.247715	0.027639	0.856016
H	1.566687	0.375349	1.996243
H	2.275912	2.374367	0.533482
C	-1.025963	1.889721	-0.158252
C	-2.061276	1.270996	-0.288756
C	-3.243756	0.432540	-0.564853
O	-3.699705	-0.221823	0.644810
C	-2.912841	-1.018651	1.359271
O	-1.774773	-1.292335	1.079328
C	-3.640478	-1.530147	2.586365
H	-4.596191	-1.990855	2.292191
H	-3.006799	-2.255776	3.112085
H	-3.871177	-0.680269	3.249058
N	2.188994	-0.459385	0.199419
S	1.600397	-1.379755	-1.032039
O	0.538008	-0.632911	-1.673719
O	2.741103	-1.859875	-1.788666
C	0.832267	-2.817201	-0.244521
H	0.458883	-3.450398	-1.063308
H	1.601685	-3.351478	0.331080
H	0.001735	-2.466707	0.387143
C	-4.438718	1.302203	-0.978274
H	-5.310256	0.658815	-1.179867
H	-4.691992	2.006185	-0.170901
H	-4.189450	1.871963	-1.886033
C	-2.904109	-0.607461	-1.647821
H	-2.758883	-0.089112	-2.608248
H	-1.970835	-1.133181	-1.404777
H	-3.741510	-1.318638	-1.746596
C	0.335889	3.983600	-0.469580
H	0.058227	4.071575	-1.533937
H	-0.366438	4.611131	0.105487
H	1.354686	4.378376	-0.336457

2c

O	-3.502993	-0.840885	-0.676922
C	-3.336756	-0.000468	0.435970
C	-2.230919	-1.140149	-1.159891
C	-1.414942	-1.464305	0.118233
C	0.082514	-1.508344	-0.050333
C	0.884079	-0.481274	-0.380374
H	-4.214754	-0.116090	1.090065
H	-3.278241	1.059300	0.117248
H	-2.301059	-1.987832	-1.858632
H	-1.780316	-0.278082	-1.697621
H	-1.743809	-2.461430	0.448727
H	0.579045	-2.476368	0.073420
C	-2.002697	-0.423442	1.129584
C	-1.082110	0.775822	1.444607
H	-1.617907	1.491647	2.087975
C	-0.647759	1.531787	0.199115
O	-1.149443	2.580127	-0.124395
C	0.482727	0.926985	-0.614101
C	1.130970	1.723099	-1.482996
H	1.981588	1.360686	-2.067137
H	0.797189	2.757437	-1.608397
H	-0.179732	0.420144	1.970548
H	-2.211174	-0.928812	2.085753
O	2.228034	-0.747422	-0.588994
C	3.092372	-0.340748	0.369864
O	2.738130	0.161048	1.395336
C	4.520048	-0.608332	-0.044446
H	4.781097	0.048143	-0.890708
H	5.187511	-0.405881	0.802721
H	4.625582	-1.649593	-0.385550

3c

O	-2.814384	-0.563461	0.374806
C	-3.599269	-0.054907	-0.681875
C	-5.050259	-0.289830	-0.365050
C	-5.995683	0.650083	-0.445937
C	-1.488224	-0.458949	0.242055
C	-0.630981	-1.095292	1.068052
C	0.825142	-1.000615	0.969621
H	-3.331655	-0.577969	-1.622919

H	-3.403811	1.025503	-0.827054
H	-5.306916	-1.316401	-0.074600
H	-7.045517	0.420512	-0.240054
H	-5.755222	1.682730	-0.724595
H	-1.126390	0.161289	-0.591512
H	0.047874	1.633359	0.902717
H	-1.056055	-1.779692	1.811526
H	1.388942	-1.926924	1.134657
C	1.567060	0.098916	0.693568
C	1.088895	1.479540	0.603466
C	1.845749	2.529034	0.241071
O	2.798206	-0.580219	-1.610422
C	3.456554	-0.392778	-0.632059
O	2.938187	-0.055698	0.570225
C	4.963803	-0.490081	-0.542790
H	5.242409	-1.215265	0.237979
H	5.366430	-0.798467	-1.515889
H	5.381187	0.486542	-0.249625
H	1.434283	3.541998	0.236981
H	2.891649	2.407082	-0.055203

3d

C	-2.769868	1.311572	-1.187739
C	-2.863318	0.749098	-2.585589
C	-2.161075	1.209636	-3.624718
C	-0.995727	-0.054922	-0.175948
C	-0.409123	-1.128207	0.403346
C	1.045299	-1.357324	0.395382
C	1.962026	-0.366494	0.579865
H	-2.044862	2.143020	-1.154715
H	-3.748702	1.697870	-0.869078
H	-3.562539	-0.087835	-2.712133
H	-2.267765	0.775583	-4.623501
H	-1.454432	2.040994	-3.514153
H	0.751635	1.104394	1.600690
H	-0.370106	0.670168	-0.707751
H	-1.028806	-1.930935	0.813898
C	1.681232	1.003242	1.030569
C	2.440800	2.109825	0.862829
O	3.312211	-0.679682	0.501308
C	3.877989	-1.024089	-0.670734
O	3.298200	-1.031934	-1.717074
C	5.338124	-1.365045	-0.469987
H	5.441892	-2.138291	0.307034
H	5.765303	-1.710418	-1.419960
H	5.874990	-0.468738	-0.118798

N	-2.347907	0.303982	-0.203330
S	-3.510108	-0.489980	0.700713
O	-3.325135	-1.920611	0.597794
O	-4.777484	0.109986	0.341406
C	-3.113970	-0.011050	2.397279
H	-2.070516	-0.285148	2.609320
H	-3.282737	1.069525	2.497782
H	-3.802780	-0.581794	3.037333
C	2.047990	3.411297	1.525003
H	2.862007	3.772418	2.181206
H	1.879289	4.201922	0.770521
H	1.137194	3.309285	2.135322
C	3.707278	2.165539	0.030447
H	4.584061	1.834998	0.616110
H	3.636037	1.537989	-0.871099
H	3.903646	3.200253	-0.295864
C	1.477072	-2.785894	0.144649
H	1.569683	-2.970649	-0.940502
H	2.447877	-3.010026	0.613374
H	0.725996	-3.487961	0.541461

3e

C	1.985383	0.628967	-0.138250
C	1.275132	-0.684015	-0.079045
C	-0.074801	-0.816661	0.002770
H	-0.457761	-1.843417	0.008649
C	-1.065022	0.249940	0.146005
C	-2.412118	0.110081	0.100638
C	3.179294	0.799722	0.782146
H	3.582594	1.822339	0.721638
H	2.899678	0.593572	1.830580
H	3.989811	0.097774	0.518529
C	1.621235	1.597015	-0.998504
H	0.787353	1.456271	-1.692619
H	-0.671195	1.254839	0.331964
H	2.159581	2.550261	-1.037771
C	2.163224	-1.913331	-0.096377
H	2.780769	-1.976355	0.817921
H	1.564798	-2.835131	-0.162076
H	2.859633	-1.887641	-0.954024
C	-3.139883	-1.186424	-0.171278
H	-3.810314	-1.435296	0.672019
H	-3.784188	-1.080722	-1.063618
H	-2.469565	-2.040267	-0.340540
C	-3.319159	1.299616	0.321051
H	-3.970838	1.465752	-0.557053

H	-3.990883	1.125873	1.182545
H	-2.749181	2.222674	0.508925

5e

C	1.730245	0.639239	0.058860
C	1.406201	-0.649254	-0.222027
C	0.053514	-1.088502	-0.669568
H	0.041143	-1.977034	-1.320508
C	-1.121857	-0.594186	-0.323913
C	-2.306041	-0.135466	0.024285
C	3.083146	1.074956	0.583281
H	2.947643	1.694453	1.489004
H	3.753363	0.246134	0.844911
H	3.597167	1.715364	-0.157849
C	0.767040	1.796343	-0.113777
H	0.025216	1.610236	-0.904239
H	0.209792	1.997245	0.820307
H	1.323001	2.716555	-0.363906
C	2.373296	-1.816317	-0.126924
H	2.062823	-2.519293	0.667510
H	2.366159	-2.386167	-1.073558
H	3.409613	-1.512993	0.069666
C	-3.013590	0.950508	-0.766466
H	-3.998415	0.589947	-1.114638
H	-3.196713	1.833984	-0.128135
H	-2.429669	1.265281	-1.644167
C	-3.038395	-0.661901	1.246242
H	-3.240920	0.160828	1.955727
H	-4.014575	-1.089493	0.953969
H	-2.456990	-1.437565	1.765943

CO

C	0.000000	0.000000	-0.643399
O	0.000000	0.000000	0.482549

E-1c

O	3.581094	0.043190	-0.008055
C	4.896561	-0.016078	-0.476450
C	5.655656	1.183022	0.024229
C	6.860290	1.126951	0.598641
C	2.772256	-0.992491	-0.474683
C	1.412342	-0.876660	0.152826
C	0.263292	-0.973048	-0.540816
H	4.901305	-0.017009	-1.590457
H	5.396198	-0.953919	-0.150538
H	5.155215	2.147707	-0.128921
H	7.383404	2.034154	0.916195
H	7.369040	0.170994	0.770064
H	2.689994	-0.974420	-1.583123
H	3.216981	-1.977433	-0.201294
H	1.391948	-0.725463	1.238747
H	0.294262	-1.108022	-1.630452
C	-1.038270	-0.920226	0.055595
C	-2.157254	-0.881494	0.525698
C	-3.505784	-0.853344	1.110151
O	-4.158545	0.391655	0.908787
C	-4.796458	0.566351	-0.259875
O	-4.877335	-0.283812	-1.099396
C	-5.376739	1.959590	-0.352620
H	-4.551988	2.689562	-0.396593
H	-5.994682	2.036769	-1.256225
H	-5.970638	2.182156	0.547211
H	-3.445137	-0.983668	2.201282
H	-4.112968	-1.665110	0.677228

IN1

O	-4.254037	1.070002	-0.131228
C	-5.516475	1.595988	0.163353
C	-6.516380	1.068207	-0.829520
C	-7.702293	0.549583	-0.499876
C	-3.241984	1.538764	0.700902
C	-1.954654	0.857142	0.333577
C	-0.782241	1.505320	0.217415
H	-5.484397	2.707638	0.102043
H	-5.825306	1.337108	1.198975
H	-6.215936	1.150331	-1.881811
H	-8.407318	0.208540	-1.264100
H	-8.012802	0.449074	0.546788
H	-3.131836	2.642804	0.628547
H	-3.480022	1.309724	1.765816
H	-2.006191	-0.227117	0.174544
H	-0.733639	2.594234	0.351775
C	0.480806	0.886953	-0.077887
C	1.661685	0.618030	-0.338201
C	3.054761	0.639974	-0.850861
O	3.520387	1.958544	-1.048775
C	3.917990	2.633657	0.044107
O	3.869498	2.171659	1.147970
C	4.419544	4.010677	-0.323758
H	3.619733	4.569761	-0.834916

H	4.735467	4.537650	0.585361
H	5.261903	3.920390	-1.027959
Rh	0.819988	-1.396284	0.138896
C	0.733673	-1.090325	2.009608
O	0.695149	-0.892971	3.127912
Cl	1.041119	-1.808268	-2.167819
C	0.541644	-3.303501	0.283601
O	0.385547	-4.423110	0.310601
H	3.055989	0.139792	-1.831146
H	3.717087	0.097596	-0.157908

IN10-diene

O	3.715494	-1.968901	0.646212
C	3.649001	-1.830689	-0.749089
C	2.423627	-1.945656	1.204302
C	1.436905	-1.817957	0.018476
C	0.106723	-1.241553	0.482853
C	-1.079295	-1.102172	-0.307452
H	3.648473	-2.819977	-1.251146
H	4.532691	-1.270721	-1.096573
H	2.238938	-2.866933	1.786110
H	2.319638	-1.080291	1.887239
H	1.243978	-2.832224	-0.378714
H	-0.136810	-1.552015	1.508286
Rh	-0.323382	0.866806	0.143769
C	2.322116	-1.096555	-1.022103
C	2.491955	0.408379	-0.756923
H	2.782089	0.583695	0.293422
C	1.236002	1.226788	-1.021890
O	1.167257	2.079638	-1.850710
Cl	0.691120	1.694250	2.100495
C	-1.110393	-0.371175	-1.518151
H	3.269496	0.824253	-1.418328
H	1.984043	-1.266302	-2.058434
O	-2.245827	-1.247156	0.412139
C	-3.365071	-1.801511	-0.141386
O	-3.400964	-2.231146	-1.251745
C	-4.490281	-1.797720	0.863390
H	-4.185044	-2.358832	1.760842
H	-4.704591	-0.763405	1.176513
H	-5.379517	-2.253738	0.410485
C	-1.047143	2.680057	-0.332085
O	-1.472587	3.695964	-0.571114
H	-2.081019	-0.160992	-1.973012
H	-0.281069	-0.479646	-2.222597

IN10

O	-3.720967	-2.012714	-0.564298
C	-3.493394	-2.034509	0.822221
C	-2.505396	-1.864638	-1.261221
C	-1.397100	-1.845500	-0.183358
C	-0.114175	-1.215000	-0.703706
C	1.098895	-1.060544	0.017590
H	-3.403110	-3.074069	1.198349
H	-4.347246	-1.558848	1.331872
H	-2.366352	-2.699817	-1.971345
H	-2.505010	-0.918462	-1.836325
H	-1.152749	-2.894479	0.069802
H	0.071588	-1.466939	-1.757501
Rh	0.207772	0.921932	-0.250218
C	-2.167513	-1.276305	1.025703
C	-2.430021	0.236295	0.947015
H	-2.861314	0.499561	-0.034624
C	-1.195001	1.102729	1.140589
O	-1.072665	1.902866	2.012808
Cl	-1.005870	1.750494	-2.105398
C	1.137057	-0.261226	1.195470
C	1.494865	-0.270940	2.473333
H	1.873615	-1.190414	2.934278
H	1.409574	0.631620	3.087127
H	-3.135564	0.539347	1.737873
H	-1.689727	-1.530628	1.986051
O	2.252164	-1.165491	-0.727003
C	3.350761	-1.739007	-0.154118
O	3.310296	-2.286104	0.904218
C	4.551660	-1.589161	-1.052894
H	4.308819	-1.942952	-2.066824
H	4.817916	-0.522010	-1.126760
H	5.390100	-2.158763	-0.632826
C	0.855468	2.733484	0.249403
O	1.259031	3.754875	0.503808

IN11

O	4.803631	-0.627741	0.202460
C	3.927981	-1.655128	-0.149428
C	4.157607	0.556030	-0.145051
C	2.724681	0.370199	0.411997
C	1.842531	1.549631	0.077840
C	0.639449	1.729194	-0.493722
H	4.179634	-2.555987	0.431249
H	4.038707	-1.894891	-1.227649

H	4.691004	1.407745	0.304753
H	4.126481	0.698696	-1.247845
H	2.856545	0.424946	1.509102
H	2.291002	2.488773	0.428458
Rh	-1.142847	-0.633110	0.152751
C	2.463057	-1.146729	0.114895
C	1.586555	-1.581162	-1.068366
H	1.663125	-0.858555	-1.901265
C	0.080129	-1.810698	-0.894355
O	-0.462922	-2.692890	-1.489604
Cl	-2.399367	-1.823140	1.817927
C	-0.329254	0.767840	-1.100316
C	-0.695638	0.995821	-2.377193
H	-0.286854	1.840429	-2.947785
H	-1.402231	0.354503	-2.914812
H	1.950410	-2.549880	-1.450787
H	2.082894	-1.631367	1.028255
O	0.196473	3.053679	-0.541821
C	-0.891121	3.341827	0.194442
O	-1.411117	2.548090	0.930838
C	-1.355670	4.758645	-0.038537
H	-0.501762	5.451604	0.000480
H	-1.795910	4.824284	-1.047478
H	-2.110714	5.022598	0.712752
C	-2.624742	-1.106155	-1.136365
O	-3.485942	-1.396729	-1.797319
C	0.005299	-0.212191	1.706841
O	0.516105	0.005304	2.686437

IN12

O	4.606253	-1.908146	-0.843708
C	3.657575	-2.671675	-0.155537
C	3.983569	-0.705291	-1.171773
C	3.254929	-0.296700	0.134719
C	2.309178	0.847223	-0.092668
C	1.043075	1.101626	0.286987
H	4.183859	-3.408375	0.470540
H	3.010065	-3.220211	-0.871002
H	4.746180	0.020776	-1.493470
H	3.244293	-0.834786	-1.992321
H	4.040437	0.082981	0.814728
H	2.779765	1.670454	-0.641521
Rh	-1.934534	-0.271765	-0.154385
C	2.782837	-1.674363	0.672908
C	1.286927	-1.969059	0.470630
H	0.986721	-1.724865	-0.563525
C	0.444898	-1.183062	1.448830
O	0.008606	-1.663921	2.464104
Cl	-0.583301	0.026217	-2.085819
C	0.128102	0.274651	1.102699
C	-0.957788	0.837296	1.733314
H	-1.207089	1.891386	1.596167
H	-1.401029	0.295075	2.571591
H	1.090056	-3.034429	0.670313
H	3.018679	-1.762552	1.745669
O	0.460820	2.305718	-0.051845
C	1.036072	3.501346	0.232829
O	2.082246	3.623754	0.794072
C	0.158717	4.624530	-0.269184
H	-0.832178	4.571509	0.209036
H	0.638234	5.585804	-0.045459
H	0.006539	4.510320	-1.354264
C	-3.147855	-0.862824	-1.503466
O	-3.854950	-1.190534	-2.323892
C	-3.126559	-0.757012	1.226470
O	-3.860029	-1.074307	2.034919

IN13

O	-3.185213	-1.953271	-0.497757
C	-3.106236	-1.385761	0.773164
C	-2.077627	-1.826436	-1.367615
C	-0.801379	-1.580137	-0.602524
C	0.404183	-1.078845	-1.191001
C	1.391310	-0.659535	-0.256057
H	-2.473262	-1.975915	1.466099
H	-4.137483	-1.422884	1.169746
H	-2.019144	-2.779581	-1.924027
H	-2.243195	-1.005167	-2.088954
H	-0.656595	-2.247187	0.256432
H	0.534455	-0.846499	-2.252910
Rh	-0.450635	0.417012	0.160254
C	-2.682206	0.064373	0.801983
C	-1.977994	0.651953	1.836740
H	-1.613853	0.048864	2.676264
C	0.259780	2.190977	0.611581
O	0.659719	3.223699	0.835837
Cl	-1.525453	1.675380	-1.682992
C	0.971649	-0.650009	1.136368
C	1.435369	-1.077959	2.308775
H	2.334723	-1.701813	2.361265
H	0.926605	-0.820158	3.243885
H	-2.056003	1.729559	2.003744

H	-3.174864	0.712362	0.067185
O	2.551682	-0.097463	-0.719727
C	3.735752	-0.625842	-0.311120
O	3.808107	-1.613765	0.354361
C	4.887165	0.201755	-0.825248
H	5.831878	-0.292450	-0.566310
H	4.799829	0.328677	-1.915524
H	4.845251	1.204397	-0.369439

IN14

O	-3.384521	-2.730410	0.018809
C	-3.561303	-1.432941	0.550633
C	-2.091113	-2.903611	-0.510455
C	-1.275430	-1.732850	0.054650
C	-0.008285	-1.351212	-0.672226
C	1.120736	-0.919029	-0.001779
H	-3.581368	-1.473471	1.658461
H	-4.522023	-1.020026	0.200845
H	-1.701191	-3.890002	-0.207719
H	-2.111047	-2.861451	-1.618748
H	-1.026342	-1.945200	1.109741
H	0.106137	-1.606321	-1.732597
Rh	-0.071463	1.021791	-0.032157
C	-2.349488	-0.625946	0.052782
C	-1.863346	0.569525	0.851136
H	-1.732456	0.332215	1.919884
C	-0.086158	2.677252	0.883838
O	-0.092199	3.661448	1.441308
Cl	-0.890980	1.914050	-2.085321
C	0.985578	-0.158301	1.238107
C	1.436407	-0.290324	2.485733
H	2.030067	-1.164512	2.776903
H	1.225644	0.468892	3.246336
H	-2.513464	1.450948	0.732429
H	-2.529030	-0.312378	-0.990724
O	2.275628	-0.769811	-0.741151
C	3.427991	-1.273041	-0.224019
O	3.450173	-1.934154	0.769509
C	4.607815	-0.887382	-1.080084
H	5.506289	-1.394602	-0.706792
H	4.414255	-1.158618	-2.129500
H	4.743927	0.205636	-1.038690

IN15

O	3.284723	0.304727	0.179856
C	4.500920	-0.009165	-0.431269
C	5.536451	1.008665	-0.033852
C	6.761153	0.708683	0.407574
C	2.236104	-0.555769	-0.178058
C	0.971119	-0.061079	0.532841
C	0.596675	1.326176	0.083011
C	-0.610406	1.491432	-0.476781
H	4.381459	-0.001901	-1.538430
H	4.838856	-1.030215	-0.151732
H	5.228628	2.056244	-0.146680
H	7.487611	1.489852	0.652085
H	7.083192	-0.331328	0.537035
H	2.089930	-0.561944	-1.276124
H	2.468953	-1.597747	0.123389
H	1.241725	-0.017501	1.607987
H	1.301121	2.158472	0.184342
Rh	-0.740448	-1.251824	0.339793
Cl	0.147502	-2.570703	-1.380082
C	-1.337952	-0.342568	1.925558
O	-1.656504	0.180049	2.872933
C	-1.499086	0.324841	-0.641238
C	-2.617116	0.318565	-1.378516
H	-2.897978	1.214729	-1.944830
H	-3.271098	-0.551238	-1.478098
O	-1.051967	2.708365	-0.951485
C	-1.924832	3.399032	-0.182894
O	-2.305097	3.014503	0.883190
C	-2.325295	4.689415	-0.859140
H	-1.425206	5.280679	-1.090069
H	-2.827719	4.465594	-1.813883
H	-2.997225	5.252410	-0.199195
C	-2.378564	-2.525244	0.020949
O	-3.189238	-3.261388	-0.237518

IN16

O	-2.490511	-2.642745	0.316743
C	-3.204744	-1.463443	0.277722
C	-2.842154	-0.467929	-0.799613
C	-1.893048	-0.601825	-1.768507
C	-1.084893	-2.631475	0.425716
C	-0.403402	-1.372844	1.010913
C	1.080558	-1.603173	0.845271
C	1.677090	-0.892260	-0.128883
H	-3.185488	-0.925082	1.254416
H	-4.265154	-1.739280	0.122589
H	-3.453185	0.445017	-0.806679

H	-1.790649	0.176273	-2.531072
H	-1.317826	-1.518602	-1.905311
H	-0.829400	-3.498256	1.063849
H	-0.639081	-2.841096	-0.564237
H	-0.673943	-1.294699	2.083300
H	1.617799	-2.399532	1.375354
Rh	-0.878539	0.469869	0.129378
Cl	-1.856312	2.617927	-0.405369
C	0.197485	1.392551	1.413728
O	0.831371	1.965166	2.150555
C	0.861219	0.133158	-0.814899
C	1.245990	0.818882	-1.902180
H	2.208792	0.602048	-2.383455
H	0.617338	1.597986	-2.344117
O	2.943813	-1.143630	-0.574225
C	4.020697	-0.364291	-0.280527
O	5.054396	-0.590800	-0.826699
C	3.812641	0.727390	0.751343
H	4.785874	1.190255	0.957938
H	3.118262	1.487427	0.357892
H	3.381053	0.316289	1.677291

IN17

O	-0.274055	4.421846	0.167996
C	0.174495	3.612468	-0.880241
C	-1.152818	3.664033	0.952712
C	-0.761648	2.161831	0.773695
C	-1.909010	1.338937	0.251584
C	-1.904874	0.020311	-0.013441
H	1.070657	4.073534	-1.323543
H	-0.598393	3.505305	-1.675007
H	-1.065866	4.003401	1.996881
H	-2.201581	3.825730	0.628703
H	-0.411913	1.746327	1.731122
H	-2.839200	1.855121	-0.014238
Rh	1.291157	-0.704146	-0.366344
C	0.455718	2.249053	-0.221729
C	0.648175	1.085498	-1.182523
H	-0.257133	0.908307	-1.790153
C	0.224786	-0.717077	1.258334
O	0.378108	-0.552929	2.412790
Cl	3.421422	0.282901	-0.200177
C	-0.814966	-0.951028	0.235234
C	-0.520646	-2.010847	-0.636362
H	-1.074561	-2.063743	-1.580200
H	-0.133820	-2.959633	-0.258442
H	1.491610	1.317069	-1.856569
H	1.371099	2.365158	0.382277
O	-3.004434	-0.513780	-0.660185
C	-3.716733	-1.487042	-0.036354
O	-3.420352	-1.919711	1.035895
C	-4.893220	-1.909053	-0.882992
H	-5.559541	-1.045708	-1.040137
H	-4.542194	-2.240506	-1.872992
H	-5.433245	-2.718168	-0.375428
C	2.409504	-2.362212	0.220367
O	3.131391	-3.168449	0.531821

IN17CO

O	-1.938462	4.070778	-0.123301
C	-1.337737	3.341838	-1.154170
C	-2.272779	3.170816	0.900415
C	-1.294738	1.954103	0.792073
C	-2.039772	0.661694	0.560188
C	-1.610498	-0.555877	0.938483
H	-0.813088	4.043214	-1.822323
H	-2.086708	2.778673	-1.753888
H	-2.189400	3.696446	1.864902
H	-3.320063	2.825696	0.789180
H	-0.684659	1.887150	1.704970
H	-2.973949	0.714303	-0.001934
Rh	1.518698	-0.131601	-0.520346
C	-0.395903	2.363983	-0.426873
C	0.133984	1.215329	-1.284236
H	-0.693078	0.586247	-1.648727
C	0.914345	-0.058716	1.390161
O	1.619157	0.424500	2.223346
Cl	0.263826	-1.943924	-1.374454
C	-0.362467	-0.809022	1.705993
C	-0.265548	-1.754564	2.657096
H	-1.121279	-2.394481	2.889763
H	0.670426	-1.913745	3.200097
H	0.648966	1.631450	-2.176370
H	0.434270	2.975119	-0.027810
O	-2.304991	-1.723710	0.737256
C	-3.025393	-1.992984	-0.377532
O	-3.346736	-1.177919	-1.189321
C	-3.348095	-3.467319	-0.435226
H	-2.417698	-4.010096	-0.671471
H	-3.711362	-3.821726	0.541215
H	-4.093913	-3.646776	-1.220033
C	2.620579	1.410435	-0.159810

O	3.253406	2.329793	0.011942
C	2.845953	-1.673882	-0.032167
O	3.486815	-2.575661	0.173496

IN18

O	-1.827151	3.135473	-0.635962
C	-0.492056	3.252995	-1.055013
C	-1.899222	2.567168	0.656108
C	-0.590839	1.769038	0.821912
C	-0.705214	0.427220	0.093897
C	-1.465295	-0.656513	0.799363
H	-0.259754	4.300408	-1.322650
H	-0.327245	2.637065	-1.963876
H	-1.970415	3.359772	1.428534
H	-2.796430	1.930246	0.710929
H	-0.311351	1.611275	1.873487
H	-1.203175	0.600446	-0.874263
Rh	1.085885	-0.638921	-0.097229
C	0.378142	2.753036	0.117831
C	1.778028	2.268501	-0.293399
H	2.269069	3.022309	-0.932827
C	0.373713	-1.295590	-1.761679
O	-0.058006	-1.666092	-2.737148
Cl	1.888823	-0.008500	2.068731
C	-1.484452	-0.891131	2.101298
C	-1.475702	-1.090812	3.393944
H	-2.238547	-0.641236	4.042532
H	-0.695729	-1.702622	3.864848
H	2.385828	2.098021	0.609174
H	0.536299	3.594519	0.814715
O	-2.121534	-1.557792	-0.046700
C	-3.371862	-1.228264	-0.451714
O	-3.925866	-0.226942	-0.109747
C	-3.933783	-2.288571	-1.369802
H	-3.916092	-3.265495	-0.861567
H	-4.960180	-2.017914	-1.647772
H	-3.305639	-2.368826	-2.271206
C	1.803451	0.961740	-1.088543
O	2.223416	0.856886	-2.197732
C	2.850987	-1.711712	-0.056962
O	3.862037	-2.202118	0.013961

IN19

O	4.328468	0.002645	0.159403
C	4.365061	-1.330038	-0.282693
C	3.411959	0.046574	1.221909
C	2.218376	-0.773542	0.707947
C	1.397135	0.013061	-0.328940
C	0.186138	0.803782	0.140059
H	5.074943	-1.917189	0.334803
H	4.726895	-1.340838	-1.323538
H	3.839139	-0.420820	2.134423
H	3.161188	1.097302	1.434532
H	1.573458	-1.176239	1.500014
H	2.088040	0.747468	-0.790948
Rh	-1.707188	-0.330135	-0.034304
C	2.924120	-1.904088	-0.120356
C	2.114361	-2.102829	-1.419266
H	2.726704	-2.105738	-2.338173
C	-2.561312	1.287442	-0.570113
O	-3.088278	2.239807	-0.885377
Cl	-0.749482	-2.401238	0.636429
C	-0.471083	0.673512	1.351655
C	-0.611892	0.846318	2.652560
H	0.181616	1.363364	3.206869
H	-1.490137	0.488331	3.196799
H	1.528867	-3.036984	-1.411437
H	2.955468	-2.840296	0.455630
O	0.043423	2.038795	-0.521587
C	0.782729	3.066743	-0.044772
O	1.513245	2.959194	0.897276
C	0.558880	4.315622	-0.862814
H	-0.512847	4.568769	-0.869865
H	1.146253	5.138426	-0.436246
H	0.863279	4.128806	-1.905141
C	1.101080	-0.964393	-1.477281
O	0.211235	-0.839674	-2.274400
C	-3.387736	-1.366629	0.097215
O	-4.316230	-1.986572	0.267934

IN2

O	-3.831348	0.946768	-0.171784
C	-5.178671	0.991511	0.194352
C	-6.032468	0.867404	-1.038778
C	-7.075594	0.041164	-1.153964
C	-2.953348	1.119433	0.897606
C	-1.541793	0.939049	0.417096
C	-0.552838	1.803088	0.698499
H	-5.401106	1.958873	0.701132
H	-5.425032	0.184655	0.917895
H	-5.751310	1.529328	-1.867815

H	-7.682246	0.012119	-2.064255
H	-7.361033	-0.637293	-0.341421
H	-3.080442	2.120175	1.366492
H	-3.163473	0.365400	1.690605
H	-1.333940	0.034096	-0.168772
H	-0.779069	2.735507	1.232037
C	0.856054	1.607120	0.350257
C	1.608856	0.518026	0.142503
C	3.034835	0.699291	-0.263959
O	3.436042	2.129289	-0.452181
C	2.650606	3.086215	-0.198665
O	1.465148	2.936440	0.208425
C	3.148642	4.476974	-0.423208
H	3.098994	4.685319	-1.506299
H	2.515566	5.195042	0.113703
H	4.199470	4.549501	-0.108173
Rh	1.019219	-1.491790	0.163740
C	0.520247	-1.328310	1.944495
O	0.227352	-1.196649	3.042202
Cl	1.731063	-1.620318	-2.138124
C	0.598506	-3.371133	0.025860
O	0.377996	-4.477376	-0.100265
H	3.223837	0.215087	-1.234959
H	3.747128	0.321364	0.485870

IN20

O	-2.818458	-1.500575	-0.975441
C	-2.582229	-2.494095	-0.019792
C	-1.790979	-1.631778	-1.919395
C	-0.500556	-1.877278	-1.087940
C	0.375117	-0.636822	-0.958569
C	1.080327	-0.337699	0.240600
H	-2.838014	-3.496267	-0.422537
H	-3.215378	-2.297917	0.859791
H	-1.988589	-2.496574	-2.585451
H	-1.750811	-0.715047	-2.526813
H	0.126580	-2.652359	-1.561416
H	0.857881	-0.330460	-1.894304
Rh	-0.585626	0.931997	0.088128
C	-1.064932	-2.402358	0.272469
C	-0.774681	-1.438922	1.440025
H	-1.467971	-0.551439	1.348936
C	0.195181	2.256467	-0.924692
O	0.685209	3.063716	-1.554439
Cl	-2.244666	2.347736	0.909994
C	0.680579	-1.011878	1.498856
C	1.474609	-1.150474	2.570974
H	2.508888	-0.796703	2.555501
H	1.103742	-1.610174	3.491651
H	-1.085144	-1.877828	2.402263
H	-0.631793	-3.383586	0.521283
O	2.329520	0.256224	0.206441
C	3.361385	-0.467248	-0.301393
O	3.234067	-1.572218	-0.735879
C	4.645347	0.324981	-0.231527
H	4.528312	1.268047	-0.788704
H	4.864116	0.586104	0.816028
H	5.462950	-0.271756	-0.655047

IN21

O	3.222473	-1.581732	0.832378
C	3.994284	-1.597992	-0.339854
C	5.354749	-1.031104	-0.039524
C	6.507731	-1.609338	-0.387402
C	1.919297	-2.038827	0.635279
C	1.147619	-1.797981	1.900700
C	-0.082790	-1.250354	1.977695
H	3.492687	-0.983388	-1.118664
H	4.087454	-2.630749	-0.738999
H	5.352867	-0.065790	0.482867
H	7.470994	-1.134705	-0.176446
H	6.529714	-2.576954	-0.902488
H	1.439340	-1.532522	-0.224774
H	1.913907	-3.133864	0.422733
H	1.651353	-2.091053	2.829740
H	-0.566718	-1.119384	2.952678
C	-0.822886	-0.797956	0.830973
C	-1.542848	-0.466371	-0.118779
C	-2.482756	-0.522102	-1.266736
O	-3.354059	-1.631070	-1.186273
C	-4.387993	-1.526704	-0.332424
O	-4.575412	-0.557491	0.345763
C	-5.241856	-2.772699	-0.360437
H	-4.633608	-3.639684	-0.056546
H	-6.092391	-2.645974	0.321143
H	-5.594143	-2.958544	-1.387335
Rh	-0.194669	1.319079	-0.012278
C	-1.095085	2.074012	1.474578
O	-1.651003	2.516695	2.361042
Cl	0.826751	0.418255	-1.953337
C	0.792413	2.925075	-0.400040
O	1.387359	3.846975	-0.675783

H	-1.882536	-0.644386	-2.180933
H	-3.057711	0.415118	-1.324931

IN22

O	1.951480	-1.975175	0.238581
C	2.842648	-1.764810	-0.825947
C	4.154311	-1.273421	-0.278786
C	5.346241	-1.793621	-0.585107
C	0.672284	-2.347325	-0.183949
C	-0.197033	-2.550887	1.027949
C	-1.362330	-1.942035	1.308263
H	2.419629	-1.005656	-1.519154
H	2.994135	-2.702998	-1.402738
H	4.086019	-0.408934	0.394598
H	6.273761	-1.368804	-0.188924
H	5.437180	-2.660252	-1.250592
H	0.246094	-1.598903	-0.877337
H	0.722133	-3.319884	-0.727406
H	0.169668	-3.302467	1.738240
H	-1.926989	-2.270515	2.190868
C	-1.976149	-0.847886	0.539327
C	-1.520092	0.327986	0.096218
C	-2.436586	1.206076	-0.691718
O	-3.805734	0.636282	-0.887381
C	-4.152180	-0.471871	-0.385150
O	-3.387396	-1.205817	0.298904
C	-5.545198	-0.947450	-0.643488
H	-5.592965	-1.320395	-1.681299
H	-5.800541	-1.759265	0.049440
H	-6.245278	-0.104163	-0.552164
Rh	0.424176	1.103935	0.222186
C	0.287478	1.162448	2.073506
O	0.170683	1.180301	3.210063
Cl	0.482246	0.942310	-2.203095
C	2.168321	1.923750	0.160563
O	3.183405	2.426889	0.080886
H	-2.038611	1.361517	-1.707201
H	-2.620102	2.178841	-0.210585

IN23

O	2.789101	-1.950674	0.728914
C	3.807545	-1.249174	0.072689
C	5.117507	-1.954175	0.296008
C	6.001706	-2.224180	-0.668266
C	1.540829	-1.353073	0.591030
C	0.520032	-2.177637	1.321297
C	-0.799959	-2.230899	1.068371
H	3.867043	-0.212826	0.478326
H	3.590908	-1.149437	-1.010867
H	5.327990	-2.230624	1.337313
H	6.956934	-2.710131	-0.446748
H	5.802552	-1.965176	-1.714731
H	1.573454	-0.317195	1.021275
H	1.259339	-1.226980	-0.473766
H	0.926709	-2.802653	2.124769
H	-1.415891	-2.927466	1.648245
C	-1.556709	-1.474799	0.056103
C	-1.326700	-0.246452	-0.419733
C	-1.839207	0.834053	-1.135387
O	-4.167014	-0.628396	0.055704
C	-3.887346	-1.697932	-0.402379
O	-2.637398	-2.208710	-0.418848
C	-4.857257	-2.670017	-1.033900
H	-4.784669	-3.648426	-0.533779
H	-5.876193	-2.270451	-0.954821
H	-4.586285	-2.818338	-2.091789
Rh	-0.134579	1.409843	0.040556
C	-1.193095	1.568549	1.627469
O	-1.818948	1.637055	2.567902
Cl	1.198572	1.179424	-1.887956
H	-1.542775	1.001594	-2.178250
H	-2.763801	1.318467	-0.794614
C	0.780719	3.200367	0.170456
O	1.271335	4.215566	0.140970

IN24

O	2.425545	-1.641089	0.135929
C	3.520050	-1.115865	-0.569784
C	4.706944	-1.035968	0.352670
C	5.922574	-1.503796	0.056584
C	1.308462	-1.945569	-0.642156
C	0.630031	-0.716616	-1.252559
C	-0.808945	-0.669685	-1.503937
C	-1.671577	-0.791751	-0.399093
H	3.282518	-0.098147	-0.950771
H	3.759108	-1.749356	-1.449823
H	4.524148	-0.533693	1.311135
H	6.761353	-1.389747	0.750094
H	6.124866	-2.013938	-0.892517
H	0.611446	-2.494348	0.005434
H	1.604125	-2.622603	-1.473614

H	1.202436	-0.262723	-2.072532
H	-1.240207	-0.369370	-2.464933
Rh	-0.088902	0.769279	0.042532
Cl	0.580562	2.545270	-1.511357
C	-1.055596	-0.794334	0.920658
C	-1.223484	-1.453353	2.065985
H	-0.668515	-1.165079	2.964267
H	-1.900355	-2.312777	2.124141
O	-3.009010	-0.580054	-0.604115
C	-3.898975	-1.492442	-0.128567
O	-3.562210	-2.526365	0.362187
C	-5.312154	-1.007802	-0.332857
H	-6.011926	-1.798639	-0.035067
H	-5.477999	-0.104433	0.276472
H	-5.464135	-0.730329	-1.387548
C	-1.189225	2.247179	0.901348
O	-1.772287	3.109940	1.332910
C	1.522430	0.955252	1.108054
O	2.458082	1.100883	1.725127

IN25

O	2.120069	-1.605467	0.327679
C	3.348976	-1.283712	-0.279452
C	4.210576	-0.550958	0.711260
C	5.420891	-0.960390	1.101653
C	1.156611	-2.120562	-0.536481
C	0.522188	-1.079940	-1.467079
C	-0.848564	-0.764398	-1.545391
C	-1.647311	-0.578621	-0.361327
H	3.182968	-0.614828	-1.147539
H	3.854765	-2.206571	-0.633517
H	3.785035	0.390443	1.081326
H	6.024647	-0.372565	1.800139
H	5.854808	-1.897191	0.732171
H	0.381528	-2.586580	0.086620
H	1.595750	-2.914225	-1.178580
H	1.083178	-0.856831	-2.381961
H	-1.292814	-0.398811	-2.478816
Rh	0.051980	0.702324	-0.212757
Cl	1.965175	1.918041	-0.879809
C	-1.000329	-0.603023	0.905352
C	-1.091182	-1.066727	2.145025
H	-0.437920	-0.690636	2.938398
H	-1.811902	-1.859419	2.376952
O	-2.937827	-0.138963	-0.537076
C	-3.938604	-0.836706	0.066098
O	-3.750917	-1.851437	0.664860
C	-5.262977	-0.145646	-0.143893
H	-6.067475	-0.778370	0.251450
H	-5.252141	0.823887	0.380487
H	-5.416822	0.056680	-1.215127
C	-0.510443	2.232081	0.850848
O	-0.855033	3.126538	1.449431

IN26

O	-2.284053	2.712676	-0.306488
C	-2.495070	1.969145	0.851603
C	-2.590542	0.481164	0.601590
C	-2.242669	-0.478988	1.544088
C	-1.021715	2.530272	-0.879170
C	-0.809459	1.108028	-1.382235
C	0.509567	0.533538	-1.567650
C	1.371543	0.452780	-0.449560
H	-3.469428	2.300902	1.252616
H	-1.720531	2.175716	1.618317
H	-3.226417	0.173004	-0.237396
H	-2.684161	-1.477051	1.473773
H	-1.829711	-0.177212	2.513689
H	-0.220306	2.825877	-0.177621
H	-0.986581	3.214952	-1.743488
H	-1.520623	0.827584	-2.170760
H	0.806427	0.011173	-2.482763
Rh	-0.585490	-0.487231	0.038574
Cl	-1.868294	-2.044787	-1.363667
C	0.804903	0.751037	0.855666
C	1.192588	1.386670	1.960799
H	0.595538	1.330659	2.877840
H	2.104635	1.993690	1.974431
O	2.558923	-0.211033	-0.613032
C	3.705215	0.384088	-0.187015
O	3.738249	1.506297	0.217038
C	4.872006	-0.561800	-0.320809
H	5.799229	-0.029217	-0.075039
H	4.729575	-1.412557	0.365417
H	4.913282	-0.963878	-1.344999
C	0.026653	-2.125915	0.939879
O	0.346757	-3.093810	1.427406

IN27

O	-2.504242	2.233180	-0.814319
C	-3.442092	2.085846	0.236466

C	-4.821263	2.323688	-0.311928
C	-5.862098	1.516952	-0.087018
C	-1.233770	1.953547	-0.519479
C	-0.243862	2.141631	-1.426185
C	1.173431	1.843886	-1.240514
C	1.755889	1.040916	-0.321935
H	-3.218554	2.831977	1.026392
H	-3.358332	1.079187	0.685500
H	-4.942559	3.237700	-0.907405
H	-6.858358	1.750894	-0.474752
H	-5.754820	0.596519	0.498625
H	-0.572037	-0.655736	-1.068685
H	-1.043306	1.573092	0.492139
H	-0.533670	2.579032	-2.387944
H	1.857780	2.315731	-1.954326
Rh	0.016449	-1.457848	0.078180
Cl	-1.706288	-1.047803	1.620594
C	1.480858	-1.796991	-1.114264
O	2.335068	-1.980560	-1.829458
C	1.080492	0.185628	0.691664
C	1.243921	0.378076	2.015368
H	0.746842	-0.260138	2.753249
H	1.864229	1.202481	2.387535
O	3.138346	0.851835	-0.432050
C	3.975275	1.519665	0.383585
O	3.614445	2.302015	1.213445
C	5.411802	1.137650	0.099643
H	6.079614	1.749821	0.718908
H	5.556972	0.069601	0.329334
H	5.634186	1.281361	-0.969159
C	-1.205393	-3.058260	-0.417792
O	-1.967422	-3.852609	-0.653029

IN28

O	3.094307	-1.999167	-0.526823
C	4.012492	-0.922612	-0.383192
C	5.263566	-1.433316	0.274624
C	6.491337	-1.254590	-0.220032
C	1.804325	-1.704538	-0.565003
C	0.866567	-2.638620	-0.868606
C	-0.566737	-2.411789	-0.900307
C	-1.325321	-1.539169	-0.179609
H	3.546700	-0.131594	0.236509
H	4.241532	-0.498798	-1.378494
H	5.116716	-1.956021	1.228129
H	7.378127	-1.609369	0.313769
H	6.654191	-0.739986	-1.174266
H	0.133649	-0.947983	1.311217
H	1.545485	-0.657017	-0.357089
H	1.222522	-3.629780	-1.169631
H	-1.133244	-3.038486	-1.599929
Rh	-0.444378	1.505100	0.169179
Cl	1.494627	1.410566	1.544688
C	-1.976091	1.601589	-0.936073
O	-2.903999	1.687364	-1.587318
C	-0.862249	-0.713573	0.925285
C	-1.620640	0.215519	1.616800
H	-1.247742	0.602401	2.569642
H	-2.685658	0.348243	1.406604
O	-2.659348	-1.402658	-0.528931
C	-3.601256	-2.003798	0.244429
O	-3.333571	-2.665028	1.200257
C	-4.984941	-1.715070	-0.289206
H	-5.729818	-2.201561	0.353025
H	-5.155141	-0.627319	-0.320659
H	-5.065742	-2.090100	-1.321948
C	0.470525	2.924240	-0.765470
O	1.044776	3.759817	-1.268622

IN3

O	-3.677598	1.143060	0.061442
C	-4.947781	1.265420	0.630522
C	-5.986684	1.210868	-0.456841
C	-7.088231	0.456929	-0.409700
C	-2.638212	1.244004	0.983577
C	-1.325822	1.040086	0.279849
C	-0.270509	1.859841	0.434204
H	-5.027973	2.237506	1.169278
H	-5.130519	0.465274	1.380240
H	-5.792664	1.862393	-1.318352
H	-7.828877	0.478601	-1.214937
H	-7.290397	-0.209482	0.437101
H	-2.649582	2.228996	1.499960
H	-2.754148	0.468244	1.775810
H	-1.264325	0.179872	-0.402173
H	-0.366713	2.778234	1.027785
C	1.058480	1.637489	-0.156146
C	1.593662	0.446319	-0.425606
C	2.640340	-0.389914	-0.747768
O	3.678581	2.204649	0.450339
C	3.017800	2.999076	-0.150616
O	1.712757	2.817485	-0.459847

C	3.493463	4.335738	-0.670774
H	2.830425	5.137154	-0.309531
H	4.525523	4.507882	-0.340077
H	3.442214	4.334361	-1.771815
Rh	0.911543	-1.488766	0.035668
C	1.446941	-1.176619	1.839086
O	1.756942	-0.966542	2.909192
Cl	0.164381	-1.826573	-2.162952
C	0.399179	-3.398662	0.290528
O	0.139276	-4.495690	0.345834
H	2.729978	-0.796316	-1.762689
H	3.527716	-0.433645	-0.103039

IN4

O	-3.396301	-0.088839	-0.766149
C	-4.141706	0.437921	0.294162
C	-5.283687	1.244571	-0.264087
C	-6.551517	1.145320	0.144548
C	-2.351768	-0.948252	-0.400331
C	-1.192165	-0.216159	0.269598
C	-0.482555	0.770073	-0.524448
C	0.689885	1.307376	0.041395
H	-3.510646	1.098509	0.928572
H	-4.527624	-0.372186	0.949369
H	-5.006479	1.962453	-1.046694
H	-7.337389	1.780587	-0.275417
H	-6.850115	0.425483	0.915690
H	-1.997087	-1.430623	-1.322623
H	-2.720634	-1.743867	0.279660
H	-1.344561	0.052537	1.322859
H	-0.731257	0.986731	-1.569180
Rh	0.805230	-0.933057	0.118498
Cl	0.443471	-2.375097	-1.844299
C	1.115658	0.699969	1.293908
C	1.526657	1.114743	2.490487
H	1.872048	0.401577	3.245808
H	1.517482	2.180729	2.742913
O	1.473426	2.135237	-0.716154
C	1.857245	3.331755	-0.194213
O	1.460901	3.733888	0.856715
C	2.808203	4.034075	-1.130157
H	3.037312	5.030446	-0.732082
H	3.731761	3.440041	-1.224349
H	2.358033	4.109859	-2.132282
C	2.732994	-1.235269	-0.397890
O	3.791244	-1.442497	-0.726248
C	0.576821	-2.400704	1.369119
O	0.409530	-3.246611	2.100074

IN5

O	-3.469702	0.318748	-0.840599
C	-4.202886	0.529484	0.333492
C	-5.313508	1.504340	0.047679
C	-6.588689	1.322372	0.401308
C	-2.412837	-0.591866	-0.726204
C	-1.209006	-0.019055	0.005426
C	-0.268763	0.767480	-0.682579
C	0.995082	1.058102	-0.062239
H	-3.551710	0.950607	1.131026
H	-4.616116	-0.426066	0.719736
H	-5.005872	2.420272	-0.472993
H	-7.350889	2.080383	0.196189
H	-6.916852	0.408923	0.911022
H	-2.121398	-0.869366	-1.751609
H	-2.731951	-1.521291	-0.215528
H	-1.285386	0.096849	1.094943
H	-0.361087	0.972399	-1.756440
Rh	0.744482	-1.060505	0.018947
Cl	-0.191305	-3.197872	-0.263808
C	1.241637	0.473234	1.213502
C	1.630506	0.732014	2.455390
H	1.840885	-0.075739	3.163608
H	1.737586	1.772320	2.783489
O	1.948716	1.712169	-0.802615
C	2.498926	2.843601	-0.282243
O	2.139090	3.323368	0.748975
C	3.585464	3.364993	-1.189393
H	3.951310	4.323697	-0.801001
H	4.408268	2.632681	-1.228738
H	3.195611	3.483143	-2.212375
C	2.537443	-1.817667	0.017144
O	3.581631	-2.249840	0.004623

IN6

O	-3.107433	-2.057350	-0.273020
C	-3.387229	-0.836764	0.345732
C	-2.036265	-2.011052	-1.177938
C	-0.754891	-1.674462	-0.445798
C	0.426376	-1.173042	-1.094292
C	1.434745	-0.682730	-0.224764
H	-4.299999	-1.004748	0.944780

H	-3.584779	-0.036116	-0.391180
H	-1.971739	-3.021143	-1.617627
H	-2.219232	-1.275703	-1.984018
H	-0.582464	-2.299546	0.438755
H	0.522504	-1.015460	-2.173436
Rh	-0.432500	0.392267	0.167989
C	-2.298879	-0.381430	1.301165
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C	0.245308	2.215382	0.389046
O	0.611800	3.279996	0.490323
Cl	-1.770276	1.453562	-1.624463
C	1.056723	-0.552045	1.174237
C	1.560950	-0.877390	2.362849
H	2.468236	-1.487502	2.438538
H	1.077120	-0.546517	3.288107
H	-1.570094	1.208572	2.560219
H	-1.915712	-1.154213	1.979218
O	2.561450	-0.126008	-0.769296
C	3.775075	-0.558641	-0.333218
O	3.902077	-1.474799	0.420431
C	4.879396	0.267428	-0.943693
H	4.768777	0.290714	-2.038954
H	4.800478	1.304612	-0.579101
H	5.849379	-0.159986	-0.660402

IN7

O	-3.504126	-1.070810	-1.022671
C	-3.208907	0.273207	-0.673035
C	-3.223331	-1.917969	0.051292
C	-2.032391	-1.250656	0.759009
C	-0.751688	-1.509505	-0.023929
C	0.491269	-1.545884	0.577638
H	-4.141649	0.863424	-0.610966
H	-2.563645	0.710656	-1.451648
H	-4.076321	-1.997742	0.758104
H	-3.006256	-2.926415	-0.338539
H	-1.897302	-1.587231	1.799520
H	-0.841342	-1.956047	-1.021796
Rh	0.386864	0.639565	0.098023
C	-2.496053	0.223440	0.704170
C	-1.375476	1.240705	0.955654
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C	1.111266	2.320755	0.627482
O	1.522440	3.325391	0.940247
Cl	-0.199960	1.599066	-2.057862
C	0.831947	-0.618006	1.643411
C	1.224266	-0.721195	2.912332
H	1.302156	-1.693169	3.415375
H	1.471997	0.168112	3.501468
H	-1.228971	1.363129	2.041885
H	-3.261222	0.348494	1.493645
O	1.531374	-2.177529	-0.106862
C	2.435456	-1.428342	-0.735572
O	2.317872	-0.227209	-0.827061
C	3.566888	-2.228979	-1.311981
H	4.108955	-2.729710	-0.493733
H	3.159815	-3.009772	-1.973538
H	4.238161	-1.563364	-1.868230

IN8

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C	3.178698	2.318755	0.580124
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C	1.150588	2.005340	-0.572249
C	-0.096700	1.223674	-0.919743
C	-1.150999	0.945984	-0.047545
H	3.157807	3.396271	0.841809
H	3.958427	1.833459	1.192451
H	2.273672	2.439503	-2.425502
H	2.402215	0.741809	-1.856212
H	0.865292	3.075434	-0.594120
H	-0.388554	1.229386	-1.978150
Rh	0.223342	-0.839087	0.177411
C	1.792322	1.677763	0.782843
C	1.879686	0.154041	0.970974
H	2.721643	-0.259361	0.390982
C	0.678721	-2.189636	1.463003
O	0.983604	-2.957055	2.233392
Cl	1.597589	-1.914789	-1.558704
C	-0.939264	0.432093	1.286543
C	-1.357695	0.702363	2.519445
H	-1.959267	1.598010	2.713351
H	-1.104712	0.051111	3.362004
H	2.052505	-0.068967	2.037369
H	1.245007	2.143142	1.616446
O	-2.372468	0.670612	-0.641128
C	-3.455796	1.341933	-0.167152
O	-3.369399	2.195468	0.662631
C	-4.718222	0.861323	-0.838165
H	-4.597006	0.887466	-1.932148
H	-4.909888	-0.184349	-0.547232

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C	-1.249613	-1.935380	-0.837913
O	-1.939274	-2.571042	-1.460866

IN9

O	-4.520995	-0.971961	-0.243981
C	-3.771540	-0.179490	-1.118398
C	-3.621208	-1.799091	0.444537
C	-2.263848	-1.035050	0.534831
C	-1.108332	-1.834620	-0.004429
C	0.173833	-1.485726	0.182465
H	-4.404746	0.647448	-1.476409
H	-3.419111	-0.760931	-1.999702
H	-4.050886	-2.033143	1.431033
H	-3.479553	-2.754107	-0.101607
H	-2.039096	-0.753999	1.576621
H	-1.302991	-2.718933	-0.622135
Rh	0.380712	1.424716	-0.175700
C	-2.565273	0.282083	-0.277826
C	-1.408875	0.876294	-1.071840
H	-1.103319	0.201059	-1.886302
C	-0.653247	2.104267	1.277708
O	-1.279123	2.488822	2.138208
Cl	1.531939	0.821846	-2.132021
C	0.599380	-0.269850	0.924673
C	1.096487	-0.286467	2.167919
H	1.233237	-1.243771	2.683200
H	1.392908	0.625613	2.698548
H	-1.736548	1.832128	-1.535288
H	-2.959313	1.020792	0.442630
O	1.165990	-2.197449	-0.465302
C	2.012520	-2.965897	0.246620
O	1.913182	-3.140027	1.426988
C	3.070653	-3.560484	-0.652402
H	2.591876	-4.101047	-1.483788
H	3.670154	-2.746700	-1.091121
H	3.708847	-4.235242	-0.068114
C	2.320520	2.029060	0.378494
O	3.400585	2.281496	0.567734

INS1

C	-4.480567	1.358019	-0.851635
C	-4.679020	2.504458	0.114093
C	-4.900723	3.769285	-0.256990
C	-1.960773	1.207309	-1.081920
C	-1.308138	2.109655	-0.063961
C	-0.051036	1.988805	0.410523
H	-5.317645	0.650738	-0.736350
H	-4.494259	1.725442	-1.893019
H	-4.651423	2.225094	1.175603
H	-5.066697	4.560890	0.480389
H	-4.932688	4.057448	-1.314804
H	-1.276270	0.406342	-1.403863
H	-2.196324	1.795134	-1.987462
H	-1.910519	2.953218	0.292374
C	0.839741	0.903706	0.026233
C	1.884387	0.285842	-0.297540
C	3.209751	0.127863	-0.996252
O	4.243773	0.800837	-0.247748
C	4.205980	2.108274	0.015860
O	3.323282	2.848594	-0.323030
C	5.423678	2.524229	0.816397
H	6.340996	2.185975	0.310300
H	5.426217	3.615411	0.933947
H	5.391238	2.038375	1.805195
Rh	0.534290	-1.250684	0.391139
C	1.022244	-0.927294	2.195707
O	1.326998	-0.704981	3.265441
Cl	0.070471	-1.705422	-1.953176
C	0.674662	-3.195924	0.528026
O	0.823074	-4.319012	0.535894
N	-3.233550	0.623522	-0.642143
S	-3.245567	-0.731484	0.279414
O	-1.946841	-0.838186	0.942259
O	-4.457172	-0.718089	1.074062
C	-3.358389	-2.114413	-0.873901
H	-3.416022	-3.025177	-0.259002
H	-4.276482	-1.990099	-1.465265
H	-2.450660	-2.115856	-1.498527
C	3.677901	-1.328901	-1.035328
H	4.660404	-1.374388	-1.530882
H	3.773829	-1.727924	-0.014015
H	2.951431	-1.936541	-1.594301
C	3.089214	0.689396	-2.424572
H	2.337020	0.092443	-2.963857
H	2.772243	1.740283	-2.410456
H	4.062832	0.599763	-2.934582
C	0.542630	2.976578	1.395802
H	0.852318	2.461822	2.321977
H	1.440191	3.444410	0.959079
H	-0.191012	3.754619	1.656382

INS10

O	-2.891556	0.586209	0.767822
C	-4.095624	0.149244	0.197675
C	-4.720515	-0.888350	1.090194
C	-5.993826	-0.862171	1.493105
C	-2.190824	1.495282	-0.015957
C	-0.869182	1.791588	0.688301
C	0.044263	0.608245	0.981353
C	1.366884	0.948868	0.727547
H	-3.892159	-0.294936	-0.802121
H	-4.792530	0.999851	0.044582
H	-4.058318	-1.711668	1.386847
H	-6.411306	-1.660339	2.114502
H	-6.667038	-0.043722	1.212051
H	-2.001651	1.081066	-1.029106
H	-2.747945	2.446379	-0.145767
H	-1.126671	2.260093	1.661226
H	-0.285248	-0.212218	1.617919
Rh	0.460453	-0.750168	-0.908037
Cl	0.604731	-2.504712	0.674973
C	0.488539	-2.151163	-2.204725
O	0.501165	-3.017099	-2.933001
C	1.450887	2.281026	0.080253
C	2.552757	2.957712	-0.269885
H	3.550796	2.534485	-0.119031
H	2.449656	3.953520	-0.714313
O	2.523168	0.377031	1.059792
C	2.804299	-0.467934	2.130953
O	3.825510	-1.064013	2.079547
C	1.842084	-0.474505	3.294637
H	2.415291	-0.770650	4.183711
H	1.360334	0.501067	3.453608
H	1.071834	-1.237505	3.099306
C	0.036337	2.784384	-0.052231
O	-0.316843	3.778033	-0.624380
C	0.361893	0.574298	-2.250885
O	0.316847	1.341477	-3.089569

INS11

C	-1.681104	1.877687	0.970565
C	-2.513595	1.305988	2.091728
C	-3.456314	2.004336	2.729276
C	-0.791174	1.668792	-1.335119
C	0.354801	2.536403	-0.870535
C	1.649724	2.218051	-0.640597
H	-2.081203	2.867900	0.688034
H	-0.642826	2.021333	1.311709
H	-2.307210	0.275466	2.400407
H	-4.006964	1.573698	3.570645
H	-3.720501	3.021617	2.420764
H	-0.439704	0.869017	-2.005031
H	-1.470295	2.339560	-1.892580
H	0.102354	3.597118	-0.760871
C	2.232011	0.852294	-0.611463
C	1.635682	-0.290915	-0.267203
C	1.916866	-1.652540	0.074211
O	4.228024	0.762769	1.232459
C	4.508039	0.778218	0.067626
O	3.598708	0.828527	-0.921257
C	5.910477	0.766678	-0.498871
H	6.632056	0.627516	0.316080
H	6.006650	-0.034378	-1.247790
H	6.102582	1.723371	-1.011431
Rh	-0.165503	-1.048728	0.245219
C	0.147092	-0.512021	2.040269
O	0.315593	-0.179473	3.109842
Cl	-0.600288	-1.797712	-2.022959
C	-1.590906	-2.451754	0.690303
O	-2.303266	-3.306683	0.869113
N	-1.576771	1.003659	-0.235450
S	-3.239204	0.678025	-0.753177
O	-3.656265	-0.499359	-0.017754
O	-3.980388	1.920104	-0.630104
C	-3.185106	0.272656	-2.509965
H	-4.222863	-0.040687	-2.701321
H	-2.942207	1.174454	-3.084436
H	-2.475214	-0.550129	-2.671369
C	2.637631	3.328343	-0.331010
H	2.132732	4.304085	-0.284392
H	3.143484	3.143213	0.631965
H	3.416274	3.376644	-1.110618
C	2.645209	-1.950659	1.386859
H	3.715057	-2.122980	1.169894
H	2.603181	-1.120320	2.104061
H	2.250607	-2.870904	1.850652
C	2.251587	-2.689700	-0.992659
H	1.882772	-3.686560	-0.697767
H	1.840042	-2.437759	-1.975009
H	3.353617	-2.749665	-1.066042

INS12

C	-2.510084	-1.277438	-0.230802
C	-1.546255	-1.375499	0.938800
C	-0.954471	-2.555173	1.291435
C	-1.970398	1.013395	-1.146274
C	-1.522731	2.071703	-0.168176
C	-0.274612	2.428832	0.190040
H	-2.065816	-1.761034	-1.117370
H	-3.415781	-1.855963	0.020160
H	-1.508109	-0.515777	1.621730
H	-0.530297	-2.703099	2.288652
H	-1.115158	-3.451207	0.681615
H	-1.130376	0.416701	-1.532040
H	-2.457696	1.510345	-2.001233
H	-2.345181	2.670756	0.243852
C	0.972777	1.787831	-0.312395
C	1.353459	0.510875	-0.325891
C	2.530621	-0.238862	-0.638239
O	3.086196	2.812463	1.065857
C	2.881800	3.185370	-0.054640
O	1.872535	2.740059	-0.821765
C	3.699878	4.217792	-0.798894
H	3.059799	5.077032	-1.055943
H	4.537258	4.543484	-0.168948
H	4.069329	3.789552	-1.743809
Rh	0.979022	-1.448707	0.232712
C	1.448265	-0.848847	1.984721
O	1.630384	-0.498928	3.045493
Cl	0.201824	-2.204838	-1.930743
C	1.787099	-3.308638	0.265362
O	2.312659	-4.302961	0.160403
N	-2.928917	0.068962	-0.556534
S	-4.456096	0.550299	-0.195196
O	-4.665560	1.810606	-0.878008
O	-5.350282	-0.573805	-0.383864
C	-4.475915	0.889769	1.587593
H	-3.748041	1.680672	1.815015
H	-5.498729	1.217231	1.827373
H	-4.241690	-0.041161	2.124714
C	3.783823	-0.111254	0.230194
H	4.472424	0.613564	-0.241543
H	3.576652	0.268404	1.240172
H	4.318637	-1.074613	0.293542
C	2.883000	-0.506778	-2.098121
H	1.998656	-0.545087	-2.743236
H	3.542891	0.313693	-2.436262
H	3.440583	-1.452422	-2.207651
C	-0.049574	3.617013	1.109071
H	-1.003623	3.980730	1.519300
H	0.629989	3.354245	1.936137
H	0.419676	4.450490	0.557588

INS13

O	0.170309	3.450674	-0.156846
C	-1.079669	2.907375	-0.416081
C	-1.575751	1.907659	0.619448
C	-2.769783	1.246615	0.456227
C	1.281385	2.613010	-0.378194
C	1.935795	2.267316	0.936838
C	2.239830	1.044933	1.400846
H	-1.147539	2.463445	-1.426685
H	-1.785634	3.756932	-0.372283
H	-1.121900	1.992120	1.615471
H	-3.336446	0.874753	1.314851
H	-3.319152	1.350202	-0.486759
H	1.001998	1.712241	-0.951189
H	2.007276	3.189961	-0.982996
H	2.209518	3.135805	1.549560
H	2.805689	0.960105	2.338215
C	1.969590	-0.255093	0.747318
C	0.811679	-0.746945	0.305194
C	0.264827	-1.964725	-0.181405
O	4.858288	-1.872833	-0.303322
C	3.916807	-1.142677	-0.350057
O	3.084705	-1.080455	0.720608
C	3.571825	-0.260881	-1.536851
H	3.548688	0.797521	-1.228348
H	4.340372	-0.411216	-2.305510
H	2.575836	-0.507042	-1.939252
Rh	-1.231756	-0.511195	0.111864
C	-1.287225	-0.939878	1.975469
O	-1.280395	-1.182087	3.080260
Cl	-0.962977	0.028365	-2.223674
C	-2.883007	-1.527363	-0.569716
O	-3.696794	-2.146736	-1.045784
H	0.324349	-2.198006	-1.251885
H	0.229869	-2.839846	0.481823

INS14

O	-1.489972	1.256996	-0.913250
C	-2.190780	2.248733	-0.196110
C	-3.358859	1.619251	0.513004
C	-3.606990	1.764015	1.819129

C	-0.543936	1.748776	-1.866160
C	0.593880	2.547175	-1.269214
C	1.726016	2.051501	-0.724677
H	-2.559994	3.007843	-0.916490
H	-1.522837	2.763383	0.523580
H	-4.035605	1.032569	-0.122041
H	-4.490014	1.315344	2.284666
H	-2.941803	2.346913	2.467372
H	-0.176159	0.848701	-2.381538
H	-1.093647	2.375176	-2.592686
H	0.515421	3.639549	-1.324031
H	2.499038	2.769093	-0.422106
C	2.103733	0.652513	-0.470604
C	1.278833	-0.373701	-0.240947
C	1.162702	-1.706607	0.238306
O	3.539183	-0.367079	1.620933
C	4.100240	-0.061851	0.608837
O	3.486827	0.485633	-0.459889
C	5.578828	-0.227505	0.337121
H	6.010916	0.730129	0.007636
H	6.078323	-0.585973	1.246121
H	5.715985	-0.952230	-0.481938
Rh	-0.690603	-0.710931	0.048135
C	-0.490579	0.038853	1.795172
O	-0.348273	0.483040	2.826576
Cl	-0.891671	-1.685189	-2.131211
C	-2.366915	-1.802863	0.423641
O	-3.238242	-2.505132	0.576125
H	1.176155	-2.538523	-0.475988
H	1.546534	-1.929283	1.243007

INS15

O	2.004868	2.884120	-1.243194
C	2.698709	1.649068	-1.270090
C	1.480791	3.127180	0.038302
C	1.348577	1.728102	0.674444
C	0.084845	1.078899	0.099488
C	-0.974031	0.694515	1.003345
H	3.718502	1.801373	-1.664992
H	2.171810	0.928238	-1.924670
H	2.161801	3.760587	0.642847
H	0.519991	3.658390	-0.064082
H	1.297627	1.754695	1.775126
H	-0.230563	1.499480	-0.860890
Rh	-0.052218	-1.034884	0.094463
C	2.704528	1.156230	0.188137
C	2.983726	-0.331492	0.429143
H	3.347579	-0.820083	-0.494133
Cl	0.931023	-1.781036	-1.946737
C	-0.634517	-0.298854	1.948377
C	-0.600524	-0.633651	3.230910
H	-0.841641	0.094553	4.014813
H	-0.308322	-1.643609	3.536491
H	3.749255	-0.490102	1.205832
H	3.476925	1.729227	0.729281
O	-2.299393	0.996887	0.877824
C	-2.922307	1.343026	-0.282001
O	-2.446550	1.157397	-1.360402
C	-4.274437	1.942072	0.011701
H	-4.144526	2.875845	0.582504
H	-4.792791	2.142942	-0.934255
H	-4.859962	1.249133	0.636190
C	1.778877	-1.174750	0.798867
O	1.833327	-2.212757	1.396462
C	-1.909133	-1.632442	-0.851598
O	-2.758988	-2.023232	-1.477006

INS2

C	4.434217	-1.647067	0.005228
C	5.734014	-1.467720	-0.742752
C	6.155454	-2.270185	-1.724992
C	3.041425	-0.038519	-1.337521
C	1.829915	-0.844791	-1.778537
C	0.499115	-0.610871	-1.649210
H	3.878346	-2.518008	-0.394035
H	4.665094	-1.848226	1.064264
H	6.344560	-0.615970	-0.415677
H	7.119841	-2.112340	-2.217728
H	5.554533	-3.123090	-2.062837
H	2.847934	1.034684	-1.297196
H	3.847312	-0.192878	-2.074508
H	2.083964	-1.806369	-2.242526
C	-0.084984	0.598079	-1.014760
C	-1.208514	0.747362	-0.287688
C	-1.376027	2.020129	0.520151
O	-0.337459	3.074253	0.136142
C	0.645809	2.820248	-0.607580
O	0.802036	1.715316	-1.201950
C	1.690429	3.864518	-0.802714
H	2.491445	3.618391	-0.081816
H	2.096336	3.809040	-1.822452
H	1.282782	4.859511	-0.581586

Rh	-2.800498	-0.664442	-0.028165
C	-3.686222	0.161841	-1.432668
O	-4.194475	0.682069	-2.316293
Cl	-1.586693	-1.756341	1.755360
C	-4.221005	-1.907315	0.344636
O	-5.039848	-2.649299	0.604752
C	-2.697756	2.753719	0.301500
H	-2.905598	2.894146	-0.771318
H	-3.511637	2.157741	0.740574
H	-2.663664	3.736696	0.798050
C	-1.073151	1.774462	2.000465
H	-1.721787	0.971735	2.382236
H	-0.024865	1.452744	2.107758
H	-1.229814	2.701140	2.576970
C	-0.475509	-1.682948	-2.089696
H	-1.285835	-1.260790	-2.705342
H	0.046397	-2.458827	-2.669313
H	-0.942585	-2.160149	-1.210610
N	3.614277	-0.437370	-0.046207
S	3.013469	0.156212	1.367606
O	4.076203	0.103521	2.349488
O	2.387948	1.438691	1.047246
C	1.716517	-0.968982	1.910900
H	2.156252	-1.971162	2.019992
H	1.370275	-0.603675	2.889450
H	0.883851	-0.972626	1.192038

INS3

C	-3.186760	2.839095	0.068517
C	-3.639299	3.069715	-1.359320
C	-3.289933	2.329648	-2.416817
C	-0.864766	1.893931	-0.147864
C	0.027576	2.221750	1.022469
C	1.315206	1.870911	1.193955
H	-2.694368	3.755316	0.447999
H	-4.059683	2.688122	0.726475
H	-4.300745	3.935768	-1.495558
H	-3.660234	2.573784	-3.417075
H	-2.619267	1.466101	-2.325854
H	-0.511965	1.028761	-0.721756
H	-0.856333	2.744918	-0.852548
H	-0.418850	2.887978	1.772762
C	2.065433	0.925490	0.316681
C	1.682905	-0.285298	-0.088100
C	2.183827	-1.492108	-0.666547
O	2.786957	3.141143	-1.041461
C	3.642180	2.432052	-0.598353
O	3.393616	1.284802	0.061765
C	5.132463	2.679965	-0.692370
H	5.557940	2.764574	0.320466
H	5.620552	1.825087	-1.186322
H	5.311914	3.602377	-1.259102
Rh	0.162117	-1.629496	0.055806
C	0.748125	-1.960623	1.837663
O	1.031609	-2.099415	2.923994
Cl	-0.829676	-1.082773	-2.103974
C	-0.790376	-3.404266	-0.249538
O	-1.239854	-4.401620	-0.530106
N	-2.272805	1.719575	0.235907
C	3.228063	-2.303286	0.099106
H	3.123362	-3.381720	-0.110152
H	4.234271	-1.994340	-0.238916
H	3.185755	-2.143969	1.186502
C	2.357052	-1.623230	-2.175457
H	2.209323	-2.667182	-2.500562
H	1.664254	-0.980506	-2.730327
H	3.396535	-1.338090	-2.423840
C	2.127878	2.438308	2.343011
H	2.655022	1.640739	2.894059
H	2.892598	3.144645	1.973708
H	1.479768	2.984241	3.045170
S	-2.838635	0.344636	0.907701
O	-1.673326	-0.503465	1.191866
O	-3.732920	0.670297	1.998465
C	-3.831119	-0.490718	-0.347243
H	-4.289988	-1.355337	0.155353
H	-4.602333	0.215093	-0.688987
H	-3.159889	-0.795057	-1.164670

INS4

C	3.253626	-1.206027	0.182948
C	3.975846	-1.606814	1.450361
C	3.791352	-2.779133	2.065698
C	1.469708	0.091376	1.344829
C	0.357680	-0.929520	1.110149
C	-0.985592	-0.691415	1.663164
C	-1.634071	0.454273	1.147401
H	3.985915	-1.090527	-0.634018
H	2.551731	-2.000540	-0.125586
H	4.686363	-0.867105	1.840607
H	4.348457	-3.042094	2.970489
H	3.084877	-3.523834	1.678441

H	1.070356	1.109873	1.379551
H	1.926834	-0.129505	2.330119
H	0.684422	-1.964751	1.282852
Rh	-0.865810	-0.811481	-0.582985
Cl	-1.090926	-3.260110	-0.638108
C	-1.000799	1.122799	0.026413
C	-0.735309	2.398273	-0.279035
O	-2.858551	0.786674	1.659236
C	-3.923555	1.094437	0.875257
O	-3.935666	0.935506	-0.307450
C	-5.056949	1.629942	1.714688
H	-5.929610	1.805186	1.073193
H	-5.302562	0.912432	2.513099
H	-4.742827	2.570020	2.196171
C	-2.436680	-0.775825	-1.886698
O	-3.250280	-0.846874	-2.662120
C	-0.135339	2.813352	-1.598472
H	-0.775310	3.560326	-2.101959
H	0.847078	3.286675	-1.418079
H	-0.012458	1.956022	-2.279142
C	-0.936862	3.516665	0.721823
H	-1.546999	4.329679	0.288935
H	-1.419016	3.165659	1.647234
H	0.047700	3.946781	0.983166
C	-1.661068	-1.678917	2.575096
H	-1.179184	-1.658513	3.567714
H	-2.731837	-1.464037	2.694103
H	-1.538808	-2.689940	2.150412
N	2.497774	0.048179	0.303299
S	3.341077	1.444455	-0.016192
O	4.717727	1.309540	0.423672
O	2.532628	2.557547	0.450015
C	3.382990	1.511412	-1.820651
H	2.356899	1.633162	-2.190901
H	4.002483	2.387074	-2.065275
H	3.845772	0.595984	-2.214433
C	0.547276	-0.828030	-1.890098
O	1.378114	-0.887287	-2.659077

INS5

C	3.473545	1.026314	-0.084382
C	4.068540	1.861408	-1.193836
C	3.978769	3.193647	-1.258861
C	1.472506	0.348977	-1.447418
C	0.526381	1.365576	-0.810416
C	-0.852077	1.534820	-1.128021
C	-1.712054	0.376340	-1.071245
H	4.295440	0.530490	0.457325
H	2.925004	1.656134	0.640029
H	4.611669	1.300197	-1.966169
H	4.451070	3.761226	-2.066843
H	3.443737	3.764664	-0.490109
H	0.957310	-0.565246	-1.760655
H	1.874666	0.830632	-2.361176
H	1.026847	2.314927	-0.578956
Rh	-0.696479	0.584494	0.827693
Cl	0.811350	1.274864	2.518654
C	-1.201334	-0.825374	-0.516042
C	-1.172336	-2.146788	-0.701005
O	-3.014605	0.567491	-1.465262
C	-4.079790	0.084950	-0.777457
O	-3.998133	-0.423372	0.299135
C	-5.350307	0.302636	-1.563821
H	-6.205611	-0.041838	-0.969086
H	-5.459244	1.369671	-1.813442
H	-5.294688	-0.256993	-2.511414
C	-1.923962	-0.086182	2.208292
O	-2.592238	-0.449234	3.042358
C	-0.762353	-3.119248	0.376372
H	-1.491986	-3.945241	0.441182
H	0.221620	-3.551491	0.121257
H	-0.696449	-2.637877	1.364126
C	-1.488302	-2.747182	-2.054226
H	-2.288519	-3.503783	-1.966187
H	-1.797813	-1.984741	-2.785339
H	-0.589406	-3.260333	-2.441383
C	-1.467212	2.903817	-1.294017
H	-1.521297	3.144987	-2.370805
H	-2.484488	2.955999	-0.881393
H	-0.835481	3.663057	-0.808681
N	2.597325	-0.022417	-0.603504
S	2.930911	-1.588771	-0.237727
O	4.369510	-1.764398	-0.262847
O	2.076398	-2.416169	-1.074553
C	2.423806	-1.817908	1.481227
H	1.336660	-1.683452	1.548478
H	2.727161	-2.838200	1.759579
H	2.936162	-1.069824	2.102982

INS6

C	2.175260	0.408524	-1.424622
C	1.490037	-0.936309	-1.313798

C	0.505097	-1.364069	-2.196169
C	1.609240	1.205204	0.832854
C	0.771634	-0.025508	1.163194
C	-0.566668	0.082580	1.734889
C	-1.516997	0.767564	0.934143
H	3.036565	0.290113	-2.100705
H	1.491809	1.155070	-1.863631
H	2.018612	-1.693656	-0.722392
H	0.333032	-2.437537	-2.314512
H	0.162959	-0.709303	-3.004492
H	0.988417	2.024232	0.441493
H	2.095567	1.555379	1.756156
H	1.379220	-0.805977	1.643111
Rh	-0.554294	-0.838700	-0.303601
Cl	-0.163658	-3.130370	0.504912
C	-1.144966	1.103188	-0.432721
C	-1.380791	2.183603	-1.191472
O	-2.759481	0.967759	1.474805
C	-3.913197	0.768635	0.789220
O	-3.961863	0.248541	-0.283615
C	-5.090392	1.271681	1.589156
H	-4.974999	2.350721	1.779059
H	-6.014806	1.078362	1.030642
H	-5.119560	0.762860	2.565634
C	-2.120863	-1.612085	-1.245793
O	-2.937015	-2.148149	-1.811747
C	-1.081884	2.222151	-2.672008
H	-0.684126	1.262985	-3.032741
H	-2.000545	2.447830	-3.244109
H	-0.355306	3.021261	-2.911089
C	-1.979389	3.455254	-0.621461
H	-2.944237	3.680856	-1.112955
H	-2.147062	3.387170	0.464421
H	-1.317489	4.319535	-0.814287
C	-0.936444	-0.641440	3.002626
H	-0.538718	-1.668878	2.945231
H	-0.475830	-0.136520	3.868982
H	-2.023897	-0.685247	3.150417
N	2.654774	0.920444	-0.147392
S	4.129619	0.388039	0.403675
O	4.614696	-0.617702	-0.521466
O	4.017598	0.112579	1.822637
C	5.202215	1.831204	0.230685
H	4.799149	2.644085	0.850268
H	6.195430	1.523162	0.589829
H	5.241048	2.114293	-0.830073

INS7

O	3.190542	0.595291	0.071578
C	4.402745	0.386401	-0.591398
C	5.388201	1.445681	-0.175986
C	6.637454	1.197441	0.226796
C	2.176449	-0.291924	-0.313510
C	0.925866	-0.020566	0.536576
C	0.555957	1.437995	0.500920
C	-0.660045	1.759031	0.052638
H	4.245085	0.442208	-1.693152
H	4.808589	-0.624429	-0.374506
H	5.019967	2.477825	-0.238643
H	7.324477	2.007927	0.489105
H	7.019018	0.172861	0.307894
H	1.954186	-0.154881	-1.397943
H	2.498601	-1.341561	-0.164806
H	1.164846	-0.320188	1.572543
H	1.272146	2.210784	0.801058
Rh	-0.592821	-1.268052	-0.151356
Cl	0.487489	-3.050485	0.925096
C	-2.035892	-0.250024	0.726718
O	-2.742469	-0.371135	1.651748
C	-1.579018	0.639935	-0.347947
C	-1.591383	0.103763	-1.638586
H	-0.985031	0.596544	-2.406883
H	-2.430480	-0.500007	-1.995249
O	-1.075243	3.055803	-0.111122
C	-2.370141	3.390995	0.069469
O	-3.216545	2.593348	0.350512
C	-2.571782	4.873196	-0.130341
H	-1.991809	5.424685	0.627242
H	-2.193864	5.171806	-1.120753
H	-3.639091	5.109065	-0.035691
C	-1.841632	-2.815835	-0.748850
O	-2.443496	-3.734384	-0.998321

INS8

O	3.147758	-0.573167	0.083392
C	4.299688	-1.209364	-0.398809
C	1.975069	-1.307946	-0.112577
C	0.807900	-0.549299	0.487833
C	0.474758	0.718235	-0.161353
C	-0.629943	1.469633	0.217189
H	4.171285	-1.449641	-1.478509
H	4.472981	-2.170805	0.129121

H	1.807697	-1.479032	-1.200302
H	2.051995	-2.307477	0.364391
H	0.852646	-0.521653	1.585974
H	0.994745	1.024905	-1.077942
Rh	-1.105404	-0.920801	-0.293663
Cl	-2.925198	-0.755856	-1.779235
C	-1.357907	-2.787372	0.015219
O	-1.511450	-3.890079	0.204461
C	-1.489456	1.114707	1.373214
C	-2.239319	1.970685	2.086532
H	-2.228169	3.046224	1.884899
H	-2.898659	1.584543	2.870223
O	-0.937560	2.623101	-0.415813
C	-0.071353	3.686414	-0.522060
O	-0.326508	4.543300	-1.302102
C	1.116396	3.701174	0.424616
H	1.489243	4.733258	0.461299
H	0.838296	3.356175	1.432784
H	1.922852	3.046956	0.057208
C	-1.651354	-0.380737	1.496493
O	-2.092748	-1.008840	2.401140
C	5.484054	-0.297748	-0.225088
H	5.356545	0.718592	-0.619312
C	6.638074	-0.663253	0.339589
H	6.782228	-1.670984	0.746505
H	7.482273	0.029234	0.412097

INS9

O	2.919858	0.904627	0.501962
C	4.083897	0.267420	0.040853
C	2.039531	0.049580	1.158754
C	0.721513	0.805701	1.340066
C	0.034032	1.251523	0.059788
C	-1.325282	1.067559	0.136748
H	3.801481	-0.545997	-0.661903
H	4.640443	-0.194865	0.882605
H	1.865556	-0.871287	0.565810
H	2.418770	-0.248510	2.158103
H	0.951011	1.709923	1.941010
H	0.544785	1.823086	-0.720374
Rh	-0.846216	-1.123763	-0.338661
Cl	0.596913	-1.536874	-2.124293
C	-0.850264	-2.985978	-0.039315
O	-0.838712	-4.104168	0.141834
C	-1.604020	0.067127	1.198441
C	-2.606949	-0.890334	1.004334
H	-3.478957	-0.647504	0.388086
H	-2.713399	-1.694246	1.740053
O	-2.281105	1.531855	-0.693982
C	-2.700637	2.845639	-0.701781
O	-3.508787	3.166504	-1.506903
C	-2.093730	3.754781	0.347358
H	-2.627082	4.713056	0.305711
H	-2.184615	3.314103	1.353387
H	-1.024054	3.923759	0.145069
C	-0.368397	-0.019034	2.061991
O	-0.229754	-0.642228	3.077970
C	4.950887	1.272485	-0.666752
H	4.449728	1.857079	-1.448864
C	6.250025	1.454546	-0.414767
H	6.766671	0.883804	0.365809
H	6.846261	2.174970	-0.983129

$Rh(CO)_2Cl_2$

Rh	1.627119	-0.000015	0.097814
Rh	-1.627012	-0.000024	0.097844
Cl	0.000090	-1.661827	0.900430
Cl	-0.000122	1.661664	0.900317
O	3.464891	2.196441	-0.854893
O	3.465517	-2.195998	-0.855227
O	-3.465573	-2.195950	-0.855086
O	-3.465368	2.195964	-0.855013
C	2.788142	1.357307	-0.502231
C	2.788535	-1.357155	-0.502425
C	-2.788426	-1.357179	-0.502348
C	-2.788252	1.357175	-0.502257

TS1

O	4.376856	-0.045097	-0.230205
C	5.611250	-0.438792	-0.759501
C	6.679641	-0.251693	0.283305
C	7.586616	-1.177520	0.606186
C	3.329001	-0.106888	-1.144308
C	2.049153	0.233447	-0.435876
C	1.106985	1.038004	-0.959345
H	5.852673	0.181888	-1.652103
H	5.580798	-1.496500	-1.097939
H	6.687179	0.730755	0.772361
H	8.363942	-0.978698	1.350286
H	7.586326	-2.168065	0.136380
H	3.492114	0.580206	-2.002900

H	3.239150	-1.134348	-1.566559
H	1.894690	-0.252630	0.535002
H	1.268805	1.552739	-1.914142
C	-0.176080	1.233681	-0.342179
C	-1.274732	0.874463	0.213800
C	-2.374181	1.784339	0.672894
O	-2.026434	3.173192	0.829924
C	-1.025068	3.753448	0.230929
O	-0.213257	3.184123	-0.485606
C	-0.949108	5.232342	0.507055
H	-0.935491	5.398245	1.595819
H	-0.049730	5.650919	0.038599
H	-1.852573	5.718463	0.104907
Rh	-1.768934	-1.224943	0.147427
C	-0.446552	-1.637471	1.390984
O	0.375399	-1.848438	2.157351
Cl	-3.471603	-0.597098	-1.387205
C	-2.423291	-3.019585	0.009503
O	-2.852338	-4.064636	-0.094764
H	-2.758043	1.478841	1.656236
H	-3.194158	1.711519	-0.061955

TS10-diene

O	1.291016	4.044770	0.548707
C	0.430957	3.178973	1.224650
C	2.301103	3.248546	0.001954
C	1.635346	1.906463	-0.442602
C	2.545582	0.735794	-0.119075
C	2.291961	-0.580655	-0.165019
H	-0.505758	3.709033	1.457440
H	0.886668	2.821548	2.176061
H	2.769733	3.796860	-0.829576
H	3.081334	3.040728	0.764663
H	1.474655	1.914812	-1.532692
H	3.580677	1.001533	0.111146
Rh	-2.028708	-0.482267	0.207986
C	0.226740	2.003197	0.246912
C	-0.337162	0.751977	0.912907
H	0.405848	0.221536	1.525469
C	-0.180692	-0.395819	-0.763269
O	-0.290658	0.131645	-1.824002
Cl	-3.109247	1.449603	-0.611437
C	0.995294	-1.317130	-0.442497
H	-1.156446	1.078851	1.591465
H	-0.497398	2.329460	-0.515164
O	3.243621	-1.540278	0.130198
C	4.530597	-1.503752	-0.296611
O	5.003901	-0.618354	-0.940979
C	5.256826	-2.746088	0.169037
H	5.220843	-2.803811	1.268714
H	4.754335	-3.642535	-0.227602
H	6.297426	-2.707295	-0.177007
C	-1.519050	-1.966567	1.282154
O	-1.278301	-2.816878	1.993866
C	-3.571972	-1.388044	-0.586582
O	-4.435914	-1.867262	-1.132341
H	1.139940	-1.959188	-1.330537
H	0.794721	-1.973288	0.417343

TS10

O	-1.591793	4.123354	-0.667579
C	-0.599569	3.345806	-1.263441
C	-2.550089	3.226861	-0.182851
C	-1.778340	1.968298	0.330871
C	-2.521446	0.702483	-0.041864
C	-2.151190	-0.592138	0.028567
H	0.283448	3.975311	-1.456522
H	-0.946483	2.915380	-2.229252
H	-3.134120	3.728106	0.603924
H	-3.243616	2.930848	-0.997469
H	-1.711330	1.996937	1.430537
H	-3.565423	0.853508	-0.337158
Rh	2.115763	-0.175716	-0.131339
C	-0.336376	2.216267	-0.244410
C	0.413053	1.030226	-0.836241
H	-0.184313	0.426627	-1.533117
C	0.226560	-0.154741	0.777053
O	0.185180	0.396037	1.841393
Cl	1.725988	-1.676683	-1.891802
C	-0.829132	-1.161310	0.371820
C	-0.575348	-2.477849	0.383110
H	-1.361323	-3.196587	0.144027
H	0.424140	-2.856741	0.605811
H	1.271567	1.426964	-1.431287
H	0.262923	2.646513	0.575180
O	-3.058535	-1.575788	-0.314462
C	-4.222146	-1.738067	0.366221
O	-4.578145	-1.032441	1.259133
C	-4.971777	-2.933949	-0.175853
H	-5.059617	-2.857393	-1.270595
H	-4.406666	-3.853107	0.049316
H	-5.962996	-2.982668	0.292504

C	2.660146	1.156452	1.168911
O	3.007636	1.955785	1.887681
C	3.482237	-1.473017	0.367534
O	4.198552	-2.296300	0.659887

TS11-diene

O	-3.097249	-2.161305	0.550918
C	-2.141450	-3.049139	1.070852
C	-2.729450	-1.858655	-0.767036
C	-1.202657	-1.656995	-0.688827
C	-0.892376	-0.303112	-0.057193
C	-0.815634	0.887409	-0.957074
H	-2.465745	-4.099066	0.927699
H	-2.053851	-2.864974	2.154923
H	-2.959776	-2.700184	-1.454815
H	-3.275833	-0.960478	-1.090735
H	-0.699277	-1.769508	-1.656380
H	-1.619615	-0.076287	0.733497
Rh	1.370810	0.364499	-0.113134
C	-0.805290	-2.791154	0.303149
C	0.369794	-2.363896	1.195914
H	0.338736	-2.828910	2.194068
C	1.126475	1.913039	1.007704
O	1.028656	2.826872	1.664090
Cl	1.978681	-1.472882	-1.553894
C	-0.255901	0.979704	-2.191335
H	1.324848	-2.602018	0.706754
H	-0.519424	-3.686952	-0.268782
O	-1.294582	2.064330	-0.388029
C	-2.638698	2.235777	-0.325305
O	-3.411043	1.448183	-0.783691
C	-2.985149	3.519662	0.387252
H	-2.432777	4.360291	-0.060162
H	-4.067564	3.687286	0.322583
H	-2.678852	3.441680	1.443213
C	0.298577	-0.852522	1.401408
O	0.191066	-0.307251	2.458155
C	3.256474	0.422515	0.107933
O	4.381565	0.403588	0.252613
H	-0.277516	1.939320	-2.713385
H	0.167021	0.105200	-2.688365

TS11

O	3.109508	-2.192848	-0.577466
C	2.145708	-3.100928	-1.050141
C	2.755515	-1.803307	0.722735
C	1.225695	-1.644140	0.660133
C	0.865096	-0.350506	-0.069898
C	0.846893	0.891190	0.788222
H	2.493048	-4.144600	-0.919880
H	2.005423	-2.922653	-2.130497
H	3.021497	-2.583756	1.467019
H	3.285671	-0.870209	0.967927
H	0.735448	-1.682864	1.641534
H	1.581588	-0.151384	-0.879469
Rh	-1.388606	0.307671	-0.046028
C	0.839926	-2.857751	-0.230228
C	-0.395147	-2.526971	-1.079546
H	-0.430465	-3.087597	-2.027005
C	-1.128118	1.729230	-1.320761
O	-1.016291	2.572556	-2.064580
Cl	-1.962681	-1.326927	1.608753
C	0.524816	0.962766	2.076090
C	0.249800	0.993591	3.353698
H	1.037625	0.828230	4.100160
H	-0.772817	1.165242	3.711209
H	-1.312430	-2.706759	-0.501462
H	0.625141	-3.726970	0.410180
O	1.231786	2.063867	0.136986
C	2.564271	2.316322	0.052310
O	3.390029	1.595936	0.526187
C	2.817366	3.594272	-0.708756
H	2.262376	4.422229	-0.240652
H	3.894309	3.804189	-0.712899
H	2.447766	3.485048	-1.741031
C	-0.315997	-1.043197	-1.431020
O	-0.217219	-0.606811	-2.538791
C	-3.280508	0.450170	-0.159649
O	-4.411970	0.469792	-0.237561

TS12

O	-3.599132	-1.333746	-0.816039
C	-3.275668	-2.017405	0.364488
C	-2.509614	-1.383936	-1.703771
C	-1.263011	-1.803628	-0.866832
C	-0.023922	-0.956117	-1.100758
C	0.967593	-0.769014	-0.105426
H	-3.437647	-3.111195	0.259745
H	-3.924613	-1.644945	1.173111
H	-2.700791	-2.110104	-2.516761
H	-2.383762	-0.385858	-2.159645

H	-1.000931	-2.850801	-1.104653
H	0.355160	-0.929237	-2.130408
Rh	-0.236991	0.935394	-0.039380
C	-1.781085	-1.721087	0.587181
C	-1.561805	-0.299335	1.108980
H	-2.309165	0.375985	0.633175
C	0.773751	2.121575	-1.259631
O	1.407576	2.802079	-1.900504
Cl	-0.955644	2.890697	1.058053
C	0.538984	-0.466693	1.238226
C	0.973235	-0.631609	2.487084
H	1.764349	-1.361749	2.686265
H	0.548439	-0.055397	3.313796
H	-1.646177	-0.182903	2.195729
H	-1.297486	-2.464072	1.238943
O	2.280675	-0.573018	-0.487197
C	3.216766	-1.418371	0.009929
O	2.945597	-2.332307	0.730000
C	4.593420	-1.029577	-0.469381
H	4.597810	-0.930632	-1.565828
H	4.859349	-0.048101	-0.043878
H	5.316438	-1.788476	-0.145023

TS13

O	-3.716334	-0.478751	-0.564540
C	-4.467974	-0.300726	0.602919
C	-5.582818	0.670933	0.327633
C	-6.862175	0.460660	0.649029
C	-2.627518	-1.328911	-0.405070
C	-1.825697	-1.300710	-1.674318
C	-0.482897	-1.316406	-1.771654
H	-3.813025	0.106028	1.404770
H	-4.877805	-1.268240	0.964889
H	-5.272709	1.608315	-0.151059
H	-7.629949	1.216537	0.457380
H	-7.188238	-0.474200	1.120054
H	-2.001051	-1.034065	0.461167
H	-2.963502	-2.376261	-0.220124
H	-2.422492	-1.262091	-2.593977
H	-0.006348	-1.321866	-2.758702
C	0.392318	-1.308622	-0.621791
C	1.114340	-0.698460	0.249000
C	1.989067	-1.341525	1.280633
O	2.298922	-2.735388	1.064305
C	1.643923	-3.525491	0.267386
O	0.672668	-3.197576	-0.405798
C	2.206523	-4.921272	0.215504
H	2.416305	-5.279614	1.234204
H	1.503448	-5.585054	-0.303347
H	3.161736	-4.887462	-0.335306
Rh	1.186331	1.445430	0.042342
C	-0.647872	1.581845	0.333060
O	-1.773114	1.622618	0.533129
Cl	3.533871	1.194411	-0.247258
C	1.463455	3.336244	-0.112925
O	1.677290	4.446891	-0.201098
H	1.521362	-1.273487	2.277192
H	2.960058	-0.825588	1.296445

TS14

O	-1.788028	1.927745	0.162917
C	-2.815962	1.783442	-0.784254
C	-4.036212	1.229491	-0.101942
C	-5.265419	1.741305	-0.211912
C	-0.592556	2.413587	-0.386172
C	0.351785	2.765880	0.732999
C	1.510392	2.156958	1.038240
H	-2.487328	1.089825	-1.587423
H	-3.052437	2.761593	-1.255041
H	-3.867289	0.328080	0.501765
H	-6.125130	1.272675	0.276819
H	-5.457015	2.645518	-0.801604
H	-0.148934	1.678446	-1.082608
H	-0.797344	3.344991	-0.959521
H	0.057206	3.627731	1.344148
H	2.140519	2.589310	1.826173
C	2.056752	0.934993	0.423821
C	1.447295	-0.213645	0.117384
C	2.046576	-1.383056	-0.409769
O	3.885301	-0.899808	-0.705874
C	4.234254	0.215086	-0.333008
O	3.454495	1.100603	0.224687
C	5.648965	0.698247	-0.508961
H	5.992608	1.189956	0.413456
H	6.298083	-0.145467	-0.775198
H	5.662883	1.447921	-1.318020
Rh	-0.494909	-1.017077	0.192738
C	-0.352324	-1.098044	2.059482
O	-0.239165	-1.122279	3.192773
Cl	-0.595909	-0.871026	-2.203233
C	-2.161981	-2.000641	0.100543
O	-3.110451	-2.613369	-0.002540

H	1.835682	-1.646121	-1.453320
H	2.303240	-2.213321	0.257721

TS16

O	-1.666698	3.391556	-0.092253
C	-2.122173	2.482738	0.856245
C	-2.200216	1.097527	0.204801
C	-2.207018	-0.048529	1.156036
C	-0.533962	2.818752	-0.651320
C	-0.858090	1.354394	-1.038821
C	0.420312	0.595469	-1.361822
C	1.373752	0.328149	-0.384091
H	-3.119026	2.797547	1.202216
H	-1.435786	2.435187	1.727407
H	-3.016460	1.016630	-0.523507
H	-3.067276	-0.720828	1.057151
H	-1.956151	0.199844	2.196983
H	0.315750	2.824555	0.059420
H	-0.251823	3.388954	-1.549999
H	-1.483588	1.310157	-1.937699
H	0.637993	0.369398	-2.409594
Rh	-0.642987	-0.725154	0.069165
Cl	-2.111348	-1.779004	-1.563032
C	0.869906	0.290815	0.985032
C	1.295552	0.720098	2.174669
H	0.741688	0.472716	3.086885
H	2.196908	1.336218	2.266738
O	2.556555	-0.241717	-0.767984
C	3.715099	0.250004	-0.255087
O	3.756682	1.242512	0.406837
C	4.881806	-0.617027	-0.655415
H	5.815159	-0.141539	-0.329014
H	4.774827	-1.607028	-0.182514
H	4.880954	-0.767764	-1.746055
C	-0.437490	-2.347934	0.978838
O	-0.320377	-3.340573	1.514192

TS17

O	-2.207744	2.076040	-0.692421
C	-3.184552	1.912525	0.322348
C	-4.537298	2.205135	-0.262863
C	-5.603920	1.416892	-0.102421
C	-0.944197	1.758770	-0.347241
C	0.078101	2.132341	-1.235533
C	1.447182	1.775591	-1.150757
C	1.995868	0.885093	-0.250552
H	-2.966870	2.623509	1.146301
H	-3.138540	0.890910	0.742264
H	-4.616520	3.142833	-0.827907
H	-6.580261	1.689610	-0.514663
H	-5.539563	0.474916	0.454457
H	-0.728082	0.330950	-0.510743
H	-0.743604	1.670943	0.729949
H	-0.255400	2.634272	-2.152253
H	2.115360	2.153864	-1.929608
Rh	-0.219662	-1.193581	0.031115
Cl	-1.518165	-1.019303	2.015643
C	0.787820	-1.423559	-1.559290
O	1.374300	-1.584622	-2.516225
C	1.276037	0.127017	0.766930
C	1.510479	0.206174	2.090012
H	0.956538	-0.414860	2.799078
H	2.245687	0.915888	2.485932
O	3.299898	0.509758	-0.519793
C	4.293581	0.847128	0.334955
O	4.137432	1.590970	1.256230
C	5.584612	0.167555	-0.054693
H	6.406110	0.578635	0.545562
H	5.488984	-0.914773	0.132417
H	5.777483	0.305573	-1.129505
C	-1.743869	-2.359623	-0.507878
O	-2.664736	-2.960799	-0.764727

TS18

O	2.363803	-2.432095	-0.790621
C	3.281403	-2.219411	0.271773
C	4.676287	-2.439220	-0.240956
C	5.681597	-1.581208	-0.047190
C	1.088840	-2.180099	-0.508790
C	0.122497	-2.200721	-1.463716
C	-1.283078	-1.863677	-1.265298
C	-1.792114	-1.035285	-0.323515
H	3.058983	-2.938936	1.086081
H	3.160789	-1.196589	0.677157
H	4.840931	-3.381114	-0.779726
H	6.692348	-1.798984	-0.405595
H	5.529303	-0.633374	0.481993
H	0.383221	-0.015720	-0.270971
H	0.858373	-1.991176	0.547005
H	0.430479	-2.492019	-2.474507
H	-1.996901	-2.270928	-1.989654

Rh	0.032563	1.479614	0.071558
Cl	1.627559	1.325700	1.809207
C	-1.155327	1.614452	-1.420108
O	-1.836093	1.710052	-2.319434
C	-1.005019	-0.251023	0.663519
C	-1.099771	-0.450125	1.994236
H	-0.502551	0.130117	2.702093
H	-1.784495	-1.213996	2.381816
O	-3.152286	-0.745047	-0.386528
C	-4.005779	-1.337566	0.472627
O	-3.667870	-2.139926	1.292664
C	-5.416421	-0.842545	0.247636
H	-5.692162	-0.960954	-0.811686
H	-6.105048	-1.403063	0.892398
H	-5.465623	0.232242	0.486773
C	1.222541	3.016301	-0.478566
O	1.988017	3.786481	-0.784796

TS19

O	-2.673563	-0.689793	-0.045530
C	-3.513047	0.408292	-0.290802
C	-4.928317	0.032518	0.053588
C	-5.737018	0.772714	0.816538
C	-1.380143	-0.545123	-0.452726
C	-0.582473	-1.739614	-0.346108
C	0.789659	-1.668205	-0.210514
H	-3.453037	0.690064	-1.364854
H	-3.191280	1.288998	0.300940
H	-5.283324	-0.907938	-0.386866
H	-6.771248	0.472066	1.009804
H	-5.394563	1.708372	1.273893
H	-1.273606	0.043480	-1.384411
H	-0.592543	0.294223	0.231032
H	-1.101069	-2.692128	-0.190494
H	1.384366	-2.578451	-0.096062
C	1.445238	-0.433910	0.020570
C	0.766242	0.776222	0.045055
C	0.882657	2.069723	-0.253448
O	3.616094	0.883849	-0.937560
C	3.724705	0.198405	0.035354
O	2.715941	-0.534887	0.555553
C	4.982497	0.011760	0.852807
H	5.204654	-1.061263	0.960910
H	5.814933	0.532494	0.362906
H	4.820785	0.421168	1.863305
H	0.189014	2.816284	0.148057
H	1.679144	2.402574	-0.929746

TS2

O	-3.786938	1.009161	-0.066600
C	-5.128666	1.109008	0.309432
C	-5.999736	0.884691	-0.897152
C	-7.056794	0.068592	-0.923046
C	-2.892073	1.264251	0.971178
C	-1.489068	1.039897	0.483682
C	-0.487686	1.911948	0.682840
H	-5.330058	2.122494	0.726721
H	-5.377466	0.376445	1.107519
H	-5.718819	1.462010	-1.787215
H	-7.675396	-0.034847	-1.819767
H	-7.342618	-0.526366	-0.047614
H	-3.007320	2.300309	1.358944
H	-3.093540	0.578312	1.826342
H	-1.303484	0.097517	-0.050198
H	-0.687105	2.883197	1.152501
C	0.912223	1.675922	0.308585
C	1.546439	0.516921	0.102046
C	2.889761	0.315270	-0.264900
O	3.578766	2.132857	-0.520384
C	2.808379	3.051525	-0.274211
O	1.577600	2.914570	0.148877
C	3.206689	4.491910	-0.457814
H	2.873331	5.085222	0.406756
H	4.293622	4.560854	-0.591719
H	2.696589	4.882480	-1.354561
Rh	0.985729	-1.513728	0.119923
C	0.869215	-1.425950	1.988863
O	0.806902	-1.338527	3.124029
Cl	1.176063	-1.555425	-2.242351
C	0.567435	-3.401930	-0.006541
O	0.336556	-4.504288	-0.130240
H	3.099969	-0.030296	-1.285141
H	3.641605	0.080126	0.497641

TS20

C	3.128573	1.218514	0.324224
C	3.290583	1.742478	1.729828
C	2.952800	2.976549	2.116286
C	0.940459	0.113906	0.590938
C	0.222034	-1.003006	1.156708
C	-1.144405	-1.167468	0.985729

C	-1.846041	-0.317755	0.081891
H	2.654373	1.989198	-0.316140
H	4.116247	0.981499	-0.098078
H	3.724997	1.034157	2.447026
H	3.114026	3.317060	3.143642
H	2.511210	3.694379	1.414664
H	0.110310	0.419238	-0.431437
H	0.751430	1.095575	1.049817
H	0.797806	-1.833957	1.573651
C	-1.264271	0.758403	-0.562067
C	-1.500870	1.999285	-1.011348
O	-3.056723	-0.804087	-0.403501
C	-4.196246	-0.450537	0.218089
O	-4.233752	0.273108	1.171270
C	-5.388921	-1.100372	-0.446260
H	-5.316291	-2.194628	-0.338276
H	-6.310463	-0.736029	0.025005
H	-5.385522	-0.871988	-1.523415
N	2.340185	-0.018623	0.308763
S	2.869353	-1.296492	-0.625597
O	2.431842	-2.530337	-0.011945
O	4.274314	-1.062986	-0.888268
C	1.975586	-1.144333	-2.193486
H	0.894629	-1.200271	-1.998473
H	2.258301	-0.194920	-2.670142
H	2.302253	-1.998613	-2.804746
C	-0.597839	2.664308	-2.025480
H	-1.147293	2.862510	-2.964387
H	-0.243188	3.642919	-1.652944
H	0.274748	2.038996	-2.271770
C	-2.655517	2.836263	-0.497406
H	-3.337890	3.099262	-1.327141
H	-3.225447	2.309350	0.281748
H	-2.280287	3.789431	-0.081030
C	-1.867036	-2.357879	1.575852
H	-2.691647	-2.023676	2.229149
H	-2.302391	-2.989367	0.783554
H	-1.179638	-2.971611	2.176498

TS21

C	1.740320	0.648476	-0.234583
C	1.410114	-0.698568	-0.015998
C	0.066775	-1.036113	0.290167
H	-0.094501	-2.011718	0.771533
C	-0.990171	-0.134266	0.300624
C	-2.311454	-0.036060	0.095570
C	3.161059	1.124759	-0.007645
H	3.198640	2.221762	0.080875
H	3.617752	0.683319	0.894817
H	3.804833	0.845474	-0.862699
C	0.686791	1.591426	-0.472414
H	0.050815	1.435860	-1.354096
H	-0.285607	1.084006	0.322701
H	0.930917	2.652772	-0.317327
C	2.496911	-1.735101	0.190389
H	3.081391	-1.535693	1.107354
H	2.070316	-2.746249	0.278888
H	3.210341	-1.741671	-0.651011
C	-3.080411	-1.057589	-0.721241
H	-3.905687	-1.488592	-0.124208
H	-3.543008	-0.583960	-1.607739
H	-2.431025	-1.876425	-1.064876
C	-3.123292	1.129122	0.618968
H	-3.648900	1.646054	-0.205833
H	-3.902530	0.777514	1.320750
H	-2.493606	1.861021	1.147852

TS4

O	-3.082863	-2.494974	-0.053985
C	-3.309081	-1.242649	0.520321
C	-1.909231	-2.378331	-0.791776
C	-0.868470	-1.673264	0.099482
C	0.338815	-1.244593	-0.732002
C	1.451556	-0.694189	-0.108345
H	-4.105271	-1.340977	1.274483
H	-3.605723	-0.496497	-0.242072
H	-1.567821	-3.386993	-1.074027
H	-2.063055	-1.767888	-1.703607
H	-0.478678	-2.346112	0.874141
H	0.379440	-1.527220	-1.788787
Rh	-0.394763	0.710145	0.044826
C	-1.992575	-0.787007	1.170868
C	-1.870764	0.686505	1.418383
H	-2.716147	1.284772	1.051730
C	-0.033605	2.529126	0.224982
O	0.188353	3.638218	0.310501
Cl	-1.947899	1.151415	-1.786520
C	1.164290	-0.015739	1.152075
C	1.712655	0.020135	2.367822
H	2.562852	-0.622258	2.622568
H	1.317544	0.689523	3.139456
H	-1.560456	0.958131	2.435242

H	-1.779779	-1.349979	2.087993
O	2.580956	-0.476468	-0.847430
C	3.789425	-0.789924	-0.308698
O	3.902538	-1.373779	0.725943
C	4.906094	-0.312253	-1.202209
H	4.741283	-0.666108	-2.231663
H	4.904154	0.789896	-1.224674
H	5.863724	-0.679786	-0.812776

TS5-diene

O	3.421852	2.151981	-0.777884
C	3.332462	2.044714	0.619059
C	2.152881	2.020993	-1.373329
C	1.143198	1.970761	-0.204487
C	-0.212969	1.439991	-0.635278
C	-1.229479	0.971940	0.173207
H	3.317269	3.045984	1.095259
H	4.213883	1.500927	0.997470
H	1.958421	2.876341	-2.044511
H	2.099940	1.090578	-1.972266
H	0.968987	3.010930	0.133864
H	-0.518019	1.722768	-1.650115
Rh	0.086860	-0.912093	0.064317
C	2.005069	1.298923	0.895514
C	2.242131	-0.221447	0.718886
H	2.603888	-0.471233	-0.291633
C	1.248274	-1.556969	1.369486
O	1.568716	-2.211085	2.274837
Cl	1.010289	-1.750809	-2.014872
C	-0.980398	0.287870	1.435876
H	3.042680	-0.512154	1.413982
H	1.641826	1.518478	1.910734
O	-2.474741	0.827342	-0.407453
C	-3.505750	1.521748	0.143025
O	-3.361568	2.265556	1.064888
C	-4.795856	1.214764	-0.576952
H	-5.018770	0.139026	-0.493558
H	-5.606128	1.807782	-0.134652
H	-4.687160	1.448356	-1.647881
C	-1.297225	-2.210215	-0.115577
O	-2.095912	-2.999947	-0.245191
H	-0.311882	0.784147	2.145702
H	-1.869342	-0.123201	1.925985

TS5

O	3.683684	2.118312	-0.774647
C	3.558030	1.740093	0.574603
C	2.420441	2.285351	-1.365182
C	1.393025	2.130216	-0.220107
C	-0.011493	1.892519	-0.708979
C	-0.999967	1.208274	-0.094599
H	3.672238	2.618091	1.242066
H	4.354001	1.018442	0.821769
H	2.350724	3.277391	-1.846542
H	2.258274	1.517612	-2.148316
H	1.359620	3.096753	0.321038
H	-0.299633	2.437927	-1.616895
Rh	0.077717	-1.191541	-0.010156
C	2.140274	1.143785	0.715366
C	2.117512	-0.311871	0.232410
H	2.166923	-0.416528	-0.865887
C	1.119033	-1.442925	1.473386
O	1.530978	-1.687674	2.519395
Cl	0.711658	-2.359623	-2.009012
C	-0.823782	0.288513	1.051324
C	-1.229559	0.458240	2.312838
H	-1.739338	1.380971	2.612430
H	-1.065187	-0.312648	3.073544
H	2.992776	-0.871131	0.595708
H	1.784171	1.216452	1.755064
O	-2.248071	1.184249	-0.708186
C	-3.254132	1.868070	-0.116616
O	-3.098788	2.532457	0.865062
C	-4.551020	1.667111	-0.863243
H	-4.408469	1.887588	-1.932422
H	-4.858189	0.611946	-0.779096
H	-5.321851	2.317807	-0.431451
C	-1.553235	-2.250850	0.017299
O	-2.466834	-2.910707	0.068150

TS6-diene

O	-4.604247	-1.031420	0.510382
C	-3.538226	-1.840047	0.093541
C	-4.113847	0.271577	0.561189
C	-3.276390	0.437500	-0.743911
C	-2.201073	1.496866	-0.691975
C	-1.041481	1.426977	-0.018868
H	-3.938542	-2.811434	-0.233304
H	-2.834552	-2.026638	0.928356
H	-4.959517	0.972729	0.622517
H	-3.473213	0.428591	1.455232

H	-3.978994	0.739675	-1.534573
H	-2.363996	2.414630	-1.266610
Rh	1.414334	-0.530645	-0.019767
C	-2.852678	-1.048885	-1.054553
C	-1.347549	-1.324630	-1.288068
H	-1.228492	-2.337236	-1.708521
C	-0.498792	-1.340048	-0.010928
O	-0.521949	-2.305545	0.727095
Cl	3.505730	-1.194250	-0.823696
C	-0.568668	0.272543	0.807467
H	-0.972880	-0.604655	-2.027726
H	-3.348304	-1.333113	-1.996425
O	-0.138126	2.461224	-0.211491
C	0.363180	3.135537	0.849246
O	0.014385	2.931022	1.974906
C	1.406650	4.131546	0.405631
H	1.032961	4.725727	-0.441892
H	1.672092	4.778530	1.251269
H	2.300510	3.583116	0.063566
C	1.901388	-1.538585	1.678095
O	2.226845	-2.110541	2.590179
C	1.325449	0.478807	-1.685923
O	1.371275	1.035313	-2.666964
H	0.122387	0.606982	1.601880
H	-1.405144	-0.150986	1.380068

TS6

O	-4.925452	-1.247587	0.236334
C	-3.804098	-2.012170	0.560119
C	-4.499167	0.081671	0.255222
C	-3.088367	0.098605	-0.404419
C	-2.208674	1.170082	0.205787
C	-0.905781	1.369813	-0.037116
H	-4.007481	-3.067541	0.321462
H	-3.569059	-1.932780	1.644671
H	-5.239372	0.699485	-0.275861
H	-4.421210	0.448597	1.301183
H	-3.204986	0.318474	-1.478777
H	-2.677378	1.877784	0.900522
Rh	1.597029	-0.492673	0.054799
C	-2.648471	-1.407309	-0.271887
C	-1.277307	-1.681942	0.365673
H	-1.124641	-1.094741	1.278573
C	-0.157896	-1.450078	-0.646245
O	0.004244	-2.128573	-1.616440
Cl	0.913865	-0.016169	2.277006
C	-0.063910	0.507792	-0.921976
C	-0.126753	0.703957	-2.255683
H	-0.659061	1.566994	-2.670936
H	0.326022	-0.005624	-2.958341
H	-1.201679	-2.755371	0.618376
H	-2.666097	-1.864772	-1.273551
O	-0.262105	2.399852	0.620794
C	0.177526	3.456556	-0.087124
O	-0.020399	3.595493	-1.260503
C	0.932068	4.414675	0.804342
H	1.811393	3.902252	1.226137
H	1.239998	5.291165	0.220436
H	0.292777	4.716353	1.648849
C	2.937421	-1.498250	1.073045
O	3.645968	-2.115479	1.699588
C	2.444470	-0.785747	-1.650473
O	2.986796	-0.936337	-2.631451

TS7

O	-3.001671	-2.668160	-0.191504
C	-3.107715	-1.737068	0.850910
C	-1.926084	-2.380330	-1.043190
C	-0.941570	-1.506907	-0.279182
C	0.292458	-1.089453	-1.003783
C	1.375616	-0.683436	-0.216418
H	-2.664675	-2.121127	1.791613
H	-4.177502	-1.537825	1.035739
H	-1.435140	-3.330202	-1.317280
H	-2.258957	-1.877380	-1.972192
H	-0.673056	-1.988104	0.670658
H	0.378614	-1.158861	-2.092354
Rh	-0.411965	0.704473	0.114594
C	-2.454804	-0.439854	0.411458
C	-2.091110	0.638326	1.327091
H	-1.907287	0.370760	2.376624
C	0.194292	2.424881	0.602065
O	0.546219	3.464621	0.882923
Cl	-1.632781	1.792720	-1.721171
C	1.014006	-0.314090	1.151953
C	1.498207	-0.559289	2.370703
H	2.338712	-1.246340	2.518584
H	1.056065	-0.081058	3.251217
H	-2.643305	1.573609	1.180859
H	-2.906863	-0.061505	-0.515812
O	2.557766	-0.374643	-0.824462
C	3.718206	-0.857709	-0.303571

O	3.744576	-1.657177	0.581520
C	4.904663	-0.253567	-1.010957
H	5.822792	-0.738745	-0.656830
H	4.793999	-0.374336	-2.099724
H	4.940191	0.827459	-0.798207

TS8

O	-3.047846	-2.464672	-0.260196
C	-3.603290	-1.351634	0.339967
C	-2.668001	-0.157785	0.182275
C	-2.253064	0.380811	-1.112676
C	-1.667340	-2.512378	-0.038918
C	-1.159532	-1.370617	0.873380
C	0.343115	-1.639508	0.957424
C	1.184787	-1.228380	-0.014435
H	-3.833810	-1.524690	1.411509
H	-4.548393	-1.102640	-0.172696
H	-2.928155	0.614367	0.936033
H	-2.710825	1.326853	-1.429825
H	-2.125475	-0.347207	-1.923724
H	-1.405328	-3.477263	0.434553
H	-1.131275	-2.460207	-1.004624
H	-1.588088	-1.448457	1.882723
H	0.667773	-2.385317	1.694183
Rh	-0.671922	0.829501	0.105500
Cl	-0.245998	2.919060	-0.842866
C	0.631348	1.398593	1.616740
O	1.283100	1.846085	2.421447
C	0.700253	-0.171486	-0.917250
C	1.143419	0.052285	-2.162595
H	1.899911	-0.609932	-2.605349
H	0.768273	0.886526	-2.760773
O	2.401108	-1.810596	-0.196257
C	3.592183	-1.139775	-0.174209
O	4.546021	-1.664656	-0.653666
C	3.601676	0.198748	0.534826
H	4.640680	0.547560	0.592078
H	2.996388	0.934284	-0.019375
H	3.184412	0.092041	1.548703

TS9-diene

O	-1.014294	4.363732	0.208636
C	-0.102257	3.709149	-0.622958
C	-2.006938	3.428571	0.503355
C	-1.298521	2.041875	0.645628
C	-2.121999	0.952397	-0.002644
C	-1.859274	-0.351275	-0.168752
H	0.814148	4.314347	-0.698125
H	-0.519288	3.568387	-1.645620
H	-2.530002	3.746047	1.418719
H	-2.748886	3.381794	-0.322299
H	-1.187899	1.806201	1.715479
H	-3.104559	1.249543	-0.389687
Rh	1.446445	-0.498851	-0.159512
C	0.127090	2.335401	0.044995
C	0.750298	1.303917	-0.893502
H	0.033096	1.024597	-1.690485
C	0.494777	-0.303469	1.379015
O	0.162610	-0.078121	2.458343
Cl	3.611074	0.098450	-0.810763
C	-0.654101	-1.190128	0.166773
H	1.637561	1.751956	-1.368200
H	0.807931	2.510902	0.895037
O	-2.826704	-1.085834	-0.857150
C	-3.470473	-2.096664	-0.239308
O	-3.243869	-2.432741	0.887129
C	-4.494878	-2.718589	-1.159904
H	-5.246329	-1.961547	-1.436037
H	-4.006971	-3.054253	-2.088561
H	-4.976100	-3.562727	-0.650145
C	2.417820	-2.292830	0.376339
O	3.069248	-3.166124	0.657700
H	-0.912430	-1.929601	0.941758
H	-0.403712	-1.788424	-0.732312

TS9

Rh	1.389609	-0.367035	-0.103618
Cl	2.890623	-0.851644	1.702735
C	2.916916	-0.189766	-1.278841
O	3.796344	-0.161269	-1.986145
C	-1.689107	-0.257061	0.824381
C	-1.726418	1.082003	0.859732
C	-0.509197	1.971601	0.939058
H	0.209610	1.579450	1.679576
H	-2.709211	1.562622	0.786034
C	-0.897217	3.429241	1.231984
H	-1.690027	3.528983	1.990737
H	-0.009307	3.996918	1.578593
O	-1.380935	3.921094	0.010513
C	-0.720341	3.293619	-1.065467
H	-0.111176	4.024138	-1.628948

H	-1.476092	2.872853	-1.753553
C	0.166196	2.170103	-0.457338
C	0.289097	0.918985	-1.326701
H	1.173235	2.587750	-0.264200
H	-0.704751	0.526046	-1.591851
H	0.817191	1.145307	-2.267197
C	0.232393	-1.650483	-0.720100
O	-0.243021	-2.467376	-1.382958
C	-0.455260	-1.093523	0.890447
C	-0.253190	-1.969857	1.893972
H	0.643299	-2.598264	1.930342
H	-0.972067	-2.058967	2.718822
O	-2.875091	-0.974260	0.764812
C	-3.362634	-1.287906	-0.457480
O	-2.842884	-0.936189	-1.475513
C	-4.614433	-2.122761	-0.336959
H	-5.047696	-2.275134	-1.333370
H	-4.357746	-3.094487	0.115403
H	-5.334392	-1.623850	0.330124

TSS1

O	-0.613052	3.657307	-0.302157
C	-1.502990	3.149028	0.619337
C	-1.935958	1.733913	0.260845
C	-2.295709	0.796247	1.308610
C	0.531335	2.869286	-0.233165
C	0.252437	1.354372	-0.301594
C	0.636243	0.487013	0.819616
C	1.924060	-0.276522	0.883893
H	-2.410215	3.777667	0.610900
H	-1.081653	3.167400	1.647939
H	-2.547237	1.731966	-0.649827
H	-3.318856	0.400610	1.314135
H	-1.923299	1.026915	2.315354
H	1.077486	3.075857	0.708992
H	1.191744	3.126499	-1.072798
H	0.457656	0.945106	-1.297449
H	0.477004	0.964718	1.797750
Rh	-1.104289	-0.417929	0.103019
Cl	-0.047389	-1.548621	-1.840318
C	2.489519	-0.582951	2.039608
C	3.022483	-0.894568	3.195430
H	2.778707	-1.839116	3.699517
H	3.737108	-0.225561	3.692447
O	2.524474	-0.729665	-0.269613
C	3.039294	0.147998	-1.150326
O	3.083499	1.330276	-0.952396
C	3.509921	-0.569307	-2.389080
H	4.020212	0.138592	-3.054285
H	4.175390	-1.401446	-2.112771
H	2.621574	-1.001208	-2.880937
C	-0.971433	-1.947882	1.277687
O	-0.834517	-2.812095	1.994799
C	-2.691348	-1.048497	-1.038138
O	-3.510923	-1.453752	-1.698851

TSS10

O	-3.123859	0.014044	0.014135
C	-4.382009	-0.519025	-0.264262
C	-5.329268	-0.167331	0.851531
C	-6.558281	0.325004	0.673739
C	-2.151393	-0.320574	-0.933925
C	-0.858674	0.366452	-0.600617
C	0.313337	-0.280928	-0.492098
H	-4.314605	-1.628473	-0.351589
H	-4.774091	-0.145047	-1.235349
H	-4.946907	-0.359718	1.862194
H	-7.217686	0.533983	1.521764
H	-6.950469	0.536568	-0.328037
H	-2.003284	-1.422059	-0.977944
H	-2.493223	-0.002535	-1.945991
H	-0.889993	1.454323	-0.466010
H	0.351370	-1.370380	-0.606170
C	1.586669	0.385734	-0.234861
C	2.029826	1.612710	-0.121632
C	3.425708	1.862895	0.167357
O	4.326633	0.575815	0.336691
C	3.827439	-0.583757	0.214145
O	2.628883	-0.834365	-0.050967
C	4.765548	-1.741460	0.430099
H	4.985548	-1.812820	1.508532
H	4.298838	-2.673304	0.085564
H	5.711822	-1.550195	-0.097439
H	3.607503	2.368829	1.128195
H	3.968509	2.388558	-0.633446

TSS15

O	-4.248849	-1.252894	0.076356
C	-4.213110	0.144927	0.256302
C	-3.024935	-1.835189	0.449768
C	-2.139787	-0.675843	0.977812

C	-0.647317	-0.968311	0.963421
C	0.213380	-1.308758	-0.099897
H	-4.654343	0.427530	1.232964
H	-4.809434	0.620140	-0.540042
H	-3.184888	-2.615079	1.215685
H	-2.554029	-2.317695	-0.429613
H	-2.390686	-0.509672	2.038459
H	-0.294760	-1.410703	1.902908
Rh	0.545248	0.751309	0.261321
C	-2.724699	0.526933	0.209737
C	-2.241529	0.637955	-1.238689
H	-2.494959	-0.285056	-1.790441
C	-0.747971	0.919280	-1.443175
O	-0.372971	1.751465	-2.234645
Cl	1.004625	1.520841	2.413331
C	0.219573	-0.562970	-1.356830
C	0.602384	-0.937520	-2.589141
H	0.793244	-1.990861	-2.823567
H	0.691855	-0.190839	-3.384534
H	-2.751513	1.472418	-1.746950
H	-2.522312	1.469754	0.743254
O	1.149528	-2.280715	0.130951
C	2.492833	-2.109982	-0.051334
O	2.987644	-1.081110	-0.389758
C	3.218179	-3.394021	0.267970
H	3.088179	-3.623349	1.338181
H	2.784785	-4.226954	-0.307040
H	4.283823	-3.272851	0.036387
C	1.740457	2.208122	-0.431734
O	2.474086	2.978538	-0.802523

TSS16

O	-0.664778	4.113421	-0.897100
C	0.184336	3.130271	-1.401909
C	-1.770913	3.446050	-0.354157
C	-1.246594	2.102276	0.249711
C	-2.180964	0.958991	-0.099200
C	-2.018377	-0.375273	0.024252
H	1.165178	3.580611	-1.622414
H	-0.219220	2.682526	-2.337647
H	-2.241202	4.102313	0.393579
H	-2.515464	3.232321	-1.148324
H	-1.208225	2.170212	1.349328
H	-3.183323	1.268517	-0.410990
Rh	2.318642	-0.683429	-0.028506
C	0.229966	2.072707	-0.282280
C	0.775477	0.718080	-0.729853
H	0.148038	0.208578	-1.472958
C	0.394934	-0.241755	0.747027
O	0.467662	0.288467	1.831015
Cl	2.024711	-2.489683	-1.434966
C	-0.796154	-1.118438	0.408478
C	-0.742210	-2.454338	0.507031
H	-1.628470	-3.060707	0.309467
H	0.193066	-2.962383	0.753472
H	1.746210	0.919948	-1.260499
H	0.875318	2.458891	0.522677
O	-3.057268	-1.227817	-0.289809
C	-4.275648	-1.134881	0.302737
O	-4.577045	-0.287580	1.085967
C	-5.165853	-2.259083	-0.175969
H	-5.160327	-2.301042	-1.276051
H	-4.773631	-3.219501	0.196440
H	-6.183425	-2.101176	0.203381
C	3.047234	0.576849	1.228429
O	3.530876	1.296816	1.955773

TSS17

O	3.767089	0.831308	-1.125720
C	4.200355	-0.409363	-0.636958
C	3.247979	1.533595	-0.037211
C	2.368957	0.500901	0.707157
C	1.018980	0.382003	0.003284
C	-0.141667	1.240989	0.316121
H	5.213594	-0.318662	-0.196334
H	4.248357	-1.119485	-1.476872
H	4.055419	1.887746	0.638825
H	2.690889	2.407638	-0.407457
H	2.241357	0.737795	1.774622
H	1.165071	0.271964	-1.080349
Rh	-0.993931	-0.610128	0.272304
C	3.184501	-0.824616	0.464423
C	2.188492	-1.942536	0.078823
H	1.948676	-1.959473	-0.992733
Cl	-0.973522	-2.731661	-0.828874
C	-0.793811	0.975515	1.544639
C	-1.119650	1.430015	2.747614
H	-0.711949	2.376293	3.123882
H	-1.794994	0.869291	3.401551
H	2.503937	-2.941264	0.413383
H	3.704321	-1.115487	1.389895
O	-0.524538	2.320921	-0.451901

C	-0.655491	2.243809	-1.798713
O	-0.451744	1.247746	-2.425620
C	-1.097750	3.574580	-2.359341
H	-0.390968	4.362903	-2.056241
H	-1.151120	3.504619	-3.453073
H	-2.084931	3.835432	-1.945014
C	0.980722	-1.508039	0.872187
O	0.728993	-1.767021	1.996316
C	-2.886080	-0.400171	0.024960
O	-3.996746	-0.258471	-0.142300

TSS2

O	-0.031280	3.591109	-0.794024
C	-0.745166	3.302134	0.352018
C	-1.408664	1.924458	0.243178
C	-1.668985	1.172399	1.496547
C	0.925294	2.593218	-0.914812
C	0.324866	1.179034	-0.700831
C	0.874914	0.385692	0.399493
C	1.548076	-0.928061	0.501976
H	-1.538829	4.057720	0.472182
H	-0.094703	3.333881	1.252731
H	-2.240234	1.972912	-0.471693
H	-2.722738	1.108309	1.800521
H	-1.022119	1.430991	2.346431
H	1.740012	2.738491	-0.178368
H	1.356030	2.640387	-1.926120
H	0.159350	0.643618	-1.644434
H	1.057548	0.987247	1.301789
Rh	-1.130142	-0.354036	0.228889
Cl	-0.820800	-1.686294	-1.859680
C	0.557786	-1.657906	0.972267
C	-0.617488	-2.286752	1.281796
H	-1.000167	-3.034477	0.576405
H	-0.934465	-2.354503	2.329558
O	2.839800	-1.297132	0.325639
C	3.815543	-0.375261	0.125711
O	3.638016	0.804320	0.199823
C	5.118879	-1.063075	-0.197177
H	5.912901	-0.311255	-0.286764
H	5.361048	-1.792958	0.591138
H	5.010379	-1.619231	-1.142636
C	-2.980031	-0.897964	-0.098195
O	-4.034559	-1.259547	-0.291191

TSS3

C	-2.281153	-2.217201	0.130771
C	-3.587689	-2.886097	0.504604
C	-3.681915	-3.894634	1.377292
C	-2.531417	-0.226397	1.575566
C	-1.356892	-0.476360	2.497681
C	-0.084109	-0.064950	2.311571
H	-1.460352	-2.565476	0.780857
H	-1.966351	-2.493158	-0.887847
H	-4.486404	-2.499301	0.005898
H	-4.642390	-4.370939	1.598202
H	-2.797323	-4.289477	1.891982
H	-2.689456	0.860362	1.497401
H	-3.439738	-0.675914	2.015904
H	-1.572053	-1.014846	3.428503
C	0.299136	0.712279	1.149816
C	0.984076	0.984507	0.111352
C	0.964758	2.193165	-0.797302
O	-0.032796	3.184907	-0.431310
C	-0.881908	3.147000	0.561554
O	-0.876730	2.326247	1.465139
C	-1.912342	4.240826	0.489707
H	-2.727433	3.844496	-0.139939
H	-2.299335	4.453842	1.495075
H	-1.496202	5.141992	0.018544
Rh	2.346184	-0.681850	-0.216279
C	3.581245	0.175621	0.885650
O	4.311427	0.723803	1.570724
Cl	0.753176	-1.775595	-1.636442
C	3.522285	-2.132949	-0.652386
O	4.193765	-2.997230	-0.949548
C	2.310270	2.928290	-0.738252
H	2.566607	3.192047	0.300502
H	3.101752	2.281326	-1.147410
H	2.251005	3.849759	-1.338989
C	0.592397	1.791742	-2.229071
H	1.279820	1.019509	-2.604261
H	-0.431326	1.390262	-2.224571
H	0.627314	2.681344	-2.878282
C	1.015593	-0.350103	3.316821
H	1.486674	0.589191	3.652460
H	0.611825	-0.879714	4.193047
H	1.802100	-0.975303	2.860764
N	-2.299306	-0.752720	0.225915
S	-3.089963	0.109074	-0.957228
O	-4.527690	-0.103305	-0.907132
O	-2.611046	1.484420	-0.853411

C	-2.469540	-0.591126	-2.497343
H	-2.970917	-1.549487	-2.685923
H	-2.773173	0.149327	-3.252555
H	-1.374566	-0.700042	-2.436926

TSS4

C	-4.377460	-1.721211	0.057710
C	-5.691696	-1.518723	0.773859
C	-6.108137	-2.255363	1.808388
C	-3.062961	0.043463	1.279766
C	-1.851785	-0.695416	1.825193
C	-0.527394	-0.427900	1.714592
H	-3.805938	-2.543191	0.532556
H	-4.587955	-2.011786	-0.984694
H	-6.317747	-0.709463	0.375867
H	-7.083249	-2.085340	2.275252
H	-5.491821	-3.064944	2.217581
H	-2.869993	1.108016	1.138436
H	-3.884761	-0.048120	2.009699
H	-2.095754	-1.619715	2.364991
C	0.025160	0.751444	0.984997
C	1.159532	0.794844	0.260087
C	1.562090	1.820008	-0.643665
O	0.213402	3.319633	-0.201258
C	-0.733324	2.995566	0.491501
O	-0.835881	1.844299	1.115587
C	-1.931396	3.876707	0.703853
H	-2.710765	3.497343	0.018761
H	-2.295698	3.798063	1.738406
H	-1.683797	4.914253	0.444492
Rh	2.776111	-0.659660	0.053896
C	3.572075	0.122287	1.547938
O	4.025876	0.607997	2.476336
Cl	1.750286	-1.678190	-1.854967
C	4.195277	-1.920028	-0.228974
O	5.014677	-2.676889	-0.433838
C	2.774361	2.676320	-0.376900
H	2.993911	2.757727	0.697190
H	3.641266	2.221741	-0.887240
H	2.608552	3.676564	-0.803843
C	1.100841	1.712248	-2.072662
H	1.634960	0.865607	-2.540191
H	0.023543	1.483013	-2.101046
H	1.307565	2.644135	-2.619763
C	0.470510	-1.405887	2.296940
H	1.198528	-0.891376	2.946168
H	-0.045668	-2.176994	2.887806
H	1.042444	-1.911696	1.498437
N	-3.591944	-0.489449	0.019873
S	-2.957761	-0.009163	-1.423896
O	-3.979226	-0.200353	-2.432399
O	-2.384599	1.315559	-1.207235
C	-1.605870	-1.138596	-1.806601
H	-2.013982	-2.158435	-1.860192
H	-1.207874	-0.841329	-2.788243
H	-0.820784	-1.057911	-1.041762

TSS5

C	-3.186679	0.841329	-1.692622
C	-2.265245	-0.072228	-2.467812
C	-1.049784	0.299092	-2.886969
C	-2.133315	0.774766	0.566021
C	-1.738127	2.156095	0.636288
C	-0.419445	2.581163	0.786487
C	0.615125	1.619535	0.733639
H	-2.834808	1.882084	-1.757183
H	-4.204266	0.802591	-2.109649
H	-2.647606	-1.083771	-2.654686
H	-0.412874	-0.391932	-3.449184
H	-0.636691	1.294486	-2.679593
H	-0.928656	0.245417	0.190647
H	-2.134155	0.168574	1.478430
H	-2.470533	2.911993	0.326372
C	0.364344	0.231306	0.734571
C	0.403884	-0.853312	1.651408
O	1.884234	2.052960	0.380106
C	2.152749	2.324598	-0.925303
O	1.301125	2.417809	-1.758983
C	3.638140	2.428088	-1.160938
H	3.824625	3.005994	-2.075782
H	4.150918	2.871531	-0.295562
H	4.017289	1.399083	-1.308643
Rh	1.917193	-1.044269	0.105308
Cl	3.739462	-1.786180	-1.214512
C	0.764347	-2.037910	-1.144464
C	3.320521	-0.208143	1.210693
O	0.202624	-2.665356	-1.895717
O	4.189676	0.210831	1.797132
N	-3.261408	0.483686	-0.262523
S	-4.356568	-0.672610	0.202376
O	-3.798256	-1.392741	1.331034
O	-4.795926	-1.370043	-0.988139

C	-5.767844	0.269868	0.824364
H	-6.159206	0.896944	0.011302
H	-6.518390	-0.470666	1.138912
H	-5.433794	0.875029	1.678457
C	-0.593243	-2.002390	1.577797
H	-1.361345	-1.893975	2.365436
H	-1.132516	-2.039308	0.619183
H	-0.090449	-2.970974	1.739565
C	0.951144	-0.636875	3.058582
H	1.531680	-1.512234	3.397932
H	1.582826	0.261366	3.127211
H	0.107340	-0.509683	3.761929
C	-0.075536	4.055404	0.735789
H	0.698470	4.309611	1.477261
H	0.307598	4.327525	-0.262768
H	-0.965751	4.668257	0.941961

TSS7

C	2.309999	0.009868	-1.425271
C	1.415976	-1.035728	-0.750102
C	0.388357	-1.636868	-1.649866
C	1.799702	1.192491	0.490357
C	0.976379	-0.087561	0.770763
C	-0.342493	0.293582	1.456210
C	-1.282097	1.035381	0.735458
H	3.084908	-0.487661	-2.023892
H	1.697468	0.651828	-2.082279
H	2.005425	-1.809045	-0.240745
H	0.420381	-2.730978	-1.712320
H	0.286191	-1.146858	-2.628171
H	1.169118	1.939713	-0.015814
H	2.165414	1.610547	1.437926
H	1.511385	-0.724935	1.485382
Rh	-0.936208	-1.027357	-0.252966
Cl	-0.632833	-3.080307	1.034189
C	-1.207505	0.934684	-0.715993
C	-1.381615	1.831409	-1.700375
O	-2.318544	1.629651	1.409471
C	-3.614016	1.338901	1.118373
O	-3.939486	0.486323	0.349811
C	-4.542307	2.224894	1.913282
H	-4.343942	3.281003	1.671144
H	-5.581108	1.965647	1.673486
H	-4.353065	2.088385	2.989779
C	-2.489862	-1.664709	-1.089564
O	-3.422671	-2.069159	-1.588600
C	-1.431030	1.433283	-3.156970
H	-1.318872	0.346779	-3.285693
H	-2.395968	1.736278	-3.603312
H	-0.640785	1.946234	-3.736048
C	-1.549406	3.312858	-1.424498
H	-2.519730	3.669589	-1.816820
H	-1.501434	3.544938	-0.349617
H	-0.767261	3.896470	-1.943882
C	-0.455585	-0.011424	2.927283
H	-0.372339	-1.103773	3.064187
H	0.360677	0.473474	3.490589
H	-1.417929	0.329867	3.332404
N	2.900598	0.853140	-0.395583
S	4.338794	0.350361	0.300213
O	4.807873	-0.811148	-0.428647
O	4.164212	0.306807	1.740005
C	5.458472	1.714867	-0.066903
H	5.060562	2.628302	0.395674
H	6.428693	1.442420	0.374395
H	5.535989	1.814967	-1.157867

TSS8

O	3.184794	0.437143	0.057961
C	4.423126	0.135413	-0.514526
C	5.387233	1.259280	-0.243694
C	6.622838	1.094586	0.236641
C	2.192515	-0.515098	-0.216301
C	0.897437	-0.115327	0.512707
C	0.569890	1.324110	0.213409
C	-0.650686	1.670636	-0.224336
H	4.308632	0.006513	-1.615294
H	4.824862	-0.821339	-0.118687
H	5.016677	2.263209	-0.488108
H	7.295855	1.944726	0.385009
H	7.007093	0.101433	0.497312
H	2.021055	-0.570242	-1.316363
H	2.510581	-1.518910	0.118650
H	1.084173	-0.229018	1.597438
H	1.354749	2.083470	0.300520
Rh	-0.694175	-1.335992	-0.063586
Cl	0.512227	-3.276963	0.420818
C	-1.796993	-0.327656	1.021600
O	-2.392657	-0.101996	1.990859
C	-1.691223	0.630909	-0.366085
C	-2.759078	0.693472	-1.188354
H	-2.908171	1.556742	-1.848351

H	-3.521798	-0.090741	-1.202719
O	-0.955000	2.954462	-0.616503
C	-1.860965	3.652485	0.114684
O	-2.415857	3.194125	1.066697
C	-2.035662	5.045073	-0.442944
H	-1.079991	5.588527	-0.366809
H	-2.303132	4.994447	-1.509980
H	-2.814185	5.567998	0.126687
C	-2.124855	-2.689839	-0.700165
O	-2.834758	-3.508371	-1.007470

TSS9

O	3.191648	0.661859	-0.160296
C	4.454455	0.166248	-0.519816
C	2.233385	-0.331313	0.033929
C	0.941732	0.357704	0.460926
C	-0.054271	0.889414	-0.532155
C	-1.282796	1.066297	0.104474
H	4.364510	-0.450286	-1.441822
H	4.861485	-0.492212	0.275762
H	2.086714	-0.926923	-0.889952
H	2.533478	-1.026345	0.847351
H	1.267516	1.179149	1.133690
H	0.168929	1.203223	-1.554664
Rh	-0.666622	-1.161267	-0.159897
Cl	-2.437859	-1.915279	-1.433434
C	-0.120264	-3.012289	-0.045009
O	0.203700	-4.095527	-0.013887
C	-1.288256	0.669573	1.531070
C	-2.250661	0.849072	2.452772
H	-3.174658	1.384714	2.214917
H	-2.120377	0.426123	3.453646
O	-2.378362	1.606565	-0.467080
C	-2.558578	2.961646	-0.594634
O	-3.543889	3.352862	-1.127128
C	-1.465829	3.846724	-0.024465
H	-1.817106	4.885257	-0.073407
H	-1.237290	3.571770	1.017970
H	-0.540081	3.747207	-0.613769
C	-0.053521	-0.178206	1.714703
O	0.343566	-0.773298	2.676259
C	5.384970	1.320576	-0.774249
H	5.006457	2.084766	-1.465103
C	6.602864	1.435331	-0.238047
H	6.994131	0.686393	0.460411
H	7.255203	2.279554	-0.481202

Z-1c

O	-3.151301	0.409359	-0.134857
C	-3.641854	-0.873477	0.119342
C	-5.090673	-0.780978	0.516280
C	-6.063392	-1.539413	0.003565
C	-1.792863	0.437272	-0.450180
C	-1.395591	1.855199	-0.748385
C	-0.194422	2.401549	-0.478253
H	-3.061757	-1.343319	0.946133
H	-3.526045	-1.530694	-0.769675
H	-5.313477	-0.039064	1.293809
H	-7.097314	-1.453510	0.351674
H	-5.860426	-2.276784	-0.782039
H	-1.172947	0.026588	0.374962
H	-1.590521	-0.194749	-1.346250
H	-2.159622	2.462325	-1.246984
H	-0.002119	3.441215	-0.767600
C	0.888290	1.709998	0.158152
C	1.828667	1.152625	0.688407
C	2.962765	0.495515	1.353720
O	3.219877	-0.800891	0.834676
C	4.011171	-0.880715	-0.248268
O	4.531310	0.071130	-0.755026
C	4.139650	-2.312932	-0.715912
H	3.157933	-2.665222	-1.072139
H	4.874967	-2.365027	-1.528852
H	4.440256	-2.958183	0.123979
H	2.737948	0.349432	2.421661
H	3.863539	1.122348	1.252174

Z-5c

O	-2.838758	-0.511224	-0.321905
C	-3.788092	0.439095	0.057201
C	-5.149373	-0.202380	0.086635
C	-6.018850	-0.082801	1.093595
C	-1.551709	0.007426	-0.466393
C	-0.642222	-1.101330	-0.915264
C	0.692482	-1.163018	-0.765074
H	-3.792450	1.280903	-0.673234
H	-3.546776	0.876034	1.050157
H	-5.408961	-0.784064	-0.807203
H	-7.010051	-0.544460	1.049461
H	-5.771393	0.483628	1.999116
H	-1.547229	0.838761	-1.209200

H	-1.179563	0.445389	0.486095
H	-1.154360	-1.934491	-1.409757
H	1.226312	-2.055525	-1.109721
C	1.566708	-0.145370	-0.154680
C	1.323101	1.155584	-0.104048
C	1.102859	2.446060	-0.129563
O	4.123641	0.883773	-0.338215
C	3.924935	-0.129555	0.258990
O	2.706991	-0.706843	0.394727
C	4.968681	-0.962593	0.969337
H	4.961879	-1.989411	0.571037
H	5.955159	-0.502764	0.829537
H	4.722277	-1.020980	2.041717
H	0.537273	2.949782	0.664685
H	1.501772	3.064844	-0.943972
H	3.853204	-0.409582	2.608926
H	4.678955	-1.549679	1.460007
H	5.460516	0.020728	1.896461
C	-1.053910	2.878260	-1.385742
H	-1.718557	3.468877	-2.040850
H	-0.281002	3.564826	-0.996615
H	-0.563652	2.100395	-1.989677
C	-2.579220	3.262478	0.668424
H	-3.206568	3.938418	0.061297
H	-3.223049	2.730955	1.383368
H	-1.854117	3.888433	1.218580
C	-1.852048	-2.148800	1.982056
H	-2.663893	-1.704299	2.584694
H	-2.308371	-2.913334	1.331623
H	-1.142181	-2.643822	2.661697

Z-5d

C	2.291482	-1.546647	-0.933326
C	1.999205	-0.998618	-2.312100
C	0.914639	-1.317019	-3.026171
C	1.015118	0.087953	0.452515
C	0.175864	-0.888806	1.238083
C	-1.156876	-1.087860	1.153398
C	-2.047500	-0.287559	0.273983
H	1.528065	-2.289015	-0.643300
H	3.270564	-2.051654	-0.935308
H	2.747899	-0.296096	-2.700204
H	0.743824	-0.899066	-4.023449
H	0.160852	-2.013646	-2.639366
H	0.487126	0.404533	-0.464797
H	1.210338	1.003651	1.033737
H	0.737194	-1.503683	1.953512
C	-1.911248	0.993369	-0.016127
C	-1.849100	2.288797	-0.237648
O	-3.112414	-1.024354	-0.242397
C	-4.384463	-0.604648	-0.061566
O	-4.689742	0.369025	0.559695
C	-5.345383	-1.547813	-0.752071
H	-5.220607	-2.566711	-0.352637
H	-6.373610	-1.199063	-0.593015
H	-5.114092	-1.582789	-1.828647
N	2.306667	-0.504079	0.098635
S	3.706573	0.336166	0.337396
O	3.366931	1.672002	0.785168
O	4.561359	0.126300	-0.816429
C	4.505146	-0.498465	1.729109

S15. References.

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