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Supporting Information

Metalla-Claisen Rearrangement in Gold-Catalyzed [4+2] Reaction: A New Elementary Reaction Suggested for Future Reaction Design

*J. Liu, Y. Yang, W. Shi, Z.-X. Yu**

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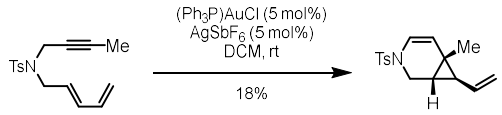
Contents

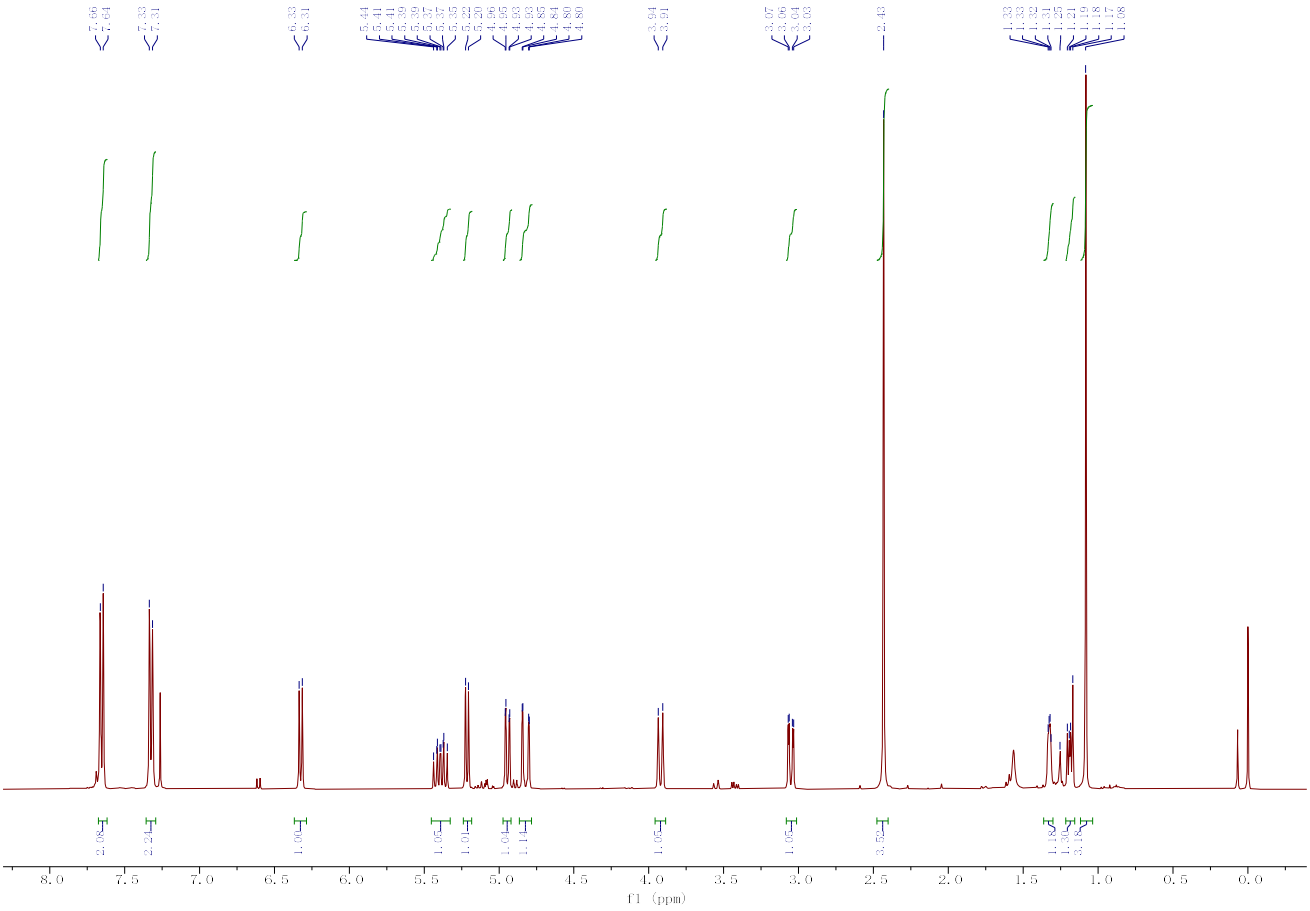
1. Reaction of 1d under Fürstner's conditions



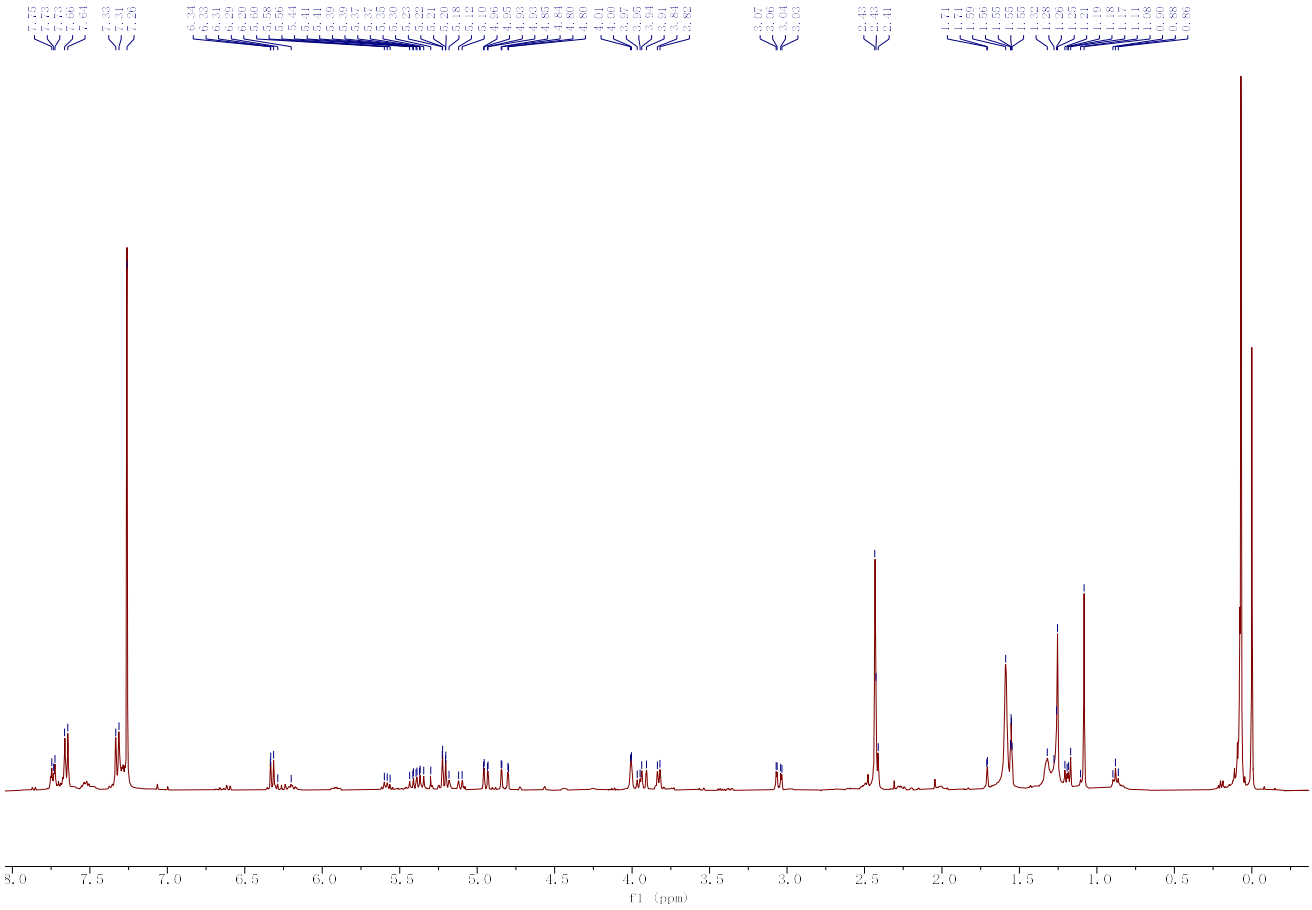
1d **3d**

In glove box $(Ph_3P)AuCl$ (9.9 mg, 0.01 mmol, 5%) and $AgSbF_6$ (6.9 mg, 0.02 mmol, 5%) were added into a flask, which was sealed tightly and moved out. 2 mL of super-dry dichloromethane was added to the mixture. After stirring for 20 min under room temperature, a solution of **1d**[1] (115.8 mg, 0.4 mmol) in super-dry dichloromethane was added. The reaction mixture was stirred under room temperature for 24 h, and then concentrated under vacuum and purified by flash column chromatography (PE/EA = 30 : 1) to yield **3d** (with some inseparable impurities) as a white solid. RUN1: 21.0 mg (18%); RUN2: 20.5 mg (18%).

The following peaks are selected as known compound **3d**:[2] ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.65 (d, *J* = 8.1 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 6.32 (d, *J* = 8.1 Hz, 1H), 5.39 (ddd, *J* = 17.0, 10.3, 8.9 Hz, 1H), 5.21 (d, *J* = 8.1 Hz, 1H), 4.94 (dd, *J* = 10.3, 1.9 Hz, 1H), 4.82 (dd, *J* = 17.0, 1.9 Hz, 1H), 3.92 (d, *J* = 11.8 Hz, 1H), 3.05 (dd, *J* = 11.8, 2.7 Hz, 1H), 2.43 (s, 3H), 1.36 – 1.30 (m, 1H), 1.22 – 1.16 (m, 1H), 1.08 (s, 3H).



^{1}H-NMR of the crude reaction mixture

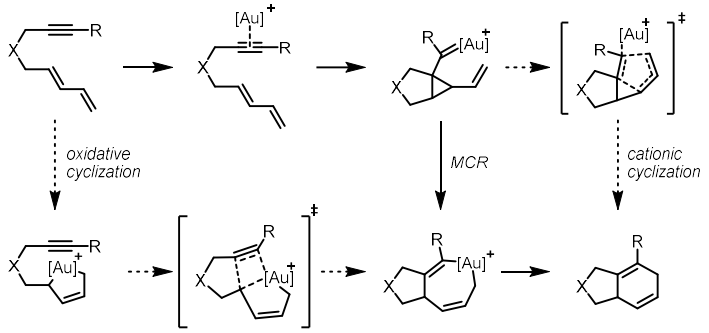


2. Computational methods

Geometry optimization at BMK-D3BJ/def2-SVP[3-5] level was carried out with *Gaussian* 09 E.01 program package[6] in vacuum, with the ULTRAFINE grid. This functional was appropriate for both Au and Rh according to our previous studies and benchmark.[7] Single point energy at ωB97M-V/def2-QZVP/SMD(DCM)[5,8,9] level was calculated with *ORCA* 5.0.3 program package[10] and the default RIJCOSX approximation[11] along with the def2/J auxiliary basis set[12] to save computation time. ωB97M-V has been shown to give a balanced description of various organic and organometallic reactions.[13] Unscaled frequency analysis was carried out to check the nature of each intermediate and transition state and Grimme's quasi-RRHO correction[14] was performed with *Shermo* 2.3.4[15] to acquire the thermal correction to Gibbs free energy at 298.15 K and 1 M. Conformational search was performed by metadynamics method, with *crest* 2.12[16] and *xtb* 6.5.0 and 6.4.1, using GFN-2 and GBSA solvent model of DCM.[17] An energy window of 3 kcal/mol was utilized. Natural bond analysis was performed with the *NBO* 3.1 built in *Gaussian*.[18] Wiberg bond indexes and orbital isosurfaces and RDG analysis were generated with *Multiwfn* 3.8(dev),[19] and visualized with *VMD* 1.9.3.[20] Intrinsic bond analysis was performed with *IBOview*.[21] Other structure picture was generated with *CYLview* 1.0b.[22] All analysis was based on the BMK/def2-SVP wavefunction.

3. Calculations of other pathways in Au-catalyzed [4 + 2] reaction

In Fürstner's original paper,[23] two other pathways were proposed, schematically shown in **Scheme S1**. The potential energy surfaces were calculated (**Figure S1**), ruling out these pathways.



Scheme S1. Reaction pathways proposed by Fürstner.

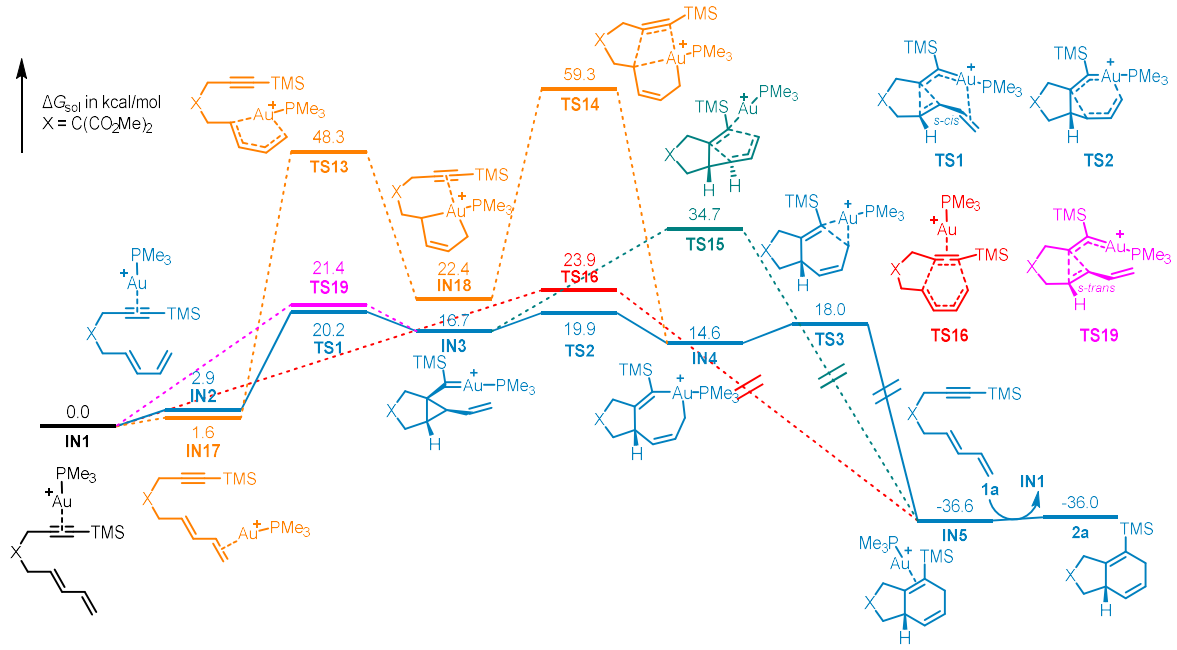


Figure S1. Potential energy surfaces of pathways for the [4 + 2] reaction computed at *ω*B97M-V/def2-QZVP/SMD(DCM)//BMK-D3BJ/def2-SVP level.

The existence of **IN2** is confirmed by an IRC calculation (**Figure S2A**) of **TS1**.

The oxidative cyclization process proceeds through **IN17** and **TS13**, but with a very high $\Delta G^{\neq}$ of 48.3 kcal/mol. The generated Au-cyclopentene **IN18** is 22.4 kcal/mol higher than **IN1**, and the followed insertion step via **TS14** is also not easy, requiring a $\Delta G^{\neq}$ of 36.9 kcal/mol (from **IN18**), giving **IN4** which is more probably formed through **TS1** in the MCR process.

Another pathway from **IN3** is the cationic cyclization via **TS15**, where the vinyl group directly interacts with the carbon atom in the Au-carbene structure in **IN3**. But the barrier is much higher than that in the MCR process, with a $\Delta\Delta G^{\neq}$ of 14.8 kcal/mol. The difference may be understood through the stabilization of Au(I) to the forming allyl cation in **TS2**, as mentioned in the main text.

Direct Diels-Alder cycloaddition of the uncoordinated C=C bond in **IN2** with the diene moiety was also considered, which requires an activation free energy of 21.0 kcal/mol (**IN2** to **TS16**) and is 2.7 kcal/mol higher than **TS1**. Thus, such a pathway can be excluded for further consideration.

The *exo*-cyclopropanation via **TS19** where the diene moiety appears to be in an *s-trans* pattern was also considered, and we found it is 1.2 kcal/mol higher in free energy than **TS1**. RDG analysis[24] (**Figure S2B)** revealed an Au-alkene interaction in **TS1** which may provide the stabilization effect. While such effect does not exist in **TS19** with an *s-trans* diene (**Figure S2C)**.

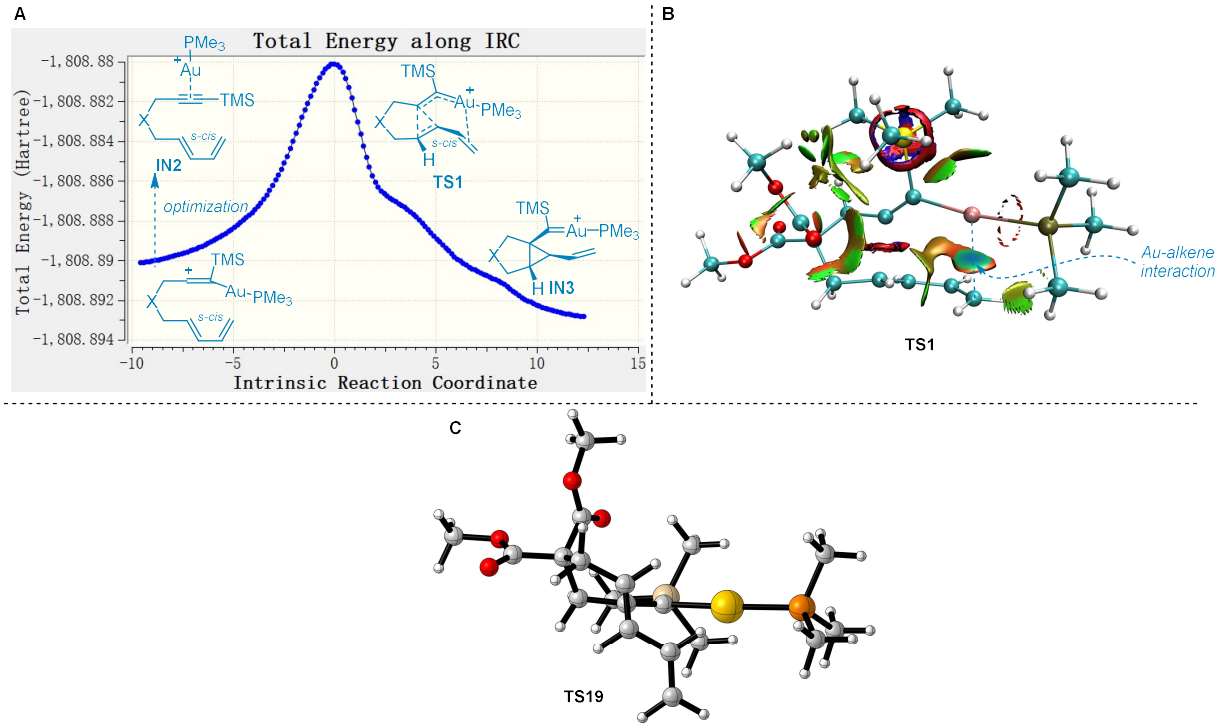


Figure S2. (A) IRC of TS1. The IRC stopped at a vinyl cation type structure but further optimization led to IN2. (B) RDG analysis of TS1, showing strong Au-alkene interaction. (C) Bottom-view of TS19, showing that no Au-alkene interaction is achievable.

4. Separated diagrams of the key IBOs for TS2

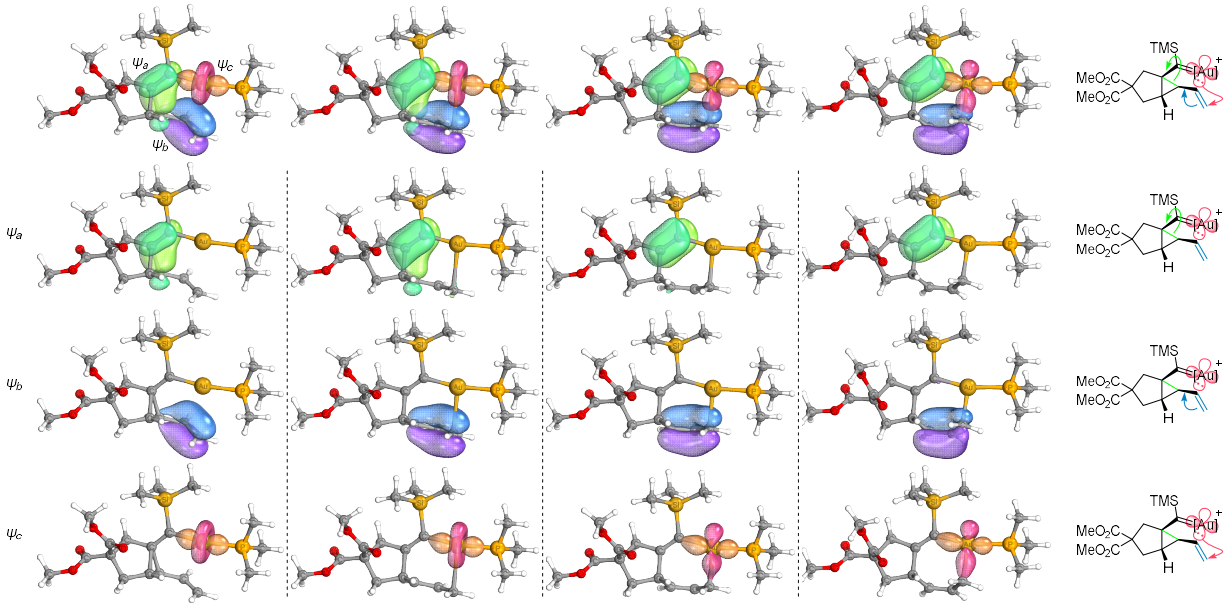
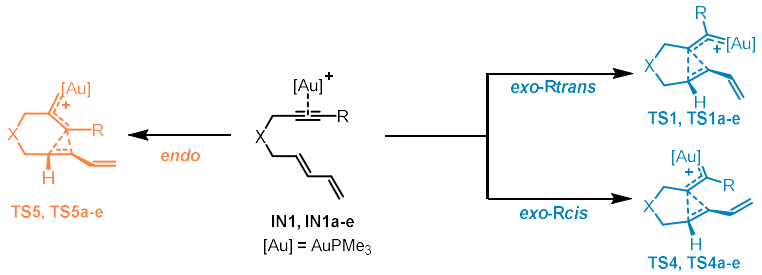


Figure S3. Key IBOs along the IRC of TS2

5. Further discussion of terminal group effects and ligand effects

Table S1. More selected transition states for *exo* and *endo* cyclization.[a]



Entry	X	R	*exo*-R*trans*	*exo*-R*cis*	*endo*
1	$C(CO_2Me)_2$	TMS	**TS1**: ***20.2***	**TS4**: 22.8	**TS5**: 27.7
2	$C(CO_2Me)_2$	Me	**TS1a**: 22.5	**TS4a**: ***16.6***	**TS5a**: 18.5
3	NMs	Me	**TS1b**: 25.9	**TS4b**: 20.2	**TS5b**: ***15.7***
4	NMs	TMS	**TS1c**: ***18.4***	**TS4c**: 19.6	**TS5c**: 19.1
5	$C(CO_2Me)_2$	^{t}Bu	**TS1d**: 26.0	**TS4d**: ***25.4***	**TS5d**: 28.7
6[b]	$C(CO_2Me)_2$	TMS	**TS1e**: ***18.5***	**TS4e**: 24.0	**TS5e**: 27.9

[a]Calculated at BMK-D3BJ/def2-TZVPP(SMD:DCM)//BMK-D3BJ/def2-SVP level in kcal/mol, relative to corresponding **IN1** derivatives. [b]The PMe_3 ligand was changed to PPh_3.

By keeping the tether X to $C(CO_2Me)_2$, we further investigated the influence of terminal R. Bulky R groups such as TMS and ^{t}Bu both disfavor **TS5** as shown in entries 1 and 5, contrast to that of R = Me. In the transition state forming a larger ring (with one more atom included in the cycle), the *endo* type cyclization suffers from more severe transannular strain than that of *exo* type (**Figure S4A**, RDG analysis[24]). Also, this steric effect between R and the vinyl group slightly destabilizes **TS4** (**Figure S4B**). However, though TMS and ^{t}Bu group are of the similar size, ^{t}Bu slightly favors **TS4** while TMS significantly favors **TS1**, which further shows the special electronic effect of TMS mentioned in the main text.

The influence of β-silicon effect on regioselectivity can be further rationalized through the resonance description. By describing the Au-alkyne complex **IN1** as resonance structures **A** and **B** (**Figure S4C**), we notice that **B** is stabilized by hyperconjugation in the β-position of silyl group and displays extra reactivity on C2. Bond lengths and WBIs both suggest similar conclusion from the resonance analysis.

As shown in entry 6 in **Table S1**, changing the ligand from PMe_3 to PPh_3 does not significantly affect the selectivity, probably due to the long P–Au bond in this system.

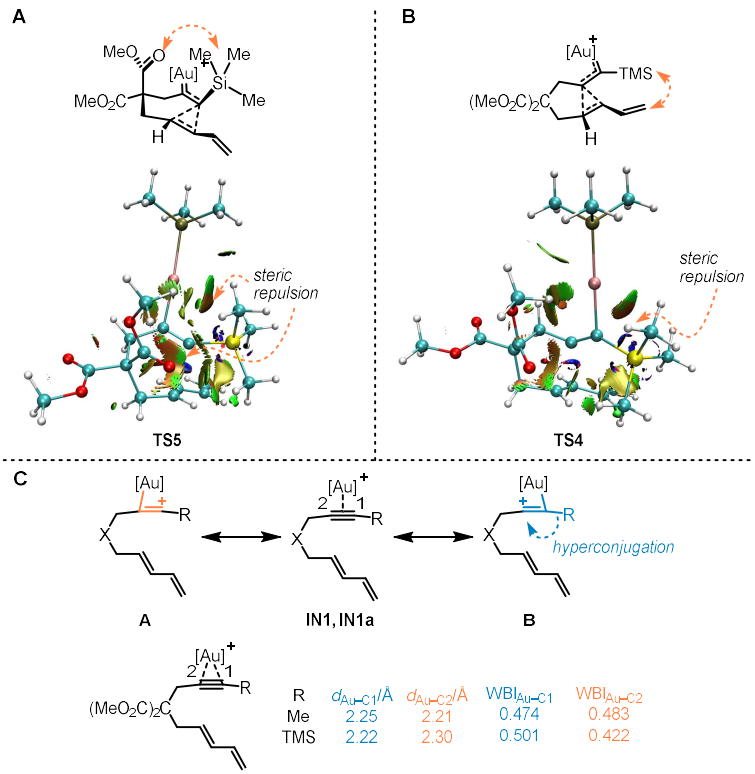


Figure S4. (A) (B) RDG analysis of TS5 and TS4, the brownish yellow and red parts indicate the steric repulsion. (C) Resonance structure and wavefunction analysis of IN1 and IN1a.

6. Further discussion on Rh-catalyzed [4 + 2] reaction

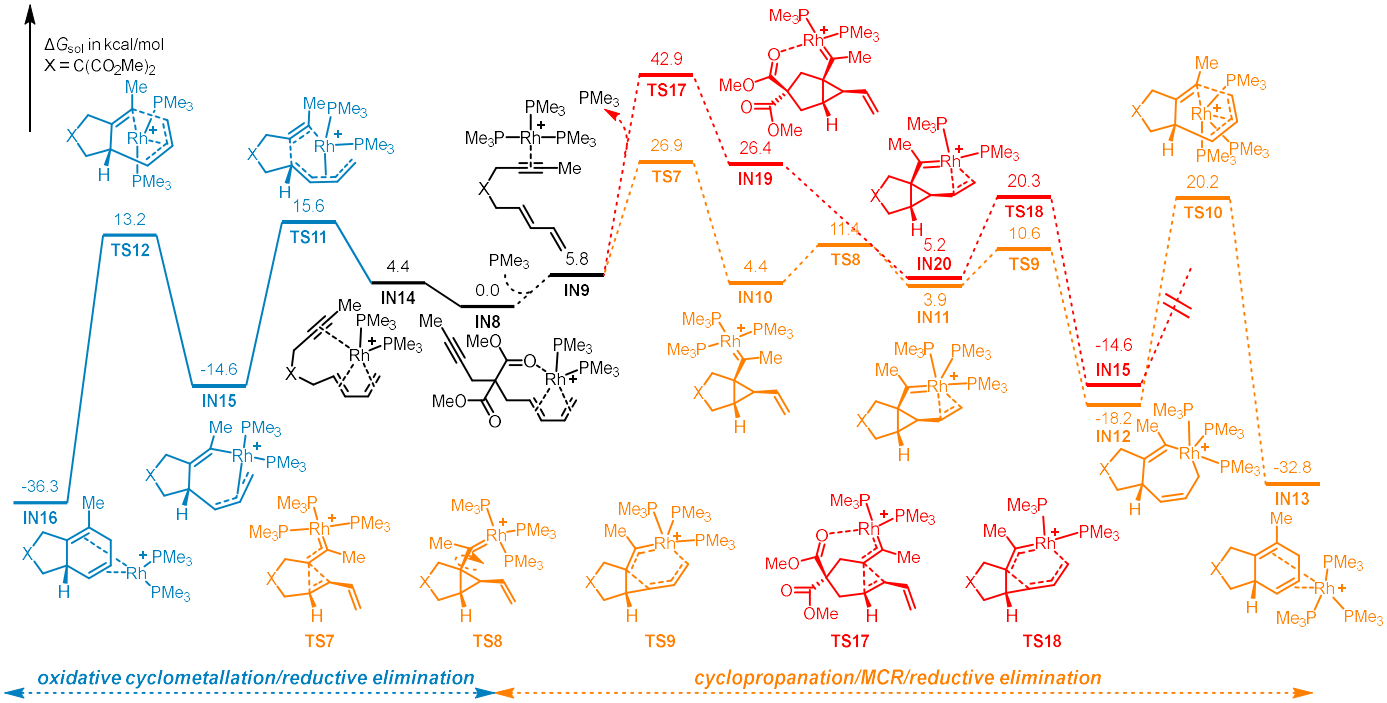
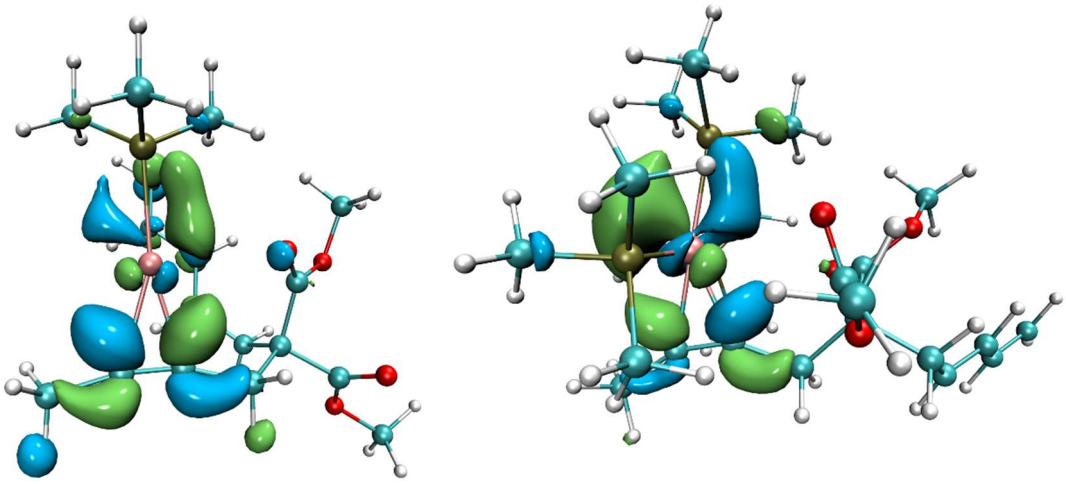


Figure S5. Full free energy diagram of Rh catalyzed [4 + 2] reaction computed at *ω*B97M-V/def2-QZVP/SMD(DCM)//BMK-D3BJ/def2-SVP level.

The full mechanism considered for cationic Rh catalyzed [4 + 2] is shown in **Figure S5**. In addition to what has been discussed in the main text, cyclopropanation with one less phosphine ligand was also considered and this reaction requires a much higher activation free energy, $\Delta G^{\neq}$ of 37.1 kcal/mol. Here MCR process was also facile with $\Delta G^{\neq}$ of 15.1 kcal/mol (**IN20** to **TS18**), but the barrier is higher than that of the MCR with one more phosphine ligand. The difference may be due to the fact that the added ligand may help stabilize the more electron-deficient formal Rh(III) generated through MCR. **TS18** leads to **IN15**, which is identical to that in the oxidative cyclization pathway, and the followed steps are the same.

7. Difference reactivity of cyclopropanation by Rh(I) and Au(I) catalysts

The difference reactivity of $Au(PR_3)^+$ and $Rh(PR_3)_3^+$ catalyst to cyclopropanation reaction is attributed to the difference in the electronic effect of the center metal. It is well known that the cyclopropanation reaction of an alkene moiety and the alkyne-metal complex mainly relate to the interaction of π(alkene) with the π*(alkyne-metal). The more electron deficient the metal catalyst is, the lower π* orbital is, and consequently the lower the cyclopropanation barrier is.



IN1a -3.53 eV **IN9** -3.16 eV

Figure S6. LUMO isosurfaces and energies of Au(I) and Rh(I) complexes with the substrate.

The lowest unoccupied Kohn-Sham orbitals (LUMOs) of Au and Rh complexes with the substrate, which has $C(CO_2Me)_2$ tether and a Me group as the terminal substituent (**IN1a** and **IN9**, respectively) were shown in **Figure S6**. Both the orbitals corresponds to π* of alkyne–metal complexes, where the Au complex has lower LUMO than that of the Rh complex, suggesting Au-catalyzed cyclopropanation is easier than that by a Rh catalyst.

8. Summary of energies and coordinates

Intermediate and transition state index for Figure 1:

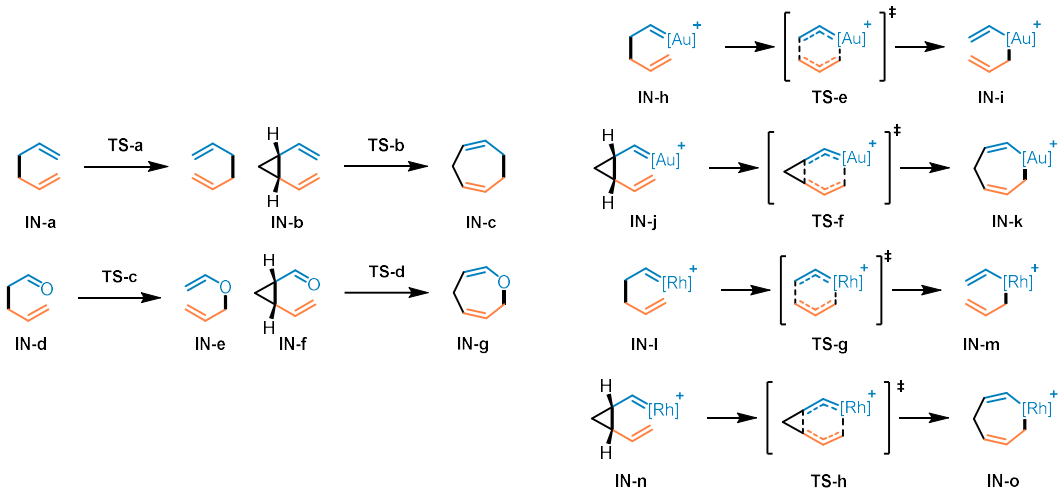


Table of solvated single point energies (*SPE*) and thermal corrections to Gibbs free energy (*TCG*)

Specie	*TCG*/ha	*SPE*/ha	Specie	*TCG*/ha	*SPE*/ha	Specie	*TCG*/ha	*SPE*/ha
IN-a	0.114822	-234.590260	**TS2**	0.433874	-1811.223228	**PMe3**	0.087903	-461.073838
TS-a	0.117089	-234.530884	**IN4**	0.436404	-1811.234243	**IN8**	0.476539	-1877.880256
IN-b	0.119402	-272.674471	**TS3**	0.434882	-1811.227330	**IN9**	0.585584	-2338.965940
TS-b	0.121623	-272.639880	**IN5**	0.437667	-1811.317051	**TS7**	0.585162	-2338.931978
IN-c	0.124411	-272.708674	**TS4**	0.431426	-1811.216267	**IN10**	0.586310	-2338.968883
IN-d	0.090706	-270.545932	**TS5**	0.431981	-1811.208884	**TS8**	0.585642	-2338.957069
TS-c	0.091684	-270.463806	**IN6**	0.432539	-1811.233351	**IN11**	0.592475	-2338.975956
IN-e	0.092544	-270.514730	**TS6**	0.428984	-1811.207786	**TS9**	0.591877	-2338.964633
IN-f	0.095878	-308.630363	**IN7**	0.435547	-1811.273199	**IN12**	0.587973	-2339.006604
TS-d	0.099434	-308.586059	**IN1a**	0.361785	-1441.885241	**TS10**	0.591474	-2338.948988
IN-g	0.101575	-308.630815	**IN1b**	0.306149	-1590.083234	**IN13**	0.594824	-2339.036792
IN-h	0.189945	-791.878756	**IN1c**	0.375923	-1959.443764	**IN14**	0.479237	-1877.875899
TS-e	0.187822	-791.830021	**IN1d**	0.443825	-1559.815788	**TS11**	0.479201	-1877.857984
IN-i	0.188508	-791.852974	**IN1e**	0.584379	-2386.509205	**IN15**	0.478696	-1877.905716
IN-j	0.196628	-829.981310	**TS1a**	0.359394	-1441.846962	**TS12**	0.481767	-1877.864408
TS-f	0.196980	-829.973469	**TS1b**	0.304346	-1590.040126	**IN16**	0.482888	-1877.944529
IN-k	0.198266	-829.981438	**TS1c**	0.376745	-1959.415237	**IN17**	0.428713	-1811.244406
IN-l	0.416707	-1689.010843	**TS1d**	0.444169	-1559.775961	**TS13**	0.429201	-1811.173366
TS-g	0.415720	-1688.951639	**TS1e**	0.583842	-2386.479213	**IN18**	0.433637	-1811.219112
IN-m	0.412794	-1688.987129	**TS4a**	0.361893	-1441.858953	**TS14**	0.434500	-1811.161147
IN-n	0.422646	-1727.096495	**TS4b**	0.304146	-1590.049099	**TS15**	0.430772	-1811.196589

TS-h	0.421197	-1727.079602	**TS4c**	0.373742	-1959.410333	**TS16**	0.431069	-1811.214036
IN-o	0.422380	-1727.107499	**TS4d**	0.444226	-1559.775434	**TS17**	0.475214	-1877.810561
1a	0.321767	-1214.579952	**TS4e**	0.586743	-2386.473247	**IN19**	0.475818	-1877.837414
2a	0.330024	-1214.645552	**TS5a**	0.360786	-1441.854828	**IN20**	0.475452	-1877.870811
IN1	0.429963	-1811.251084	**TS5b**	0.304114	-1590.056185	**TS18**	0.476726	-1877.848077
IN2	0.430487	-1811.246957	**TS5c**	0.374388	-1959.411759	**TS19**	0.430416	-1811.217415
TS1	0.431446	-1811.220444	**TS5d**	0.443460	-1559.769033			
IN3	0.432166	-1811.226602	**TS5e**	0.587083	-2386.467471			

Calculated at ωB97M-V/def2-QZVP/SMD(DCM)//BMK-D3BJ/def2-SVP level with a standard state of 298.15 K, 1 M.

Cartesian coordinates

IN-a

C	-0.757683	-1.066988	0.246151
C	0.749443	-1.096324	-0.099323
C	-1.483924	0.073265	-0.419544
H	-0.889440	-1.003011	1.341294
C	1.484893	0.117698	0.406657
H	1.191231	-2.005793	0.348962
C	-2.162873	1.031062	0.219131
H	-1.423268	0.104721	-1.516889
C	2.170777	0.975253	-0.355195
H	1.425198	0.297455	1.489688
H	-2.239143	1.042217	1.312728
H	-2.664191	1.836988	-0.325597
H	2.246420	0.838096	-1.440258
H	2.678635	1.843443	0.075956
H	-1.206782	-2.025197	-0.075434
H	0.881109	-1.181863	-1.193005

IN-b

C	-0.779393	0.605556	-0.404807
C	-0.000012	1.678802	0.353895
C	0.779300	0.605565	-0.404885
H	-0.000042	2.699879	-0.039818
H	0.000045	1.615193	1.448301
C	-1.546437	-0.428669	0.331314
H	-1.231754	0.914044	-1.354365
C	1.546416	-0.428660	0.331163
H	1.231564	0.914050	-1.354490
C	-2.664829	-1.007741	-0.122754
H	-1.159397	-0.718514	1.316507
C	2.664701	-1.007816	-0.123060
H	1.159523	-0.718426	1.316437
H	-3.087208	-0.744097	-1.098943
H	-3.193375	-1.762716	0.466214
H	3.086934	-0.744240	-1.099332
H	3.193309	-1.762784	0.465860

IN-c

C	-1.447351	0.745975	0.203312
C	-1.538141	-0.748836	0.019735
C	-0.307759	-1.602077	-0.166110
H	-2.096578	-1.165885	0.882858
H	-2.215450	-0.933053	-0.839716
C	-0.416132	1.583157	0.022920
H	-2.403802	1.202403	0.490410
C	0.991212	-1.303306	-0.022721
H	-0.544082	-2.643882	-0.419995
C	1.000340	1.245604	-0.385532
H	-0.623367	2.649076	0.179958
C	1.612608	0.029018	0.331941
H	1.697408	-2.129723	-0.171625
H	1.042202	1.071823	-1.477446
H	1.637184	2.124963	-0.191231
H	2.688422	-0.015313	0.092142
H	1.548930	0.191176	1.424616

IN-d

C	0.420528	0.244639	0.350715
C	-0.493838	-0.770666	-0.346289
C	1.860418	-0.198871	0.355781
C	-1.956542	-0.376838	-0.321403
H	-0.415279	-1.775459	0.114962

H	-0.201308	-0.915801	-1.404531
H	0.322174	1.225521	-0.143596
H	0.060793	0.382271	1.386432
C	2.864759	0.453481	-0.238926
H	2.076315	-1.138425	0.884701
O	-2.381273	0.615132	0.201577
H	-2.650415	-1.091327	-0.838381
H	2.693278	1.393261	-0.776854
H	3.891540	0.076543	-0.203771

IN-e

O	-0.363877	-0.091329	0.493444
C	0.382626	0.138077	-0.664815
C	-1.685166	0.109927	0.439469
C	1.839736	-0.139043	-0.414700
H	0.012189	-0.505897	-1.490149
H	0.250360	1.188054	-1.001173
C	-2.416723	0.515905	-0.610699
H	-2.145410	-0.105405	1.409439
C	2.350686	-0.547417	0.749071
H	2.491686	0.020331	-1.282781
H	-1.992586	0.739447	-1.591478
H	-3.494659	0.630335	-0.482351
H	1.706543	-0.708076	1.617980
H	3.423552	-0.729889	0.858444

IN-f

C	0.801169	-0.633595	-0.387031
C	0.006261	-1.688928	0.353304
C	-0.765244	-0.622307	-0.430991
H	-0.009427	-2.711587	-0.034722
H	-0.021166	-1.617024	1.447451
C	1.567847	0.402568	0.352455
H	1.253234	-0.939218	-1.337419
C	-1.519235	0.418904	0.319155
H	-1.229252	-0.901865	-1.382469
C	2.651999	1.018277	-0.133602
H	1.218967	0.651327	1.362650
O	-2.510166	0.957568	-0.091091
H	-1.104973	0.673748	1.330472
H	3.034900	0.793224	-1.135349
H	3.191302	1.766077	0.454564

IN-g

O	1.552817	0.130288	0.256369
C	0.844507	1.152132	-0.409889
C	1.057883	-1.115844	0.207061
C	-0.487669	1.504437	0.217000
H	1.514733	2.023383	-0.409554
H	0.689691	0.839935	-1.462765
C	-0.187464	-1.542707	-0.072284
H	1.840707	-1.848513	0.431773
C	-1.512498	0.644599	0.253786
H	-0.606844	2.505759	0.645325
C	-1.471494	-0.766155	-0.296213
H	-0.292303	-2.632630	-0.092676
H	-2.458128	0.971313	0.703293
H	-2.288230	-1.343871	0.169226
H	-1.728708	-0.741616	-1.377032

IN-h

Au	-0.396841	-2.272942	-1.491535
P	1.490101	-3.683927	-1.305249
C	-2.101129	-1.143306	-1.649941
C	2.579683	-3.629573	-2.750032
C	1.037905	-5.425952	-1.110045
C	2.550050	-3.301079	0.111638
C	-2.756863	-0.393042	-0.601359
H	-2.689178	-1.163090	-2.583440
H	2.020327	-3.924005	-3.652975
H	3.435629	-4.313284	-2.619618
H	2.958992	-2.605342	-2.897904
H	0.444802	-5.759640	-1.977075
H	1.939626	-6.056272	-1.028183
H	0.425551	-5.556393	-0.202948
H	1.972404	-3.385589	1.046533
H	3.407379	-3.993981	0.156382
H	2.928409	-2.268991	0.031316
H	-2.392357	-0.514526	0.423773
C	-1.995000	0.765604	-1.399153
C	-2.949555	1.728052	-2.049450
H	-1.322134	0.336223	-2.204856
C	-3.084846	1.872355	-3.370511
H	-3.561387	2.319383	-1.357110
H	-2.485223	1.294599	-4.084134
H	-3.804117	2.583265	-3.787313
H	-1.258405	1.192052	-0.699993
H	-3.841788	-0.244008	-0.673362

IN-i

Au	0.284474	-0.223164	-0.913317
P	2.744072	-0.082489	-0.821715
C	-1.666056	-0.642381	-0.625004
C	3.413737	-1.258906	0.385379
C	3.374469	1.532602	-0.304043
C	3.597356	-0.462201	-2.371967
C	-2.152584	-1.855695	-0.911892
H	-2.279696	0.121982	-0.128062
H	2.998570	-1.054611	1.386207
H	4.513281	-1.183839	0.436280
H	3.142090	-2.289450	0.102888
H	2.957747	1.804599	0.679512
H	4.475381	1.517919	-0.233521
H	3.074173	2.301017	-1.034583
H	3.336393	0.288949	-3.134092
H	4.690830	-0.456037	-2.224963
H	3.293604	-1.455653	-2.740607
H	-1.583256	-2.619297	-1.455266
C	1.264708	2.628537	-3.076702
C	0.641409	1.442964	-3.223412
H	2.080741	2.928928	-3.742148
C	-0.519129	1.048211	-2.406492
H	0.960587	0.747333	-4.008956
H	-0.973114	1.857571	-1.816196
H	-1.274198	0.448884	-2.928762
H	0.947199	3.348926	-2.313214
H	-3.164158	-2.138771	-0.590757

IN-j

Au	0.097302	-0.099329	0.411440
P	2.246674	0.295038	-0.509852
C	-1.680170	-0.466240	1.320760
C	2.847800	1.981080	-0.231305
C	2.365173	0.040599	-2.299976
C	3.515026	-0.783197	0.203653
C	-2.836924	-1.060590	0.848919
H	-1.752412	-0.204153	2.390759
H	3.858109	2.113058	-0.654324
H	2.881544	2.191384	0.850183
H	2.164559	2.707501	-0.700595
H	3.392310	0.227929	-2.656362
H	2.084213	-0.995111	-2.551615
H	1.677081	0.723430	-2.824473
H	4.505146	-0.566882	-0.232114
H	3.562332	-0.633177	1.294621
H	3.261636	-1.838883	0.013443
C	-2.940706	-1.734465	-0.540954
H	-3.699605	-1.212623	1.507433
C	-3.423977	-0.377627	-0.716523
H	-3.670999	-2.550946	-0.548068
H	-1.973630	-1.979173	-0.994389
C	-2.706425	0.678311	-1.429804
H	-4.479265	-0.179663	-0.493923
C	-3.293475	1.854768	-1.706864
H	-1.699296	0.452364	-1.794486
H	-4.304018	2.088919	-1.353394
H	-2.785380	2.614185	-2.308288

IN-k

Au	-0.065660	0.496411	-0.066893
P	2.245021	-0.288748	0.050567
C	-1.866306	1.413311	-0.039895
C	3.293701	0.707153	1.140057
C	3.089246	-0.311602	-1.550635
C	2.362609	-1.981635	0.685093
C	-3.131195	1.001334	0.068641
H	-1.697751	2.504878	-0.085547
H	4.320046	0.303564	1.172664
H	2.879874	0.712375	2.161896
H	3.333100	1.747763	0.777908
H	4.120120	-0.691059	-1.447992
H	2.543777	-0.954876	-2.260717
H	3.123661	0.707312	-1.970173
H	1.803192	-2.675062	0.034887
H	3.413263	-2.315820	0.726455
H	1.933322	-2.033022	1.699372
C	-3.720786	-0.418758	0.002573
H	-3.906504	1.773712	0.170110
C	-2.912420	-1.483240	0.673856
H	-3.856292	-0.660662	-1.069840
H	-4.729528	-0.390518	0.437711
C	-1.672462	-1.864744	0.270856
H	-3.334003	-1.955031	1.568868
C	-1.014220	-1.240456	-0.864647
H	-1.123487	-2.619348	0.843614
H	-1.665721	-0.815912	-1.638088

H	-0.148061	-1.770268	-1.281196

IN-l

Rh	0.255768	-0.179125	-0.445918
P	-1.578953	-1.613902	0.054106
P	1.198398	0.161469	1.672960
C	-2.882006	-1.050172	1.198230
C	-1.130629	-3.204490	0.824122
C	-2.541783	-2.133310	-1.399112
P	-1.137724	1.822076	-0.254792
C	1.273917	-1.688833	-0.953512
C	2.587304	-0.965488	2.008857
C	1.951476	1.794349	1.944165
C	0.164254	-0.073817	3.152207
H	-3.408243	-0.173102	0.791548
H	-3.626076	-1.846895	1.366370
H	-2.441461	-0.771851	2.169178
H	-0.564209	-3.028703	1.754254
H	-2.030876	-3.793752	1.066128
H	-0.500984	-3.806965	0.151450
H	-2.947200	-1.244212	-1.909512
H	-1.873393	-2.644183	-2.111358
H	-3.373160	-2.808431	-1.133436
C	-0.296755	3.352359	-0.773552
C	-1.843907	2.357178	1.340006
C	-2.600895	1.795084	-1.338424
C	2.547259	-1.516071	-1.721036
H	1.025501	-2.746780	-0.759261
H	2.227810	-2.007303	1.984168
H	3.049136	-0.765880	2.990905
H	3.352473	-0.851656	1.223987
H	1.182917	2.583342	1.919731
H	2.674197	1.998711	1.136714
H	2.475283	1.844849	2.913905
H	0.738833	0.101406	4.077821
H	-0.216269	-1.108908	3.170332
H	-0.699119	0.609040	3.137387
H	0.078752	3.267389	-1.805189
H	0.564748	3.548112	-0.114598
H	-0.983496	4.213757	-0.721979
H	-2.436491	1.555092	1.804123
H	-1.035846	2.635037	2.035875
H	-2.492957	3.238527	1.203093
H	-3.300703	1.007263	-1.016037
H	-2.291235	1.565760	-2.370933
H	-3.134208	2.760576	-1.330114
C	2.992659	-0.047687	-1.685968
H	2.345178	-1.866167	-2.758074
C	1.752278	0.832574	-1.607645
H	3.611845	0.209554	-2.564022
C	0.649870	0.544179	-2.468889
H	1.924712	1.873054	-1.309556
H	0.720591	-0.257452	-3.210387
H	-0.036484	1.340549	-2.769280
H	3.623425	0.124142	-0.796635
H	3.323364	-2.213057	-1.351083

IN-m

Rh	-0.071601	-0.286834	-0.121019
P	2.292365	-0.476827	-0.524414
P	-2.390800	-0.725140	0.124528
C	3.115091	-1.867061	0.299440
C	3.481691	0.876784	-0.269128
C	2.500362	-0.846203	-2.294116
P	-0.348398	2.125674	-0.400910
C	0.048272	-2.323888	-0.103630
C	-3.533583	0.543790	0.757709
C	-3.131229	-1.201969	-1.461388
C	-2.760661	-2.104511	1.242368
H	3.044582	-1.740670	1.391268
H	2.627097	-2.810918	0.017854
H	4.178744	-1.905756	0.012383
H	3.291242	1.702916	-0.967946
H	3.420585	1.254139	0.763013
H	4.505642	0.507177	-0.445774
H	1.941718	-1.761528	-2.546853
H	2.113935	-0.015561	-2.908563
H	3.563451	-1.001285	-2.544475
C	1.064654	3.189957	-0.828979
C	-1.052413	3.041052	1.005929
C	-1.484515	2.486761	-1.780972
C	-0.089891	-3.080920	-1.205419
H	0.241683	-2.851814	0.845556
H	-4.560654	0.142662	0.784846
H	-3.534364	1.448973	0.132412
H	-3.251998	0.823780	1.786449
H	-3.051721	-0.373878	-2.185694
H	-4.195378	-1.465613	-1.340928

H	-2.592983	-2.073843	-1.865841
H	-2.308292	-3.030648	0.859755
H	-3.849918	-2.242587	1.341371
H	-2.337649	-1.894857	2.239250
H	0.734545	4.232420	-0.974875
H	1.538660	2.842032	-1.760797
H	1.816002	3.169879	-0.024005
H	-2.004464	2.601121	1.333054
H	-0.354892	3.004930	1.859056
H	-1.223395	4.097860	0.740317
H	-1.644537	3.571204	-1.905433
H	-2.461814	2.003901	-1.624796
H	-1.059636	2.087979	-2.717992
C	2.213690	0.021147	3.148293
H	-0.283821	-2.643565	-2.196387
C	1.255575	0.571075	2.385765
H	3.088497	0.593538	3.472831
C	0.028509	-0.129665	1.922755
H	1.371093	1.621785	2.084566
H	-0.025439	-1.145346	2.347689
H	-0.868509	0.436570	2.231965
H	2.135832	-1.015031	3.497482
H	-0.012637	-4.176146	-1.184735

IN-n

Rh	-0.239129	0.037654	0.397617
P	1.455669	1.686892	-0.118433
P	1.362878	-1.710290	0.551345
C	2.314487	1.683959	-1.726520
C	2.862662	1.749131	1.039587
C	0.838037	3.396448	-0.042221
P	-0.859257	-0.292134	-1.852025
C	-1.677097	-1.150146	1.043189
C	0.727886	-3.382369	0.196682
C	2.873639	-1.709845	-0.472413
C	2.035063	-1.885424	2.231824
H	1.596033	1.835356	-2.547741
H	3.061664	2.494001	-1.770144
H	2.830061	0.724881	-1.889458
H	3.435049	0.809029	1.009532
H	3.544730	2.579700	0.791653
H	2.500509	1.887567	2.070102
H	-0.000856	3.524305	-0.746273
H	0.469593	3.620039	0.971925
H	1.631359	4.120463	-0.292429
C	-2.236792	-1.456702	-2.111855
C	0.355198	-0.986518	-3.021504
C	-1.428101	1.204943	-2.720963
C	-2.968608	-0.700242	1.363765
H	-1.521736	-2.206225	1.324387
H	0.332420	-3.425901	-0.832500
H	-0.089315	-3.648456	0.884884
H	1.521180	-4.141694	0.299278
H	2.610646	-1.705865	-1.541802
H	3.486613	-2.603624	-0.266459
H	3.489325	-0.821065	-0.267595
H	2.527101	-0.944306	2.528209
H	2.757521	-2.715131	2.314248
H	1.204927	-2.055773	2.936832
H	-2.485532	-1.555384	-3.182046
H	-3.134734	-1.133487	-1.564048
H	-1.948178	-2.447219	-1.721385
H	1.272494	-0.381589	-3.052227
H	0.624113	-2.007603	-2.703769
H	-0.064821	-1.043693	-4.040009
H	-2.275201	1.652484	-2.176013
H	-1.741329	0.989975	-3.756921
H	-0.620610	1.954944	-2.744018
C	-3.643448	0.504902	0.653782
C	-2.798782	0.973381	1.732875
H	-3.642480	-1.300441	1.984731
H	-4.729816	0.510670	0.787719
H	-3.293341	0.694566	-0.364443
C	-1.425546	1.458501	1.445981
H	-3.251578	1.154171	2.716173
C	-0.355235	0.988664	2.302845
H	-1.414975	2.481771	1.050052
H	-0.618114	0.341598	3.148666
H	0.468585	1.668410	2.544504

IN-o

Rh	-0.042477	-0.060675	-0.191525
P	2.164756	0.806100	-0.566098
P	-2.122963	-1.195372	-0.346696
C	2.038408	1.860421	-2.050281
C	3.478404	-0.345850	-1.047719
C	3.020911	1.847600	0.653521
P	-1.028301	2.102198	0.407389

C	0.681107	-1.769070	-1.023484
C	-2.144290	-2.926380	0.195126
C	-3.648315	-0.578159	0.434196
C	-2.563136	-1.282985	-2.108122
H	3.021883	2.263322	-2.346473
H	1.645606	1.259437	-2.888522
H	1.349142	2.703482	-1.884980
H	3.648943	-1.073995	-0.240569
H	3.183263	-0.905542	-1.947125
H	4.409918	0.210104	-1.246529
H	3.868597	2.373031	0.182263
H	2.348536	2.589262	1.103875
H	3.414564	1.204695	1.455970
C	-2.147672	2.644958	-0.926627
C	-0.026530	3.606958	0.656182
C	-2.044847	2.172282	1.915909
C	1.258130	-2.885996	-0.557860
H	0.587275	-1.725778	-2.130085
H	-3.105556	-3.396768	-0.070014
H	-2.021558	-2.982281	1.289304
H	-1.317610	-3.472436	-0.282546
H	-4.502945	-1.212501	0.144502
H	-3.872397	0.458871	0.142452
H	-3.547395	-0.622078	1.531201
H	-1.772884	-1.823172	-2.654327
H	-2.647510	-0.269437	-2.535655
H	-3.521006	-1.808974	-2.257487
H	-1.563685	2.802604	-1.849818
H	-2.661957	3.588010	-0.675107
H	-2.906400	1.876015	-1.141416
H	-0.681788	4.490376	0.742092
H	0.551440	3.520763	1.590109
H	0.675766	3.775952	-0.174355
H	-1.392348	2.056981	2.797479
H	-2.790487	1.366935	1.942743
H	-2.563483	3.142494	1.995776
C	1.484038	-3.228759	0.920278
C	2.180882	-2.145270	1.702535
H	1.594556	-3.654882	-1.267202
H	2.061941	-4.162118	0.986276
H	0.500850	-3.440506	1.382800
C	1.587157	-0.990810	2.070889
H	3.235952	-2.301297	1.956933
C	0.175148	-0.666609	1.770465
H	2.176251	-0.246444	2.618865
H	-0.461710	-1.556170	1.882367
H	-0.211013	0.134525	2.416838

TS-a

C	-0.271742	-0.891504	-1.218919
C	0.271742	0.891504	-1.218919
C	0.227663	-1.418964	0.000000
H	0.156775	-1.282847	-2.151006
C	-0.227663	1.418964	0.000000
H	1.357091	0.750004	-1.292253
C	-0.271742	-0.891504	1.218919
H	1.237806	-1.848049	0.000000
C	0.271742	0.891504	1.218919
H	-1.237806	1.848049	0.000000
H	-1.357091	-0.750004	1.292253
H	0.156775	-1.282847	2.151006
H	1.357091	0.750004	1.292253
H	-0.156775	1.282847	2.151006
H	-1.357091	-0.750004	-1.292253
H	-0.156775	1.282847	-2.151006

TS-b

C	0.259531	-1.031309	0.952012
C	-0.850526	-1.370252	0.000000
C	0.259531	-1.031309	-0.952012
H	-1.168465	-2.419563	0.000000
H	-1.710848	-0.689665	0.000000
C	0.498011	0.254889	1.469467
H	0.912504	-1.852617	1.261230
C	0.498011	0.254889	-1.469467
H	0.912504	-1.852617	-1.261230
C	-0.280407	1.357457	1.133035
H	1.476016	0.418949	1.937065
C	-0.280407	1.357457	-1.133035
H	1.476016	0.418949	-1.937065
H	-1.357709	1.236278	1.016538
H	0.038174	2.354539	1.453924
H	-1.357709	1.236278	-1.016538
H	0.038174	2.354539	-1.453924

TS-c

C	-0.340946	-1.054337	-1.235172
C	0.332426	1.037958	-1.195685

C	0.248203	-1.337070	-0.008208
H	0.075440	-1.495577	-2.147547
C	-0.226252	1.448578	0.009632
H	1.397600	0.791063	-1.245406
H	1.257812	-1.800564	-0.008080
C	0.282540	0.900716	1.208310
H	-1.252164	1.833246	0.012030
H	1.361579	0.732591	1.291703
H	-0.208204	1.133487	2.156864
H	-1.390358	-0.752734	-1.264475
H	-0.114596	1.338617	-2.149005
O	-0.192325	-0.845503	1.084609

TS-d

C	-0.434763	0.971375	-1.014041
C	0.562845	1.495429	-0.031185
C	-0.434927	-0.332274	-1.511246
C	-0.409932	0.974918	1.000076
H	0.677342	2.585830	-0.028422
H	1.536325	0.989607	-0.016463
H	-1.249186	1.649202	-1.291047
C	0.522002	-1.242688	-1.038160
H	-1.348928	-0.703754	-1.985374
C	-0.462188	-0.376978	1.344794
H	-1.150342	1.656871	1.427670
H	0.403234	-2.306285	-1.263857
H	1.554703	-0.923558	-0.895143
O	0.298304	-1.267622	0.861306
H	-1.301581	-0.701935	1.992317

TS-e

Au	0.553357	0.039493	0.251822
P	2.948636	-0.171506	0.215513
C	-1.467978	0.238005	0.523173
C	3.563484	-1.501577	1.280168
C	3.772400	1.330573	0.805650
C	3.687049	-0.496805	-1.409304
C	-2.321190	1.074989	-0.109229
H	-1.868449	-0.292580	1.404615
H	3.223931	-1.337303	2.316068
H	4.665889	-1.541517	1.267720
H	3.165286	-2.471673	0.940371
H	3.438219	1.563136	1.830174
H	4.868420	1.204584	0.808038
H	3.510434	2.183715	0.158640
H	3.434941	0.314896	-2.112187
H	4.785943	-0.561396	-1.333298
H	3.310989	-1.450615	-1.815583
H	-1.970792	1.829078	-0.827227
C	-2.252993	-0.084225	-2.324458
C	-0.933490	0.179531	-2.665068
H	-3.072276	0.558067	-2.662339
C	0.074282	-0.656084	-2.193826
H	-0.676761	1.106367	-3.188106
H	-0.177884	-1.639321	-1.781024
H	1.115973	-0.490238	-2.484820
H	-2.528632	-1.030270	-1.850369
H	-3.383130	1.138424	0.161815

TS-f

Au	0.027056	-0.483276	0.074117
P	-2.249382	0.235830	0.069255
C	1.869590	-1.364214	-0.020511
C	-3.404187	-1.147415	0.250599
C	-2.757801	1.074308	-1.454765
C	-2.681198	1.383255	1.404823
C	3.133949	-0.955292	0.190279
H	1.791018	-2.442374	-0.252077
H	-3.261963	-1.863738	-0.575115
H	-4.448992	-0.793302	0.242562
H	-3.211623	-1.675071	1.199101
H	-2.600404	0.406078	-2.317264
H	-3.822830	1.359025	-1.412158
H	-2.155097	1.983521	-1.613236
H	-2.081922	2.305649	1.329998
H	-3.749561	1.655161	1.361375
H	-2.472493	0.916254	2.381414
C	3.546520	0.394104	0.859650
H	3.991015	-1.581689	-0.088134
C	3.316026	1.173344	-0.350256
H	4.599547	0.338857	1.161735
H	2.906966	0.631020	1.717475
C	2.112607	1.829266	-0.663399
H	4.099221	1.147188	-1.117889
C	1.059922	1.901884	0.230766
H	1.980958	2.213927	-1.679219
H	1.193291	1.699639	1.297634
H	0.144676	2.430637	-0.051945

TS-g

Rh	0.143733	-0.379234	-0.281007
P	1.498327	0.375660	1.520062
P	-0.263393	1.703924	-1.212256
C	2.845584	1.509944	1.048871
C	2.392775	-0.965974	2.363065
C	0.802240	1.283079	2.940912
P	-2.020206	-0.490962	0.863784
C	1.882969	-0.554699	-1.271847
C	1.134989	2.512335	-2.046255
C	-1.515596	1.736305	-2.527327
C	-0.811539	2.988760	-0.045033
H	2.427360	2.484306	0.746301
H	3.524270	1.681814	1.901211
H	3.423746	1.098324	0.207144
H	3.064853	-1.472564	1.653460
H	2.996572	-0.579710	3.202066
H	1.675710	-1.709082	2.749427
H	1.614716	1.705695	3.555818
H	0.152028	2.105564	2.604357
H	0.207818	0.611001	3.575810
C	-2.288208	0.214885	2.521908
C	-2.562018	-2.209899	1.128792
C	-3.461992	0.189937	-0.023542
C	2.638181	-1.717504	-1.194393
H	2.232767	0.169080	-2.024581
H	2.033593	2.517662	-1.411044
H	0.875334	3.551475	-2.309061
H	1.376002	1.970444	-2.974703
H	-1.202224	1.051476	-3.331895
H	-1.627214	2.751718	-2.943878
H	-2.491268	1.393987	-2.156071
H	-1.122299	3.909494	-0.567066
H	0.018924	3.240173	0.635661
H	-1.653575	2.627297	0.567127
H	-1.667471	-0.313258	3.261944
H	-3.345078	0.105707	2.817776
H	-2.024432	1.283643	2.548210
H	-3.535829	-2.235045	1.645913
H	-2.666017	-2.731681	0.163995
H	-1.821958	-2.753096	1.738690
H	-4.394260	-0.062659	0.508872
H	-3.520932	-0.225015	-1.042138
H	-3.397362	1.287419	-0.095996
C	1.135985	-3.084233	-1.588562
H	2.694117	-2.276828	-0.259249
C	-0.088268	-2.569860	-1.084649
H	1.589705	-3.941046	-1.081842
C	-0.787443	-1.526360	-1.802697
H	-0.539104	-3.096647	-0.238861
H	-0.438219	-1.340384	-2.826618
H	-1.882432	-1.501114	-1.746314
H	1.317669	-3.052772	-2.667287
H	3.509632	-1.859470	-1.851153

TS-h

Rh	0.252889	-0.198802	0.270836
P	0.726788	1.280350	-1.556917
P	-1.199837	-1.849610	-0.628729
C	2.327448	1.056118	-2.399440
C	0.841510	3.040503	-1.097160
C	-0.424442	1.288131	-2.969530
P	-1.601083	1.165031	1.007938
C	1.834501	-1.204630	-0.339979
C	-0.432177	-2.910331	-1.897046
C	-1.772866	-3.076584	0.587174
C	-2.749654	-1.378745	-1.470169
H	2.366153	0.076371	-2.903019
H	2.493564	1.843048	-3.154192
H	3.144514	1.091372	-1.660289
H	1.599745	3.152808	-0.304183
H	1.131233	3.666571	-1.958218
H	-0.115881	3.414072	-0.703946
H	-0.138792	2.029971	-3.734836
H	-0.427851	0.287791	-3.435253
H	-1.448507	1.506007	-2.628642
C	-2.676590	2.013323	-0.195601
C	-1.110925	2.533402	2.103089
C	-2.829741	0.274359	2.014950
C	3.125337	-1.105226	0.217853
H	1.854281	-1.632705	-1.357987
H	-0.073539	-2.298970	-2.742635
H	-1.147372	-3.656227	-2.282431
H	0.431089	-3.444914	-1.468977
H	-0.894427	-3.554336	1.051117
H	-2.409000	-3.854395	0.131190
H	-2.336480	-2.574615	1.389968

H	-3.256542	-2.259766	-1.899029
H	-2.533169	-0.665937	-2.283303
H	-3.445303	-0.895965	-0.765854
H	-2.113840	2.771162	-0.761752
H	-3.512032	2.519549	0.316646
H	-3.093103	1.290184	-0.913387
H	-1.989635	3.100600	2.452643
H	-0.572033	2.145600	2.982363
H	-0.434121	3.219021	1.568294
H	-3.568317	0.966188	2.453593
H	-2.327811	-0.276418	2.825950
H	-3.368669	-0.456710	1.391352
C	3.417147	-1.298713	1.735914
C	2.996598	0.063712	1.483039
H	4.018641	-1.190109	-0.412828
H	4.481341	-1.491406	1.900633
H	2.756458	-1.982373	2.270702
C	1.583577	0.501929	1.740348
H	3.767288	0.833657	1.372881
C	0.629575	-0.429344	2.332921
H	1.510582	1.566179	1.991101
H	0.948296	-1.423736	2.654775
H	-0.120589	-0.019463	3.017391

1a

C	2.571351	0.941956	1.386230
C	1.229079	0.561676	1.961037
C	0.754071	2.198124	-0.714522
C	2.120048	1.791639	-1.040529
C	2.705408	0.666284	-0.143092
H	2.781206	2.011726	1.556082
H	3.355727	0.369516	1.901559
H	0.375806	1.209425	1.736791
H	2.159329	1.445988	-2.087170
H	2.780277	2.673522	-0.952951
C	1.034530	-0.552779	2.690292
H	1.885694	-1.214722	2.900958
C	-0.268665	-0.957781	3.218582
H	-1.110857	-0.289977	2.997306
C	-0.475302	-2.078191	3.930997
H	0.349705	-2.760604	4.165625
H	-1.469130	-2.345243	4.301133
C	-0.375038	2.556103	-0.432388
Si	-2.105034	2.922164	0.058921
C	-2.505799	1.806037	1.515878
H	-3.549458	1.943375	1.849293
H	-2.370370	0.747957	1.231920
H	-1.843842	2.023757	2.372387
C	-2.236484	4.725993	0.556549
H	-3.265604	4.972277	0.872279
H	-1.556403	4.953397	1.395219
H	-1.969512	5.386600	-0.286066
C	-3.234052	2.546584	-1.388875
H	-2.980803	3.178163	-2.257483
H	-3.133088	1.491690	-1.695986
H	-4.290139	2.731848	-1.124822
C	2.028238	-0.670314	-0.470259
C	4.169961	0.541505	-0.586219
O	1.091971	-0.813017	-1.200630
O	4.505957	0.000910	-1.602992
O	5.012752	1.153749	0.235593
O	2.606897	-1.656779	0.206880
C	1.994483	-2.928447	0.110596
H	1.920793	-3.245520	-0.940854
H	2.628147	-3.622199	0.677611
H	0.981783	-2.891273	0.545458
C	6.380299	1.135139	-0.133932
H	6.918835	1.682468	0.649814
H	6.745862	0.098813	-0.201533
H	6.522550	1.621178	-1.111736

2a

C	-1.849730	-1.810324	0.444507
C	-1.433392	-1.664602	-1.029998
C	-1.886018	0.571795	-0.080590
C	-2.677852	-0.522883	0.687998
H	-2.441289	-2.714385	0.648273
H	-0.958603	-1.790745	1.093870
H	-1.170247	1.043178	0.608796
H	-2.552949	1.360600	-0.462791
C	-1.128140	-0.180499	-1.167883
C	-0.245398	0.325181	-2.049565
C	-0.305006	-2.527160	-1.527906
H	-0.243912	-3.562439	-1.173055
C	0.574473	-2.056494	-2.420312
H	1.368759	-2.709210	-2.800555
C	0.528057	-0.639412	-2.947731
H	0.090608	-0.642097	-3.968636

H	-2.336288	-1.888465	-1.635069
Si	0.031051	2.176421	-2.242315
C	-1.495199	2.943592	-3.033796
H	-2.391601	2.770925	-2.413299
H	-1.376424	4.034103	-3.161672
H	-1.686153	2.501331	-4.026931
C	1.513828	2.451714	-3.367145
H	1.663986	3.530599	-3.547998
H	2.441838	2.055471	-2.918503
H	1.375862	1.963923	-4.347880
C	0.362314	3.028157	-0.594873
H	-0.552810	3.141227	0.008999
H	1.102623	2.469610	0.004147
H	0.767090	4.040069	-0.774962
H	1.560425	-0.272549	-3.087068
C	-2.841068	-0.258721	2.183725
C	-4.093766	-0.690497	0.119625
O	-3.844130	-0.479093	2.805115
O	-4.562216	-1.720531	-0.277380
O	-4.747068	0.465013	0.113345
O	-1.720393	0.191377	2.739351
C	-6.097584	0.425240	-0.305455
H	-6.469798	1.455969	-0.248788
H	-6.173234	0.044361	-1.335972
H	-6.683126	-0.230579	0.357491
C	-1.747735	0.398059	4.139254
H	-0.753776	0.771813	4.415719
H	-2.523557	1.132493	4.405988
H	-1.963969	-0.545144	4.665068

IN1

C	2.528248	0.844916	1.417462
C	1.174232	0.525403	2.007401
C	0.410113	1.657565	-0.669899
C	1.817551	1.430788	-1.032318
C	2.654222	0.517240	-0.097143
H	2.767564	1.910295	1.553840
H	3.311330	0.271843	1.936206
H	0.468835	1.355267	2.125184
H	1.871424	1.021561	-2.054417
H	2.285255	2.432030	-1.050568
C	0.766885	-0.702751	2.381830
H	1.453862	-1.556020	2.301831
C	-0.570558	-0.962778	2.917079
H	-1.249912	-0.100832	2.960346
C	-0.986350	-2.161574	3.361781
H	-0.320050	-3.032232	3.357428
H	-1.985437	-2.300776	3.785384
C	-0.709520	2.102848	-0.368773
Au	-1.088899	-0.079600	-0.517361
P	-2.078577	-2.183749	-0.584399
C	-3.485775	-2.394322	0.530428
H	-4.275938	-1.667120	0.283216
H	-3.898237	-3.414662	0.453983
H	-3.151259	-2.214808	1.564843
C	-2.682108	-2.623002	-2.232091
H	-1.849127	-2.578592	-2.952632
H	-3.109856	-3.639865	-2.236719
H	-3.454128	-1.905553	-2.554013
C	-0.894525	-3.473998	-0.143047
H	-1.348608	-4.475922	-0.223468
H	-0.022340	-3.393655	-0.811195
H	-0.561344	-3.303637	0.893937
Si	-2.241860	3.031973	0.202108
C	-2.682454	2.274285	1.855454
H	-3.563291	2.779191	2.289719
H	-2.927469	1.203528	1.742861
H	-1.853381	2.369981	2.578255
C	-1.755993	4.826153	0.336499
H	-2.617549	5.426079	0.679422
H	-0.935428	4.967907	1.059810
H	-1.432417	5.226444	-0.639115
C	-3.562995	2.719402	-1.077074
H	-3.246070	3.072097	-2.073214
H	-3.794687	1.642974	-1.151365
H	-4.493178	3.250507	-0.809126
C	2.309589	-0.958835	-0.340899
C	4.102367	0.675160	-0.614036
O	1.423193	-1.361577	-1.049458
O	4.444005	0.233585	-1.674825
O	4.869202	1.369505	0.199891
O	3.117941	-1.741557	0.344968
C	2.956331	-3.144605	0.204048
H	3.020594	-3.431618	-0.856210
H	3.768103	-3.607246	0.777877
H	1.978850	-3.453714	0.608456
C	6.215002	1.586633	-0.214683
H	6.686435	2.178472	0.578722

H	6.731331	0.623238	-0.340116
H	6.234809	2.130379	-1.171070

IN2

C	2.542421	0.824353	1.465812
C	1.365616	0.173710	2.145980
C	0.446995	1.673633	-0.560612
C	1.828155	1.385570	-0.975105
C	2.670902	0.472743	-0.044550
H	2.502557	1.920367	1.571404
H	3.465943	0.485647	1.961635
H	1.395051	-0.921831	2.213740
H	1.822346	0.949118	-1.987310
H	2.328918	2.368754	-1.038226
C	0.343672	0.829763	2.720550
H	0.349153	1.927293	2.704722
C	-0.797559	0.188240	3.396921
H	-1.301810	0.788398	4.163979
C	-1.255687	-1.048480	3.142274
H	-0.796879	-1.668607	2.364926
H	-2.078550	-1.479423	3.720320
C	-0.648776	2.167783	-0.247600
Au	-1.077147	-0.006185	-0.320487
P	-2.120733	-2.084331	-0.455876
C	-3.590834	-2.272467	0.580082
H	-4.348231	-1.527085	0.287896
H	-4.021069	-3.282893	0.476041
H	-3.324395	-2.094579	1.634117
C	-2.662820	-2.447299	-2.143595
H	-1.793560	-2.421506	-2.820961
H	-3.136588	-3.441923	-2.200808
H	-3.383446	-1.684324	-2.479535
C	-1.015606	-3.449353	-0.023503
H	-1.498692	-4.421749	-0.217909
H	-0.096676	-3.354667	-0.624800
H	-0.743001	-3.395208	1.043087
Si	-2.164918	3.197231	0.178487
C	-2.683524	2.693709	1.899531
H	-3.622070	3.205977	2.175856
H	-2.853877	1.605149	1.962172
H	-1.920984	2.967265	2.648382
C	-1.630744	4.980340	0.072388
H	-2.480517	5.643684	0.312580
H	-0.818622	5.199809	0.785833
H	-1.279895	5.233732	-0.942198
C	-3.459276	2.747215	-1.090289
H	-3.096067	2.930955	-2.115697
H	-3.739339	1.682752	-1.008901
H	-4.371828	3.350398	-0.939737
C	2.315279	-1.002868	-0.267195
C	4.109160	0.633043	-0.579323
O	1.397103	-1.405831	-0.935843
O	4.476276	0.095279	-1.585593
O	4.833867	1.459680	0.146390
O	3.134098	-1.780304	0.408845
C	2.964974	-3.184938	0.288718
H	3.041137	-3.487730	-0.766320
H	3.767943	-3.642580	0.878531
H	1.982518	-3.484104	0.686996
C	6.164242	1.708037	-0.298785
H	6.599544	2.412777	0.419485
H	6.737590	0.769206	-0.317922
H	6.152197	2.140368	-1.310621

IN3

C	2.534419	-1.984345	-0.276349
C	1.070411	-1.796022	0.115819
C	2.462457	-0.008177	1.174990
C	3.232167	-0.624130	-0.015417
H	2.997420	-2.766506	0.345832
H	2.621716	-2.278048	-1.330531
H	2.613015	1.075936	1.239683
H	2.856708	-0.440847	2.108621
C	1.002523	-0.374088	0.910773
C	-0.072282	0.475772	0.736093
C	0.655037	-2.001940	1.471943
H	1.443559	-2.152097	2.219022
C	-0.697501	-2.404454	1.902540
H	-0.980014	-2.142027	2.927908
C	-1.522885	-3.130982	1.135508
H	-1.247634	-3.435247	0.120209
H	0.316475	-1.865542	-0.673061
Si	0.121557	2.359623	1.013790
C	0.733800	2.637379	2.764771
H	1.728657	2.205138	2.957190
H	0.795953	3.722733	2.961241
H	0.027219	2.209379	3.496840
C	-1.553027	3.174262	0.806184

H	-1.476867	4.256072	1.016432
H	-1.930135	3.058299	-0.224775
H	-2.300468	2.749527	1.498695
C	1.289385	3.010634	-0.302395
H	2.344512	2.773467	-0.094528
H	1.024517	2.584184	-1.285487
H	1.196323	4.109145	-0.365727
H	-2.490277	-3.469835	1.517798
Au	-1.930127	-0.036772	0.042585
P	-4.090477	-0.406284	-0.840524
C	-4.178308	-1.706408	-2.100634
H	-3.854659	-2.667786	-1.669751
H	-5.205206	-1.816432	-2.488427
H	-3.503721	-1.460954	-2.937176
C	-5.319758	-0.883719	0.403876
H	-5.390494	-0.101105	1.176778
H	-6.313202	-1.027047	-0.053995
H	-5.013027	-1.821588	0.894269
C	-4.790071	1.061730	-1.639911
H	-5.800461	0.858914	-2.033567
H	-4.846422	1.888551	-0.913126
H	-4.138035	1.379679	-2.469859
C	4.717412	-0.806017	0.297021
C	3.046558	0.274223	-1.245070
O	2.149467	0.151097	-2.034085
O	5.225549	-0.540463	1.348489
O	5.346707	-1.338918	-0.736772
O	3.969900	1.217024	-1.297837
C	6.743888	-1.561540	-0.595349
H	7.262484	-0.609155	-0.407552
H	6.939972	-2.245823	0.244022
H	7.081304	-2.004080	-1.540252
C	3.966024	2.079605	-2.428097
H	3.054514	2.695480	-2.437889
H	4.855061	2.714032	-2.330042
H	4.012133	1.487502	-3.354370

IN4

C	-2.422831	-1.546546	-2.230076
C	-1.062242	-1.423802	-1.517008
C	-2.392930	0.654374	-1.273147
C	-3.332714	-0.539417	-1.499107
H	-2.336428	-1.241128	-3.286754
H	-2.821190	-2.569793	-2.185275
H	-2.792315	1.377300	-0.550467
H	-2.272161	1.178561	-2.238519
C	-1.076241	0.013966	-0.864886
C	-0.165804	0.513273	-0.029320
C	0.134762	-1.620740	-2.365882
H	0.028212	-1.481791	-3.448480
C	1.370253	-1.865470	-1.851223
H	2.234818	-1.907823	-2.521714
C	1.600092	-1.992344	-0.423551
H	0.764923	-2.396309	0.164573
H	-1.059529	-2.113133	-0.658101
Si	-0.507571	2.023650	1.082530
C	-0.809817	3.532560	0.018529
H	-1.691988	3.423428	-0.632425
H	-0.971710	4.417966	0.659104
H	0.062423	3.734379	-0.626692
C	1.006159	2.371583	2.166589
H	0.788512	3.255427	2.794566
H	1.238233	1.541208	2.857311
H	1.909714	2.623051	1.579846
C	-1.945389	1.589943	2.201860
H	-2.848593	1.326597	1.625596
H	-1.683153	0.724890	2.835483
H	-2.198618	2.435630	2.865267
H	2.566249	-2.422394	-0.135993
Au	1.731095	-0.028613	0.417497
P	4.058192	-0.053754	1.170266
C	4.915051	-1.640176	0.991017
H	4.946270	-1.937325	-0.070523
H	5.950585	-1.572764	1.365171
H	4.386640	-2.423870	1.559278
C	5.096677	1.142710	0.290407
H	4.688683	2.158842	0.419473
H	6.133153	1.125589	0.668109
H	5.104344	0.912871	-0.787717
C	4.222847	0.377713	2.922249
H	5.281123	0.387376	3.233916
H	3.789263	1.375863	3.100629
H	3.673801	-0.350486	3.541918
C	-4.549445	-0.161414	-2.341864
C	-3.765180	-1.092173	-0.137772
O	-3.368999	-2.117357	0.344353
O	-4.634190	0.841534	-2.991686
O	-5.465597	-1.114017	-2.297287

O	-4.589257	-0.252755	0.472284
C	-6.648785	-0.907603	-3.057147
H	-7.168378	-0.000557	-2.712612
H	-6.403315	-0.794036	-4.123979
H	-7.274199	-1.794179	-2.897816
C	-5.070591	-0.638360	1.751727
H	-4.233649	-0.731528	2.461518
H	-5.760630	0.151777	2.071694
H	-5.592895	-1.604874	1.687202

IN5

C	-2.016932	-1.907167	0.237906
C	-1.573051	-1.630217	-1.207858
C	-2.164276	0.531638	-0.240205
C	-2.766556	-0.607548	0.644364
H	-2.674657	-2.781861	0.331329
H	-1.127795	-2.051327	0.875681
H	-1.723854	1.328470	0.367906
H	-2.951316	0.997205	-0.859024
C	-1.173186	-0.166093	-1.157848
C	-0.171136	0.379788	-1.947822
C	-0.508555	-2.516489	-1.792507
H	-0.546312	-3.587472	-1.566966
C	0.431020	-2.017765	-2.607244
H	1.176683	-2.681205	-3.057833
C	0.499110	-0.550709	-2.968609
H	0.004580	-0.388319	-3.948681
H	-2.484260	-1.682953	-1.842716
Si	0.143758	2.247113	-2.214394
C	-0.808739	2.721363	-3.753020
H	-1.892592	2.561038	-3.620736
H	-0.653070	3.789700	-3.985604
H	-0.481307	2.139513	-4.631486
C	1.990101	2.454455	-2.468025
H	2.233981	3.523570	-2.598169
H	2.564378	2.086502	-1.598915
H	2.353129	1.926533	-3.365990
C	-0.397779	3.282473	-0.747196
H	-1.493567	3.341662	-0.647004
H	0.022952	2.919306	0.207053
H	-0.029193	4.313064	-0.897356
H	1.548168	-0.248080	-3.118749
Au	0.856428	-0.030627	0.021165
P	2.316226	-0.274167	1.819933
C	3.964573	-0.859562	1.363032
H	4.444878	-0.136798	0.683717
H	4.597330	-0.987236	2.257749
H	3.884347	-1.825167	0.837854
C	2.580690	1.255188	2.748428
H	1.613644	1.655393	3.093009
H	3.232626	1.080977	3.621182
H	3.048275	2.010715	2.096232
C	1.677689	-1.478056	3.008615
H	2.337581	-1.558537	3.889013
H	0.670047	-1.173326	3.332690
H	1.598774	-2.466383	2.526791
C	-2.619405	-0.387359	2.147904
C	-4.267367	-0.754449	0.342703
O	-3.389686	-0.804933	2.960917
O	-4.769590	-1.723729	-0.149479
O	-4.912893	0.355306	0.653583
O	-1.498847	0.269958	2.470694
C	-6.323616	0.351942	0.472284
H	-6.675490	1.341678	0.787011
H	-6.574284	0.168409	-0.583591
H	-6.780922	-0.434389	1.091396
C	-1.311812	0.517153	3.856628
H	-0.364880	1.065027	3.948594
H	-2.139423	1.124071	4.254391
H	-1.273029	-0.428481	4.419826

IN6

C	-3.641037	-2.661208	0.918936
C	-2.095757	-2.604870	0.805455
H	-1.640745	-2.962740	1.743664
H	-1.750886	-3.333507	0.040202
C	-4.342199	-1.629971	0.014227
H	-5.392737	-1.525461	0.327870
H	-4.358092	-2.028780	-1.012385
C	-3.649343	-0.278427	-0.000521
H	-4.161329	0.465783	-0.622744
C	-3.007086	0.279458	1.210721
H	-2.852825	-0.377771	2.071060
C	-2.918197	1.712660	1.512674
H	-3.158453	2.419451	0.712635
C	-2.614881	2.152230	2.744171
H	-2.379922	1.453843	3.555172
H	-2.606403	3.220766	2.978200

C	-1.408377	-1.351507	0.341432
C	-2.128726	-0.254356	-0.189947
Si	-1.271333	1.024391	-1.322033
C	-0.030006	2.063511	-0.377421
H	0.489891	2.742023	-1.076926
H	-0.509658	2.680851	0.399136
H	0.734441	1.437948	0.115068
C	-0.423502	0.041897	-2.675536
H	0.394833	-0.587439	-2.285830
H	-1.139912	-0.618516	-3.194551
H	0.005217	0.726742	-3.428426
C	-2.584225	2.101441	-2.116490
H	-3.309620	1.494254	-2.685921
H	-3.146114	2.735020	-1.410795
H	-2.095893	2.780552	-2.838036
Au	0.633257	-1.342876	0.442293
P	2.995981	-1.289566	0.586559
C	3.653388	-1.715722	2.219828
H	3.341874	-2.737325	2.492099
H	4.755116	-1.660583	2.230225
H	3.251419	-1.022580	2.976697
C	3.824942	-2.417473	-0.564176
H	3.537499	-2.173531	-1.599900
H	4.921598	-2.344372	-0.468993
H	3.514900	-3.454916	-0.358227
C	3.682965	0.346327	0.215314
H	4.784830	0.338580	0.270245
H	3.376800	0.658440	-0.796706
H	3.294776	1.086044	0.934769
C	-4.065310	-2.477853	2.388292
C	-4.086102	-4.078905	0.508319
O	-3.338310	-2.119866	3.276749
O	-4.673687	-4.349743	-0.497380
O	-5.346308	-2.746597	2.541090
O	-3.679215	-4.962832	1.406807
C	-5.884490	-2.648847	3.853953
H	-6.945202	-2.913135	3.769497
H	-5.363802	-3.344886	4.528585
H	-5.770348	-1.623871	4.237760
C	-4.009625	-6.325099	1.167283
H	-3.571811	-6.663517	0.215959
H	-3.593939	-6.893572	2.007861
H	-5.102262	-6.447640	1.120152

IN7

C	1.600809	-1.274505	0.221267
C	0.876293	-0.605400	-0.938422
H	0.804506	-1.200308	-1.856612
H	0.390093	1.192235	-1.976958
C	1.593670	-0.422457	1.513894
H	2.412648	-0.772731	2.160349
H	0.642321	-0.608430	2.044021
C	1.711634	1.076874	1.288930
H	1.591751	1.647487	2.218238
C	2.665504	1.693398	0.303917
H	3.190921	1.012926	-0.371277
C	3.422417	2.926031	0.618132
H	3.008088	3.581942	1.391230
C	4.585127	3.243405	0.034977
H	5.034604	2.600738	-0.729906
H	5.130879	4.149069	0.314026
C	0.694898	0.772969	-1.007980
C	1.069238	1.725617	0.059051
Si	0.127598	3.371192	0.122641
C	0.828989	4.506460	-1.186396
H	1.898352	4.706702	-1.005283
H	0.737219	4.063007	-2.193592
H	0.295039	5.472631	-1.199204
C	-1.694115	3.045815	-0.242405
H	-2.236508	4.007311	-0.282822
H	-1.847666	2.533801	-1.208371
H	-2.151650	2.435501	0.555831
C	0.221314	4.110504	1.842299
H	-0.426722	5.004082	1.884385
H	-0.148090	3.401551	2.604001
H	1.232648	4.432747	2.136827
Au	-1.279480	-0.332230	-0.440814
P	-3.551577	-0.464484	0.109797
C	-3.890293	-0.034574	1.834626
H	-3.568425	1.000709	2.034248
H	-4.967663	-0.122245	2.055614
H	-3.330347	-0.707174	2.504340
C	-4.600758	0.630660	-0.875211
H	-4.500518	0.382833	-1.944417
H	-5.659040	0.531569	-0.579623
H	-4.279638	1.675403	-0.730856
C	-4.214643	-2.131548	-0.115922
H	-5.276722	-2.177687	0.178517

H	-4.119112	-2.429162	-1.172780
H	-3.634035	-2.844744	0.491469
C	3.048175	-1.593477	-0.224364
C	0.926666	-2.619978	0.549559
O	4.035348	-1.222547	0.337261
O	-0.219645	-2.887288	0.295242
O	3.032373	-2.339370	-1.317664
O	1.747440	-3.414223	1.198723
C	4.292050	-2.766032	-1.824686
H	4.075698	-3.368502	-2.714943
H	4.912296	-1.895881	-2.087395
H	4.819979	-3.366613	-1.068789
C	1.254638	-4.684862	1.608545
H	0.930831	-5.265206	0.731665
H	2.087538	-5.184200	2.117189
H	0.403161	-4.558606	2.293919

IN17

C	0.960863	0.020053	-1.617571
C	-0.447953	0.323505	-2.084252
C	3.582713	-0.758219	-0.414834
C	2.593759	-1.760619	-0.814415
C	1.151921	-1.193119	-0.662972
H	1.541130	-0.191083	-2.534027
H	1.411401	0.903026	-1.140582
H	-0.959105	-0.476109	-2.640656
H	2.743416	-2.067971	-1.861711
H	2.695601	-2.661306	-0.187637
C	-0.958236	1.609362	-2.204964
H	-0.363121	2.445096	-1.809290
C	-2.129088	1.962872	-3.022388
H	-2.675817	1.137940	-3.495356
C	-2.516821	3.234602	-3.209924
H	-1.979356	4.069085	-2.745858
H	-3.376232	3.477860	-3.840775
C	4.353506	0.113973	-0.055177
Au	-1.838166	0.629816	-0.330193
P	-2.842476	0.160638	1.730584
C	-4.614840	0.481775	1.883428
H	-4.974707	0.216539	2.892028
H	-4.819898	1.548331	1.697154
H	-5.166605	-0.111883	1.136749
C	-2.614789	-1.583218	2.147050
H	-1.549293	-1.848953	2.061452
H	-2.981905	-1.792365	3.166098
H	-3.155278	-2.211377	1.421021
C	-2.036489	1.095600	3.051019
H	-2.393826	0.770713	4.042867
H	-0.946660	0.947093	2.969873
H	-2.243767	2.171200	2.928058
Si	5.536514	1.437043	0.478257
C	5.916607	1.167837	2.291967
H	6.365168	0.173850	2.459342
H	6.631218	1.928320	2.653039
H	5.003426	1.241694	2.906501
C	7.076871	1.288782	-0.571758
H	7.811839	2.063688	-0.291356
H	7.553513	0.302829	-0.438057
H	6.842344	1.412410	-1.642632
C	4.679947	3.082840	0.209347
H	5.333449	3.915585	0.523657
H	4.431718	3.230861	-0.855564
H	3.746467	3.143012	0.794738
C	0.100814	-2.263699	-0.976345
C	0.961716	-0.771738	0.805434
O	-0.945986	-2.362970	-0.387522
O	0.642774	0.328663	1.175835
O	1.219553	-1.773152	1.622194
O	0.439834	-3.006012	-2.008299
C	-0.476075	-4.016641	-2.419258
H	-0.637553	-4.735058	-1.601897
H	-1.440974	-3.566392	-2.697265
H	-0.016530	-4.511452	-3.282830
C	1.204126	-1.504759	3.016205
H	0.196093	-1.197288	3.336882
H	1.489664	-2.439854	3.512404
H	1.920406	-0.704779	3.255702

IN18

C	-1.831395	1.147350	-1.362775
C	-0.704046	0.225322	-1.890471
C	0.048250	1.564999	0.725271
C	-1.359616	1.587416	1.132271
C	-2.303878	0.908133	0.094761
H	-1.531750	2.205078	-1.429630
H	-2.710637	1.037665	-2.017280
H	-0.059894	0.832600	-2.553932
H	-1.485319	1.115648	2.118887

H	-1.636608	2.652657	1.228828
C	-1.203698	-0.963246	-2.678476
H	-1.968010	-0.796675	-3.448527
C	-0.659264	-2.163026	-2.465211
H	-0.909762	-3.039979	-3.075082
C	0.319892	-2.317831	-1.331816
H	1.279412	-2.768222	-1.644523
H	-0.104199	-2.943357	-0.526158
C	1.212402	1.659613	0.325912
Au	0.629993	-0.491134	-0.444409
P	1.963781	-1.500344	1.348702
C	1.246723	-3.091625	1.824133
H	1.395742	-3.831845	1.021663
H	1.706828	-3.474598	2.750291
H	0.162586	-2.954856	1.979966
C	3.721460	-1.826129	1.059282
H	4.256590	-0.884225	0.857748
H	4.185026	-2.318897	1.930778
H	3.836165	-2.479259	0.178284
C	1.873248	-0.506065	2.857677
H	2.314148	0.489042	2.693915
H	0.811029	-0.370124	3.122471
H	2.391400	-1.003683	3.694502
Si	2.910932	2.219517	-0.253509
C	4.049806	2.183957	1.228007
H	3.651732	2.801543	2.051380
H	4.224507	1.166490	1.613677
H	5.032654	2.600998	0.944365
C	3.461205	1.038879	-1.594731
H	2.746533	1.026485	-2.435612
H	4.439112	1.360870	-1.994440
H	3.575377	0.003786	-1.231363
C	2.667814	3.948366	-0.904088
H	3.626840	4.355169	-1.270900
H	1.950662	3.961426	-1.741987
H	2.291788	4.623347	-0.116802
C	-2.417060	-0.592647	0.396423
C	-3.702330	1.525894	0.295882
O	-1.709771	-1.195738	1.166623
O	-4.280487	2.189321	-0.511948
O	-4.153652	1.242154	1.508968
O	-3.364920	-1.139578	-0.328610
C	-3.537278	-2.547059	-0.245184
H	-2.659238	-3.049758	-0.681200
H	-3.662268	-2.856874	0.802597
H	-4.434718	-2.780492	-0.830011
C	-5.439531	1.746888	1.852758
H	-5.639231	1.405295	2.875376
H	-5.443424	2.846269	1.803622
H	-6.197826	1.355603	1.158030

TS1

C	-2.747421	-2.055854	0.356329
C	-1.251188	-2.065633	0.118245
C	-1.094481	-0.316480	-0.951222
C	-2.540179	-0.254112	-1.295459
C	-3.320258	-0.671778	-0.038875
H	-3.230849	-2.823079	-0.269283
H	-2.966689	-2.272037	1.411943
H	-0.620783	-1.776334	0.963604
H	-2.793303	0.764645	-1.620127
H	-2.800597	-0.934323	-2.122929
C	-0.694454	-2.698155	-0.979549
H	-1.368444	-3.001387	-1.790589
C	0.710771	-2.971617	-1.167430
H	1.034997	-3.219694	-2.183608
C	1.631500	-2.916139	-0.173776
H	1.346463	-2.783887	0.874660
H	2.681703	-3.142119	-0.380523
C	-0.006646	0.351888	-0.782221
Au	1.903622	-0.097069	-0.133812
P	4.124527	-0.256495	0.630106
C	5.308165	-0.767930	-0.643669
H	6.331344	-0.826438	-0.235323
H	5.027775	-1.754631	-1.046999
H	5.293966	-0.044956	-1.475575
C	4.781994	1.305091	1.272389
H	4.749430	2.075246	0.484613
H	4.161898	1.650565	2.115617
H	5.823466	1.187834	1.616834
C	4.357494	-1.441024	1.982671
H	3.721294	-1.159767	2.837928
H	4.065131	-2.452249	1.655398
H	5.409940	-1.466633	2.312433
Si	-0.051533	2.271238	-0.819424
C	0.188515	2.741594	0.979992
H	-0.464801	2.129749	1.627314

H	1.230458	2.568828	1.300282
H	-0.044262	3.808446	1.146419
C	1.353655	2.863619	-1.905363
H	1.277779	2.435228	-2.919877
H	1.330288	3.963504	-2.001542
H	2.333766	2.576742	-1.487824
C	-1.660678	2.977985	-1.465693
H	-1.865938	2.673680	-2.506580
H	-2.533386	2.720745	-0.844266
H	-1.565264	4.079150	-1.464035
C	-3.053133	0.351927	1.070349
C	-4.817628	-0.771880	-0.332862
O	-2.274012	0.190509	1.968983
O	-5.292882	-0.694543	-1.429235
O	-5.495149	-1.001626	0.777665
O	-3.747013	1.459414	0.867251
C	-3.597087	2.511586	1.811731
H	-2.586316	2.943326	1.739373
H	-4.352266	3.264112	1.554520
H	-3.755981	2.133464	2.832431
C	-6.907140	-1.129962	0.657944
H	-7.158981	-1.964012	-0.014312
H	-7.283998	-1.322033	1.669544
H	-7.338781	-0.201937	0.253514

TS2

C	-3.205667	-1.820649	-2.524223
C	-1.747635	-1.475585	-2.171183
C	-3.160208	0.563112	-2.059553
C	-4.080699	-0.670526	-1.972867
H	-3.326724	-1.883628	-3.616776
H	-3.491001	-2.787008	-2.088067
H	-3.518508	1.405889	-1.455130
H	-3.146062	0.909408	-3.107390
C	-1.799232	0.058480	-1.610536
C	-0.924922	0.556087	-0.717599
C	-0.901461	-0.972251	-3.216251
H	-1.394806	-0.447462	-4.043066
C	0.522623	-1.053398	-3.248641
H	1.046266	-0.442192	-3.990238
C	1.242011	-1.800393	-2.363140
H	0.768484	-2.507131	-1.676059
H	-1.289317	-2.124176	-1.419615
Si	-1.457960	1.999957	0.423627
C	-1.624104	3.523062	-0.658129
H	-2.405361	3.421646	-1.428719
H	-1.880802	4.395900	-0.031279
H	-0.670371	3.743433	-1.167744
C	-0.134253	2.314032	1.719874
H	-0.452483	3.140391	2.380731
H	0.033638	1.426727	2.355210
H	0.826419	2.604316	1.259831
C	-3.046253	1.546504	1.311244
H	-3.934061	1.597491	0.661691
H	-2.969627	0.519828	1.710145
H	-3.212159	2.235104	2.158212
H	2.334219	-1.823609	-2.420484
Au	0.975106	-0.038346	-0.204700
P	3.145627	-0.421456	0.665904
C	3.619864	-2.164906	0.824879
H	3.622444	-2.650487	-0.164683
H	4.624291	-2.265434	1.269975
H	2.891991	-2.692248	1.463142
C	4.482797	0.335202	-0.297163
H	4.318764	1.422928	-0.367973
H	5.464711	0.150140	0.170502
H	4.492564	-0.074128	-1.320450
C	3.339077	0.257796	2.334937
H	4.359885	0.093078	2.719474
H	3.128811	1.339935	2.322683
H	2.617131	-0.221267	3.016567
C	-5.353244	-0.491658	-2.799468
C	-4.419722	-0.948829	-0.504537
O	-3.769962	-1.667328	0.205143
O	-5.586174	0.463339	-3.484175
O	-6.130529	-1.556018	-2.692959
O	-5.483806	-0.269609	-0.116410
C	-7.358976	-1.530929	-3.408006
H	-7.980527	-0.690051	-3.064675
H	-7.172446	-1.419004	-4.486886
H	-7.854932	-2.486539	-3.199686
C	-5.949958	-0.482360	1.209606
H	-5.206086	-0.127832	1.938610
H	-6.879812	0.091571	1.301761
H	-6.137114	-1.553757	1.376430

TS3

C	-3.623414	-2.354519	-0.111958

C	-2.348695	-2.080538	-0.919371
C	-3.165884	-0.006069	0.154145
C	-4.332485	-0.983089	-0.085530
H	-4.250198	-3.126972	-0.579628
H	-3.379004	-2.653983	0.921178
H	-2.900585	-0.033861	1.225051
H	-3.410605	1.032319	-0.106023
C	-1.989796	-0.588285	-0.620435
C	-0.934040	0.116661	-1.041658
C	-1.214072	-3.028611	-0.787782
H	-1.273772	-3.843825	-0.058564
C	-0.090460	-2.835829	-1.522541
H	0.775002	-3.495496	-1.401280
C	0.040962	-1.661052	-2.381200
H	-0.858051	-1.309415	-2.893375
H	-2.647925	-2.031537	-1.984016
Si	-0.985715	1.975144	-1.484263
C	-2.491706	2.227816	-2.569311
H	-3.429116	1.915648	-2.079679
H	-2.591674	3.293693	-2.840956
H	-2.387890	1.651740	-3.505340
C	0.552335	2.435956	-2.455247
H	0.436572	3.456306	-2.862694
H	1.460595	2.431492	-1.828275
H	0.716480	1.755964	-3.309258
C	-1.060396	2.963433	0.104682
H	-1.947337	2.719734	0.712104
H	-0.165574	2.773894	0.722162
H	-1.095501	4.044117	-0.121486
H	0.919885	-1.618347	-3.039459
Au	1.075759	-0.371811	-0.858019
P	3.281511	-0.154603	-0.023092
C	4.479363	-1.295945	-0.760849
H	4.513967	-1.147985	-1.852472
H	5.487562	-1.130293	-0.344320
H	4.176754	-2.336945	-0.562508
C	3.961790	1.497729	-0.320606
H	3.329771	2.256591	0.169340
H	4.989424	1.580450	0.072431
H	3.975491	1.706267	-1.403191
C	3.418980	-0.413994	1.763552
H	4.461056	-0.284219	2.101654
H	2.775870	0.304613	2.297090
H	3.082560	-1.431671	2.020485
C	-5.434531	-0.959214	0.975771
C	-4.987611	-0.682559	-1.442555
O	-6.580975	-1.205997	0.735615
O	-5.000813	-1.432202	-2.378321
O	-5.496325	0.538885	-1.456851
O	-4.959575	-0.697347	2.184817
C	-6.202672	0.926306	-2.627824
H	-6.573884	1.941131	-2.440912
H	-5.532363	0.911921	-3.501350
H	-7.041052	0.236599	-2.807296
C	-5.897230	-0.725642	3.254268
H	-5.333658	-0.484365	4.163639
H	-6.692411	0.015423	3.082866
H	-6.354208	-1.723656	3.334962

TS4

C	3.685492	0.137809	0.069738
C	3.000652	1.486530	0.033612
C	1.138976	0.858383	-0.679522
C	1.673083	-0.428911	-1.224782
C	2.613615	-0.963338	-0.131441
H	4.420746	0.062350	-0.747557
H	4.198992	-0.005766	1.030597
H	2.724704	1.932743	0.991449
H	0.840434	-1.120801	-1.412385
H	2.233564	-0.312650	-2.165074
C	2.883579	2.231145	-1.122609
H	3.226699	1.785088	-2.065869
C	2.428937	3.611665	-1.200020
H	2.153460	4.110731	-0.267105
C	2.383912	4.279048	-2.366517
H	2.666454	3.798702	-3.310066
H	2.072718	5.326841	-2.411432
C	0.094338	1.360082	-0.102814
Au	-1.511401	0.009296	-0.299254
P	-3.303407	-1.478933	-0.449133
C	-3.890225	-2.043931	1.169317
H	-4.212939	-1.179130	1.771776
H	-4.734713	-2.746202	1.065363
H	-3.069574	-2.547190	1.705822
C	-4.767500	-0.796371	-1.267086
H	-4.510821	-0.486899	-2.293291
H	-5.581088	-1.540375	-1.307723
H	-5.120137	0.092731	-0.719480

C	-2.911610	-2.992747	-1.363222
H	-3.776304	-3.677343	-1.389306
H	-2.623638	-2.738520	-2.396379
H	-2.058935	-3.505307	-0.889019
Si	-0.372446	2.812295	1.017857
C	-0.946092	4.224973	-0.065089
H	-1.801928	3.900962	-0.682181
H	-1.283210	5.069388	0.561713
H	-0.161468	4.589929	-0.745408
C	-1.799811	2.234807	2.092803
H	-2.041379	3.013136	2.838637
H	-2.713330	2.042172	1.504642
H	-1.538314	1.315020	2.644702
C	1.015600	3.251482	2.203921
H	1.389385	2.335651	2.696925
H	1.871101	3.791686	1.771007
H	0.592262	3.899237	2.992393
C	1.809246	-1.137620	1.164972
C	3.252141	-2.286234	-0.554992
O	1.937520	-0.458148	2.143735
O	3.174262	-2.744879	-1.658637
O	3.922371	-2.822812	0.448712
O	0.903224	-2.096879	1.035257
C	0.036298	-2.305369	2.138148
H	-0.612343	-1.423624	2.276416
H	-0.561664	-3.193319	1.895758
H	0.613716	-2.472523	3.059674
C	4.594371	-4.051638	0.196617
H	5.335510	-3.922677	-0.606545
H	5.087626	-4.328656	1.135830
H	3.871411	-4.824734	-0.104542

TS5

C	2.579987	-0.912983	-0.314148
C	1.445728	-0.693048	-1.348084
H	1.876425	-0.306009	-2.287891
H	0.963888	-1.648842	-1.585667
C	3.568330	0.273015	-0.312970
H	4.121147	0.231076	-1.267519
H	4.288073	0.116580	0.503784
C	2.964584	1.656060	-0.166202
H	3.059220	2.127520	0.814668
C	2.578530	2.415981	-1.239482
H	2.549356	1.941642	-2.230073
C	2.265586	3.839635	-1.214610
H	2.369839	4.367342	-0.261711
C	1.898897	4.512482	-2.319623
H	1.799514	4.007159	-3.286850
H	1.697478	5.587206	-2.291691
C	0.483092	0.290844	-0.737700
C	0.686631	1.411457	-0.131320
Si	0.023828	2.582677	1.213446
C	1.403657	3.289306	2.255235
H	1.990702	2.466220	2.698874
H	2.086018	3.987071	1.748793
H	0.931254	3.843238	3.086495
C	-1.038583	3.868413	0.377307
H	-1.518562	4.519777	1.128703
H	-0.449730	4.501937	-0.305356
H	-1.834764	3.383345	-0.213629
C	-0.970133	1.493558	2.372859
H	-1.230962	2.073614	3.276221
H	-1.906191	1.120327	1.927087
H	-0.346930	0.637417	2.684872
Au	-1.506037	-0.270904	-0.441569
P	-3.720069	-1.007301	-0.227311
C	-3.888730	-2.809746	-0.202268
H	-3.321920	-3.227047	0.645511
H	-4.947290	-3.105642	-0.107732
H	-3.478002	-3.235685	-1.132171
C	-4.521806	-0.434268	1.293152
H	-5.557504	-0.808685	1.361039
H	-3.955122	-0.785858	2.170858
H	-4.538969	0.667827	1.313027
C	-4.798147	-0.448979	-1.570499
H	-5.829251	-0.814320	-1.427397
H	-4.808220	0.652433	-1.608508
H	-4.414895	-0.821188	-2.534564
C	3.353804	-2.187193	-0.683278
C	1.964190	-1.086799	1.082187
O	3.221922	-2.780984	-1.714501
O	2.141554	-0.349312	2.012232
O	4.199660	-2.515865	0.278362
O	1.162352	-2.141241	1.107020
C	4.999952	-3.673094	0.068286
H	5.620069	-3.783226	0.965857
H	4.359767	-4.557122	-0.072066
H	5.630689	-3.543360	-0.824139

C	0.459450	-2.395718	2.311689
H	-0.009926	-3.380041	2.193711
H	1.146603	-2.394134	3.170608
H	-0.311458	-1.621458	2.464156

TS6

C	2.830084	-0.537955	-0.465644
C	1.398268	-1.009817	-0.446407
H	1.221592	-2.092079	-0.499108
H	0.512530	-0.654608	-1.559615
C	2.971080	0.699978	-1.394741
H	2.792221	0.369200	-2.431689
H	4.008025	1.057620	-1.328266
C	1.998875	1.789175	-0.964018
H	2.470953	2.644484	-0.472718
C	0.711066	2.099232	-1.728954
H	0.507235	1.462226	-2.601875
C	0.227682	3.493861	-1.873927
H	0.499134	4.190298	-1.071422
C	-0.485501	3.933216	-2.917458
H	-0.763809	3.266114	-3.741075
H	-0.805724	4.976509	-2.987476
C	0.324358	-0.109679	-0.436441
C	0.653146	1.348931	-0.364410
Si	0.043674	2.158004	1.249239
C	-1.692999	2.821717	1.008427
H	-1.727829	3.569557	0.198399
H	-2.397719	2.012813	0.746768
H	-2.058181	3.300095	1.934256
C	0.043742	0.818242	2.571710
H	-0.007282	1.276140	3.575061
H	-0.815142	0.132249	2.474425
H	0.961307	0.206324	2.532158
C	1.254167	3.491274	1.748885
H	1.329183	4.317991	1.023200
H	0.944734	3.929993	2.713885
H	2.258492	3.051066	1.880228
Au	-1.678621	-0.649016	-0.227633
P	-3.955581	-1.138761	0.079431
C	-4.817156	-1.611120	-1.441626
H	-4.738714	-0.799227	-2.182871
H	-4.352123	-2.513926	-1.869924
H	-5.882975	-1.815265	-1.243063
C	-4.265849	-2.492063	1.241667
H	-3.833803	-2.247281	2.225609
H	-5.348180	-2.670482	1.358872
H	-3.787263	-3.415372	0.876594
C	-4.883976	0.272430	0.733151
H	-5.948431	0.017230	0.871308
H	-4.460511	0.581664	1.702854
H	-4.806581	1.124392	0.037735
C	3.728480	-1.683576	-0.955935
C	3.235457	-0.155648	0.978571
O	3.312340	-2.669506	-1.495631
O	3.610731	0.925360	1.320532
O	4.995494	-1.409056	-0.732538
O	3.093368	-1.202269	1.774339
C	5.957469	-2.368998	-1.161312
H	5.891029	-2.510580	-2.250383
H	6.936978	-1.962795	-0.883350
H	5.778649	-3.332168	-0.660481
C	3.493012	-1.041912	3.132969
H	4.560880	-0.781638	3.182142
H	2.904561	-0.243408	3.610144
H	3.306213	-2.005499	3.621241

TS13

C	-0.324961	-1.440152	-1.814264
C	0.110047	-0.018885	-1.462281
C	-2.741474	-0.931869	-0.160562
C	-1.611990	-1.668723	0.404755
C	-0.786955	-2.387059	-0.691559
H	-1.223844	-1.273548	-2.437070
H	0.404958	-1.944268	-2.461679
H	-0.599860	0.497268	-0.798631
H	-0.943017	-0.983151	0.950184
H	-1.957235	-2.418386	1.134729
C	0.670315	0.771423	-2.508937
H	0.147977	1.685453	-2.822640
C	1.804246	0.284628	-3.145808
H	1.987134	0.419915	-4.221010
C	2.774472	-0.336172	-2.291099
H	3.313963	0.460356	-1.715523
H	3.502174	-1.022529	-2.746283
C	-3.659570	-0.329205	-0.688131
Au	2.098261	-0.559241	-0.216909
P	2.149673	-0.631602	2.170798
C	3.055692	-2.075114	2.779124

H	4.064288	-2.108210	2.335706
H	3.150434	-2.037475	3.877796
H	2.497993	-2.980352	2.490613
C	3.053040	0.804754	2.811014
H	2.523747	1.733845	2.542669
H	3.145370	0.752474	3.909197
H	4.062649	0.845116	2.370513
C	0.593115	-0.646189	3.090805
H	-0.037121	0.211416	2.804866
H	0.063063	-1.584766	2.868516
H	0.799512	-0.589023	4.173240
Si	-5.088636	0.520008	-1.512546
C	-6.211741	-0.815544	-2.185136
H	-5.672499	-1.462466	-2.897827
H	-6.600831	-1.450847	-1.371404
H	-7.074082	-0.369422	-2.711009
C	-5.950320	1.573598	-0.229284
H	-5.269132	2.335214	0.186792
H	-6.813098	2.097174	-0.677417
H	-6.323776	0.955686	0.604884
C	-4.385731	1.574478	-2.894370
H	-5.198117	2.097352	-3.429214
H	-3.694612	2.339736	-2.501578
H	-3.842474	0.955825	-3.629003
C	0.372917	-3.135142	-0.023538
C	-1.678726	-3.468433	-1.352314
O	0.552470	-3.206927	1.164565
O	-2.077938	-3.424101	-2.478198
O	-1.946129	-4.432856	-0.489655
O	1.158523	-3.703958	-0.920656
C	2.273234	-4.439714	-0.439080
H	1.943537	-5.226282	0.255935
H	2.756481	-4.879170	-1.319674
H	2.972784	-3.764920	0.082164
C	-2.789933	-5.487204	-0.940087
H	-3.773350	-5.086810	-1.228333
H	-2.338220	-5.990626	-1.808041
H	-2.887789	-6.181097	-0.096840

TS14

C	2.258238	-1.363293	0.832349
C	1.002985	-1.034536	1.668492
C	0.702596	0.706532	1.120575
C	2.156065	1.076411	1.011124
C	2.763846	-0.061201	0.167973
H	3.029256	-1.783596	1.499680
H	2.023251	-2.119687	0.071395
H	1.297661	-0.543359	2.608156
H	2.272229	2.057310	0.528860
H	2.667810	1.106539	1.987285
C	0.381123	-2.353066	2.183069
H	0.856597	-2.696580	3.110349
C	-0.474510	-3.156900	1.542480
H	-0.695590	-4.138628	1.981958
C	-1.137454	-2.757313	0.248454
H	-2.155513	-3.168795	0.192677
H	-0.579588	-3.138676	-0.628014
C	-0.425815	1.278196	0.768433
Au	-1.040959	-0.671011	0.379870
P	-3.035148	-0.303181	-0.696493
C	-3.842510	-1.790271	-1.312536
H	-4.162499	-2.429857	-0.475453
H	-4.729828	-1.505946	-1.903861
H	-3.149616	-2.362587	-1.949727
C	-4.235692	0.512433	0.368422
H	-3.811158	1.445518	0.766276
H	-5.160863	0.734193	-0.190853
H	-4.476544	-0.151136	1.215152
C	-2.750223	0.720748	-2.150937
H	-2.307513	1.683335	-1.858032
H	-2.044483	0.202184	-2.821000
H	-3.697384	0.901331	-2.687218
Si	-0.615240	3.086916	0.302617
C	0.151214	3.254250	-1.404779
H	0.075296	4.290738	-1.777878
H	1.221699	2.986229	-1.368718
H	-0.333868	2.591326	-2.141465
C	-2.408670	3.637746	0.301734
H	-3.035715	3.164380	-0.470356
H	-2.874671	3.465445	1.287924
H	-2.440722	4.726334	0.116337
C	0.311375	4.115503	1.560802
H	-0.105386	3.966621	2.571928
H	1.385525	3.870386	1.598952
H	0.223924	5.188755	1.315519
C	2.211238	0.056013	-1.259477
C	4.290311	0.016963	0.154217
O	1.273298	-0.567246	-1.685438

O	4.932759	0.775907	0.820820
O	4.792656	-0.896714	-0.658589
O	2.857227	0.980180	-1.945100
C	2.482090	1.175747	-3.301570
H	3.157018	1.943725	-3.697944
H	2.593236	0.235954	-3.863211
H	1.436854	1.513850	-3.363586
C	6.209762	-0.954521	-0.765905
H	6.601467	0.003412	-1.140310
H	6.659312	-1.164285	0.216446
H	6.431026	-1.764134	-1.471609

TS15

Au	1.730904	0.231414	-0.017285
P	3.318424	1.995383	0.039020
C	0.343630	-1.238497	0.000122
C	4.017905	2.392359	-1.584883
C	4.748650	1.674340	1.103279
C	2.615478	3.551564	0.642658
C	-1.053891	-0.887549	-0.391360
Si	0.742001	-2.823551	0.973161
H	4.739987	3.223084	-1.509877
H	3.211560	2.681279	-2.278599
H	4.530455	1.509066	-1.999569
H	5.282823	0.776573	0.751769
H	4.412225	1.491233	2.136798
H	5.444650	2.530240	1.099209
H	2.232164	3.416180	1.667186
H	3.373696	4.352846	0.645815
H	1.773129	3.854815	-0.000495
C	-1.832146	-0.000711	0.576615
C	-2.023432	-1.780388	-1.160831
C	-1.208410	-0.721617	-1.913853
C	2.485908	-3.348916	0.563229
C	-0.508037	-4.189032	0.724970
C	0.612379	-2.139717	2.723107
C	-3.295941	-0.061583	0.061200
H	-1.459319	1.033932	0.599341
H	-1.766360	-0.429984	1.591276
C	-3.430149	-1.394182	-0.728613
H	-1.829532	-2.836434	-1.366208
C	0.099561	-1.137646	-2.514856
H	-1.683239	0.168548	-2.334572
H	2.783898	-4.203448	1.195717
H	2.575515	-3.665408	-0.489541
H	3.202187	-2.528578	0.739641
H	-1.534894	-3.831815	0.912253
H	-0.469297	-4.631045	-0.284930
H	-0.304563	-5.003904	1.442610
H	0.874601	-2.947892	3.430276
H	-0.411281	-1.808175	2.965123
H	1.305443	-1.299298	2.892282
C	-4.256089	-0.026072	1.259903
C	-3.597756	1.151455	-0.830064
H	-3.828983	-2.156834	-0.041567
H	-4.139914	-1.298004	-1.564969
C	0.668387	-2.358994	-2.405868
H	0.678370	-0.334451	-2.987862
O	-4.329449	1.199748	1.756105
O	-4.814129	-0.979305	1.720426
O	-4.868679	1.154106	-1.188885
O	-2.794381	1.973958	-1.177908
H	0.129955	-3.223417	-2.007758
H	1.681653	-2.531417	-2.779624
C	-5.171552	1.387795	2.885219
C	-5.314718	2.232648	-1.998588
H	-6.208227	1.114945	2.635978
H	-5.105106	2.451449	3.143908
H	-4.831922	0.762968	3.725296
H	-4.768740	2.245975	-2.954200
H	-6.384683	2.064786	-2.170245
H	-5.151453	3.189552	-1.480150

TS16

Au	-1.043643	0.540751	-0.075142
P	-1.193261	2.850590	-0.319936
C	-0.280969	3.699815	0.990529
C	-2.853358	3.568644	-0.327935
C	-0.397558	3.383019	-1.852707
H	-0.287248	4.792445	0.839067
H	-0.716763	3.467271	1.975393
H	0.756339	3.328660	0.962458
H	-2.807634	4.664482	-0.446258
H	-3.370077	3.329706	0.615692
H	-3.439903	3.143322	-1.158415
H	-0.927042	2.960556	-2.721803
H	-0.386619	4.483069	-1.934370
H	0.635692	2.998593	-1.849699

C	5.310050	-1.014720	-2.256284
O	4.132073	-0.690983	-1.525097
H	5.356924	-0.305173	-3.090947
H	5.254662	-2.048471	-2.629289
H	6.195904	-0.914671	-1.611220
C	3.868970	-1.426953	-0.455996
C	2.549111	-0.971780	0.199537
O	4.530855	-2.348541	-0.081010
C	1.384024	-1.532810	-0.644439
C	2.436307	-1.536619	1.641818
C	2.555235	0.562066	0.215840
C	0.066734	-1.484023	0.059412
H	1.316755	-1.013343	-1.612965
H	1.587683	-2.601168	-0.845034
C	0.985327	-1.651196	2.037284
H	2.921753	-2.523727	1.641647
H	2.999656	-0.892414	2.333519
O	3.580644	1.012549	0.909721
O	1.747833	1.279677	-0.322594
C	-1.204279	-1.646302	0.064481
C	0.289465	-0.678317	2.733040
H	0.563860	-2.660824	2.015645
C	3.780624	2.415424	0.975269
Si	-2.765875	-2.278148	-0.767530
C	-1.120082	-0.748711	2.882273
H	0.801663	0.252705	3.005414
H	4.734431	2.565409	1.495094
H	3.820686	2.844381	-0.037090
H	2.965871	2.891245	1.543633
C	-2.390942	-2.320341	-2.599984
C	-3.103341	-3.983328	-0.083797
C	-4.164978	-1.087836	-0.412411
C	-1.862083	-1.785434	2.359081
H	-1.643028	0.134371	3.265400
H	-2.122354	-1.315686	-2.970276
H	-1.554101	-3.004076	-2.822404
H	-3.270534	-2.666587	-3.171186
H	-2.232078	-4.648012	-0.213364
H	-3.953298	-4.438451	-0.622754
H	-3.364267	-3.958435	0.987275
H	-3.982220	-0.107742	-0.886216
H	-4.312346	-0.923933	0.667685
H	-5.109791	-1.484640	-0.824280
H	-2.954877	-1.744050	2.386028
H	-1.429508	-2.774136	2.196054

TS1a

C	-2.651634	-1.649639	0.706382
C	-1.162690	-1.767975	0.530060
C	-1.112010	-0.290328	-1.393696
C	-2.565345	-0.457282	-1.474726
C	-3.184802	-0.417426	-0.067969
H	-3.153178	-2.547454	0.309859
H	-2.906372	-1.540983	1.770791
H	-0.529157	-1.226496	1.242849
H	-2.916362	0.410699	-2.066649
H	-2.883608	-1.371248	-2.001082
C	-0.587286	-2.560938	-0.421543
H	-1.233015	-3.094271	-1.132306
C	0.843887	-2.827327	-0.515884
H	1.468054	-2.491391	0.319041
C	1.395911	-3.488153	-1.548260
H	0.786459	-3.848466	-2.384545
H	2.469650	-3.692040	-1.588317
C	-0.049347	0.412646	-1.548484
Au	1.666012	0.242454	-0.381452
P	3.574795	0.226323	0.972116
C	3.915856	-1.389146	1.720372
H	4.068038	-2.143438	0.931016
H	4.819238	-1.350366	2.352732
H	3.061327	-1.702260	2.342769
C	5.097787	0.669693	0.099326
H	5.001676	1.681912	-0.326054
H	5.964792	0.646758	0.781136
H	5.272687	-0.034686	-0.730122
C	3.472633	1.375686	2.367373
H	3.345497	2.404350	1.992670
H	2.598316	1.129196	2.991589
H	4.384448	1.328162	2.986588
C	-2.762416	0.872914	0.650559
C	-4.712360	-0.479618	-0.176213
O	-2.057695	0.911805	1.619281
O	-5.301640	-0.717478	-1.190973
O	-5.270180	-0.273245	1.001794
O	-3.252994	1.932300	0.031235
C	-2.964125	3.204416	0.597142
H	-3.454222	3.944850	-0.046237
H	-3.359812	3.261600	1.622308

H	-1.876806	3.371543	0.623495
C	-6.692193	-0.316754	1.061867
H	-6.959795	-0.118207	2.106369
H	-7.122485	0.448333	0.398315
H	-7.055717	-1.307475	0.750126
C	-0.052943	1.578458	-2.549596
H	-1.031226	1.715050	-3.036391
H	0.226539	2.507332	-2.029565
H	0.706612	1.386908	-3.323649

IN1a

C	2.465046	0.798986	1.435322
C	1.118428	0.420882	2.007162
C	0.358647	1.643548	-0.673149
C	1.784977	1.433419	-1.006374
C	2.616934	0.507104	-0.083342
H	2.666444	1.869084	1.596068
H	3.260418	0.242220	1.952671
H	0.372162	1.216280	2.110868
H	1.858144	1.046960	-2.036024
H	2.245540	2.437336	-0.993815
C	0.784137	-0.819406	2.414616
H	1.523999	-1.629291	2.354905
C	-0.529285	-1.150468	2.969552
H	-1.260168	-0.331422	3.013833
C	-0.863035	-2.365434	3.438608
H	-0.144909	-3.193825	3.432528
H	-1.845633	-2.561429	3.878114
C	-0.746113	2.167548	-0.467277
Au	-1.038157	-0.065492	-0.493765
P	-2.074903	-2.161999	-0.518344
C	-3.443549	-2.373783	0.642387
H	-4.232985	-1.633377	0.435617
H	-3.869653	-3.388088	0.559988
H	-3.072786	-2.219059	1.667873
C	-2.743821	-2.571889	-2.148705
H	-1.938485	-2.526131	-2.899938
H	-3.180979	-3.584782	-2.149811
H	-3.521375	-1.843937	-2.431448
C	-0.888971	-3.471179	-0.142510
H	-1.359802	-4.465496	-0.221046
H	-0.042771	-3.392308	-0.843370
H	-0.513532	-3.323215	0.883243
C	2.296423	-0.968117	-0.360521
C	4.069724	0.696352	-0.576281
O	1.412256	-1.369212	-1.074100
O	4.432045	0.281421	-1.640929
O	4.814390	1.386067	0.261680
O	3.117879	-1.753685	0.304646
C	2.975996	-3.155881	0.133582
H	3.042918	-3.418698	-0.932709
H	3.795338	-3.618909	0.696196
H	2.003540	-3.487366	0.532136
C	6.161952	1.633155	-0.130228
H	6.613820	2.214143	0.682332
H	6.694820	0.680894	-0.270467
H	6.185418	2.198701	-1.073805
C	-1.893698	3.060714	-0.234092
H	-1.542160	4.105332	-0.262793
H	-2.659905	2.922441	-1.012491
H	-2.348692	2.866552	0.749698

IN1b

C	-3.503465	-2.437065	-0.526659
C	-3.594492	-1.307781	0.478611
C	-1.964339	0.221774	-1.557365
C	-2.452871	-0.985428	-2.297975
H	-3.275835	-3.382054	-0.010476
H	-4.464452	-2.567295	-1.050904
H	-4.396058	-0.571729	0.337976
H	-3.484984	-0.774146	-2.626961
H	-1.828168	-1.108012	-3.194649
C	-2.696116	-1.118448	1.460993
H	-1.883601	-1.846484	1.595743
C	-2.691557	0.074660	2.307425
H	-3.549310	0.752363	2.207618
C	-1.693697	0.383940	3.153015
H	-0.835917	-0.285462	3.275471
H	-1.712518	1.293944	3.759244
C	-1.779594	1.363413	-1.116857
Au	-0.176300	-0.007076	-0.258843
P	1.677128	-0.980729	0.781144
C	1.270484	-2.121274	2.120411
H	0.577841	-2.884230	1.729919
H	2.186105	-2.608890	2.496001
H	0.789519	-1.585215	2.953536
C	2.614316	-1.959649	-0.412016
H	2.975664	-1.311846	-1.226783

H	3.472156	-2.452337	0.075640
H	1.945746	-2.714442	-0.853825
C	2.841468	0.215196	1.479818
H	3.709666	-0.301938	1.922468
H	3.195277	0.899679	0.691958
H	2.343725	0.812877	2.260571
C	-1.791236	2.776882	-0.709491
H	-2.637841	3.282890	-1.202345
H	-1.912123	2.860352	0.382076
H	-0.857327	3.279169	-1.005948
N	-2.458006	-2.223313	-1.543368
S	-1.064830	-3.104024	-1.448261
O	-0.745774	-3.358211	-0.050141
O	-0.087200	-2.428783	-2.285470
C	-1.474266	-4.685078	-2.200713
H	-0.574255	-5.311951	-2.116702
H	-2.309462	-5.134674	-1.645263
H	-1.736136	-4.504397	-3.251963

IN1c

C	2.587398	0.424516	1.559961
C	1.245045	0.351925	2.240662
C	0.624436	2.274453	-0.244945
C	2.100335	2.079544	-0.247692
H	3.223965	1.201874	2.022672
H	3.107030	-0.539069	1.651357
H	0.664924	1.280143	2.326820
H	2.510284	2.324657	-1.242298
H	2.546529	2.810628	0.452914
C	0.717916	-0.789498	2.718459
H	1.310446	-1.713141	2.671694
C	-0.629355	-0.881848	3.281934
H	-1.212874	0.048439	3.312004
C	-1.168912	-2.024966	3.740046
H	-0.599557	-2.962250	3.741280
H	-2.179979	-2.053954	4.156727
C	-0.576132	2.576133	-0.170741
Au	-0.611604	0.324522	-0.356151
P	-1.116498	-1.932854	-0.588421
C	-2.627607	-2.453961	0.252126
H	-3.492979	-1.901046	-0.147464
H	-2.794467	-3.535602	0.112368
H	-2.532836	-2.236658	1.328505
C	-1.330404	-2.425241	-2.317336
H	-0.411114	-2.228004	-2.892352
H	-1.563440	-3.501462	-2.385596
H	-2.151353	-1.849439	-2.774299
C	0.205411	-2.976359	0.068810
H	0.069875	-4.022895	-0.252650
H	1.202351	-2.619053	-0.246839
H	0.162372	-2.932700	1.168044
Si	-2.326418	3.222817	0.118086
C	-2.876548	2.354876	1.681304
H	-3.898868	2.665272	1.960346
H	-2.882074	1.258513	1.545072
H	-2.209461	2.598100	2.526478
C	-2.183335	5.068238	0.311174
H	-3.180563	5.502802	0.502648
H	-1.529557	5.335576	1.158254
H	-1.779975	5.537601	-0.601828
C	-3.330738	2.703018	-1.364950
H	-2.917586	3.124484	-2.297059
H	-3.357542	1.604149	-1.464788
H	-4.371356	3.058802	-1.265495
N	2.447885	0.722011	0.124390
S	3.312846	-0.181797	-0.978818
O	4.439269	0.583452	-1.459214
O	3.480746	-1.484313	-0.367191
C	2.184771	-0.368424	-2.378356
H	1.353041	-1.017288	-2.080530
H	1.829118	0.613149	-2.722732
H	2.793182	-0.842405	-3.163584

IN1d

C	2.382537	0.827470	1.459758
C	1.048577	0.424368	2.043965
C	0.238507	1.649093	-0.589135
C	1.656356	1.467975	-0.968365
C	2.521278	0.551555	-0.063989
H	2.568582	1.899238	1.626571
H	3.193092	0.279058	1.962662
H	0.294294	1.208790	2.166835
H	1.712336	1.084763	-1.999923
H	2.101638	2.478675	-0.962381
C	0.722841	-0.824639	2.429919
H	1.462366	-1.632849	2.351291
C	-0.590690	-1.165247	2.979073
H	-1.320597	-0.345666	3.032446

C	-0.927594	-2.387183	3.427122
H	-0.210240	-3.216096	3.410767
H	-1.911825	-2.588650	3.860390
C	-0.861431	2.137372	-0.289859
Au	-1.123833	-0.095296	-0.442406
P	-2.116788	-2.208163	-0.522664
C	-3.492435	-2.463477	0.621559
H	-4.292891	-1.733843	0.418742
H	-3.900514	-3.483554	0.521383
H	-3.132837	-2.316729	1.652381
C	-2.762577	-2.602368	-2.166226
H	-1.950165	-2.529254	-2.907652
H	-3.182357	-3.622273	-2.190259
H	-3.548920	-1.882299	-2.444782
C	-0.911842	-3.502573	-0.156080
H	-1.360656	-4.504675	-0.259951
H	-0.057866	-3.392216	-0.843340
H	-0.553344	-3.366312	0.877401
C	-2.478684	2.572351	1.523586
H	-3.317688	3.214448	1.837527
H	-2.821005	1.523646	1.538004
H	-1.664363	2.688953	2.257859
C	-1.522939	4.447780	0.109033
H	-2.351562	5.109826	0.409350
H	-0.693327	4.586162	0.820767
H	-1.183137	4.750598	-0.894146
C	-3.168252	2.805737	-0.903950
H	-2.840742	3.060368	-1.924559
H	-3.536885	1.766631	-0.903912
H	-4.003299	3.470411	-0.629198
C	2.228739	-0.927343	-0.350906
C	3.962920	0.778082	-0.570968
O	1.351501	-1.340033	-1.066330
O	4.336667	0.348444	-1.625723
O	4.684451	1.520427	0.242890
O	3.065959	-1.702229	0.307457
C	2.952079	-3.105051	0.123137
H	3.022530	-3.356172	-0.945759
H	3.781518	-3.556969	0.679992
H	1.987175	-3.460162	0.519805
C	6.018240	1.810350	-0.165585
H	6.451236	2.432503	0.626555
H	6.588745	0.876887	-0.282315
H	6.013067	2.348541	-1.125339
C	-2.017991	2.983465	0.108510

IN1e

C	-3.801847	0.141964	-1.171728
C	-2.634544	0.715238	-1.933416
C	-2.024169	1.596848	0.966698
C	-3.146477	0.704044	1.293572
C	-3.489135	-0.395187	0.254875
H	-4.589185	0.905981	-1.060773
H	-4.233610	-0.690907	-1.747853
H	-2.281907	1.711852	-1.649306
H	-2.927652	0.217995	2.259374
H	-4.034887	1.344192	1.426137
C	-2.055429	0.114734	-2.989935
H	-2.407888	-0.874175	-3.312892
C	-0.988368	0.740384	-3.773413
H	-0.579660	1.679698	-3.376456
C	-0.511005	0.245281	-4.927393
H	-0.919536	-0.674923	-5.360766
H	0.278768	0.754597	-5.486513
C	-1.239041	2.532564	0.738539
Au	0.048781	0.748649	0.499625
Si	-0.281936	4.106093	0.356360
C	0.541698	3.805618	-1.295523
H	1.091995	4.705939	-1.621084
H	1.259206	2.967136	-1.251036
H	-0.211891	3.578322	-2.070008
C	-1.535761	5.483958	0.283548
H	-1.032326	6.442214	0.064185
H	-2.282615	5.304983	-0.508192
H	-2.067022	5.593302	1.244029
C	0.947522	4.317186	1.744633
H	0.431670	4.479705	2.706168
H	1.589925	3.427207	1.856113
H	1.598185	5.189249	1.557302
C	-2.408152	-1.485810	0.244231
C	-4.750778	-1.107725	0.795591
O	-1.546850	-1.578963	1.084624
O	-4.767108	-2.242394	1.179208
O	-5.795225	-0.298524	0.795791
O	-2.562690	-2.317578	-0.755641
C	-1.778294	-3.504389	-0.745419
H	-2.135583	-4.165407	0.059400
H	-1.925587	-3.978840	-1.722696

H	-0.718603	-3.265164	-0.584914
C	-7.024406	-0.834719	1.275038
H	-7.762002	-0.027498	1.194168
H	-7.325492	-1.697868	0.662755
H	-6.915963	-1.159004	2.321005
P	1.905166	-0.627097	0.201311
C	3.317428	0.276398	-0.455223
C	2.422073	-1.396797	1.741462
C	1.579846	-1.965823	-0.956728
C	3.534449	1.601008	-0.029285
C	4.221207	-0.324566	-1.349520
C	3.766063	-1.419017	2.151381
C	1.428808	-2.015666	2.529098
C	0.918029	-1.646350	-2.156323
C	1.989328	-3.287722	-0.711703
C	4.647903	2.312314	-0.484150
H	2.828861	2.074184	0.660942
C	5.331617	0.394426	-1.806916
H	4.055415	-1.349738	-1.692677
C	4.115953	-2.061992	3.345371
H	4.538062	-0.936171	1.545953
C	1.790821	-2.660231	3.714626
H	0.381617	-1.999247	2.206219
C	0.679604	-2.637325	-3.109805
H	0.594208	-0.620254	-2.349904
C	1.739494	-4.279780	-1.669328
H	2.496988	-3.544693	0.222078
C	5.546591	1.709090	-1.374840
H	4.813244	3.339322	-0.147501
H	6.030466	-0.074879	-2.504773
C	3.132251	-2.682489	4.124181
H	5.161253	-2.076988	3.666020
H	1.022457	-3.143435	4.324426
C	1.089164	-3.956423	-2.866783
H	0.172702	-2.375003	-4.042266
H	2.057677	-5.308360	-1.477917
H	6.414876	2.267427	-1.735975
H	3.410143	-3.183276	5.055956
H	0.899991	-4.734245	-3.612165

TS1b

C	-3.398889	-1.632324	-0.123536
C	-1.888007	-1.756818	-0.058899
C	-1.545728	0.373818	-1.075517
C	-2.988444	0.337771	-1.416502
H	-3.791770	-2.252865	-0.946736
H	-3.879567	-1.975167	0.805720
H	-1.387675	-1.596660	0.905024
H	-3.279702	1.397319	-1.555547
H	-3.172020	-0.193643	-2.366395
C	-1.144724	-2.178688	-1.124534
H	-1.648197	-2.349789	-2.086591
C	0.272961	-2.506475	-1.061139
H	0.734168	-2.525602	-0.067396
C	0.991930	-2.830848	-2.151011
H	0.542270	-2.838619	-3.150162
H	2.047883	-3.106713	-2.076329
C	-0.464760	1.023414	-0.840832
Au	1.331866	0.278567	-0.104003
P	3.404838	-0.400572	0.756181
C	4.746085	0.760889	0.398807
H	4.516026	1.743543	0.841835
H	5.702903	0.396464	0.809614
H	4.848418	0.891554	-0.690804
C	3.424705	-0.614085	2.554061
H	4.421533	-0.934600	2.901601
H	3.163251	0.337649	3.044726
H	2.680786	-1.370199	2.853173
C	3.966106	-1.987757	0.084647
H	3.233468	-2.778394	0.318200
H	4.065612	-1.911750	-1.010752
H	4.942524	-2.275099	0.510705
N	-3.781967	-0.247022	-0.371952
S	-4.303911	0.708454	0.894621
O	-5.335088	-0.044546	1.560079
O	-4.515275	2.013816	0.312046
C	-2.919733	0.849406	2.054732
H	-2.059522	1.299109	1.540514
H	-3.280517	1.506516	2.860686
H	-2.687472	-0.146192	2.458938
C	-0.463021	2.547641	-1.079342
H	-1.455519	2.933068	-1.359663
H	-0.123310	3.060128	-0.166622
H	0.254651	2.779248	-1.881986

TS1c

C	-3.354491	-2.176279	-0.448653
C	-1.855883	-2.143424	-0.161124

C	-1.508359	-0.213707	-0.846886
C	-2.872579	-0.096489	-1.459955
H	-3.547852	-2.767147	-1.360249
H	-3.920406	-2.640691	0.374251
H	-1.557577	-1.909800	0.865950
H	-3.153441	0.963065	-1.539377
H	-2.850321	-0.519924	-2.480497
C	-0.958921	-2.809124	-0.979191
H	-1.321175	-3.157959	-1.954649
C	0.427249	-3.018739	-0.690709
H	1.040374	-3.449390	-1.489400
C	1.032090	-2.671693	0.486685
H	0.455567	-2.363458	1.364663
H	2.083402	-2.917117	0.655897
C	-0.429641	0.385255	-0.503862
Au	1.514154	-0.134897	-0.044066
P	3.850770	-0.131235	0.319060
C	4.357697	1.079994	1.567839
H	5.453651	1.085937	1.694465
H	4.027935	2.086977	1.263881
H	3.886533	0.842298	2.535606
C	4.584811	-1.694785	0.868992
H	4.409813	-2.480547	0.115414
H	5.672935	-1.587617	1.016191
H	4.130981	-2.012825	1.822290
C	4.781443	0.314254	-1.170213
H	4.585118	-0.419252	-1.969178
H	4.458257	1.304670	-1.530107
H	5.865428	0.342776	-0.966861
Si	-0.423462	2.312552	-0.317410
C	0.933214	2.993529	-1.412808
H	1.932531	2.710794	-1.039823
H	0.835827	2.621185	-2.447206
H	0.879619	4.096213	-1.445925
C	-2.062180	3.072620	-0.787276
H	-2.269546	2.987367	-1.868044
H	-2.932185	2.679292	-0.233841
H	-1.994946	4.153235	-0.562816
C	-0.059064	2.619142	1.494622
H	0.944228	2.255242	1.774937
H	-0.101164	3.702259	1.707087
H	-0.793382	2.125157	2.153608
N	-3.833471	-0.819514	-0.666503
S	-4.628693	-0.023844	0.561593
O	-5.646596	-0.928638	1.030077
O	-4.916900	1.294653	0.042129
C	-3.442038	0.190847	1.915784
H	-2.572214	0.753486	1.548786
H	-3.978198	0.763197	2.687996
H	-3.159746	-0.796157	2.308898

TS1d

C	2.452146	-2.055928	-0.104408
C	0.980995	-1.991211	0.210955
C	1.042743	0.115688	1.164478
C	2.503116	-0.024533	1.306832
C	3.066415	-0.639092	0.017536
H	2.965089	-2.716663	0.612905
H	2.611579	-2.438199	-1.122641
H	0.293220	-1.849440	-0.630281
H	2.901416	0.992322	1.449349
H	2.812800	-0.628521	2.174227
C	0.480452	-2.214758	1.467127
H	1.185201	-2.364045	2.295811
C	-0.932666	-2.379024	1.787710
H	-1.632517	-2.456955	0.949657
C	-1.378169	-2.476359	3.052339
H	-0.691377	-2.416569	3.904066
H	-2.439138	-2.621114	3.274801
C	0.004147	0.853952	0.955224
Au	-1.742632	0.146969	0.044860
P	-3.662362	-0.542372	-1.098584
C	-3.558323	-0.283972	-2.888011
H	-4.475927	-0.629879	-3.393389
H	-3.412837	0.787756	-3.100167
H	-2.692700	-0.831682	-3.294900
C	-4.033313	-2.306266	-0.902768
H	-4.937754	-2.588293	-1.468321
H	-3.185466	-2.910034	-1.266449
H	-4.194850	-2.538698	0.162715
C	-5.174263	0.311727	-0.583949
H	-5.061229	1.396381	-0.743750
H	-6.046754	-0.046708	-1.156072
H	-5.352992	0.141396	0.490213
C	1.334524	2.938332	1.750049
H	2.120893	2.834746	0.984299
H	1.228102	4.012302	1.972976
H	1.660111	2.437978	2.676693

C	-0.373473	3.121323	-0.062035
H	-1.377288	2.840005	-0.420557
H	-0.358353	4.211122	0.106079
H	0.354428	2.883557	-0.854754
C	-1.093799	2.633588	2.314841
H	-0.860524	2.089376	3.244465
H	-1.149082	3.710265	2.548311
H	-2.084617	2.303112	1.961430
C	2.647292	0.210439	-1.190784
C	4.593698	-0.722700	0.097752
O	1.930636	-0.169330	-2.072951
O	5.220263	-0.551023	1.103504
O	5.105971	-1.044813	-1.075746
O	3.160019	1.428333	-1.108740
C	2.911095	2.307562	-2.197852
H	1.829789	2.391096	-2.384258
H	3.335014	3.278338	-1.913968
H	3.399253	1.926504	-3.107979
C	6.521449	-1.178642	-1.149771
H	7.006460	-0.231064	-0.870953
H	6.864753	-1.971045	-0.467757
H	6.749610	-1.438996	-2.190071
C	-0.010081	2.390093	1.245485

TS1e

Au	0.517551	0.010350	-0.369639
P	2.802392	-0.087419	0.181228
C	-1.431843	0.419492	-0.902504
C	3.585418	-1.523398	-0.581793
C	3.120280	-0.202763	1.949881
C	3.723568	1.353955	-0.391092
Si	-1.488545	2.337226	-0.914227
C	-2.510650	-0.268112	-1.027812
C	3.406472	-1.701999	-1.969807
C	4.289402	-2.487827	0.157007
C	2.108977	-0.678632	2.804074
C	4.374877	0.148944	2.484033
C	4.976795	1.251052	-1.019307
C	3.162239	2.625378	-0.159349
C	-0.167718	2.966718	-2.080805
C	-3.146570	3.024941	-1.450481
C	-1.161080	2.784400	0.878063
C	-3.966945	-0.238159	-1.323264
C	3.938801	-2.823816	-2.608238
H	2.846032	-0.959505	-2.549126
C	4.813567	-3.617281	-0.487963
H	4.426222	-2.365547	1.234605
C	2.353374	-0.817868	4.174770
H	1.124294	-0.928408	2.395969
C	4.614329	0.009464	3.854150
H	5.160073	0.538625	1.828781
C	5.658834	2.410393	-1.409972
H	5.420362	0.269411	-1.207643
C	3.849911	3.778378	-0.544905
H	2.184480	2.709377	0.327153
H	-0.318102	2.557717	-3.095201
H	-0.213264	4.067800	-2.153999
H	0.847741	2.687363	-1.751926
H	-3.401655	2.742437	-2.486526
H	-3.078823	4.127761	-1.423482
H	-3.976860	2.727056	-0.790192
H	-1.377737	3.849853	1.072004
H	-1.793882	2.167054	1.540986
H	-0.111151	2.592276	1.159795
C	-4.694742	-0.699674	-0.050960
H	-4.256285	0.779563	-1.620848
H	-4.234929	-0.911714	-2.154004
C	4.641268	-3.785832	-1.865732
H	3.803291	-2.952934	-3.685672
H	5.359308	-4.366198	0.092602
C	3.606010	-0.476103	4.698871
H	1.562506	-1.184631	4.834672
H	5.589023	0.285496	4.265900
C	5.098879	3.671123	-1.173334
H	6.632201	2.325850	-1.901103
H	3.410178	4.762213	-0.359939
C	-4.079824	-2.080477	0.285760
C	-6.199076	-0.821890	-0.292381
C	-4.405049	0.301997	1.072547
H	5.052244	-4.667903	-2.364817
H	3.795891	-0.579791	5.770961
H	5.634496	4.573540	-1.481118
C	-2.588171	-2.041919	0.022903
H	-4.274538	-2.338775	1.337048
H	-4.556001	-2.837964	-0.357288
O	-6.831584	-1.088347	0.837098
O	-6.717176	-0.730464	-1.368175
O	-5.120800	1.404138	0.919205

O	-3.593622	0.133067	1.940690
C	-2.021278	-2.683669	-1.064647
H	-1.960018	-1.721743	0.858661
C	-8.243785	-1.241366	0.765053
C	-4.943534	2.439447	1.876861
C	-0.610352	-2.909872	-1.257855
H	-2.692099	-3.020086	-1.865525
H	-8.504578	-2.064630	0.082916
H	-8.707478	-0.313161	0.398125
H	-8.580360	-1.463615	1.784712
H	-5.050334	2.039442	2.895999
H	-3.942962	2.887576	1.767693
H	-5.719680	3.185884	1.668850
C	0.315590	-2.808586	-0.270148
H	-0.280957	-3.166610	-2.270321
H	0.024387	-2.668028	0.775412
H	1.373735	-2.998338	-0.472198

TS4a

C	3.842406	0.193877	0.020211
C	3.299566	1.551826	0.401594
C	1.212445	1.182054	-0.365751
C	1.683205	0.041900	-1.186585
C	2.671267	-0.759637	-0.325195
H	4.488753	0.283721	-0.867854
H	4.429178	-0.230303	0.847546
H	3.098351	1.729788	1.464719
H	0.817282	-0.576997	-1.465310
H	2.172315	0.362728	-2.119534
C	3.193292	2.585085	-0.493821
H	3.441946	2.392040	-1.546662
C	2.867899	3.966197	-0.156451
H	2.775405	4.219730	0.904969
C	2.733705	4.921202	-1.093377
H	2.834293	4.690915	-2.160029
H	2.527570	5.960555	-0.822068
C	0.291568	1.718181	0.352886
Au	-1.432591	0.542324	0.024844
P	-3.420026	-0.653692	-0.261417
C	-3.318542	-2.392765	0.234481
H	-3.065108	-2.459902	1.305006
H	-4.279120	-2.907853	0.062609
H	-2.531266	-2.900331	-0.346816
C	-4.803573	0.028268	0.685607
H	-5.723522	-0.556120	0.514421
H	-4.564258	0.015575	1.761396
H	-4.981431	1.073904	0.385850
C	-3.986964	-0.686368	-1.980551
H	-4.932815	-1.246937	-2.071991
H	-4.142528	0.343215	-2.341828
H	-3.223768	-1.162091	-2.617733
C	1.962800	-1.194442	0.965469
C	3.170384	-1.984262	-1.095068
O	2.275102	-0.845347	2.066519
O	2.964201	-2.170330	-2.260433
O	3.875443	-2.775761	-0.308738
O	0.917701	-1.966359	0.692093
C	0.135669	-2.386775	1.798714
H	0.767214	-2.872301	2.557657
H	-0.366633	-1.517116	2.255429
H	-0.601544	-3.096442	1.403079
C	4.429209	-3.948476	-0.895361
H	5.111957	-3.677819	-1.714815
H	4.972719	-4.463149	-0.094254
H	3.627357	-4.588229	-1.293791
C	0.228307	2.866451	1.315908
H	1.177245	2.963934	1.865951
H	0.044743	3.801280	0.759843
H	-0.584646	2.737097	2.043385

TS4b

C	3.479418	1.242360	-1.174320
C	3.421603	-0.272412	-1.208280
C	1.146835	-0.124830	-0.578690
C	1.301175	1.298999	-0.105733
H	4.519134	1.581606	-1.046349
H	3.101206	1.663191	-2.121013
H	3.477057	-0.762285	-2.188654
H	0.716019	1.925985	-0.803420
H	0.870383	1.382514	0.903873
C	3.472005	-1.034188	-0.076994
H	3.465561	-0.547781	0.905404
C	3.564449	-2.487691	-0.061205
H	3.683600	-3.003260	-1.021571
C	3.550688	-3.188594	1.086886
H	3.446716	-2.685383	2.054831
H	3.655727	-4.277395	1.092889
C	0.452708	-1.122246	-0.946638

Au	-1.498900	-0.459853	-0.428926
P	-3.725912	0.031636	0.094875
C	-4.254264	1.684344	-0.421091
H	-4.129080	1.794818	-1.510506
H	-5.313305	1.853730	-0.161873
H	-3.637005	2.448959	0.077753
C	-4.889400	-1.110703	-0.690169
H	-5.928317	-0.857172	-0.418907
H	-4.782097	-1.061950	-1.786012
H	-4.676482	-2.143048	-0.368108
C	-4.082234	-0.059331	1.866698
H	-5.144829	0.162787	2.063932
H	-3.849988	-1.068778	2.243348
H	-3.455957	0.663725	2.414063
C	0.630705	-2.490526	-1.519995
H	0.577901	-3.242855	-0.715643
H	-0.150668	-2.718147	-2.259670
H	1.615451	-2.563323	-2.006790
N	2.673803	1.748775	-0.073473
S	3.390781	2.048443	1.410736
O	4.771658	1.633918	1.301749
O	2.516274	1.489499	2.424100
C	3.352966	3.839516	1.563831
H	2.306362	4.172541	1.547356
H	3.822541	4.072774	2.531201
H	3.931358	4.269082	0.734670

TS4c

C	-3.307646	-0.069565	-1.674806
C	-2.951940	1.214306	-0.948438
C	-1.021076	0.277905	-0.336059
C	-1.568058	-1.130444	-0.363736
H	-4.387037	-0.112883	-1.883955
H	-2.769232	-0.127378	-2.635142
H	-2.654697	2.078710	-1.551078
H	-0.893423	-1.694575	-1.033593
H	-1.504842	-1.560746	0.648799
C	-3.178442	1.376455	0.392058
H	-3.518948	0.522511	0.990004
C	-3.007815	2.618382	1.125813
H	-2.717371	3.514894	0.569257
C	-3.238747	2.690546	2.450470
H	-3.545031	1.806025	3.020461
H	-3.140915	3.633314	2.996802
C	-0.002741	1.040550	-0.301199
Au	1.679707	-0.231406	-0.052369
P	3.621278	-1.486881	0.256068
C	3.716357	-2.297657	1.871519
H	2.866201	-2.987938	1.995368
H	4.657805	-2.864145	1.971768
H	3.664124	-1.542311	2.672439
C	3.838262	-2.812010	-0.958544
H	3.860470	-2.387483	-1.975401
H	4.778617	-3.359799	-0.776839
H	2.994647	-3.518487	-0.897836
C	5.123057	-0.483234	0.136125
H	6.023423	-1.104255	0.280819
H	5.173863	-0.002292	-0.854318
H	5.107038	0.307865	0.903444
Si	0.536590	2.853178	-0.342857
C	2.267767	2.900168	-1.062764
H	2.587017	3.947811	-1.207031
H	3.001692	2.419679	-0.392610
H	2.313432	2.398004	-2.044837
C	-0.582115	3.837118	-1.479208
H	-0.129790	4.834058	-1.629409
H	-0.654590	3.357568	-2.470890
H	-1.599555	3.997742	-1.093589
C	0.559884	3.463873	1.421208
H	0.891816	4.516604	1.455838
H	-0.431287	3.394557	1.895727
H	1.267058	2.867381	2.022968
N	-2.934148	-1.200520	-0.838473
S	-4.093666	-1.906161	0.144993
O	-5.317105	-1.160068	-0.049651
O	-3.509104	-2.050215	1.465017
C	-4.316356	-3.549511	-0.547929
H	-5.077453	-4.042715	0.075103
H	-4.666634	-3.442201	-1.583419
H	-3.359690	-4.086544	-0.493285

TS4d

C	-3.435009	0.819645	0.277715
C	-3.289859	-0.691801	0.299210
C	-1.292234	-0.792078	-0.434661
C	-1.409220	0.557366	-1.077219
C	-2.069499	1.475593	-0.038683
H	-4.149409	1.111359	-0.508664

H	-3.811650	1.175616	1.246616
H	-3.198526	-1.167612	1.277627
H	-0.418909	0.927817	-1.373874
H	-2.027613	0.540158	-1.987549
C	-3.561107	-1.459316	-0.815202
H	-3.703510	-0.937091	-1.771078
C	-3.799584	-2.893020	-0.855852
H	-3.791826	-3.450377	0.085158
C	-4.099095	-3.522967	-2.007569
H	-4.130813	-2.983578	-2.961018
H	-4.327991	-4.592397	-2.028636
C	-0.427004	-1.587459	0.115476
Au	1.419768	-0.571844	-0.211674
P	3.384193	0.646186	-0.503790
C	3.016748	2.310777	-1.118855
H	2.587599	2.240459	-2.132056
H	2.262005	2.786978	-0.471181
H	3.922940	2.938683	-1.155998
C	4.330488	0.894849	1.020066
H	5.228392	1.508131	0.833547
H	3.701390	1.398543	1.771323
H	4.639613	-0.079918	1.431235
C	4.566119	-0.053570	-1.682270
H	4.896443	-1.045562	-1.333489
H	4.083033	-0.179215	-2.664812
H	5.447248	0.600772	-1.794305
C	0.966755	-3.039176	1.636941
H	1.129764	-2.206378	2.341511
H	0.973108	-3.978680	2.213220
H	1.810189	-3.075301	0.927592
C	-1.493763	-2.946460	1.973567
H	-1.482924	-2.035003	2.594632
H	-2.491726	-3.066101	1.535556
H	-1.323214	-3.814396	2.630925
C	-0.518891	-4.056165	-0.105769
H	0.302399	-4.028341	-0.840515
H	-0.468068	-5.018322	0.431339
H	-1.470268	-4.008075	-0.654516
C	-1.207978	1.510239	1.229827
C	-2.245769	2.887527	-0.597434
O	-1.494798	0.972456	2.260394
O	-2.007853	3.195850	-1.730543
O	-2.720239	3.700175	0.329403
O	-0.070736	2.168618	1.026125
C	0.826701	2.219376	2.124094
H	0.333247	2.651082	3.007789
H	1.176557	1.203276	2.372843
H	1.665081	2.855951	1.810978
C	-2.954356	5.051348	-0.050179
H	-3.691396	5.095783	-0.866152
H	-3.337839	5.558080	0.843337
H	-2.017298	5.518508	-0.388950
C	-0.385370	-2.894504	0.902400

TS4e

Au	0.195513	-0.940374	-0.142555
P	2.334072	-0.011561	-0.154167
C	-1.837492	-1.506266	-0.140956
C	3.678150	-1.083061	-0.680347
C	2.781601	0.617767	1.475570
C	2.330595	1.413847	-1.262701
Si	-2.166658	-3.008242	0.955773
C	-2.481217	-0.569426	-0.763994
C	3.419045	-2.053226	-1.667071
C	4.978865	-0.939570	-0.164191
C	2.558997	-0.213683	2.590587
C	3.305166	1.908393	1.662246
C	3.353946	1.636904	-2.198696
C	1.239877	2.307061	-1.194109
C	-2.212345	-4.530993	-0.128867
C	-3.699749	-2.759728	2.011337
C	-0.721162	-3.121499	2.148102
C	-2.291192	0.834005	-1.252041
C	4.455295	-2.862489	-2.142032
H	2.404226	-2.172490	-2.061857
C	6.010677	-1.756491	-0.639367
H	5.183241	-0.194511	0.610329
C	2.855250	0.242583	3.877165
H	2.140722	-1.216577	2.448676
C	3.594610	2.363937	2.955370
H	3.476231	2.562614	0.802813
C	3.284267	2.742913	-3.056814
H	4.199958	0.947504	-2.266857
C	1.172162	3.403529	-2.056449
H	0.439163	2.154537	-0.462806
H	-1.261568	-4.628385	-0.680790
H	-2.336227	-5.435757	0.492009
H	-3.028786	-4.503229	-0.867155

H	-3.691900	-3.520379	2.812371
H	-3.657523	-1.767474	2.496243
H	-4.662967	-2.855895	1.487100
H	-0.597693	-2.176239	2.705886
H	-0.901200	-3.924249	2.885238
H	0.226158	-3.348197	1.628954
C	-2.957637	1.718022	-0.182036
H	-1.222042	1.054700	-1.364916
H	-2.768506	1.025448	-2.226044
C	5.750729	-2.714307	-1.628096
H	4.251385	-3.614243	-2.909420
H	7.020482	-1.645689	-0.234701
C	3.368157	1.535509	4.060954
H	2.680944	-0.406835	4.739556
H	3.998619	3.370215	3.097299
C	2.196702	3.621100	-2.990153
H	4.082028	2.911476	-3.785560
H	0.304748	4.067295	-2.003564
C	-4.437481	1.262204	-0.153890
C	-2.774794	3.200077	-0.509801
C	-2.322329	1.436302	1.194128
H	6.559641	-3.351962	-1.995799
H	3.592458	1.895675	5.069006
H	2.142485	4.475211	-3.671170
C	-4.466429	-0.251397	-0.221581
H	-4.929907	1.611941	0.763854
H	-4.955767	1.694423	-1.024781
O	-3.488094	3.953084	0.305590
O	-2.061708	3.613118	-1.382016
O	-1.101760	1.940937	1.273070
O	-2.852651	0.811322	2.068607
C	-4.583545	-0.951675	-1.405831
H	-4.531875	-0.791214	0.725831
C	-3.386723	5.363417	0.145637
C	-0.377572	1.687710	2.472785
C	-4.824403	-2.384287	-1.516081
H	-4.579077	-0.390807	-2.349885
H	-3.693040	5.654983	-0.870198
H	-2.349651	5.689935	0.316127
H	-4.057025	5.804731	0.892664
H	-0.940586	2.059548	3.341395
H	-0.209117	0.604917	2.582810
H	0.581851	2.210503	2.371510
C	-4.963519	-2.991978	-2.706977
H	-4.925879	-2.955528	-0.589150
H	-4.876305	-2.434005	-3.646041
H	-5.176401	-4.062584	-2.778241

TS5a

C	2.274986	-1.053050	0.134917
C	1.367584	-0.467140	-0.969006
H	1.995209	-0.099150	-1.798470
H	0.721614	-1.252546	-1.378420
C	3.458792	-0.108275	0.419964
H	4.104954	-0.114556	-0.473899
H	4.036380	-0.525609	1.260020
C	3.114584	1.325674	0.768025
H	2.956449	1.539878	1.831646
C	3.333661	2.358063	-0.106902
H	3.550044	2.115434	-1.156886
C	3.392271	3.766242	0.259336
H	3.278566	4.015096	1.320957
C	3.629689	4.738048	-0.640897
H	3.764507	4.507740	-1.703780
H	3.709338	5.786727	-0.340219
C	0.564802	0.658471	-0.368246
C	0.922770	1.693443	0.301871
Au	-1.513841	0.377996	-0.222761
P	-3.805249	-0.084536	-0.187090
C	-4.509770	-0.253055	1.472716
H	-4.358493	0.678889	2.041215
H	-5.590310	-0.469979	1.420023
H	-4.006695	-1.071243	2.012587
C	-4.805849	1.187127	-0.999164
H	-4.483634	1.302582	-2.046831
H	-5.875555	0.917715	-0.978810
H	-4.669105	2.154496	-0.489164
C	-4.217447	-1.628211	-1.038178
H	-3.888113	-1.574257	-2.088656
H	-3.695534	-2.472298	-0.559194
H	-5.304531	-1.814323	-1.011073
C	2.832529	-2.402480	-0.342718
C	1.460815	-1.272249	1.415816
O	2.728136	-2.816040	-1.461436
O	1.684471	-0.744907	2.468155
O	3.460541	-3.024130	0.640436
O	0.440473	-2.090598	1.192537
C	4.044122	-4.286311	0.339824

H	3.272228	-4.987701	-0.011160
H	4.808834	-4.175227	-0.443769
H	4.496849	-4.643765	1.272312
C	-0.440888	-2.317724	2.279420
H	0.108933	-2.703900	3.150891
H	-0.937658	-1.374382	2.562528
H	-1.175755	-3.054470	1.932101
C	0.569631	2.901695	1.068743
H	1.027961	2.892384	2.069868
H	0.854884	3.822441	0.538800
H	-0.525374	2.900245	1.193490

TS5b

C	-1.191271	-1.032037	-0.561288
H	-1.001021	-1.573024	0.377857
H	-0.761049	-1.630465	-1.386134
C	-3.075085	0.043074	-1.757512
H	-4.124519	-0.185527	-2.007289
H	-2.478625	-0.123043	-2.670608
C	-2.995692	1.499252	-1.337431
H	-2.997375	2.233102	-2.154716
C	-3.170668	1.941461	-0.060457
H	-3.214398	1.223632	0.766041
C	-3.330668	3.345450	0.295606
H	-3.335410	4.079934	-0.519469
C	-3.506783	3.745637	1.568243
H	-3.524328	3.021367	2.390541
H	-3.657116	4.799462	1.820090
C	-0.425505	0.272462	-0.517933
C	-0.677102	1.512606	-0.660570
Au	1.659696	0.140903	-0.186686
P	3.933261	-0.193122	0.245959
C	4.557681	0.800552	1.624009
H	5.627052	0.594457	1.801060
H	4.431106	1.872688	1.402522
H	3.990165	0.568546	2.539928
C	4.311421	-1.908372	0.682328
H	4.023915	-2.578368	-0.144191
H	5.388926	-2.030767	0.885391
H	3.741689	-2.201302	1.579222
C	5.010223	0.194108	-1.156268
H	4.891528	1.252228	-1.440611
H	6.067106	0.007559	-0.900202
H	4.734994	-0.428399	-2.023107
C	-0.350484	2.944163	-0.739698
H	0.747773	3.042234	-0.764074
H	-0.752424	3.394447	-1.660400
H	-0.733705	3.493193	0.133812
N	-2.615562	-0.885127	-0.742363
S	-3.642963	-1.361349	0.478490
O	-2.948009	-1.172247	1.737441
O	-4.908453	-0.715124	0.212262
C	-3.846448	-3.132855	0.228281
H	-2.865271	-3.621821	0.305084
H	-4.512277	-3.478718	1.033144
H	-4.306321	-3.291484	-0.756432

TS5c

C	-1.279952	-1.522066	-0.692616
H	-1.116619	-2.196470	0.162040
H	-0.866853	-2.016021	-1.592784
C	-3.107341	-0.141367	-1.638736
H	-4.164617	-0.262688	-1.926800
H	-2.514142	-0.129638	-2.568416
C	-2.976225	1.185434	-0.909279
H	-3.053854	2.081041	-1.536470
C	-3.088049	1.313181	0.445956
H	-3.054205	0.416910	1.075216
C	-3.301144	2.566170	1.154137
H	-3.408111	3.483086	0.564799
C	-3.438282	2.607298	2.492710
H	-3.360008	1.696230	3.096708
H	-3.648140	3.544421	3.016548
C	-0.478130	-0.264087	-0.476951
C	-0.680015	1.002183	-0.445301
Si	0.020968	2.764619	-0.395172
C	0.255327	3.237459	1.392659
H	0.897954	2.498775	1.902306
H	0.747466	4.223863	1.461258
H	-0.701618	3.289081	1.934518
C	1.679606	2.682531	-1.272763
H	2.041371	3.712161	-1.446589
H	2.440262	2.159123	-0.669410
H	1.602123	2.180025	-2.251903
C	-1.075424	3.930891	-1.354782
H	-2.054456	4.113669	-0.889369
H	-0.558440	4.904932	-1.422102
H	-1.234716	3.571641	-2.385985

Au	1.585455	-0.455606	-0.112902
P	3.847434	-0.844360	0.351721
C	4.938537	-0.494407	-1.049881
H	4.831131	0.559319	-1.354847
H	5.992421	-0.686441	-0.785752
H	4.660951	-1.129224	-1.907010
C	4.482817	0.163926	1.715140
H	3.908765	-0.043641	2.632822
H	5.548623	-0.053037	1.900510
H	4.372658	1.233861	1.474470
C	4.199796	-2.556681	0.819295
H	5.274088	-2.692423	1.030332
H	3.619989	-2.826060	1.717116
H	3.905769	-3.235870	0.002626
N	-2.697636	-1.286170	-0.849124
S	-3.760225	-1.970428	0.234445
O	-3.068852	-2.106026	1.503123
O	-4.989047	-1.216758	0.124372
C	-4.050106	-3.628574	-0.404501
H	-4.740964	-4.111057	0.303051
H	-4.506333	-3.540235	-1.399695
H	-3.094784	-4.170732	-0.439077

TS5d

C	-2.179461	1.267397	-0.151064
C	-1.327427	0.578489	-1.241064
H	-1.985293	0.226923	-2.052898
H	-0.641755	1.307105	-1.689626
C	-3.421540	0.422468	0.193699
H	-4.162595	0.600471	-0.604118
H	-3.846237	0.802672	1.133279
C	-3.251194	-1.087272	0.318483
H	-3.387006	-1.506895	1.320573
C	-3.393323	-1.906083	-0.775942
H	-3.317672	-1.441802	-1.768406
C	-3.788502	-3.306618	-0.790486
H	-4.074897	-3.770413	0.157327
C	-3.896338	-3.999768	-1.939806
H	-3.632902	-3.549410	-2.903505
H	-4.255575	-5.032858	-1.950219
C	-0.592250	-0.564075	-0.586591
C	-1.016285	-1.554664	0.119223
C	-1.647744	-3.703822	1.417438
H	-1.212484	-4.381147	2.167979
H	-2.571278	-3.292232	1.846789
H	-1.887017	-4.296686	0.524696
C	0.628638	-3.354171	0.516078
H	0.394741	-3.785520	-0.469827
H	1.492636	-2.680287	0.408671
H	0.913065	-4.170072	1.200002
C	-0.222719	-1.898275	2.425048
H	0.592486	-1.176413	2.251694
H	-1.076809	-1.339474	2.837394
H	0.114602	-2.642994	3.164476
Au	1.477842	-0.213658	-0.388464
P	3.738842	0.359005	-0.280923
C	4.743027	-0.803193	0.678731
H	4.679131	-1.808325	0.230882
H	5.799935	-0.487506	0.701550
H	4.363181	-0.862192	1.711701
C	4.532021	0.445397	-1.905664
H	4.019490	1.194122	-2.531423
H	5.596079	0.721094	-1.811500
H	4.456154	-0.531666	-2.410023
C	4.037668	1.977133	0.476166
H	5.115414	2.212837	0.493605
H	3.509272	2.757645	-0.095592
H	3.654509	1.981261	1.509568
C	-2.651303	2.633239	-0.672594
C	-1.338359	1.492341	1.111698
O	-2.527421	3.002683	-1.804756
O	-1.568025	1.009913	2.184099
O	-3.235953	3.325142	0.290719
O	-0.298004	2.277100	0.856704
C	-3.744309	4.608735	-0.051759
H	-2.930299	5.256353	-0.411088
H	-4.504615	4.519207	-0.842314
H	-4.187036	5.016963	0.864575
C	0.587447	2.528014	1.933702
H	1.061307	1.586248	2.259405
H	1.340791	3.231077	1.556537
H	0.046907	2.964716	2.787070
C	-0.603567	-2.616546	1.108233

TS5e

Au	-0.227567	0.202813	-0.618887
P	-2.496582	-0.122999	-0.153727
C	1.832700	0.346411	-0.915539

C	-3.369537	1.423323	0.149444	H	5.337189	-0.721624	-1.080993
C	-2.650924	-1.088342	1.366604	O	4.512885	-3.355490	0.435182
C	-3.402162	-1.023213	-1.421053	O	3.681128	-3.387334	-1.639237
C	2.541862	-0.873298	-1.441894	O	1.618001	-2.133079	0.975081
C	2.289265	1.392353	-0.306879	O	2.983948	-0.681511	1.981674
C	-2.978086	2.567334	-0.572488	H	0.657593	4.128998	-0.767156
C	-4.445624	1.506420	1.053538	H	1.077759	5.108860	0.664737
C	-2.281168	-0.488495	2.587558	H	2.322242	4.733274	-0.564062
C	-3.022719	-2.443020	1.343014	H	3.420051	1.992855	2.656858
C	-4.802026	-0.925339	-1.528426	H	2.845734	3.650902	2.975755
C	-2.693041	-1.878215	-2.285135	H	4.155591	3.393870	1.808284
C	3.455213	-1.383747	-0.297898	H	0.476078	1.167418	2.239778
H	1.842299	-1.661051	-1.744951	H	0.213155	2.857424	2.757157
H	3.161631	-0.634461	-2.323530	H	-0.591042	2.260157	1.282897
Si	1.847876	2.776143	0.924930	H	-5.261280	4.798509	0.639643
C	-3.659778	3.775890	-0.398913	H	-2.649434	-3.177008	4.662062
H	-2.138289	2.507725	-1.273177	H	-5.308295	-3.130615	-4.087960
C	-5.121830	2.718857	1.225824	C	4.467984	1.804642	-1.196215
H	-4.750334	0.627297	1.628846	H	4.626703	1.433973	0.893362
C	-2.284267	-1.236807	3.766685	C	4.976781	-4.692462	0.295508
H	-1.990839	0.566922	2.614336	C	0.752946	-2.125913	2.101245
C	-3.018552	-3.190291	2.528833	C	4.605768	3.255670	-1.181556
H	-3.316059	-2.918682	0.403193	H	4.408278	1.341483	-2.190560
C	-5.481866	-1.682942	-2.486684	H	4.131676	-5.369141	0.097927
H	-5.359080	-0.251358	-0.871269	H	5.692607	-4.762752	-0.537465
C	-3.379221	-2.639114	-3.237801	H	5.463126	-4.948401	1.244374
H	-1.602440	-1.946144	-2.211636	H	1.268766	-2.532515	2.984352
C	4.723001	-0.511910	-0.188150	H	0.427048	-1.097012	2.316870
C	3.878887	-2.828331	-0.599010	H	-0.113060	-2.746119	1.835589
C	2.686537	-1.354255	1.033342	C	4.609375	3.986841	-2.309889
C	1.449901	4.331756	-0.026088	H	4.752423	3.742162	-0.211777
C	3.212982	2.970779	2.186613	H	4.477390	3.518583	-3.291706
C	0.335950	2.199994	1.877242	H	4.752344	5.070987	-2.285899
C	-4.731093	3.852105	0.500578				
H	-3.352882	4.660129	-0.964127	**IN8**			
H	-5.956128	2.778951	1.930191	C	1.201502	1.413297	0.321744
C	-2.647989	-2.591685	3.738222	C	0.153535	1.698683	-0.739649
H	-2.003010	-0.763220	4.711469	C	3.640014	-0.333881	0.525059
H	-3.312017	-4.243475	2.504692	C	2.615103	-0.321571	1.567240
C	-4.772628	-2.541189	-3.338431	C	1.179703	0.044678	1.058260
H	-6.568940	-1.601054	-2.571573	H	2.172344	1.487307	-0.197431
H	-2.824363	-3.302546	-3.906762	H	1.169564	2.202614	1.087887
C	4.504900	0.985967	-0.095357	H	0.351340	1.263231	-1.727941
H	5.287177	-0.835928	0.698502	H	2.570258	-1.300831	2.069272

H	2.893332	0.414945	2.342585	H	1.001014	-3.043454	-1.557388
C	-0.779860	2.720357	-0.651670	H	-0.312455	-1.978704	-2.165204
H	-0.872807	3.258823	0.302478	C	-0.271386	-0.727573	4.390063
C	-1.515633	3.273745	-1.799608	H	0.188241	-1.450401	5.074268
H	-1.346533	2.802824	-2.775836	H	-0.293636	0.276128	4.839972
C	-2.347483	4.321911	-1.682423	H	-1.298591	-1.034264	4.142796
H	-2.522399	4.805101	-0.714646				
H	-2.867051	4.733286	-2.552275	**IN9**			
C	4.507937	-0.327578	-0.329694	C	-1.240867	0.901678	-1.709788
Au	-1.872858	0.728048	-0.303788	C	-3.260218	1.899382	-0.547055
P	-3.333027	-1.020651	0.210720	C	-4.295349	0.933781	-1.060150
C	-5.089843	-0.618151	0.063681	C	-5.295928	0.452814	-0.298721
H	-5.712652	-1.479932	0.357889	C	-6.284015	-0.525014	-0.755153
H	-5.332783	0.238810	0.712668	C	-7.267111	-1.001881	0.026377
H	-5.325948	-0.341743	-0.976695	H	-1.244452	1.834121	-2.300585
C	-3.059534	-2.500226	-0.788499	H	-1.918900	0.193666	-2.215734
H	-2.019269	-2.829529	-0.629750	H	-3.593463	2.317596	0.414479
H	-3.748403	-3.306446	-0.483837	H	-3.115613	2.738939	-1.245057
H	-3.216906	-2.276499	-1.856035	H	-4.210061	0.592124	-2.099930
C	-3.062573	-1.539543	1.919279	H	-5.392031	0.805056	0.738033
H	-3.753712	-2.352169	2.200102	H	-6.192387	-0.874142	-1.791449
H	-2.020771	-1.892874	2.000288	H	-7.988127	-1.735401	-0.345005
H	-3.204929	-0.679581	2.593518	H	-7.384218	-0.662605	1.062003
Si	5.865774	-0.320459	-1.590596	Rh	1.457172	-0.404055	-0.312768
C	6.546217	1.421095	-1.685588	P	1.768709	-0.908363	2.015180
H	6.945298	1.743145	-0.708711	P	0.708370	-2.628393	-0.762139
H	7.366788	1.475442	-2.422539	C	0.132712	0.330262	-1.758752
H	5.767122	2.140114	-1.991139	C	1.152628	-0.056408	-2.393715
C	7.171426	-1.536186	-1.028593	C	-0.135799	-3.743901	0.406596
H	8.005773	-1.568571	-1.751191	H	0.415567	-3.852676	1.351987
H	7.582759	-1.248853	-0.046064	H	-1.133004	-3.328801	0.618138
H	6.756170	-2.554472	-0.940502	H	-0.249758	-4.743892	-0.044438
C	5.120723	-0.838679	-3.231541	C	2.194169	-3.585074	-1.216953
H	4.316755	-0.148984	-3.540153	H	2.892030	-3.638742	-0.365127
H	5.892001	-0.834891	-4.021767	H	1.942273	-4.611576	-1.533731
H	4.702695	-1.857873	-3.172283	H	2.719253	-3.076879	-2.042432
C	0.667928	-1.100460	0.171265	C	-0.356266	-2.813132	-2.222535
C	0.224199	0.124868	2.267052	H	0.121263	-2.384380	-3.115068
O	-0.092669	-1.958163	0.547327	H	-0.571878	-3.878623	-2.406218
O	-0.702397	0.894392	2.331406	H	-1.298149	-2.276265	-2.031361
O	0.533502	-0.725094	3.218318	C	2.739764	-2.401709	2.408120
O	1.155811	-1.034483	-1.047974	H	2.721498	-2.616284	3.490316
C	0.769480	-2.048493	-1.964765	H	2.360141	-3.282728	1.869917
H	1.340240	-1.865991	-2.882302	H	3.787251	-2.245902	2.099356

C	2.488369	0.279460	3.188473
H	1.916239	1.218734	3.151842
H	2.438801	-0.127200	4.212793
H	3.542418	0.485776	2.946786
C	0.148870	-1.186171	2.787361
H	0.255052	-1.516156	3.834889
H	-0.396828	-0.228476	2.752567
H	-0.424205	-1.930056	2.219432
C	-1.860968	1.220434	-0.330911
C	-0.961586	2.169392	0.467243
C	-2.126218	-0.062099	0.466129
O	-0.286295	1.867132	1.416994
O	-1.018122	3.395806	-0.031158
O	-1.923686	-1.175712	0.058882
O	-2.724414	0.199840	1.613822
C	-0.340363	4.437686	0.654371
C	-3.324323	-0.887275	2.301051
H	-0.515065	4.360688	1.737766
H	0.741034	4.388590	0.455801
H	-0.746724	5.378565	0.263140
H	-4.056693	-1.384137	1.644250
H	-2.566875	-1.618691	2.618326
H	-3.823094	-0.457012	3.178205
C	1.988481	-0.315439	-3.587171
H	2.268957	-1.380950	-3.651539
H	1.454956	-0.040690	-4.512718
H	2.929375	0.260367	-3.548406
P	2.643401	1.652287	-0.337740
C	2.077285	2.834039	-1.605384
H	1.012574	3.075817	-1.457547
H	2.673171	3.761080	-1.568489
H	2.172417	2.390294	-2.607298
C	4.358947	1.312682	-0.852351
H	4.851547	0.676169	-0.098435
H	4.362208	0.762637	-1.807101
H	4.944497	2.240493	-0.970456
C	2.906996	2.747355	1.096888
H	3.306280	3.721222	0.766479
H	1.961044	2.897684	1.637595
H	3.636607	2.300446	1.786908

IN10

Rh	1.585681	-0.120152	0.159145
P	2.331012	1.584936	-1.358032
P	2.436166	-1.857270	-1.128873
C	1.354018	3.111324	-1.149383
C	1.949643	1.205789	-3.101979
C	4.042977	2.201490	-1.461367
P	1.684809	1.300863	2.012790
C	0.399701	-1.276402	1.146862
C	1.487042	-2.382246	-2.594423
C	2.644556	-3.450531	-0.270802
C	4.111579	-1.578314	-1.788301
H	1.534329	3.814824	-1.979744
H	1.611444	3.619714	-0.207614
H	0.277227	2.869483	-1.111489
H	2.105444	2.088770	-3.744532
H	2.582750	0.388005	-3.479309
H	0.894838	0.893467	-3.183308
H	4.143273	3.004101	-2.211807
H	4.722826	1.376627	-1.729573
H	4.363804	2.588550	-0.481382
C	1.851949	0.481859	3.631622
C	0.204124	2.326949	2.284090
C	3.063336	2.489718	2.097384
C	0.739108	-2.279356	2.205940
C	-0.997344	-1.074440	0.782294
H	1.346934	-1.541461	-3.290698
H	0.487935	-2.715336	-2.267104
H	1.982021	-3.211621	-3.128609
H	3.184173	-3.309375	0.679206
H	1.654788	-3.881891	-0.051000
H	3.203457	-4.165434	-0.898260
H	4.486725	-2.466301	-2.324967
H	4.794998	-1.347878	-0.954300
H	4.119233	-0.723172	-2.481255
H	0.958179	-0.124625	3.843904
H	1.967005	1.227686	4.436328
H	2.731088	-0.182672	3.634897
H	-0.647942	1.647627	2.461376
H	0.312425	2.997077	3.154050
H	-0.041325	2.917095	1.386674
H	3.019074	3.214452	1.271349
H	4.017699	1.942026	2.025038
H	3.045076	3.048050	3.048721
H	1.773178	-2.165059	2.556814
H	0.639225	-3.289134	1.767749
H	0.050506	-2.250988	3.069249

C	-1.326124	-0.014212	-0.271567
C	-2.776271	0.456346	-0.022710
H	-0.658256	0.849581	-0.124782
H	-1.198211	-0.371124	-1.304902
C	-3.082364	0.102758	1.460559
C	-2.889641	1.976543	-0.220185
C	-3.730023	-0.181401	-1.049189
C	-2.195625	-1.088062	1.784078
H	-2.792499	0.945728	2.110802
H	-4.151690	-0.094940	1.617254
O	-4.151456	2.349696	-0.300434
O	-1.958661	2.736861	-0.256278
O	-4.839321	-0.663879	-0.520413
O	-3.468974	-0.221326	-2.220209
C	-2.112148	-2.235614	0.832298
H	-1.999226	-1.308733	2.839491
C	-4.416080	3.737267	-0.463430
C	-5.795660	-1.203400	-1.422426
C	-1.842389	-3.619190	1.298045
H	-2.738255	-2.202255	-0.065177
H	-5.506957	3.836290	-0.511650
H	-3.953360	4.105228	-1.391524
H	-4.013992	4.304988	0.389197
H	-6.144099	-0.423092	-2.115862
H	-6.625580	-1.569890	-0.806431
H	-5.352712	-2.024480	-2.006172
C	-1.922042	-4.688930	0.495223
H	-1.618854	-3.760819	2.360839
H	-2.165269	-4.588269	-0.568583
H	-1.763522	-5.700414	0.880165

TS8

Rh	1.338349	0.141368	0.116666
P	1.880724	-2.125381	-0.568194
P	1.794996	-0.273436	2.348509
C	0.975112	-2.466133	-2.109816
C	1.272273	-3.475144	0.492602
C	3.579340	-2.679415	-0.938524
P	2.830447	1.066610	-1.391030
C	0.338510	1.720206	0.404107
C	0.613204	-1.243235	3.337752
C	2.039548	1.196547	3.391674
C	3.374288	-1.151464	2.585563
H	1.225881	-1.726299	-2.885038
H	-0.101088	-2.392495	-1.882968
H	1.186042	-3.479604	-2.491857
H	1.808603	-3.501415	1.454126
H	0.197760	-3.314269	0.677088
H	1.403419	-4.452200	-0.002911
H	4.025232	-2.073453	-1.742943
H	3.591978	-3.736623	-1.253631
H	4.214568	-2.573536	-0.042970
C	2.778117	2.863720	-1.679866
C	2.982175	0.455087	-3.103457
C	4.518761	0.854677	-0.736369
C	0.721599	3.075259	0.908055
C	-1.100627	1.491558	0.040189
H	-0.335151	-0.684813	3.407645
H	0.988282	-1.437837	4.357401
H	0.397479	-2.202199	2.841164
H	2.353754	0.910868	4.409929
H	2.813128	1.846813	2.951971
H	1.103020	1.772812	3.457911
H	3.324173	-2.163131	2.154880
H	3.633543	-1.238761	3.654451
H	4.176003	-0.599274	2.067178
H	2.879293	3.403947	-0.726487
H	1.815114	3.145626	-2.136704
H	3.595309	3.178307	-2.350930
H	3.197938	-0.624439	-3.115699
H	2.032755	0.617453	-3.640674
H	3.789060	0.977941	-3.645185
H	4.594152	1.386922	0.226507
H	5.281080	1.257042	-1.425540
H	4.727968	-0.210558	-0.552473
H	-0.010390	3.429114	1.657681
H	0.668718	3.815861	0.091476
H	1.736541	3.097148	1.327171
C	-1.760173	0.234278	0.642372
C	-2.800109	-0.291055	-0.382309
H	-1.003791	-0.552321	0.786208
H	-2.221740	0.434546	1.622937
C	-2.406483	0.334609	-1.749434
C	-2.718536	-1.815754	-0.503171
C	-4.234976	0.079680	0.017249
C	-1.618836	1.585192	-1.410222
H	-1.747528	-0.358301	-2.302319
H	-3.300821	0.531900	-2.359979

O	-3.801625	-2.309772	-1.065213
O	-1.760093	-2.478353	-0.194886
O	-4.552604	-0.493936	1.170331
O	-4.966716	0.796312	-0.603019
C	-2.143269	2.576036	-0.376847
H	-0.960439	1.998531	-2.182820
C	-3.850596	-3.711975	-1.288614
C	-5.869944	-0.272984	1.653930
C	-1.827771	4.017692	-0.558219
H	-3.153391	2.404161	0.010437
H	-4.835031	-3.917202	-1.725593
H	-3.728333	-4.253080	-0.338330
H	-3.052095	-4.016151	-1.982261
H	-5.949332	-0.829228	2.595853
H	-6.609363	-0.638969	0.925502
H	-6.041949	0.800760	1.824220
C	-2.555839	5.012834	-0.038509
H	-0.975258	4.261152	-1.204714
H	-3.431184	4.811493	0.588685
H	-2.308456	6.059990	-0.234164

IN11

Rh	1.547142	0.099210	0.196154
P	3.050934	2.006442	0.021332
P	3.463988	-1.315782	0.697764
C	3.441832	2.611602	1.697484
C	2.576134	3.590417	-0.759284
C	4.707197	1.816527	-0.732699
P	1.168832	-1.060571	-1.859498
C	-0.109868	1.079584	-0.255221
C	4.621651	-0.738836	1.985828
C	4.625565	-1.774422	-0.633176
C	3.002007	-2.934482	1.395285
H	3.794195	1.789870	2.337019
H	2.514015	3.000474	2.149117
H	4.197363	3.415848	1.685259
H	2.458789	3.482070	-1.848924
H	1.630150	3.964398	-0.340423
H	3.360499	4.342681	-0.569774
H	5.308517	1.061506	-0.206350
H	5.263801	2.768852	-0.710805
H	4.600471	1.497665	-1.783620
C	-0.497206	-0.973423	-2.595508
C	1.308235	-2.877435	-1.753341
C	2.239677	-0.640630	-3.272758
C	-0.207746	2.135616	-1.320988
C	-1.384586	0.585421	0.220586
H	5.177782	0.152135	1.659365
H	5.350014	-1.530471	2.229129
H	4.067682	-0.478698	2.901768
H	5.022451	-0.870816	-1.120117
H	5.470899	-2.360387	-0.234861
H	4.125120	-2.376583	-1.405501
H	2.327001	-3.477900	0.718266
H	2.475098	-2.786338	2.351999
H	3.896285	-3.551811	1.583047
H	-1.255060	-1.303233	-1.863037
H	-0.557385	-1.629562	-3.480040
H	-0.737343	0.052017	-2.912289
H	1.050992	-3.343424	-2.719513
H	2.316755	-3.205795	-1.468726
H	0.598236	-3.239906	-0.990998
H	3.296985	-0.773963	-2.991907
H	2.092829	0.422365	-3.528812
H	2.024366	-1.253597	-4.164828
H	0.711268	2.241586	-1.905993
H	-0.403835	3.097769	-0.806053
H	-1.055718	1.985174	-2.006459
C	-2.704115	0.838754	-0.509920
C	-3.829889	0.381538	0.439929
H	-2.811390	1.923710	-0.673441
H	-2.778643	0.326168	-1.480192
C	-3.283479	0.670314	1.857366
C	-5.103419	1.193650	0.158086
C	-4.157372	-1.099715	0.212333
C	-1.772349	0.526523	1.785007
H	-3.557262	1.701713	2.126098
H	-3.723647	-0.000555	2.613019
O	-5.718762	0.731983	-0.920223
O	-5.460982	2.146668	0.787498
O	-5.129854	-1.492053	1.014639
O	-3.604705	-1.817563	-0.578655
C	-1.188323	-0.673533	1.164122
H	-1.179138	1.108801	2.490902
C	-6.904462	1.403667	-1.322766
C	-5.583957	-2.831208	0.881592
C	0.263409	-1.013812	1.429615
H	-1.835849	-1.524992	0.942669

H	-7.264857	0.880574	-2.216728
H	-6.688216	2.458139	-1.552442
H	-7.656753	1.361781	-0.520516
H	-4.766810	-3.536780	1.095992
H	-5.949193	-3.008108	-0.141345
H	-6.396619	-2.953046	1.607705
C	1.094721	-0.159172	2.251641
H	0.444426	-2.093362	1.459224
H	0.681490	0.722767	2.746579
H	1.875021	-0.628461	2.860281

IN12

Rh	1.677051	0.020029	-0.118130
P	1.068217	2.330156	0.024441
P	4.077293	0.485657	0.132237
C	1.330007	3.164968	1.618508
C	-0.660904	2.751368	-0.318958
C	1.965839	3.364753	-1.177538
P	2.030559	-2.321383	-0.452299
C	-0.178985	-0.299518	-0.808810
C	5.183425	-0.807903	0.785211
C	4.616173	1.896301	1.153168
C	4.823708	0.856184	-1.489544
H	0.564759	2.826950	2.335661
H	1.230005	4.256971	1.501738
H	2.317686	2.935319	2.042283
H	-0.964018	2.373379	-1.307175
H	-1.321377	2.295766	0.435641
H	-0.791523	3.846373	-0.290481
H	3.047475	3.365192	-0.970863
H	1.606972	4.407495	-1.154675
H	1.810533	2.966056	-2.194790
C	0.588531	-3.337405	-0.871311
C	2.838069	-3.313665	0.851705
C	3.093760	-2.569887	-1.914324
C	0.046080	-0.113014	-2.302805
C	-1.361084	-0.571305	-0.257185
H	4.911170	-1.041037	1.828075
H	6.232110	-0.465761	0.770174
H	5.112090	-1.734539	0.195854
H	4.270835	1.757941	2.191606
H	5.716304	1.976846	1.160243
H	4.203345	2.843651	0.774920
H	4.320805	1.723254	-1.948277
H	4.690034	-0.001538	-2.169421
H	5.901781	1.075761	-1.407378
H	0.893241	-4.388955	-1.003886
H	0.118696	-2.977589	-1.798623
H	-0.152616	-3.262095	-0.062335
H	2.068781	-3.882412	1.396155
H	3.551748	-4.031876	0.414632
H	3.365039	-2.678950	1.577269
H	2.665564	-2.032775	-2.778174
H	3.176161	-3.638353	-2.175906
H	4.107238	-2.177273	-1.734829
H	1.093490	0.208588	-2.529551
H	-0.610004	0.660184	-2.743417
H	-0.110567	-1.042342	-2.879613
C	-2.676515	-0.752598	-0.991784
C	-3.743348	-0.414016	0.070709
H	-2.768282	-0.130910	-1.897332
H	-2.834390	-1.802590	-1.298858
C	-3.127977	-0.971905	1.374128
C	-3.905882	1.102483	0.162333
C	-5.091505	-1.070287	-0.222516
C	-1.618507	-0.669887	1.264477
H	-3.591900	-0.532066	2.268161
H	-3.292248	-2.063481	1.391327
O	-4.516417	1.584308	-0.910002
O	-3.492771	1.791604	1.057796
O	-6.046177	-0.539266	0.528213
O	-5.256778	-1.979828	-0.984978
C	-0.739424	-1.668900	1.965222
H	-1.431412	0.332514	1.691123
C	-4.745699	2.982269	-0.947052
C	-7.351507	-1.077837	0.385087
C	0.564786	-1.461066	2.234288
H	-1.190381	-2.630586	2.241618
H	-5.281347	3.182809	-1.883013
H	-3.790312	3.530081	-0.926390
H	-5.350429	3.294932	-0.082198
H	-7.703678	-0.956171	-0.650763
H	-7.992623	-0.518783	1.077512
H	-7.354647	-2.149396	0.636945
C	1.296439	-0.208141	1.905627
H	1.124575	-2.263953	2.726575
H	0.688488	0.659920	2.199285
H	2.258749	-0.154808	2.441272

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Rh	-1.257521	-0.180636	-0.124009
P	-1.612051	2.202863	-0.537241
P	-3.486566	-0.936593	-0.651495
C	-0.490280	3.249987	0.446637
C	-3.246392	2.979146	-0.280786
C	-1.255965	2.801826	-2.224171
P	-1.635562	-0.042285	2.131107
C	0.220119	-1.703049	0.047099
C	-3.711972	-2.741863	-0.736103
C	-3.995661	-0.385279	-2.315088
C	-4.944861	-0.419760	0.315783
H	-0.673494	3.110073	1.524349
H	-0.599486	4.321559	0.207437
H	0.550123	2.944426	0.238060
H	-3.964331	2.556099	-1.004026
H	-3.633007	2.787751	0.730255
H	-3.203041	4.070090	-0.440799
H	-1.451900	3.884701	-2.303587
H	-1.889503	2.274927	-2.956858
H	-0.200195	2.623833	-2.482262
C	-2.854359	1.181688	2.704880
C	-0.214885	0.420997	3.162827
C	-2.263642	-1.571506	2.883024
C	0.560057	-2.610121	1.211345
C	0.806278	-0.367161	-0.059475
H	-3.492236	-3.188800	0.248052
H	-2.999183	-3.169353	-1.460167
H	-4.734952	-3.023721	-1.038879
H	-4.064531	0.715392	-2.327104
H	-3.251235	-0.680338	-3.070618
H	-4.976136	-0.800335	-2.604086
H	-5.873161	-0.808600	-0.136004
H	-5.004119	0.680744	0.341722
H	-4.887799	-0.789483	1.352004
H	-3.022216	1.062068	3.788271
H	-3.815951	1.064387	2.186644
H	-2.480183	2.202074	2.528689
H	-0.530475	0.550016	4.211491
H	0.579407	-0.335558	3.122562
H	0.206584	1.370170	2.794875
H	-1.585262	-2.407652	2.662435
H	-3.250138	-1.811046	2.454272
H	-2.370093	-1.468437	3.975973
H	1.559513	-3.054877	1.048832
H	-0.169359	-3.433418	1.294560
H	0.605357	-2.092891	2.178318
C	1.991899	0.080165	0.773881
C	3.198989	-0.029891	-0.235687
H	1.879100	1.125838	1.104639
H	2.194755	-0.545507	1.651240
C	2.592195	-0.310378	-1.650954
C	3.918294	1.315729	-0.228034
C	4.136047	-1.174219	0.143228
C	1.141312	0.160969	-1.455146
H	3.141514	0.230732	-2.433698
H	2.622997	-1.389150	-1.870171
O	4.776129	1.401673	0.775090
O	3.666945	2.217299	-0.981680
O	5.215182	-1.166405	-0.621561
O	3.903868	-2.011752	0.972373
C	0.001602	-0.251063	-2.359309
H	1.183705	1.262737	-1.411177
C	5.473812	2.628531	0.926781
C	6.169141	-2.194645	-0.403647
C	-0.561973	-1.485885	-2.235520
H	-0.363458	0.430676	-3.133287
H	4.766405	3.455290	1.094149
H	6.065406	2.845397	0.024388
H	6.131230	2.502876	1.795612
H	6.978048	-2.021103	-1.123667
H	5.713035	-3.183175	-0.566538
H	6.553431	-2.146390	0.626665
C	-0.000752	-2.482197	-1.250127
H	-1.372401	-1.780924	-2.911129
H	-0.715037	-3.302969	-1.077644
H	0.932402	-2.947936	-1.631369

IN14

C	1.731712	-0.877641	1.113430
C	1.842446	0.701066	-1.001702
C	0.564526	0.107326	-1.573630
C	0.341376	-1.325813	-1.588711
C	-0.952052	-1.779734	-1.912935
C	-1.928275	-0.759618	-2.258030
H	2.273653	-0.901500	2.071517
H	1.579260	-1.919047	0.796660

H	1.588065	1.683438	-0.570389
H	2.559374	0.893380	-1.815525
H	0.240280	0.646862	-2.473135
H	1.081276	-2.039803	-1.223385
H	-1.200093	-2.839040	-1.792910
H	-2.964958	-1.091994	-2.370787
H	-1.635864	-0.032071	-3.024218
Rh	-1.177645	-0.225933	-0.380459
P	-2.954371	-1.386145	0.768978
P	-1.892338	2.000579	-0.613181
C	0.429537	-0.246831	1.364929
C	-0.512402	0.386374	1.840299
C	-3.540556	2.476503	-0.001789
H	-4.301227	1.864081	-0.513840
H	-3.640558	2.305695	1.080739
H	-3.748622	3.539551	-0.210531
C	-2.005681	2.548938	-2.343403
H	-1.053560	2.372832	-2.869398
H	-2.798518	1.992521	-2.867747
H	-2.237513	3.626018	-2.393363
C	-0.785361	3.260470	0.093765
H	-0.560264	3.059566	1.152019
H	0.168920	3.242754	-0.457334
H	-1.219457	4.270142	0.002218
C	-2.301096	-2.496205	2.053676
H	-1.587153	-3.199261	1.593001
H	-1.752022	-1.922593	2.817192
H	-3.104179	-3.071561	2.544005
C	-4.282083	-0.486995	1.633016
H	-3.873479	0.223133	2.366728
H	-4.880665	0.080577	0.903016
H	-4.949608	-1.189934	2.159862
C	-3.933517	-2.516943	-0.267841
H	-4.529058	-1.944340	-0.996989
H	-3.276778	-3.204687	-0.823861
H	-4.623778	-3.114075	0.351403
C	2.607255	-0.103017	0.083060
C	3.549324	-1.122440	-0.574336
C	3.460876	0.918937	0.855961
O	3.509695	-1.448609	-1.726830
O	4.380592	-1.629178	0.321995
O	3.278691	1.237941	1.996710
O	4.392776	1.431347	0.071346
C	5.320826	-2.592582	-0.136369
C	5.256543	2.405726	0.641446
H	5.917083	-2.878941	0.738203
H	4.799953	-3.467903	-0.553308
H	5.962422	-2.154727	-0.915807
H	5.955482	2.696911	-0.151752
H	4.677339	3.276176	0.985220
H	5.799501	1.977772	1.497647
C	-1.336914	1.100780	2.832049
H	-1.885834	0.381395	3.462287
H	-0.673016	1.685125	3.490510
H	-2.064656	1.782175	2.372693

IN15

Rh	1.851792	-0.264345	-0.585722
P	3.650749	-0.798769	0.828239
P	1.531322	2.050105	-0.292113
C	3.581612	-2.484024	1.498742
C	4.149700	0.206561	2.256670
C	5.154064	-0.803909	-0.197263
C	0.421617	-0.564712	0.785002
C	1.996677	2.898429	-1.833099
C	2.487704	2.961893	0.956688
C	-0.170748	2.577664	0.008373
H	3.519029	-3.205537	0.669465
H	2.683034	-2.612292	2.123212
H	4.474247	-2.708789	2.106195
H	5.009133	-0.258320	2.768623
H	4.444590	1.214193	1.927545
H	3.322848	0.303486	2.976826
H	6.036223	-1.117692	0.386585
H	5.030815	-1.495886	-1.046581
H	5.343785	0.205355	-0.599925
C	0.673013	-0.281365	2.241810
C	-0.760947	-0.922175	0.273589
H	1.868318	3.990848	-1.745523
H	1.369716	2.533924	-2.663124
H	3.050621	2.689538	-2.082892
H	3.565491	2.875220	0.743890
H	2.296690	2.563197	1.965690
H	2.217172	4.031286	0.947305
H	-0.236765	3.676503	0.073064
H	-0.804545	2.227891	-0.821598
H	-0.574105	2.132355	0.931794
H	-0.270384	-0.316327	2.809802

H	1.360998	-1.009102	2.703015
H	1.108543	0.721733	2.387764
C	-1.008398	-1.018979	-1.217095
C	-2.100853	-1.112761	0.943583
C	-2.338716	-0.254153	-1.393628
C	0.157468	-0.542001	-2.070095
H	-1.196026	-2.083663	-1.460488
C	-3.084054	-0.390197	-0.027216
H	-2.344099	-2.189094	0.987612
H	-2.167068	-0.700329	1.957998
H	-2.957101	-0.658265	-2.207376
H	-2.140041	0.806526	-1.615919
C	1.257401	-1.386358	-2.340697
H	-0.055736	0.236626	-2.812104
C	-4.372195	-1.206214	-0.165141
C	-3.414040	1.004746	0.504892
C	1.759203	-2.313235	-1.385013
H	1.914672	-1.106073	-3.177675
O	-5.063846	-1.164679	0.964143
O	-4.688435	-1.838715	-1.131664
O	-4.402706	1.548137	-0.184559
O	-2.826070	1.563728	1.392107
H	1.071871	-2.826379	-0.701929
H	2.666500	-2.868512	-1.644857
C	-6.278073	-1.900483	1.002580
C	-4.821403	2.850763	0.191842
H	-6.084080	-2.970246	0.830517
H	-6.969594	-1.535944	0.227733
H	-6.701773	-1.742338	2.001750
H	-3.995260	3.569064	0.076114
H	-5.153306	2.856603	1.241176
H	-5.651852	3.111227	-0.475440

IN16

C	-1.908656	-1.358300	0.448174
C	-2.023153	-0.597537	-1.905442
C	-0.857083	-1.602501	-1.784271
C	0.519505	-1.115171	-2.195496
C	1.621366	-1.872099	-1.758626
C	1.360861	-3.095354	-0.897778
H	-2.653198	-2.175510	0.486470
H	-1.720143	-1.016024	1.473559
H	-2.889789	-1.053469	-2.405327
H	-1.748907	0.299451	-2.480823
H	-1.111167	-2.546135	-2.307590
H	0.612662	-0.408579	-3.025501
H	2.599449	-1.760973	-2.235808
H	2.292548	-3.442767	-0.425511
H	0.941376	-3.945043	-1.476737
Rh	1.122336	-0.473805	-0.233540
P	1.409723	0.235151	2.081453
P	2.512791	1.236103	-1.001463
C	-0.684803	-1.850129	-0.283706
C	0.376330	-2.612243	0.168685
C	1.520771	2.016891	2.445812
H	2.352400	2.504803	1.918463
H	0.575657	2.487173	2.133165
H	1.661383	2.174378	3.528393
C	0.146782	-0.235261	3.303484
H	0.446918	0.106452	4.308339
H	-0.802260	0.250575	3.029162
H	0.003093	-1.323557	3.336121
C	2.940282	-0.437220	2.805858
H	2.905635	-1.539055	2.789794
H	3.813551	-0.126467	2.210412
H	3.080959	-0.104167	3.848269
C	4.103848	1.552944	-0.175539
H	4.720999	0.640439	-0.232227
H	4.647715	2.375712	-0.669767
H	3.974999	1.809354	0.885589
C	3.064674	1.047995	-2.724904
H	2.204352	0.959376	-3.406016
H	3.664634	1.919991	-3.034763
H	3.686484	0.144496	-2.832231
C	1.664794	2.843692	-1.040995
H	2.326270	3.654377	-1.390389
H	0.808867	2.758722	-1.731965
H	1.270496	3.092906	-0.044349
C	-2.456198	-0.223726	-0.458727
C	-3.985763	-0.157734	-0.323014
C	-1.899862	1.143314	-0.062351
O	-4.765770	-0.601652	-1.112762
O	-4.318569	0.408280	0.829050
O	-1.078992	1.352824	0.797607
O	-2.437882	2.096416	-0.798532
C	-5.707553	0.509796	1.117854
C	-2.117359	3.441478	-0.480898
H	-5.782722	1.000051	2.095953

H	-6.214218	1.107422	0.345015
H	-6.164980	-0.490587	1.150992
H	-2.675621	4.065501	-1.189001
H	-2.419771	3.669209	0.552644
H	-1.036179	3.615683	-0.586236
C	0.440774	-3.256065	1.528377
H	0.358264	-4.350423	1.398729
H	1.403794	-3.066581	2.030437
H	-0.383990	-2.937909	2.180283

IN19

Rh	-1.093718	-0.007131	0.161606
P	-2.983190	1.086278	-0.534984
P	-2.145762	-2.217336	0.087637
C	-0.146781	1.655774	0.471113
C	-3.931411	0.247941	-1.846738
C	-2.756377	2.730398	-1.282860
C	-4.257191	1.390146	0.730615
C	-3.785141	-2.401211	0.864067
C	-1.177566	-3.474654	0.981122
C	-2.355229	-3.012722	-1.539377
C	-0.652112	2.751125	1.364908
C	1.219382	1.754163	-0.012523
H	-4.778612	0.872107	-2.177586
H	-4.331302	-0.712355	-1.488761
H	-3.276566	0.051227	-2.711586
H	-2.038765	2.656754	-2.116209
H	-3.711888	3.128156	-1.664035
H	-2.352817	3.438988	-0.545284
H	-4.570673	0.434843	1.181367
H	-5.141452	1.894439	0.304646
H	-3.845764	2.018744	1.536997
H	-4.541798	-1.791605	0.345245
H	-3.731037	-2.056395	1.910372
H	-4.121464	-3.451949	0.853899
H	-0.981375	-3.131530	2.009271
H	-1.709245	-4.440536	1.012028
H	-0.210192	-3.611840	0.473502
H	-1.374585	-3.068184	-2.040354
H	-3.025310	-2.421770	-2.182276
H	-2.764563	-4.032858	-1.441895
H	0.017182	2.875168	2.236564
H	-1.661365	2.544428	1.744825
H	-0.647101	3.722266	0.837959
C	1.740245	0.681761	-0.983165
C	2.703424	-0.159942	-0.120878
H	0.923702	0.085878	-1.416906
H	2.312170	1.131625	-1.810234
C	3.467448	0.906141	0.707652
C	1.912574	-1.061238	0.820367
C	3.632058	-1.011234	-0.990904
C	2.429141	1.993151	0.989009
H	3.892393	0.484297	1.629595
H	4.300181	1.279794	0.091171
O	2.694125	-1.774002	1.587099
O	0.699190	-1.112071	0.905039
O	3.030931	-2.135092	-1.359732
O	4.724839	-0.675221	-1.340000
C	2.156770	3.059851	-0.008047
H	2.177627	2.214956	2.032090
C	2.109513	-2.651638	2.541858
C	3.766504	-3.003265	-2.214513
C	1.714683	4.419942	0.397401
H	2.786380	3.053076	-0.905690
H	1.412395	-2.099418	3.189716
H	2.941449	-3.059517	3.127827
H	1.571584	-3.461732	2.028036
H	4.701284	-3.316263	-1.725480
H	4.011398	-2.492040	-3.157725
H	3.120752	-3.869422	-2.402427
C	1.677588	5.455163	-0.451070
H	1.466185	4.576247	1.452523
H	1.937813	5.337898	-1.509023
H	1.397170	6.456464	-0.111703

IN20

Rh	-1.840466	-0.256125	0.453149
P	-1.743425	1.923283	-0.495149
P	-4.183978	-0.696996	-0.084159
C	-0.019967	-0.139440	1.132146
C	-0.177853	2.819816	-0.297369
C	-2.949328	3.184306	0.027251
C	-1.964551	1.857937	-2.300239
C	-5.345681	0.595000	-0.635049
C	-5.071549	-1.394262	1.343901
C	-4.389144	-1.957577	-1.381155
C	0.289221	0.570593	2.412633
C	1.016307	-0.887846	0.498004

H	0.680198	2.230825	-0.659574
H	-0.013709	3.027193	0.773567
H	-0.197651	3.781712	-0.837240
H	-2.871871	3.347251	1.115120
H	-2.761050	4.143153	-0.485291
H	-3.975872	2.861597	-0.198433
H	-1.185959	1.219206	-2.748521
H	-1.903621	2.862593	-2.752186
H	-2.942753	1.413906	-2.545682
H	-6.330826	0.159417	-0.873353
H	-4.967802	1.109183	-1.533753
H	-5.484229	1.342017	0.163124
H	-4.548279	-2.287398	1.719727
H	-5.098125	-0.652680	2.159733
H	-6.107218	-1.668565	1.081201
H	-3.836417	-2.874662	-1.121934
H	-3.988937	-1.575696	-2.335360
H	-5.451909	-2.216921	-1.522042
H	1.165805	1.233700	2.279546
H	0.574871	-0.167237	3.186269
H	-0.558395	1.164232	2.788917
C	2.448461	-1.107447	0.970896
C	3.336617	-0.524513	-0.154508
H	2.659437	-0.625900	1.936636
H	2.680910	-2.178096	1.085725
C	2.568415	-0.808826	-1.473355
C	3.450515	0.987760	0.050317
C	4.731329	-1.154386	-0.179491
C	1.087778	-0.720141	-1.124167
H	2.842226	-0.080452	-2.247941
H	2.818836	-1.820945	-1.831928
O	4.237260	1.274255	1.071876
O	2.862030	1.812071	-0.598179
O	5.523737	-0.492035	-1.007034
O	5.043273	-2.137734	0.427851
C	0.415590	-1.893222	-0.554140
H	0.483110	0.089347	-1.538362
C	4.461803	2.647114	1.359298
C	6.852945	-0.975476	-1.152924
C	-1.085088	-1.968642	-0.471848
H	0.953746	-2.849825	-0.608848
H	4.912323	3.148398	0.489394
H	5.146386	2.673281	2.215489
H	3.514196	3.148980	1.607778
H	7.346445	-0.305249	-1.866902
H	6.844855	-2.007902	-1.534062
H	7.372266	-0.957718	-0.182742
C	-1.678503	-2.371085	0.766625
H	-1.587032	-2.200473	-1.420676
H	-1.023030	-2.642017	1.603286
H	-2.623189	-2.923353	0.760150

PMe_3

P	0.000000	0.000000	-0.701280
C	0.000000	1.618103	0.175667
C	-1.401318	-0.809051	0.175667
H	-0.888922	2.202601	-0.116983
H	0.888922	2.202601	-0.116983
H	0.000000	1.503194	1.274995
C	1.401318	-0.809051	0.175667
H	-1.463047	-1.871130	-0.116983
H	-2.351969	-0.331471	-0.116983
H	-1.301804	-0.751597	1.274995
H	2.351969	-0.331471	-0.116983
H	1.463047	-1.871130	-0.116983
H	1.301804	-0.751597	1.274995

TS7

Rh	1.671128	0.108944	-0.236573
P	3.427264	-0.790173	1.004205
P	1.744375	2.139360	0.927082
C	4.732817	0.290847	1.691005
C	4.530840	-2.034975	0.246269
C	2.831336	-1.657106	2.495055
P	1.385901	-1.881893	-1.449071
C	0.180151	0.979121	-1.463529
C	1.674469	2.050189	2.750849
C	0.379401	3.314635	0.630112
C	3.169311	3.227150	0.590872
H	5.448695	-0.303928	2.283112
H	4.326075	1.080413	2.338109
H	5.281725	0.770679	0.863801
H	3.978249	-2.906460	-0.130513
H	5.069500	-1.576081	-0.599446
H	5.273502	-2.388282	0.981396
H	2.282801	-0.947615	3.136108
H	3.655994	-2.104443	3.076146
H	2.121893	-2.448697	2.203573

C	-0.122986	-1.989972	-2.466665
C	1.227269	-3.440119	-0.515810
C	2.657963	-2.228647	-2.710551
C	0.552302	1.672773	-2.730805
C	-0.922344	0.735961	-0.846285
H	0.724610	1.570082	3.041194
H	1.719288	3.052846	3.209520
H	2.491013	1.439557	3.163259
H	0.306182	3.566657	-0.438960
H	-0.583083	2.874766	0.933005
H	0.541042	4.242079	1.205022
H	3.157745	3.495406	-0.478734
H	4.119528	2.713530	0.792020
H	3.126536	4.152502	1.190415
H	-0.175373	-1.152109	-3.178997
H	-0.997757	-1.945983	-1.802125
H	-0.144025	-2.941733	-3.023649
H	1.149837	-4.305731	-1.195925
H	2.074584	-3.605295	0.165293
H	0.304491	-3.375980	0.085337
H	3.660317	-2.283162	-2.263171
H	2.664905	-1.402889	-3.441405
H	2.451723	-3.172352	-3.243994
H	0.892468	2.699756	-2.505439
H	-0.296638	1.744888	-3.432321
H	1.389071	1.162408	-3.231752
C	-1.548705	0.188871	0.391517
C	-2.930030	-0.465483	0.114920
H	-0.863526	-0.569973	0.800406
H	-1.639125	0.982471	1.152950
C	-3.346998	-0.258271	-1.369236
C	-2.863306	-1.977080	0.375732
C	-3.965480	0.152682	1.062594
C	-2.672274	0.949029	-1.976327
H	-3.066381	-1.143526	-1.958862
H	-4.442798	-0.156695	-1.421489
O	-4.070959	-2.503772	0.348048
O	-1.850931	-2.607758	0.524279
O	-3.751212	-0.244384	2.306171
O	-4.815913	0.931598	0.734801
C	-2.710616	2.208457	-1.427499
H	-2.325393	0.853269	-3.012297
C	-4.179208	-3.908740	0.540357
C	-4.629259	0.256786	3.306254
C	-2.241368	3.409199	-2.101690
H	-3.155212	2.341510	-0.433027
H	-5.249636	-4.141640	0.494850
H	-3.762837	-4.190396	1.519166
H	-3.633706	-4.444888	-0.250844
H	-5.666698	-0.031760	3.079685
H	-4.567457	1.354591	3.355281
H	-4.302853	-0.190569	4.252743
C	-2.235815	4.616529	-1.507043
H	-1.912391	3.310213	-3.142358
H	-2.571340	4.739368	-0.471064
H	-1.912071	5.514836	-2.040470

TS9

Rh	-1.547767	0.128804	-0.212428
P	-2.919686	2.027547	0.210817
P	-3.510753	-1.155907	-0.825773
C	-3.378120	2.834274	-1.359172
C	-2.305646	3.489769	1.114584
C	-4.530427	1.814195	1.049164
P	-1.172065	-1.306756	1.737922
C	0.186903	1.074038	0.379043
C	-4.696525	-0.384706	-1.978960
C	-4.642766	-1.760544	0.470926
C	-3.117241	-2.672941	-1.755641
H	-3.807720	2.112068	-2.066928
H	-2.459839	3.236120	-1.818781
H	-4.090621	3.662523	-1.204757
H	-2.125233	3.266043	2.176276
H	-1.367549	3.847479	0.664369
H	-3.053846	4.297839	1.050693
H	-5.198221	1.154743	0.475777
H	-5.042487	2.781972	1.184551
H	-4.369885	1.358963	2.041557
C	0.487845	-1.331555	2.493930
C	-1.329445	-3.090886	1.373986
C	-2.242808	-1.086340	3.197672
C	0.256034	1.778233	1.722413
C	1.429555	0.857895	-0.192548
H	-5.452048	-1.121887	-2.298294
H	-4.170985	-0.013044	-2.872837
H	-5.219342	0.462696	-1.511389
H	-4.982130	-0.922304	1.098708
H	-5.526179	-2.247209	0.024493

H	-4.144761	-2.489979	1.125842
H	-4.032042	-3.242466	-1.989886
H	-2.429397	-3.317645	-1.188441
H	-2.625358	-2.400689	-2.704226
H	1.275402	-1.400814	1.723126
H	0.579556	-2.201050	3.166191
H	0.655800	-0.424303	3.090527
H	-1.110869	-3.695844	2.270146
H	-2.330082	-3.362340	1.011486
H	-0.598351	-3.353916	0.590575
H	-3.302714	-1.178958	2.911935
H	-2.091996	-0.070001	3.599842
H	-2.022057	-1.816256	3.995399
H	-0.656427	1.656547	2.319523
H	0.399278	2.859156	1.540848
H	1.117728	1.463969	2.330430
C	2.771455	0.994641	0.521785
C	3.833343	0.414305	-0.433948
H	2.979106	2.067164	0.691699
H	2.794467	0.482045	1.494671
C	3.257231	0.661539	-1.845737
C	5.175393	1.130140	-0.236426
C	4.038016	-1.082075	-0.174599
C	1.733141	0.623467	-1.712869
H	3.572654	1.665671	-2.166384
H	3.638590	-0.057589	-2.586672
O	5.740049	0.739868	0.896923
O	5.625094	1.961600	-0.969957
O	5.054043	-1.545184	-0.876621
O	3.348068	-1.764182	0.538751
C	1.054906	-0.615546	-1.404316
H	1.203932	1.297233	-2.391069
C	6.987384	1.332475	1.231656
C	5.383152	-2.918994	-0.727393
C	-0.350995	-0.822354	-1.681711
H	1.634917	-1.462014	-1.024749
H	6.880164	2.423794	1.326011
H	7.733557	1.114627	0.452442
H	7.290126	0.890915	2.188809
H	5.623303	-3.139674	0.323593
H	6.255570	-3.095950	-1.367624
H	4.539708	-3.552156	-1.042455
C	-1.184377	0.238002	-2.261667
H	-0.613061	-1.876790	-1.810920
H	-0.708045	1.152351	-2.627623
H	-1.989625	-0.079483	-2.935490

TS10

Rh	1.928253	0.049419	0.011685
P	2.444419	2.383344	-0.373653
P	4.185278	-0.502294	-0.166162
C	3.164195	3.309556	1.021290
C	0.986738	3.418090	-0.733920
C	3.499088	2.802455	-1.799465
P	1.346095	-2.264853	0.093803
C	-0.297388	0.419665	-0.208467
C	4.811763	-0.725555	-1.865018
C	4.822158	-1.984751	0.691602
C	5.392477	0.687038	0.518224
H	3.401638	4.345422	0.725966
H	4.073029	2.830581	1.410262
H	2.425225	3.347892	1.839376
H	0.607827	3.205884	-1.744189
H	0.172900	3.224287	-0.018195
H	1.259969	4.485149	-0.682909
H	3.566415	3.895722	-1.930477
H	3.054064	2.368985	-2.711202
H	4.518099	2.401829	-1.697203
C	-0.386285	-2.761254	-0.170415
C	1.729477	-3.239110	1.585490
C	2.098719	-3.204419	-1.281840
C	-0.073175	0.588588	-1.724676
C	-1.558512	0.139305	0.158425
H	4.268180	-1.542015	-2.366010
H	5.891755	-0.951215	-1.880374
H	4.630487	0.192432	-2.446911
H	4.322634	-2.912584	0.385110
H	5.902168	-2.093726	0.496185
H	4.677751	-1.858116	1.777306
H	6.416297	0.292317	0.406124
H	5.191506	0.835491	1.591932
H	5.348560	1.663598	0.018432
H	-0.763337	-2.350084	-1.119023
H	-1.022197	-2.399133	0.647813
H	-0.447115	-3.861465	-0.213634
H	1.016720	-2.946827	2.373132
H	1.614522	-4.319533	1.394387
H	2.744219	-3.044261	1.957542

H	1.751394	-2.761826	-2.231183
H	1.787358	-4.262268	-1.255925
H	3.195997	-3.165401	-1.277443
H	-0.411959	-0.328177	-2.237667
H	0.965749	0.754825	-2.053246
H	-0.687490	1.421821	-2.106995
C	-2.693956	-0.063203	-0.834724
C	-3.972645	-0.183241	0.024647
H	-2.773983	0.759918	-1.560397
H	-2.539181	-0.999861	-1.403001
C	-3.459311	-0.763293	1.357289
C	-4.555971	1.210035	0.278644
C	-5.007656	-1.083576	-0.644852
C	-2.129348	-0.026312	1.572228
H	-4.176585	-0.630234	2.180860
H	-3.300030	-1.846232	1.219857
O	-5.745105	1.129438	0.851732
O	-3.986356	2.240724	0.042675
O	-5.579232	-0.461164	-1.666150
O	-5.233381	-2.217013	-0.328922
C	-1.156563	-0.648942	2.528998
H	-2.349528	1.004311	1.925345
C	-6.400811	2.350485	1.157762
C	-6.560557	-1.185519	-2.392125
C	0.107439	-0.202078	2.501996
H	-1.479141	-1.454594	3.197932
H	-5.799031	2.943560	1.863416
H	-7.362905	2.078141	1.608310
H	-6.556933	2.939454	0.241124
H	-6.123600	-2.098680	-2.824602
H	-6.914080	-0.515217	-3.185059
H	-7.392092	-1.470488	-1.729537
C	0.486252	0.885696	1.566048
H	0.889748	-0.627387	3.138931
H	-0.211382	1.731823	1.577681
H	1.483929	1.275243	1.824955

TS11

Rh	1.383031	-0.522562	-0.312060
P	3.541795	-0.309617	0.490938
P	1.048680	1.865286	-0.450918
C	4.802793	-0.112403	-0.800332
C	3.903587	1.020114	1.677671
C	4.128412	-1.760839	1.414986
C	0.506687	-0.728155	1.540529
C	0.731647	2.725311	1.114781
C	2.439378	2.766445	-1.213356
C	-0.306030	2.485416	-1.498917
H	4.751967	-0.973965	-1.486585
H	4.610611	0.798835	-1.388485
H	5.818825	-0.059746	-0.374011
H	4.958164	0.966736	1.995653
H	3.720895	2.018448	1.256510
H	3.265049	0.897131	2.566876
H	4.235364	-2.627338	0.746524
H	3.402841	-2.028849	2.199006
H	5.105890	-1.555039	1.882144
C	0.872980	-0.455631	2.961250
C	-0.554045	-1.060797	0.896326
H	-0.204896	2.325023	1.541328
H	0.623215	3.812680	0.963926
H	1.550470	2.547519	1.828584
H	2.590168	2.386586	-2.238207
H	2.228810	3.848065	-1.267766
H	3.379038	2.626345	-0.660326
H	-0.231234	2.070258	-2.517079
H	-0.256661	3.585545	-1.566996
H	-1.282923	2.211146	-1.081309
H	1.047276	0.624122	3.102567
H	0.064276	-0.760050	3.644607
H	1.792235	-0.987262	3.254759
C	-2.008702	-1.341754	1.017180
C	-2.758335	-0.525580	-0.052299
H	-2.207193	-2.416909	0.863786
H	-2.341743	-1.064599	2.028810
C	-1.957739	-0.633166	-1.379365
C	-4.183784	-1.081008	-0.207732
C	-2.855453	0.935246	0.396862
C	-0.608080	-1.298451	-1.154923
H	-2.540058	-1.257162	-2.076600
H	-1.842915	0.350394	-1.853104
O	-4.895092	-0.812291	0.875169
O	-4.580184	-1.706513	-1.147426
O	-3.645715	1.623487	-0.410955
O	-2.269149	1.414552	1.329654
C	0.440414	-1.048895	-2.175445
H	-0.711259	-2.373043	-0.957364
C	-6.238235	-1.279990	0.899257

C	-3.880317	2.987395	-0.090631
C	1.630864	-1.803680	-2.098023
H	0.254473	-0.348915	-2.995437
H	-6.262066	-2.376647	0.810943
H	-6.807631	-0.841956	0.065621
H	-6.656104	-0.961640	1.861801
H	-2.938025	3.557167	-0.115998
H	-4.576230	3.365395	-0.849021
H	-4.319270	3.071262	0.914900
C	1.822863	-2.548034	-0.873781
H	2.419226	-1.667456	-2.845096
H	1.008858	-3.173972	-0.489346
H	2.804738	-3.011011	-0.738953

TS12

Rh	1.246204	-0.209729	-0.584030
P	2.854000	-0.761189	1.080245
P	1.636531	2.144957	-0.325365
C	3.674015	-2.365632	0.811350
C	4.327231	0.304901	1.201388
C	2.314184	-0.812837	2.821113
C	0.115741	-1.949436	-0.421579
C	3.203593	2.858361	-0.918040
C	0.423813	3.186526	-1.187598
C	1.470980	2.724737	1.390087
H	2.952895	-3.191273	0.748835
H	4.391042	-2.579574	1.621750
H	4.230327	-2.322931	-0.140136
H	4.067351	1.319976	1.535719
H	5.044970	-0.120760	1.922972
H	4.819515	0.373996	0.217876
H	1.989204	0.196712	3.124384
H	1.460775	-1.495543	2.955643
H	3.131858	-1.132967	3.489163
C	0.356596	-3.090344	0.530224
C	-1.094519	-1.646503	-0.935338
H	3.314861	2.639155	-1.993050
H	3.210191	3.953273	-0.781623
H	4.069795	2.431409	-0.394207
H	-0.588900	2.857502	-0.910874
H	0.556815	4.243320	-0.901302
H	0.553687	3.106033	-2.278368
H	1.579673	3.820431	1.455874
H	2.219552	2.259143	2.049574
H	0.462418	2.437945	1.731580
H	0.972881	-3.867206	0.044361
H	0.863725	-2.791274	1.456882
H	-0.599217	-3.566153	0.801083
C	-1.280441	-0.672239	-2.091893
C	-2.451555	-1.847486	-0.313203
C	-2.492680	0.201686	-1.638509
C	-0.003733	0.092292	-2.384819
H	-1.582004	-1.254825	-2.984832
C	-2.892831	-0.359476	-0.245146
H	-3.152767	-2.371035	-0.986650
H	-2.457014	-2.337237	0.668241
H	-3.335709	0.086964	-2.335743
H	-2.240950	1.268506	-1.566078
C	1.246611	-0.514565	-2.643919
H	-0.142600	1.110791	-2.755906
C	-4.393268	-0.216635	0.012261
C	-2.088813	0.345055	0.852099
C	1.503777	-1.829391	-2.075863
H	2.041440	0.034086	-3.158193
O	-4.675622	0.960010	0.550683
O	-5.203219	-1.047610	-0.279809
O	-2.237874	-0.251201	2.020527
O	-1.361499	1.292239	0.685103
H	2.554761	-2.135438	-2.006837
H	0.844765	-2.664105	-2.331006
C	-6.047258	1.238928	0.803211
C	-1.508534	0.280829	3.111528
H	-6.464293	0.497122	1.501088
H	-6.621790	1.207682	-0.134883
H	-6.080137	2.243418	1.241879
H	-1.810145	1.321322	3.307099
H	-0.428302	0.255036	2.890444
H	-1.737579	-0.352357	3.977263

TS17

Rh	-1.181539	-0.030293	0.162979
P	-2.733274	1.377061	-0.713791
P	-2.507809	-1.929687	0.038274
C	0.014566	1.647907	0.699375
C	-2.014813	2.805126	-1.590325
C	-3.830421	2.167134	0.507259
C	-3.920440	0.772154	-1.957947
C	-4.132550	-1.807678	0.855969

C	-1.755181	-3.347282	0.900339
C	-2.913610	-2.661620	-1.581176
C	-0.316936	2.614260	1.786980
C	1.088961	1.406031	0.011745
H	-2.798636	3.473312	-1.985320
H	-1.395328	2.444630	-2.428145
H	-1.360235	3.377930	-0.915255
H	-4.527365	2.882700	0.038266
H	-4.411021	1.393611	1.036777
H	-3.222445	2.698062	1.257614
H	-3.374347	0.350435	-2.817746
H	-4.568006	1.590239	-2.316178
H	-4.563024	-0.016364	-1.535974
H	-4.683572	-2.763038	0.822089
H	-4.750104	-1.030376	0.377574
H	-3.983863	-1.516214	1.908880
H	-2.424743	-4.223775	0.898839
H	-0.809510	-3.613506	0.400736
H	-1.526667	-3.064831	1.940479
H	-3.509847	-3.583737	-1.471338
H	-1.977817	-2.903195	-2.111716
H	-3.477156	-1.947409	-2.200519
H	-1.083349	2.199942	2.458925
H	-0.720905	3.544791	1.347670
H	0.566059	2.892797	2.387646
C	1.638494	0.405437	-0.958905
C	2.507631	-0.538594	-0.109735
H	0.808372	-0.117601	-1.459857
H	2.270939	0.870561	-1.731821
C	3.535729	0.405335	0.580733
C	1.655777	-1.288288	0.924362
C	3.123183	-1.624201	-1.003970
C	2.843308	1.690027	1.005667
H	4.004098	-0.090858	1.442973
H	4.320539	0.629183	-0.155406
O	2.398483	-1.986370	1.739764
O	0.444515	-1.262854	1.012409
O	4.188749	-1.199380	-1.653149
O	2.626037	-2.708388	-1.132956
C	2.820136	2.825217	0.218132
H	2.532952	1.782235	2.053288
C	1.748220	-2.811250	2.701570
C	4.789145	-2.110300	-2.569895
C	2.393958	4.145876	0.665188
H	3.215823	2.762030	-0.803761
H	1.118899	-3.553647	2.188890
H	1.124741	-2.197367	3.368577
H	2.546932	-3.307524	3.264743
H	5.109501	-3.021008	-2.042415
H	5.652142	-1.587575	-2.998817
H	4.070547	-2.385800	-3.356416
C	2.323864	5.200683	-0.166165
H	2.158547	4.268959	1.727858
H	2.561210	5.103210	-1.231489
H	2.035750	6.191873	0.195280

TS18

Rh	1.783825	0.111191	0.063748
P	3.718949	1.518393	0.337545
P	3.031422	-1.878521	-0.116044
C	0.055237	-0.877406	0.449175
C	4.399158	1.395453	2.019068
C	3.375048	3.295548	0.162193
C	5.171043	1.294047	-0.736307
C	4.508550	-2.221426	0.895068
C	3.676824	-1.918568	-1.817525
C	2.125262	-3.453233	-0.019787
C	0.051049	-1.651659	1.754815
C	-1.195641	-0.538964	-0.031378
H	3.610938	1.635048	2.752354
H	5.244776	2.087489	2.170590
H	4.741766	0.366863	2.216443
H	2.995562	3.513409	-0.850382
H	2.603923	3.597894	0.889861
H	4.280107	3.902056	0.333944
H	5.595375	0.285344	-0.608656
H	5.956368	2.034280	-0.507855
H	4.876633	1.410105	-1.793011
H	5.248901	-1.413093	0.782193
H	4.986807	-3.171439	0.601436
H	4.230045	-2.282654	1.960551
H	2.829796	-1.915120	-2.522889
H	4.285268	-1.023701	-2.020073
H	4.288608	-2.818660	-1.998294
H	1.188443	-3.371887	-0.595281
H	1.869671	-3.694312	1.023382
H	2.730114	-4.278922	-0.430805
H	1.058568	-1.880717	2.131787

H	-0.513630	-2.598420	1.661291
H	-0.464526	-1.060090	2.534283
C	-2.529555	-0.816600	0.641664
C	-3.615165	-0.148672	-0.238175
H	-2.682318	-1.910723	0.676261
H	-2.571115	-0.437953	1.674114
C	-2.963333	0.039716	-1.631828
C	-4.857492	-1.045194	-0.322773
C	-4.031750	1.208555	0.343195
C	-1.452850	0.117725	-1.407016
H	-3.195703	-0.850707	-2.235646
H	-3.366032	0.914260	-2.165033
O	-5.486920	-1.064063	0.841940
O	-5.184826	-1.677581	-1.284696
O	-5.114562	1.662727	-0.257964
O	-3.429302	1.807170	1.194538
C	-0.868599	1.226748	-0.657521
H	-0.844695	-0.267175	-2.230569
C	-6.660070	-1.861335	0.927048
C	-5.622778	2.918676	0.171098
C	0.506489	1.654615	-0.805924
H	-1.524298	1.825334	-0.016246
H	-6.423637	-2.915511	0.716638
H	-7.409941	-1.513087	0.200565
H	-7.034762	-1.747671	1.951455
H	-4.873836	3.709363	0.012092
H	-5.879446	2.878729	1.240404
H	-6.517495	3.109089	-0.433503
C	1.409019	1.025726	-1.739220
H	0.729550	2.641075	-0.388911
H	1.021203	0.325707	-2.487441
H	2.243510	1.625569	-2.121994

TS19

C	-2.626678	-2.053224	0.629470
C	-1.138018	-2.052074	0.359913
C	-1.041766	-0.325076	-0.815474
C	-2.497052	-0.328400	-1.133310
C	-3.266143	-0.730351	0.135215
H	-3.114180	-2.870413	0.076715
H	-2.832804	-2.199637	1.699566
H	-0.454586	-1.796825	1.178142
H	-2.770086	0.684350	-1.459827
H	-2.730460	-1.034276	-1.948085
C	-0.603532	-2.589653	-0.791726
H	-1.287865	-2.890538	-1.595982
C	0.807785	-2.876174	-0.996808
H	1.480644	-2.717222	-0.147790
C	1.280817	-3.355994	-2.160974
H	0.617641	-3.533887	-3.014939
H	2.340115	-3.593191	-2.293089
C	0.018246	0.405658	-0.712947
Au	1.927869	0.018185	-0.023391
P	4.114224	-0.261346	0.771734
C	5.291018	0.889740	0.014427
H	6.308966	0.735905	0.410916
H	5.304471	0.744835	-1.078172
H	4.979471	1.927267	0.217952
C	4.285973	0.001895	2.556064
H	3.655387	-0.717349	3.103557
H	5.334432	-0.122322	2.876049
H	3.948994	1.018649	2.815827
C	4.819724	-1.904749	0.475135
H	5.853680	-1.967150	0.854941
H	4.209883	-2.672595	0.978734
H	4.823895	-2.118179	-0.606130
Si	-0.066499	2.281141	-1.115656
C	0.190832	3.144452	0.522272
H	-0.624243	2.869476	1.212318
H	1.156115	2.872476	0.982149
H	0.173351	4.240009	0.384105
C	1.355866	2.588955	-2.301144
H	1.354305	3.642365	-2.633162
H	2.331827	2.384180	-1.828266
H	1.272569	1.952749	-3.199412
C	-1.664041	2.845761	-1.908158
H	-1.552061	3.911987	-2.175982
H	-1.900473	2.301257	-2.838333
H	-2.508024	2.765812	-1.204312
C	-3.169368	0.390448	1.180590
C	-4.748303	-0.954859	-0.213995
O	-2.655063	1.459295	0.993615
O	-5.225972	-2.022386	-0.467695
O	-5.397711	0.194776	-0.253788
O	-3.731734	0.022330	2.316279
C	-3.783915	0.987496	3.358791
H	-2.766545	1.265121	3.673800
H	-4.311103	1.889614	3.013862

H	-4.326806	0.515484	4.186337	H	-7.132610	1.185557	-0.578517
C	-6.778005	0.148269	-0.598577	H	-6.905117	-0.285906	-1.601663
H	-7.329590	-0.464864	0.129884				

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