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Supporting Information

Computational Study of Mechanisms and Tether Length Effects of Rh-Catalyzed [3+2] and [3+2+1] Reactions of Ene/Yne-Vinylcyclopropanes

Guan-Yu Zhang, Mu Lin, and Zhi-Xiang Yu*This manuscript is part of a joint special collection on Mechanisms and Selectivities of Organic Reactions – In Celebration of Prof. Kendall N. Houk's 80th birthday.

Supporting Information

Computational study of Mechanisms and Tether Length Effects of Rh-Catalyzed [3+2] and [3+2+1] Reactions of Ene/Yne-Vinylcyclopropanes

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1. Estimation of CO Concentration

In our [3+2+1] reactions, we used 0.2 atm CO gas, 80 °C and solvent toluene as the standard conditions. To estimate the CO concentration in solution phase under such conditions, the Henry's law constant K_H of CO at 353 K (80 °C) is found to be 11.53 MPa m^3/kmol according to the literature[1].

The concentration of CO is given by the equation

$$c = \frac{P}{K_H} = \frac{0.2 \times 0.101\ \text{MPa}}{11.53\ \text{MPa} \cdot \text{m}^3 \cdot \text{kmol}^{-1}} \approx 0.0018\ \text{mol} \cdot \text{L}^{-1}$$

Thus, the free energy change from the original standard state 1 atm (1 mol/24.5 L) to this new standard state is given by the equation

$$\Delta G = RT \ln \frac{c_1}{c_0} = RT \ln(0.0018 \times 24.5) = -1.85\ \text{kcal/mol}$$

2. Disscussions about the [3+2+1] Reaction of Ene-VCP with an Elongated Tether

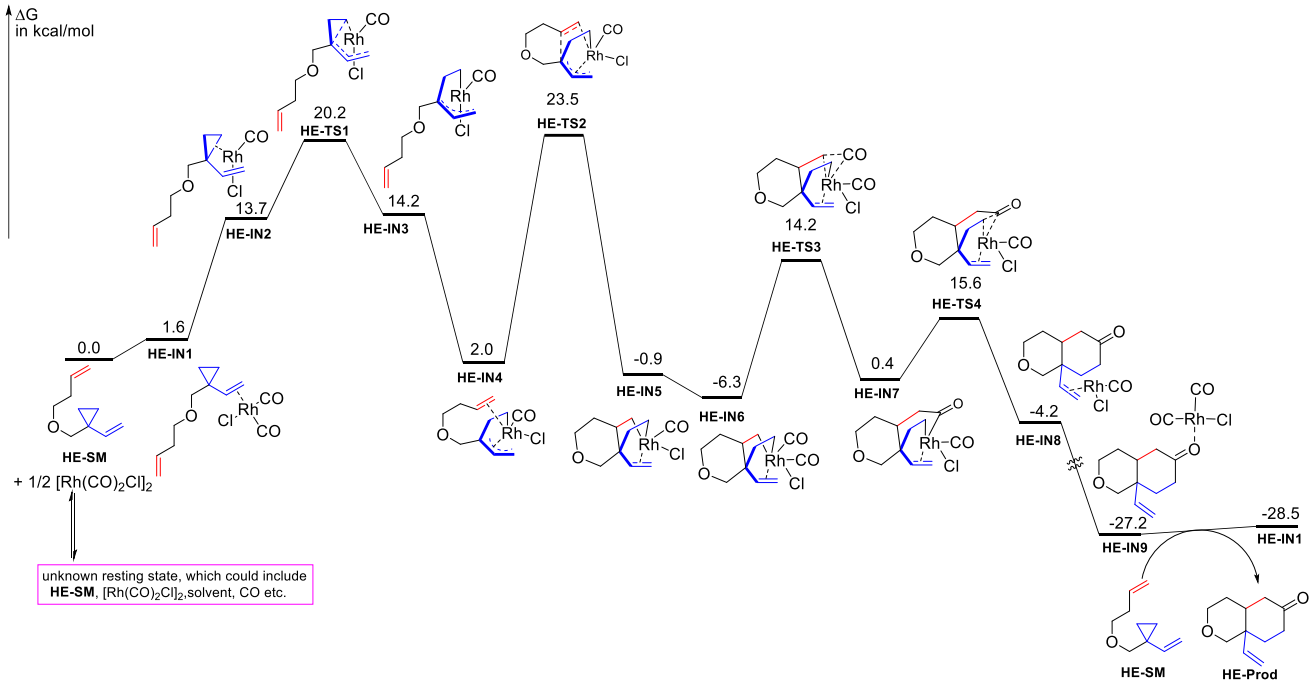

Figure S1. Energy profile for the [3+2+1] reaction of ene-VCP with an elongated tether.

Here we showed the computed free energy profile for the [3+2+1] reaction of ene-VCP with an elongated tether (Fig. S1). The energy barrier for the reaction seems reasonable, with the alkene insertion step **HE-TS2** being the rate-determining step. The activation energy of the reaction is 23.5 kcal/mol or higher (the resting state is estimated to have contribution and the exact vale is not known). The possible [3+1+2] pathway for this substrate is disfavored compared to the [3+2+1] pathway because CO insertion is more difficult, as can be understood by checking similar processes in Figures 1–3 (all these CO insertions via [3+1+2] pathway require activation free energies about 26 kcal/mol with respect to their substrates). Experimentally, such a reaction led to a complex mixture,[2] suggesting other unknown competing reaction pathways would occur simultaneously. Some possible side reaction pathways are presented and discussed below (Fig. S2).

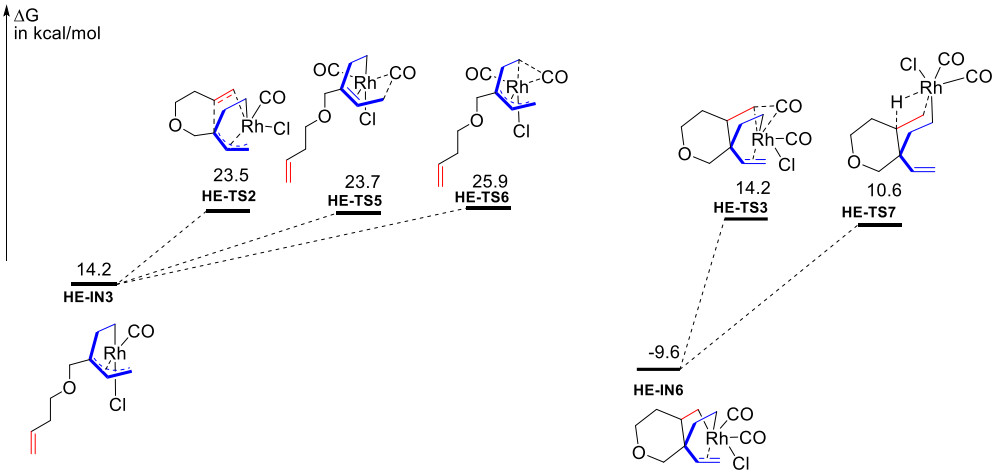

Figure S2. Possible side reaction pathways for the [3+2+1] reactions of ene-VCP with an elongated tether.

We proposed that as the transition state **HE-TS2** is more energy demanding than **E-TS2**, now the side reactions such as carbonyl insertion via **HE-TS5** and **HE-TS6** and β-H elimination via **HE-TS7** are comparable in energy, and all of them could lead to competing side reactions. These preliminary results may help understand the behavior of Ene-VCPs with elongated tethers in the [3+2+1] reaction.

3. Discussions on the isomers of IN2

For **Y-IN2**, there is also an isomer **Y-IN2'**, which is 5.6 kcal/mol lower than **Y-IN2** in energy. However, this intermediate is an off-cycle intermediate and is non-productive, which means it must convert back to **Y-IN2** to continue the catalytic cycle. Therefore, the structure **Y-IN2'** is not included in the free energy profiles of the reactions.

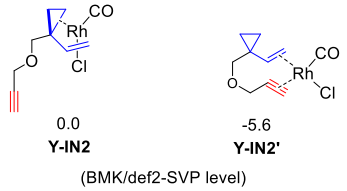

Figure S3. Comparison of **Y-IN2** and **Y-IN2'**

4. Alkyne/alkene insertion step in the [3+2] reaction of ene/yne-VCPs

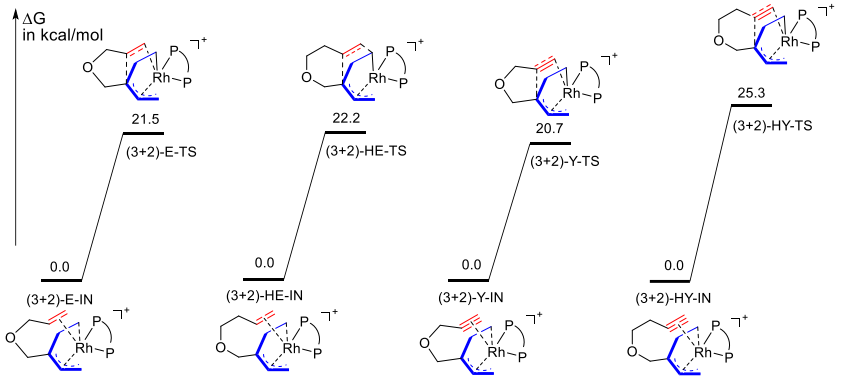

Figure S4. Comparison of intramolecular alkyne/alkene insertion transition states for [3+2] reaction of yne/ene-VCPs with different tethers and their activation free energies

5. Computed Energies of the Stationary Points

Table S1 Computed energy data

Name	TCG	SPE(low)	SPE(scrf)	SPE(dlpno)
CO	-0.013860	-113.172745	-113.168349	-113.158173
$[Rh(CO)_2Cl]_2$	-0.007654	-1592.916752	-1592.918084	-1593.122137
		[3+2+1] reaction of 1-yne-VCP		
Y-SM	0.147771	-424.631946	-424.641528	-424.511159
Y-Prod	0.166348	-537.938622	-537.951214	-537.778986
Y-IN1	0.155910	-1221.085160	-1221.098414	-1221.076107
Y-IN2	0.152255	-1107.882177	-1107.899134	-1107.884008
Y-TS1	0.150712	-1107.869179	-1107.884881	-1107.872435
Y-IN3	0.150798	-1107.876880	-1107.893759	-1107.878411
Y-IN4	0.159017	-1107.914148	-1107.927965	-1107.915791
Y-IN4'	0.157503	-1221.093399	-1221.107320	-1221.080598
Y-TS2	0.159762	-1107.887533	-1107.901949	-1107.884931
Y-TS2'	0.158814	-1221.056607	-1221.074608	-1221.037058
Y-IN5	0.160997	-1107.940270	-1107.954656	-1107.933375
Y-IN6	0.167356	-1221.136674	-1221.150209	-1221.117493
Y-TS3	0.168096	-1221.116892	-1221.132761	-1221.092357
Y-IN7	0.169713	-1221.152775	-1221.171180	-1221.120388
Y-TS4	0.168622	-1221.126415	-1221.143131	-1221.091904
Y-IN8	0.171853	-1221.188254	-1221.206374	-1221.152620
Y-IN9	0.173191	-1334.397859	-1334.412180	-1334.342907
		[3+2+1] reaction of 1-ene-VCP		
E-SM	0.171548	-425.887977	-425.896699	-425.765213
E-Prod	0.188549	-539.157028	-539.169438	-539.001594
E-IN1	0.178525	-1222.341647	-1222.354069	-1222.330134
E-IN2	0.174611	-1109.132705	-1109.149355	-1109.133894
E-TS1	0.174193	-1109.122791	-1109.137686	-1109.124555
E-IN3	0.173818	-1109.130865	-1109.146646	-1109.131211
E-IN4	0.185087	-1109.165514	-1109.178592	-1109.168649
E-IN4'	0.180754	-1222.348244	-1222.360915	-1222.334219
E-TS2	0.184526	-1109.135954	-1109.149390	-1109.136309
E-TS2'	0.182871	-1222.310354	-1222.327328	-1222.289796
E-IN5	0.184681	-1109.163149	-1109.178700	-1109.160101
E-IN6	0.190072	-1222.356937	-1222.370533	-1222.341607
E-TS3	0.190736	-1222.337426	-1222.353024	-1222.316759
E-IN7	0.194499	-1222.370368	-1222.389038	-1222.342715
E-TS4	0.191392	-1222.344175	-1222.360374	-1222.312932
E-IN8	0.193288	-1222.379814	-1222.398262	-1222.346760
E-IN9	0.197713	-1335.616504	-1335.629716	-1335.566335

	[3+2+1] reaction of 1-yne-VCP with elongated tethers			
HY-SM	0.174846	-463.895873	-463.906259	-463.760234
HY-Prod	0.196390	-577.200823	-577.214349	-577.027646
HY-IN1	0.182559	-1260.349157	-1260.363330	-1260.324848
HY-IN2	0.178483	-1147.141548	-1147.159449	-1147.128141
HY-TS1	0.178003	-1147.129854	-1147.146643	-1147.117948
HY-IN3	0.177335	-1147.138676	-1147.156031	-1147.126354
HY-IN4	0.184396	-1260.356124	-1260.370618	-1260.329256
HY-IN4'	0.186266	-1147.164467	-1147.178577	-1147.150286
HY-TS2	0.184906	-1260.317523	-1260.336394	-1260.284362
HY-TS2'	0.186567	-1147.122866	-1147.136924	-1147.108448
HY-IN5	0.187971	-1260.361502	-1260.381650	-1260.328211
HY-IN6	0.194350	-1260.370749	-1260.386671	-1260.333525
HY-TS3	0.195265	-1260.337921	-1260.352782	-1260.294569
HY-IN7	0.196896	-1260.380779	-1260.396767	-1260.329667
HY-IN8	0.205604	-1373.568340	-1373.583038	-1373.509253
HY-TS4	0.203842	-1373.543082	-1373.558896	-1373.486661
HY-IN9	0.202943	-1373.661034	-1373.675483	-1373.592682
	[3+2] reaction catalysed by cationic Rh catalysts			
(3+2)-E-IN	0.408933	-1495.336881	-1495.411971	-1495.005319
(3+2)-HE-IN	0.436787	-1534.592006	-1534.664349	-1534.246447
(3+2)-Y-IN	0.382074	-1494.088890	-1494.161249	-1493.753233
(3+2)-HY-IN	0.409551	-1533.338225	-1533.411411	-1532.988413
(3+2)-E-TS	0.407665	-1495.306466	-1495.380836	-1494.970482
(3+2)-HE-TS	0.436038	-1534.558674	-1534.631239	-1534.210023
(3+2)-Y-TS	0.382844	-1494.060532	-1494.132484	-1493.721395
(3+2)-HY-TS	0.410279	-1533.299463	-1533.371890	-1532.949571

Table S2 Computed energy data for the the [3+2+1] reactions of 1-ene-VCPs with elongated tethers.

Name	G
HE-SM	-464.946004
HE-Prod	-578.194271
HE-IN1	-1261.392390
HE-IN2	-1148.188056
HE-TS1	-1148.177080
HE-IN3	-1148.186826
HE-IN4	-1148.206815
HE-TS2	-1148.174819
HE-IN5	-1148.215222
HE-IN6	-1261.407744
HE-TS3	-1261.378863
HE-IN7	-1261.405666

HE-TS4	-1261.385432
HE-IN8	-1261.416677
HE-IN9	-1374.647022
HE-TS5	-1261.358589
HE-TS6	-1261.358160
HE-TS7	-1261.378782

6. Cartesian Coordinates of the Stationary Points

CO

C	0.000000	0.000000	-0.643398
O	0.000000	0.000000	0.482549

$[Rh(CO)_2Cl]_2$

Rh	-1.803691	-1.245108	1.371685
Rh	0.263230	0.821813	-0.059018
Cl	-2.194588	0.714188	-0.063876
Cl	0.155605	-1.636005	-0.063876
C	-3.314623	-0.836537	2.420948
C	-1.395120	-2.756040	2.420948
C	0.227535	2.705622	-0.030900
C	2.147039	0.786118	-0.030900
O	3.279831	0.732427	-0.011791
O	0.173844	3.838414	-0.011791
O	-1.122206	-3.669609	3.035256
O	-4.228192	-0.563623	3.035256

Y-SM

H	1.570513	-3.834444	0.087299
C	2.397073	-3.313867	-0.418962
C	3.207713	-4.020194	-1.215425
H	3.066310	-5.096576	-1.353121
H	4.038283	-3.551785	-1.753885
C	3.785829	-1.083326	-0.359999
C	3.335169	-1.394282	1.069130
C	1.149819	-1.130462	-0.343581
H	3.716522	-0.038962	-0.679016
H	4.646819	-1.626243	-0.760988
H	3.878392	-2.166190	1.623668
H	2.948501	-0.559404	1.662239
H	0.800792	-1.306865	-1.380895
H	0.395662	-1.574665	0.333096
C	1.227328	1.067779	-1.191551
H	0.241751	1.046784	-1.702837
H	1.983257	0.736117	-1.933358
C	2.485097	-1.849014	-0.129034
C	1.529658	2.453825	-0.804826
C	1.781859	3.599256	-0.510809
O	1.222706	0.240146	-0.065462
H	2.004428	4.616730	-0.242001

Y-Prod

C	0.858875	-1.428587	-0.928072
C	-0.257820	0.671463	-0.356748
C	-0.507958	-1.205213	-1.635676
C	1.079526	-2.817093	-0.314834
C	2.195008	-2.784951	0.745476
H	0.136895	-3.136817	0.163941
H	1.307523	-3.561231	-1.096236
H	3.171771	-2.577183	0.271795
H	2.292520	-3.747131	1.272791
H	-1.099467	0.820813	0.349471
H	0.234284	1.648667	-0.508372
H	-1.306572	-1.744421	-1.082561
H	-0.516982	-1.529973	-2.687231
C	1.954734	-0.965872	-1.880982
C	2.979478	-1.688440	-2.346162
H	3.156125	-2.727209	-2.050790
H	3.686071	-1.252272	-3.058910
H	1.834758	0.066207	-2.234538
C	0.686995	-0.389273	0.177581
C	1.193035	-0.511396	1.415992
C	1.999051	-1.701615	1.808776
O	2.476223	-1.802315	2.913718
H	1.011885	0.228123	2.204035
O	-0.705031	0.184227	-1.597564

Y-IN1

H	1.513362	-1.012859	1.983418
C	1.946179	-0.040690	1.709892
C	3.288467	0.138231	1.971453
C	0.959282	1.003890	1.312397
H	3.840569	-0.645216	2.499625
H	3.763820	1.121110	1.894326
C	1.376705	2.467744	1.161326
C	0.586565	2.045711	2.392833
C	-0.187966	0.457663	0.456544

H	0.844683	3.066499	0.415916
H	2.431268	2.732916	1.284773
H	1.110639	1.985758	3.351984
H	-0.467086	2.338475	2.437063
H	0.225584	-0.017975	-0.455222
H	-0.706738	-0.334675	1.027514
C	-1.082729	1.882524	-1.196187
H	-1.466003	1.095678	-1.878708
H	-0.044625	2.111617	-1.515270
C	-1.899844	3.093382	-1.358293
C	-2.560993	4.093833	-1.512197
Rh	3.236070	-0.849156	-0.065995
C	3.577153	-1.850619	-1.691534
O	3.771199	-2.484095	-2.607720
Cl	3.160108	-2.951460	0.986637
C	3.322392	0.828041	-0.928384
O	3.388581	1.837793	-1.450527
O	-1.119117	1.448774	0.133986
H	-3.154358	4.981399	-1.644799

Y-IN2

H	-0.522849	-0.446556	-1.594260
C	-1.497176	0.032568	-1.452057
C	-2.650819	-0.383216	-2.160031
H	-2.567195	-1.232411	-2.845145
H	-3.456740	0.317964	-2.410624
C	-2.963538	1.673053	0.076431
C	-2.285547	2.504136	-0.992181
C	-0.305923	1.466484	0.275754
H	-2.912421	1.987183	1.122292
H	-3.921113	1.205383	-0.207130
H	-2.755416	2.524853	-1.980661
H	-1.849793	3.459398	-0.682493
H	-0.521481	2.237144	1.042054
H	-0.065680	0.521447	0.805487
C	1.964053	2.064803	0.125184
H	2.733224	2.223138	-0.647878
H	2.253649	1.166257	0.709177
C	1.946586	3.231764	1.035012
C	1.935048	4.180179	1.786450
C	-1.515008	1.271840	-0.621565
Rh	-2.777709	-0.788518	-0.064040
Cl	-3.455432	-1.002169	2.172144
C	-2.632743	-2.631089	-0.253663
O	-2.535064	-3.755983	-0.381612
O	0.756716	1.859021	-0.544957
H	1.930896	5.025061	2.452886

Y-TS1

H	0.331237	-1.783683	0.672280
C	1.055605	-1.172787	1.220602
C	2.103524	-1.759758	1.989732
H	2.123923	-2.850837	2.075520
H	2.539486	-1.233657	2.846439
C	2.955322	0.980788	1.274635
C	1.636107	1.216370	1.997822
C	0.232562	0.836761	-0.119009
H	3.219136	1.749354	0.539075
H	3.809115	0.690213	1.912079
H	1.602763	0.859710	3.035562
H	1.211015	2.226051	1.929401
H	0.860386	1.556199	-0.685788
H	-0.077330	0.039981	-0.826568
C	-1.667982	2.135783	-0.490161
H	-2.060433	1.422718	-1.246293
H	-1.075554	2.896694	-1.041898
C	-2.799444	2.797505	0.172630
C	-3.738153	3.350090	0.696785
C	1.051743	0.249548	1.013291
Rh	2.848606	-0.861751	0.202051
Cl	4.209044	0.084983	-1.478634
C	2.897205	-2.535430	-0.850347
O	2.901147	-3.465355	-1.494283
H	-4.571820	3.840329	1.168068
O	-0.870976	1.475034	0.450014

Y-IN3

Rh	1.415602	-0.094206	-0.090502
Cl	2.402239	-1.742918	-1.413405
O	1.923324	-2.236349	2.248121
C	1.708100	-1.423965	1.495535
C	1.050974	1.094078	-1.712368
C	0.184235	2.165434	-1.031489
C	0.048141	1.622219	0.397041
C	1.153700	1.576270	1.254989
C	2.480642	1.504975	0.682691
H	0.483124	0.480463	-2.430147
H	1.958675	1.474925	-2.205595

H	-0.814817	2.255987	-1.484470
H	0.643533	3.169428	-1.013227
H	0.996223	1.301650	2.305396
H	2.762438	2.182960	-0.130562
H	3.305447	1.269192	1.364786
C	-1.340188	1.374875	0.938368
H	-1.872579	2.351262	1.010347
H	-1.292841	0.945436	1.961783
O	-2.014789	0.519791	0.066810
C	-3.355011	0.319287	0.410755
H	-3.439398	-0.121595	1.427083
H	-3.903011	1.285697	0.430797
C	-4.003811	-0.578007	-0.553555
C	-4.554312	-1.316620	-1.336067
H	-5.034943	-1.975513	-2.037857

Y-IN4

C	1.622921	-0.834041	0.815132
C	1.075264	0.865644	-1.521536
C	2.898715	-0.013840	0.764259
C	1.536593	-2.110818	-0.032815
C	0.158644	-2.042277	-0.723328
Rh	-0.361004	-0.151502	-0.046294
H	2.354379	-2.085326	-0.770810
H	1.687818	-3.006776	0.598048
H	-0.529561	-2.842164	-0.409501
H	0.245525	-2.070212	-1.820019
H	2.893418	1.832387	-1.917922
H	2.159847	2.185630	-0.312510
C	0.686425	-0.552798	1.828030
C	-0.625561	-1.130482	1.830660
H	-0.758407	-2.199968	1.640906
H	-1.343955	-0.690333	2.529994
H	0.840469	0.360697	2.413692
C	2.383200	1.386660	-1.048430
C	0.033888	0.624525	-2.139197
O	3.234773	0.418395	-0.526298
H	3.744335	-0.641254	1.096533
H	2.815951	0.852333	1.450109
Cl	-0.661642	2.140519	0.868554
C	-2.230152	-0.228201	-0.514213
O	-3.334494	-0.280413	-0.754898
H	-0.706690	0.554372	-2.921021

Y-IN4'

C	0.060460	1.562039	-0.271216
C	-0.894365	2.611553	0.310003
C	-2.169245	1.828725	0.678854
Rh	-1.525303	-0.058112	0.060079
H	-0.429648	3.076641	1.196269
H	-1.063935	3.420560	-0.423723
H	-3.064605	2.170139	0.137323
H	-2.384499	1.875198	1.757078
C	-0.241353	0.885822	-1.464839
C	-1.599708	0.762127	-1.917434
H	-2.262252	1.634414	-1.902911
H	-1.772626	0.063160	-2.742042
H	0.520464	0.199728	-1.849804
C	1.475291	1.571668	0.265287
H	1.450053	1.438031	1.368819
H	1.891449	2.591803	0.085806
C	3.564070	0.549732	0.145388
H	4.056427	1.542410	0.060020
H	3.568246	0.276434	1.221981
O	2.256734	0.604186	-0.344721
Cl	-0.630810	-2.244891	-0.672901
C	-0.980101	-0.611400	1.875963
O	-0.636821	-0.963093	2.892953
C	-3.282343	-0.880758	-0.022298
O	-4.299403	-1.364516	-0.110030
C	4.353941	-0.437056	-0.602001
C	5.021721	-1.245012	-1.203680
H	5.603854	-1.972126	-1.741994

Y-TS2

C	1.493788	-0.526131	0.535970
C	1.237220	0.658770	-1.091760
C	2.887847	0.069844	0.783826
C	1.421137	-1.891529	-0.170973
C	-0.012998	-1.968615	-0.744697
Rh	-0.685699	-0.121937	-0.050205
H	2.195064	-1.928345	-0.953796
H	1.650816	-2.690886	0.557640
H	-0.587599	-2.828285	-0.365167
H	-0.010478	-2.019728	-1.843163
H	2.967080	1.346534	-2.142746
H	2.586328	2.246977	-0.630730
C	0.595389	-0.366687	1.709206

C	-0.433692	-1.225524	2.053762
H	-0.485276	-2.258436	1.705744
H	-1.084896	-0.944468	2.886830
H	0.669203	0.586161	2.246702
C	2.625223	1.242137	-1.101690
C	0.114115	0.673972	-1.724282
O	3.495607	0.404279	-0.417532
H	3.508171	-0.693284	1.282101
H	2.802026	0.953597	1.449299
Cl	-1.287221	2.092237	0.881632
C	-2.496524	-0.337074	-0.553831
O	-3.581104	-0.453451	-0.858894
H	-0.282309	1.032011	-2.672344

Y-TS2'

O	-0.751756	-2.518194	-0.066814
C	-0.044746	-1.640536	0.007360
O	1.389007	0.505917	-2.828207
C	1.469039	0.427870	-1.672013
Rh	1.237593	-0.220646	0.078064
C	0.301580	0.814828	1.884529
C	1.558750	0.508855	2.374599
C	0.103431	1.482100	0.609186
C	1.152321	2.490251	0.090595
C	2.263749	1.694048	-0.648537
H	0.667357	3.188157	-0.611948
H	2.660308	2.212658	-1.530378
H	1.577563	3.095781	0.909202
H	3.141239	1.428996	-0.034424
Cl	3.047917	-1.815685	-0.022844
H	2.441852	1.107753	2.130152
H	-0.573308	0.299507	2.297936
H	1.667300	-0.195431	3.203215
C	-1.324312	1.713374	0.150474
H	-1.332514	1.896401	-0.944983
H	-1.733076	2.630347	0.635162
O	-2.109618	0.607790	0.475630
C	-3.456069	0.753165	0.123272
H	-3.893072	1.650341	0.610630
H	-3.560944	0.895014	-0.973035
C	-4.222576	-0.431767	0.529334
C	-4.870891	-1.398640	0.854734
H	-5.441389	-2.264323	1.142746

Y-IN5

C	3.155990	-0.180950	0.693651
C	1.318781	-1.841687	-0.152068
C	-0.138890	-1.855933	-0.685838
Rh	-1.237180	-0.258066	0.104096
H	2.046127	-2.057613	-0.951788
H	1.463357	-2.611948	0.626529
H	-0.683879	-2.759560	-0.350759
H	-0.142958	-1.864377	-1.785651
H	2.840852	1.201017	-2.173757
H	2.838276	2.190640	-0.677421
C	0.714245	-0.112030	1.571328
C	-0.195346	-0.942185	2.156210
H	-0.223623	-2.017207	1.955883
H	-0.850722	-0.558747	2.942999
H	0.757889	0.927902	1.922629
C	2.705008	1.164391	-1.081455
C	0.094424	0.745395	-1.013018
O	3.653318	0.281852	-0.532905
H	3.719198	-1.081134	0.984591
H	3.277213	0.586246	1.488538
Cl	-2.853187	0.873003	1.469667
C	-2.443067	-0.231523	-1.356752
O	-3.152535	-0.220109	-2.236015
H	-0.235599	1.404898	-1.825868
C	1.654671	-0.452826	0.437402
C	1.367581	0.585495	-0.650844

Y-IN6

C	-0.271668	-0.649192	-0.044023
C	0.902787	1.406718	0.584231
C	1.224374	-0.833093	0.301366
C	-0.626962	-0.826011	-1.537472
C	-2.066955	-0.324050	-1.832262
H	0.119534	-0.275430	-2.134597
H	-0.521047	-1.892085	-1.808577
H	-2.569709	-0.991673	-2.552699
H	-2.025020	0.674536	-2.291566
H	1.071692	2.346840	0.035059
H	1.081305	1.598369	1.663504
H	1.740188	-1.561025	-0.344363
H	1.338814	-1.154127	1.359335
C	-1.260039	-1.404245	0.825631
C	-2.134707	-2.369793	0.416110

H	-2.104507	-2.791799	-0.592209
H	-2.776794	-2.858506	1.155341
H	-1.253605	-1.141689	1.890772
C	-0.473961	0.803499	0.360640
C	-1.740660	1.214737	0.481504
Cl	-4.288520	-0.212625	2.169530
C	-4.095986	1.332492	-0.604890
O	-4.609833	2.284189	-0.928003
Rh	-3.162516	-0.214868	-0.025439
C	-4.649167	-1.546834	-0.513832
O	-5.507317	-2.250026	-0.710500
O	1.794205	0.431433	0.092038
H	-1.990450	2.231938	0.811047

Y-TS3

C	-0.324277	-0.690467	0.076266
C	0.747518	1.407421	0.718565
C	1.173414	-0.793367	0.492590
C	-0.612676	-1.144307	-1.372841
C	-2.081054	-0.856417	-1.762404
H	0.099747	-0.630110	-2.039088
H	-0.388435	-2.223029	-1.441510
H	-2.543803	-1.737459	-2.234404
H	-2.129272	-0.045204	-2.504850
H	0.957644	2.392832	0.275059
H	0.750702	1.509505	1.826312
H	1.735291	-1.516418	-0.118078
H	1.256101	-1.090091	1.559617
C	-1.271020	-1.378423	1.062940
C	-2.054172	-2.465888	0.824418
H	-2.017053	-3.023936	-0.115084
H	-2.672319	-2.871082	1.631092
H	-1.298719	-0.944109	2.070805
C	-0.567508	0.806399	0.247835
C	-1.762757	1.423900	0.130105
Cl	-4.218800	0.126913	2.146316
C	-3.265811	1.334546	-0.803953
O	-3.616018	2.231450	-1.447777
Rh	-3.144349	-0.330609	0.002336
C	-4.687144	-1.377613	-0.486594
O	-5.622958	-1.948641	-0.760778
H	-1.851130	2.456597	0.490416
O	1.709585	0.484157	0.288692

Y-IN7

C	0.482471	-0.767693	-0.277468
C	-1.341894	0.838722	-0.512694
C	-0.875301	-1.359931	-0.750896
C	0.803934	-1.127229	1.192906
C	2.102437	-0.434390	1.658569
H	-0.064376	-0.861175	1.820571
H	0.900728	-2.225680	1.256194
H	2.599887	-1.048680	2.432998
H	1.864286	0.531609	2.133890
H	-1.777923	1.527496	0.229074
H	-1.609438	1.207432	-1.526177
H	-1.081801	-2.350983	-0.318519
H	-0.895099	-1.441949	-1.858936
C	1.642214	-1.125444	-1.181485
C	2.556699	-2.110306	-0.946144
H	2.507392	-2.750803	-0.058798
H	3.300761	-2.361268	-1.706393
H	1.667672	-0.624172	-2.158351
C	0.167972	0.711760	-0.398277
C	1.072929	1.700230	-0.438637
Cl	5.257970	-0.552249	-1.500428
C	2.549460	1.531409	-0.275570
O	3.268154	2.491020	-0.315502
Rh	3.452382	-0.224132	0.073722
C	4.712179	0.766569	1.168201
O	5.464291	1.321692	1.797212
O	-1.837449	-0.453826	-0.292512
H	0.770602	2.748724	-0.548305

Y-TS4

C	-2.018075	-0.450319	0.153949
C	-3.690233	0.845981	-1.065676
C	-3.417258	-1.117598	0.015916
C	-1.639963	-0.072184	1.607003
C	-0.289937	0.676839	1.626023
H	-2.447441	0.550522	2.024580
H	-1.590454	-0.984092	2.225172
H	0.460630	0.173130	2.265280
H	-0.368613	1.683163	2.058526
H	-4.181318	1.827317	-0.980795
H	-3.755712	0.510689	-2.124419
H	-3.724996	-1.665459	0.920108
H	-3.414764	-1.822887	-0.841639

C	-0.902676	-1.249341	-0.498391
C	-0.071060	-2.098809	0.199232
H	-0.174431	-2.261088	1.276343
H	0.581222	-2.787503	-0.343544
H	-0.912616	-1.304200	-1.594545
C	-2.247895	0.840370	-0.608288
C	-1.294899	1.774964	-0.699764
Cl	2.295083	-1.219054	-1.656970
C	0.019700	1.635602	-0.003275
O	0.792533	2.567502	0.043502
Rh	1.023750	-0.160463	-0.002712
C	2.725403	0.789602	0.462222
O	3.708191	1.275588	0.724484
O	-4.317791	-0.067162	-0.204374
H	-1.436650	2.738138	-1.201354

Y-IN8

C	1.004437	-1.385477	-0.947979
C	-0.512207	0.405914	-0.229152
C	-0.265213	-1.168368	-1.815535
C	0.987122	-2.759490	-0.248830
C	1.954686	-2.885129	0.943850
H	-0.047931	-2.898754	0.109266
H	1.184730	-3.556442	-0.986903
H	2.942147	-3.268788	0.638617
H	1.577202	-3.625789	1.669246
H	-1.086202	0.653732	0.677133
H	-0.383731	1.323483	-0.839566
H	-0.690332	-2.104302	-2.209368
H	-0.036180	-0.493293	-2.666735
C	2.293324	-0.972398	-1.652544
C	3.573571	-1.133097	-1.190695
H	3.839829	-1.731824	-0.318812
H	4.402074	-0.748698	-1.792573
H	2.174057	-0.469953	-2.621464
C	0.836795	-0.248469	0.074804
C	1.547868	-0.334858	1.298269
C	2.194782	-1.605648	1.762830
O	2.840433	-1.648036	2.780366
Rh	2.642986	0.783461	-0.205548
C	2.213341	2.426154	0.707490
O	1.976363	3.400493	1.229617
Cl	4.095000	2.037580	-1.550513
H	1.274163	0.314795	2.138971
O	-1.199203	-0.579665	-0.954998

Y-IN9

C	0.683099	0.342944	0.291526
C	1.601567	-1.611550	-0.855955
C	2.160805	0.007692	0.645941
C	-0.251235	0.626386	1.473180
C	-1.730998	0.464954	1.082738
H	-0.022490	-0.091715	2.279701
H	-0.076593	1.633685	1.884518
H	-2.067091	1.285174	0.419966
H	-2.383758	0.472634	1.971451
H	1.724327	-2.622603	-0.415554
H	1.624111	-1.715820	-1.955020
H	2.195955	-0.583303	1.585713
H	2.797512	0.898087	0.755618
C	0.693559	1.412976	-0.795445
C	0.115461	2.617682	-0.742603
H	-0.470407	2.960838	0.115509
H	0.224804	3.319650	-1.574943
H	1.282641	1.148201	-1.682694
C	0.316001	-0.991257	-0.346272
C	-0.920313	-1.526249	-0.330218
C	-2.025623	-0.812916	0.324896
H	-1.155810	-2.498772	-0.774423
O	2.623252	-0.740714	-0.448532
O	-3.165289	-1.263222	0.222081
Rh	-5.014718	-0.732906	1.194328
C	-6.579074	-0.333207	2.130667
C	-5.808908	-0.393035	-0.488785
Cl	-3.978390	-1.159832	3.266767
O	-7.507526	-0.093250	2.738593
O	-6.273907	-0.192158	-1.508238

E-SM

H	1.763371	-3.855132	0.067443
C	2.518057	-3.198501	-0.390370
C	3.506190	-3.754162	-1.100912
H	3.577283	-4.840238	-1.215361
H	4.275615	-3.148124	-1.590550
C	3.469358	-0.751062	-0.283478
C	2.960407	-1.117593	1.114531
C	0.915078	-1.269513	-0.515446
H	3.217595	0.246317	-0.655253

H	4.448299	-1.130413	-0.591709
H	3.584739	-1.773078	1.730417
H	2.378273	-0.364400	1.653318
H	0.762084	-1.418030	-1.607642
H	0.166240	-1.907457	0.006279
C	-0.528551	0.571057	-0.499390
H	-1.327724	0.021011	0.042068
H	-0.721017	0.433802	-1.587704
C	2.316236	-1.737175	-0.138691
O	0.734475	0.069040	-0.176223
C	-0.584729	2.037034	-0.162992
H	0.248136	2.637979	-0.550017
C	-1.568628	2.613205	0.532957
H	-1.578241	3.690980	0.722380
H	-2.402879	2.027503	0.936760

E-Prod

C	0.975617	-1.313898	-0.954498
C	-0.316448	0.664489	-0.361933
C	-0.436287	-1.162248	-1.615610
C	1.053365	-2.632854	-0.156383
C	2.197153	-2.630830	0.865411
H	0.094052	-2.775569	0.370616
H	1.148797	-3.484138	-0.850777
H	3.176845	-2.530477	0.363487
H	2.240118	-3.564648	1.451722
H	-0.766948	1.216659	0.477641
H	-0.147930	1.373655	-1.200154
H	-0.947476	-2.128818	-1.746930
H	-0.342741	-0.677515	-2.609940
C	2.050783	-1.182683	-2.014999
C	2.909643	-2.114492	-2.443598
H	2.939688	-3.126959	-2.028988
H	3.625855	-1.887862	-3.239213
H	2.088455	-0.191263	-2.490346
C	0.998127	-0.059065	0.011207
C	1.012818	-0.440097	1.504849
C	2.083659	-1.466944	1.849800
O	2.785211	-1.377825	2.822893
H	1.157918	0.442765	2.146811
O	-1.185373	-0.359843	-0.752149
H	1.875779	0.572159	-0.203746
H	0.034035	-0.888199	1.762407

E-IN1

H	1.505855	-1.036804	1.896491
C	1.822185	-0.012890	1.655075
C	3.102323	0.344355	2.017877
C	0.741076	0.891108	1.168155
H	3.713235	-0.359108	2.591952
H	3.445403	1.382579	1.968626
C	0.972425	2.393372	1.021724
C	0.153597	1.883000	2.201726
C	-0.232169	0.206462	0.214992
H	0.424350	2.885214	0.213057
H	1.969826	2.799408	1.217491
H	0.613248	1.896713	3.195170
H	-0.929286	2.031852	2.170151
H	0.309985	-0.096196	-0.708549
H	-0.605288	-0.727765	0.690439
C	-2.229335	0.509553	-0.966160
H	-2.702938	-0.391318	-0.522354
H	-1.724819	0.184102	-1.903417
Rh	3.359020	-0.638066	-0.018418
C	3.989165	-1.564975	-1.595684
O	4.358984	-2.156196	-2.486162
Cl	3.458388	-2.742137	1.031952
C	3.309861	1.046241	-0.873208
O	3.302978	2.062601	-1.385482
O	-1.285737	1.060819	-0.091167
C	-3.273088	1.543858	-1.290342
H	-2.884564	2.514889	-1.623078
C	-4.589790	1.331261	-1.217022
H	-4.996611	0.371117	-0.878518
H	-5.309198	2.107057	-1.496486

E-IN2

H	-0.294776	-0.438752	-1.548780
C	-1.237251	0.095976	-1.391076
C	-2.391404	-0.165570	-2.168434
H	-2.344293	-0.951847	-2.928100
H	-3.134979	0.614363	-2.375693
C	-2.629259	1.696180	0.238922
C	-1.862185	2.567627	-0.733612
C	0.000381	1.271108	0.488010
H	-2.594589	1.914582	1.309588
H	-3.604016	1.315268	-0.111084
H	-2.295854	2.708258	-1.728782

H	-1.374805	3.459565	-0.327258
H	-0.176837	1.990729	1.315672
H	0.131247	0.267846	0.945260
C	2.313826	1.626799	0.469407
H	2.536807	0.612233	0.861342
H	2.217723	2.301856	1.349549
C	-1.193206	1.254889	-0.451435
Rh	-2.627561	-0.751619	-0.126746
Cl	-3.414045	-1.112461	2.054699
C	-2.611624	-2.573100	-0.488049
O	-2.593841	-3.685143	-0.721342
O	1.117429	1.632053	-0.260453
C	3.433427	2.108139	-0.413011
H	3.235534	3.044643	-0.949967
C	4.607623	1.485426	-0.545766
H	4.818898	0.544067	-0.025050
H	5.402190	1.895714	-1.176453

E-TS1

H	0.220925	-1.644144	0.479265
C	0.939079	-1.109110	1.108919
C	1.879361	-1.798993	1.930266
H	1.817937	-2.891119	1.971550
H	2.280339	-1.336264	2.839169
C	2.976970	0.896084	1.398645
C	1.624923	1.196587	2.031988
C	0.360895	1.006065	-0.196094
H	3.347196	1.672209	0.718914
H	3.758133	0.525671	2.085908
H	1.488562	0.801221	3.047129
H	1.278028	2.236622	1.979095
H	1.074019	1.709685	-0.675989
H	0.064911	0.262747	-0.965237
C	-1.438556	2.433034	-0.645208
H	-1.834516	1.779103	-1.450461
H	-0.743899	3.157917	-1.125880
C	1.050620	0.316094	0.964597
Rh	2.828066	-0.894068	0.247003
Cl	4.409157	-0.005240	-1.263972
C	2.842710	-2.526916	-0.867956
O	2.836313	-3.430042	-1.549148
O	-0.744295	1.683506	0.314907
C	-2.562266	3.176023	0.024515
H	-2.279709	3.747267	0.917944
C	-3.823254	3.186983	-0.415927
H	-4.125796	2.614855	-1.300845
H	-4.598395	3.771426	0.089039

E-IN3

Rh	1.385777	-0.097097	-0.108924
Cl	2.266038	-1.793059	-1.449597
O	2.025831	-2.168462	2.259233
C	1.769889	-1.381239	1.492561
C	0.926825	1.055583	-1.734635
C	0.085453	2.131553	-1.028761
C	0.030566	1.611307	0.412842
C	1.179849	1.596521	1.213563
C	2.475388	1.528761	0.574672
H	0.330637	0.425965	-2.414352
H	1.806360	1.435394	-2.277471
H	-0.936999	2.203108	-1.429521
H	0.534587	3.139960	-1.052607
H	1.080033	1.340645	2.275689
H	2.706178	2.191101	-0.266951
H	3.337697	1.314857	1.216425
C	-1.326273	1.354178	1.026307
H	-1.860972	2.327919	1.117503
H	-1.222289	0.936849	2.051044
O	-2.036713	0.486877	0.201094
C	-3.360712	0.269304	0.605694
H	-3.373987	-0.120413	1.648364
H	-3.935465	1.219568	0.604782
C	-4.003176	-0.732693	-0.314618
H	-3.434181	-1.657485	-0.473282
C	-5.190368	-0.557766	-0.901230
H	-5.629643	-1.330804	-1.539065
H	-5.767766	0.364011	-0.763479

E-IN4

C	1.364544	-0.583576	1.368417
C	1.412607	0.943483	-1.070480
C	2.738327	0.223172	-1.020430
C	2.620518	0.257417	1.399206
C	1.438877	-2.009832	0.807990
C	0.370474	-2.019342	-0.305252
C	0.426589	0.648730	-1.998518
Rh	-0.365403	-0.097760	-0.012562
H	2.455797	-2.207797	0.434609

H	1.239410	-2.739693	1.612404
H	-0.384977	-2.809760	-0.172583
H	0.810428	-2.138948	-1.308038
H	-0.300018	1.422171	-2.262134
H	0.545604	-0.195093	-2.687597
H	2.625372	-0.792978	-1.444919
H	3.422475	0.775360	-1.691957
H	3.286257	-0.114778	2.198967
H	2.356039	1.305103	1.643753
C	0.218646	-0.166946	2.073739
C	-1.035808	-0.834106	1.883608
H	-1.078588	-1.927134	1.836929
H	-1.917976	-0.348167	2.312120
H	1.354177	1.915724	-0.565148
H	0.211934	0.840208	2.505911
Cl	-1.121615	2.222338	0.463528
C	-2.044092	-0.387361	-0.927531
O	-3.039940	-0.562259	-1.434661
O	3.380606	0.176517	0.225261

E-IN4'

C	0.036307	1.652481	-0.287544
C	-0.960343	2.628377	0.348596
C	-2.177587	1.759749	0.724144
Rh	-1.444832	-0.066858	0.029709
H	-0.499964	3.094243	1.236550
H	-1.197707	3.446201	-0.355691
H	-3.105576	2.064751	0.216849
H	-2.365625	1.760014	1.808444
C	-0.260033	0.996784	-1.494074
C	-1.620282	0.808187	-1.917740
H	-2.331981	1.638991	-1.859258
H	-1.774157	0.126289	-2.760251
H	0.529332	0.365176	-1.914606
C	1.461278	1.697078	0.221212
H	1.457734	1.564889	1.325596
H	1.853010	2.725740	0.034589
C	3.551240	0.643042	0.091944
H	4.106830	1.593203	-0.057210
H	3.522868	0.447113	1.187255
O	2.243820	0.741700	-0.399204
Cl	-0.425976	-2.169435	-0.790487
C	-0.815441	-0.638960	1.812011
O	-0.422402	-0.999877	2.807639
C	-3.155428	-0.984484	-0.031674
O	-4.147455	-1.519721	-0.107838
C	4.250271	-0.493122	-0.604662
H	3.684616	-1.432712	-0.641661
C	5.474038	-0.409026	-1.133255
H	5.951856	-1.274960	-1.601521
H	6.044401	0.527232	-1.114937

E-TS2

C	0.059718	-0.593178	1.265065
C	0.174419	0.475442	-0.366079
C	1.620561	0.061984	-0.608312
C	1.423577	-0.041173	1.689584
C	0.073934	-2.079050	0.843961
C	-1.167588	-2.290085	-0.051813
C	-0.807366	0.243231	-1.445591
Rh	-1.951819	-0.381960	0.123533
H	1.021017	-2.308084	0.331470
H	0.061744	-2.697556	1.759609
H	-1.832280	-3.089245	0.314636
H	-0.888748	-2.538260	-1.087992
H	-1.264115	1.151586	-1.854602
H	-0.538959	-0.513483	-2.194872
H	1.668235	-0.866881	-1.207499
H	2.100914	0.865898	-1.195402
H	1.826037	-0.678926	2.495907
H	1.318747	0.989863	2.082420
C	-1.050736	-0.226607	2.189550
C	-2.117530	-1.034749	2.501065
H	-2.119483	-2.110617	2.314772
H	-2.924259	-0.628807	3.118226
H	0.080668	1.481192	0.066820
H	-1.073681	0.816091	2.529119
Cl	-2.640019	1.967698	0.482137
C	-3.545043	-0.755814	-0.790574
O	-4.500135	-0.975105	-1.361702
O	2.296103	-0.101914	0.606180

E-TS2'

O	-0.878019	-2.437810	0.055941
C	-0.124206	-1.596339	0.099313
O	1.350370	0.403110	-2.815137
C	1.437008	0.359320	-1.657993
Rh	1.210878	-0.227048	0.113586

C	0.319842	0.880332	1.899464
C	1.577081	0.565236	2.383364
C	0.116894	1.510725	0.606011
C	1.175294	2.484680	0.044474
C	2.266585	1.645514	-0.677435
H	0.693894	3.165574	-0.676823
H	2.661083	2.126370	-1.581313
H	1.618329	3.110717	0.837838
H	3.146354	1.386742	-0.064114
Cl	2.984752	-1.866677	0.039983
H	2.468233	1.138945	2.109519
H	-0.559651	0.393761	2.337373
H	1.683106	-0.115407	3.231872
C	-1.315474	1.730501	0.153619
H	-1.330721	1.906376	-0.943222
H	-1.727868	2.648229	0.633485
O	-2.087845	0.621646	0.489297
C	-3.444311	0.734672	0.148687
H	-3.920290	1.574587	0.696339
H	-3.536766	0.954919	-0.937713
C	-4.142070	-0.560891	0.462562
H	-3.669974	-1.461863	0.050414
C	-5.271317	-0.652070	1.170213
H	-5.757451	-1.616853	1.344260
H	-5.753822	0.235072	1.597007

E-IN5

C	1.825360	0.410603	0.300909
C	1.530578	-0.250078	-1.081677
C	2.806781	-1.084438	-1.281199
C	3.314555	0.735839	0.083020
C	1.606093	-0.579492	1.466591
C	0.143360	-1.097826	1.541600
C	0.160028	-0.920888	-1.126411
Rh	-1.048301	0.019968	0.255515
H	2.327570	-1.407433	1.365264
H	1.883698	-0.060157	2.401403
H	-0.272066	-0.968738	2.559616
H	0.109139	-2.178155	1.329259
H	-0.343190	-0.768998	-2.095621
H	0.228950	-2.001926	-0.926522
H	2.701665	-2.089458	-0.827299
H	3.061748	-1.216469	-2.346905
H	3.866937	0.841754	1.031885
H	3.433164	1.675513	-0.494659
C	0.874647	1.575342	0.391625
C	0.029925	1.861007	1.419187
H	0.083515	1.347903	2.383746
H	-0.658090	2.706922	1.330738
H	1.543668	0.566865	-1.825174
H	0.829164	2.226561	-0.492356
Cl	-2.536426	1.618007	-0.758645
C	-2.271750	-1.382801	-0.008950
O	-2.997321	-2.236133	-0.165875
O	3.831288	-0.363003	-0.630408

E-IN6

C	-1.648968	0.227531	0.484889
C	-1.467662	-0.843486	-0.609631
C	-2.774477	-0.687169	-1.398042
C	-3.131169	-0.026691	0.815074
C	-1.426029	1.667058	-0.035126
C	0.014474	1.934192	-0.556788
C	-0.088947	-0.730767	-1.274661
Rh	1.234326	0.329428	0.012473
H	-2.179839	1.878115	-0.812361
H	-1.662670	2.357837	0.793923
H	0.399269	2.885720	-0.151482
H	0.007349	2.041926	-1.652501
H	0.340874	-1.725814	-1.470075
H	-0.176330	-0.203690	-2.240703
H	-2.683454	0.088703	-2.183866
H	-3.100794	-1.624225	-1.881138
H	-3.628344	0.843510	1.276024
H	-3.241498	-0.893125	1.499043
C	-0.612789	-0.131054	1.523994
C	0.185794	0.736583	2.206552
H	0.050614	1.820247	2.147932
H	0.879338	0.349633	2.959442
H	-1.515151	-1.820208	-0.094622
H	-0.501247	-1.199385	1.751317
Cl	2.447755	-1.669981	0.807847
C	2.206093	0.356589	-1.604184
O	2.760962	0.344610	-2.588161
O	-3.733572	-0.289133	-0.433975
C	2.657280	1.349785	1.102546
O	3.497377	1.835144	1.676065

E-TS3

C	-1.919201	0.653369	-0.009949
C	-1.861406	-0.753141	0.652544
C	-3.296947	-1.294617	0.415021
C	-3.387307	1.010128	0.308343
C	-1.644698	0.597878	-1.533254
C	-0.172925	0.216034	-1.871366
C	-0.764289	-1.753196	0.177124
Rh	0.802749	0.038630	-0.024433
H	-2.360720	-0.109578	-1.985678
H	-1.892606	1.585951	-1.958939
H	0.291602	0.980130	-2.514639
H	-0.125299	-0.729957	-2.433949
H	-0.694520	-2.556120	0.927850
H	-1.076179	-2.193526	-0.783920
H	-3.331175	-1.988720	-0.445541
H	-3.673553	-1.837249	1.301843
H	-3.795119	1.778578	-0.368604
H	-3.472526	1.383520	1.350867
C	-0.919094	1.545480	0.706892
C	-0.073949	2.444334	0.137643
H	-0.093028	2.676386	-0.930510
H	0.590382	3.040130	0.771157
H	-1.714765	-0.597309	1.734499
H	-0.888600	1.446497	1.799745
Cl	1.584958	-0.095715	2.289322
C	0.971788	-1.793945	-0.251502
O	1.463198	-2.815441	-0.495173
O	-4.106887	-0.179139	0.132339
C	2.438735	0.796054	-0.648317
O	3.427959	1.202173	-1.016021

E-IN7

C	1.918850	-0.502668	-0.052771
C	2.222835	0.801435	0.737847
C	3.608850	1.172797	0.196888
C	3.329462	-1.129753	0.048520
C	1.529057	-0.288063	-1.531458
C	0.104589	0.274136	-1.733026
C	1.118076	1.863718	0.718953
Rh	-1.104574	-0.207125	-0.152908
H	2.279642	0.355292	-2.023316
H	1.606307	-1.266572	-2.035268
H	-0.377016	-0.178963	-2.615308
H	0.120756	1.363663	-1.886318
H	1.298412	2.638221	1.482257
H	1.048794	2.340649	-0.271514
H	3.532606	1.800710	-0.712764
H	4.216161	1.722089	0.937104
H	3.516588	-1.880038	-0.737338
H	3.469489	-1.618458	1.034853
C	0.828888	-1.282554	0.652504
C	-0.025802	-2.192428	0.075814
H	0.041225	-2.488086	-0.974053
H	-0.678524	-2.807653	0.701741
H	2.351506	0.491068	1.792110
H	0.820694	-1.211756	1.749236
Cl	-2.807692	-1.697915	-1.085410
C	-0.198306	1.151541	1.048696
O	-0.761463	1.294015	2.102191
O	4.225336	-0.057760	-0.115850
C	-2.368910	1.140260	-0.727043
O	-3.122305	1.893063	-1.098452

E-TS4

C	1.930883	-0.531997	-0.090636
C	2.178017	0.673203	0.845602
C	3.684204	0.974641	0.633468
C	3.314600	-1.209061	0.002165
C	1.609634	-0.058537	-1.528089
C	0.190885	0.554982	-1.631769
C	1.228770	1.839817	0.576633
Rh	-1.099935	-0.286621	-0.007890
H	2.377560	0.667152	-1.842350
H	1.705058	-0.912285	-2.219428
H	-0.470194	-0.013691	-2.311075
H	0.202308	1.564159	-2.068260
H	1.032435	2.437882	1.480866
H	1.666481	2.535362	-0.162923
H	3.839741	1.851038	-0.022827
H	4.195836	1.180212	1.591897
H	3.530151	-1.870279	-0.853329
H	3.377670	-1.813047	0.932418
C	0.805949	-1.383055	0.455621
C	-0.001397	-2.178976	-0.332567
H	0.138070	-2.258268	-1.415143
H	-0.655204	-2.920754	0.133741
H	2.026415	0.320438	1.880001

H	0.790288	-1.546513	1.541060
Cl	-2.338654	-1.408946	1.628519
C	-0.161563	1.526417	-0.002314
O	-0.987481	2.407982	-0.020352
O	4.240423	-0.159121	0.008093
C	-2.847924	0.615456	-0.499463
O	-3.842012	1.065718	-0.780766

E-IN9

C	0.741203	0.431844	0.084971
C	1.423386	-1.792946	-0.646847
C	2.085745	-0.128106	0.659017
C	-0.247124	0.707183	1.239245
C	-1.693340	0.832657	0.744995
H	-0.174350	-0.121796	1.963900
H	0.050304	1.617104	1.785136
H	-1.820358	1.714314	0.090244
H	-2.417708	0.952356	1.570248
H	1.106024	-2.846603	-0.679546
H	2.176658	-1.628113	-1.444844
H	2.266926	0.187594	1.698488
H	2.937177	0.213932	0.034617
C	1.013359	1.643186	-0.784188
C	0.691390	2.919995	-0.548496
H	0.142300	3.241641	0.342184
H	0.972581	3.703684	-1.258278
H	1.568043	1.414228	-1.705442
C	0.256620	-0.789660	-0.796398
C	-1.065427	-1.414554	-0.300052
C	-2.115931	-0.363650	-0.079784
H	-1.429734	-2.175268	-1.005176
O	1.971247	-1.518293	0.612038
H	0.102504	-0.490198	-1.844925
H	-0.886780	-1.889416	0.684704
O	-3.256361	-0.423302	-0.516978
Rh	-4.079614	-1.659219	-2.088102
C	-4.720517	-2.648855	-3.536875
C	-5.482868	-2.221341	-0.950550
Cl	-2.300887	-0.929044	-3.454532
O	-5.072660	-3.239388	-4.440022
O	-6.319748	-2.550817	-0.253397

E-IN8

C	1.837641	0.417786	0.312786
C	1.946187	-0.486616	-0.976893
C	3.446587	-0.363790	-1.355001
C	3.273462	1.017087	0.380528
C	1.562031	-0.447609	1.557080
C	0.270741	-1.256982	1.386590
C	1.514673	-1.950766	-0.745223
Rh	-1.180215	0.451409	0.156345
H	2.409351	-1.137168	1.705697
H	1.511804	0.178606	2.462413
H	-0.684812	-0.642427	1.582466
H	0.129434	-1.979081	2.212624
H	1.357006	-2.482882	-1.695652
H	2.312822	-2.481880	-0.191528
H	3.891779	-1.310590	-1.698599
H	3.579841	0.395267	-2.152458
H	3.604852	1.223337	1.410412
H	3.318586	1.961100	-0.202522
C	0.775459	1.491008	0.134499
C	-0.003538	2.047242	1.137425
H	0.101524	1.766214	2.190292
H	-0.569303	2.960415	0.932724
H	1.309741	-0.065534	-1.771160
H	0.785863	2.001833	-0.837361
Cl	-2.128890	2.013484	-1.271909
C	0.250457	-2.080652	0.089391
O	-0.659648	-2.820230	-0.180787
O	4.098399	0.042635	-0.182642
C	-2.790964	-0.639926	-0.139289
O	-3.754005	-1.202687	-0.316272

HY-SM

H	-0.176067	1.244363	-1.994712
C	-0.135213	1.455573	-0.915870
C	-1.269221	1.769467	-0.279188
C	1.228253	1.357081	-0.306314
H	-2.219999	1.831918	-0.817452
H	-1.288028	1.975085	0.796212
C	1.544539	2.043187	1.017280
C	2.109345	2.618942	-0.285529
C	1.904981	0.025339	-0.610495
H	2.248698	1.532086	1.680007
H	0.749427	2.598417	1.523716
H	1.666285	3.543057	-0.670724
H	3.178131	2.486128	-0.475927

H	1.306359	-0.797436	-0.161677
H	1.909543	-0.138766	-1.711408
C	3.883157	-1.191314	-0.336285
H	3.955298	-1.411605	-1.422173
H	3.351664	-2.043591	0.136710
O	3.207364	0.005806	-0.112825
C	5.289922	-1.060866	0.260910
H	5.200306	-0.831212	1.336955
H	5.799381	-0.202856	-0.211205
C	6.085055	-2.279265	0.073785
C	6.723163	-3.294335	-0.092033
H	7.297413	-4.192285	-0.234769

HY-Prod

C	-1.781529	0.676769	-0.589711
C	-2.702920	-0.344391	-1.283362
C	-2.384495	-1.796564	-0.903689
H	-3.743226	-0.127533	-0.980298
H	-2.659885	-0.205055	-2.376510
H	-1.366274	-2.072890	-1.234656
H	-3.086014	-2.510671	-1.362722
C	-0.390817	0.780578	-1.207126
C	0.073236	0.127282	-2.278225
H	-0.519363	-0.604673	-2.835012
H	1.087643	0.316014	-2.643110
H	0.266024	1.512364	-0.722233
C	-1.636029	0.355745	0.903924
C	-1.978064	-0.841224	1.426745
H	-1.905316	-1.030359	2.503772
C	-2.443893	2.089128	-0.686646
H	-3.493987	2.008065	-0.331367
H	-2.455165	2.413427	-1.739809
C	-1.103233	1.481875	1.762506
H	-1.224798	1.240793	2.831080
H	-0.020337	1.599483	1.572325
C	-1.799978	2.811796	1.421079
H	-1.296899	3.655207	1.918371
H	-2.852645	2.780617	1.774001
O	-1.760891	3.057087	0.044884
C	-2.420150	-1.999625	0.606545
O	-2.742351	-3.048293	1.113236

HY-IN1

H	-0.292041	0.981289	-1.856500
C	-0.193202	1.364656	-0.831764
C	-1.266869	2.060616	-0.320964
C	1.170894	1.258579	-0.238176
H	-2.124951	2.271586	-0.966530
H	-1.197156	2.616493	0.619344
C	1.520859	1.966460	1.068572
C	2.026876	2.548171	-0.246715
C	1.868949	-0.057099	-0.563832
H	2.254875	1.462288	1.703638
H	0.735758	2.505573	1.607940
H	1.551886	3.458164	-0.627014
H	3.087847	2.426918	-0.481661
H	1.305986	-0.894941	-0.096971
H	1.840218	-0.220982	-1.663602
C	3.886306	-1.217137	-0.325233
H	3.929794	-1.455167	-1.408222
H	3.391702	-2.072200	0.180434
Rh	-1.760884	-0.115951	0.116458
C	-2.607561	-1.820059	0.473269
O	-3.123898	-2.814086	0.628755
Cl	-2.694805	-0.306172	-2.034843
C	-1.039450	0.031881	1.856330
O	-0.623854	0.128935	2.911452
O	3.182627	-0.032629	-0.103200
C	5.305763	-1.036299	0.225906
H	5.242672	-0.783119	1.298603
H	5.780160	-0.178455	-0.281778
C	6.124020	-2.240017	0.043798
C	6.780342	-3.244042	-0.116592
H	7.370738	-4.132270	-0.255215

HY-IN2

Rh	1.820362	-0.187568	0.016028
Cl	1.303266	-2.299970	-0.864695
O	3.870670	-1.370121	1.850651
C	3.092417	-0.928934	1.150073
C	0.156747	0.891170	-1.442118
C	-0.241337	2.324921	-1.145255
C	-0.024950	1.500282	0.086836
C	1.217315	1.563162	0.912309
C	2.475590	1.820595	0.310889
H	-0.622144	0.188284	-1.744387
H	1.135591	0.750443	-1.932886
H	-1.278490	2.586755	-1.371485

H	0.493279	3.106383	-1.364244
H	1.095000	1.551900	2.001576
H	2.554306	2.297891	-0.673723
H	3.341213	1.986980	0.959350
C	-1.249631	1.007963	0.849451
H	-1.513115	1.783620	1.603407
H	-0.988818	0.080366	1.399626
O	-2.310397	0.789882	-0.020360
C	-3.464913	0.302273	0.598736
C	-4.526570	0.080341	-0.484529
H	-3.256166	-0.652065	1.123258
H	-3.840712	1.023325	1.353986
C	-5.788314	-0.411373	0.079276
H	-4.137994	-0.641550	-1.223783
H	-4.698512	1.031704	-1.017599
C	-6.819309	-0.817013	0.566006
H	-7.738795	-1.180724	0.989127

HY-TS1

Rh	1.574420	-0.117786	-0.144426
Cl	0.958401	-2.161270	-1.154885
O	3.145054	-1.861362	1.893260
C	2.601769	-1.208297	1.145898
C	0.480983	0.912633	-1.656892
C	-0.006854	2.242671	-1.093456
C	0.145126	1.611809	0.256302
C	1.379494	1.620933	0.987977
C	2.609915	1.689424	0.262531
H	-0.325581	0.245710	-1.977254
H	1.310097	0.976788	-2.383258
H	-1.040478	2.509452	-1.346720
H	0.670912	3.091196	-1.256652
H	1.356999	1.443503	2.068596
H	2.684825	2.270289	-0.663633
H	3.541985	1.636584	0.834222
C	-1.114681	1.185211	0.984302
H	-1.510826	2.095933	1.494728
H	-0.874590	0.440134	1.769626
O	-2.045284	0.688910	0.083969
C	-3.246287	0.284202	0.672537
C	-4.151917	-0.269194	-0.433143
H	-3.065512	-0.498447	1.437208
H	-3.743963	1.137572	1.179172
C	-5.454271	-0.694740	0.090944
H	-3.642788	-1.119333	-0.919333
H	-4.292541	0.509296	-1.203056
C	-6.522020	-1.038555	0.545173
H	-7.473219	-1.350375	0.938390

HY-IN3

Rh	-1.426611	0.107140	-0.086936
Cl	-2.252132	1.858924	-1.390372
O	-1.895376	2.197446	2.306311
C	-1.701880	1.398800	1.533452
C	-1.073605	-1.046720	-1.737763
C	-0.232335	-2.147388	-1.070155
C	-0.106571	-1.628375	0.367961
C	-1.222313	-1.597043	1.217165
C	-2.538297	-1.494542	0.631211
H	-0.492551	-0.432331	-2.443431
H	-1.987438	-1.400758	-2.240025
H	0.770454	-2.246999	-1.512562
H	-0.708555	-3.143465	-1.075860
H	-1.074415	-1.349659	2.275616
H	-2.818604	-2.141913	-0.206857
H	-3.369374	-1.259837	1.305941
C	1.277839	-1.412923	0.934474
H	1.785524	-2.401873	1.011263
H	1.219583	-0.990160	1.959984
O	1.992196	-0.568981	0.086712
C	3.326862	-0.387753	0.456066
C	3.978395	0.554500	-0.562449
H	3.400902	0.048604	1.473919
H	3.866600	-1.357570	0.472382
C	5.391516	0.798862	-0.253822
H	3.423912	1.508899	-0.574455
H	3.882283	0.113460	-1.569734
C	6.555250	0.986032	0.020621
H	7.590401	1.160077	0.254877

HY-IN4

C	-0.404232	-1.672386	0.354043
C	0.245827	-2.008778	1.701444
C	1.408451	-1.005792	1.838831
Rh	1.149056	-0.020011	0.016900
H	-0.497441	-1.889683	2.508043
H	0.568086	-3.065582	1.716093
H	2.394183	-1.487965	1.924509

H	1.277740	-0.339694	2.704955
C	0.297545	-1.853072	-0.848954
C	1.734554	-1.879539	-0.868641
H	2.281104	-2.463246	-0.119877
H	2.205645	-1.835552	-1.855777
H	-0.246617	-1.649646	-1.776468
C	-5.510278	-0.188508	-2.570162
C	-6.692707	0.044267	-2.682294
H	-7.741118	0.255927	-2.793989
C	-1.906571	-1.492246	0.348442
H	-2.184213	-0.738090	1.116508
H	-2.361053	-2.455423	0.682481
C	-4.081620	-0.477385	-2.405461
H	-3.781432	-1.293773	-3.085036
H	-3.479066	0.406330	-2.678129
C	-3.742548	-0.880974	-0.965980
H	-4.323036	-1.782233	-0.677456
H	-4.027402	-0.065657	-0.269139
O	-2.370608	-1.129822	-0.903652
Cl	0.688433	1.086850	-2.149617
C	0.137293	1.475241	0.819715
O	-0.460315	2.341255	1.230200
C	2.917907	0.779117	-0.057450
O	3.954883	1.220712	-0.133621

HY-IN4'

C	1.068420	-1.519900	0.454667
C	0.411541	-2.653431	-0.335796
C	-0.783164	-1.965015	-1.020272
Rh	-0.708501	-0.112387	-0.061019
H	1.129195	-3.087988	-1.052512
H	0.108713	-3.465433	0.347241
H	-1.733199	-2.499841	-0.861229
H	-0.621433	-1.867205	-2.105097
C	0.438038	-0.989549	1.580764
C	-0.996262	-1.162930	1.728592
H	-1.435989	-2.151507	1.551464
H	-1.469587	-0.592471	2.534154
H	0.960235	-0.217346	2.155663
C	0.915490	1.161887	-1.423286
C	0.019456	0.741225	-2.150884
H	-0.616944	0.494664	-2.985561
C	2.502701	-1.199250	0.091293
H	2.590669	-1.222049	-1.013266
H	3.131318	-2.030755	0.473471
C	1.992111	1.856009	-0.698004
H	2.322927	2.690979	-1.343242
H	1.532573	2.293132	0.207093
C	3.229967	1.022955	-0.313302
H	3.945567	1.710483	0.165316
H	3.713437	0.616616	-1.224117
O	2.984015	0.001029	0.605597
Cl	-0.692771	2.010350	1.242519
C	-2.538929	0.352461	-0.445513
O	-3.627147	0.609053	-0.621184

HY-TS2

O	1.861145	1.977330	2.006507
C	1.175664	1.395436	1.321034
O	-0.173169	-2.165588	1.762080
C	-0.244117	-1.297141	0.994754
Rh	0.086120	0.350115	0.149067
C	-1.363578	2.043515	-0.327252
C	-0.865587	1.756211	-1.586224
C	-1.875918	1.015665	0.561644
C	-2.553368	-0.242466	-0.024671
C	-1.442974	-1.274725	-0.368920
H	-3.235694	-0.669971	0.728519
H	-1.736126	-2.313355	-0.171270
H	-3.159956	-0.003349	-0.914821
H	-1.085474	-1.254468	-1.412410
Cl	2.034421	-0.401015	-1.064950
H	-1.222581	0.904639	-2.174084
H	-1.110947	3.002845	0.138608
H	-0.275582	2.501370	-2.125711
C	-2.342883	1.441260	1.941773
O	-1.486136	2.408539	2.463718
H	-2.382032	0.550941	2.604235
H	-3.380863	1.842333	1.878968
C	-1.873951	2.901101	3.713837
H	-2.879968	3.365419	3.658153
H	-1.927262	2.082118	4.459997
C	-0.842835	3.944965	4.157913
H	-0.784907	4.739018	3.393125
H	0.152565	3.470802	4.208696
C	-1.184962	4.529955	5.458880
C	-1.487013	4.999265	6.532603
H	-1.745175	5.421834	7.487415

HY-TS2'

C	1.241332	-1.012967	0.257256
C	0.720306	-2.293201	-0.421749
C	-0.757353	-2.053176	-0.764937
Rh	-0.867136	-0.111970	-0.059686
H	1.321768	-2.475755	-1.326696
H	0.891667	-3.149793	0.257628
H	-1.446675	-2.740039	-0.248589
H	-0.946876	-2.131255	-1.845574
C	0.610512	-0.634809	1.538272
C	-0.558041	-1.181364	2.045152
H	-0.913934	-2.173172	1.760232
H	-0.993579	-0.732952	2.943066
H	1.032350	0.254013	2.023243
C	1.056181	0.464616	-1.206364
C	-0.083224	0.480870	-1.826707
H	-0.492708	0.883697	-2.752066
C	2.782436	-0.992138	0.268628
H	3.136514	-1.333026	-0.724896
H	3.078554	-1.756305	1.010268
C	2.115816	1.509669	-0.967293
H	2.217161	2.084514	-1.904473
H	1.653594	2.187137	-0.222816
C	3.488576	1.066805	-0.471413
H	4.057293	1.947559	-0.136094
H	4.062298	0.576698	-1.285149
O	3.386531	0.198917	0.621480
Cl	-0.870312	2.189705	0.888111
C	-2.730468	0.064199	-0.337719
O	-3.842490	0.189573	-0.516310

HY-IN5

Rh	-1.584237	-0.246927	-0.367491
C	-0.148674	0.865063	-1.521605
C	-1.435260	1.459423	-1.723724
C	0.467070	0.609621	-0.268860
C	0.458875	1.525438	0.953884
C	-0.918384	2.091411	1.304471
H	0.816930	0.917985	1.801543
H	-1.001199	2.377424	2.365692
H	1.199350	2.331265	0.812834
H	-1.159301	2.992905	0.713692
H	-1.743265	2.370660	-1.205394
H	0.214232	0.234444	-2.346513
C	-2.042914	1.092848	1.007397
O	-3.111268	1.108280	1.527742
H	-1.853007	1.370015	-2.732185
C	-3.493403	-0.773748	-0.532728
O	-4.573877	-1.083013	-0.621643
Cl	-1.101773	-2.082378	1.026070
O	2.827919	0.380015	-0.238400
C	3.974108	-0.404672	-0.107758
H	3.944267	-1.000511	0.827953
H	4.063416	-1.121811	-0.950552
C	1.637989	-0.356875	-0.266185
H	1.601715	-1.016323	-1.159078
H	1.557381	-1.014315	0.623552
C	5.187282	0.533389	-0.094766
H	5.081285	1.241828	0.745237
H	5.183300	1.130619	-1.023281
C	6.452477	-0.199091	0.024686
C	7.484453	-0.823666	0.123573
H	8.405457	-1.371832	0.212114

HY-IN6

Rh	0.662614	-0.123306	0.088748
C	-0.220888	0.524893	1.966627
C	1.207699	0.714160	1.957592
C	-1.121979	1.045666	1.018373
C	-1.079673	2.424587	0.364431
C	0.304052	2.880594	-0.102223
H	-1.755556	2.378443	-0.503604
H	0.247071	3.692221	-0.845864
H	-1.522139	3.152906	1.070278
H	0.913509	3.258886	0.736656
H	1.659843	1.699555	1.828408
H	-0.564577	-0.364863	2.505902
C	1.061331	1.695566	-0.724300
O	1.819096	1.857376	-1.646989
H	1.765811	0.052125	2.628315
C	2.431962	-0.788946	-0.386759
O	3.463564	-1.188392	-0.607881
Cl	0.304255	-2.411878	1.046323
O	-3.090569	0.469764	-0.264288
C	-3.385655	-0.739535	-0.889753
H	-4.162582	-1.304150	-0.334492
H	-3.806618	-0.468280	-1.870770

C	-2.521316	0.427338	1.015448
H	-3.168277	1.016612	1.696189
H	-2.473621	-0.604161	1.409815
C	-2.175573	-1.681665	-1.084278
H	-2.462371	-2.486587	-1.784923
H	-1.869535	-2.178857	-0.145479
C	-0.980098	-1.018292	-1.614755
C	0.000894	-0.516367	-2.153658
H	0.737519	-0.111053	-2.832259

HY-TS3

Rh	0.534714	-0.254036	0.096950
C	-0.165782	0.378468	2.076400
C	1.237558	0.513022	2.134459
C	-1.035883	0.927204	1.072732
C	-0.979378	2.350923	0.516592
C	0.410400	2.823973	0.098013
H	-1.654560	2.370108	-0.353745
H	0.358379	3.669949	-0.609849
H	-1.409466	3.044293	1.262931
H	1.005564	3.182659	0.954585
H	1.771641	1.430918	1.884036
H	-0.565852	-0.493585	2.607188
C	1.248344	1.724250	-0.561768
O	2.399733	1.883390	-0.864150
H	1.772718	-0.170239	2.801135
C	2.150342	-1.267555	-0.438373
O	3.042032	-1.891884	-0.735363
Cl	-0.262856	-2.485443	0.749461
O	-3.066025	0.316397	-0.185615
C	-2.895692	-0.877011	-0.903460
H	-2.566859	-1.689690	-0.235191
H	-3.870488	-1.150358	-1.343513
C	-2.472818	0.385647	1.082541
H	-3.101489	1.076621	1.675905
H	-2.491724	-0.603785	1.574032
C	-1.871254	-0.746308	-2.053921
H	-2.299628	-0.179006	-2.898037
H	-1.622246	-1.763016	-2.408480
C	-0.625316	-0.078762	-1.604028
C	0.248317	0.837024	-1.857658
H	0.738939	1.308757	-2.708829

HY-IN7

Rh	0.574386	0.486821	0.183292
C	0.751190	-0.486522	2.175684
C	1.110827	0.823300	2.498340
C	-0.457291	-0.848104	1.469748
C	-1.712304	0.010090	1.670540
C	-1.692643	1.347617	0.853732
H	-2.605392	-0.555894	1.359704
H	-2.151112	2.159910	1.441229
H	-1.833094	0.249209	2.741547
H	-0.670353	1.821322	0.679389
H	0.363357	1.586417	2.740155
H	1.553467	-1.233816	2.168356
C	-2.448968	1.261657	-0.484720
O	-3.505773	1.834671	-0.606042
H	2.129594	1.021411	2.842267
C	1.482635	1.896684	-0.910915
O	2.010051	2.607527	-1.610055
Cl	2.428738	-0.801656	-0.456975
O	-1.193694	-2.601259	-0.126121
C	-0.281260	-2.673820	-1.196858
H	0.739248	-2.824448	-0.808438
H	-0.555000	-3.557737	-1.797823
C	-0.661371	-2.329782	1.133117
H	-1.371593	-2.754439	1.867579
H	0.305128	-2.854563	1.265788
C	-0.286126	-1.425781	-2.133535
H	-1.036756	-1.562114	-2.931680
H	0.711491	-1.353779	-2.596737
C	-0.632349	-0.199521	-1.335350
C	-1.867832	0.342316	-1.473815
H	-2.554584	0.017018	-2.266389

HY-IN8

Rh	-0.671448	-0.505866	0.143647
C	-0.432251	0.139792	2.280565
C	-0.736960	-1.197086	2.514838
C	0.636221	0.640069	1.422462
C	2.043536	0.046042	1.588146
C	3.041003	0.202791	0.414587
H	2.499077	0.551229	2.462072
H	1.979428	-1.020280	1.866199
H	0.020283	-1.987058	2.507671
H	-1.232182	0.850222	2.515198
C	2.622226	-0.513250	-0.874136

O	3.110224	-1.566632	-1.201664
H	-1.683611	-1.442523	3.004890
C	0.464145	-2.072400	0.045119
O	0.911761	-3.107927	0.022696
C	-2.032905	-1.433692	-0.992375
O	-2.809096	-1.851269	-1.696347
Cl	-2.527080	1.065751	0.208313
O	0.992391	2.683155	-0.001045
C	-0.017358	2.921705	-0.953773
H	-0.958637	3.176032	-0.439872
H	0.309341	3.804658	-1.526994
C	0.606762	2.177308	1.242340
H	1.312351	2.604837	1.981946
H	-0.406236	2.538742	1.496664
C	-0.280876	1.741913	-1.960967
H	0.212496	1.967988	-2.922502
H	-1.363943	1.666296	-2.135160
C	0.327612	0.479453	-1.395279
C	1.620561	0.257635	-1.686564
H	2.101761	0.884102	-2.456737
H	3.163392	1.275915	0.190452
H	4.009257	-0.222571	0.724842

HY-TS4

Rh	-0.960047	-0.401593	0.221423
C	-0.180627	0.687767	1.951952
C	-0.768596	-0.413883	2.586586
C	0.996159	0.748002	1.079191
C	2.095142	-0.264160	1.441398
C	3.140042	-0.635168	0.383490
H	2.623856	0.180045	2.306194
H	1.645261	-1.189788	1.829942
H	-0.224136	-1.330986	2.827415
H	-0.765913	1.611332	1.996822
C	2.545615	-1.193651	-0.903133
O	2.915322	-2.231992	-1.393730
H	-1.693089	-0.242827	3.144560
C	-0.114248	-2.119071	0.347611
O	0.287338	-3.174813	0.411971
C	-2.256709	-1.135938	-0.986827
O	-3.049206	-1.509807	-1.705971
Cl	-2.501315	1.468922	0.069646
O	1.729138	2.726109	-0.356552
C	0.547965	2.938235	-1.085786
H	-0.267546	3.251277	-0.406588
H	0.741623	3.757585	-1.795600
C	1.504179	2.219654	0.911392
H	2.468148	2.277325	1.447088
H	0.788278	2.875533	1.444970
C	0.117860	1.667148	-1.855494
H	0.622881	1.647796	-2.836736
H	-0.969424	1.700118	-2.013072
C	0.576868	0.447464	-1.082847
C	1.617590	-0.249378	-1.589999
H	1.934651	-0.028486	-2.621105
H	3.714347	0.264753	0.093125
H	3.843698	-1.377605	0.791587

HY-IN9

C	3.119684	-0.214622	0.572830
C	1.834587	-0.885867	1.091381
C	0.633525	0.067021	1.130299
H	1.563217	-1.720691	0.421084
H	2.013484	-1.321356	2.087435
H	0.827862	0.925711	1.801798
H	-0.276825	-0.448398	1.467071
C	3.834170	0.650447	1.608126
C	3.460490	0.874564	2.872789
H	2.548771	0.458632	3.311724
H	4.082073	1.491339	3.529283
H	4.776827	1.088330	1.259702
C	2.833276	0.648186	-0.659891
C	1.579974	1.005899	-1.030314
H	1.395795	1.565894	-1.952972
C	4.118373	-1.329605	0.118219
H	3.583704	-2.019670	-0.568470
H	4.446578	-1.899875	1.001897
C	4.040085	1.041255	-1.477080
H	3.730681	1.484526	-2.437242
H	4.610307	1.810560	-0.924605
C	4.962215	-0.173763	-1.705991
H	5.917410	0.144821	-2.150059
H	4.473373	-0.882057	-2.407210
O	5.254017	-0.811405	-0.497893
C	0.397919	0.657559	-0.237378
O	-0.720969	0.900348	-0.689190
Rh	-2.615316	0.026273	-0.183392
C	-4.215895	-0.862738	0.184670

C	-3.411048	1.736698	-0.054471
Cl	-1.557817	-2.081656	-0.344519
O	-5.166173	-1.442133	0.409803
O	-3.873954	2.773827	0.020103

(3+2)-E-IN

C	1.970780	-0.742067	1.539837
C	2.003858	0.701946	-0.952224
C	3.344331	0.013307	-0.833883
C	3.203325	0.130747	1.583528
C	2.098892	-2.172465	1.011771
C	1.049996	-2.227247	-0.115732
C	1.040873	0.324296	-1.884347
Rh	0.235581	-0.312793	0.107595
H	3.126532	-2.353172	0.662155
H	1.907453	-2.890678	1.827725
H	0.320012	-3.039542	0.031763
H	1.507465	-2.363497	-1.108419
H	0.360308	1.074289	-2.298811
H	1.216687	-0.559368	-2.508126
H	3.259995	-1.032174	-1.183545
H	4.023327	0.530419	-1.536828
H	3.868179	-0.233074	2.388139
H	2.916253	1.171022	1.838841
C	0.795483	-0.353714	2.210779
C	-0.431121	-1.071525	1.998130
H	-0.412685	-2.166047	1.967129
H	-1.331091	-0.660714	2.467502
P	-0.809968	1.917540	0.505505
C	-1.874517	2.012466	1.982336
C	0.274202	3.370087	0.712684
H	0.995146	3.201555	1.530663
H	-2.322435	3.015685	2.084186
C	-3.062081	1.515237	-1.217914
C	-2.596621	0.280728	-2.015323
H	-1.963058	0.603237	-2.862483
H	-3.475111	-0.218448	-2.463271
H	-3.634224	1.203168	-0.324847
H	-3.780322	2.067455	-1.846790
P	-1.669974	-1.000160	-1.091062
C	-1.359149	-2.238431	-2.382708
H	-0.699366	-1.823428	-3.161805
C	-2.947187	-1.787032	-0.064068
H	-2.517659	-2.660388	0.454180
H	1.987527	1.725345	-0.560016
H	-2.305056	-2.552480	-2.855448
H	-0.866631	-3.124414	-1.951702
H	-3.310698	-1.087598	0.706614
H	-3.802783	-2.122739	-0.674349
H	-2.688329	1.270936	1.921646
H	-1.294657	1.798668	2.895862
H	0.844735	3.562844	-0.211302
H	-0.312370	4.275158	0.946097
H	0.782023	0.624360	2.708087
C	-1.938439	2.493884	-0.819974
H	-1.324531	2.734647	-1.708219
H	-2.383179	3.449929	-0.488478
O	3.970451	0.085343	0.415248

(3+2)-HE-IN

C	-1.857037	1.656589	0.716900
C	-1.404086	2.938337	0.014994
C	-0.157232	2.504491	-0.779666
Rh	-0.035828	0.509639	-0.167452
H	-2.209683	3.318495	-0.634081
H	-1.198588	3.729637	0.757243
H	0.725764	3.108940	-0.526768
H	-0.319831	2.583585	-1.867600
C	-1.041028	1.073288	1.698178
C	0.368393	1.352036	1.755511
H	0.714066	2.383932	1.624875
H	0.943919	0.789982	2.499095
H	-1.463917	0.241260	2.271476
C	-1.643476	0.063212	-1.772627
C	-0.367218	-0.153826	-2.276874
H	-0.004722	-1.178776	-2.412565
C	-3.321414	1.246687	0.631619
H	-3.774895	1.709980	-0.264135
H	-3.840953	1.679613	1.508656
C	-2.615643	-1.061861	-1.467393
H	-3.004630	-1.424818	-2.439390
H	-2.083327	-1.912366	-1.018274
C	-3.837903	-0.701828	-0.610344
H	-4.411035	-1.622035	-0.411078
H	-4.504045	-0.024399	-1.180291
O	-3.537572	-0.132323	0.635313
H	0.109563	0.612180	-2.894403
H	-2.094900	1.045896	-1.959000

P	2.285450	0.385844	-0.608774
C	2.837750	-0.514378	-2.093007
C	3.105632	1.993437	-0.809899
C	3.287046	-0.379531	0.721302
H	3.939366	-0.528743	-2.152338
H	2.474275	-1.554540	-2.088405
H	2.447427	-0.026098	-3.000633
H	2.677712	2.534998	-1.668790
H	2.962092	2.611684	0.091170
H	4.187010	1.855768	-0.978152
C	2.969811	-1.842756	1.088477
H	3.184598	0.261682	1.615514
H	4.344647	-0.309513	0.407830
C	1.611667	-2.074140	1.780910
H	3.058620	-2.487813	0.195322
H	3.759508	-2.188528	1.776761
H	1.519960	-1.401376	2.653182
H	1.578029	-3.103661	2.181823
P	0.125180	-1.835771	0.731186
C	-1.198828	-2.418408	1.843534
C	0.304752	-3.224191	-0.445177
H	-1.103871	-1.917081	2.821604
H	-1.134360	-3.506798	2.011363
H	-2.191126	-2.159117	1.438362
H	-0.612535	-3.374677	-1.036300
H	1.128570	-3.036720	-1.153180
H	0.519960	-4.162410	0.094821

(3+2)-Y-IN

C	-2.333702	-0.486611	-1.027559
C	-1.588265	0.238168	1.676294
C	-3.452006	0.499228	-0.677000
C	-2.482364	-1.978496	-0.695915
C	-1.159476	-2.347270	-0.001558
Rh	-0.297504	-0.444752	-0.012561
H	-3.347292	-2.113942	-0.026811
H	-2.694119	-2.560886	-1.610870
H	-0.585922	-3.104718	-0.555387
H	-1.319721	-2.710696	1.024973
H	-3.685799	0.452083	1.889921
H	-2.740913	1.942970	2.162935
C	-1.320301	-0.043365	-1.902716
C	-0.119150	-0.798668	-2.119255
H	-0.184070	-1.879374	-2.284957
H	0.661939	-0.304896	-2.709549
H	-1.355839	1.006587	-2.216771
C	-2.831714	1.054324	1.516285
C	-0.636944	-0.379158	2.184730
O	-3.061744	1.505088	0.223447
H	-4.316390	-0.057310	-0.266806
H	-3.785856	1.024941	-1.585556
H	-0.031788	-0.834275	2.956065
P	1.878398	-1.287683	0.331264
C	2.521765	-1.311627	2.034573
C	2.108949	-3.008483	-0.198864
C	3.200850	-0.419668	-0.591334
H	3.571911	-1.649641	2.053515
H	2.466254	-0.311169	2.494953
H	1.928463	-2.008371	2.650265
H	1.469424	-3.677847	0.398427
H	1.829123	-3.121737	-1.259053
H	3.160829	-3.315929	-0.073031
C	3.391641	1.083266	-0.300669
H	3.000293	-0.568866	-1.668342
H	4.143872	-0.953441	-0.373684
C	2.293690	2.004765	-0.867701
H	3.511760	1.252390	0.785361
H	4.351224	1.387413	-0.751495
H	2.154445	1.792318	-1.944605
H	2.624899	3.057137	-0.799945
P	0.652408	1.868123	-0.065594
C	-0.291436	3.183876	-0.899574
C	0.941396	2.572765	1.589185
H	-0.290875	3.019371	-1.990328
H	0.146642	4.177422	-0.703701
H	-1.337410	3.165144	-0.548977
H	-0.022949	2.736743	2.097240
H	1.524208	1.877500	2.216095
H	1.476527	3.535788	1.528942

(3+2)-HY-IN

C	-1.909220	1.567325	0.922389
C	-1.452381	2.929601	0.409852
C	-0.271962	2.565530	-0.504207
Rh	-0.066854	0.512691	-0.077011
H	-2.270743	3.439317	-0.123469
H	-1.164741	3.580150	1.252894
H	0.627352	3.149763	-0.263995

H	-0.521914	2.732416	-1.563416
C	-1.110174	0.859677	1.824623
C	0.307308	1.152000	1.908549
H	0.626792	2.201098	1.926508
H	0.893428	0.519718	2.586295
H	-1.532959	-0.037097	2.288368
C	-1.588207	-0.424202	-1.656492
C	-0.700173	0.223118	-2.224762
H	-0.171741	0.705197	-3.035088
C	-3.352020	1.185504	0.659522
H	-3.664704	1.648120	-0.294589
H	-3.968083	1.653073	1.454327
C	-2.709738	-1.334238	-1.338568
H	-3.059922	-1.754422	-2.300103
H	-2.333591	-2.180934	-0.743539
C	-3.923898	-0.738299	-0.598697
H	-4.636917	-1.561645	-0.427604
H	-4.426583	0.007307	-1.242110
O	-3.605805	-0.187911	0.643798
P	2.196143	0.541122	-0.753761
C	2.607586	-0.220085	-2.358947
C	2.952504	2.185326	-0.913490
C	3.355895	-0.273333	0.407097
H	3.700303	-0.300884	-2.490075
H	2.160464	-1.222113	-2.458087
H	2.213935	0.402731	-3.179474
H	2.414348	2.785359	-1.664315
H	2.907604	2.721474	0.048403
H	4.008024	2.092796	-1.220266
C	3.153217	-1.779039	0.662634
H	3.293210	0.279427	1.362724
H	4.375687	-0.107207	0.014809
C	1.883729	-2.140254	1.457020
H	3.182622	-2.335707	-0.291776
H	4.022744	-2.139203	1.237981
H	1.859776	-1.560670	2.397964
H	1.924143	-3.205428	1.749570
P	0.291710	-1.859632	0.591571
C	-0.884174	-2.584964	1.784270
C	0.380810	-3.111923	-0.733897
H	-0.727632	-2.126094	2.775252
H	-0.736839	-3.673756	1.884718
H	-1.926562	-2.380619	1.488293
H	-0.560179	-3.172303	-1.301480
H	1.174740	-2.850546	-1.451577
H	0.602621	-4.108978	-0.316281

(3+2)-E-TS

C	0.036621	-0.530282	1.226053
C	0.147526	0.543671	-0.354915
C	1.598539	0.135506	-0.612308
C	1.397138	0.010779	1.688333
C	0.072182	-2.007823	0.787202
C	-1.154282	-2.199651	-0.126724
C	-0.842761	0.359896	-1.451324
Rh	-1.987415	-0.301549	0.110313
H	1.026900	-2.232623	0.289049
H	0.048704	-2.638611	1.692906
H	-1.796797	-3.036425	0.196092
H	-0.858398	-2.392208	-1.170317
H	-1.194512	1.293358	-1.912694
H	-0.567285	-0.388392	-2.208096
H	1.648557	-0.794461	-1.208461
H	2.073085	0.939877	-1.202483
H	1.791726	-0.654628	2.475548
H	1.296008	1.028886	2.116582
C	-1.093638	-0.215750	2.151429
C	-2.145380	-1.060016	2.438736
H	-2.118053	-2.128613	2.219347
H	-2.933857	-0.716604	3.115512
P	-2.964301	1.939359	0.475529
C	-3.984771	2.075177	1.979713
C	-1.833958	3.362900	0.629132
H	-1.146806	3.225852	1.481339
H	-4.451424	3.071302	2.068155
C	-5.221608	1.537488	-1.228905
C	-4.752861	0.291094	-2.004741
H	-4.095656	0.598378	-2.839696
H	-5.626532	-0.205860	-2.464427
H	-5.798728	1.241252	-0.333464
H	-5.934689	2.082420	-1.869853
P	-3.853811	-0.989138	-1.056897
C	-3.534933	-2.241550	-2.330649
H	-2.792664	-1.862694	-3.052434
C	-5.137227	-1.748796	-0.017290
H	-4.714120	-2.620029	0.510051
H	0.118630	1.550612	0.082533
H	-4.462928	-2.493630	-2.871159

H	-3.130140	-3.157254	-1.872067
H	-5.488835	-1.034214	0.745165
H	-5.999787	-2.083290	-0.618736
H	-4.779796	1.310832	1.975884
H	-3.364062	1.902777	2.875502
H	-1.227562	3.470164	-0.286454
H	-2.392051	4.302251	0.784217
H	-1.088434	0.787563	2.598797
C	-4.093826	2.515402	-0.844189
H	-3.476910	2.734177	-1.735978
H	-4.529805	3.479079	-0.523612
O	2.268616	-0.014755	0.604473

(3+2)-HE-TS

C	-1.263549	1.067222	0.255117
C	-0.707268	2.404346	-0.255007
C	0.755611	2.106658	-0.648020
Rh	0.840692	0.109333	-0.044034
H	-1.311261	2.762497	-1.105522
H	-0.803814	3.167696	0.537308
H	1.469162	2.764012	-0.128261
H	0.918166	2.231050	-1.731195
C	-0.625577	0.603163	1.528288
C	0.493079	1.151278	2.123523
H	0.886621	2.132450	1.853426
H	0.852738	0.722535	3.064466
H	-1.116153	-0.255566	2.000842
C	-1.156768	-0.087060	-1.322567
C	0.185205	-0.400045	-1.900202
H	0.331048	-1.457906	-2.161414
C	-2.802189	1.049643	0.408991
H	-3.250714	1.495117	-0.503018
H	-3.048706	1.706265	1.260800
C	-2.065079	-1.299233	-1.091000
H	-2.218441	-1.786404	-2.071268
H	-1.544613	-2.030362	-0.453627
C	-3.436863	-0.983811	-0.489966
H	-3.956142	-1.913248	-0.210898
H	-4.064623	-0.459628	-1.239566
O	-3.334115	-0.202459	0.667235
H	0.508327	0.266993	-2.709561
H	-1.658837	0.716329	-1.879855
P	3.111727	0.044333	-0.490630
C	3.529646	-0.750951	-2.071609
C	3.938703	1.655726	-0.613456
C	4.167548	-0.824900	0.724142
H	4.621271	-0.782075	-2.228427
H	3.134278	-1.779009	-2.109450
H	3.068238	-0.186932	-2.898962
H	3.482296	2.258278	-1.414382
H	3.838306	2.210034	0.333904
H	5.010828	1.520870	-0.835198
C	3.843956	-2.307414	0.987687
H	4.107945	-0.256408	1.671099
H	5.210858	-0.735433	0.370157
C	2.522445	-2.555701	1.738846
H	3.864207	-2.879653	0.042079
H	4.661962	-2.723744	1.599425
H	2.488486	-1.919931	2.643355
H	2.490357	-3.602745	2.091327
P	0.980543	-2.237620	0.797774
C	-0.259017	-2.812252	2.009867
C	0.987419	-3.584026	-0.433831
H	-0.183733	-2.212744	2.932659
H	-0.092892	-3.870688	2.273816
H	-1.284774	-2.703835	1.620439
H	0.014866	-3.640972	-0.950250
H	1.758278	-3.405439	-1.202013
H	1.184862	-4.559938	0.041951

(3+2)-Y-TS

C	-2.365340	-0.381866	-0.657397
C	-1.939967	0.199262	1.223617
C	-3.695944	0.423867	-0.654242
C	-2.442537	-1.903238	-0.443661
C	-1.019739	-2.319531	-0.014372
Rh	-0.139913	-0.419457	-0.074736
H	-3.195249	-2.123501	0.330295
H	-2.788011	-2.390055	-1.373868
H	-0.569396	-3.052925	-0.700431
H	-1.012453	-2.751885	0.997951
H	-3.973702	0.358280	1.912530
H	-2.998694	1.853209	2.120219
C	-1.455384	0.047226	-1.756151
C	-0.516648	-0.746947	-2.400673
H	-0.573129	-1.836324	-2.402324
H	0.103074	-0.288849	-3.178222
H	-1.510996	1.109568	-2.022340

C	-3.202727	1.007305	1.447294
C	-0.843992	-0.166135	1.810805
O	-3.629437	1.497359	0.223164
H	-4.503639	-0.277220	-0.361330
H	-3.920397	0.816168	-1.656739
H	-0.472377	-0.176279	2.836522
P	1.976798	-1.287109	0.275969
C	2.497545	-1.316740	2.016633
C	2.206380	-3.005716	-0.258443
C	3.342543	-0.423886	-0.583959
H	3.519111	-1.719372	2.124592
H	2.466997	-0.303828	2.450482
H	1.803440	-1.951389	2.592545
H	1.516888	-3.664372	0.293340
H	1.985848	-3.101598	-1.334324
H	3.242378	-3.337080	-0.074876
C	3.550713	1.070562	-0.261451
H	3.171479	-0.550976	-1.669500
H	4.270355	-0.976755	-0.348326
C	2.478391	2.022406	-0.831351
H	3.651660	1.216144	0.829696
H	4.523539	1.368362	-0.687329
H	2.359495	1.835799	-1.915242
H	2.820689	3.068298	-0.728242
P	0.822228	1.868562	-0.067633
C	-0.136818	3.175231	-0.899842
C	1.058362	2.558763	1.600996
H	-0.142731	3.010995	-1.990513
H	0.286148	4.175516	-0.705078
H	-1.181850	3.154933	-0.542390
H	0.079963	2.647690	2.101435
H	1.684430	1.890661	2.215487
H	1.530444	3.555413	1.566453

(3+2)-HY-TS

C	-1.382351	1.011924	0.412225
C	-0.989063	2.352457	-0.223684
C	0.463446	2.194274	-0.693674
Rh	0.720078	0.202892	-0.131281
H	-1.671807	2.559313	-1.062379
H	-1.139075	3.160342	0.517109
H	1.153687	2.883178	-0.183982
H	0.560857	2.357457	-1.778170
C	-0.591426	0.593588	1.592261
C	0.595634	1.169930	2.031373
H	0.877942	2.191395	1.771613
H	1.089298	0.736678	2.907419
H	-0.975724	-0.292574	2.112843
C	-1.258185	-0.288267	-1.227741
C	-0.142940	-0.243962	-1.899637
H	0.165098	-0.528352	-2.907861
C	-2.907717	0.902474	0.634298
H	-3.407253	1.449150	-0.188495
H	-3.114967	1.448355	1.571462
C	-2.388147	-1.293068	-1.209218
H	-2.588596	-1.563843	-2.261374
H	-1.980036	-2.199300	-0.723199
C	-3.690279	-0.938231	-0.493744
H	-4.279927	-1.852938	-0.330003
H	-4.301295	-0.244381	-1.103625
O	-3.428593	-0.373222	0.757953
P	2.965861	0.301903	-0.703780
C	3.318380	-0.277908	-2.390441
C	3.717148	1.953968	-0.672554
C	4.119179	-0.659937	0.342582
H	4.398726	-0.244318	-2.612015
H	2.957793	-1.310065	-2.532135
H	2.789061	0.365637	-3.112948
H	3.205027	2.615295	-1.389128
H	3.622529	2.396544	0.332567
H	4.786023	1.899005	-0.939581
C	3.880602	-2.180109	0.439923
H	4.089534	-0.211645	1.353473
H	5.136253	-0.477158	-0.049785
C	2.645393	-2.594894	1.263935
H	3.837144	-2.626544	-0.570475
H	4.768462	-2.626236	0.918649
H	2.683590	-2.104895	2.254911
H	2.674716	-3.683876	1.451419
P	1.024361	-2.181198	0.519247
C	-0.131629	-2.879816	1.744745
C	0.903989	-3.348205	-0.875261
H	0.002289	-2.374759	2.716380
H	0.037295	-3.960536	1.890674
H	-1.176576	-2.722965	1.426938
H	-0.080550	-3.252730	-1.363056
H	1.668001	-3.113266	-1.635122
H	1.039665	-4.393770	-0.549889

HE-SM

C	0.082888	1.034756	-1.565170
C	-0.546392	2.402756	-1.281997
C	-0.094449	1.495609	-0.123383
C	1.082495	1.925249	0.695233
C	2.366161	1.632436	0.457257
H	-0.587811	0.244143	-1.913584
H	1.091831	1.009077	-1.987559
H	-1.623382	2.505089	-1.443089
H	0.056246	3.294730	-1.481895
H	0.835578	2.542399	1.571831
H	2.667015	1.010423	-0.392279
H	3.161147	2.008681	1.108432
C	-1.179135	0.832510	0.718257
H	-1.457696	1.512039	1.555118
H	-0.767928	-0.094075	1.176623
O	-2.295929	0.536744	-0.059627
C	-3.329342	-0.087294	0.638649
C	-4.495904	-0.342854	-0.319307
H	-2.978323	-1.047924	1.076301
H	-3.669851	0.546349	1.485745
H	-4.105127	-0.923146	-1.175402
H	-4.855821	0.622271	-0.713982
C	-5.619481	-1.095851	0.346294
H	-5.375520	-2.100961	0.719381
C	-6.861069	-0.629056	0.517025
H	-7.149947	0.366663	0.160346
H	-7.633006	-1.226510	1.012119

HE-Prod

C	3.124456	0.278666	-0.453376
C	2.784427	1.528861	-1.302279
C	1.380421	2.130312	-1.019696
H	3.540544	2.307328	-1.101304
H	2.879149	1.277776	-2.370306
H	0.923245	2.567135	-1.920277
H	1.477448	2.943671	-0.275293
C	2.705583	-1.025833	-1.115690
C	1.871350	-1.182776	-2.150162
H	1.372582	-0.345832	-2.649530
H	1.646215	-2.182101	-2.535838
H	3.159896	-1.920575	-0.672258
C	2.437391	0.410449	0.945698
C	0.907129	0.371625	0.806144
H	0.420362	0.799585	1.702858
H	2.732996	1.406038	1.334106
H	0.535957	-0.662340	0.709312
C	4.656512	0.220399	-0.211086
H	4.985391	1.199839	0.201892
H	5.187311	0.054558	-1.163417
C	2.967295	-0.641728	1.934396
H	2.587319	-0.433564	2.950628
H	2.596761	-1.642429	1.649545
C	4.500737	-0.651542	1.943799
H	4.889147	-1.483433	2.551959
H	4.875968	0.297214	2.386771
O	5.023660	-0.811076	0.653259
C	0.388768	1.147574	-0.406482
O	-0.736580	1.019299	-0.811450

HE-IN1

H	-0.603926	1.040113	-1.895527
C	-0.605470	1.441285	-0.872911
C	-1.788546	1.982776	-0.418657
C	0.732603	1.533144	-0.221254
H	-2.637787	2.066681	-1.103763
H	-1.838941	2.551481	0.515224
C	0.920158	2.286106	1.093729
C	1.393610	2.932988	-0.202811
C	1.626172	0.331562	-0.508849
H	1.690829	1.894707	1.763830
H	0.043131	2.706774	1.595691
H	0.809691	3.764632	-0.610007
H	2.470274	2.964388	-0.390745
H	1.169861	-0.578260	-0.059449
H	1.663469	0.163861	-1.608082
C	3.783497	-0.520164	-0.201403
H	3.880551	-0.745173	-1.284645
H	3.395268	-1.440843	0.286344
Rh	-1.987257	-0.235771	0.027387
C	-2.591993	-2.042391	0.371964
O	-2.963956	-3.100331	0.518780
Cl	-2.779248	-0.581369	-2.161660
C	-1.383547	0.035137	1.796706
O	-1.041792	0.204146	2.869159
O	2.902017	0.545097	0.001689
C	5.151614	-0.154238	0.378849

H	5.003889	0.123748	1.438692
H	5.538738	0.736608	-0.143971
C	6.130476	-1.296392	0.274991
H	5.867019	-2.212534	0.822725
C	7.265806	-1.270997	-0.431145
H	7.934163	-2.136846	-0.468885
H	7.569256	-0.379107	-0.991978

HE-IN2

Rh	-1.121249	-0.693453	-1.350345
Cl	-2.248814	1.340310	-1.027290
O	-3.709927	-2.189911	-1.525153
C	-2.732078	-1.614494	-1.460137
C	1.051533	0.436277	-1.224094
C	2.296639	-0.411703	-1.047112
C	1.119088	-0.924598	-0.276846
C	0.274852	-2.069182	-0.726994
C	0.050747	-2.307537	-2.106970
H	0.977463	1.370784	-0.664525
H	0.618016	0.456326	-2.239177
H	3.097234	0.038298	-0.453899
H	2.630530	-0.999554	-1.908094
H	-0.039607	-2.789576	0.037015
H	0.722402	-1.906236	-2.875887
H	-0.468847	-3.224538	-2.401389
C	1.080356	-0.677917	1.227325
H	1.573719	-1.543930	1.724217
H	0.023634	-0.656139	1.565935
O	1.730946	0.506153	1.542980
C	1.688869	0.838100	2.902350
C	2.437209	2.155278	3.116653
H	0.635045	0.937438	3.239072
H	2.153595	0.034724	3.512449
H	1.984966	2.910743	2.448290
H	3.488928	2.028292	2.808878
C	2.356917	2.618776	4.549330
H	1.350431	2.842491	4.930629
C	3.404984	2.764477	5.366962
H	4.426703	2.555917	5.028232
H	3.280211	3.104904	6.399613

HE-TS1

Rh	-0.012831	0.221483	0.075084
Cl	-0.976393	2.360258	0.350487
O	-2.885238	-0.882393	0.513298
C	-1.838093	-0.497954	0.322935
C	1.876407	1.157090	-0.235738
C	2.978170	0.195505	0.196686
C	1.934605	-0.471476	1.039029
C	1.068227	-1.499816	0.540102
C	0.756148	-1.522750	-0.855567
H	1.864185	2.095160	0.328190
H	1.768593	1.300880	-1.325139
H	3.792431	0.647557	0.776637
H	3.370505	-0.448307	-0.601884
H	0.562128	-2.158902	1.253723
H	1.500078	-1.226068	-1.603486
H	0.047039	-2.279492	-1.206272
C	1.975530	-0.232730	2.535892
H	2.705608	-0.967245	2.954487
H	0.987225	-0.451920	2.989253
O	2.380571	1.064473	2.804573
C	2.434111	1.373536	4.168465
C	2.905993	2.819418	4.332565
H	1.431703	1.244443	4.629840
H	3.128722	0.684952	4.695809
H	2.227210	3.462041	3.742927
H	3.916075	2.920909	3.901080
C	2.901482	3.247931	5.778217
H	1.922679	3.254726	6.278712
C	3.985399	3.605293	6.475223
H	4.980890	3.617425	6.015911
H	3.915298	3.907012	7.524939

HE-IN3

Rh	1.511994	-0.119580	-0.159556
Cl	2.263654	-1.890050	-1.483503
O	2.168404	-2.152754	2.238119
C	1.911588	-1.374216	1.462990
C	1.034938	0.999270	-1.802926
C	0.235803	2.108945	-1.099627
C	0.215900	1.619615	0.353998
C	1.389258	1.609277	1.121864
C	2.661426	1.499846	0.446001
H	0.408947	0.367041	-2.452132
H	1.908291	1.347492	-2.376232
H	-0.796756	2.192436	-1.470865
H	0.703301	3.107382	-1.159860

H	1.317729	1.382327	2.192770
H	2.878625	2.132653	-0.421443
H	3.539322	1.282863	1.065151
C	-1.124518	1.408174	1.019711
H	-1.627802	2.397727	1.119284
H	-0.991693	1.001061	2.045088
O	-1.892721	0.551960	0.236352
C	-3.200308	0.371870	0.699171
C	-3.945336	-0.558840	-0.259865
H	-3.191704	-0.061374	1.723328
H	-3.726956	1.347865	0.764748
H	-3.359965	-1.492421	-0.347145
H	-3.974297	-0.095666	-1.260370
C	-5.340101	-0.863930	0.225251
H	-5.415132	-1.394541	1.185269
C	-6.464711	-0.532281	-0.417853
H	-6.438232	-0.005938	-1.379264
H	-7.449710	-0.782305	-0.011471

HE-IN4

C	1.179645	1.450490	-0.378380
C	0.647378	2.521773	0.579589
C	-0.581155	1.856746	1.231341
Rh	-0.684005	0.136438	0.072068
H	1.424686	2.801747	1.310935
H	0.392840	3.438254	0.019051
H	-1.484383	2.486187	1.186460
H	-0.394500	1.605759	2.288998
C	0.445306	1.109905	-1.523171
C	-0.960771	1.411986	-1.594202
H	-1.322991	2.389258	-1.256011
H	-1.509900	0.978238	-2.435789
H	0.879199	0.374127	-2.209740
C	2.638916	1.044242	-0.251578
H	2.947550	1.132476	0.808873
H	3.233451	1.795621	-0.810615
C	1.794258	-1.850716	0.726379
H	2.091938	-2.657397	1.425448
H	1.225587	-2.323034	-0.092129
C	3.093723	-1.238562	0.188458
H	3.665710	-2.034543	-0.314590
H	3.714715	-0.871397	1.033232
O	2.942258	-0.213115	-0.756114
Cl	-0.832054	-1.866025	-1.406950
C	-2.570470	-0.180440	0.327106
O	-3.682234	-0.357536	0.440031
C	0.877333	-0.914121	1.491453
H	1.344619	-0.076622	2.026839
C	-0.413968	-1.251655	1.854153
H	-0.836794	-2.206760	1.524474
H	-0.906281	-0.737859	2.684783

HE-TS2

C	-1.235737	1.010186	0.201237
C	-0.703608	2.320495	-0.406189
C	0.768008	2.044648	-0.787368
Rh	0.898852	0.112855	-0.044598
H	-1.319530	2.597721	-1.279235
H	-0.822468	3.135177	0.331458
H	1.473594	2.751958	-0.322380
H	0.922307	2.089666	-1.876939
C	-0.608105	0.633824	1.501868
C	0.495740	1.240512	2.058910
H	0.855722	2.221785	1.743476
H	0.912499	0.825652	2.981403
H	-1.017696	-0.263447	1.979940
C	-1.082099	-0.306699	-1.290633
C	0.264758	-0.609995	-1.836432
H	0.507176	-1.678124	-1.899479
C	-2.775582	0.965394	0.302425
H	-3.202159	1.292106	-0.670288
H	-3.061352	1.714037	1.062311
C	-1.915016	-1.518289	-0.871785
H	-2.024225	-2.163748	-1.762517
H	-1.339993	-2.097523	-0.128502
C	-3.313661	-1.189975	-0.350011
H	-3.791932	-2.098747	0.046025
H	-3.948381	-0.804843	-1.177329
O	-3.299202	-0.252322	0.692552
Cl	0.933259	-2.160933	0.944514
C	2.752157	-0.066020	-0.290211
O	3.868187	-0.187787	-0.450428
H	0.572951	-0.025980	-2.711569
H	-1.621808	0.426754	-1.906271

HE-IN5

C	1.679090	-0.296127	0.596744
C	1.091831	-1.389198	1.506967

C	-0.393537	-1.665209	1.163244
Rh	-1.223815	-0.032809	0.184125
H	1.703741	-2.302918	1.399935
H	1.198486	-1.073753	2.560515
H	-0.992237	-1.818632	2.082207
H	-0.477951	-2.593796	0.575388
C	0.873393	0.982208	0.743934
C	-0.007677	1.275063	1.743370
H	-0.150917	0.624634	2.612137
H	-0.516076	2.243453	1.752316
H	1.052619	1.763027	-0.005623
C	1.524705	-0.734668	-0.892587
C	0.035513	-0.691098	-1.307770
H	-0.139051	0.073905	-2.086381
C	3.172159	-0.050829	0.923672
H	3.684872	-1.038141	0.936102
H	3.272067	0.395965	1.926721
C	2.396141	0.130821	-1.828759
H	2.422906	-0.322367	-2.835370
H	1.945977	1.132832	-1.945587
C	3.817298	0.291450	-1.281851
H	4.401066	0.993638	-1.897283
H	4.342713	-0.688589	-1.292622
O	3.796770	0.807115	0.021274
Cl	-2.496258	1.961398	-0.298725
C	-2.595325	-1.087495	-0.602607
O	-3.401039	-1.723465	-1.075541
H	-0.290388	-1.664267	-1.705915
H	1.900164	-1.774172	-0.948387

HE-IN6

Rh	1.057685	0.002936	-0.107502
C	-1.811325	0.636079	-0.364625
C	-1.161149	1.344275	-1.568863
C	0.257090	0.805163	-1.869420
H	-1.821803	1.222978	-2.447013
H	-1.126950	2.430509	-1.367913
H	0.891510	1.603829	-2.290126
H	0.198851	0.013721	-2.634037
C	-0.908463	0.780665	0.851489
C	0.006698	1.780407	1.060506
H	0.099582	2.631890	0.380367
H	0.528322	1.835821	2.020931
H	-1.070472	0.080973	1.679507
C	-1.867774	-0.895650	-0.608330
C	-0.445055	-1.482956	-0.393993
H	-0.191074	-2.157939	-1.227727
H	-2.200809	-1.052118	-1.651729
H	-0.399496	-2.080890	0.530511
C	-3.219889	1.230269	-0.116778
H	-3.747964	1.264544	-1.095512
H	-3.134858	2.264728	0.256465
C	-2.891423	-1.583179	0.323445
H	-3.067988	-2.619049	-0.015969
H	-2.479028	-1.651935	1.345807
C	-4.207089	-0.805536	0.395701
H	-4.894031	-1.255737	1.129314
H	-4.715327	-0.808967	-0.593581
O	-3.973505	0.514136	0.808300
Cl	1.835152	-0.942402	2.043563
C	2.586578	1.337858	0.139682
O	3.459729	2.028950	0.316075
C	2.086580	-1.281739	-1.070622
O	2.669052	-2.069743	-1.632110

HE-TS3

Rh	-1.163583	-0.043254	-0.016835
C	1.686699	-0.728831	-0.247239
C	1.030130	-1.523275	-1.398440
C	-0.444052	-1.140112	-1.662543
H	1.639635	-1.372903	-2.307295
H	1.111370	-2.598649	-1.160247
H	-1.054757	-2.045028	-1.812196
H	-0.527844	-0.564317	-2.597961
C	0.887601	-0.908785	1.041339
C	-0.004421	-1.902132	1.308540
H	-0.194252	-2.727844	0.616772
H	-0.489246	-1.944643	2.288377
H	1.079646	-0.187473	1.846587
C	1.767955	0.797326	-0.599152
C	0.454674	1.595307	-0.368217
H	0.554275	2.589946	-0.827338
H	2.045840	0.856737	-1.667879
H	0.295980	1.800930	0.704300
C	3.126588	-1.296637	-0.069838
H	3.588883	-1.359104	-1.079818
H	3.066043	-2.317895	0.339560
C	2.858820	1.523735	0.226185

H	3.031990	2.530908	-0.192261
H	2.501435	1.665411	1.262060
C	4.167746	0.735439	0.282709
H	4.888273	1.222091	0.958060
H	4.630226	0.678070	-0.726637
O	3.935461	-0.551946	0.778748
Cl	-1.869406	1.060068	2.055238
C	-2.884891	-0.837426	-0.164023
O	-3.922895	-1.277954	-0.256608
C	-1.092033	1.379943	-1.211538
O	-1.440192	2.029220	-2.110706

HE-IN7

Rh	-1.399094	-0.525027	0.167588
C	1.686240	-0.643311	-0.255035
C	1.019602	-1.507254	-1.359005
C	-0.514040	-1.356739	-1.529359
H	1.540346	-1.296756	-2.310522
H	1.257083	-2.561876	-1.127674
H	-0.970467	-2.352499	-1.683213
H	-0.740821	-0.776980	-2.438596
C	0.910660	-0.757298	1.045735
C	0.146724	-1.818984	1.422478
H	0.059238	-2.721511	0.806932
H	-0.313185	-1.836503	2.414712
H	1.051053	0.037816	1.788672
C	1.801645	0.872480	-0.630280
C	0.525248	1.706677	-0.360414
H	0.602109	2.676755	-0.878550
H	2.027626	0.914762	-1.711913
H	0.446464	1.916637	0.720127
C	3.119002	-1.241951	-0.081744
H	3.554683	-1.357714	-1.098792
H	3.035383	-2.244887	0.366971
C	2.949460	1.582244	0.130522
H	3.130751	2.572603	-0.322618
H	2.639070	1.762507	1.175959
C	4.235047	0.761436	0.166801
H	4.994693	1.246764	0.798875
H	4.659982	0.650786	-0.854445
O	3.974250	-0.497865	0.718723
Cl	-2.400273	0.070684	2.271473
C	-3.101270	-0.345591	-0.705085
O	-4.114676	-0.279416	-1.195984
C	-0.822997	1.117864	-0.772756
O	-1.536740	1.653266	-1.565481

HE-TS4

Rh	1.292737	-0.212380	0.174027
C	-1.803573	0.036935	0.637977
C	-1.139550	0.803192	1.797067
C	0.252629	1.342017	1.414854
H	-1.803484	1.632621	2.095474
H	-1.063994	0.142865	2.677609
H	1.028818	1.096078	2.163674
H	0.266338	2.440213	1.392827
C	-0.890347	-1.094163	0.174578
C	-0.095933	-1.822644	1.022624
H	-0.063432	-1.631227	2.100221
H	0.396692	-2.731908	0.669595
H	-1.025484	-1.473331	-0.845656
C	-2.081068	1.009171	-0.538167
C	-0.792291	1.454688	-1.252282
H	-0.929446	2.433772	-1.740308
H	-2.564880	1.899795	-0.093211
H	-0.547613	0.737648	-2.057881
C	-3.157025	-0.537559	1.135241
H	-3.724070	0.288772	1.619907
H	-2.974890	-1.316752	1.893504
C	-3.072144	0.404198	-1.554313
H	-3.377419	1.174844	-2.284207
H	-2.577190	-0.400101	-2.127816
C	-4.299772	-0.181452	-0.853195
H	-4.949951	-0.709997	-1.567297
H	-4.896709	0.632360	-0.386410
O	-3.917119	-1.112319	0.121872
Cl	2.280996	-1.959567	-1.034900
C	3.088528	0.570748	0.183249
O	4.142388	0.973841	0.204112
C	0.516681	1.568569	-0.452298
O	1.341027	2.396292	-0.759576

HE-IN8

Rh	1.235604	-0.386310	0.065888
C	-1.777422	0.089775	0.662797
C	-1.144695	0.938531	1.777425
C	0.204109	1.514973	1.319337
H	-1.823621	1.772829	2.026932

H	-1.012836	0.358670	2.706415
H	1.054934	0.747321	1.500634
H	0.585536	2.285043	2.011870
C	-0.854548	-1.065090	0.258178
C	-0.059226	-1.779486	1.151196
H	-0.012232	-1.536525	2.218743
H	0.319577	-2.765366	0.867884
H	-1.075833	-1.550113	-0.699122
C	-2.082021	1.037866	-0.533916
C	-0.811164	1.681076	-1.113269
H	-1.047543	2.534529	-1.770716
H	-2.709459	1.849876	-0.115391
H	-0.270176	0.944981	-1.742095
C	-3.133893	-0.498014	1.132931
H	-3.762878	0.330008	1.531670
H	-2.969015	-1.226881	1.943306
C	-2.926211	0.326380	-1.604365
H	-3.247545	1.049053	-2.375223
H	-2.323807	-0.444043	-2.117097
C	-4.155970	-0.324301	-0.957805
H	-4.705105	-0.944427	-1.682871
H	-4.846749	0.468722	-0.595883
O	-3.799065	-1.163786	0.106684
Cl	1.750599	-2.064462	-1.454587
C	3.106122	0.185680	-0.111943
O	4.207278	0.426698	-0.201220
C	0.195731	2.180149	-0.074778
O	0.967023	3.072122	-0.316809

HE-IN9

Rh	-2.455492	0.005245	-0.033285
C	3.137776	0.276023	-0.455858
C	2.789861	1.509000	-1.324081
C	1.379032	2.103415	-1.064496
H	3.531576	2.302432	-1.131057
H	2.888767	1.242878	-2.387566
H	0.908536	2.499797	-1.976694
H	1.466336	2.951961	-0.356417
C	2.732232	-1.038594	-1.106193
C	1.862661	-1.209677	-2.107811
H	1.337161	-0.381418	-2.595436
H	1.619832	-2.211264	-2.473331
H	3.206921	-1.924330	-0.667263
C	2.437267	0.417194	0.936202
C	0.911747	0.351951	0.776575
H	0.387192	0.705057	1.686194
H	2.716729	1.418058	1.324354
H	0.557438	-0.680048	0.595196
C	4.667369	0.241255	-0.197663
H	4.981273	1.227989	0.210579
H	5.208739	0.072988	-1.143441
C	2.961361	-0.627932	1.934957
H	2.568525	-0.419970	2.946111
H	2.602091	-1.631435	1.647177
C	4.494898	-0.620197	1.961228
H	4.884189	-1.445643	2.577062
H	4.854591	0.334169	2.405135
O	5.034903	-0.778957	0.677912
Cl	-1.351400	-1.927806	-0.796535
C	-3.872845	-1.090348	0.495587
O	-4.709279	-1.791530	0.807232
C	0.402469	1.178204	-0.378770
O	-0.771905	1.178294	-0.721466
C	-3.310809	1.579403	0.571385
O	-3.814523	2.535525	0.929787

HE-TS5

C	0.252298	-1.732025	0.181603
C	0.099763	-1.791535	-1.328577
C	-0.548815	-0.467262	-1.790348
Rh	-1.537789	0.315710	-0.110278
H	1.079048	-1.949660	-1.808137
H	-0.536945	-2.655320	-1.593833
H	-1.171176	-0.593631	-2.690540
H	0.250013	0.255319	-2.020250
C	-0.859320	-1.689874	0.975998
C	-2.252746	-1.769027	0.431370
H	-2.372686	-2.540119	-0.342495
H	-3.011417	-1.835630	1.220888
H	-0.756895	-1.542642	2.056275
C	1.638300	-1.685238	0.768878
H	2.135059	-2.668074	0.594994
H	1.588278	-1.530190	1.866410
C	4.377811	0.565946	-0.183289
H	3.784342	1.482221	-0.009364
H	4.352465	0.357002	-1.266099
C	3.692756	-0.580071	0.564073
H	3.740946	-0.402348	1.660319

H	4.226977	-1.534025	0.366239
O	2.361123	-0.667685	0.144570
Cl	-2.138680	1.211429	2.062854
C	-3.123552	-0.468842	-0.650884
O	-4.134346	-0.661533	-1.167218
C	-1.412427	2.089835	-0.793050
O	-1.402633	3.145726	-1.200314
C	5.796458	0.771977	0.284348
H	5.922943	1.054857	1.339172
C	6.884188	0.628528	-0.480203
H	6.805878	0.350295	-1.537813
H	7.889354	0.791610	-0.079107

HE-TS6

O	0.650157	-2.505622	0.350138
C	-0.058115	-1.642937	0.170495
O	-1.773723	0.607296	2.757208
C	-1.731420	0.483425	1.603272
Rh	-1.326138	-0.235798	-0.086421
C	-0.204878	0.718610	-1.828339
C	-1.409923	0.399289	-2.429254
C	-0.127180	1.436286	-0.568067
C	-1.212601	2.471035	-0.199438
C	-2.403666	1.712120	0.450038
H	-0.794436	3.190961	0.523463
H	-2.882906	2.267186	1.266174
H	-1.544321	3.048355	-1.079393
H	-3.216137	1.428575	-0.240400
Cl	-3.151397	-1.819423	-0.106171
H	-2.306602	1.013792	-2.300282
H	0.701793	0.181921	-2.130430
H	-1.442322	-0.338189	-3.235175
C	1.250592	1.674594	0.023041
O	2.058219	0.558953	-0.178153
H	1.148462	1.899897	1.106021
H	1.710308	2.573333	-0.450000
C	3.365309	0.699792	0.304821
H	3.859251	1.576568	-0.164226
H	3.351141	0.881399	1.401023
C	4.154890	-0.572574	-0.009542
H	4.188935	-0.715241	-1.102890
H	3.602219	-1.428923	0.418104
C	5.550176	-0.521739	0.560314
H	5.625084	-0.453173	1.654941
C	6.674139	-0.547650	-0.163667
H	6.647269	-0.619182	-1.257400
H	7.659605	-0.507315	0.310669

HE-TS7

C	-2.078018	-0.641020	0.182699
C	-1.318163	-1.807578	0.886622
C	0.217407	-1.865911	0.700946
Rh	1.021489	-0.009675	0.167343
H	-1.522714	-1.701665	1.966539
H	-1.767399	-2.774405	0.609390
H	0.474406	-2.570944	-0.108047
H	0.669371	-2.282328	1.616066
C	-3.195312	-1.065655	-0.771547
C	-3.333582	-2.241978	-1.391112
H	-2.627821	-3.068703	-1.259025
H	-4.177540	-2.418054	-2.065381
H	-3.939885	-0.279365	-0.953056
C	-1.148099	0.268307	-0.659526
C	-0.262396	-0.272490	-1.598081
H	-0.293945	-1.343340	-1.817653
C	-2.737102	0.219169	1.305116
H	-1.973901	0.421572	2.085745
H	-3.548518	-0.368319	1.765705
C	-1.593169	1.712376	-0.844512
H	-0.726511	2.327710	-1.136832
H	-2.304891	1.697647	-1.691479
C	-2.301716	2.293419	0.377633
H	-2.804243	3.237486	0.118647
H	-1.562836	2.508539	1.177617
O	-3.285162	1.412510	0.850113
Cl	1.872279	2.174523	-0.633961
C	1.995906	0.194098	1.825123
O	2.519226	0.341941	2.814891
H	0.118599	0.384974	-2.386894
H	-0.109334	0.692734	1.026869
C	2.500853	-0.808993	-0.987281
O	3.324508	-1.186438	-1.657090

7. References

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