

Supporting Information

Control the chemoselectivity by coordinated water and relative size of ligands to metal cations of Lewis acid catalysts for cycloaddition of aryloxiranyldicarboxylate with aldehyde: Theoretical and experimental study

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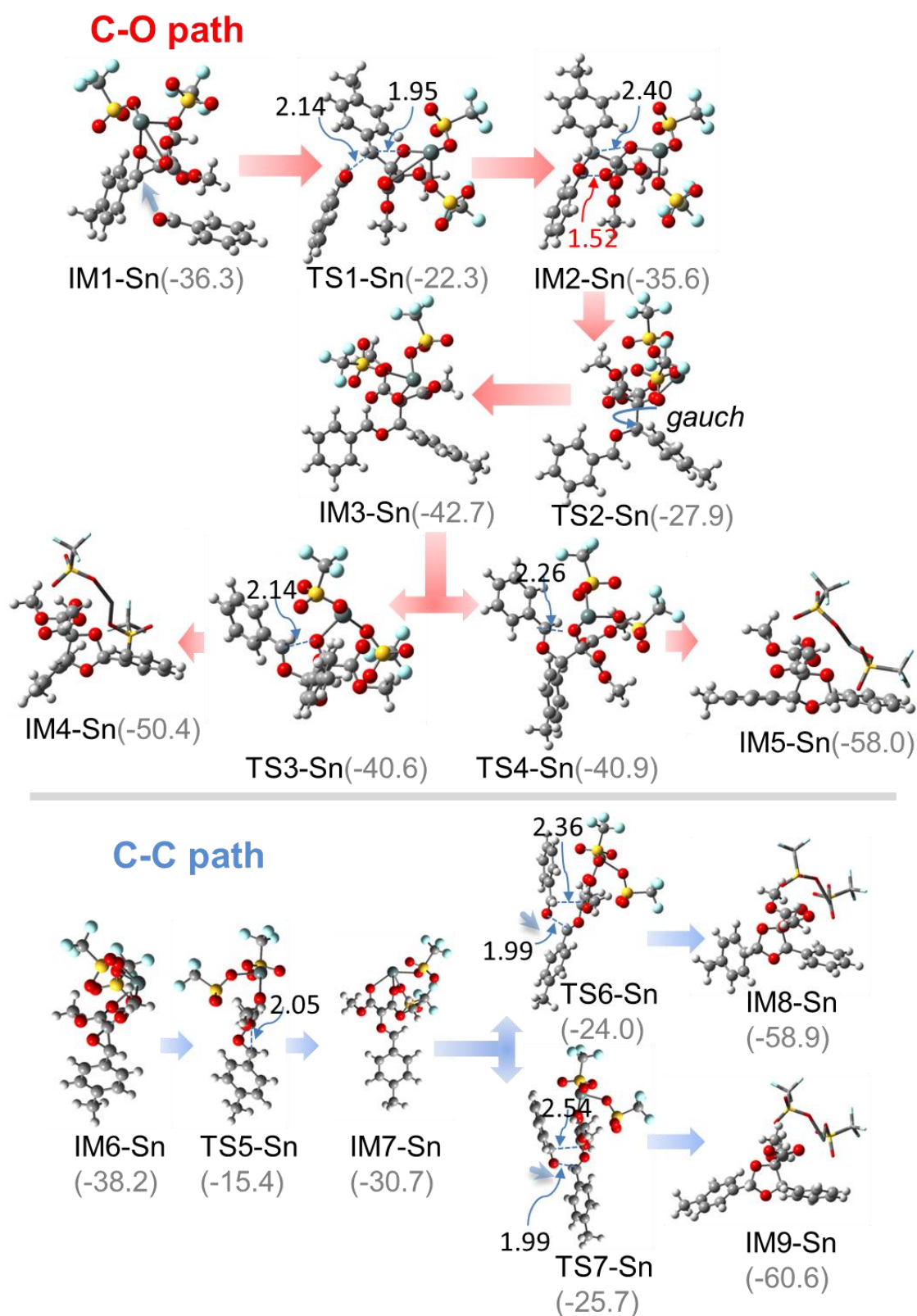


Figure S1. The optimized structures of the species on the $\text{Sn}(\text{OTf})_2$ -catalyzed paths at M06-2X/6-31+G(d)/LANL2DZ level. The Gibbs free energies (kcal/mol) of these

structures are calculated at M06-2X/6-311++G(d,p)/SDD level with SMD solvation model and listed in brackets.

M06-2X functional may overestimates weak interaction, leading to some unreasonable structures, such as **IM2-Sn**. The bond, which is marked in red, is obviously impossible.

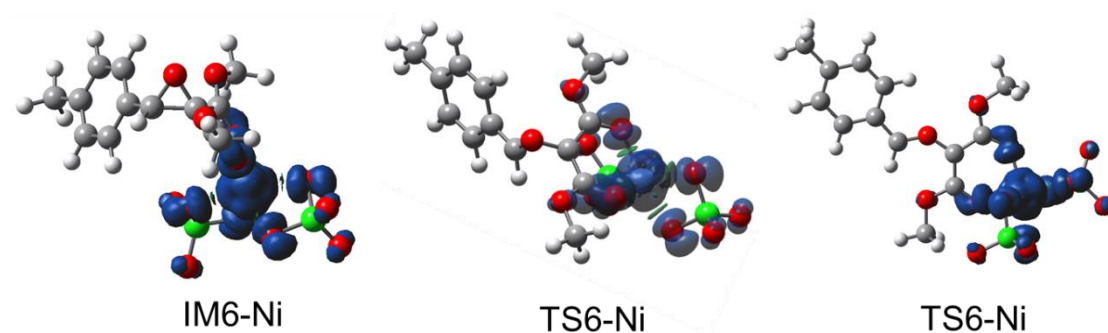


Figure S2. The spin density distributions of several nickelous complexes of high spin states on C-C cleaved paths.

It is interesting that two catalysts which lead to C-C bond cleavage, $\text{Ni}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ and $\text{Cu}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$, are with non-zero spin. Whether non-zero spin has influence on the formation of ylide intermediate is studied from the distributions of the spin density. Evidently, there is no spin interaction between the dipole and metallic center, thus we supposed that C-C bond cleavage is not obviously promoted by the non-zero spin of catalyst. The experimental observation on $\text{Mn}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ -catalyzed reactions, that the C-O cleaved products are mainly yielded, is also confirmed the little influence on C-C bond cleavage from spin.

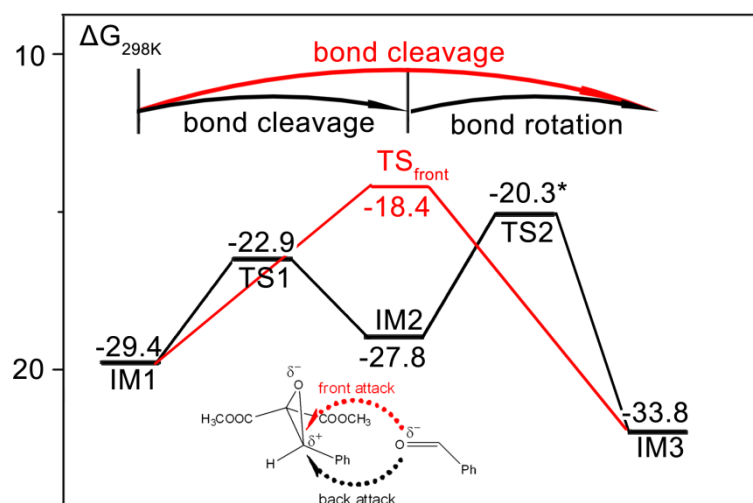


Figure S3. The energy profile of the front and back attacks of R2 for the $\text{Sn}(\text{OTf})_2$ -catalyzed C-O cleaved path.

Some recent study on the cycloaddition of cyclopropane derivative with aldehyde showed that the front attack was favorable. (Zhang, J. S.; Shen, W.; Li, M. *Eur J Org Chem* **2007**, 4855-4866.) We also calculate a front attack pathway through the transition state TS_{front} , connecting **IM1-Sn** and **IM3-Sn** directly. The energy barrier for the front attacking is 11.0 kcal/mol, and much higher than those from the back attacking.

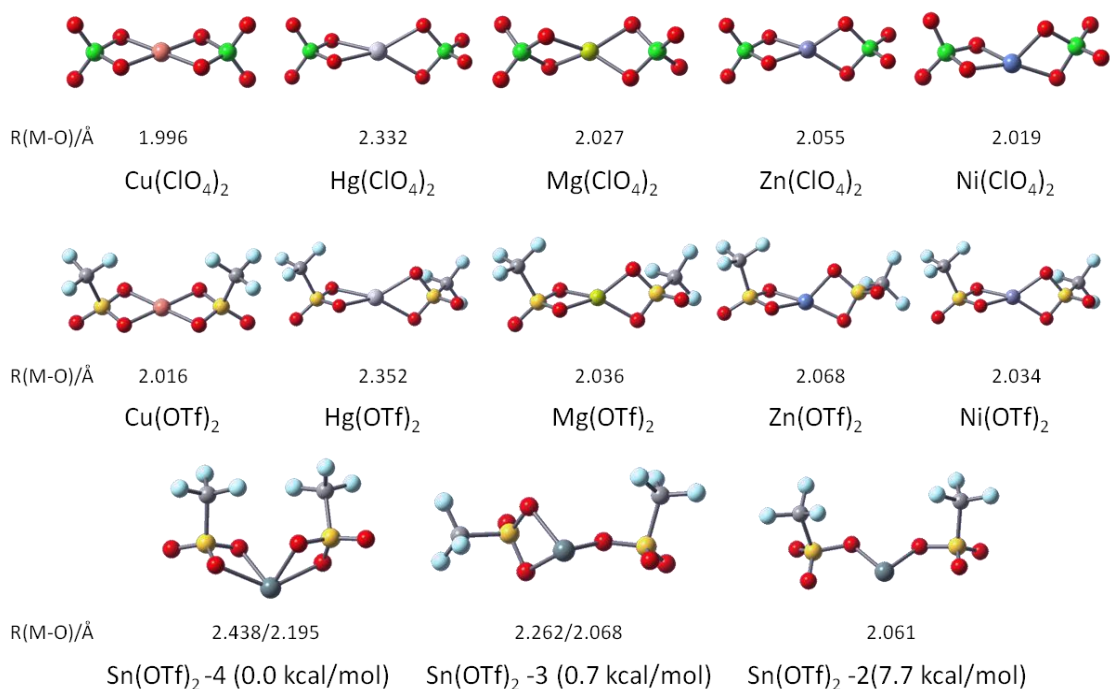


Figure S4. The structures of various Lewis acid catalysts labeled in Figure 1. It should be noticed that the Cu^{2+} and Sn^{2+} are different from the other listed cations. Cu^{2+} has 9 electrons in its 3d orbital. In $\text{Cu}(\text{ClO}_4)_2$ or $\text{Cu}(\text{OTf})_2$, the Cu^{2+} is at the center of a planar square, as the same as in most cupreous complexes. The coordination mode of the Sn^{2+} is more complicated than Cu^{2+} . Two electrons from its 5s orbital form a non-bonding electron pair, with influence on the structure. Several local minimums could be obtained from the $\text{Sn}(\text{OTf})_2$ optimization. The coordination number of Sn cation may be 2, 3 or 4. In the most stable structure, both the OTf^- anions are chelating ligands and the complex has a distorted pyramid form.

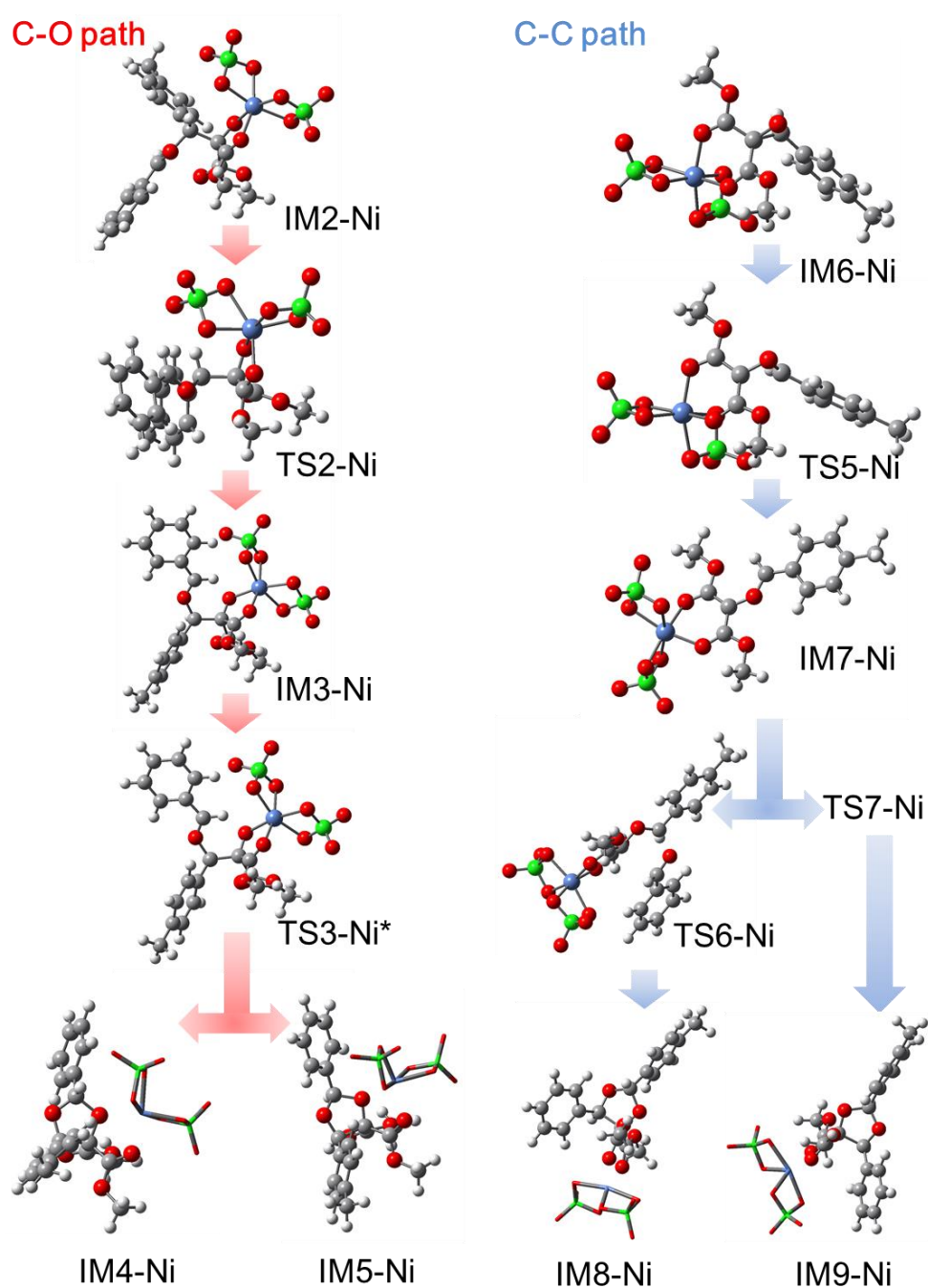


Figure S5. The optimized structures on Ni(CIO₄)₂-catalyzed path. **IM1-Ni**, **TS1-Ni**,

IM6-Ni, **TS5-Ni**, **IM7-Ni** and **TS7-Ni** have been shown in Figure 7.

Here, **IM6-Ni**, **IM7-Ni** and **TS5-Ni** are pictured again from another point of view to see the coordination octahedron clearly. The transition state **TS4-Ni**, which leads to **IM5-Ni**, is almost the same as **TS3-Ni**, as mentioned in article and omitted above.

Table S1. The influence of water coordination on the reaction barriers of the $\text{Ni}(\text{ClO}_4)_2 \cdot n\text{H}_2\text{O}$ -catalyzed reactions. All the energies (in kcal/mol) are computed at UB3LYP/6-311++G(d,p)/SDD level with SMD model for CH_2Cl_2 solvent. $\Delta E_{\text{H}_2\text{O}}^{\text{IM1}}$ and $\Delta E_{\text{H}_2\text{O}}^{\text{IM6}}$ are the energy changes caused by the water replacing the chelating ClO_4^- sites. $\Delta\Delta G_{\text{IMi}}^{\text{TSi}}$ is change in the energy barrier from IMi to TSi. To compare the binding ability of water with the central Ni^{2+} , we define $\Delta E_{\text{H}_2\text{O}}^{\text{IM1}}$ and $\Delta E_{\text{H}_2\text{O}}^{\text{IM6}}$ as the energy differences generated by the water coordination. The populations of different complexes (labeled in the brackets behind $\Delta E_{\text{H}_2\text{O}}^{\text{IMi}}$) are computed by the Boltzmann Distribution to obtain the weighted average values of the energy barriers.

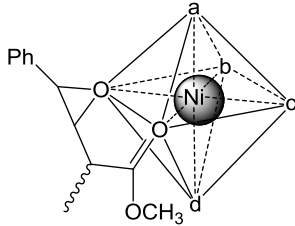
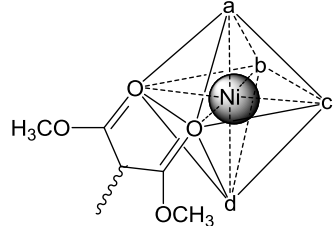
		C-O cleavage		C-C cleavage			
							
Catalyst composition	Water Site(s)	$\Delta E_{H_2O}^{IM1}$ (%)	C-O cleavage $\Delta\Delta G_{IM1}^{TS1}$	$\Delta E_{H_2O}^{IM6}$ (%)	C-C cleavage $\Delta\Delta G_{IM6}^{TS5}$	[3+2] addition $\Delta\Delta G_{IM7}^{TS6}$ $\Delta\Delta G_{IM7}^{TS7}$	
n=0							
Ni(η^2 -ClO ₄) ₂ -R1	-	0.0	11.2	0.0	13.7	15.8	8.8
n=1							
Ni(η^2 -ClO ₄) (ClO ₄)OH ₂ -R1	a	12.2(1)	13.0	11.1(2)	11.0	15.7	10.0
	b	13.2(6)	11.6	13.3(97)	10.0	19.1	8.8
	c	14.8(91)	13.9	10.5(1)	11.4	19.2	8.7
	d	12.4(2)	12.4	8.3(0)	10.8	16.1	14.9
	Average	14.6	13.7	13.2	10.0	19.0	8.8
n=2							
Ni(ClO ₄) ₂ (OH ₂) ₂ -R1	ab	26.8(35)	13.9	28.6(99)	11.6	16.8	9.3
	ac	26.3(15)	13.4	25.7(1)	13.7	20.8	7.5
	ad	26.3(15)	13.5	21.5(0)	13.7	16.8	12.7
	bc	25.6(5)	13.7	25.2(0)	9.5	20.2	8.5
	bd	23.6(0)	12.0	25.3(0)	12.5	17.2	13.3
	cd	26.7(30)	13.3	22.9(0)	12.5	18.8	10.2
	Average	26.6	13.6	28.6	11.6	16.8	9.3

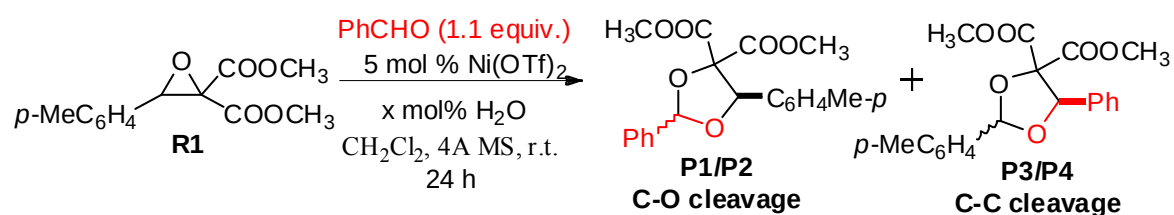
Table S2. The influence of water coordination on the reaction barriers of the $\text{Mg}(\text{ClO}_4)_2 \cdot n\text{H}_2\text{O}$ -catalyzed reactions. The energies (in kcal/mol) are computed at B3LYP/6-311++G(d,p) level with SMD model for CH_2Cl_2 solvent.

Catalyst composition	Water Site(s)	$\Delta E_{H_2O}^{IM1}$	C-O cleavage	$\Delta E_{H_2O}^{IM6}$	C-C cleavage	[3+2] addition	
		(%)	$\Delta\Delta G_{IM1}^{TS1}$	(%)	$\Delta\Delta G_{IM6}^{TS5}$	$\Delta\Delta G_{IM7}^{TS6}$	$\Delta\Delta G_{IM7}^{TS7}$
n=0							
Mg(η^2 -ClO ₄) ₂ -R1	-	0.0	12.7	0.0	13.1	17.7	10.2
n=1							
Mg(η^2 -ClO ₄) (ClO ₄)OH ₂ -R1	a	11.6(2)	14.0	12.2(5)	13.2	18.4	9.9
	b	13.2(28)	13.9	13.8(88)	10.6	19.4	10.8
	c	13.8(69)	14.0	11.6(2)	11.9	19.9	9.3
	d	11.1(1)	12.5	12.1(5)	13.5	17.6	11.5
	<i>Average</i>	<i>13.6</i>	<i>13.9</i>	<i>13.6</i>	<i>10.9</i>	<i>19.3</i>	<i>10.8</i>
n=2							
Mg(ClO ₄) ₂ (OH ₂) ₂ -R1	ab	25.4(22)	14.8	29.4(96)	12.1	16.2	9.8
	ac	25.6(30)	15.6	27.5(4)	13.6	19.2	7.2
	ad	25.7(35)	15.6	25.6(0)	13.6	18.2	15.1
	bc	30.4	19.9	25.5(0)	10.1	19.2	8.2
	bd	24.3(3)	15.6	25.9(0)	11.7	17.3	13.5
	cd	24.9(10)	13.4	25.9(0)	14.3	15.0	11.0
	<i>Average</i>	<i>25.5</i>	<i>15.2</i>	<i>29.3</i>	<i>12.1</i>	<i>16.2</i>	<i>9.8</i>

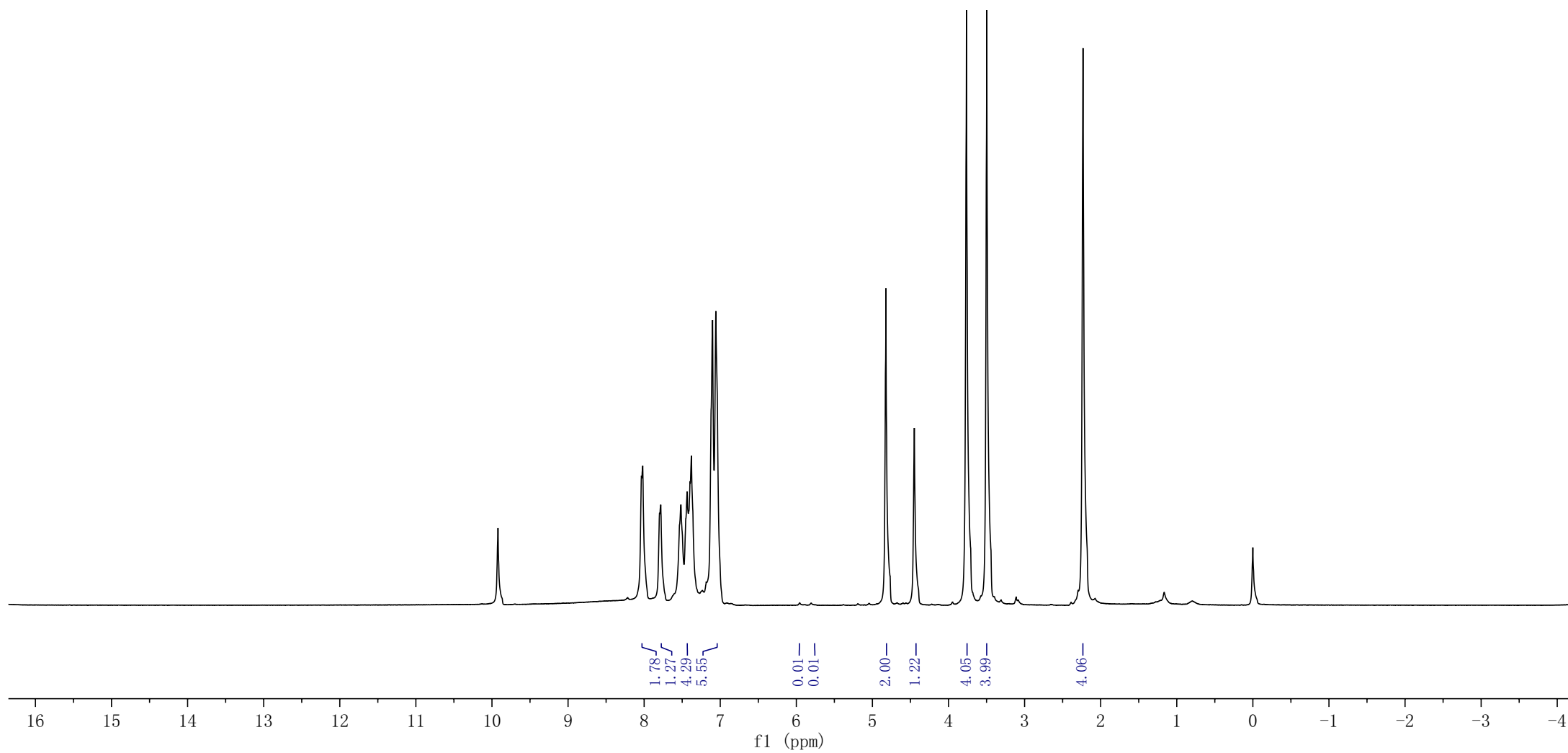
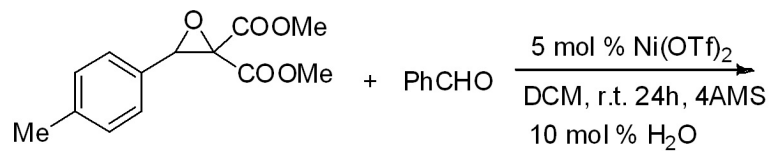
Table S3. Energy barriers of pathways catalyzed by some Lewis acids. The energies (in kcal/mol) are computed at (U)B3LYP/6-31+G(d,p)/LANL2DZ//((U)B3LYP/6-311++G(d,p)/SDD level with SMD model for CH₂Cl₂ solvent.

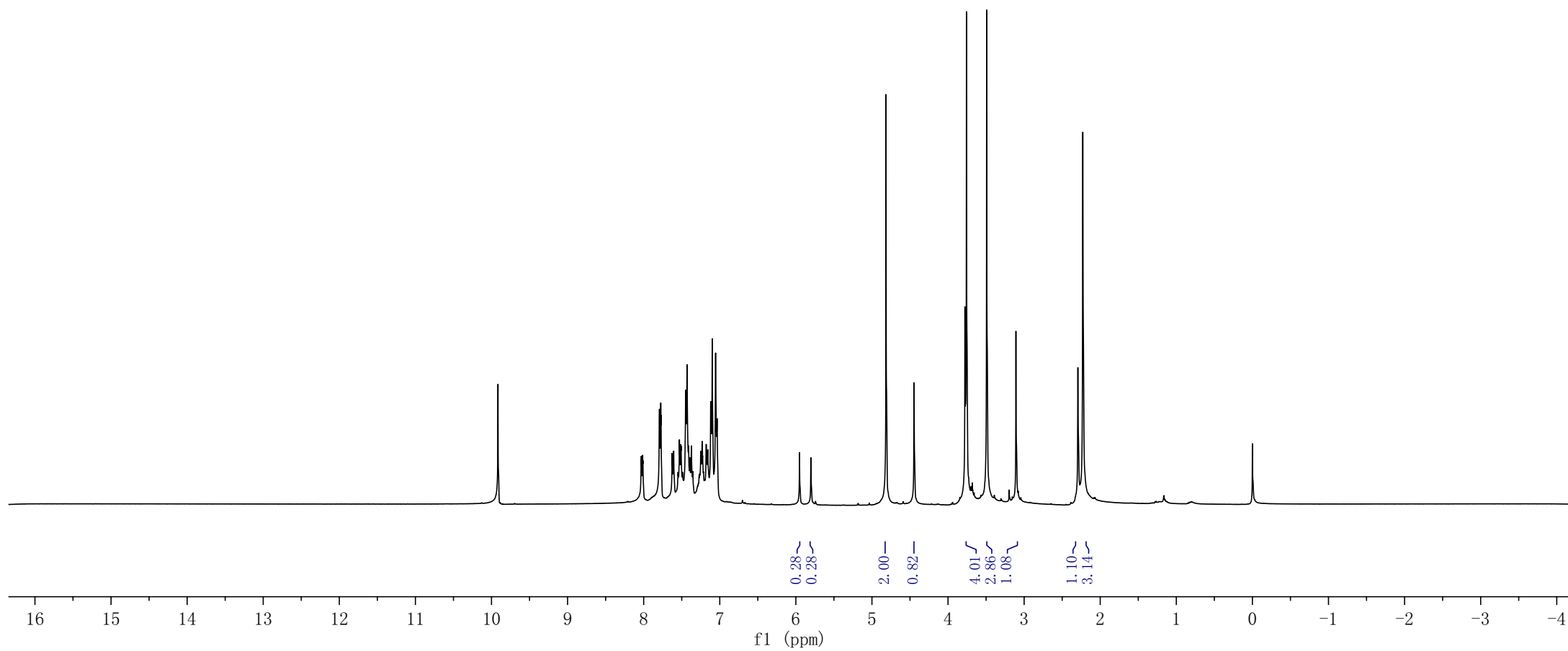
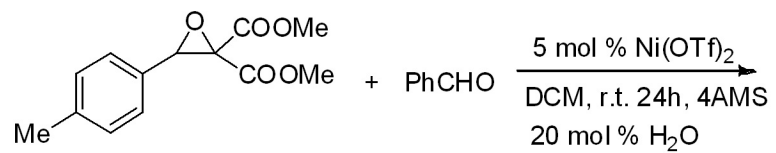
		IM			TS			E _a (kcal/mol)	
	M	U-gas(a.u.)	thermal	U-PCM(a.u.)	U-gas(a.u.)	thermal	U-PCM(a.u.)	gas	PCM
L=ClO ₄ ⁻									
C-O cleave	Cu	-2943.1669	0.3128	-2944.9374	-2943.1411	0.3142	-2944.9288	17.1	6.3
	Hg	-2789.7373	0.3079	-2901.0650	-2789.7179	0.3110	-2901.0502	14.1	11.2
	Zn	-2812.6665	0.3128	-2974.7632	-2812.6404	0.3147	-2974.7537	17.6	7.2
	Mn	-2851.0368	0.3095	-2852.0463	-2851.0097	0.3123	-2852.0352	18.8	8.7
C-C cleave	Cu	-2597.5791	0.2152	-2599.2568	-2597.5563	0.2184	-2599.2403	16.3	12.4
	Hg	-2444.1596	0.2107	-2555.3799	-2444.1353	0.2131	-2555.3590	16.8	14.6
	Zn	-2467.0816	0.2172	-2629.0863	-2467.0577	0.2153	-2629.0665	13.8	11.2
	Mn	-2505.4522	0.2129	-2506.3708	-2505.4280	0.2115	-2506.3500	14.3	12.2
cis addition	Cu	-2943.1682	0.3142	-2944.9514	-2943.1647	0.3183	-2944.9457	4.8	6.2
	Hg	-2789.7444	0.3052	-2901.0609	-2789.7333	0.3112	-2901.0570	10.8	6.3
	Zn	-2812.6704	0.3122	-2974.7777	-2812.6647	0.3193	-2974.7704	8.1	9.0
	Mn	-2851.0372	0.3077	-2852.0593	-2851.0320	0.3153	-2852.0523	8.0	9.1
L=OTf ⁻									
C-O cleave	Cu	-3344.6105	0.3245	-3346.5329	-3344.5861	0.3319	-3346.5245	19.9	9.9
	Hg	-3191.1921	0.3249	-3302.6607	-3191.1652	0.3228	-3302.6498	15.6	5.5
	Zn	-3214.1085	0.3276	-3376.3618	-3214.0914	0.3313	-3376.3542	13.0	7.1
	Mn	-3252.4806	0.3235	-3253.6419	-3252.4572	0.3289	-3253.6327	18.1	9.2
C-C cleave	Cu	-2999.0258	0.2319	-3000.8553	-2999.0041	0.2321	-3000.8354	13.7	12.6
	Hg	-2845.6072	0.2291	-2956.9756	-2845.5826	0.2277	-2956.9538	14.6	12.9
	Zn	-2868.5301	0.2336	-3030.6848	-2868.5100	0.2330	-3030.6667	12.2	11.0
	Mn	-2906.8969	0.2277	-2907.9671	-2906.8768	0.2307	-2907.9490	14.6	13.3
cis addition	Cu	-3344.6168	0.3308	-3346.5465	-3344.6129	0.3330	-3346.5404	3.8	5.2
	Hg	-3191.1919	0.3239	-3302.6648	-3191.1863	0.3276	-3302.6587	5.8	6.2
	Zn	-3214.1203	0.3287	-3376.3736	-3214.1154	0.3335	-3376.3689	6.1	6.0
	Mn	-3252.4866	0.3264	-3253.6550	-3252.4817	0.3308	-3253.6502	5.8	5.7

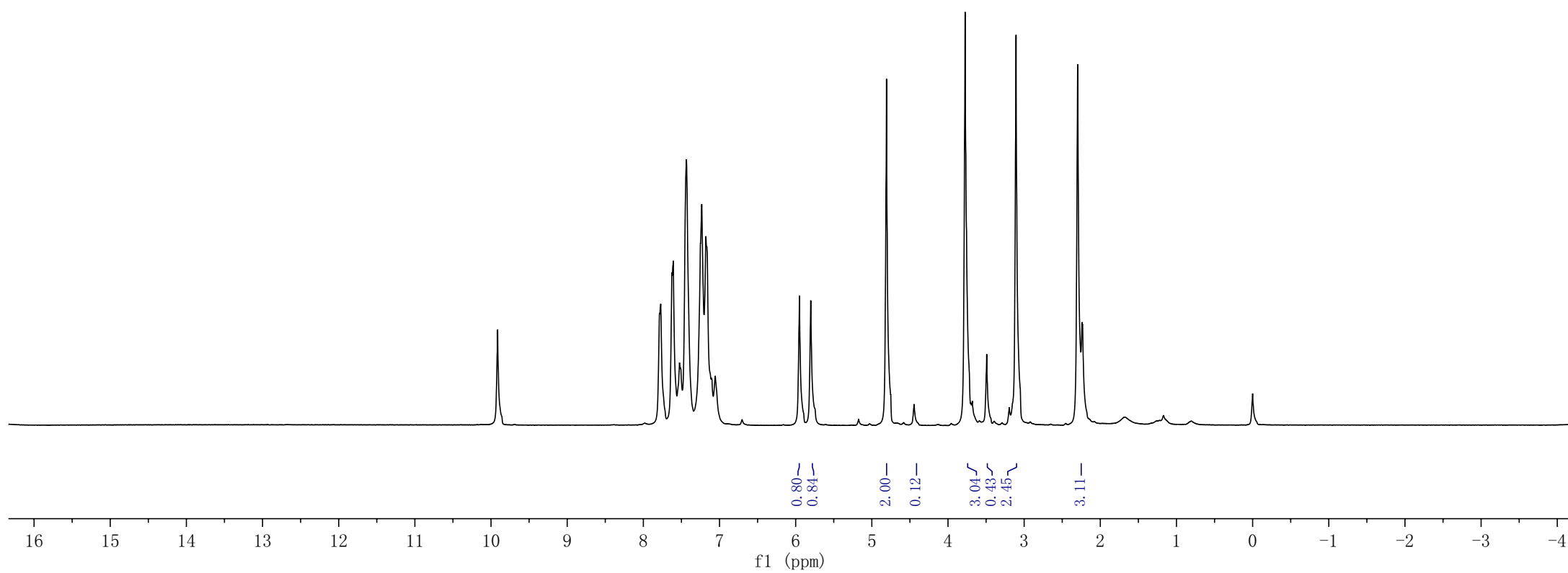
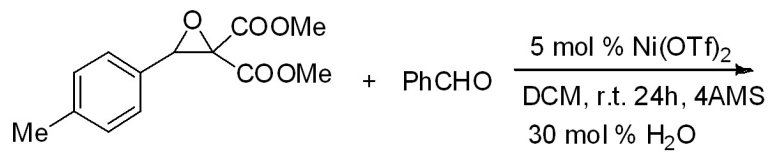
Water effect on Ni(OTf)₂ catalyzed [3+2] cycloaddition reaction



In an inert atmosphere glovebox, a flame-dried vial was charged with 5 mol % $\text{Ni}(\text{ClO}_4)_2$, 100 mg of activated 4 Å molecular sieve (M.S.), and a magnetic stir bar. Outside of the glovebox, the vial was placed under an N_2 atmosphere and charged with 1 mL of DCM followed by the benzaldehyde **R2** (56 μL , 0.55 mmol). Afterwards, **R1** (125 mg, 0.5 mmol) and 4 mL of DCM containing x mol% H_2O were added. The reaction was stirred at room temperature for 24 hours. The reaction mixture was then passed over a plug of silica with 30 mL of Et_2O . The solvent was removed under reduced pressure and the residue was estimated by ^1H NMR spectroscopy using dibromomethane as the internal reference.







The optimized structures for all stationary points discussed in the paper.

Reactants

R1

C	-3.92061200	-0.42404000	-0.17005500
C	-3.19078300	-1.15921700	-1.11473400
C	-1.82336000	-1.38521300	-0.95019400
C	-1.14489200	-0.86849600	0.16105200
C	-1.86512600	-0.13465600	1.11420300
C	-3.23257700	0.08136100	0.94397700
H	-3.69822600	-1.56542200	-1.98717500
H	-1.28075500	-1.96599100	-1.69371300
H	-1.35238600	0.25901100	1.98618800
H	-3.77616800	0.65173600	1.69464000
C	-5.40809600	-0.20558800	-0.32685000
H	-5.73763400	-0.41161000	-1.35080300
H	-5.97765600	-0.86470700	0.34210900
H	-5.69010000	0.82515400	-0.08193700
C	0.31642100	-1.13185300	0.30182900
H	0.66574200	-2.06858400	-0.13199600
C	1.34883600	-0.04951500	0.39087200
O	0.95426000	-0.79658400	1.53672600
C	2.77258400	-0.27876500	-0.08064400
C	0.92920100	1.41112200	0.36551600
O	3.08602400	-1.58327000	-0.12180300
O	0.81974700	1.83235400	-0.90279000
C	4.44664500	-1.89237800	-0.48776200
H	4.51134900	-2.97981800	-0.45496600
H	4.66167700	-1.51829700	-1.49190100
H	5.13927300	-1.44027200	0.22650600
C	0.49998900	3.22713900	-1.08109600
H	1.27618700	3.84870600	-0.62752600
H	0.46510500	3.37747400	-2.15998100
H	-0.46702700	3.45330900	-0.62487900
O	3.53559900	0.62065200	-0.36463300
O	0.71577300	2.08433700	1.34734300

R2

C	1.73367300	1.06630200	-0.00000300
C	0.35573700	1.29014200	-0.00000100

C	-0.53573100	0.20704400	0.00000500
C	-0.03914900	-1.10746900	0.00000700
C	1.33546500	-1.32961300	0.00000100
C	2.22212300	-0.24368200	-0.00000400
H	2.42317900	1.90621900	-0.00000600
H	-0.03418000	2.30640600	-0.00000100
H	-0.74453500	-1.93341700	0.00001300
H	1.72202700	-2.34536400	0.00000000
H	3.29469300	-0.42090000	-0.00000800
C	-1.99354000	0.46626200	0.00001000
H	-2.27654600	1.54150400	0.00002400
O	-2.85701300	-0.39354600	-0.00001400

Products

P1

C	-0.03876700	-0.54334300	-0.00824400
O	0.56879100	-1.29175100	-1.05979300
C	1.70199000	-0.55787000	-1.47418700
C	0.24422200	0.94577400	-0.47886100
H	0.51368700	-0.69612000	0.92600400
O	1.34095600	0.81917600	-1.36169600
C	-1.47301100	-0.98175900	0.17591900
C	-2.25783900	-1.38102900	-0.91525600
C	-2.04019400	-1.00660700	1.45483000
C	-3.57873100	-1.78649600	-0.72333000
H	-1.82889000	-1.37991500	-1.91187000
C	-3.36477600	-1.40927500	1.63907800
H	-1.44497600	-0.70411900	2.31234200
C	-4.15749800	-1.80904000	0.55503800
H	-4.16886500	-2.09591300	-1.58398900
H	-3.78451500	-1.41973300	2.64298900
C	-5.57871000	-2.28402300	0.75487700
H	-6.24073000	-1.91412100	-0.03679900
H	-5.63500800	-3.38091100	0.73736200
H	-5.98212800	-1.95020500	1.71698200
C	0.63903800	1.91593000	0.65468400
C	-0.94132600	1.53606600	-1.27797000
O	0.14990300	1.53583700	1.84908700
O	-1.75446100	2.24934800	-0.48055600
O	1.30670600	2.90867400	0.47755700
O	-1.11748600	1.35079300	-2.45808700
H	1.85065300	-0.77281100	-2.53743700
C	2.95222300	-0.88339800	-0.66264600
C	3.22746200	-2.21647000	-0.32640000

C	3.85819600	0.11998600	-0.29743100
C	4.39035900	-2.54065900	0.37579000
H	2.52314100	-2.99567900	-0.60554600
C	5.02250700	-0.20719000	0.40495200
H	3.64480500	1.15257000	-0.55631100
C	5.29140700	-1.53585700	0.74322800
H	4.59195500	-3.57654900	0.63731900
H	5.71800100	0.57902700	0.68821700
H	6.19697100	-1.78819500	1.28938500
C	0.41940300	2.42988900	2.94890100
H	-0.00134500	3.41668300	2.74035100
H	-0.06458500	1.97621400	3.81393600
H	1.49697800	2.51800300	3.10793800
C	-2.93113100	2.80168000	-1.10637500
H	-3.45169900	3.33962200	-0.31420900
H	-2.64297300	3.47987500	-1.91341000
H	-3.55469300	1.99780400	-1.50495000
P2			
O	-1.02714200	2.64517900	-1.70064000
O	-0.02424000	3.47427600	0.14586200
O	0.14629600	0.26528100	2.15887200
O	-1.69804800	1.37324800	1.45785000
O	1.47199300	1.09991400	-0.11406500
O	0.84295900	-0.87467800	-1.02689200
C	3.22166400	-0.98947900	0.95270600
H	2.38269600	-0.75923700	1.60235700
C	4.36175200	-1.62127800	1.45021500
H	4.40936300	-1.89691400	2.50078200
C	5.44318200	-1.89670100	0.60487800
H	6.32983700	-2.38807500	0.99808700
C	5.38441400	-1.53489500	-0.74288000
H	6.22278800	-1.74247900	-1.40286700
C	4.24374400	-0.89920800	-1.24234400
H	4.19687200	-0.61343900	-2.29132100
C	3.16040500	-0.63009300	-0.40051300
C	1.92822300	0.02573300	-0.96119900
H	2.12410900	0.43963900	-1.96374600
C	0.05422000	1.11830800	-0.12363300
C	-0.32409300	-0.06296100	-1.10520200
H	-0.40602500	0.38562500	-2.10368400
C	-1.56619900	-0.86693100	-0.81086000
C	-2.78774100	-0.48554700	-1.38349800
H	-2.82680400	0.38341500	-2.03618900

C	-3.95061500	-1.20647100	-1.11584200
H	-4.88844500	-0.89374900	-1.57141200
C	-3.92946200	-2.33428800	-0.27985600
C	-2.70189800	-2.71094600	0.28053600
H	-2.65394900	-3.58676700	0.92452500
C	-1.53253800	-1.98961900	0.02309900
H	-0.58995500	-2.30609700	0.45818900
C	-5.19229400	-3.12139100	-0.01197800
H	-5.01124000	-3.94025700	0.69222400
H	-5.59217100	-3.55907000	-0.93579700
H	-5.98003100	-2.48424400	0.40979100
C	-0.41788900	2.48340300	-0.66298400
C	-0.36022200	4.81198500	-0.27364500
H	0.04286300	5.46399200	0.50104000
H	-1.44520800	4.92111300	-0.34974700
H	0.09846300	5.02991900	-1.24150800
C	-0.46200400	0.87016000	1.30646300
C	-2.33879700	1.12058100	2.72489900
H	-3.31083200	1.60897600	2.65742500
H	-1.74470100	1.54513400	3.53809300
H	-2.45528600	0.04456600	2.87570200
P3			
C	4.98161300	-0.91497800	0.13361700
C	4.08594700	-1.98727700	0.01567800
C	2.79411200	-1.80023600	-0.48044500
C	2.36049400	-0.52632800	-0.86626300
C	3.24929300	0.55036600	-0.76076000
C	4.54087200	0.35446700	-0.26786700
H	4.40200600	-2.98453100	0.31566400
H	2.11615400	-2.64504600	-0.56353100
H	2.92701800	1.54365300	-1.06019900
H	5.21697000	1.20404900	-0.19266200
O	0.44809500	0.96707600	-1.17602200
C	-1.92338200	1.32551400	-0.70295600
C	-0.18834900	1.71069700	1.04410300
O	-2.09129600	1.06598500	-2.00371700
O	0.03654400	2.97752600	0.68167600
C	-3.37523800	1.43020100	-2.55158300
H	-3.32091900	1.16507700	-3.60746500
H	-4.16922300	0.87204900	-2.04902100
H	-3.54659700	2.50253100	-2.42847500
C	0.36467400	3.89265900	1.74663900
H	1.27867600	3.57145400	2.25275800

H	0.50871500	4.85721800	1.26005100
H	-0.45721300	3.93866300	2.46555700
O	-2.75248000	1.84545200	0.01466200
O	-0.09783900	1.29153100	2.17886900
C	0.97627900	-0.33512800	-1.47240800
H	1.00442900	-0.43253700	-2.56325300
C	-0.55746800	0.84574400	-0.18090500
C	-0.55178100	-0.69150500	0.17622700
H	0.12751800	-0.81078500	1.02808000
C	-1.87737400	-1.34647400	0.49222600
C	-2.60640800	-2.02787800	-0.49084300
C	-2.38414800	-1.27239700	1.79711300
C	-3.83026500	-2.62301300	-0.17190500
H	-2.20465100	-2.10302800	-1.49602900
C	-3.61089400	-1.86039000	2.11056000
H	-1.82037800	-0.74385700	2.56132300
C	-4.33771800	-2.53806700	1.12727900
H	-4.38416000	-3.15794200	-0.93968200
H	-3.99637400	-1.79205200	3.12464100
H	-5.29006000	-3.00099200	1.37361700
O	0.02403900	-1.25896700	-0.99941300
C	6.36863100	-1.11676300	0.70002900
H	7.07619000	-0.38214900	0.29983900
H	6.36863800	-1.00888600	1.79334800
H	6.75341100	-2.11699700	0.47177600

P4

O	2.32246000	2.10472900	-1.59332100
O	1.48384000	3.15716900	0.22094900
O	0.31484000	0.08254900	2.12120900
O	2.42987000	0.64310900	1.54422900
O	-0.59996000	1.30711900	-0.17950100
O	-0.50523000	-0.75037100	-1.12227100
C	-2.91896000	-0.22723100	0.75456900
H	-2.08451000	-0.25374100	1.44893900
C	-4.21056000	-0.52313100	1.18267900
H	-4.37762000	-0.79261100	2.22400900
C	-5.30325000	-0.47695100	0.29886900
C	-5.05994000	-0.12161100	-1.03304100
H	-5.88793000	-0.07614000	-1.73723100
C	-3.76630000	0.18006900	-1.46992100
H	-3.59915000	0.45676900	-2.50912100
C	-2.68942000	0.12456900	-0.58338100
C	-1.29994000	0.41685900	-1.07422100

H	-1.32466000	0.88480900	-2.07172100
C	0.76319000	0.92310900	-0.12382100
C	0.84309000	-0.29717100	-1.12608100
H	1.09666000	0.12849900	-2.10566100
C	1.79708000	-1.42305100	-0.80646100
C	3.10806000	-1.37117100	-1.29979100
H	3.41912000	-0.52474100	-1.90730100
C	4.01272000	-2.39442100	-1.00908100
H	5.02686000	-2.34375100	-1.39745100
C	3.61202000	-3.48453100	-0.23062100
C	2.30224000	-3.54476100	0.25395900
H	1.98001000	-4.39519100	0.84980900
C	1.39684000	-2.51877100	-0.03028100
H	0.37615000	-2.57057100	0.33463900
C	1.63077000	2.10716900	-0.59543100
C	2.20834000	4.35076900	-0.13806100
H	1.96543000	5.07648900	0.63785900
H	3.28205000	4.14711900	-0.15962100
H	1.88365000	4.70832900	-1.11860100
C	1.11244000	0.51024900	1.31909900
C	2.90584000	0.19773900	2.83083900
H	3.97955000	0.38448900	2.81978900
H	2.41932000	0.76529900	3.62815900
H	2.69908000	-0.86775100	2.95712900
C	-6.69974000	-0.79072000	0.78540900
H	-7.42007000	-0.79437000	-0.03940100
H	-7.03951000	-0.05086000	1.52193900
H	-6.74141000	-1.77289000	1.27265900
H	4.31332000	-4.28570100	-0.01064100

Sn-path

Sn(OTf)₂

C	3.26647100	1.25346000	-0.27356500
F	2.53231400	1.33934000	-1.40001100
F	2.98625900	2.29531300	0.50743000
F	4.55986000	1.26593300	-0.59417600
O	3.08424400	-1.43046100	-0.38191100
O	1.29814100	-0.17656700	0.75896900
Sn	0.01521700	-1.22693500	-0.46523600
O	-1.42834400	-0.40990300	0.75872500
C	-3.19482000	1.37716400	-0.04363700
F	-2.29325900	1.77088700	-0.96154400
F	-3.03556100	2.10019300	1.06307500
F	-4.42271900	1.56236400	-0.52953300

O	-3.82127100	-0.80143100	1.41821400
S	-2.94219900	-0.45080000	0.31900600
O	-3.01412800	-1.14608400	-0.97597600
S	2.85637700	-0.35990400	0.60102400
O	3.53640500	-0.34455600	1.88165300

IM1-Sn

O	1.76660900	2.36719700	0.28752400
O	-1.44759700	0.19119500	2.91781500
O	0.82299700	0.14236000	2.90179300
O	-0.47122000	0.88784800	0.04299300
C	-0.21829700	1.51857500	1.31418500
C	-1.43980500	1.90314800	0.55795200
C	1.03819800	2.35641300	1.27503600
C	-0.37358100	0.54546800	2.49032600
C	0.85231600	-0.92886800	3.87533600
H	1.90923100	-1.08635400	4.08523300
H	0.40271600	-1.82035400	3.43384500
H	0.30906900	-0.62927400	4.77473800
Sn	1.33236900	0.54701900	-1.54636700
O	1.24484000	3.04108700	2.37586600
C	2.50735400	3.76215600	2.47402100
H	2.54682800	4.53601400	1.70478800
H	2.49718500	4.20019600	3.47064700
H	3.33090500	3.05595200	2.35321000
O	0.37737100	-1.33509800	-1.57972900
O	2.64880800	-0.32993500	-0.16724600
S	-0.27245800	-2.36378600	-0.61724700
S	4.07550300	0.14846200	0.22473500
O	0.13099200	-2.17124800	0.77564400
O	4.14647400	0.59260700	1.61606500
O	-1.68983500	-2.55764000	-0.93028500
O	4.66187400	0.97444300	-0.83579900
C	0.59457600	-3.92475600	-1.20519600
C	4.96258700	-1.50751600	0.17029100
F	1.91698100	-3.82477600	-1.02292600
F	0.35076800	-4.13459200	-2.50576800
F	0.13669100	-4.97170200	-0.50398000
F	6.25556500	-1.31839300	0.46720300
F	4.87250600	-2.04162300	-1.05507400
F	4.43171400	-2.35552000	1.05702700
C	-4.33403500	-0.62176600	0.40814800
H	-3.34569400	-1.03910700	0.14393100
O	-4.45503000	0.57252600	0.66219600

C	-5.43859400	-1.60028300	0.41823000
C	-6.74603100	-1.22249700	0.77139200
C	-5.16158800	-2.93127500	0.06466100
C	-7.76482500	-2.17140600	0.77088800
H	-6.93890700	-0.18869900	1.04337400
C	-6.18682500	-3.87951800	0.06313400
H	-4.14671800	-3.21053900	-0.20923500
C	-7.48526800	-3.49970700	0.41645000
H	-8.77669100	-1.88494100	1.04566100
H	-5.97479400	-4.90927700	-0.21153600
H	-8.28362600	-4.23778700	0.41704500
H	-2.33666900	1.39570000	0.91111800
C	-1.72167100	3.15619500	-0.18994800
C	-3.05362200	3.59916000	-0.14731200
C	-0.78719600	3.90978800	-0.92273200
C	-3.43314100	4.77632100	-0.79517500
H	-3.79558300	3.00808700	0.38180600
C	-1.18046800	5.07549700	-1.57544000
H	0.24656300	3.59506300	-0.99958600
C	-2.50705600	5.53633100	-1.51979800
H	-4.47080700	5.09748600	-0.74536900
H	-0.44185500	5.63785800	-2.14289300
C	-2.91121200	6.80806300	-2.22753000
H	-2.65421600	6.76939400	-3.29332000
H	-3.98822100	6.98586400	-2.14701000
H	-2.39507800	7.67854800	-1.80245900

IM2-Sn

O	-0.31028000	-1.81504400	-2.34134700
O	2.12426300	-0.68551000	1.42178600
O	-0.08168700	-1.02347000	1.22879500
O	0.11058900	0.49681000	-1.06727700
C	1.00759400	-0.49459500	-0.79796400
C	2.38455900	-0.06353200	-1.42286200
C	0.55235700	-1.82070500	-1.48452900
C	1.09294800	-0.74734400	0.73968600
C	-0.23473100	-1.17018900	2.66238500
H	-1.26201700	-1.50464700	2.79339500
H	-0.07785800	-0.19659300	3.12869800
H	0.47548800	-1.91054300	3.03721100
Sn	-1.83225800	0.50706300	-1.72666200
O	1.19014100	-2.90324100	-1.05086300
C	0.72098900	-4.17759900	-1.57873400
H	0.86690200	-4.20361600	-2.66105600

H	1.33600000	-4.92837200	-1.08315800
H	-0.33402400	-4.29840800	-1.32753500
O	-2.20341600	1.86067500	-0.05327200
O	-2.53570300	-1.02234600	-0.36477100
S	-1.35817100	2.71871500	0.89312200
S	-3.13510400	-2.42056100	-0.57246500
O	-0.50196700	1.93430500	1.79797300
O	-2.21815800	-3.48230600	-0.13472600
O	-0.76073500	3.88524600	0.23445000
O	-3.82621400	-2.56582000	-1.85583800
C	-2.72581700	3.39509300	1.99001600
C	-4.47771800	-2.38005400	0.74095700
F	-3.36541400	2.39973300	2.62271400
F	-3.61723500	4.09021700	1.26971700
F	-2.19127700	4.21250700	2.91369100
F	-5.12838200	-3.55344500	0.75154100
F	-5.35885600	-1.40222200	0.49272100
F	-3.94422100	-2.17883000	1.95917100
C	3.96151700	-0.67961500	0.27695500
H	3.98467800	0.36605200	0.57286200
O	3.43945900	-0.98943300	-0.85806600
C	4.78861500	-1.63724600	0.96839200
C	4.86981200	-2.98233100	0.55258200
C	5.52484300	-1.19325400	2.08434600
C	5.69013300	-3.86466400	1.24585200
H	4.28706900	-3.31363100	-0.30062200
C	6.34218400	-2.08445000	2.77458200
H	5.44492300	-0.15792400	2.40545100
C	6.42459800	-3.41678600	2.35394900
H	5.75936000	-4.90219100	0.93249800
H	6.91034800	-1.74690100	3.63611900
H	7.06172600	-4.11277100	2.89308200
H	2.38461200	-0.36638300	-2.47043000
C	2.79719200	1.38064900	-1.32442000
C	3.68267700	1.86304900	-2.30209300
C	2.37355500	2.25657400	-0.31143900
C	4.14347700	3.17903600	-2.26344100
H	4.01002800	1.20614900	-3.10622300
C	2.83035500	3.57354600	-0.28682700
H	1.65401600	1.94349500	0.43540000
C	3.72151900	4.05937900	-1.25615900
H	4.82369500	3.53043900	-3.03589800
H	2.45697700	4.23928600	0.48698900
C	4.17772700	5.49896000	-1.23017800

H	4.56471100	5.77702800	-0.24249300
H	4.96413500	5.68585100	-1.96879200
H	3.34233000	6.17597400	-1.45002700
IM3-Sn			
O	-0.79302800	-2.62896600	0.08677100
O	1.33522600	0.53171900	2.75231200
O	-0.78163500	-0.20916700	2.46376300
O	0.53617900	-0.33678400	-0.18666800
C	0.82944100	-1.05847300	0.94841000
C	2.31762900	-1.53272900	0.98168400
C	-0.04127400	-2.34233400	1.00432400
C	0.50649600	-0.16326900	2.18733600
C	-1.31122400	0.75217100	3.40944800
H	-2.36609800	0.49750600	3.49594900
H	-1.17950300	1.75563000	3.00073000
H	-0.79697500	0.65128000	4.36827900
Sn	-1.06385200	-0.61589400	-1.50118800
O	0.10926700	-3.05888000	2.10663000
C	-0.80554000	-4.18021400	2.27394900
H	-0.63216300	-4.91563500	1.48534500
H	-0.56699400	-4.59091700	3.25421800
H	-1.83227800	-3.81112100	2.23378200
O	-1.03176300	1.60461700	-1.57890200
O	-2.60215600	-0.32179500	-0.02645000
S	-0.32621400	2.67853700	-0.76032300
S	-3.75300700	-1.24334500	0.41584900
O	-0.73822700	2.74760900	0.64485600
O	-3.56544100	-1.75848900	1.77710300
O	1.12605600	2.73466900	-1.03541700
O	-4.17020200	-2.16820400	-0.64273500
C	-1.02077400	4.22365300	-1.57194900
C	-5.12466800	0.03141000	0.56528500
F	-2.34831300	4.28615800	-1.41550900
F	-0.73734900	4.24375000	-2.88304900
F	-0.46849700	5.30910300	-1.00061100
F	-6.25857700	-0.57792000	0.94660500
F	-5.33936400	0.63990900	-0.60928200
F	-4.81087400	0.96039800	1.48166100
C	3.07081900	0.80600000	0.73257400
H	2.11144100	1.08612000	0.29772900
O	3.31390700	-0.42035700	1.01148300
C	4.09980800	1.77958900	0.92635100
C	5.35758200	1.44361800	1.48494000

C	3.81432300	3.11332300	0.55265200
C	6.31153200	2.43349000	1.66028700
H	5.56062200	0.41767600	1.77414100
C	4.78293100	4.09725700	0.73798400
H	2.84577700	3.34654400	0.11873200
C	6.02318800	3.75873000	1.28754900
H	7.27904000	2.18882400	2.08862200
H	4.57174600	5.12383100	0.45447300
H	6.77629700	4.52934200	1.43122300
H	2.50446000	-2.00248400	1.94885200
C	2.72632700	-2.46694800	-0.12876100
C	3.05877100	-3.79171300	0.18044900
C	2.78499100	-2.05081500	-1.46879700
C	3.42139100	-4.68833100	-0.82748900
H	3.03339800	-4.12866800	1.21443900
C	3.15628400	-2.94889800	-2.46712400
H	2.53928400	-1.02689000	-1.73085000
C	3.47369500	-4.28470300	-2.16796400
H	3.67304100	-5.71322100	-0.56485800
H	3.19695500	-2.60752900	-3.49919000
C	3.84814600	-5.25278100	-3.26555100
H	4.58527000	-4.81611700	-3.94961500
H	4.26908500	-6.17782700	-2.85855800
H	2.96980200	-5.52328000	-3.86626200

IM4-Sn

O	-0.46893700	0.12428400	-0.66819800
O	1.81353200	-3.21205300	-0.39065900
O	1.85806000	-2.51861800	-2.54372800
O	1.72987100	-0.68966200	0.54484100
C	1.75784500	-0.81932700	-0.86145700
C	3.09531500	-0.10403200	-1.28893600
C	0.47174200	-0.20120700	-1.40754500
C	1.80439400	-2.33946800	-1.22454400
C	1.79257900	-3.89331400	-2.99774600
H	1.83110900	-3.83389900	-4.08496700
H	0.85460000	-4.33913100	-2.66089200
H	2.64234800	-4.45712900	-2.60588400
Sn	-0.99581300	-0.29205600	1.45594200
O	0.44037400	-0.03636800	-2.69467200
C	-0.78787600	0.49299900	-3.28296300
H	-1.02472700	1.45817000	-2.83270200
H	-0.55888500	0.59028700	-4.34243500
H	-1.59261800	-0.22182600	-3.10987200

O	-2.08429200	-1.92503200	0.66685700
O	-2.61076700	1.03823800	0.86194000
S	-2.19855700	-2.87978400	-0.54509000
S	-2.19216900	2.49696400	0.58587800
O	-1.21247500	-2.55689800	-1.58987200
O	-2.61782600	2.99770300	-0.71651500
O	-2.36683300	-4.26563600	-0.12872500
O	-0.78387900	2.67561900	1.00498600
C	-3.85751500	-2.34418800	-1.25070100
C	-3.22559100	3.41631200	1.85688000
F	-3.79784700	-1.07065000	-1.66991200
F	-4.81938400	-2.45453000	-0.32983000
F	-4.16091400	-3.12648600	-2.29683700
F	-2.94613200	4.72450000	1.79559300
F	-2.94296500	2.96973400	3.09094000
F	-4.52813500	3.23583300	1.61820700
C	3.01302900	-0.15712600	1.00311500
H	2.86399900	0.91124100	1.20252900
O	3.87191500	-0.33475400	-0.10034500
C	3.51896100	-0.85608400	2.23381600
C	3.46373700	-2.25093000	2.36177800
C	4.07973100	-0.08309800	3.25767200
C	3.97676000	-2.86077300	3.50766800
H	3.00779100	-2.84528200	1.57695300
C	4.59883900	-0.69723000	4.40064000
H	4.11478400	1.00007700	3.16084500
C	4.54724100	-2.08791500	4.52569700
H	3.92802100	-3.94189400	3.60792000
H	5.03570500	-0.09173300	5.19023800
H	4.94502900	-2.56891900	5.41567000
H	3.58605400	-0.66847800	-2.08196400
C	3.02171100	1.35535100	-1.69317000
C	3.83834000	1.78362800	-2.74774500
C	2.21580100	2.31123600	-1.05052800
C	3.85543500	3.12129500	-3.14848300
H	4.46861200	1.06360500	-3.26555300
C	2.23354500	3.64549600	-1.45653800
H	1.54465200	2.04013800	-0.24083400
C	3.05599900	4.07789700	-2.50889400
H	4.49742200	3.42211200	-3.97345000
H	1.58751400	4.35638500	-0.94648700
C	3.07594400	5.52941900	-2.92824200
H	3.57026900	6.15176600	-2.17076400
H	3.61315400	5.66661900	-3.87238700

H	2.06007100	5.92195500	-3.05503400
IM5-Sn			
O	1.17389600	-0.95779900	-1.30531800
O	1.56708700	-0.15703600	3.24949900
O	0.35702900	-1.53914700	1.92162800
O	0.67214600	0.99647800	0.35125300
C	1.67366600	0.08107800	0.82058500
C	2.92976500	1.01004300	1.04752800
C	1.81407300	-1.00147700	-0.25601700
C	1.20179000	-0.55077300	2.16316000
C	-0.25742100	-2.19319300	3.06025900
H	-0.85755700	-2.99170100	2.62757200
H	-0.88302200	-1.47358800	3.58903400
H	0.52064800	-2.59151100	3.71576500
Sn	-0.99857200	0.31681100	-1.40874900
O	2.64812800	-1.95776700	0.06865300
C	2.76390400	-3.08830000	-0.84385900
H	3.10777800	-2.73579200	-1.81817600
H	3.50346400	-3.73881300	-0.37994200
H	1.79262400	-3.57887800	-0.92698400
O	-2.26770600	1.19674300	0.06039300
O	-1.59318300	-1.52399200	-0.55042500
S	-2.39375100	1.47935900	1.57537300
S	-1.52764000	-2.93169200	-1.19388600
O	-2.10672700	0.30818800	2.40213800
O	-0.60014500	-3.81871000	-0.48896400
O	-1.78657400	2.76513700	1.93719500
O	-1.47583800	-2.84713000	-2.65725300
C	-4.25152200	1.74652100	1.67127500
C	-3.24491300	-3.55134400	-0.74992300
F	-4.90508200	0.64907200	1.27009200
F	-4.61781200	2.77689900	0.89419200
F	-4.59345100	2.01784900	2.93781300
F	-3.40848400	-4.78185200	-1.25416800
F	-4.18204900	-2.74386400	-1.26395700
F	-3.39470000	-3.60328500	0.57924600
C	1.29157000	2.36660800	0.27961300
H	1.03384800	2.83048400	1.23826100
O	2.64952300	2.09849500	0.16846200
C	0.77543400	3.15050100	-0.89354400
C	1.37374100	3.02644500	-2.15807800
C	-0.30760600	4.02245800	-0.71572000
C	0.88197600	3.76120600	-3.23718100

H	2.22490300	2.36581200	-2.28778700
C	-0.80084300	4.75064500	-1.80196900
H	-0.77519700	4.10815900	0.26067000
C	-0.20840600	4.62126500	-3.06110900
H	1.34900000	3.66521700	-4.21366700
H	-1.64596100	5.41865600	-1.66114700
H	-0.59116400	5.19154700	-3.90348000
H	2.85167300	1.34396000	2.08887800
C	4.30504900	0.45032100	0.79263000
C	5.01634400	-0.12688700	1.84989100
C	4.89539500	0.49305300	-0.47793400
C	6.28603200	-0.66922000	1.63591000
H	4.57618000	-0.15733000	2.84394300
C	6.16716000	-0.04141000	-0.68131500
H	4.36967600	0.96279400	-1.30392200
C	6.88482500	-0.63600200	0.36955100
H	6.82187700	-1.11478100	2.47091100
H	6.61365500	0.00972000	-1.67249800
C	8.27019400	-1.19513300	0.13881800
H	8.63563500	-1.73547200	1.01810900
H	8.28621600	-1.88646900	-0.71265200
H	8.98844700	-0.39471700	-0.08174000

IM6-Sn

C	-6.01727100	1.71084000	0.56543800
C	-5.66138100	1.41705000	-0.76100100
C	-4.85531300	0.32103400	-1.06285400
C	-4.36876900	-0.50541100	-0.03857800
C	-4.72693200	-0.23099800	1.28735000
C	-5.54486800	0.86250400	1.57757600
H	-6.02347900	2.05124000	-1.56693200
H	-4.60224800	0.10887400	-2.09989600
H	-4.37427800	-0.87981200	2.08234800
H	-5.82355200	1.05705500	2.61084900
C	-6.86968400	2.91490600	0.89058800
H	-6.25388100	3.82156200	0.96241800
H	-7.62359600	3.09447800	0.11609000
H	-7.38729200	2.79302900	1.84788900
C	-3.52127300	-1.67536400	-0.39889800
H	-3.83446200	-2.22211500	-1.29156600
O	-2.99717300	-2.50892100	0.62439400
C	-2.03357800	-1.78773300	-0.11320100
C	-1.19320700	-2.55732900	-1.10799600
C	-1.31775600	-0.66260300	0.58725500

O	-1.51802400	-3.83178900	-1.16777300
O	-1.63019500	-0.53532900	1.84209200
C	-0.72914000	-4.66471000	-2.06170700
H	-1.15433700	-5.66136200	-1.95460700
H	-0.82579400	-4.30241800	-3.08747800
H	0.31589800	-4.64400900	-1.74590900
C	-0.94479600	0.50639800	2.60535700
H	-1.12857000	1.48229900	2.15610800
H	-1.37260800	0.43369900	3.60335600
H	0.12401500	0.29095200	2.61229600
O	-0.34005800	-2.02827400	-1.81425400
O	-0.53928100	0.11308500	0.00973600
Sn	1.05706100	0.19287900	-1.57019600
O	1.86869500	1.56789200	-0.09998600
O	2.25717400	-1.20486500	-0.52902300
S	1.22926500	2.95869300	0.09633300
S	2.07129000	-2.43243400	0.38589300
O	0.85646700	3.22001400	1.48549800
O	0.25441800	3.22275400	-0.97589500
O	2.45093500	-3.68052700	-0.27271100
O	0.78807300	-2.38403200	1.10803900
C	2.70239600	4.06987400	-0.25311200
F	2.32733300	5.35215400	-0.15879200
F	3.16659500	3.84543600	-1.49357900
F	3.68604500	3.83867200	0.62377500
C	3.39421400	-2.08574600	1.67508400
F	4.59516000	-1.99239600	1.09550300
F	3.12568900	-0.94208000	2.31700000
F	3.41230700	-3.08888700	2.56281400

IM7-Sn

C	-7.42415900	-0.29951700	-1.44132200
C	-6.78860100	0.87199500	-0.99509800
C	-5.49898700	0.82852400	-0.48050600
C	-4.81029000	-0.40397100	-0.40322800
C	-5.44540600	-1.59071700	-0.84800500
C	-6.72971700	-1.52832100	-1.35671200
H	-7.31186400	1.82208200	-1.05623600
H	-5.00844500	1.73820300	-0.14383100
H	-4.91722800	-2.53681100	-0.78502900
H	-7.21740800	-2.43771300	-1.69873100
O	-2.78124700	-1.46208100	0.13494300
C	-1.35382800	-0.99115000	2.07915100
C	-0.43012300	-1.85609800	-0.08961100

O	-2.52413100	-0.72666200	2.70159600
O	-0.77851300	-2.37319300	-1.26109900
C	-2.42813700	-0.21135000	4.04630600
H	-3.46025400	-0.06681000	4.36652700
H	-1.92033500	-0.93032900	4.69308900
H	-1.88587800	0.73705800	4.04629600
C	0.29094000	-2.69419200	-2.19274600
H	0.93923400	-3.46333800	-1.76940100
H	-0.22506400	-3.06359700	-3.07846800
H	0.87406800	-1.80128900	-2.42024400
O	-0.26387700	-0.88054500	2.67138100
O	0.79506800	-1.77637600	0.22905300
Sn	1.91563600	-0.45802300	1.52525200
O	2.92121400	-0.02640000	-0.39969000
O	0.77149300	1.30691600	0.95041400
S	3.86002900	-1.05387700	-1.04643500
S	-0.34343400	1.80743800	0.03483900
O	3.50947100	-1.36013100	-2.43396000
O	4.14185700	-2.16153000	-0.11651400
O	-1.59076100	2.07270900	0.78275500
O	-0.47750200	1.05714100	-1.21851700
C	5.45109800	-0.06095000	-1.14369300
F	6.42820400	-0.81877100	-1.66397900
F	5.82853000	0.33819600	0.08393600
F	5.29199500	1.02376700	-1.91447100
C	0.32170000	3.50279700	-0.42445900
F	0.50635600	4.24538000	0.67618800
F	1.48106600	3.39106200	-1.07575800
F	-0.56758600	4.12237100	-1.21761600
C	-3.48291800	-0.38503200	0.10230500
H	-3.01767100	0.54103000	0.44909200
C	-1.49143900	-1.41871800	0.72988200
C	-8.82033000	-0.26101300	-2.00423700
H	-9.24251000	0.74738000	-1.97491100
H	-8.82768100	-0.60349400	-3.04695500
H	-9.48674400	-0.92872700	-1.44399900
IM8-Sn			
C	-6.59433700	-0.85542300	-2.67073400
C	-6.61032900	-1.44995000	-1.40223600
C	-5.81579000	-0.95892900	-0.36180100
C	-4.97383500	0.13792600	-0.57370000
C	-4.94920400	0.74262000	-1.83816400
C	-5.74986000	0.24946800	-2.86818600

H	-7.25130700	-2.31012400	-1.22168700
H	-5.84508100	-1.43599700	0.61379800
H	-4.29358600	1.58955600	-2.01629500
H	-5.71557300	0.72839900	-3.84487900
O	-2.94920800	1.32396100	0.10036800
C	-1.10962700	1.38764400	1.69212700
C	-0.86278500	0.28791300	-0.55533800
O	-1.84716200	2.34255300	2.21421300
O	-1.33674400	0.48367300	-1.74835900
C	-1.21724300	3.16392700	3.23598900
H	-1.97664400	3.89555000	3.50779800
H	-0.94350000	2.54282300	4.09153200
H	-0.33210900	3.64789100	2.81818000
C	-0.45352000	0.20798700	-2.88078600
H	-0.08395100	-0.81683500	-2.83431900
H	-1.07981000	0.37347000	-3.75535900
H	0.37854000	0.91254400	-2.84806000
O	0.02209700	1.11476100	2.07957700
O	0.24762900	-0.22655000	-0.35527500
Sn	1.97760700	-0.21029600	1.08590400
O	2.92588300	-0.91910100	-0.77123500
O	2.45495600	1.72658000	0.35388300
S	2.53763800	-2.29732600	-1.33087200
S	1.70911600	3.04098200	0.04816600
O	2.06830800	-2.24909900	-2.71531100
O	1.74492200	-3.04686400	-0.33622500
O	1.82698000	4.02066200	1.12692800
O	0.37662100	2.79487200	-0.52859800
C	4.21367500	-3.14259600	-1.38833600
F	4.06962700	-4.39635800	-1.83795500
F	4.75105800	-3.18498200	-0.15759800
F	5.04799100	-2.48270600	-2.19976100
C	2.76332600	3.67887300	-1.37061200
F	4.03229500	3.83430100	-0.98061700
F	2.72253600	2.81907400	-2.39820700
F	2.28204400	4.86176000	-1.77629000
C	-4.16383400	0.71113400	0.57656400
H	-4.72495800	1.47266200	1.12816200
C	-1.84183500	0.61522300	0.57423300
C	-2.49680900	-0.74736700	1.11185000
H	-2.60739200	-1.39658400	0.23142000
C	-1.80477300	-1.49950900	2.21811800
C	-2.06917700	-1.21610100	3.56550600
C	-0.88172400	-2.50378900	1.89217900

C	-1.40780000	-1.92269300	4.57239400
H	-2.80577200	-0.46032900	3.82075900
C	-0.21295100	-3.20122200	2.90228600
H	-0.67549900	-2.75016600	0.85354400
C	-0.47495000	-2.91193600	4.24423800
H	-1.62504800	-1.70320900	5.61456000
H	0.50337700	-3.97203200	2.63237900
H	0.03798000	-3.45967100	5.03040300
O	-3.76167600	-0.26035100	1.52414200
C	-7.46139000	-1.37575400	-3.79452000
H	-8.21530000	-0.63458900	-4.09001600
H	-6.86529000	-1.60312400	-4.68696300
H	-7.98964400	-2.28917800	-3.50228400

IM9-Sn

C	7.43907400	-0.18525700	2.09509700
C	7.67151200	0.05811200	0.73578200
C	6.61377200	0.10198200	-0.17729600
C	5.30078600	-0.10408000	0.25161500
C	5.05425100	-0.34473500	1.61040400
C	6.11171900	-0.38378100	2.51536300
H	8.68829500	0.21936400	0.38519500
H	6.81725100	0.29601100	-1.22840000
H	4.03335800	-0.48636700	1.95031300
H	5.90741500	-0.56736200	3.56835500
O	3.04873500	0.64987200	-0.26742500
C	1.27903700	1.05501600	-1.90490200
C	0.85433000	-0.19270400	0.24732500
O	2.11922000	1.98723500	-2.30016500
O	1.36388100	-0.28753600	1.44170200
C	1.63684200	2.92732600	-3.29955500
H	2.48697300	3.57866700	-3.49675200
H	1.33451900	2.38888200	-4.20046500
H	0.79683300	3.49130800	-2.88939200
C	0.43980900	-0.55541500	2.54270500
H	-0.06024200	-1.51149000	2.38743900
H	1.07260100	-0.56983000	3.42821600
H	-0.29660200	0.24710700	2.59223300
O	0.16936900	0.87507800	-2.39786600
O	-0.34531400	-0.41652600	0.03236600
Sn	-2.07373300	-0.02075900	-1.32168800
O	-3.09574700	-0.30248500	0.57074200
O	-2.12912700	2.01150000	-0.73661700
S	-3.31430600	-1.70176200	1.18137100

S	-1.16058800	3.11631500	-0.26878600
O	-2.76260600	-1.82050800	2.53066300
O	-3.01967700	-2.74736500	0.18855100
O	-1.06994900	4.21151300	-1.23326900
O	0.08790500	2.55714600	0.27446100
C	-5.18025200	-1.69311100	1.39431200
F	-5.57868000	-2.87231000	1.89039900
F	-5.78126300	-1.49910300	0.20872700
F	-5.55576500	-0.71991700	2.23220800
C	-2.10525000	3.78556200	1.21152700
F	-3.32149500	4.19917100	0.84159200
F	-2.22964200	2.83468300	2.14570200
F	-1.42984900	4.81954600	1.73096900
C	4.18236400	-0.09318700	-0.74682300
H	4.50737500	0.34229000	-1.70426600
C	1.88758900	0.12608100	-0.84211100
C	2.41147900	-1.21898200	-1.59410100
H	2.54716100	-0.94272500	-2.65076400
C	1.55851700	-2.45615600	-1.49949900
C	1.67081800	-3.33276300	-0.41131000
C	0.62713800	-2.72891900	-2.51098000
C	0.84469100	-4.45600900	-0.33030300
H	2.41415200	-3.14225500	0.35670600
C	-0.20323700	-3.84902500	-2.42294600
H	0.55074100	-2.06533600	-3.36982300
C	-0.09953100	-4.71158900	-1.32874200
H	0.93620700	-5.13071700	0.51660300
H	-0.92805100	-4.04803400	-3.20761000
H	-0.75170600	-5.57689600	-1.25359700
O	3.66670700	-1.39624400	-0.97654100
C	8.57450700	-0.22339400	3.09185200
H	8.48034800	0.58207400	3.83151700
H	8.58643200	-1.17038800	3.64576300
H	9.54518600	-0.11110200	2.59808100
TS1-Sn			
O	0.87495300	-2.06335000	-2.14584500
O	2.00498900	-0.01965600	1.71050600
O	-0.19840200	-0.50062000	1.55350700
O	-0.09530000	0.36196700	-1.07895200
C	0.97368800	-0.30302800	-0.48234800
C	1.98822600	0.53725300	-1.21262700
C	1.06938100	-1.77956700	-0.98368100
C	0.99947700	-0.25036300	1.06040600

C	-0.34779600	-0.47393300	2.98913600
H	-1.37303200	-0.79329200	3.16931900
H	-0.19239500	0.54417200	3.35171600
H	0.36614300	-1.16012900	3.45120200
Sn	-2.04346600	-0.01593500	-1.65795000
O	1.38485500	-2.63088000	-0.01449600
C	1.42356600	-4.03658300	-0.37393900
H	2.10818500	-4.18555900	-1.21204900
H	1.78229300	-4.54430700	0.52097000
H	0.41635300	-4.36824300	-0.63314500
O	-2.65768200	1.04258800	0.13517700
O	-1.98236400	-1.78981200	-0.47156300
S	-2.23562800	2.47001000	0.51978900
S	-2.82474100	-3.08041100	-0.58914900
O	-1.29912300	2.50631700	1.64982100
O	-1.99424700	-4.27239600	-0.41652800
O	-1.93863300	3.29152600	-0.66137500
O	-3.78255500	-3.00588500	-1.69602400
C	-3.86047300	3.11244900	1.20893600
C	-3.84630400	-2.94923000	0.98305300
F	-4.26193300	2.37039100	2.25013400
F	-4.81334700	3.08648500	0.26647500
F	-3.69720200	4.37952000	1.62086200
F	-4.66867600	-4.00315900	1.07432500
F	-4.57952800	-1.82709200	0.96978000
F	-3.05071400	-2.93030100	2.06515400
C	4.56333700	-0.35844700	0.18913500
H	4.23606000	0.45223200	0.85802800
O	3.88944900	-0.63384100	-0.80568400
C	5.79902100	-1.05606400	0.55559400
C	6.31679700	-2.09346700	-0.24296100
C	6.46903800	-0.66975900	1.72943300
C	7.49404400	-2.73202700	0.13369300
H	5.78683800	-2.38006800	-1.14637500
C	7.64762600	-1.31464400	2.10488500
H	6.05870200	0.12811700	2.34431600
C	8.15841100	-2.34331600	1.30654200
H	7.89882900	-3.53274200	-0.47892600
H	8.16475500	-1.02011700	3.01357800
H	9.07670600	-2.84669100	1.59758600
H	2.19697500	0.14900000	-2.20327800
C	2.34026100	1.89945400	-0.97156100
C	3.20352900	2.51800200	-1.91286400
C	1.84306100	2.68216000	0.10160100

C	3.58118300	3.84377900	-1.76927000
H	3.58049500	1.93381900	-2.74862300
C	2.20783400	4.01434000	0.21720300
H	1.13061500	2.27479800	0.80654700
C	3.08363100	4.61912400	-0.70451200
H	4.25225800	4.29579000	-2.49508700
H	1.79036000	4.60586600	1.02764700
C	3.44080000	6.07638400	-0.57358400
H	3.62987600	6.34814300	0.47094300
H	4.32436600	6.33298700	-1.16610400
H	2.60984300	6.70400000	-0.92356700

TS2-Sn

O	-0.80087700	-1.68972800	-2.18030300
O	1.70456800	-1.14627300	1.69937500
O	-0.33902500	-1.95636100	1.16951000
O	0.20206900	0.28127200	-0.69540800
C	0.85723500	-0.92547900	-0.59668000
C	2.33143000	-0.84347000	-1.10732100
C	0.14779900	-1.99125100	-1.47440500
C	0.81409100	-1.37811300	0.89793800
C	-0.66654300	-2.20643900	2.55844800
H	-1.63105800	-2.71012400	2.52516800
H	-0.73824300	-1.25017400	3.07974100
H	0.09896500	-2.84094500	3.01164500
Sn	-1.66895600	0.65410200	-1.54759800
O	0.65684100	-3.20881200	-1.37641500
C	-0.07783700	-4.26878000	-2.05389100
H	-0.06715800	-4.09132400	-3.13147900
H	0.45587200	-5.18393300	-1.80059800
H	-1.10321900	-4.28680300	-1.67932500
O	-1.84781900	2.08834000	0.14021300
O	-2.75971000	-0.66926300	-0.24887200
S	-1.03739900	2.33279600	1.40695500
S	-3.66142400	-1.87307100	-0.57613000
O	-1.04994200	1.22416600	2.36603600
O	-3.06253700	-3.14841600	-0.16576800
O	0.27236900	2.96035300	1.12660700
O	-4.27462900	-1.77064500	-1.90410000
C	-2.05728400	3.69974900	2.19423500
C	-5.04145500	-1.56598100	0.66079900
F	-3.29042800	3.26659700	2.48142100
F	-2.14944700	4.75917300	1.37640600
F	-1.46281800	4.09335200	3.33499100

F	-5.97023100	-2.52772300	0.53886600
F	-5.62270800	-0.37866300	0.44081500
F	-4.56684400	-1.58824800	1.91598000
C	4.58143000	-0.90677000	-0.09120400
H	4.99831000	-0.36539800	-0.94037400
O	3.35182200	-1.26564000	-0.10163600
C	5.40891100	-1.29455100	1.00840700
C	4.89561500	-2.00244100	2.12299800
C	6.77444900	-0.93030100	0.95714000
C	5.74422700	-2.34016000	3.16531200
H	3.84422800	-2.26912100	2.15274500
C	7.61381800	-1.27476300	2.01425000
H	7.14796200	-0.39455500	0.08868000
C	7.10156800	-1.97555400	3.11031200
H	5.36251300	-2.88164500	4.02583000
H	8.66333500	-0.99838200	1.98327200
H	7.75946700	-2.24207400	3.93359400
H	2.46982200	-1.60741700	-1.87427700
C	2.76030500	0.50020100	-1.63977000
C	3.04924300	0.63424400	-3.00347000
C	2.88021500	1.62676000	-0.80983500
C	3.42903800	1.87010300	-3.53239800
H	2.97621700	-0.23037800	-3.65952900
C	3.26827000	2.85378000	-1.34359800
H	2.66900800	1.54460600	0.25134700
C	3.54231600	3.00136800	-2.71390400
H	3.64613700	1.95185900	-4.59488900
H	3.35660900	3.71469900	-0.68453700
C	3.93568500	4.34500600	-3.28133800
H	4.70865100	4.82621600	-2.67065700
H	4.31871300	4.25283600	-4.30277700
H	3.07492200	5.02605100	-3.30921800
TS3-Sn			
O	0.67843100	-2.58663700	-0.30648400
O	1.08015800	0.27171000	3.27425800
O	-0.65828300	-0.75623700	2.25022400
O	0.87658700	0.06337000	-0.03601600
C	1.35749700	-0.68203000	1.01925600
C	2.87581800	-0.36556600	1.24935500
C	1.16898800	-2.19051800	0.73871500
C	0.58670800	-0.32375600	2.33662700
C	-1.57137800	-0.40489600	3.31429200
H	-2.47647700	-0.97201100	3.10316200

H	-1.76329700	0.66879200	3.27357500
H	-1.14447700	-0.68682700	4.27986400
Sn	-0.47140800	-0.55237300	-1.54260800
O	1.55578800	-2.96789800	1.73698000
C	1.24750800	-4.38515000	1.60901700
H	1.79555500	-4.80444400	0.76241900
H	1.57814000	-4.82774500	2.54770400
H	0.17165400	-4.50474600	1.46650300
O	-1.41702000	1.38144200	-1.26295200
O	-2.02890900	-1.33244800	-0.30945100
S	-1.55027000	2.53050700	-0.25461300
S	-2.60360900	-2.75926200	-0.20099700
O	-1.45076100	2.11014800	1.14659400
O	-2.24538900	-3.41105400	1.06283700
O	-0.79171700	3.71470900	-0.67851100
O	-2.47504100	-3.51022900	-1.45327500
C	-3.35591700	2.98159800	-0.51618100
C	-4.42534600	-2.33161500	-0.03168300
F	-4.15349300	1.95061900	-0.20753600
F	-3.57822500	3.33163600	-1.79238700
F	-3.67483800	4.02182000	0.27331200
F	-5.13828700	-3.46362600	0.07485400
F	-4.85558200	-1.65216900	-1.10333800
F	-4.63775000	-1.58792200	1.06517900
C	2.71751800	1.78427600	0.19500700
H	2.86537700	1.29258500	-0.76266000
O	2.92554400	1.12047500	1.27467300
C	2.43012700	3.17620700	0.25621700
C	2.13099300	3.81483400	1.48463000
C	2.43399900	3.91301000	-0.95034300
C	1.85936700	5.17377600	1.49261600
H	2.09225500	3.22750100	2.39635400
C	2.16965100	5.27545100	-0.92709400
H	2.63353900	3.40668400	-1.89117600
C	1.88142200	5.90076900	0.29166500
H	1.61040800	5.67240600	2.42428200
H	2.16037200	5.84634300	-1.85009800
H	1.65356400	6.96326800	0.30643200
H	3.13538000	-0.60374300	2.27858500
C	3.89638900	-0.95114700	0.30627000
C	5.15727000	-1.27625200	0.83136400
C	3.67071700	-1.17462300	-1.06310300
C	6.16094800	-1.80090300	0.01686000
H	5.35452600	-1.11947900	1.88963900

C	4.67764500	-1.70208800	-1.87158400
H	2.70203400	-0.95781200	-1.49866100
C	5.93989500	-2.02490000	-1.34982300
H	7.12760000	-2.04479600	0.45126000
H	4.47332900	-1.87324700	-2.92625500
C	7.01318900	-2.61617800	-2.23319000
H	7.12054400	-2.04863400	-3.16500400
H	7.98518600	-2.62966000	-1.72991300
H	6.76768200	-3.64954300	-2.51096000

TS4-Sn

O	1.14741200	-2.05902100	-0.83070900
O	0.87363200	0.30109600	3.19358100
O	-0.33887200	-1.35499100	2.23549700
O	0.63249700	0.38599700	0.05423800
C	1.38214400	-0.39859100	0.90506300
C	2.81138100	0.26721400	1.17363100
C	1.53317100	-1.81397600	0.30319300
C	0.62648500	-0.45778600	2.27219700
C	-1.27593300	-1.40261700	3.34073300
H	-1.86917100	-2.29722800	3.15852400
H	-1.90454100	-0.51112000	3.30984600
H	-0.73156200	-1.46823100	4.28550300
Sn	-0.57978000	-0.20628600	-1.55319300
O	2.07559100	-2.69073900	1.12575400
C	2.12234300	-4.07172300	0.66856200
H	2.74391200	-4.13927200	-0.22691100
H	2.56720800	-4.62303400	1.49594500
H	1.10621300	-4.41253500	0.46071900
O	-1.94857200	1.31492100	-0.72898100
O	-1.72563300	-1.61448700	-0.43789100
S	-2.44533100	1.77251400	0.64548100
S	-1.98753300	-3.11202000	-0.69422800
O	-3.11888100	0.73271900	1.42266300
O	-1.38737900	-3.96204000	0.33914900
O	-1.46290900	2.61911500	1.34916900
O	-1.81560500	-3.47076600	-2.10565600
C	-3.79191800	2.96546000	0.10286400
C	-3.83571600	-3.16685200	-0.36112500
F	-4.72065200	2.34021300	-0.63019900
F	-3.26755600	3.96577400	-0.63107900
F	-4.38168800	3.50037300	1.18342400
F	-4.27995300	-4.41811700	-0.56139000
F	-4.48971600	-2.34167500	-1.18972400

F	-4.10162800	-2.81487000	0.90336600
C	1.76970300	2.41705300	0.78665400
H	0.98371600	2.17787100	1.49878900
O	2.78846100	1.64259300	0.64193000
C	1.77080200	3.67197100	0.09371800
C	2.81432400	4.02477600	-0.79746400
C	0.71106300	4.57374800	0.34169900
C	2.79179100	5.26252600	-1.42167100
H	3.62326900	3.32530900	-0.98117400
C	0.70214100	5.81389300	-0.29263000
H	-0.10167500	4.27353900	0.99481900
C	1.73688200	6.15653700	-1.16826800
H	3.58726300	5.54171700	-2.10630100
H	-0.11381100	6.50683600	-0.11152700
H	1.72471600	7.12380800	-1.66397000
H	2.93063300	0.36234700	2.25318600
C	4.02210600	-0.37776900	0.55443400
C	5.02960400	-0.89267900	1.37648400
C	4.17130400	-0.47262700	-0.83862700
C	6.15975200	-1.49808500	0.82077800
H	4.93043400	-0.82902200	2.45783300
C	5.30320700	-1.07200200	-1.38653100
H	3.40038900	-0.08056400	-1.49662800
C	6.31822800	-1.59665300	-0.56775600
H	6.92951000	-1.89524900	1.47832300
H	5.39901000	-1.13888100	-2.46818100
C	7.54611800	-2.23418800	-1.17562500
H	8.16955700	-2.71078100	-0.41241300
H	7.27471800	-2.99687700	-1.91546800
H	8.16395400	-1.48849500	-1.69271500
TS5-Sn			
C	7.01225400	-1.79930200	0.92055400
C	6.87198700	-1.70925100	-0.47817700
C	5.87892700	-0.92286100	-1.04154500
C	4.98812600	-0.19835400	-0.21128700
C	5.11507500	-0.29717400	1.19862700
C	6.11945400	-1.07811200	1.74323200
H	7.55070100	-2.26398500	-1.12008200
H	5.78081800	-0.85639100	-2.12238800
H	4.41483000	0.23733600	1.83076400
H	6.21841700	-1.14871000	2.82355700
C	8.09040700	-2.64904200	1.53862400
H	7.66068700	-3.38334500	2.23120700

H	8.66696100	-3.18880000	0.78214600
H	8.78581800	-2.03037900	2.12057600
C	4.02239800	0.64416900	-0.81548700
H	3.98247700	0.75018400	-1.89829600
O	3.23562400	1.44660800	-0.10076100
C	2.00526900	1.02534600	-0.67563600
C	1.33214000	1.96362900	-1.54390700
C	1.34201600	-0.10171700	-0.09517000
O	2.06404700	3.05131400	-1.80678000
O	2.00583300	-0.72728300	0.87155400
C	1.39744200	4.10266600	-2.54775600
H	2.13452300	4.90194400	-2.61954600
H	1.11334600	3.74219900	-3.53928100
H	0.51167200	4.43328800	-2.00082300
C	1.31899100	-1.82729500	1.53339300
H	1.10184400	-2.62228700	0.81889700
H	2.01978700	-2.16490200	2.29637300
H	0.39016400	-1.47305100	1.98053000
O	0.20396400	1.79317800	-2.02771800
O	0.20515600	-0.51236500	-0.43639200
Sn	-1.60722800	0.11056900	-1.51818800
O	-2.47745600	-1.19116800	0.03652300
O	-2.12680600	1.62437900	-0.12691400
S	-2.27735600	-2.71280300	0.03630400
S	-1.42058900	2.66842500	0.76004000
O	-1.77165000	-3.22455000	1.31152500
O	-1.63939700	-3.16360700	-1.21311000
O	-1.49117600	4.01792700	0.19801300
O	-0.12540300	2.18496400	1.26000500
C	-4.05828300	-3.29947100	-0.06707700
F	-4.09148600	-4.64000100	-0.11117800
F	-4.64165000	-2.82049200	-1.17976200
F	-4.76117700	-2.88628300	0.99551900
C	-2.57979900	2.65794500	2.23887200
F	-3.82654000	2.96727400	1.86105500
F	-2.58598300	1.45391500	2.82174300
F	-2.16025600	3.56850500	3.13185800
TS6-Sn			
C	7.62379800	0.46961300	1.78187800
C	7.63519000	0.32762800	0.38656700
C	6.44468200	0.26081400	-0.33741200
C	5.21218100	0.32993200	0.32473400
C	5.18557800	0.47362700	1.72169300

C	6.37944400	0.54338100	2.43337600
H	8.58516200	0.27535700	-0.13952200
H	6.47471100	0.15550300	-1.41959600
H	4.23270000	0.54877700	2.23617100
H	6.34904100	0.66313600	3.51404900
O	2.88590100	0.69272400	0.17407400
C	1.20986000	0.96975200	-1.63364400
C	0.61530900	0.19459100	0.64608800
O	2.20524500	1.54555500	-2.33341200
O	1.08903400	0.05231600	1.88799200
C	1.82582300	2.17547400	-3.58080900
H	2.74588500	2.62144700	-3.95878800
H	1.43876000	1.42964500	-4.27892100
H	1.06908300	2.94084600	-3.39594700
C	0.11250100	-0.08078900	2.95824000
H	-0.48985000	-0.98097100	2.83394400
H	0.71293600	-0.12987600	3.86654300
H	-0.53805000	0.79545300	2.96915900
O	0.06607300	0.87188300	-2.11924800
O	-0.61515400	0.00470300	0.43809700
Sn	-2.03955300	0.06420500	-1.18615600
O	-3.34095000	-0.50172700	0.60154100
O	-2.42135700	2.09672800	-0.70995800
S	-3.15597100	-1.84617700	1.29273600
S	-1.56765200	3.36990400	-0.52428600
O	-2.91096200	-1.75152300	2.73475100
O	-2.27952600	-2.74385700	0.50716300
O	-1.45851600	4.15283000	-1.75608700
O	-0.35134000	3.12010800	0.25963400
C	-4.87445100	-2.58613200	1.13339700
F	-4.89005700	-3.81546200	1.67530800
F	-5.22459500	-2.68927600	-0.16088700
F	-5.78174700	-1.82879300	1.76290400
C	-2.71530700	4.33686800	0.60635500
F	-3.89940600	4.54386700	0.01619000
F	-2.91189000	3.67674600	1.75562300
F	-2.15796400	5.52642600	0.88372200
C	3.96748800	0.23315800	-0.46603600
H	4.04007100	0.48746100	-1.52068500
C	1.59057400	0.49471700	-0.33910800
C	2.71471600	-1.98105200	-0.23629900
H	2.42041900	-1.62525200	0.75401200
C	2.03938600	-3.12792200	-0.78732600
C	2.47989700	-3.74603700	-1.98055400

C	0.88188400	-3.60036700	-0.13071300
C	1.77152700	-4.82327800	-2.49415000
H	3.36855900	-3.37197500	-2.47910000
C	0.16329000	-4.66523600	-0.66779700
H	0.51930500	-3.10988700	0.76795500
C	0.61301300	-5.27873900	-1.84130700
H	2.10637400	-5.30896300	-3.40621000
H	-0.75140800	-4.98966800	-0.18297500
H	0.05461600	-6.11177200	-2.26014300
O	3.70284600	-1.43081900	-0.81621900
C	8.90839200	0.54926500	2.57189800
H	8.96836200	1.48900600	3.13489200
H	8.97523300	-0.26804900	3.30096000
H	9.78561000	0.49135800	1.91999000

TS7-Sn

C	-7.77844100	0.08245900	-1.36287100
C	-7.69522200	-0.17740700	0.01365800
C	-6.45853000	-0.27506400	0.64845400
C	-5.27442600	-0.11276800	-0.08606900
C	-5.34341600	0.14451600	-1.46757800
C	-6.58240900	0.24131100	-2.08888000
H	-8.60699900	-0.30122500	0.59243200
H	-6.41152400	-0.47799800	1.71598700
H	-4.42756800	0.27386300	-2.03532600
H	-6.62955500	0.44559700	-3.15605000
O	-2.94565200	0.26658900	-0.02315500
C	-1.34744900	0.80668600	1.76724000
C	-0.65739100	-0.28366100	-0.36881500
O	-2.39610900	1.41262400	2.35604200
O	-1.08329300	-0.62284500	-1.57700500
C	-2.08130600	2.30280200	3.45663600
H	-3.03742600	2.74555000	3.74008800
H	-1.65010700	1.74072300	4.29055300
H	-1.38361700	3.07069000	3.11490200
C	-0.06637900	-0.89083800	-2.58158400
H	0.54583000	-1.74608700	-2.29409200
H	-0.63251800	-1.09781600	-3.48954200
H	0.56279200	-0.00813100	-2.70500500
O	-0.21606000	0.83354800	2.28579700
O	0.56842700	-0.39725000	-0.08458600
Sn	2.02983800	0.34396500	1.32299500
O	3.31581500	-0.12825600	-0.45842900
O	1.86792400	2.29852200	0.49236300

S	3.61251500	-1.58825900	-0.80321200
S	0.79135900	3.18819200	-0.16011400
O	3.27601400	-1.94951800	-2.18234100
O	3.17668000	-2.48878300	0.28375400
O	0.00956400	3.93594400	0.83217700
O	0.07123400	2.50088300	-1.24039000
C	5.48907800	-1.60352800	-0.73190600
F	5.94241100	-2.84307100	-0.98149200
F	5.91413800	-1.23341800	0.48909900
F	6.01055100	-0.76606000	-1.63816400
C	1.90383300	4.45178200	-0.99781200
F	2.66689200	5.08084900	-0.09213300
F	2.69641400	3.85859200	-1.89974100
F	1.14128600	5.36291400	-1.62477700
C	-3.99463100	-0.23179800	0.60266000
H	-3.99150800	-0.19801500	1.68944700
C	-1.66802400	0.13809700	0.54089500
C	-2.55421100	-2.34428100	1.21149700
H	-2.43319900	-1.91330400	2.21486000
C	-1.57301500	-3.32293400	0.79116900
C	-1.67617700	-3.97366300	-0.45664400
C	-0.47668800	-3.59062900	1.63736800
C	-0.68757300	-4.86972500	-0.84610900
H	-2.52261100	-3.75576200	-1.10005800
C	0.51594300	-4.47793300	1.23351600
H	-0.39793900	-3.07893800	2.59402200
C	0.41065600	-5.11394100	-0.00807400
H	-0.75559800	-5.36907700	-1.80836500
H	1.38188400	-4.65378700	1.86323700
H	1.19623000	-5.79064700	-0.33185200
O	-3.57792200	-2.05052800	0.53244400
C	-9.11347600	0.19933300	-2.05714200
H	-9.94318200	0.00211300	-1.37144800
H	-9.25232400	1.20481000	-2.47436300
H	-9.18764600	-0.50831500	-2.89209800

Ni-Path

Ni(ClO₄)₂

O	-1.72603200	-0.84642200	0.88385200
O	-1.43000200	0.64637200	-0.93698800
O	1.72595600	-0.84565600	-0.88458800
O	3.59491500	-0.59199300	0.75772600
O	1.43010000	0.64558900	0.93743200
O	-3.59491500	-0.59132300	-0.75840100

Ni	0.00001300	-0.42818800	-0.00000100
O	-3.11753800	1.23323500	0.81465500
O	3.11751700	1.23393800	-0.81370000
Cl	-2.58911300	0.14469200	0.00019500
Cl	2.58909100	0.14468100	-0.00018700

IM1-Ni

O	-0.97417200	-1.73934500	-0.34428900
O	1.84233400	-0.24424300	2.66895900
O	-0.20882400	0.52068800	3.26078600
O	-0.93613200	0.76154300	0.59227900
C	0.12628900	-0.11708200	1.00895100
C	0.36559200	0.92617200	-0.04241300
C	-0.12186800	-1.52554600	0.51939800
C	0.69579600	0.04813000	2.40621700
C	0.23705500	0.70802400	4.62426900
H	-0.63436000	1.08777300	5.15605100
H	1.05888500	1.42756300	4.65097600
H	0.56567300	-0.24609700	5.04292900
O	0.59460200	-2.45911100	1.09058100
C	0.35827600	-3.82555300	0.64353300
H	0.65007800	-3.91422900	-0.40454000
H	0.99224000	-4.43713800	1.28319900
H	-0.69726200	-4.07388200	0.76876400
C	3.59514900	-1.31655300	-0.24950500
H	3.52160600	-1.13547300	0.84046000
O	2.60628600	-1.16749100	-0.95797100
C	4.92310100	-1.73103000	-0.74258700
C	5.13982700	-1.99490800	-2.10701700
C	5.98018500	-1.86212000	0.17240400
C	6.40231300	-2.38549200	-2.54515000
H	4.31076400	-1.88838700	-2.80069300
C	7.24517900	-2.25412600	-0.26882200
H	5.80564300	-1.65506800	1.22635900
C	7.45447800	-2.51526700	-1.62680400
H	6.57360900	-2.59037000	-3.59848400
H	8.06315000	-2.35554800	0.43909000
H	8.43858900	-2.82061300	-1.97305200
H	0.39396200	0.54932800	-1.06168000
C	1.08545400	2.20105500	0.20811500
C	2.22323300	2.48819300	-0.55848800
C	0.65131300	3.12753800	1.16533600
C	2.92664600	3.67425500	-0.35172100
H	2.55723500	1.78260700	-1.31502200

C	1.35783200	4.31481800	1.35658600
H	-0.25007800	2.93130900	1.73756400
C	2.50655000	4.60946600	0.60634100
H	3.80939600	3.88131200	-0.95248700
H	1.00265200	5.03081700	2.09449100
C	3.24449900	5.91441600	0.79476400
H	3.15435600	6.28176800	1.82283500
H	4.30993900	5.81072800	0.56215200
H	2.83935200	6.69207600	0.13319600
Ni	-2.48477200	-0.29032400	-0.48263800
Cl	-2.94940700	1.70579600	-2.25172400
Cl	-4.22106100	-2.07753200	0.58435300
O	-3.61616000	1.42998000	-0.87930900
O	-1.95665800	0.50000600	-2.32638800
O	-3.93399100	-1.76133500	-0.90336500
O	-3.32195000	-1.01196700	1.28510600
O	-2.20109300	2.97166900	-2.22181300
O	-3.92726000	1.64129900	-3.34129300
O	-5.63310100	-1.86089400	0.91198000
O	-3.75578800	-3.43283000	0.93056500

IM2-Ni

O	-1.27543400	-1.81494100	-0.85851200
O	2.37450100	-0.98715400	1.78999500
O	0.40833200	-1.89351800	2.40458700
O	-0.74978800	0.11398000	0.90702000
C	0.33050500	-0.55085200	0.44938500
C	1.14266200	0.46027800	-0.44011400
C	-0.12572700	-1.75124200	-0.44379300
C	1.17391100	-1.15876700	1.61035300
C	1.03169000	-2.49676200	3.55742300
H	0.23529100	-3.05448400	4.04866500
H	1.42444700	-1.72020000	4.21836300
H	1.84175700	-3.16100900	3.24476700
O	0.78511900	-2.68352800	-0.69601600
C	0.33166400	-3.83419700	-1.46088600
H	0.02562500	-3.51750500	-2.46028700
H	1.19199100	-4.50128700	-1.50440000
H	-0.50960400	-4.30708400	-0.95042000
C	3.51950300	-0.09144100	-0.28262600
H	3.57375400	0.69355800	0.46965400
O	2.43797800	-0.23956500	-0.93071900
C	4.68306300	-0.87288700	-0.58962500
C	4.66913300	-1.87905800	-1.58167500

C	5.86595400	-0.60188200	0.13069500
C	5.82925500	-2.59490300	-1.84545100
H	3.75184200	-2.07954400	-2.12551600
C	7.02280400	-1.32731500	-0.13832100
H	5.86370400	0.16815600	0.89770900
C	7.00281000	-2.31972600	-1.12530100
H	5.83003700	-3.36817600	-2.60785700
H	7.93485300	-1.12454000	0.41465300
H	7.90634700	-2.88531000	-1.33671600
H	0.60877200	0.55898800	-1.38524000
C	1.45038100	1.82169000	0.11478200
C	1.79210000	2.82638100	-0.80690900
C	1.41555600	2.15098700	1.47704100
C	2.11642400	4.11136600	-0.37929000
H	1.78144700	2.60619600	-1.87245500
C	1.73049100	3.44346000	1.89766200
H	1.10266200	1.42056800	2.21184600
C	2.08527400	4.44569000	0.98327600
H	2.36416400	4.87269400	-1.11538400
H	1.67871500	3.68054800	2.95779800
C	2.37084200	5.85534700	1.44343600
H	2.72691400	5.87637700	2.47902000
H	3.12288800	6.34083500	0.81158300
H	1.46045900	6.46785800	1.39672800
Ni	-2.42701400	-0.17415800	-0.11941100
Cl	-2.58800700	2.33776800	-1.22680900
Cl	-4.61554100	-1.74446200	0.38771000
O	-3.18731400	1.83188500	0.09405900
O	-1.89622600	1.05447400	-1.77356600
O	-4.23893100	-0.99115200	-0.90675200
O	-3.46611300	-1.31378600	1.33438900
O	-1.57628100	3.38550100	-0.98438800
O	-3.63758300	2.78595000	-2.15442300
O	-5.91646200	-1.29276800	0.90457200
O	-4.57793800	-3.20455500	0.16916800
IM3-Ni			
C	-2.02854200	-0.11151100	-0.99229600
C	-1.08674100	2.04233900	-0.15324800
H	-0.12930500	1.56747800	0.05625400
O	-2.03242100	1.35039600	-0.66387600
C	-1.29989100	3.43141800	0.10581700
C	-2.50250100	4.09103900	-0.25160600
C	-0.25767800	4.14082200	0.74734200

C	-2.64930800	5.43926100	0.03278200
H	-3.29178000	3.53702400	-0.74940700
C	-0.42220500	5.49346000	1.03205800
H	0.65896800	3.61980300	1.00541700
C	-1.61041900	6.13813600	0.67417300
H	-3.56290300	5.95795000	-0.24194700
H	0.37474200	6.04481600	1.52129700
H	-1.73293400	7.19633000	0.88992900
H	-2.00458400	-0.09632000	-2.08310900
C	-3.37254200	-0.62377500	-0.52038800
C	-4.10545000	-1.47953400	-1.35225700
C	-3.93094600	-0.24756600	0.71085300
C	-5.35156500	-1.96622100	-0.94856800
H	-3.69731700	-1.77339800	-2.31488100
C	-5.18020400	-0.72535900	1.10031000
H	-3.39798100	0.42909100	1.37344700
C	-5.91254300	-1.60070400	0.28133500
H	-5.89971900	-2.63127600	-1.61195600
H	-5.59529000	-0.41169900	2.05611900
C	-7.25823000	-2.12914300	0.72114700
H	-7.89498900	-1.32724600	1.11341400
H	-7.79011100	-2.60833900	-0.10717100
H	-7.14869200	-2.87505700	1.51963800
O	0.57527800	-0.87619600	1.44273300
O	-1.20834300	-2.31986300	-2.51458200
O	-0.07987000	-3.16344100	-0.74516000
O	0.36678100	-0.13687900	-1.07841800
C	-0.70093600	-0.85430200	-0.60949400
C	-0.48598300	-1.17636700	0.89386000
C	-0.74018000	-2.21000700	-1.40053600
C	0.22942700	-4.37242500	-1.47470600
H	0.81071700	-4.97947500	-0.78238200
H	0.82007700	-4.12486000	-2.35907200
H	-0.69447700	-4.87748700	-1.76755000
O	-1.45631600	-1.81442000	1.51657200
C	-1.18039000	-2.26816900	2.86856400
H	-1.00026500	-1.41088500	3.52082000
H	-2.07602000	-2.80975700	3.16976900
H	-0.30436700	-2.91984300	2.86202100
Ni	2.02727700	-0.26285800	0.00800100
Cl	2.91107000	2.26648100	-0.66364600
Cl	3.81693100	-2.23295900	0.66027700
O	3.20834200	0.94448000	-1.36584600
O	2.05615400	1.79834100	0.56097000

O	3.68817000	-0.80344200	1.22938800
O	2.70786300	-2.22485900	-0.42443100
O	2.08199400	3.15294700	-1.50913900
O	4.13701400	2.93033300	-0.20191600
O	5.13905300	-2.44761800	0.05517100
O	3.50348100	-3.23791100	1.69500200

IM4-Ni

C	-2.10628900	1.27442400	-1.08463400
C	-0.38215900	1.98417900	0.32807300
H	-0.63330700	1.64546700	1.33740400
O	-1.50537500	2.38464300	-0.39916000
C	0.67748200	3.04900800	0.33568500
C	0.92640400	3.81936700	-0.81060700
C	1.41808600	3.27462500	1.50186400
C	1.92069500	4.79697700	-0.78885300
H	0.33214300	3.66545600	-1.70594300
C	2.41440500	4.25497200	1.51922500
H	1.21992700	2.68747100	2.39307000
C	2.66850700	5.01398200	0.37486900
H	2.10867800	5.39489200	-1.67683900
H	2.98784700	4.42332500	2.42656900
H	3.44253900	5.77706100	0.38874500
H	-2.51259500	1.69198400	-2.00642300
C	-3.21418400	0.59016000	-0.31224400
C	-4.52268700	0.69540700	-0.80107700
C	-3.00483000	-0.11474000	0.88504200
C	-5.59383700	0.11374500	-0.11887600
H	-4.70955100	1.24073700	-1.72389000
C	-4.07863200	-0.69163500	1.56270600
H	-2.01243300	-0.23052100	1.30791000
C	-5.39210000	-0.58786900	1.07703800
H	-6.59960200	0.21205800	-0.52126900
H	-3.88755400	-1.23201200	2.48729500
C	-6.54652800	-1.20206600	1.83428700
H	-6.73336000	-0.66327900	2.77236400
H	-7.47036000	-1.17666900	1.24718200
H	-6.34098900	-2.24636700	2.09841100
O	-0.40025100	-1.84365800	-0.74327300
O	-0.60049300	1.83853500	-3.44106200
O	0.80728800	0.09836300	-3.09083300
O	0.08641900	0.74157900	-0.38343800
C	-0.83847000	0.43867200	-1.43417700
C	-1.02505300	-1.07436400	-1.46990700

C	-0.21587000	0.89344000	-2.79060100
C	1.59241500	0.43360000	-4.25869100
H	2.37419000	-0.32327000	-4.29680100
H	2.02115500	1.43097000	-4.13866300
H	0.96341000	0.40156500	-5.15160400
O	-1.88748000	-1.46304600	-2.38033100
C	-2.10538100	-2.89589100	-2.51943800
H	-2.51680600	-3.29144000	-1.58911800
H	-2.81828800	-2.98919600	-3.33674700
H	-1.15965100	-3.38702500	-2.75592400
Ni	1.05606000	-1.01227300	0.47840200
Cl	0.95041300	-0.46839300	3.14769100
Cl	3.07683900	-2.48213500	-0.56941400
O	2.03410700	-0.08563800	2.11140800
O	-0.09710600	-1.15941400	2.22204800
O	2.10969200	-2.82749800	0.59205600
O	2.59737200	-1.04132100	-0.92041500
O	0.36088000	0.74628200	3.74278900
O	1.46232000	-1.40252300	4.15133100
O	4.47112300	-2.47187700	-0.11542800
O	2.85648400	-3.37999400	-1.71566700

IM5-Ni

C	-2.23534400	-0.08248800	1.59652800
C	-0.14439400	-0.75364100	2.25067200
H	-0.13785500	-0.18864600	3.19284500
O	-1.42480000	-1.21401800	1.95208000
C	0.90650700	-1.81999500	2.26141100
C	0.60944600	-3.14292400	1.92014900
C	2.19828700	-1.47714500	2.68841300
C	1.60585200	-4.11868300	2.00161700
H	-0.39186000	-3.40499000	1.59622400
C	3.19322900	-2.45124100	2.75244400
H	2.42729300	-0.44875400	2.95927900
C	2.89539500	-3.77553900	2.41292400
H	1.37497600	-5.14456700	1.72921900
H	4.19690500	-2.17879100	3.06666500
H	3.66958300	-4.53646800	2.46591200
H	-2.73144100	0.30771200	2.48986500
C	-3.25505900	-0.49171600	0.56351300
C	-4.59991000	-0.15358100	0.74587200
C	-2.88510700	-1.20831800	-0.58528100
C	-5.55903400	-0.51544300	-0.20399500
H	-4.90410600	0.39517500	1.63484700

C	-3.84804200	-1.56725200	-1.52773500
H	-1.85008800	-1.49579300	-0.74688700
C	-5.20123700	-1.23041400	-1.35509000
H	-6.60017400	-0.24534500	-0.04149400
H	-3.54131600	-2.12426600	-2.41047500
C	-6.23831500	-1.65611000	-2.36876700
H	-6.47304900	-2.72395300	-2.26594700
H	-7.17335000	-1.09965600	-2.24513300
H	-5.88321200	-1.50175300	-3.39433100
O	-0.47050800	1.44216200	-1.11497300
O	-1.49349400	2.10196300	3.32807200
O	-0.32458300	3.15534800	1.70060000
O	0.08759100	0.26433400	1.19712700
C	-1.14525600	0.99558700	1.16622200
C	-1.29958300	1.59647100	-0.22284500
C	-1.03809800	2.15166000	2.20635400
C	-0.02003700	4.26052500	2.58437800
H	0.58262700	4.94147600	1.98538200
H	0.54277800	3.89783600	3.44729600
H	-0.94585500	4.73653500	2.91618700
O	-2.38675300	2.32052200	-0.35175300
C	-2.61395200	2.94958800	-1.64387000
H	-2.70868700	2.17817300	-2.41010200
H	-3.54463200	3.50119600	-1.52321300
H	-1.78164900	3.61652300	-1.87671800
Ni	1.20095500	0.27583100	-0.76801900
Cl	1.61100300	-2.19758100	-1.80382400
Cl	2.98604600	2.27130800	-1.22145200
O	2.46645300	-1.41850500	-0.77294700
O	0.36479900	-1.25679600	-1.89027600
O	2.29587800	1.32981600	-2.23789400
O	2.40603700	1.72111900	0.11763200
O	1.21297800	-3.51156100	-1.28222600
O	2.28643400	-2.28216300	-3.10309100
O	4.44446500	2.11874500	-1.25622700
O	2.55355900	3.66474500	-1.42270600
IM6-Ni			
C	5.44805600	-0.77296600	-0.14451600
C	4.45002900	-1.12361200	-1.06964200
C	3.35583400	-0.29353300	-1.29725200
C	3.22321600	0.90864700	-0.58469200
C	4.20861600	1.27100800	0.34130200
C	5.30894700	0.43659700	0.55064200

H	4.52770600	-2.06139400	-1.61459800
H	2.59116800	-0.59113300	-2.01033200
H	4.11501300	2.20429700	0.88741600
H	6.07294700	0.73365900	1.26565600
C	6.63582400	-1.67820500	0.08389600
H	6.31565400	-2.68168100	0.39046900
H	7.22761800	-1.79457800	-0.83290100
H	7.29774300	-1.28316900	0.86131600
C	2.06763600	1.80013000	-0.87435300
H	1.85572400	1.97698700	-1.93098200
O	1.83467200	2.93072400	-0.04936100
C	0.83257800	1.93424500	0.00979300
C	-0.47346900	2.25063900	-0.67870600
C	0.72612100	1.10617000	1.26502200
O	-0.43667100	3.37472300	-1.36127000
O	1.60105200	1.43395800	2.18736400
C	-1.64077600	3.72965900	-2.09951100
H	-1.39666300	4.67358100	-2.58362700
H	-1.86608600	2.95173400	-2.83151900
H	-2.47621200	3.84166400	-1.40624400
C	1.60342000	0.62971300	3.40039200
H	1.81458300	-0.41105600	3.14846800
H	2.39471900	1.05861000	4.01262500
H	0.63289900	0.70858900	3.89375700
O	-1.46878800	1.52827000	-0.64327900
O	-0.09249500	0.19884800	1.41373800
Ni	-1.61166100	-0.39767100	0.12753200
O	-3.17397000	0.07418300	1.41828100
O	-1.23656200	-2.44546800	0.55281700
Cl	-4.30124000	-0.17783100	0.37104000
Cl	-0.22271500	-2.62769700	-0.59544600
O	-5.22061000	-1.22006700	0.83868800
O	-3.46100400	-0.67090300	-0.83542800
O	-0.25502600	-1.20616400	-1.24500500
O	1.12472500	-2.90415500	-0.06726500
O	-4.98586600	1.08405900	0.04537900
O	-0.67311400	-3.63904800	-1.55712900

IM7-Ni

C	7.45168500	-0.39329700	0.30643600
C	7.11340800	0.78342700	-0.38191800
C	5.78718100	1.08809500	-0.66715300
C	4.75318400	0.21345400	-0.26575600
C	5.08653300	-0.97488600	0.42993800

C	6.41264500	-1.26274100	0.70480500
H	7.89929400	1.46520400	-0.69558000
H	5.54288300	2.00359800	-1.20048300
H	4.29660900	-1.65106300	0.74188700
H	6.66106100	-2.17643300	1.23938100
C	8.88671200	-0.73181600	0.61775800
H	9.17760100	-1.67784800	0.14346900
H	9.57110700	0.04662100	0.26817400
H	9.03537800	-0.85626800	1.69773600
C	3.40704900	0.57001900	-0.58400200
H	3.16254300	1.48227400	-1.11729800
O	2.45100700	-0.21166600	-0.22922400
C	1.08414600	-0.16698000	-0.36958100
C	0.41977500	-1.29904900	0.22836100
C	0.37624000	0.88373200	-1.03689000
O	1.24365300	-2.23802700	0.71102500
O	1.15074100	1.86870400	-1.53076700
C	0.60435900	-3.37977500	1.33401200
H	1.42822500	-4.01746900	1.65385200
H	0.00514200	-3.05614200	2.18768400
H	-0.03333100	-3.89477000	0.61274600
C	0.44268000	2.98518600	-2.14005400
H	-0.24618200	3.42265000	-1.41537400
H	1.22643900	3.68889500	-2.41991300
H	-0.10538300	2.63954700	-3.01846200
O	-0.81135100	-1.44079700	0.31220900
O	-0.85499300	0.92684300	-1.19325600
Ni	-2.25595500	-0.03172300	-0.05132800
O	-3.20351600	-1.14236900	-1.55425700
O	-3.40567400	1.78483600	-0.01758800
Cl	-4.14624400	-1.91069000	-0.58557100
Cl	-2.65777500	2.37382500	1.19187400
O	-5.55348500	-1.65822100	-0.92116500
O	-3.76876900	-1.25733200	0.76641000
O	-1.73820000	1.18709300	1.59580700
O	-1.83008900	3.53016700	0.78214200
O	-3.81644600	-3.34691000	-0.57934300
O	-3.58036600	2.71067200	2.28256700
IM8-Ni			
C	7.15503900	-1.47171700	0.34652000
C	6.87807400	-0.36456200	1.15721300
C	5.62983800	0.26422100	1.11204000
C	4.63261300	-0.20451700	0.25447500

C	4.89702200	-1.31397600	-0.56114000
C	6.14194400	-1.93445600	-0.51342600
H	7.64367000	0.01292100	1.83100300
H	5.43620700	1.12315400	1.75123800
H	4.12431100	-1.68197600	-1.22884600
H	6.33667200	-2.79346600	-1.15244200
C	8.50181100	-2.15626800	0.38462300
H	8.99706600	-2.11247200	-0.59371400
H	9.16764500	-1.68994400	1.11784600
H	8.40156500	-3.21659400	0.64851400
C	3.29626000	0.47449900	0.22474400
H	3.28948900	1.36092200	0.87233400
O	2.25132200	-0.41106700	0.67598900
C	1.04629100	-0.03744300	0.06757500
C	0.11973600	0.68101800	1.06562900
C	0.39488300	-1.30070100	-0.53121800
O	0.79222800	1.32997700	1.98823800
O	1.28105000	-2.07735800	-1.11559600
C	0.01008600	2.08366500	2.96080000
H	0.74467000	2.45878800	3.67129400
H	-0.50330400	2.90185800	2.45227400
H	-0.71481100	1.42504500	3.44181700
C	0.76956100	-3.27097500	-1.77426900
H	0.04240400	-2.98892200	-2.53817200
H	1.64831000	-3.74054700	-2.21304200
H	0.30184300	-3.92291800	-1.03420200
O	-1.10696100	0.70627100	1.00810400
O	-0.80333200	-1.57048200	-0.53309400
Ni	-2.48119300	-0.57716700	0.15179600
O	-2.66408500	-1.62844600	1.94547300
O	-3.69226400	-1.72165800	-1.16222500
Cl	-3.77508600	-0.70616700	2.53121500
Cl	-3.54461600	-0.74607000	-2.34916700
O	-4.97855200	-1.47821900	2.85311100
O	-4.02044900	0.24392400	1.33283800
O	-2.72868300	0.40540600	-1.67730600
O	-2.74919700	-1.35287500	-3.43223900
O	-3.25181500	0.04158200	3.68951200
O	-4.84727700	-0.25492500	-2.80685500
C	1.49845100	0.94823600	-1.14606600
H	1.17148000	0.50455400	-2.09157900
C	1.00244700	2.38441400	-1.08191400
C	1.84128000	3.43177300	-0.67828700
C	-0.30798300	2.67395400	-1.49046900

C	1.36772700	4.74644800	-0.65933100
H	2.87215500	3.22757200	-0.40859200
C	-0.78136900	3.98790100	-1.46481600
H	-0.96738400	1.88076600	-1.83310700
C	0.05410200	5.02748900	-1.04608800
H	2.03063400	5.55150800	-0.35287100
H	-1.79981000	4.19456300	-1.78181600
H	-0.31143300	6.05091400	-1.03434300
O	2.90677200	0.81899000	-1.09448100

IM9-Ni

C	-7.19781300	-0.73339800	0.90675500
C	-6.98679800	-1.19308900	-0.39910700
C	-5.72573600	-1.10607700	-0.99609500
C	-4.65058700	-0.54997500	-0.29928400
C	-4.84855700	-0.08676400	1.00903400
C	-6.10634700	-0.17863600	1.59890000
H	-7.81413200	-1.62603600	-0.95651900
H	-5.58389400	-1.47140500	-2.01106300
H	-4.01259800	0.33467500	1.55820200
H	-6.24799100	0.18235900	2.61563700
C	-8.55175500	-0.84520300	1.56883300
H	-8.84405700	0.09946800	2.04276600
H	-9.32976000	-1.11626200	0.84781800
H	-8.54470100	-1.61261100	2.35413700
C	-3.31142800	-0.43840300	-0.96258200
H	-3.28632700	-0.99659700	-1.90950400
O	-2.25763100	-0.94041800	-0.11244000
C	-1.06684900	-0.27577400	-0.42697400
C	-0.10979700	-1.18006000	-1.21970800
C	-0.42457100	0.29032800	0.84951700
O	-0.75243400	-2.09270000	-1.91337400
O	-1.32011400	0.66080000	1.73798100
C	0.05651600	-2.99789500	-2.72389700
H	-0.66012600	-3.70345700	-3.14073000
H	0.55800700	-2.43099200	-3.51099900
H	0.79078100	-3.49700900	-2.08994700
C	-0.81141000	1.27397400	2.95524300
H	-0.27748600	2.19278800	2.70601200
H	-1.69865000	1.48010600	3.55182400
H	-0.14456600	0.57736400	3.46644000
O	1.10873100	-1.03163200	-1.29782500
O	0.77995800	0.44983100	1.03214800
Ni	2.44236900	-0.43519100	0.17184700

O	2.09283900	-2.22077900	1.21311600
O	3.77755500	0.56298000	1.44931600
Cl	3.17869400	-3.04445300	0.45786700
Cl	4.11776000	1.67875700	0.42933700
O	4.16434700	-3.59048600	1.39456600
O	3.79746900	-1.95708000	-0.44618400
O	3.23793800	1.23404000	-0.77987000
O	3.67497800	2.99138500	0.92530900
O	2.53162300	-4.09235400	-0.35817600
O	5.53960200	1.65661500	0.07037600
C	-1.55346300	0.93075200	-1.41579900
H	-1.32655800	0.59835000	-2.43975200
C	-0.97012900	2.30196300	-1.18074100
C	-1.64748500	3.25188300	-0.40278900
C	0.26695000	2.63075800	-1.75132700
C	-1.08524600	4.51423500	-0.19748500
H	-2.61608700	3.00493000	0.01893700
C	0.83291400	3.88767000	-1.53140800
H	0.80174300	1.90469600	-2.35887600
C	0.15653800	4.83279700	-0.75600000
H	-1.62072800	5.25053700	0.39646100
H	1.80243300	4.12192100	-1.96021900
H	0.59608200	5.81206000	-0.58684600
O	-2.94450300	0.91014900	-1.19475700

TS1-Ni

O	-1.29118200	-1.77881400	-0.78714600
O	2.21651800	-1.02387600	2.02323100
O	0.17116100	-1.75771600	2.63564800
O	-0.83604600	0.20672900	0.94208100
C	0.25299700	-0.54325800	0.61179800
C	0.99229900	0.49069700	-0.23304800
C	-0.18252600	-1.75753800	-0.26563700
C	1.01579300	-1.12153400	1.83085400
C	0.72213700	-2.36141000	3.82419500
H	-0.12485600	-2.83463700	4.31957800
H	1.16430500	-1.59332200	4.46372900
H	1.48226900	-3.09938500	3.55460000
O	0.69082500	-2.74341000	-0.37779100
C	0.26042800	-3.90640600	-1.13688100
H	0.08067600	-3.62216300	-2.17587200
H	1.08501300	-4.61376100	-1.05836600
H	-0.65427800	-4.31270600	-0.70071900
C	3.57895300	-0.26181700	-0.35856900

H	3.65786900	0.44692500	0.47384100
O	2.48740300	-0.38862100	-0.94358300
C	4.77129300	-0.99476800	-0.74196900
C	4.76561200	-1.90469000	-1.81908300
C	5.95359500	-0.77119100	-0.01058000
C	5.93404400	-2.57844200	-2.15467300
H	3.84709500	-2.06434800	-2.37505100
C	7.12077000	-1.45237400	-0.35035300
H	5.94667900	-0.07195900	0.82193300
C	7.10909100	-2.35277100	-1.42113100
H	5.93924000	-3.27864000	-2.98495400
H	8.03387000	-1.28485700	0.21305300
H	8.01928900	-2.88308500	-1.68836800
H	0.53378100	0.56553400	-1.21451800
C	1.46745100	1.78104700	0.27005300
C	1.63600300	2.80873600	-0.68036900
C	1.74511600	2.07180600	1.62165200
C	2.08358800	4.06988500	-0.30126700
H	1.38870000	2.61910800	-1.72132300
C	2.17801300	3.33976300	1.99298100
H	1.60332000	1.32039600	2.38655300
C	2.35592500	4.36167400	1.04366900
H	2.19158200	4.84700600	-1.05353300
H	2.36917700	3.54751700	3.04333700
C	2.78390700	5.74358300	1.47176900
H	3.57495900	5.70245500	2.22943200
H	3.14781100	6.33340700	0.62453100
H	1.93890500	6.28791300	1.91431200
Ni	-2.46807900	-0.11645500	-0.16993600
Cl	-2.58259300	2.36967200	-1.33488800
Cl	-4.67280400	-1.67415600	0.27581300
O	-3.23458300	1.88904300	-0.02961700
O	-1.86120100	1.07773200	-1.82121200
O	-4.23973100	-0.95035900	-1.01855000
O	-3.56481900	-1.21673800	1.26109500
O	-1.58513300	3.42693900	-1.07168600
O	-3.59205600	2.79243300	-2.31595700
O	-5.99448900	-1.21251900	0.72478500
O	-4.62221400	-3.13837000	0.09493000
TS2-Ni			
O	1.29415700	-0.32159500	1.55861800
O	-1.77144400	-3.40774900	-0.11050200
O	-0.20697300	-3.33325400	1.51946200

O	0.50743500	-1.48849100	-0.68762500
C	-0.48200600	-1.34428800	0.24915900
C	-1.58337500	-0.39149300	-0.40604400
C	0.13427900	-0.72444100	1.53547600
C	-0.95557700	-2.79586700	0.53860100
C	-0.32213500	-4.75983100	1.69707000
H	0.37101400	-5.00560200	2.50151700
H	-0.04007500	-5.27180700	0.77379000
H	-1.34697700	-5.02672500	1.96838200
O	-0.65569900	-0.68850100	2.59872700
C	-0.05100600	-0.25887600	3.84435800
H	0.31462700	0.76646100	3.75211500
H	-0.84690800	-0.32939400	4.58535500
H	0.77819500	-0.92317000	4.09704200
C	-1.48349800	1.98102900	-0.07134900
H	-1.21353400	2.00891000	-1.12785100
O	-1.73252900	0.84780900	0.46098100
C	-1.57901900	3.19653100	0.67333400
C	-2.00631400	3.22865100	2.02166200
C	-1.22593100	4.39261100	0.00804900
C	-2.07813400	4.44489100	2.68485600
H	-2.28153300	2.30375300	2.51848400
C	-1.29614400	5.60552500	0.68563200
H	-0.88564700	4.35453100	-1.02328700
C	-1.72093700	5.62969300	2.01894000
H	-2.40889300	4.48312000	3.71842700
H	-1.01685200	6.52631700	0.18319900
H	-1.77516900	6.57744600	2.54782600
H	-1.11852000	-0.06073800	-1.33303100
C	-2.98730600	-0.87037600	-0.64254000
C	-3.43813600	-1.01827000	-1.95741900
C	-3.87292300	-1.13208200	0.41471700
C	-4.74554700	-1.44147700	-2.21219500
H	-2.76256900	-0.82279900	-2.78672600
C	-5.17694000	-1.54016600	0.15263500
H	-3.53956700	-1.02415500	1.44425600
C	-5.63581000	-1.70988600	-1.16593500
H	-5.07379400	-1.56384000	-3.24166400
H	-5.85071300	-1.74081100	0.98319700
C	-7.04433800	-2.18578400	-1.43588200
H	-7.77934900	-1.61536200	-0.85509500
H	-7.30301400	-2.09059500	-2.49541900
H	-7.16202900	-3.24183000	-1.15926400
Ni	2.10773300	-0.39354000	-0.38135800

Cl	1.43244000	1.59618000	-2.26791700
Cl	4.70563200	-0.97546300	0.22073100
O	2.21331200	0.33799800	-2.56051800
O	1.20283100	1.52785400	-0.72604200
O	3.99884500	0.40084500	0.11565300
O	3.54587300	-1.92807900	-0.16865500
O	0.08680200	1.57793900	-2.91582000
O	2.17518700	2.81527900	-2.61797900
O	5.81109300	-1.07135300	-0.74342800
O	5.14140500	-1.22787100	1.60590300

TS3/4-Ni

C	-2.05448700	-0.10393200	-1.01043900
C	-1.11961400	2.02321300	-0.11903500
H	-0.21476400	1.52046200	0.21427000
O	-2.03503000	1.35890700	-0.71330100
C	-1.29452200	3.42849100	0.07653000
C	-2.42942000	4.12198800	-0.41342200
C	-0.28997900	4.11881000	0.79425300
C	-2.54809400	5.48305900	-0.18169600
H	-3.19097500	3.58301800	-0.96765600
C	-0.42482100	5.48528200	1.02276000
H	0.58143100	3.57480900	1.14449600
C	-1.54705200	6.16262400	0.53565900
H	-3.41046000	6.02652400	-0.55607200
H	0.34596300	6.02213300	1.56690900
H	-1.64654900	7.23106900	0.70859000
H	-2.07129300	-0.10316700	-2.10133500
C	-3.38073800	-0.60588300	-0.48370200
C	-4.14001000	-1.48039100	-1.27082200
C	-3.89384000	-0.20552100	0.75920400
C	-5.36901400	-1.96147600	-0.81140400
H	-3.76570900	-1.79316800	-2.24129100
C	-5.12641800	-0.67802800	1.20432000
H	-3.33921600	0.48731500	1.38719100
C	-5.88526200	-1.57204100	0.43086900
H	-5.93922500	-2.64176700	-1.43983900
H	-5.50760100	-0.34519200	2.16769200
C	-7.21141300	-2.09567300	0.93179500
H	-7.83192700	-1.28959300	1.34099100
H	-7.77671700	-2.58461500	0.13181400
H	-7.06825000	-2.83245400	1.73347300
O	0.53379900	-0.96665300	1.40662100
O	-1.26325700	-2.24711900	-2.61186500

O	0.00437900	-3.10674300	-0.94742800
O	0.34829400	-0.09958900	-1.07842900
C	-0.71699600	-0.84860000	-0.66016300
C	-0.51300500	-1.25715100	0.82471200
C	-0.73786700	-2.16192000	-1.52104500
C	0.33047300	-4.26769400	-1.74447400
H	0.98755400	-4.86626000	-1.11554300
H	0.84741100	-3.95364000	-2.65361900
H	-0.58181100	-4.81286100	-1.99955800
O	-1.47226200	-1.96013600	1.39103000
C	-1.20496300	-2.48404800	2.71937900
H	-1.06541300	-1.66089400	3.42339200
H	-2.08745500	-3.07052900	2.97104300
H	-0.30770500	-3.10559400	2.69220600
Ni	1.99492200	-0.26993400	0.03400700
Cl	2.90869100	2.27458200	-0.52688600
Cl	3.80044500	-2.23452600	0.65408000
O	3.22164000	0.96787500	-1.25339000
O	2.00012700	1.78201200	0.64688200
O	3.61654000	-0.84316800	1.29680600
O	2.73881200	-2.18549400	-0.47695900
O	2.12846900	3.19489300	-1.38185100
O	4.12183100	2.90820200	0.00664200
O	5.15114600	-2.38984000	0.09622700
O	3.46449300	-3.30252700	1.61635000

TS5-Ni

C	6.27095500	-0.43446400	-0.11203000
C	5.48037300	-0.74387200	-1.23602100
C	4.22942400	-0.17005300	-1.40211800
C	3.73077300	0.73991400	-0.43541000
C	4.51512700	1.04067500	0.70939500
C	5.76639900	0.46816100	0.85206800
H	5.85473300	-1.44474200	-1.97806500
H	3.62040900	-0.42183100	-2.26985900
H	4.11784600	1.71431500	1.45975000
H	6.36908100	0.70327200	1.72464100
C	7.62988700	-1.05530800	0.07529300
H	7.65180800	-1.68326000	0.98071800
H	7.91189900	-1.67987200	-0.77956700
H	8.40013800	-0.27820000	0.20528400
C	2.47675800	1.35291400	-0.66536000
H	1.92496000	1.15264200	-1.58077700
O	1.97134200	2.27619100	0.15684700

C	0.70939300	1.64399200	0.34090600
C	-0.42338400	2.20003400	-0.35382000
C	0.59227000	0.60185500	1.32272100
O	-0.13145700	3.29171400	-1.06602100
O	1.69175500	0.38134900	2.05595000
C	-1.23377800	3.90260000	-1.78005300
H	-0.79374100	4.76181900	-2.28407200
H	-1.65618100	3.19721300	-2.49852400
H	-2.00801900	4.21500900	-1.07560900
C	1.61789200	-0.72684700	2.98970700
H	1.39333300	-1.65223000	2.45375500
H	2.60537900	-0.76725400	3.44989500
H	0.84765900	-0.53355900	3.73989700
O	-1.57817100	1.73542500	-0.33637000
O	-0.45073300	-0.04634400	1.53476700
Ni	-1.94016400	-0.22974400	0.15658500
O	-3.57036400	0.07384900	1.42531900
O	-1.63511200	-2.39817800	0.22352300
Cl	-4.64014300	0.00415900	0.29805500
Cl	-0.54368300	-2.38849300	-0.85077500
O	-5.58429400	-1.09343700	0.54464800
O	-3.74259500	-0.29852100	-0.92938100
O	-0.56727000	-0.90491500	-1.31888200
O	0.78330500	-2.69040400	-0.26332100
O	-5.31143300	1.30501700	0.14321600
O	-0.87024800	-3.28604900	-1.96620400

TS6-Ni

C	7.27759500	-1.21204900	0.08006800
C	6.90869600	-0.02172600	0.72405600
C	5.57311500	0.37293500	0.78651800
C	4.57446900	-0.42156900	0.20509200
C	4.93191900	-1.61500200	-0.44806700
C	6.26600100	-1.99868800	-0.50378800
H	7.67394600	0.59984900	1.18190400
H	5.30562500	1.29770400	1.29270900
H	4.16017600	-2.22703600	-0.90367700
H	6.53534300	-2.92316200	-1.00942100
C	8.72000200	-1.65209900	0.01577400
H	9.03367000	-1.82970200	-1.02020000
H	9.38970700	-0.90259400	0.44857600
H	8.86839900	-2.59192200	0.56286100
C	3.18549900	0.02301700	0.27037600
H	2.94877900	0.86507000	0.91282800

O	2.26919200	-0.93212600	0.17128400
C	0.91946200	-0.61964000	0.05832200
C	0.22973500	0.06598600	1.12035900
C	0.20557600	-1.45121700	-0.88565100
O	1.02084600	0.49176000	2.11537800
O	0.99276500	-2.21116500	-1.65177600
C	0.35435700	1.13253700	3.23483100
H	1.14798900	1.31919600	3.95801900
H	-0.10668900	2.06705600	2.90883500
H	-0.40740700	0.46839800	3.64728000
C	0.32136800	-3.05545800	-2.61843300
H	-0.26065500	-2.44665500	-3.31356200
H	1.12635600	-3.57834000	-3.13427100
H	-0.33839800	-3.76028100	-2.10774300
O	-0.98992200	0.30615200	1.14869800
O	-1.02923500	-1.47342900	-1.04113300
Ni	-2.48163700	-0.53705400	0.03773400
O	-2.77837500	-2.06908900	1.45007900
O	-3.92845100	-1.03932800	-1.46568300
Cl	-3.73831200	-1.24302000	2.35131700
Cl	-3.72233100	0.25095800	-2.27726500
O	-5.02253400	-1.93513400	2.51494700
O	-3.89984300	0.04537800	1.51396600
O	-2.71593500	1.02157100	-1.36662400
O	-3.09478800	-0.03618800	-3.58109700
O	-3.09083500	-0.94602800	3.64461400
O	-4.97311800	1.00864000	-2.41061200
C	1.67785600	1.34105700	-1.42200600
H	1.05597200	0.93044300	-2.22610600
C	1.19360600	2.54263100	-0.75178700
C	2.06425800	3.36621400	-0.00615100
C	-0.15931300	2.91000000	-0.89922700
C	1.58123000	4.52561400	0.59278800
H	3.11774700	3.10986000	0.05809700
C	-0.63791200	4.06703600	-0.28721400
H	-0.83857300	2.27950200	-1.46639400
C	0.22900600	4.87349600	0.45818000
H	2.25457900	5.16861400	1.15315000
H	-1.68513800	4.33476700	-0.39168900
H	-0.14434900	5.77979300	0.92780500
O	2.86279900	0.88193200	-1.30937800
TS7-Ni			
C	-6.95921300	-1.84341200	-0.02606600

C	-6.35566700	-1.58387900	-1.26519700
C	-4.99575000	-1.28563900	-1.35061800
C	-4.20959000	-1.24312700	-0.19193800
C	-4.80092600	-1.49905800	1.05579100
C	-6.15819300	-1.79426300	1.12974600
H	-6.95446300	-1.61901100	-2.17186100
H	-4.54567400	-1.09082400	-2.32178900
H	-4.19197000	-1.47100800	1.95372800
H	-6.60833500	-1.99301800	2.09972300
C	-8.42669300	-2.18462800	0.07344800
H	-8.92704200	-1.57009600	0.83130500
H	-8.94129100	-2.03309000	-0.88057100
H	-8.56609800	-3.23369200	0.36536500
C	-2.77735500	-0.92050200	-0.30496400
H	-2.33303200	-0.99711900	-1.29712100
O	-2.02504000	-1.32480100	0.70495900
C	-0.61669700	-1.18682100	0.58986000
C	0.07956500	-1.97554000	-0.35970600
C	0.03140300	-0.46557900	1.62745600
O	-0.70564100	-2.78380100	-1.11033200
O	-0.79192500	0.07103200	2.54493900
C	-0.02219500	-3.63230800	-2.06007600
H	-0.81569700	-4.19652400	-2.55114500
H	0.53544600	-3.03063100	-2.78161000
H	0.66588900	-4.30332500	-1.54144500
C	-0.15895000	0.83247500	3.59726500
H	0.40901400	1.66493800	3.17567900
H	-0.98379200	1.19271100	4.21305300
H	0.50712000	0.19270400	4.18107900
O	1.31607600	-1.96490500	-0.56486100
O	1.27159000	-0.31152400	1.74067000
Ni	2.55949400	-0.56789700	0.20790400
O	3.93891400	-1.89870200	1.06647200
O	3.50340100	1.35964900	0.70305900
Cl	4.81081900	-2.04046600	-0.21081400
Cl	2.50437400	2.19254000	-0.09051000
O	6.18962500	-1.60222600	0.04973200
O	4.09036800	-1.06194400	-1.17000500
O	1.64479700	1.10586300	-0.79946000
O	1.64188200	2.99388300	0.80828600
O	4.74783900	-3.41826100	-0.72940800
O	3.16892400	3.03798800	-1.09811000
C	-1.85039400	1.47639000	-0.81881700
H	-1.13988400	0.92431300	-1.44534700

C	-1.70205500	2.90430200	-0.73182600
C	-2.56476700	3.69036800	0.06648800
C	-0.67261300	3.51319600	-1.48049600
C	-2.39250800	5.06624800	0.10455600
H	-3.34789400	3.20666300	0.64174500
C	-0.51006400	4.89478900	-1.43692300
H	0.00394700	2.89767400	-2.06626500
C	-1.36687700	5.66634400	-0.64625100
H	-3.04563100	5.68026500	0.71772000
H	0.29275700	5.36387400	-1.99680900
H	-1.23361300	6.74414600	-0.60422100
O	-2.76913900	0.84909500	-0.22724200

Ni-1H₂O path

IM1a

O	-0.50995600	-1.86881600	-0.38155800
O	2.18071600	0.01410700	2.53452700
O	0.06511000	0.54037800	3.15881800
O	-0.73882300	0.63616200	0.50674300
C	0.42530100	-0.10500000	0.91487700
C	0.51763100	0.93169600	-0.16546600
C	0.32936800	-1.54301800	0.45736800
C	1.00137000	0.16042500	2.29371100
C	0.51049600	0.81048300	4.50855300
H	-0.38888600	1.10423000	5.04808400
H	1.24736600	1.61716100	4.50277700
H	0.95015200	-0.09085900	4.94213100
O	1.16412600	-2.37474700	1.02887700
C	1.06926200	-3.77084900	0.62390300
H	1.36121900	-3.86007000	-0.42426700
H	1.76980600	-4.29345500	1.27303400
H	0.04677800	-4.12468800	0.76766200
C	3.97779100	-0.93328400	-0.35730000
H	3.85693400	-0.69947800	0.71793400
O	3.00540600	-0.88692300	-1.10256700
C	5.34532000	-1.28820600	-0.78470700
C	5.62753200	-1.61265900	-2.12373900
C	6.37447900	-1.30196800	0.17064100
C	6.92647700	-1.94733700	-2.49676500
H	4.81955600	-1.59648700	-2.84954500
C	7.67623000	-1.63773700	-0.20524600
H	6.14892600	-1.04857500	1.20459200
C	7.95036700	-1.96029600	-1.53817400
H	7.14850600	-2.19900500	-3.53032600

H	8.47237800	-1.64833300	0.53402300
H	8.96306700	-2.22253800	-1.83356300
H	0.56821800	0.53007000	-1.17445800
C	1.08696400	2.28923300	0.03729800
C	2.19532300	2.67316500	-0.72960000
C	0.53616000	3.19745400	0.95177400
C	2.75536700	3.94020600	-0.56604300
H	2.62092900	1.97915400	-1.45007300
C	1.09925500	4.46483400	1.09904700
H	-0.34475100	2.92166800	1.52317400
C	2.21786100	4.85868400	0.34811300
H	3.61830900	4.22219800	-1.16506600
H	0.65337700	5.16451200	1.80259400
C	2.79920000	6.24580100	0.49323800
H	2.75965800	6.59063200	1.53258500
H	3.84269600	6.28020700	0.16263400
H	2.23809000	6.97102900	-0.11139100
Ni	-2.22167400	-0.58962000	-0.45995300
Cl	-3.59224900	-2.67600500	0.61317800
O	-3.58582100	0.90663800	-0.22485900
O	-3.44692300	-2.23714100	-0.87061800
O	-2.82549400	-1.53512700	1.33506100
O	-3.24857600	2.06602100	-2.38038500
O	-4.92688600	2.86568700	-0.77825300
O	-4.99964200	-2.70562200	1.01618500
O	-2.90854800	-3.96436200	0.83595400
O	-1.68671400	-0.06626500	-2.38367000
H	-1.94419000	-0.75151700	-3.02266300
H	-2.22732600	0.74962800	-2.59376300
Cl	-4.31654200	1.66852000	-1.37153900
O	-5.29485400	0.76143100	-2.00352800
IM1b			
O	-1.17610500	-1.66985600	-0.45114300
O	1.69272400	-0.85900200	2.78386800
O	-0.34639000	-0.13372300	3.45933900
O	-0.94425900	0.66303200	0.85168100
C	0.03159500	-0.35841200	1.13471400
C	0.39033200	0.80605600	0.26438700
C	-0.31606000	-1.65121100	0.42808100
C	0.56829200	-0.47407400	2.55018000
C	0.06191100	-0.24363800	4.84287000
H	-0.81029800	0.06044500	5.42029700
H	0.91094800	0.41685300	5.03502600

H	0.33872300	-1.27621500	5.06816500
O	0.33598000	-2.70836900	0.84240400
C	0.02415800	-3.96571700	0.17702500
H	0.31939700	-3.89831700	-0.87170000
H	0.61524800	-4.71108300	0.70647800
H	-1.04509500	-4.16893300	0.26022500
C	3.47991200	-1.50244700	-0.24263000
H	3.41225300	-1.51735100	0.86288100
O	2.48650600	-1.23859400	-0.90864700
C	4.80825600	-1.81191600	-0.80774800
C	5.01653600	-1.82977500	-2.19844300
C	5.87328700	-2.09150100	0.06346100
C	6.27903400	-2.12508700	-2.70601900
H	4.18137000	-1.61062800	-2.85753400
C	7.13830800	-2.38723200	-0.44735500
H	5.70505900	-2.07485900	1.13851000
C	7.33937100	-2.40375400	-1.83134700
H	6.44377400	-2.13953200	-3.78001700
H	7.96256000	-2.60320300	0.22686900
H	8.32344900	-2.63369200	-2.23181800
H	0.40418100	0.59273400	-0.80067200
C	1.20829400	1.96175400	0.70979500
C	2.30392200	2.33914000	-0.07937800
C	0.91456200	2.69509200	1.86695300
C	3.10433900	3.41552800	0.29985800
H	2.52413900	1.79259500	-0.99253500
C	1.71691200	3.77629700	2.23204900
H	0.04694600	2.43746200	2.46727400
C	2.82567600	4.15453700	1.45983700
H	3.95053100	3.69440100	-0.32405100
H	1.47147300	4.34195400	3.12828700
C	3.67230500	5.34647200	1.84101400
H	3.57894300	5.58106500	2.90671500
H	4.73177700	5.17186700	1.62228300
H	3.36714500	6.23961800	1.27929600
Ni	-2.55019400	-0.07538200	-0.40305600
Cl	-1.76629700	1.99565500	-2.79634300
Cl	-4.45688900	-1.85193400	0.40775100
O	-2.16321100	2.98473100	-1.72102700
O	-1.66328900	0.59250900	-2.11388000
O	-4.12332200	-1.37029600	-1.01858000
O	-3.46061900	-0.99708100	1.25472900
O	-0.41907600	2.31213000	-3.30531000
O	-2.78692200	1.93272200	-3.85538300

O	-5.84159500	-1.52647600	0.77191500
O	-4.14720900	-3.28307500	0.56886700
O	-3.77036800	1.54787800	-0.14401100
H	-3.91765800	1.79312900	0.78308300
H	-3.34367900	2.30619600	-0.61783600

IM1c

O	-0.85385600	-1.57508800	-0.90961900
O	1.77628200	-0.53606100	2.40949700
O	-0.31085700	0.09040100	3.03466200
O	-0.98503300	0.72136800	0.43558300
C	0.12730300	-0.14219400	0.72432200
C	0.31327200	1.09984500	-0.10098900
C	0.01774800	-1.44043100	-0.04388200
C	0.63430900	-0.21745700	2.15388900
C	0.06143300	0.00256100	4.42940600
H	-0.83965200	0.27227500	4.97858200
H	0.87689700	0.69792400	4.64309200
H	0.37010900	-1.01835100	4.66539100
O	0.89395200	-2.35588700	0.26138100
C	0.77065300	-3.63672700	-0.41894500
H	0.89293600	-3.49120600	-1.49376900
H	1.57553100	-4.24376200	-0.00804400
H	-0.20675300	-4.06494000	-0.19188200
C	3.74717700	-0.80326200	-0.52593000
H	3.51091700	-0.81750200	0.55517800
O	2.90516500	-0.41794500	-1.32862100
C	5.09871400	-1.27397700	-0.89124200
C	5.51854100	-1.30774800	-2.23290200
C	5.97004100	-1.69662800	0.12550200
C	6.79686000	-1.76077200	-2.54811200
H	4.83129500	-0.97680600	-3.00627400
C	7.25140200	-2.15047000	-0.19237300
H	5.63857700	-1.66699000	1.16154700
C	7.66300900	-2.18229400	-1.52858400
H	7.12461500	-1.78848000	-3.58386200
H	7.92551400	-2.47738300	0.59459200
H	8.66016600	-2.53550200	-1.77877600
H	0.40401900	0.92829300	-1.17066900
C	0.91866100	2.35505800	0.41464700
C	0.37263200	3.05329200	1.49920700
C	2.05912000	2.86138400	-0.22568700
C	0.97088300	4.23474600	1.93928700
H	-0.52769200	2.68470400	1.98054600

C	2.65239300	4.03788800	0.22905200
H	2.48158400	2.32941200	-1.07408900
C	2.11910100	4.74664900	1.31725200
H	0.53076300	4.77321400	2.77568400
H	3.53888700	4.41658900	-0.27505200
C	2.74362600	6.04342600	1.77720900
H	3.83699700	6.00769800	1.71161000
H	2.40748000	6.88341800	1.15439200
H	2.47230000	6.27397100	2.81285100
Ni	-2.45229900	-0.26392800	-0.79412900
Cl	-3.16216100	1.94285900	-2.23603100
Cl	-3.21007800	-2.48377500	1.40113400
O	-3.82258300	1.32701100	-0.97152800
O	-1.95606800	0.98335800	-2.42904900
O	-3.74740200	-3.27013400	0.23117100
O	-3.20441800	-0.98681500	0.98754900
O	-2.69823300	3.31066700	-1.97291000
O	-4.08035600	1.85436900	-3.38204400
O	-4.07720100	-2.61791200	2.57958400
O	-1.80715600	-2.89207000	1.69061700
O	-3.65640600	-1.52975400	-1.89177500
H	-4.50434400	-1.10815500	-2.11248000
H	-3.85562400	-2.27424600	-1.27243500
IM1d			
O	-1.08923900	-1.46734600	0.16657900
O	2.17231200	0.04859400	2.65541800
O	0.32526100	1.20766800	3.27273300
O	-0.66168000	1.11302800	0.67754600
C	0.32958500	0.18026800	1.13831500
C	0.57899000	1.02956400	-0.07581600
C	-0.11085800	-1.24198100	0.88123500
C	1.05693600	0.46929000	2.43767100
C	0.94961000	1.53996000	4.53492800
H	0.20913500	2.13389300	5.06944300
H	1.86138800	2.11573500	4.35918300
H	1.18895500	0.62677600	5.08489200
O	0.59199000	-2.17684300	1.46607900
C	0.19125500	-3.55444900	1.19736800
H	0.40528900	-3.78672600	0.15256800
H	0.80260800	-4.15338500	1.87003900
H	-0.87410100	-3.67783700	1.39725100
C	3.55682400	-1.57753000	-0.20024000
H	3.57661100	-1.26598000	0.86215400

O	2.56130400	-1.35590000	-0.87940900
C	4.77519500	-2.24796300	-0.69525700
C	4.86461300	-2.69853000	-2.02451200
C	5.85580400	-2.43546200	0.18165200
C	6.02501000	-3.32859900	-2.46602300
H	4.01871100	-2.54609800	-2.68862600
C	7.01854200	-3.06713000	-0.26298000
H	5.77994300	-2.08378000	1.20868700
C	7.10144800	-3.51305700	-1.58598000
H	6.09746100	-3.67851400	-3.49224000
H	7.85485800	-3.21179300	0.41539900
H	8.00545500	-4.00580200	-1.93465500
H	0.47036300	0.51222800	-1.02553000
C	1.45936400	2.22657900	-0.07818600
C	2.56433900	2.24239100	-0.94129700
C	1.20751700	3.33955900	0.73377700
C	3.41245100	3.34811500	-0.97316400
H	2.75908900	1.38761400	-1.58378700
C	2.05858400	4.44426900	0.68661300
H	0.33483300	3.35057600	1.37916400
C	3.17427400	4.46963000	-0.16329700
H	4.26708300	3.34424400	-1.64608900
H	1.84345800	5.30744500	1.31266400
C	4.07018300	5.68407900	-0.23804900
H	4.02868800	6.27117000	0.68560400
H	5.11403700	5.40267800	-0.41649700
H	3.76568200	6.34496800	-1.06086100
Ni	-2.44433700	0.07712700	-0.11189500
Cl	-2.79952600	2.01417000	-1.98673500
Cl	-4.43995600	-2.43874500	-0.04454700
O	-3.41194300	1.87686400	-0.56239000
O	-1.94180400	0.71842100	-2.05347000
O	-4.00109200	-1.10813300	-0.72144700
O	-4.52835800	-2.16493200	1.44966100
O	-1.93185800	3.20095900	-2.05549700
O	-3.84668900	2.00768600	-3.01022600
O	-5.76154100	-2.78568700	-0.58261800
O	-3.42380200	-3.48137900	-0.30232600
O	-3.01104400	-0.02645300	1.87718900
H	-3.52390100	0.76279700	2.11892000
H	-3.64555600	-0.79838000	1.89405900
IM6a			
C	5.59534300	0.32853400	-0.41767400

C	4.86111900	1.00551000	0.56700100
C	3.73674800	0.42430100	1.15437700
C	3.30955700	-0.84897600	0.75416600
C	4.03489100	-1.53804700	-0.22805800
C	5.16443500	-0.95272300	-0.79896000
H	5.17121900	1.99946200	0.87993500
H	3.18561900	0.97049200	1.91704600
H	3.71584200	-2.52973200	-0.53222700
H	5.72381100	-1.50271100	-1.55307200
C	6.81891500	0.95031900	-1.04998400
H	6.69781000	1.04922800	-2.13603900
H	7.01693000	1.94723800	-0.64369300
H	7.71076200	0.33430100	-0.87906400
C	2.12020500	-1.45202700	1.41648200
H	2.07666500	-1.33215700	2.50150400
O	1.61477800	-2.70003100	0.96146500
C	0.75596500	-1.59678300	0.76582200
C	-0.43913800	-1.48648500	1.68351900
C	0.54731700	-1.10129600	-0.64367300
O	-0.50320000	-2.46286800	2.55860700
O	1.13927500	-1.82975400	-1.55267100
C	-1.62764700	-2.44657300	3.47920200
H	-1.48724300	-3.32973500	4.10012300
H	-1.60547000	-1.53285300	4.07648100
H	-2.55774400	-2.50584200	2.91112200
C	0.95622500	-1.42236900	-2.94195100
H	1.39146600	-0.43218500	-3.08959800
H	1.48753700	-2.17809400	-3.51789300
H	-0.10972700	-1.41427300	-3.17463100
O	-1.23392300	-0.54517500	1.67570900
O	-0.08876900	-0.07906200	-0.90940300
Ni	-1.53928500	0.84580300	0.19493100
O	-3.10573900	-0.14903900	-0.65247400
O	-1.47309300	2.60201000	-1.06473600
Cl	-0.72187700	3.43917100	-0.01447000
O	-2.10030400	-2.40275500	-0.49701700
O	-0.21832400	2.34600800	0.95891000
O	0.39140800	4.18851600	-0.60070400
O	-4.43044700	-2.10944300	-1.22519800
O	-1.69070500	4.31340800	0.69974000
Cl	-3.05853800	-1.57732300	-1.29945900
O	-2.57884100	-1.43441300	-2.69411700
O	-3.10715900	1.73264300	1.28097600
H	-3.05568900	2.70926400	1.25725600

H	-3.91801000	1.47302600	0.80718200
IM6b			
C	5.28945500	-0.64335700	-1.26933100
C	4.53521100	0.53625200	-1.39121700
C	3.55907100	0.86784400	-0.45410100
C	3.30211300	0.01151300	0.62858700
C	4.04333300	-1.16860600	0.76164000
C	5.02610700	-1.48519900	-0.17954100
H	4.71749100	1.20534500	-2.22927500
H	2.98190000	1.78177800	-0.57137800
H	3.85620700	-1.82753600	1.60364100
H	5.60142900	-2.40051200	-0.05967700
C	6.36883400	-0.97543400	-2.27338000
H	6.70031100	-2.01449300	-2.17737800
H	6.01942900	-0.82398300	-3.30143400
H	7.24812100	-0.33286700	-2.13294900
C	2.27204600	0.40466200	1.62938700
H	2.27566900	1.45326000	1.93136900
O	1.93923700	-0.49550100	2.68082300
C	0.91245600	-0.25623000	1.74084100
C	-0.24314400	0.60949400	2.18100900
C	0.55594700	-1.36086300	0.77464100
O	-0.06020300	1.15904600	3.36011200
O	1.07242800	-2.52326700	1.08058000
C	-1.08874000	2.08723300	3.81189100
H	-0.73557500	2.43586800	4.78079000
H	-1.17744200	2.90793200	3.09752800
H	-2.04036000	1.56049300	3.90256800
C	0.75494800	-3.64084700	0.19646800
H	1.20790400	-3.46372500	-0.78114300
H	1.20021600	-4.50653700	0.68362800
H	-0.32834000	-3.73521600	0.11022300
O	-1.24296700	0.81169800	1.49356900
O	-0.14072800	-1.17139400	-0.22475600
Ni	-1.43919300	0.41714800	-0.54120900
O	-3.17321300	-0.60140100	-0.14877100
O	-2.20491500	2.42118000	-0.77406600
Cl	-0.81931100	3.06120900	-0.94325200
O	-2.59568700	-2.90617300	0.53030800
O	0.10742100	1.80179200	-0.93101100
O	-0.70172600	3.76335200	-2.22709200
O	-4.82675900	-2.38134200	-0.34344500
O	-0.48665800	3.92266300	0.20837400

Cl	-3.38626400	-2.11300800	-0.44676900
O	-2.88130000	-2.36697300	-1.84879000
O	-1.62975800	-0.04563900	-2.53827900
H	-0.78420700	-0.13430200	-3.00603200
H	-2.07779900	-0.92817900	-2.54807800

IM6c

C	5.43378400	-0.55533000	-1.04178500
C	4.29978000	-0.85615900	-1.81523500
C	3.14795200	-0.07932300	-1.73524200
C	3.09406900	1.01566600	-0.85798500
C	4.21816900	1.33058700	-0.08499500
C	5.37288400	0.55138500	-0.18323200
H	4.31869100	-1.71162500	-2.48649600
H	2.28062100	-0.33471500	-2.33838300
H	4.19006000	2.18815900	0.57929000
H	6.24296600	0.81241500	0.41510400
C	6.68120100	-1.40087100	-1.14720100
H	6.46624100	-2.45264900	-0.92136500
H	7.09807700	-1.36747400	-2.16183300
H	7.45748100	-1.05910100	-0.45499000
C	1.87103300	1.85852600	-0.83963400
H	1.43318700	2.06707900	-1.81807100
O	1.77465500	2.94182200	0.06702400
C	0.82430800	1.91215700	0.27810600
C	-0.59313100	2.21861800	-0.14312300
C	0.96589000	1.05885900	1.51188100
O	-0.70280500	3.33338800	-0.82751200
O	2.08298900	1.26794400	2.16956300
C	-2.03126600	3.66660700	-1.33801000
H	-1.85657500	4.48195700	-2.03780600
H	-2.47952100	2.79634700	-1.81885000
H	-2.65690200	3.99337100	-0.50483100
C	2.35207400	0.38700400	3.29637900
H	2.34728500	-0.64998600	2.95588900
H	3.33727400	0.68626800	3.64976100
H	1.59463200	0.53674400	4.06818100
O	-1.55703600	1.49000600	0.10021700
O	0.11841800	0.24215900	1.88182500
Ni	-1.46530200	-0.49645400	0.68561400
O	-4.75210800	0.31084600	0.45855200
O	-0.83553200	-2.48614100	1.06596100
Cl	-4.27912800	-0.29491200	-0.84878500
Cl	0.25403200	-2.49801500	-0.02599400

O	-5.27629500	-1.23110100	-1.38497900
O	-2.99813900	-1.11505900	-0.52913000
O	0.02508300	-1.10826700	-0.69277300
O	1.59824200	-2.54135200	0.58338400
O	-3.94260500	0.77971600	-1.81295000
O	0.03820400	-3.57835300	-0.99235100
O	-2.80585100	-0.26457600	2.23224400
H	-2.61720700	0.47570300	2.82979200
H	-3.65946300	-0.05662600	1.76650000

IM6d

C	-6.08801400	0.80944000	-0.18715200
C	-5.44669200	0.42981800	-1.37789400
C	-4.34866300	-0.42790100	-1.36015900
C	-3.84977100	-0.91751700	-0.14303300
C	-4.48680500	-0.55503700	1.05028300
C	-5.59410200	0.29422600	1.02049800
H	-5.81735500	0.80326100	-2.32974700
H	-3.88047000	-0.72102000	-2.29811100
H	-4.12076300	-0.94762300	1.99309700
H	-6.08621800	0.55694000	1.95418100
C	-7.26644100	1.75440000	-0.20978700
H	-6.93008900	2.79855800	-0.26444500
H	-7.90832800	1.57414700	-1.07919400
H	-7.87857700	1.65328600	0.69234900
C	-2.70002300	-1.86139200	-0.16657800
H	-2.73837300	-2.62286900	-0.94889200
O	-2.13703900	-2.32593800	1.04524900
C	-1.27201200	-1.52403600	0.26271300
C	-0.17285800	-2.24191900	-0.48979500
C	-0.94794300	-0.13659200	0.76002300
O	-0.32338300	-3.54664600	-0.48092400
O	-1.59734600	0.20068600	1.84495500
C	0.69467700	-4.33388100	-1.16820900
H	0.40433700	-5.36766100	-0.98929000
H	0.68064300	-4.09738300	-2.23418200
H	1.67285700	-4.11033700	-0.73989700
C	-1.33525100	1.53770400	2.37556100
H	-1.64502600	2.28601700	1.64527500
H	-1.93251400	1.58923700	3.28394800
H	-0.27046300	1.64605700	2.58286600
O	0.72840700	-1.67387300	-1.10835700
O	-0.17035400	0.62176000	0.17755800
Ni	1.71099300	0.12487900	-0.55894200

O	2.21842400	-0.86266800	1.24196200
O	2.61448600	1.87760700	-0.00295000
Cl	3.53687800	-1.48013700	0.69194200
Cl	1.99844100	3.29955900	-0.14077300
O	4.68828900	-1.05652900	1.49075900
O	3.57711600	-0.87512400	-0.72828300
O	1.33299300	3.36019300	-1.50297200
O	0.98947800	3.50024800	0.92389700
O	3.40500900	-2.95122700	0.62282300
O	3.10364000	4.26364200	-0.05467000
O	1.47589300	0.85934800	-2.46405000
H	0.65023100	0.59225900	-2.89715000
H	1.43036100	1.84463100	-2.32910400

IM7a

C	7.37996500	-0.48257400	0.03421400
C	6.94455600	0.04125200	1.26229900
C	5.58883600	0.15351400	1.55090200
C	4.62319100	-0.26043200	0.60750700
C	5.05465600	-0.78797500	-0.63412300
C	6.40866000	-0.89349700	-0.90440600
H	7.67738200	0.36416200	1.99691100
H	5.26881900	0.56265200	2.50610800
H	4.31692200	-1.10372300	-1.36521700
H	6.73258000	-1.29885000	-1.86003900
C	8.84728700	-0.60342600	-0.28846800
H	9.10733800	0.00675300	-1.16295700
H	9.47339800	-0.27903500	0.54791800
H	9.11288100	-1.64006300	-0.53091000
C	3.24221000	-0.12578500	0.95048400
H	2.92030300	0.28992300	1.89878300
O	2.34997000	-0.51373500	0.11209300
C	0.97805100	-0.52144800	0.12023800
C	0.41516400	-0.95527700	-1.13056800
C	0.17931500	-0.01921900	1.19659200
O	1.31404800	-1.38083100	-2.02805500
O	0.86856200	0.43916200	2.25489000
C	0.78846000	-1.76956400	-3.31755700
H	1.66276500	-2.06974700	-3.89510200
H	0.09018100	-2.60207100	-3.20686600
H	0.28262800	-0.92342300	-3.78770200
C	0.07650200	1.06820500	3.30186500
H	-0.59579000	0.33384300	3.74923400
H	0.80972800	1.42052400	4.02723700

H	-0.49368700	1.89550400	2.87605900
O	-0.79716200	-0.95832400	-1.41220500
O	-1.06347000	0.00426600	1.21480300
Ni	-2.34612200	-0.20821000	-0.33263900
O	-2.31865200	1.73225600	-0.99897800
O	-4.08754700	-0.02262400	0.96592700
Cl	-4.41150000	-1.52343800	0.90613300
O	0.08902800	2.26090000	-0.92540400
O	-3.09705400	-2.11876300	0.36429800
O	-4.74775300	-2.06636900	2.22616700
O	-1.55701700	3.96620200	-1.58560100
O	-5.49496000	-1.74947300	-0.09367600
Cl	-1.26410800	2.84232100	-0.67464400
O	-1.41156700	3.22279000	0.75307700
O	-3.66848300	-0.36539800	-1.97347300
H	-4.51481200	-0.77319800	-1.69750800
H	-3.85852000	0.56252200	-2.20215200

IM7b

C	-6.93897500	-2.32213800	-0.19231400
C	-6.65095200	-0.95257800	-0.32170000
C	-5.34204300	-0.49105200	-0.25342800
C	-4.28173300	-1.40278100	-0.04627200
C	-4.56255000	-2.78624000	0.08047500
C	-5.87216700	-3.22692800	0.00968600
H	-7.46261600	-0.24744600	-0.47859200
H	-5.12301200	0.56922900	-0.35064300
H	-3.74686200	-3.48747600	0.22625200
H	-6.08719600	-4.28836900	0.10481500
C	-8.35476400	-2.83068400	-0.27054100
H	-8.63527700	-3.34891400	0.65524600
H	-9.06858000	-2.01864400	-0.43572900
H	-8.46558200	-3.55446800	-1.08786600
C	-2.96492300	-0.87123100	0.03676900
H	-2.77246900	0.19615600	-0.10178800
O	-1.97302000	-1.64003200	0.31581300
C	-1.53459200	2.93871600	0.05425800
H	-0.55122100	2.46692500	-0.13042500
C	-1.49986500	4.39367400	0.26274900
C	-2.67192700	5.11677000	0.55371000
C	-0.26534000	5.05914400	0.16657900
C	-2.60488000	6.49269300	0.74812300
H	-3.61603900	4.58443100	0.62459600
C	-0.20459100	6.44064600	0.36033500

H	0.63548400	4.49646100	-0.06702800
C	-1.37079500	7.15433300	0.65143300
H	-3.50604500	7.05615100	0.97525000
H	0.74844600	6.95638900	0.28412900
H	-1.32269900	8.22969400	0.80381600
O	-2.55364400	2.24959800	0.07543400
C	-0.65118500	-1.14070100	0.24685400
C	-0.20908300	-0.52659000	-0.95621100
C	0.19603200	-1.53930800	1.31756800
O	-1.14981900	-0.42006700	-1.91808500
O	-0.41660300	-2.26180400	2.26450700
C	-0.70565200	0.09626000	-3.19411600
H	-1.59925600	0.09994600	-3.81845300
H	-0.30633900	1.10579900	-3.07726100
H	0.06245500	-0.55559700	-3.61598400
C	0.42890700	-2.81338900	3.29831600
H	0.87808100	-2.01056100	3.88832500
H	-0.24174100	-3.41255000	3.91450700
H	1.20782300	-3.43376000	2.85025300
O	0.94634900	-0.11160600	-1.17577900
O	1.40628200	-1.24170100	1.43298900
Ni	2.57446300	-0.39443900	0.00348600
O	2.97841500	-2.14480600	-1.04892100
O	3.63697200	1.06569000	-1.23119500
Cl	3.25554200	2.26260500	-0.35666700
O	1.75142100	-3.99409700	0.03768200
O	2.45204900	1.59411300	0.79010700
O	4.44671900	2.94228800	0.17730300
O	3.66457900	-4.45389400	-1.42598800
O	2.37317100	3.19777100	-1.09346400
Cl	3.09877900	-3.55128500	-0.40933000
O	4.02505400	-3.43028300	0.77990500
O	4.25854000	-0.72998400	1.16757600
H	4.10868100	-0.43801500	2.08081700
H	4.35030100	-1.71472100	1.18337300
IM7c			
C	-1.36835000	2.19757500	-0.13739800
H	-0.54267000	1.64041400	0.33720400
C	-1.25970400	3.66357800	-0.05639200
C	-2.25289400	4.50484000	-0.59033000
C	-0.12950300	4.21773800	0.56889800
C	-2.11312500	5.88620700	-0.49676800
H	-3.11926900	4.05825100	-1.06977000

C	0.00737000	5.60415600	0.65961400
H	0.63803300	3.56314300	0.97500300
C	-0.98287000	6.43546400	0.12793900
H	-2.87740300	6.54095200	-0.90726200
H	0.88253100	6.03220400	1.14003200
H	-0.87668300	7.51517800	0.19746500
O	-2.28919700	1.59089300	-0.68409300
C	-7.13333500	-1.15889900	-0.27598700
C	-6.58223700	-0.50267100	-1.38842000
C	-5.20815000	-0.49143200	-1.60234100
C	-4.34399200	-1.14271200	-0.69729100
C	-4.89087500	-1.80511100	0.42758900
C	-6.26158100	-1.80814200	0.62500200
H	-7.23853500	0.00596500	-2.08952400
H	-4.79245800	0.03123400	-2.45965900
H	-4.22868400	-2.30503500	1.12761700
H	-6.67652400	-2.31879500	1.49076100
C	-8.62134600	-1.17317200	-0.03552700
H	-8.86848000	-0.68717900	0.91700400
H	-9.16442700	-0.65408900	-0.83076700
H	-9.00080300	-2.20114700	0.02149600
C	-2.93980500	-1.09859300	-0.95883200
H	-2.53842900	-0.61320200	-1.83838500
O	-2.13662900	-1.67227800	-0.13941500
C	-0.75131200	-1.74253100	-0.13313300
C	0.07085800	-1.48055600	-1.26996400
C	-0.20922500	-2.18999600	1.11662700
O	-0.58054300	-1.26764100	-2.42559700
O	-1.11879700	-2.52193000	2.04029000
C	0.24716300	-1.01783100	-3.59649900
H	-0.45106900	-0.67596600	-4.36038100
H	1.00666500	-0.26776500	-3.37478200
H	0.73229100	-1.94737600	-3.90301700
C	-0.60270600	-2.86540400	3.34962300
H	-0.01483400	-2.03611700	3.74781200
H	-1.48990600	-3.04532300	3.95682800
H	0.01305400	-3.76564800	3.28857600
O	1.31944400	-1.47244700	-1.25034400
O	1.01218000	-2.28831100	1.36600500
Ni	2.42906200	-1.10418900	0.42784400
O	4.67672800	-1.60236200	-2.08418100
O	3.13146700	-0.39572700	2.35463100
Cl	4.38913100	-0.12063500	-1.94425600
Cl	2.07240700	0.70401100	2.48579400

O	5.63068200	0.66347700	-2.04612700
O	3.81556700	0.10086400	-0.52149300
O	1.34290400	0.60871600	1.11625600
O	1.12179800	0.39577800	3.57648500
O	3.38416000	0.29946600	-2.95074200
O	2.68096300	2.03324900	2.64362300
O	3.67874100	-2.72590400	0.16783300
H	3.17058700	-3.53222500	-0.01367100
H	4.17507900	-2.49936600	-0.66186600

IM7d

C	-2.02456300	2.93751400	0.43256300
H	-2.02555200	2.67988500	1.51180100
C	-0.82895500	3.66673500	-0.03305400
C	-0.72715900	4.12234600	-1.35959500
C	0.22610600	3.89165400	0.86665300
C	0.42095000	4.78972200	-1.77827800
H	-1.55426500	3.94501600	-2.04092900
C	1.38004200	4.55589000	0.44368300
H	0.14448200	3.54019600	1.89318000
C	1.47581000	5.00360100	-0.87920700
H	0.50325900	5.14241600	-2.80259800
H	2.19637400	4.72829700	1.13981100
H	2.37339900	5.51849000	-1.21102000
O	-2.97115300	2.61215900	-0.27299900
C	-7.34618000	-1.35306000	0.91031500
C	-7.17013100	-0.69143200	-0.31606200
C	-5.90078300	-0.33940300	-0.76103400
C	-4.76483700	-0.64164700	0.02045200
C	-4.93383400	-1.30795200	1.25850500
C	-6.20492400	-1.65244500	1.68606100
H	-8.03796000	-0.45158600	-0.92448900
H	-5.77893900	0.17778000	-1.70930600
H	-4.06287200	-1.54511500	1.86139700
H	-6.32891200	-2.16575000	2.63656200
C	-8.71775300	-1.74539700	1.39639300
H	-8.92429900	-1.31133200	2.38266700
H	-9.50105700	-1.41427600	0.70831800
H	-8.79805900	-2.83482500	1.50284000
C	-3.48383600	-0.25407100	-0.47772000
H	-3.36672700	0.23070000	-1.43928800
O	-2.43948000	-0.49828700	0.22745400
C	-1.10295100	-0.21934400	0.00153800
C	-0.54696800	0.03470300	-1.29140900

C	-0.29469500	-0.33284400	1.18397700
O	-1.42900400	0.02053300	-2.30682600
O	-0.97361400	-0.58911800	2.30848600
C	-0.86573300	0.11364900	-3.64341100
H	-1.72219900	0.01433600	-4.31027900
H	-0.38007300	1.08276300	-3.77375200
H	-0.14547600	-0.69140300	-3.79807300
C	-0.17116500	-0.77706800	3.50503500
H	0.33205000	0.15470700	3.77047200
H	-0.88851900	-1.06705300	4.27259800
H	0.57896000	-1.55214500	3.34323300
O	0.65797400	0.25839700	-1.51380700
O	0.94106900	-0.17798200	1.21697900
Ni	2.23140100	-0.44967200	-0.35163800
O	1.58084300	-2.43101600	-0.81385600
O	3.79446300	-1.10980700	0.83829200
Cl	2.39324000	-2.53629000	-2.12947300
Cl	4.19307400	-0.53978600	2.22154300
O	3.29493700	-3.69368900	-2.10059500
O	3.17881000	-1.21062600	-2.11751600
O	4.12060300	0.97449500	2.11863000
O	3.24198500	-1.01940000	3.25131300
O	1.46885300	-2.58052900	-3.28654600
O	5.57275300	-0.97286800	2.49679900
O	3.03220700	1.45468800	-0.30124300
H	2.33868900	2.13285500	-0.24523300
H	3.52052900	1.46765000	0.56380000

IM8a

C	-6.52655100	-2.89932500	0.26449800
C	-6.27364000	-2.22550700	-0.94111000
C	-4.98756100	-1.81123000	-1.27152800
C	-3.91324000	-2.06379100	-0.39335500
C	-4.15954400	-2.74080100	0.82461800
C	-5.44588100	-3.14767400	1.13800100
H	-7.09469000	-2.02289100	-1.62367200
H	-4.80640300	-1.27861400	-2.20130200
H	-3.33540300	-2.93371000	1.50422500
H	-5.62921700	-3.66813700	2.07506500
C	-7.91807800	-3.34813600	0.63214100
H	-8.26289600	-2.84533700	1.54488700
H	-8.63636000	-3.13152700	-0.16411400
H	-7.94449500	-4.42680500	0.83084200
C	-2.61018200	-1.61519600	-0.77624600

H	-2.42987000	-1.12294100	-1.72218400
O	-1.62645500	-1.82566900	0.01838000
C	-0.28724200	-1.48054900	-0.05956500
C	0.35680800	-1.04778000	-1.25843100
C	0.40347900	-1.65998800	1.18333200
O	-0.40405100	-1.09829000	-2.36934100
O	-0.35496300	-2.13813900	2.17721100
C	0.24118400	-0.69095600	-3.60240400
H	-0.52558600	-0.80892900	-4.36802500
H	0.56506600	0.34906800	-3.52929000
H	1.10214100	-1.33083000	-3.80497900
C	0.27071500	-2.23067800	3.47539800
H	0.60673600	-1.24307200	3.79812200
H	-0.51152900	-2.60795600	4.13438500
H	1.11391500	-2.92494000	3.44297900
O	1.53662300	-0.66186800	-1.34336900
O	1.61423400	-1.41973800	1.37952600
Ni	2.88016200	-0.39661200	0.15840200
O	4.05269600	-2.04104400	-0.49331500
O	1.28906400	3.40740000	1.88464500
Cl	4.89728400	-1.21840200	-1.50755000
Cl	1.47121100	1.94189700	1.93565400
O	6.32544200	-1.29391400	-1.16047000
O	4.34646600	0.20365700	-1.28688500
O	2.05034500	1.49592600	0.57772000
O	2.44811100	1.55625000	3.01455100
O	4.63003300	-1.67778400	-2.88267800
O	0.16826800	1.24928100	2.15297000
C	-2.21972400	2.08117600	-0.29109000
H	-1.41747400	1.85871800	0.43423500
C	-2.48059100	3.51151400	-0.52906800
C	-3.52548000	3.93258500	-1.37210400
C	-1.65953000	4.46096600	0.10319100
C	-3.74686200	5.29137700	-1.57505200
H	-4.14859200	3.18347500	-1.85218500
C	-1.88329800	5.82337300	-0.10712000
H	-0.84612500	4.13248500	0.74626300
C	-2.92504700	6.23684400	-0.94246600
H	-4.55460000	5.62183700	-2.22291700
H	-1.24586200	6.55766400	0.37734300
H	-3.09989400	7.29759100	-1.10453000
O	-2.82690200	1.16056000	-0.83619800
O	4.21812300	-0.11583900	1.72310100
H	4.44652100	-0.95715900	2.14920000

H	3.75097100	0.44407200	2.38601100
IM8b			
C	0.79493300	2.83157900	-0.03813200
H	-0.11289000	2.20713600	0.05270800
C	0.55409300	4.21115900	-0.49397500
C	1.61228000	5.12291000	-0.66126600
C	-0.76709900	4.60902500	-0.75946000
C	1.34630100	6.41959300	-1.09114700
H	2.62664100	4.79680800	-0.45003800
C	-1.02950200	5.91082400	-1.19030000
H	-1.57725600	3.89663900	-0.62487000
C	0.02548400	6.81322500	-1.35534400
H	2.15968200	7.12854000	-1.22181200
H	-2.05100000	6.22019900	-1.39288900
H	-0.17820000	7.82751300	-1.68951600
O	1.89757700	2.36157900	0.23199100
C	7.30515100	-1.17884600	0.07613800
C	6.87936000	-0.16834600	0.95410300
C	5.52626900	0.09229700	1.13909500
C	4.55646200	-0.65852600	0.43937900
C	4.97767900	-1.68096800	-0.44587400
C	6.32913300	-1.92732400	-0.61773500
H	7.61785000	0.41695900	1.49533500
H	5.20905200	0.88074200	1.81679700
H	4.23496400	-2.26518300	-0.98003700
H	6.64729400	-2.71461200	-1.29686700
C	8.76971900	-1.46992300	-0.12748000
H	9.05465200	-1.32854200	-1.17785400
H	9.40067300	-0.81962600	0.48543900
H	9.00218700	-2.51099700	0.12975500
C	3.18116700	-0.34162200	0.65019100
H	2.87091900	0.43073800	1.34386500
O	2.28318400	-0.97045700	-0.01627800
C	0.90342700	-0.80630800	0.06188900
C	0.24008500	-0.51235900	1.28955200
C	0.22508800	-1.13920700	-1.15213000
O	1.04690100	-0.39012000	2.36167500
O	1.02624100	-1.55197200	-2.14058000
C	0.38705200	-0.20535000	3.63825400
H	1.19884500	-0.13827900	4.36262200
H	-0.20555200	0.71151400	3.62633400
H	-0.25876900	-1.05916700	3.85328100
C	0.37356700	-2.01249000	-3.34527600

H	-0.17717200	-1.19308500	-3.81369900
H	1.18675400	-2.34553900	-3.99036600
H	-0.30272100	-2.83684200	-3.11042100
O	-0.99149200	-0.39540600	1.43333100
O	-1.00627600	-1.03590900	-1.34252900
Ni	-2.44726800	-0.71759500	0.05283000
O	-2.59843500	-2.69204200	0.68663700
O	-3.88289000	0.20057200	1.39214900
Cl	-3.69419900	1.61839000	0.84083500
O	-0.91580100	-4.03336100	-0.52767000
O	-2.65462100	1.38927300	-0.29694900
O	-4.94760100	2.14771600	0.27884800
O	-2.86581100	-5.10859500	0.50040300
O	-3.11790300	2.51650700	1.86134600
Cl	-2.36696000	-3.92667900	-0.22145600
O	-3.14848200	-3.70362400	-1.49720000
O	-3.91976400	-1.08563000	-1.36147200
H	-3.76476700	-0.57436400	-2.17150000
H	-3.80049900	-2.04126200	-1.58747100

IM8c

C	-1.36714500	2.19904100	-0.13254200
H	-0.54374000	1.64068900	0.34458600
C	-1.25639900	3.66486800	-0.05127000
C	-2.24685300	4.50777600	-0.58767400
C	-0.12681700	4.21716300	0.57681100
C	-2.10502300	5.88891200	-0.49374500
H	-3.11278600	4.06265500	-1.06927400
C	0.01214300	5.60334000	0.66786300
H	0.63866200	3.56123900	0.98466900
C	-0.97540900	6.43629200	0.13375400
H	-2.86719800	6.54492400	-0.90612100
H	0.88686200	6.02993900	1.15037000
H	-0.86759100	7.51582800	0.20353400
O	-2.28724700	1.59375500	-0.68204100
C	-7.13431400	-1.15525900	-0.27652000
C	-6.58310500	-0.49691500	-1.38764000
C	-5.20904200	-0.48584100	-1.60175700
C	-4.34502700	-1.13937300	-0.69819700
C	-4.89201600	-1.80380500	0.42544100
C	-6.26268700	-1.80662800	0.62306700
H	-7.23928500	0.01355400	-2.08752000
H	-4.79324000	0.03848900	-2.45800500
H	-4.22991400	-2.30535800	1.12438600

H	-6.67771900	-2.31876000	1.48791000
C	-8.62237300	-1.17029800	-0.03638200
H	-8.86912100	-0.69613100	0.92212900
H	-9.16461500	-0.64076700	-0.82527900
H	-9.00315000	-2.19848500	0.00752200
C	-2.94085600	-1.09527000	-0.95986900
H	-2.53940800	-0.60812600	-1.83842000
O	-2.13780500	-1.67114000	-0.14184100
C	-0.75252700	-1.74210800	-0.13597800
C	0.06955900	-1.47800400	-1.27236400
C	-0.21043000	-2.19265400	1.11269200
O	-0.58190500	-1.26206100	-2.42738000
O	-1.12002700	-2.52622000	2.03575100
C	0.24572100	-1.00969300	-3.59778400
H	-0.45252300	-0.66584700	-4.36076500
H	1.00541800	-0.26032700	-3.37437900
H	0.73059800	-1.93862100	-3.90656200
C	-0.60392000	-2.87279300	3.34427700
H	-0.01549800	-2.04470000	3.74412900
H	-1.49113500	-3.05348400	3.95123100
H	0.01127700	-3.77328300	3.28119400
O	1.31817000	-1.47071300	-1.25293900
O	1.01095300	-2.29209900	1.36163700
Ni	2.42816200	-1.10643800	0.42582100
O	4.67666000	-1.59912000	-2.08675100
O	3.13070400	-0.40255700	2.35415400
Cl	4.38852500	-0.11777400	-1.94388700
Cl	2.07182100	0.69705400	2.48794200
O	5.62981100	0.66697500	-2.04423500
O	3.81491200	0.10070500	-0.52068400
O	1.34263600	0.60554300	1.11801300
O	1.12087400	0.38611700	3.57758700
O	3.38338600	0.30394000	-2.94953800
O	2.68059300	2.02574000	2.64949100
O	3.67762600	-2.72768800	0.16224100
H	3.16970500	-3.53367100	-0.02140300
H	4.17436100	-2.49917900	-0.66669100

IM8d

C	-6.77989600	-2.67959700	-0.10382400
C	-6.26676900	-2.20321500	-1.32158600
C	-4.92307900	-1.86982200	-1.44698300
C	-4.05341000	-2.00525300	-0.34414500
C	-4.56203800	-2.48420600	0.88689700

C	-5.90284900	-2.81224600	0.99494700
H	-6.92968900	-2.09200200	-2.17535000
H	-4.53889000	-1.48956800	-2.38972400
H	-3.89461200	-2.59237400	1.73595900
H	-6.28949100	-3.18163800	1.94170600
C	-8.23520000	-3.04379100	0.04020400
H	-8.72160200	-2.41727300	0.79881600
H	-8.77870700	-2.91929100	-0.90092100
H	-8.34910600	-4.08573300	0.36454300
C	-2.68678000	-1.63657600	-0.51956600
H	-2.30975100	-1.31939000	-1.48360300
O	-1.87779600	-1.69997500	0.47323400
C	-0.50635200	-1.41112700	0.41625400
C	0.30872200	-1.86529200	-0.65922300
C	0.01391200	-0.82717500	1.61026600
O	-0.34457300	-2.54650700	-1.62549100
O	-0.89406200	-0.64614100	2.58297200
C	0.47432800	-3.07654300	-2.69578700
H	-0.22926500	-3.57296900	-3.36432500
H	0.99650000	-2.26518100	-3.20688500
H	1.20118400	-3.78771100	-2.29784200
C	-0.41373800	-0.03087900	3.79792000
H	-0.00747100	0.96084600	3.58649300
H	-1.29190600	0.03856100	4.44015100
H	0.35807000	-0.65113800	4.25962000
O	1.54266400	-1.71403000	-0.74095600
O	1.20012200	-0.48155700	1.78961300
Ni	2.66444300	-0.43337500	0.37601900
O	3.87981600	-2.02795600	1.17330700
O	3.05942600	1.94966400	-2.45860400
Cl	5.05356800	-1.75768200	0.20978400
Cl	2.30926800	2.36821600	-1.25981700
O	6.11565000	-1.00769500	0.93192500
O	4.40356900	-0.83951600	-0.84116100
O	1.65840500	1.12371300	-0.59701200
O	3.22069900	2.99704200	-0.23868100
O	5.55291800	-2.99969000	-0.39169500
O	1.19584600	3.29105600	-1.59424200
C	-2.09516500	2.03848900	-0.68210900
H	-1.02339100	1.97358500	-0.93818600
C	-2.55420300	3.35268800	-0.19875400
C	-3.89555700	3.56396000	0.17085900
C	-1.62465900	4.40338600	-0.11001700
C	-4.29959800	4.81548900	0.62576400

H	-4.59851500	2.73952000	0.09330600
C	-2.03570900	5.65718600	0.34804000
H	-0.59253300	4.23227500	-0.40554500
C	-3.36902200	5.86228800	0.71453000
H	-5.33451400	4.98423400	0.91198900
H	-1.31872500	6.47066100	0.41592900
H	-3.68839000	6.83907100	1.06951900
O	-2.82247100	1.05300300	-0.80297400
O	3.79835700	0.92169900	1.48994000
H	4.73424900	0.64636100	1.52984000
H	3.76775300	1.77311400	0.99297400

TS1a

O	-0.85815000	-2.07371300	-0.80028100
O	2.46616200	-0.62440600	2.02237300
O	0.53352200	-1.62936900	2.61697200
O	-0.64132800	0.09147000	0.74808500
C	0.52183300	-0.57820000	0.50630500
C	1.15984600	0.43451300	-0.43821000
C	0.22320600	-1.90532600	-0.25305600
C	1.30884600	-0.93380200	1.79161200
C	1.10227000	-2.02222100	3.88305900
H	0.31599200	-2.58623700	4.38342500
H	1.37065600	-1.13577500	4.46323300
H	1.98887100	-2.64118200	3.72226900
O	1.18853800	-2.81070300	-0.24589700
C	0.89111800	-4.07670500	-0.89464000
H	0.74665600	-3.91659100	-1.96542900
H	1.76288400	-4.70183700	-0.70534300
H	-0.01149100	-4.51076600	-0.46022900
C	3.83326200	0.02997800	-0.35815700
H	3.76539000	0.84957400	0.36672300
O	2.80961900	-0.31862900	-0.97439200
C	5.13260000	-0.58240800	-0.56854200
C	5.31547300	-1.62927700	-1.49507500
C	6.22398300	-0.10080900	0.17940300
C	6.57943300	-2.18146600	-1.66657600
H	4.46433000	-1.98936700	-2.06444400
C	7.48804200	-0.66073900	0.00471100
H	6.07180200	0.70232900	0.89625900
C	7.66342600	-1.69808000	-0.91754500
H	6.72942500	-2.98702500	-2.37953500
H	8.33166600	-0.29401600	0.58185900
H	8.64903200	-2.13472800	-1.05555200

H	0.76017400	0.31847300	-1.44118200
C	1.43198100	1.82804400	-0.08783600
C	1.54525500	2.74411900	-1.15460300
C	1.55319000	2.31907700	1.22777700
C	1.78076400	4.09395600	-0.91906800
H	1.42972000	2.38977300	-2.17632600
C	1.77625500	3.67265000	1.45393400
H	1.44165900	1.65433300	2.07368500
C	1.88985800	4.58576300	0.39147700
H	1.85154700	4.78066100	-1.75888800
H	1.84322800	4.03396600	2.47734200
C	2.07311100	6.05908900	0.65670600
H	2.69035200	6.23438500	1.54470000
H	2.53802400	6.56788900	-0.19413500
H	1.10083900	6.53784600	0.83555500
Ni	-2.24796200	-0.48741400	-0.29029300
Cl	-4.17911700	-2.40960000	0.04109800
O	-3.37586300	1.11725200	0.41309100
O	-3.84114200	-1.54012200	-1.20004700
O	-3.18581900	-1.85533300	1.08395800
O	-2.31337700	2.80658300	-1.04790500
O	-3.84487500	3.48943600	0.74448900
O	-5.56959400	-2.19559200	0.46269500
O	-3.89145100	-3.83053300	-0.24131100
O	-1.69694800	0.45548900	-2.09969400
H	-2.34884600	0.20632400	-2.77689900
H	-1.87472400	1.41596000	-1.88184600
Cl	-3.59532800	2.47186000	-0.29043900
O	-4.71318900	2.34395200	-1.25317300
TS1b			
O	-1.34199500	-1.68335000	-0.75039300
O	2.17713300	-1.38486300	2.10212100
O	0.09810000	-2.05564700	2.67196200
O	-0.83480100	0.09734800	1.18158100
C	0.23563400	-0.65180100	0.77725300
C	0.99382100	0.45575400	0.05752700
C	-0.23510500	-1.74642200	-0.23201200
C	0.97122900	-1.38950900	1.92226600
C	0.62916900	-2.82301100	3.77198700
H	-0.23788900	-3.29611100	4.23168300
H	1.13188400	-2.16159800	4.48235900
H	1.33510200	-3.57170200	3.40304200
O	0.61648000	-2.73279600	-0.45390200

C	0.16671300	-3.78331100	-1.35279000
H	-0.00876000	-3.36636600	-2.34668800
H	0.97956800	-4.50822400	-1.36600800
H	-0.75455300	-4.22619800	-0.96912400
C	3.58221100	-0.39741900	-0.28854500
H	3.71920400	0.15797500	0.64785100
O	2.46520200	-0.40379100	-0.83055700
C	4.73903200	-1.07938200	-0.84503000
C	4.66354200	-1.78323400	-2.06410600
C	5.95579000	-1.01363900	-0.14022500
C	5.79757300	-2.41213100	-2.56515500
H	3.71984600	-1.81878100	-2.59940500
C	7.08824600	-1.64904000	-0.64636600
H	6.00389700	-0.47059200	0.80058100
C	7.00732100	-2.34561300	-1.85697500
H	5.74871200	-2.95314000	-3.50571400
H	8.02810500	-1.60256100	-0.10424300
H	7.89031400	-2.83936700	-2.25410800
H	0.52812400	0.65702000	-0.90182200
C	1.54706300	1.65055400	0.69232900
C	1.62943900	2.80924400	-0.11255200
C	1.98908300	1.73367800	2.02950200
C	2.13948800	3.99755300	0.39891900
H	1.25437900	2.78234800	-1.13215300
C	2.49250300	2.93053900	2.53067700
H	1.93699400	0.87207200	2.68155600
C	2.57816800	4.08258800	1.73034800
H	2.17829900	4.87699300	-0.23930100
H	2.82068000	2.97475600	3.56668400
C	3.08915400	5.38529800	2.29439300
H	3.69933300	5.22631500	3.18911200
H	3.68970100	5.93212600	1.55965700
H	2.25232300	6.03723800	2.57738200
Ni	-2.48436300	-0.06992700	0.03262100
Cl	-1.89364600	2.41063100	-2.15404500
Cl	-4.73908600	-1.60324200	0.29161000
O	-2.33727400	3.27484500	-0.99818200
O	-1.65392400	0.98037000	-1.60875400
O	-4.30731000	-0.67338700	-0.86610000
O	-3.56489200	-1.41957800	1.28635000
O	-0.58382300	2.88759600	-2.67064300
O	-2.92274100	2.36711500	-3.20590200
O	-6.00530000	-1.15056500	0.88803800
O	-4.80562000	-3.00416500	-0.16630200

O	-3.27186500	1.60434300	0.95910900
H	-2.72523300	1.72261400	1.75426900
H	-3.05081400	2.35556800	0.35632200
TS1c			
O	-1.24058600	-1.32304300	-1.26047400
O	2.11921900	-1.13829400	1.80999500
O	-0.00799800	-1.64440200	2.37154300
O	-0.80209400	0.42192100	0.72271100
C	0.24926700	-0.38274900	0.39613200
C	1.08716800	0.65531000	-0.34494700
C	-0.21719700	-1.48894800	-0.60040900
C	0.91555800	-1.08864800	1.60373400
C	0.44002200	-2.38480700	3.52457600
H	-0.46743700	-2.79828600	3.96259800
H	0.94147700	-1.71432200	4.22759600
H	1.12501400	-3.17958300	3.21843200
O	0.52297200	-2.57396900	-0.66800200
C	0.00857400	-3.66307200	-1.48943500
H	-0.02643500	-3.34797600	-2.53458300
H	0.71861300	-4.47664300	-1.34707900
H	-0.98817800	-3.93236100	-1.13634200
C	3.60164200	-0.28532300	-0.38095300
H	3.69318200	0.36884300	0.49289300
O	2.54734300	-0.26518400	-1.04484900
C	4.73826500	-1.11725300	-0.72786800
C	4.71652300	-1.97007300	-1.85037300
C	5.88244300	-1.05348700	0.09030000
C	5.83185400	-2.74545700	-2.14497100
H	3.82761700	-2.00852000	-2.47211400
C	6.99583300	-1.83609500	-0.20870200
H	5.88660300	-0.39897100	0.95838700
C	6.96891500	-2.67886900	-1.32515300
H	5.82406700	-3.40373700	-3.00885100
H	7.87848300	-1.79268500	0.42244500
H	7.83690100	-3.28934200	-1.55982200
H	0.67828800	0.82418000	-1.33630900
C	1.60992900	1.87922100	0.26934200
C	1.86058800	2.96805900	-0.59131500
C	1.86097100	2.04622600	1.64495600
C	2.35611500	4.17029100	-0.10006100
H	1.64148400	2.87120700	-1.65168000
C	2.34603000	3.25758600	2.12940500
H	1.66010000	1.24407800	2.34270300

C	2.60077800	4.34065700	1.27230300
H	2.52895800	4.99745400	-0.78428800
H	2.51682900	3.37001800	3.19745600
C	3.07767400	5.66530200	1.81475800
H	3.60459300	5.54489700	2.76714400
H	3.74765900	6.17067000	1.11058700
H	2.22582600	6.33570000	1.99226700
Ni	-2.41110500	0.21828500	-0.44523600
Cl	-2.59478100	2.91489600	-1.04870200
Cl	-3.79925200	-2.46597400	0.79142600
O	-3.31099500	2.10003500	0.05065800
O	-1.75199600	1.83321400	-1.75813000
O	-4.58480900	-2.52659900	-0.50017700
O	-3.34583700	-1.00537500	0.99244400
O	-1.72446400	3.94868900	-0.46228000
O	-3.58828000	3.48278900	-1.98119300
O	-4.64736100	-2.83926000	1.93741900
O	-2.59661600	-3.33947000	0.69330700
O	-3.98577800	-0.17365700	-1.75433100
H	-4.67210800	0.50843500	-1.66371800
H	-4.37948500	-1.02312500	-1.43445600
TS1d			
O	-1.27826200	-1.68873100	-0.28119200
O	2.51040400	-0.86070600	2.09561400
O	0.50517400	-1.31627200	3.02390500
O	-0.57463900	0.44662600	1.15586400
C	0.44044100	-0.40576600	0.83929400
C	1.15223300	0.45820300	-0.19979700
C	-0.13803300	-1.68942400	0.16583000
C	1.29180700	-0.87351700	2.04600700
C	1.15812500	-1.81357100	4.21018500
H	0.34972300	-2.14280900	4.86242300
H	1.73671700	-1.01583500	4.68308900
H	1.81941000	-2.64628700	3.95631600
O	0.65105900	-2.74884600	0.13111000
C	0.08177400	-3.95455100	-0.45386500
H	-0.13308000	-3.78268800	-1.51050200
H	0.84806500	-4.71756800	-0.32403300
H	-0.83918300	-4.21857400	0.06899300
C	3.65708900	-0.50204700	-0.49734900
H	3.87528300	0.29110600	0.22715800
O	2.49915800	-0.61403900	-0.93996600
C	4.74917800	-1.36209700	-0.91369000

C	4.56278100	-2.38616800	-1.86503000
C	6.01952200	-1.14623500	-0.34589300
C	5.64058200	-3.18037000	-2.23850000
H	3.57853000	-2.53833100	-2.29670000
C	7.09500800	-1.94826200	-0.72235100
H	6.15243500	-0.35695800	0.38994200
C	6.90388300	-2.96207000	-1.66748000
H	5.50634400	-3.96947600	-2.97263800
H	8.07565100	-1.78663300	-0.28478200
H	7.74227600	-3.58708500	-1.96345200
H	0.59807800	0.44778600	-1.13311800
C	1.76200100	1.75956200	0.08004500
C	1.89280600	2.64473100	-1.01085200
C	2.20880600	2.19175700	1.34415500
C	2.46251100	3.90183600	-0.84981700
H	1.52033600	2.34591500	-1.98697300
C	2.76477600	3.45817100	1.49882700
H	2.10827100	1.55368600	2.21167800
C	2.90132600	4.33648400	0.41122700
H	2.53858400	4.56804000	-1.70552400
H	3.08867700	3.77743000	2.48662300
C	3.45853600	5.72577600	0.59937800
H	4.09934100	5.78727300	1.48532800
H	4.04099900	6.04697600	-0.27161900
H	2.64369200	6.45052500	0.73105900
Ni	-2.32120000	0.08489100	0.18659200
Cl	-2.33593500	2.55225900	-1.04864000
Cl	-4.96871600	-1.65451100	-0.53651200
O	-2.96422400	2.12057900	0.29199700
O	-1.72014200	1.22352900	-1.55495600
O	-4.01308000	-0.48841400	-0.88225300
O	-5.41605800	-1.45664200	0.90003700
O	-1.26839000	3.54960800	-0.82642200
O	-3.36205700	3.03975700	-1.97971300
O	-6.12147400	-1.57512900	-1.44836300
O	-4.23440800	-2.93774000	-0.66356400
O	-3.13012800	-0.56666500	1.98858500
H	-3.17000900	0.18409600	2.60247400
H	-4.06182500	-0.85922200	1.79983800
TS5a			
C	6.64591400	0.77776400	-0.52333900
C	6.11176800	1.64097700	0.45298700
C	4.88817700	1.36997100	1.04641600

C	4.15712100	0.21509500	0.67368000
C	4.68217300	-0.64921400	-0.32157700
C	5.91042300	-0.36902500	-0.89470300
H	6.66679700	2.52892700	0.74266500
H	4.48600600	2.04046700	1.80208100
H	4.10623300	-1.51634800	-0.62497100
H	6.31361700	-1.03598900	-1.65276200
C	7.97617600	1.06448700	-1.16805300
H	7.87632100	1.13038900	-2.25876200
H	8.40935200	2.00181300	-0.80754300
H	8.69016200	0.25674800	-0.96152600
C	2.93994500	-0.06987100	1.34100000
H	2.58009100	0.57885000	2.13759600
O	2.26551900	-1.19856400	1.13046200
C	0.99939600	-0.60223900	0.87583700
C	-0.00743900	-0.77256800	1.89038200
C	0.70415800	-0.16623400	-0.46297900
O	0.47148600	-1.30739200	3.01892600
O	1.69860200	-0.31209100	-1.34316900
C	-0.49669400	-1.58829100	4.05608900
H	0.08325100	-2.03031600	4.86588700
H	-0.98298400	-0.66495100	4.37909900
H	-1.24617500	-2.29020600	3.68406400
C	1.37342000	0.00079300	-2.72312100
H	1.11938100	1.05879000	-2.81853800
H	2.28146900	-0.23312900	-3.27887200
H	0.53684900	-0.61846000	-3.05136000
O	-1.20394000	-0.44544800	1.79955300
O	-0.38898300	0.30660800	-0.82294100
Ni	-2.15912000	0.27669300	0.15599800
O	-2.87083700	-1.46668800	-0.64132600
O	-3.06695500	1.63667100	-1.29738100
Cl	-3.02221100	2.83809200	-0.34280900
O	-0.90951600	-2.89761100	-0.19859100
O	-2.03090700	2.36201900	0.73801200
O	-2.54525900	4.05413600	-1.01091100
O	-2.93330100	-3.82157500	-1.25134400
O	-4.36574400	3.02075000	0.27704100
Cl	-2.01535000	-2.66789700	-1.17444000
O	-1.47214200	-2.29398400	-2.50429900
O	-4.03445900	0.18424200	1.12779300
H	-4.54665200	1.00556800	0.98455100
H	-4.49553600	-0.53133300	0.65337100

TS5b

C	-6.74033400	-0.40164200	-0.74448700
C	-6.13871600	-1.67428900	-0.79060200
C	-4.87004300	-1.87797700	-0.26918100
C	-4.16134100	-0.80121800	0.31867600
C	-4.75598700	0.48665000	0.35388600
C	-6.02732700	0.66894300	-0.16162600
H	-6.67782400	-2.50444700	-1.23848900
H	-4.41578700	-2.86524800	-0.30353500
H	-4.19992000	1.31370900	0.78121100
H	-6.48476500	1.65471400	-0.12664700
C	-8.11600400	-0.17299900	-1.31250600
H	-8.07648900	0.53097600	-2.15392000
H	-8.56844900	-1.10250100	-1.66944200
H	-8.78198100	0.26704300	-0.55996000
C	-2.89740000	-1.05419700	0.90758300
H	-2.48686400	-2.06201900	0.92727400
O	-2.23418100	-0.12069600	1.58715200
C	-0.99632800	-0.25605400	0.89522200
C	0.06775900	-0.92306400	1.60277100
C	-0.80423500	0.48616700	-0.32142500
O	-0.34331700	-1.51961900	2.72801300
O	-1.87038300	1.18068900	-0.73072800
C	0.68434200	-2.17757700	3.51007200
H	0.15741300	-2.58739700	4.37145400
H	1.15730000	-2.96693700	2.92162200
H	1.43725900	-1.44999800	3.82079100
C	-1.66806700	2.05389400	-1.86763100
H	-1.41307000	1.46752300	-2.75411500
H	-2.62442800	2.55926400	-2.00295300
H	-0.87578100	2.77027800	-1.64341300
O	1.25099000	-0.99781400	1.23811200
O	0.25615300	0.50803600	-0.97645200
Ni	2.12642700	-0.04272800	-0.34363400
O	2.41718100	1.62839700	0.87320300
O	3.94052000	-1.12954500	0.05497300
Cl	3.59633300	-2.29488000	-0.88967500
O	0.36400800	2.99845400	0.83839600
O	2.23445700	-1.82523600	-1.48133000
O	4.59654500	-2.42488700	-1.96133700
O	2.51381300	3.98707600	1.48624200
O	3.41423000	-3.54920200	-0.13671700
Cl	1.83284600	3.03500100	0.59520000
O	2.10095500	3.36340300	-0.85665800

O	3.00325300	0.99778400	-1.90615600
H	2.64561200	0.73209300	-2.76803500
H	2.76008200	1.94272500	-1.75221400
TS5c			
C	6.21773300	-0.16253800	-0.79239900
C	5.26224800	-0.48162800	-1.77617500
C	3.98199200	0.04626600	-1.71771800
C	3.62145700	0.91870000	-0.65997300
C	4.57553300	1.23131700	0.34365700
C	5.85146800	0.70402900	0.26221200
H	5.53174100	-1.15373800	-2.58565900
H	3.24617300	-0.21096700	-2.47505500
H	4.28694200	1.87872700	1.16450400
H	6.58549600	0.94971900	1.02572200
C	7.60560900	-0.74321300	-0.84342300
H	7.76537900	-1.43326500	-0.00409700
H	7.78159600	-1.29507200	-1.77119600
H	8.36496900	0.04393300	-0.75906800
C	2.32207700	1.47452000	-0.65783100
H	1.62816200	1.25760900	-1.46805600
O	1.92021300	2.35103000	0.26657800
C	0.74260300	1.64593900	0.64965100
C	-0.51896600	2.11704900	0.14392500
C	0.84768100	0.57179000	1.59393400
O	-0.43126200	3.21557200	-0.60455000
O	2.06036100	0.40539500	2.13689800
C	-1.67808800	3.72194100	-1.15633800
H	-1.37272700	4.48212000	-1.87512800
H	-2.24132300	2.91625900	-1.62828000
H	-2.27512300	4.16350200	-0.35499800
C	2.21849900	-0.74929100	2.99906000
H	1.95731100	-1.65901800	2.45515200
H	3.27255500	-0.74516100	3.27683700
H	1.58620100	-0.64571000	3.88338600
O	-1.61565200	1.56076200	0.35465200
O	-0.10981800	-0.15340600	1.93749600
Ni	-1.70547700	-0.47805300	0.64417400
O	-4.93081500	0.57800200	0.58231100
O	-1.19317400	-2.58627700	0.60361100
Cl	-4.51997600	0.11793200	-0.80230900
Cl	-0.14536600	-2.45073100	-0.50844000
O	-5.58907600	-0.67677300	-1.42711300
O	-3.29264200	-0.81577300	-0.62473300

O	-0.29176100	-0.95836200	-0.90799000
O	1.22055400	-2.67899100	0.02372600
O	-4.13384200	1.28299000	-1.63313600
O	-0.44394000	-3.32824600	-1.64638600
O	-3.01641800	-0.38481300	2.23018800
H	-2.72658400	0.27054400	2.88449700
H	-3.84750400	-0.03458400	1.81340200

TS5d

C	6.84033300	0.81090200	-0.32949000
C	6.54423900	0.32677900	0.95969600
C	5.34208400	-0.31423800	1.21702600
C	4.39222000	-0.48950200	0.18024500
C	4.67916700	0.00923400	-1.11686900
C	5.88803600	0.63770500	-1.35799400
H	7.26817300	0.45764900	1.75918700
H	5.12501300	-0.68971900	2.21415600
H	3.93978400	-0.10323700	-1.90181300
H	6.10794000	1.01473400	-2.35365100
C	8.14560400	1.50325600	-0.61785300
H	7.97412800	2.50055800	-1.04198500
H	8.75565400	1.61437900	0.28316800
H	8.72862100	0.93846900	-1.35711400
C	3.20252300	-1.20686900	0.45779700
H	3.03315200	-1.63540900	1.44459700
O	2.32498100	-1.52326200	-0.49258700
C	1.17319600	-0.99683400	0.16310100
C	0.26806300	-1.94573800	0.76241000
C	0.84124700	0.39217500	-0.01856300
O	0.76216300	-3.18462000	0.81533000
O	1.75536000	1.12443700	-0.66105300
C	-0.13923400	-4.21618200	1.29666300
H	0.42236600	-5.14375400	1.19087500
H	-0.39432100	-4.03038200	2.34242400
H	-1.04337700	-4.22730000	0.68518900
C	1.40636800	2.51721700	-0.89854200
H	1.37982900	3.05846300	0.04993900
H	2.20284400	2.89330000	-1.54037300
H	0.43120400	2.58957400	-1.38081200
O	-0.84768000	-1.67004400	1.24037100
O	-0.22113200	0.90581900	0.37966100
Ni	-2.01600200	-0.10144600	0.49737600
O	-1.85062500	-1.01447500	-1.41992400
O	-3.15045500	1.46638500	-0.23506000

Cl	-3.08052900	-1.94298100	-1.23364800
Cl	-2.96544900	2.96683500	0.10309100
O	-4.06701500	-1.72679300	-2.29720900
O	-3.61408900	-1.47502400	0.13497800
O	-2.67826700	3.05725400	1.59083900
O	-1.81947800	3.50905100	-0.66501500
O	-2.63544500	-3.35286000	-1.16160900
O	-4.22527100	3.65261000	-0.22541500
O	-2.46799400	0.50277700	2.41798400
H	-1.71987000	0.37732700	3.02225100
H	-2.60495700	1.48285400	2.32080200
TS6a			
C	7.39743900	-0.98371500	-0.19665100
C	6.95992300	-0.05177400	0.75564900
C	5.60604900	0.25597100	0.88614100
C	4.65790200	-0.36949000	0.06479400
C	5.08388100	-1.30347300	-0.89606800
C	6.43550700	-1.60201900	-1.01812500
H	7.68524600	0.43535400	1.40239300
H	5.28606700	0.97808000	1.63395300
H	4.35056700	-1.78520000	-1.53477400
H	6.75732000	-2.32660800	-1.76273800
C	8.86059600	-1.32514600	-0.34349900
H	9.21511800	-1.11308300	-1.35994800
H	9.47957400	-0.75430400	0.35550000
H	9.03697700	-2.39193900	-0.15685100
C	3.24482300	-0.02002600	0.21164700
H	2.95860500	0.58890600	1.06348800
O	2.38417600	-0.95945100	-0.16648900
C	1.01535700	-0.70896200	-0.20682700
C	0.29041800	-0.36655000	0.98856100
C	0.35919200	-1.27540000	-1.35851200
O	1.05709200	-0.19259300	2.07572200
O	1.20479200	-1.71711400	-2.29964100
C	0.35291700	0.09239500	3.31351500
H	1.13331700	0.12104300	4.07378000
H	-0.15781100	1.05457400	3.23893400
H	-0.37283400	-0.69600700	3.52135500
C	0.61503000	-2.30338200	-3.47794000
H	-0.01380000	-1.57339400	-3.99351000
H	1.46218200	-2.58931400	-4.10129100
H	0.02143700	-3.18093700	-3.20958500
O	-0.93764900	-0.19476300	1.05834200

O	-0.87381300	-1.35693600	-1.53848100
Ni	-2.37867100	-0.86490200	-0.22653400
O	-2.36886000	-2.72168700	0.81969100
O	-4.33433500	2.41325900	-0.32232400
Cl	-3.42194100	-2.27985100	1.86910200
Cl	-3.69372200	1.85628800	-1.53081100
O	-4.58844100	-3.17269500	1.84461500
O	-3.79138400	-0.86718800	1.36439400
O	-2.44772400	1.02605700	-1.10377100
O	-4.62960900	0.92270400	-2.25652200
O	-2.80217000	-2.20623200	3.20766500
O	-3.19648000	2.91163200	-2.43977200
C	1.72970900	1.70348100	-1.01935900
H	1.09599100	1.55519900	-1.90106700
C	1.25903900	2.62879700	-0.00111800
C	2.14632400	3.20095400	0.93826100
C	-0.10147500	3.00002500	0.00601900
C	1.67126300	4.11452700	1.87282400
H	3.20415700	2.95885000	0.89281700
C	-0.57224300	3.90570900	0.95487400
H	-0.78971800	2.55461400	-0.70560000
C	0.31125800	4.46152500	1.88625700
H	2.35515900	4.56995400	2.58391100
H	-1.62494800	4.17225500	0.96445300
H	-0.05508300	5.17529200	2.61957400
O	2.90661100	1.21194300	-1.06163200
O	-3.80379100	-1.58174700	-1.55416400
H	-3.35785300	-1.99713500	-2.30970600
H	-4.26542100	-0.78056500	-1.90682200
TS6b			
C	7.17131700	-0.91283700	0.03939700
C	6.79699800	0.28221700	0.67159100
C	5.46071400	0.67622600	0.72145000
C	4.46692900	-0.12335400	0.13852000
C	4.82970700	-1.32254600	-0.50129300
C	6.16442900	-1.70573100	-0.54393000
H	7.55845900	0.90725400	1.13111800
H	5.18840500	1.60426600	1.21910200
H	4.06082600	-1.94116800	-0.95264600
H	6.43750500	-2.63625100	-1.03641300
C	8.61541800	-1.34856800	-0.01812100
H	8.95978700	-1.43534900	-1.05644200
H	9.27123500	-0.63917300	0.49594600

H	8.74931500	-2.33244300	0.44857700
C	3.07748300	0.32047100	0.19015700
H	2.83050200	1.15480000	0.83897100
O	2.16362900	-0.63136100	0.05768400
C	1.57839200	1.65865000	-1.47925200
H	0.96044200	1.27344000	-2.29875400
C	1.09722300	2.84522800	-0.77503400
C	1.99132300	3.66987200	-0.05947900
C	-0.26530100	3.19726300	-0.85113600
C	1.52478900	4.81840900	0.57338300
H	3.04877200	3.42218200	-0.04604700
C	-0.72910000	4.34057800	-0.20230300
H	-0.96674500	2.56256300	-1.38606100
C	0.16419200	5.15079300	0.50741000
H	2.21721000	5.46244000	1.10894800
H	-1.78582400	4.58428400	-0.24176300
H	-0.19804500	6.04633500	1.00568200
O	2.76943800	1.20971200	-1.38435800
C	0.81898100	-0.31996600	-0.09756700
C	0.08803100	0.32328400	0.96564700
C	0.15173100	-1.14245100	-1.08376100
O	0.85564200	0.77179100	1.96870700
O	0.97673700	-1.88485000	-1.81837400
C	0.16101000	1.37871800	3.08692800
H	0.94769000	1.63214600	3.79730600
H	-0.37370200	2.27151800	2.75704400
H	-0.54111400	0.66390700	3.52062400
C	0.36417700	-2.80902100	-2.74720800
H	-0.21163200	-2.26428200	-3.49946000
H	1.20132200	-3.33288900	-3.20841900
H	-0.27991200	-3.50341500	-2.20417900
O	-1.13955700	0.51512300	0.98562900
O	-1.07596700	-1.14544000	-1.31082700
Ni	-2.56098400	-0.49273800	-0.08015700
O	-2.40858300	-2.02018100	1.32605300
O	-4.11749100	0.69048200	0.84681600
Cl	-4.20238100	1.71190800	-0.29472500
O	-0.57451600	-3.51894300	0.63572600
O	-3.10079400	1.19430200	-1.26736400
O	-5.51725300	1.67788100	-0.95217300
O	-2.29854100	-4.29471000	2.19941200
O	-3.85162600	3.06575400	0.17932000
Cl	-2.01563400	-3.48512500	1.00422800
O	-2.85708900	-3.93486800	-0.16793700

O	-3.97090800	-1.61759000	-1.10314600
H	-3.92690300	-1.48037300	-2.06264900
H	-3.72942800	-2.55867600	-0.92139000
TS6c			
C	-1.34072600	0.32518400	1.63683400
H	-0.67364800	-0.47090600	1.98100300
C	-0.85949600	1.69290400	1.68647700
C	-1.75607700	2.78727500	1.64894800
C	0.52525200	1.93089800	1.83471800
C	-1.27021200	4.08624300	1.73496000
H	-2.82533100	2.60247600	1.60516500
C	1.00489300	3.23752900	1.89724800
H	1.21418600	1.09347100	1.87949200
C	0.11093800	4.31186500	1.84714700
H	-1.95948200	4.92630400	1.72723200
H	2.07295600	3.41349800	1.97243800
H	0.48758800	5.32973900	1.90496400
O	-2.53820300	-0.00593800	1.34319600
C	-7.31849300	-0.16986300	-0.23843400
C	-6.74206200	1.10519600	-0.14807800
C	-5.35693900	1.26857400	-0.17986700
C	-4.51779200	0.15390800	-0.30781700
C	-5.08264200	-1.12958100	-0.40118500
C	-6.46412500	-1.28120400	-0.36768300
H	-7.38283300	1.97828700	-0.05246800
H	-4.93012200	2.26677500	-0.11168900
H	-4.43288400	-1.99365500	-0.49751300
H	-6.89338100	-2.27808000	-0.43918100
C	-8.81618800	-0.35725000	-0.19737200
H	-9.11108400	-0.98778700	0.65085500
H	-9.33925200	0.59940800	-0.10311600
H	-9.17794300	-0.85189700	-1.10743600
C	-3.06201000	0.34422500	-0.30837700
H	-2.68916900	1.36174800	-0.38111400
O	-2.38030200	-0.58418300	-0.97696700
C	-0.98824600	-0.63563500	-0.96298700
C	-0.18012700	0.46190900	-1.39243500
C	-0.44960400	-1.96952300	-0.90242800
O	-0.85580700	1.55774800	-1.77550100
O	-1.35745000	-2.92838500	-0.70469400
C	-0.05943400	2.68506200	-2.22701900
H	-0.76903300	3.50767800	-2.31556300
H	0.73207100	2.90974200	-1.51160600

H	0.38256300	2.45367800	-3.19922400
C	-0.84713200	-4.27685900	-0.56589200
H	-0.13569700	-4.32578300	0.26085600
H	-1.72853500	-4.88530600	-0.36368200
H	-0.36273700	-4.59363800	-1.49254700
O	1.07067000	0.46171100	-1.41400700
O	0.76044900	-2.26360100	-1.03234100
Ni	2.27671100	-0.95968300	-0.56290800
O	4.31532300	1.22143300	-2.23009600
O	3.26053600	-2.48303400	0.59101000
Cl	4.19217700	1.65414100	-0.78554500
Cl	2.44416700	-2.27366500	1.87261700
O	5.50240700	2.04864400	-0.24202800
O	3.70169200	0.42922600	0.02614100
O	1.54949200	-1.06010500	1.47704900
O	1.58780700	-3.44460400	2.15299600
O	3.19486000	2.74798900	-0.66227600
O	3.30211800	-1.92539500	3.01190000
O	3.29978100	-1.29740600	-2.32568600
H	2.69453400	-1.42874700	-3.07240400
H	3.77582800	-0.44191300	-2.48336100
TS6d			
C	-2.15502600	1.83814700	-0.39020100
H	-2.12201400	1.85286700	0.70544100
C	-1.23391400	2.72196100	-1.10065900
C	-1.31426300	2.89438100	-2.49622800
C	-0.25602300	3.42085100	-0.36623100
C	-0.42393000	3.74713600	-3.14296200
H	-2.07808800	2.35981100	-3.05232400
C	0.63454900	4.27333200	-1.01934600
H	-0.19034600	3.28954700	0.71102600
C	0.55089300	4.43606800	-2.40796900
H	-0.48495100	3.87934100	-4.21948800
H	1.38722600	4.81068800	-0.44913500
H	1.24471300	5.09955300	-2.91690900
O	-3.14525300	1.28740000	-0.96947700
C	-7.27273300	-0.81998000	1.34830200
C	-7.12126600	-0.82457500	-0.04649500
C	-5.85997700	-0.71726000	-0.62979000
C	-4.71748600	-0.59475100	0.17549400
C	-4.85666400	-0.58454300	1.57560900
C	-6.11885700	-0.69902700	2.14591800
H	-7.99897300	-0.91829800	-0.68087700

H	-5.76110100	-0.72440200	-1.71274400
H	-3.97380000	-0.50057600	2.20152900
H	-6.21752800	-0.69742700	3.22905000
C	-8.63322000	-0.95585700	1.98774400
H	-8.81296600	-0.15257700	2.71242800
H	-9.43366800	-0.92566400	1.24213600
H	-8.71726100	-1.90549800	2.53186800
C	-3.41267000	-0.46775600	-0.47029700
H	-3.32997200	-0.74150100	-1.51583300
O	-2.36735800	-0.72238800	0.30956100
C	-1.07224500	-0.31514700	-0.00752100
C	-0.45247100	-0.63787800	-1.27106700
C	-0.26756600	0.01996300	1.14492400
O	-1.27437500	-1.20495200	-2.16400800
O	-0.94966100	0.10662500	2.29107900
C	-0.66854900	-1.63535900	-3.41430800
H	-1.47907600	-2.11760400	-3.96032800
H	-0.28874900	-0.76987900	-3.96097800
H	0.14308300	-2.33511000	-3.20853500
C	-0.16134300	0.38245800	3.48229700
H	0.30078200	1.36855400	3.41231600
H	-0.87928200	0.33882700	4.30081800
H	0.62104400	-0.36883400	3.59666200
O	0.72628900	-0.38054500	-1.57082800
O	0.94558000	0.29353900	1.11220300
Ni	2.33345800	-0.38634300	-0.23475800
O	1.93660500	-2.44785100	0.13671800
O	3.90429900	-0.31067500	1.11324500
Cl	2.82025000	-2.96620800	-1.02738100
Cl	4.16800200	0.81453700	2.14447500
O	3.85799500	-3.87863100	-0.53532100
O	3.43042600	-1.65330600	-1.55907400
O	3.92174400	2.13647200	1.43555700
O	3.23174200	0.67582600	3.28401800
O	1.96820300	-3.59652100	-2.06142600
O	5.57413900	0.70752600	2.56460500
O	2.90428600	1.45895700	-0.96358900
H	2.13205200	2.01218600	-1.16612700
H	3.36107200	1.87721500	-0.18677300
TS7a			
C	-6.65134500	-2.40410200	-0.42882800
C	-5.95670500	-1.90982400	-1.54253100
C	-4.65009900	-1.43728400	-1.42003700

C	-4.01045200	-1.45086500	-0.17392700
C	-4.69354700	-1.94218100	0.94977900
C	-5.99710200	-2.41017300	0.81653600
H	-6.44071400	-1.89966900	-2.51591000
H	-4.12638400	-1.06360000	-2.29736000
H	-4.19640800	-1.96172700	1.91430400
H	-6.51842500	-2.79186300	1.69153600
C	-8.05927600	-2.93480600	-0.55808200
H	-8.72373800	-2.48680700	0.19043400
H	-8.47665700	-2.72965400	-1.54879700
H	-8.08461800	-4.02132000	-0.40312000
C	-2.62815200	-0.94891700	-0.07071900
H	-2.06082000	-0.86873100	-0.99889100
O	-1.94465500	-1.35720500	0.98904100
C	-0.53749600	-1.16885800	0.93821900
C	0.22187000	-2.06616000	0.14568200
C	0.04111400	-0.22966600	1.82200700
O	-0.50945000	-2.99724400	-0.50391000
O	-0.82408900	0.36954700	2.66882800
C	0.22817000	-3.92111800	-1.33339700
H	-0.53110900	-4.56954800	-1.77167600
H	0.77851200	-3.38319700	-2.10889300
H	0.92773600	-4.50049500	-0.72658000
C	-0.25162800	1.30112000	3.60746600
H	0.23831000	2.12672000	3.08499500
H	-1.09701600	1.66145000	4.19502300
H	0.47626100	0.79870300	4.24924500
O	1.46784300	-2.05446800	0.01059800
O	1.25963500	0.07622400	1.86837800
Ni	2.55877900	-0.39543500	0.38612800
O	4.05206200	-1.42469700	1.55794700
O	2.30029400	0.60108200	-3.27358700
Cl	5.07567700	-1.47054700	0.40741400
Cl	1.70564900	1.45317500	-2.23011300
O	6.07786800	-0.38525100	0.60450300
O	4.20447200	-1.13954300	-0.81708400
O	1.28869200	0.59090600	-1.01540900
O	2.67932000	2.48892100	-1.73992000
O	5.70072800	-2.79212300	0.28919100
O	0.45123900	2.11166200	-2.70259000
C	-2.06242500	1.61223300	-0.28779200
H	-1.25762100	1.27922600	-0.95520800
C	-2.16136400	3.01804800	0.02263100
C	-3.14929100	3.50462500	0.90993600

C	-1.24873600	3.90594000	-0.58706500
C	-3.21671500	4.86430600	1.17860400
H	-3.84069400	2.80734300	1.37242500
C	-1.32757900	5.26945100	-0.30800300
H	-0.50077800	3.52027200	-1.27461700
C	-2.30607900	5.74526800	0.57010700
H	-3.97099400	5.24846900	1.85926800
H	-0.62793900	5.95688700	-0.77375300
H	-2.36456100	6.80898300	0.78603000
O	-2.87396300	0.77423000	0.18607200
O	3.65207200	1.38123000	0.64940200
H	4.60940200	1.18737200	0.69029400
H	3.50436600	1.92030000	-0.15962900

TS7b

C	1.89320100	1.79671100	0.08592600
H	1.23146100	1.53246300	0.91853800
C	1.61277400	3.01371300	-0.63955200
C	2.45267400	3.45483700	-1.68729400
C	0.48380200	3.77243700	-0.26303100
C	2.16328900	4.64534900	-2.34049800
H	3.31649500	2.85880900	-1.96535200
C	0.20199100	4.96411600	-0.92856700
H	-0.17441100	3.40502800	0.51908800
C	1.03992200	5.39924600	-1.96053600
H	2.80434200	4.99482300	-3.14467800
H	-0.66828500	5.54845000	-0.64528200
H	0.81970500	6.33036000	-2.47652800
O	2.87747100	1.05993400	-0.19287900
C	7.00542500	-1.75398200	0.14895100
C	6.53838600	-1.04649400	1.26667600
C	5.19828700	-0.67531700	1.36972700
C	4.29547300	-1.00685400	0.35051500
C	4.74980900	-1.71235800	-0.77605800
C	6.08849100	-2.07816400	-0.86792300
H	7.22923100	-0.78749300	2.06503500
H	4.85373600	-0.12972400	2.24548100
H	4.05024900	-1.97410200	-1.56341400
H	6.43275500	-2.62755600	-1.74114100
C	8.45059800	-2.17745800	0.04026600
H	8.87031500	-1.91158000	-0.93712200
H	9.06677900	-1.70907200	0.81406500
H	8.54863000	-3.26558300	0.14831700
C	2.88996100	-0.60054000	0.48092700

H	2.54463300	-0.31537900	1.47345000
O	2.02927800	-1.26371900	-0.27546100
C	0.64984400	-0.99175700	-0.09819700
C	0.02360300	-1.39262500	1.11515400
C	-0.06616900	-0.59776700	-1.25968200
O	0.85945000	-1.94114500	2.02262300
O	0.66689600	-0.55459200	-2.38665700
C	0.25418700	-2.36839100	3.26601900
H	1.07967700	-2.77490200	3.85103200
H	-0.20892400	-1.51932100	3.77379500
H	-0.49840200	-3.13587400	3.07313400
C	-0.04967500	-0.26231300	-3.60452800
H	-0.43764300	0.76006500	-3.58553200
H	0.69154800	-0.37344900	-4.39667200
H	-0.87355200	-0.96673400	-3.73925000
O	-1.18733200	-1.26922400	1.39356400
O	-1.28159000	-0.28361900	-1.29918400
Ni	-2.50652600	-0.19183900	0.31496900
O	-3.65873400	-1.87750900	0.01491200
O	-3.35183900	0.52935900	2.24173200
Cl	-2.37014300	1.68401500	2.38871100
O	-2.91920000	-2.92632500	-2.09986600
O	-1.56387200	1.61567200	1.05452300
O	-3.06270900	2.98160500	2.47980500
O	-5.10310600	-3.47511800	-1.12567800
O	-1.44462200	1.47048000	3.52290600
Cl	-4.10488500	-2.42033900	-1.36891000
O	-4.72665900	-1.26007200	-2.12081800
O	-3.87587200	0.92932700	-0.76936600
H	-3.40498100	1.52148900	-1.37682900
H	-4.33089800	0.25353600	-1.33690300
TS7c			
C	-1.78617200	1.37555000	-0.87609900
H	-1.00526400	0.78680800	-1.36907300
C	-1.74736800	2.80494400	-1.02234300
C	-2.71547500	3.63846800	-0.41593500
C	-0.71573100	3.36456600	-1.80594900
C	-2.64449300	5.01160500	-0.60069600
H	-3.50042900	3.19419400	0.18765300
C	-0.65375400	4.74340500	-1.98445400
H	0.04099100	2.71978300	-2.24261500
C	-1.61512300	5.56200400	-1.38365400
H	-3.38046600	5.66216100	-0.13853000

H	0.14994700	5.17744800	-2.57043400
H	-1.56192200	6.63924500	-1.51692200
O	-2.68701800	0.78236700	-0.22308000
C	-6.79844300	-2.01220000	-0.42582500
C	-6.00055800	-1.86145200	-1.56909600
C	-4.65230800	-1.51992800	-1.46093500
C	-4.07323100	-1.32424300	-0.20082600
C	-4.86000300	-1.47167700	0.95280400
C	-6.20403000	-1.81096200	0.83371900
H	-6.43628200	-2.01781500	-2.55269700
H	-4.04879600	-1.41469200	-2.36005000
H	-4.41153100	-1.32763300	1.93085400
H	-6.80631500	-1.92587800	1.73231700
C	-8.25595700	-2.39237900	-0.53337400
H	-8.89423900	-1.66748900	-0.01316800
H	-8.58254700	-2.44271700	-1.57690400
H	-8.44212300	-3.37245700	-0.07586800
C	-2.64576100	-0.96136600	-0.11528000
H	-2.04822700	-1.13585600	-1.01033800
O	-2.05654300	-1.24565700	1.03711800
C	-0.64226300	-1.13145200	1.09379200
C	0.15382500	-2.03628700	0.35068700
C	-0.09872000	-0.25955900	2.07045600
O	-0.53083200	-2.95064800	-0.36765300
O	-1.00354300	0.39510400	2.81845600
C	0.26319000	-3.89792900	-1.12602200
H	-0.45650600	-4.42155400	-1.75611300
H	1.02167400	-3.38410200	-1.71836400
H	0.75161100	-4.59789700	-0.44319900
C	-0.47617300	1.33342300	3.78200500
H	0.13111100	2.09063500	3.28153500
H	-1.35715100	1.77998500	4.24458700
H	0.12636900	0.81217800	4.53008500
O	1.40976700	-2.03165800	0.30991800
O	1.13091200	-0.08330300	2.27580300
Ni	2.47725500	-0.36136400	0.75039200
O	4.73112000	-2.73536100	-0.20555300
O	3.22793400	1.67317300	1.03309700
Cl	4.36591800	-1.87335400	-1.39629700
Cl	2.14242500	2.34867100	0.20214700
O	5.56477100	-1.53636500	-2.18341300
O	3.78893700	-0.54752300	-0.84062700
O	1.34769900	1.14087400	-0.36470900
O	1.24969400	3.16785100	1.05531100

O	3.33623500	-2.54998100	-2.22245000
O	2.70905500	3.14147600	-0.90338600
O	3.79951800	-1.38379300	1.96412000
H	3.30103200	-1.96246700	2.56299200
H	4.27372800	-1.97372500	1.32236200

TS7d

C	-6.65134500	-2.40410200	-0.42882800
C	-5.95670500	-1.90982400	-1.54253100
C	-4.65009900	-1.43728400	-1.42003700
C	-4.01045200	-1.45086500	-0.17392700
C	-4.69354700	-1.94218100	0.94977900
C	-5.99710200	-2.41017300	0.81653600
H	-6.44071400	-1.89966900	-2.51591000
H	-4.12638400	-1.06360000	-2.29736000
H	-4.19640800	-1.96172700	1.91430400
H	-6.51842500	-2.79186300	1.69153600
C	-8.05927600	-2.93480600	-0.55808200
H	-8.72373800	-2.48680700	0.19043400
H	-8.47665700	-2.72965400	-1.54879700
H	-8.08461800	-4.02132000	-0.40312000
C	-2.62815200	-0.94891700	-0.07071900
H	-2.06082000	-0.86873100	-0.99889100
O	-1.94465500	-1.35720500	0.98904100
C	-0.53749600	-1.16885800	0.93821900
C	0.22187000	-2.06616000	0.14568200
C	0.04111400	-0.22966600	1.82200700
O	-0.50945000	-2.99724400	-0.50391000
O	-0.82408900	0.36954700	2.66882800
C	0.22817000	-3.92111800	-1.33339700
H	-0.53110900	-4.56954800	-1.77167600
H	0.77851200	-3.38319700	-2.10889300
H	0.92773600	-4.50049500	-0.72658000
C	-0.25162800	1.30112000	3.60746600
H	0.23831000	2.12672000	3.08499500
H	-1.09701600	1.66145000	4.19502300
H	0.47626100	0.79870300	4.24924500
O	1.46784300	-2.05446800	0.01059800
O	1.25963500	0.07622400	1.86837800
Ni	2.55877900	-0.39543500	0.38612800
O	4.05206200	-1.42469700	1.55794700
O	2.30029400	0.60108200	-3.27358700
Cl	5.07567700	-1.47054700	0.40741400
Cl	1.70564900	1.45317500	-2.23011300

O	6.07786800	-0.38525100	0.60450300
O	4.20447200	-1.13954300	-0.81708400
O	1.28869200	0.59090600	-1.01540900
O	2.67932000	2.48892100	-1.73992000
O	5.70072800	-2.79212300	0.28919100
O	0.45123900	2.11166200	-2.70259000
C	-2.06242500	1.61223300	-0.28779200
H	-1.25762100	1.27922600	-0.95520800
C	-2.16136400	3.01804800	0.02263100
C	-3.14929100	3.50462500	0.90993600
C	-1.24873600	3.90594000	-0.58706500
C	-3.21671500	4.86430600	1.17860400
H	-3.84069400	2.80734300	1.37242500
C	-1.32757900	5.26945100	-0.30800300
H	-0.50077800	3.52027200	-1.27461700
C	-2.30607900	5.74526800	0.57010700
H	-3.97099400	5.24846900	1.85926800
H	-0.62793900	5.95688700	-0.77375300
H	-2.36456100	6.80898300	0.78603000
O	-2.87396300	0.77423000	0.18607200
O	3.65207200	1.38123000	0.64940200
H	4.60940200	1.18737200	0.69029400
H	3.50436600	1.92030000	-0.15962900

Ni-2H₂O path

IM1ab

O	-0.70880200	-1.60124500	0.43437600
O	2.19195200	1.23004800	2.10068800
O	0.19483200	2.30326000	2.00510300
O	-0.49985200	0.96329400	-0.29436900
C	0.50612800	0.44812500	0.59085100
C	0.80206400	0.64632800	-0.86592500
C	0.18210600	-0.97173100	1.00693600
C	1.07412500	1.37653900	1.65142500
C	0.58084700	3.20275600	3.06948600
H	-0.30704100	3.80250400	3.26202400
H	1.42025500	3.82304700	2.74466300
H	0.86154600	2.62864400	3.95511600
O	0.90607400	-1.44870000	1.98705300
C	0.61176000	-2.80812300	2.41366400
H	0.83964800	-3.49904300	1.59981800
H	1.26443600	-2.97605600	3.26862600
H	-0.44031100	-2.88344200	2.69405400
C	3.94159400	-1.29854700	0.37376700

H	3.77461600	-0.51859700	1.14101100
O	3.03995500	-1.58902100	-0.40456400
C	5.27934100	-1.92342100	0.37555900
C	5.61004400	-2.93463500	-0.54406200
C	6.22951000	-1.49515900	1.31660100
C	6.87879800	-3.50753100	-0.51801800
H	4.86214100	-3.25410800	-1.26408800
C	7.50119000	-2.07057400	1.34101600
H	5.96677100	-0.71222000	2.02516200
C	7.82413900	-3.07582700	0.42397200
H	7.13774200	-4.28972100	-1.22657800
H	8.23632700	-1.73917500	2.06923100
H	8.81349100	-3.52585900	0.44134300
H	0.80011600	-0.26572000	-1.45706500
C	1.58959800	1.78255100	-1.41102900
C	2.70310100	1.50393600	-2.21395000
C	1.23918600	3.11878000	-1.16424600
C	3.46547500	2.54667200	-2.74383200
H	2.97665900	0.47195900	-2.41874200
C	2.00307900	4.15082400	-1.70578500
H	0.36048700	3.34561500	-0.56842200
C	3.13116300	3.88611500	-2.50016600
H	4.32915800	2.31348300	-3.36217200
H	1.71390900	5.18204500	-1.51400900
C	3.94349800	5.01809100	-3.08512700
H	4.28108900	5.71067200	-2.30428300
H	4.82875000	4.64628400	-3.61096500
H	3.35070100	5.60261800	-3.80045200
Ni	-2.19239500	-0.37610600	-0.42867700
Cl	-4.46183600	-2.27407000	-1.58736600
Cl	-3.40856200	1.26646900	2.12664200
O	-5.16092700	-1.03491300	-2.06850900
O	-3.61268800	-1.88554200	-0.35367700
O	-4.72112500	0.66385000	2.42107500
O	-2.46963900	0.15853400	1.55404500
O	-3.51381400	-2.76130300	-2.65624200
O	-5.40542200	-3.32323600	-1.19628100
O	-3.53655200	2.33596400	1.06602500
O	-2.74569800	1.80916700	3.32859400
O	-3.44058900	1.01166600	-1.28835400
H	-3.65812100	1.64680000	-0.56019100
H	-4.26602600	0.53709300	-1.53684700
O	-1.58420300	-0.85449900	-2.38466500
H	-1.89269600	-0.13049000	-2.95750000

H	-2.11829900	-1.64575100	-2.65370500
IM1ac			
O	-0.70951300	-1.77049300	0.17959600
O	2.19984600	0.38545000	2.62068100
O	0.20720500	1.38062400	3.04384100
O	-0.67395900	0.87415700	0.47851700
C	0.42267700	0.13599800	1.04344800
C	0.59169500	0.90619900	-0.23628600
C	0.19653200	-1.35093600	0.90097200
C	1.05316100	0.64562300	2.32537200
C	0.73298100	1.93790300	4.27082000
H	-0.09228400	2.50509500	4.69944300
H	1.58238600	2.58829500	4.04933800
H	1.04609000	1.13428700	4.94165800
O	0.99810200	-2.12288000	1.58943600
C	0.80334100	-3.55962500	1.43726000
H	1.04357300	-3.84594400	0.41181900
H	1.49684700	-4.00701800	2.14719400
H	-0.23133800	-3.81993400	1.66564500
C	3.89669500	-1.29172800	-0.07472700
H	3.83397500	-0.93875000	0.97306400
O	2.90055600	-1.25893200	-0.78789300
C	5.22147700	-1.77692900	-0.50844500
C	5.42586800	-2.25709700	-1.81446400
C	6.28818800	-1.75590700	0.40455500
C	6.68571100	-2.70929700	-2.19740500
H	4.58923000	-2.26741600	-2.50712800
C	7.55060400	-2.20986100	0.01877100
H	6.12319700	-1.38272500	1.41334900
C	7.74765300	-2.68585800	-1.28144100
H	6.84728100	-3.08122300	-3.20556700
H	8.37600400	-2.19332600	0.72512900
H	8.72969300	-3.04009700	-1.58423500
H	0.59238000	0.29395700	-1.13485600
C	1.28813300	2.21654500	-0.32425400
C	2.46332200	2.30128600	-1.08505200
C	0.79084800	3.36436200	0.30616800
C	3.14122500	3.51469000	-1.19174200
H	2.84574500	1.41703900	-1.58841400
C	1.47502900	4.57463800	0.18389400
H	-0.14247700	3.31713800	0.85730300
C	2.65947100	4.67275200	-0.56090200
H	4.05407500	3.56512700	-1.78131800

H	1.07021400	5.46195700	0.66541200
C	3.37333900	5.99530700	-0.71805300
H	3.17589000	6.66093200	0.12907300
H	4.45756100	5.85943700	-0.79955500
H	3.03998200	6.51472900	-1.62670000
Ni	-2.26641300	-0.41892400	-0.22217700
Cl	-3.81082300	-3.25747800	-0.31748600
O	-3.74342200	1.02237200	-0.31706700
O	-3.57586400	-1.84361700	-0.94141300
O	-3.88044700	-3.06761700	1.18269500
O	-2.79019500	2.31848400	-2.18582300
O	-2.81164900	3.27671300	0.07531000
O	-5.09006000	-3.75358400	-0.84479500
O	-2.67148500	-4.13168500	-0.67027900
O	-1.71528000	-0.16333600	-2.20144100
H	-2.21706400	-0.84478500	-2.68372800
H	-2.11050000	0.71390100	-2.44317000
Cl	-3.57103000	2.46189100	-0.89934400
O	-4.91772100	2.99319800	-1.15202200
O	-2.86624900	-0.62969400	1.75259100
H	-3.54150400	0.06203700	1.87253600
H	-3.34450600	-1.49952700	1.74437700

IM1ad

O	-0.70955300	-1.77048300	0.17922600
O	2.19991800	0.38501900	2.62066800
O	0.20747300	1.38056900	3.04380200
O	-0.67393200	0.87409900	0.47852500
C	0.42267800	0.13584900	1.04340700
C	0.59176600	0.90622500	-0.23619900
C	0.19645600	-1.35106000	0.90071900
C	1.05324100	0.64528900	2.32539700
C	0.73350200	1.93793300	4.27062300
H	-0.09154400	2.50544000	4.69923600
H	1.58307200	2.58804100	4.04893500
H	1.04644800	1.13433800	4.94156500
O	0.99788700	-2.12314200	1.58918600
C	0.80302500	-3.55985700	1.43679700
H	1.04329800	-3.84603500	0.41132800
H	1.49644400	-4.00739800	2.14672200
H	-0.23169400	-3.82012900	1.66505200
C	3.89676800	-1.29199300	-0.07467700
H	3.83400700	-0.93904300	0.97310300
O	2.90064900	-1.25918200	-0.78790600

C	5.22153000	-1.77726900	-0.50845300
C	5.42592600	-2.25716400	-1.81456300
C	6.28831600	-1.75630700	0.40445100
C	6.68583000	-2.70907900	-2.19767000
H	4.58926500	-2.26740700	-2.50719700
C	7.55076900	-2.21002300	0.01848500
H	6.12340000	-1.38326500	1.41330900
C	7.74786200	-2.68572900	-1.28181700
H	6.84737300	-3.08071800	-3.20594400
H	8.37620700	-2.19346100	0.72480000
H	8.72993900	-3.03975900	-1.58476400
H	0.59254400	0.29411000	-1.13485200
C	1.28822500	2.21658700	-0.32393100
C	2.46343300	2.30141600	-1.08463000
C	0.79099400	3.36432000	0.30676300
C	3.14141100	3.51484500	-1.19107200
H	2.84583300	1.41726700	-1.58818400
C	1.47515800	4.57458600	0.18464600
H	-0.14232800	3.31701800	0.85789500
C	2.65967000	4.67279000	-0.56009000
H	4.05429300	3.56534000	-1.78058300
H	1.07036700	5.46184000	0.66631900
C	3.37337400	5.99547200	-0.71691400
H	3.18211300	6.65791300	0.13414200
H	4.45690200	5.85923600	-0.80632000
H	3.03409400	6.51871700	-1.62116900
Ni	-2.26641200	-0.41887200	-0.22243600
Cl	-3.81115400	-3.25728300	-0.31701500
O	-3.74335900	1.02249400	-0.31737900
O	-3.57596900	-1.84363800	-0.94134400
O	-3.88113700	-3.06693600	1.18307900
O	-2.79058800	2.31830300	-2.18652800
O	-2.81134900	3.27680200	0.07453200
O	-5.09028600	-3.75348500	-0.84449700
O	-2.67179000	-4.13169600	-0.66922600
O	-1.71519100	-0.16327200	-2.20166700
H	-2.21671300	-0.84483500	-2.68406800
H	-2.11055600	0.71387900	-2.44348100
Cl	-3.57104000	2.46193100	-0.89984900
O	-4.91775900	2.99331100	-1.15222300
O	-2.86621700	-0.62946800	1.75237900
H	-3.34447300	-1.49930300	1.74422200
H	-3.54144600	0.06230100	1.87222400

IM1bc

O	-0.75781400	-1.36695400	-1.50542100
O	1.83839400	-1.85105900	1.87404700
O	0.05418700	-0.94933000	2.93405500
O	-0.97690100	0.13971600	0.67023500
C	0.18093500	-0.70926700	0.58583600
C	0.27237100	0.76235700	0.26994100
C	0.08102600	-1.60654200	-0.62907200
C	0.78149000	-1.25311900	1.86832100
C	0.54123200	-1.44686000	4.19934600
H	-0.18881700	-1.11044300	4.93446100
H	1.53115000	-1.03431600	4.40954100
H	0.58760100	-2.53780200	4.17218200
O	0.92113800	-2.60479500	-0.68245100
C	0.82638200	-3.48500700	-1.83219600
H	1.05650500	-2.92452900	-2.74063700
H	1.57004300	-4.25887900	-1.64898700
H	-0.17793400	-3.90953200	-1.88620100
C	3.79086600	-0.83929400	-0.78752300
H	3.52450900	-1.43297900	0.10733000
O	2.91682900	-0.23237300	-1.39635000
C	5.22038900	-0.84590400	-1.15817800
C	5.68545300	-0.13778100	-2.28053700
C	6.12303800	-1.57650100	-0.36872300
C	7.03952000	-0.16351500	-2.60413600
H	4.97348300	0.42140200	-2.88082300
C	7.48019500	-1.60142100	-0.69483000
H	5.75615100	-2.12131600	0.49889800
C	7.93677300	-0.89480500	-1.81198100
H	7.40253500	0.38266100	-3.47068600
H	8.17812700	-2.16662500	-0.08323600
H	8.99306300	-0.91214600	-2.06817100
H	0.31847900	0.98838800	-0.79160400
C	0.85269400	1.79373600	1.16970900
C	1.99637300	2.48236200	0.73520400
C	0.27699000	2.12950100	2.40068400
C	2.56388500	3.47212800	1.53454100
H	2.43894200	2.23849800	-0.22720800
C	0.84800700	3.13240200	3.18676900
H	-0.61706700	1.61471600	2.73499100
C	1.99953600	3.81678600	2.77383400
H	3.45268600	3.99381700	1.18607100
H	0.38411200	3.39089500	4.13603800
C	2.60402400	4.91529200	3.61728000

H	2.17213600	4.93205200	4.62325700
H	3.68923300	4.79239000	3.71622500
H	2.42992900	5.90058000	3.16502600
Ni	-2.45334500	-0.27108200	-0.88669800
Cl	-2.68092500	2.66171400	-2.17196400
Cl	-3.20686900	-2.49161800	1.29877300
O	-3.35184900	3.15651400	-0.93127200
O	-1.74023100	1.49030800	-1.76834200
O	-4.13309700	-3.62688400	1.43092300
O	-3.17615100	-2.08074800	-0.19893600
O	-1.85941300	3.70251300	-2.80191400
O	-3.69553900	2.09920700	-3.12742900
O	-3.68174100	-1.29656600	2.07894400
O	-1.81818500	-2.85840400	1.68976600
O	-4.01537800	0.63538800	0.06940500
H	-4.09808600	0.21438600	0.95291900
H	-3.93284400	1.60705500	0.14810500
O	-3.57699400	-0.62929500	-2.59923600
H	-3.07294200	-1.11579100	-3.27166800
H	-3.76994500	0.26098200	-2.97794400

IM1bd

O	-1.24363500	-1.40485200	-0.10562000
O	1.91868900	-0.18713000	2.83752900
O	-0.26750600	0.10951400	3.37210100
O	-0.63613300	1.06625400	0.71980600
C	0.26780700	0.00706400	1.08223500
C	0.68507600	1.03840500	0.08649000
C	-0.22019800	-1.33022900	0.56620600
C	0.76882300	-0.01729800	2.51492700
C	0.06335900	0.05210900	4.78404500
H	-0.88336200	0.18502300	5.30629500
H	0.76260900	0.85332100	5.03177400
H	0.50841900	-0.91703600	5.01949300
O	0.50543800	-2.36075400	0.92724200
C	0.06596300	-3.66550400	0.43652800
H	0.24675300	-3.71363400	-0.63885900
H	0.68460500	-4.38324300	0.97235200
H	-0.99595400	-3.80097200	0.64751700
C	3.73071900	-1.38841100	-0.19671100
H	3.73912600	-1.09890000	0.87334100
O	2.76838300	-1.10268300	-0.89676100
C	4.92659700	-2.11409900	-0.66888500
C	5.03613300	-2.53303400	-2.00690400

C	5.96434600	-2.38580400	0.23697800
C	6.17322600	-3.21764100	-2.42756000
H	4.22487600	-2.31190500	-2.69450600
C	7.10365000	-3.07220700	-0.18666400
H	5.87395500	-2.05688700	1.27043000
C	7.20635400	-3.48748700	-1.51825300
H	6.26133900	-3.54273100	-3.46067600
H	7.90672400	-3.28244000	0.51436300
H	8.09236900	-4.02216600	-1.85093300
H	0.64886000	0.72163900	-0.95065900
C	1.59638000	2.17191400	0.38734200
C	2.67447700	2.40750500	-0.47723900
C	1.40129200	3.02245300	1.48173600
C	3.55311900	3.46077200	-0.23191600
H	2.81789100	1.76808300	-1.34368600
C	2.28103100	4.08043200	1.71399000
H	0.54620000	2.87843300	2.13672300
C	3.37346700	4.31622500	0.86681900
H	4.38373800	3.63085500	-0.91344700
H	2.11116200	4.73853600	2.56314100
C	4.31612900	5.47256300	1.10624500
H	4.13456300	5.94404200	2.07761100
H	5.36284900	5.14654600	1.07876400
H	4.19739800	6.24420400	0.33441000
Ni	-2.52768500	0.25296000	-0.13990300
Cl	-1.74456000	1.74385100	-2.92631800
Cl	-4.66413300	-2.12683500	0.25116400
O	-2.94267400	2.63301400	-2.69681200
O	-1.96580200	0.42949800	-2.12511300
O	-4.16437100	-0.92167300	-0.58926800
O	-4.83633000	-1.64007600	1.68060600
O	-0.51692900	2.39846500	-2.39814400
O	-1.62158400	1.38305400	-4.34453400
O	-5.95604800	-2.54564700	-0.30746600
O	-3.65028200	-3.20866400	0.21639300
O	-3.64837400	1.97081400	-0.19130100
H	-3.45735100	2.60749800	0.51460400
H	-3.51819500	2.41758800	-1.06721400
O	-2.96852500	0.24129400	1.91259100
H	-2.24977200	0.08016100	2.54856300
H	-3.67689200	-0.44795300	2.03903500
IM1cd			
O	-0.65936500	-1.70831800	1.17982200

O	1.99173600	1.44777200	2.45009700
O	-0.11216400	2.27946900	2.57050400
O	-0.94424200	0.82982800	0.40821600
C	0.27825600	0.48808600	1.07603000
C	0.28069400	0.83910400	-0.38628900
C	0.30768700	-0.98461300	1.42628700
C	0.82937600	1.45762100	2.10773500
C	0.32367900	3.26238200	3.53791300
H	-0.57440600	3.82270600	3.79509600
H	1.07809700	3.91457800	3.09153400
H	0.73878800	2.76348600	4.41685200
O	1.40802800	-1.41175600	1.99059900
C	1.49848900	-2.84340900	2.23899000
H	1.39875800	-3.37839400	1.29299900
H	2.48562800	-2.98506700	2.67543800
H	0.71254600	-3.14699300	2.93344900
C	4.17529300	-0.27173500	0.32475400
H	3.99263900	0.33654700	1.23198300
O	3.27323500	-0.44498600	-0.48267100
C	5.53722700	-0.83177400	0.19034100
C	5.88142700	-1.63934600	-0.90802900
C	6.49351800	-0.55092700	1.17884700
C	7.17025300	-2.15677000	-1.01103700
H	5.12782800	-1.84824300	-1.66202500
C	7.78550000	-1.06969900	1.07363300
H	6.22034600	0.07550300	2.02590600
C	8.12215300	-1.87222000	-0.02123700
H	7.43917100	-2.78185400	-1.85834900
H	8.52595500	-0.85053800	1.83815900
H	9.12725100	-2.27764700	-0.10574700
H	0.36604200	-0.01236200	-1.05577900
C	0.71409900	2.15246600	-0.93080800
C	1.77051200	2.17845900	-1.85460000
C	0.07426500	3.34918600	-0.58533800
C	2.19020800	3.38913400	-2.40085600
H	2.26491000	1.25215600	-2.13230200
C	0.49895000	4.55492200	-1.14774400
H	-0.76879300	3.33320600	0.09756300
C	1.56293000	4.59878400	-2.05917500
H	3.01223200	3.39391400	-3.11355200
H	-0.01650800	5.47516800	-0.88220000
C	2.01180500	5.90120600	-2.68020600
H	1.49771700	6.75748200	-2.23164100
H	3.09129000	6.05156400	-2.55583600

H	1.80573900	5.91622600	-3.75830400
Ni	-2.33607300	-0.79858300	0.30958500
Cl	-1.11235100	-2.58957600	-2.05842200
Cl	-5.23986800	0.47872700	0.01062200
O	-1.21527400	-2.66431600	-3.52273800
O	-1.74052400	-1.23078700	-1.61868600
O	-3.79364500	0.42052600	-0.53250000
O	-5.78426200	-0.91974100	0.01499900
O	0.29762300	-2.61437600	-1.59098000
O	-1.90794700	-3.68704500	-1.39887800
O	-5.17063800	0.99732400	1.42693400
O	-6.02583600	1.37304800	-0.84280500
O	-3.51395800	-2.48312700	0.46419100
H	-4.41520200	-2.22452400	0.16750800
H	-3.13524400	-3.10439400	-0.20369000
O	-2.93150700	-0.31634400	2.26897800
H	-3.72914800	0.26589200	2.18171200
H	-3.25586600	-1.14614300	2.65954600

IM6ab

C	5.23863900	-0.47718800	-1.21593600
C	4.62477300	0.62932800	-0.61125700
C	3.61840600	0.46650200	0.34170700
C	3.18972000	-0.81970900	0.69791300
C	3.79443900	-1.93624900	0.10222900
C	4.80822000	-1.76010800	-0.83875700
H	4.93495400	1.63436800	-0.88617900
H	3.15743000	1.34292200	0.78983000
H	3.47483500	-2.93399100	0.38566600
H	5.27671900	-2.63487100	-1.28550000
C	6.33782700	-0.30277500	-2.23834100
H	6.07373600	-0.77782500	-3.19155800
H	6.53663200	0.75541800	-2.43519300
H	7.27410500	-0.76245300	-1.89703500
C	2.13264100	-0.96676000	1.73557300
H	2.22644900	-0.31329900	2.60479000
O	1.62697000	-2.26026600	2.04151100
C	0.69957800	-1.37841500	1.44182500
C	-0.37912600	-0.81353700	2.33443500
C	0.28919600	-1.63655700	0.01304400
O	-0.22037400	-1.14260200	3.59973800
O	0.73930200	-2.76676200	-0.47093800
C	-1.18728700	-0.60290000	4.54094000
H	-0.87185100	-0.98631100	5.50986700

H	-1.15778900	0.48825000	4.51589300
H	-2.18719200	-0.95601800	4.28175800
C	0.38613200	-3.07851100	-1.85156100
H	0.83837300	-2.33791400	-2.51421300
H	0.80744000	-4.06764900	-2.02266900
H	-0.69970400	-3.07768100	-1.95413900
O	-1.29745700	-0.09419000	1.94476300
O	-0.38641600	-0.84259500	-0.64181300
Ni	-1.54857700	0.72836700	0.04812900
O	-3.34317600	-0.28074700	-0.18546300
O	0.20847500	1.80388000	0.46871800
Cl	0.49963300	3.18132300	-0.18352800
O	-2.90327400	-2.61242500	-0.86820500
O	-0.63761400	4.09312600	0.17167600
O	1.77834900	3.66922900	0.35963600
O	-5.06806600	-1.55623700	-1.34133500
O	0.56765600	2.98621000	-1.66423900
Cl	-3.61053600	-1.36847100	-1.26791200
O	-3.05907400	-0.85151400	-2.57204400
O	-2.69335200	2.28608100	0.81370900
H	-2.18678800	3.10892800	0.62521200
H	-3.51624400	2.33134700	0.29763000
O	-1.80460800	1.49493700	-1.85237100
H	-0.98107200	1.87140900	-2.22278500
H	-2.13220600	0.75485700	-2.41216300

IM6ac

C	-5.07809200	-2.02242300	1.02214900
C	-4.18068500	-1.29976200	1.82665000
C	-3.40156600	-0.27361500	1.29795300
C	-3.48816000	0.04357400	-0.06782000
C	-4.37982200	-0.66653200	-0.88115300
C	-5.16593300	-1.68405500	-0.33563500
H	-4.09263600	-1.53971900	2.88384200
H	-2.72209500	0.27223500	1.94626300
H	-4.46331400	-0.41348600	-1.93327000
H	-5.86349000	-2.21907300	-0.97645400
C	-5.92827800	-3.12180100	1.61506000
H	-5.30683300	-3.90056300	2.07464100
H	-6.58832400	-2.73215700	2.40036300
H	-6.55682900	-3.59746300	0.85515900
C	-2.68453300	1.17750100	-0.59879000
H	-2.66921900	2.07863600	0.01334300
O	-2.66481200	1.42486500	-1.99388900

C	-1.41485300	1.03979600	-1.44382600
C	-0.38074900	2.13362500	-1.31053500
C	-0.89700800	-0.32686100	-1.79186300
O	-0.89583900	3.33243400	-1.45765500
O	-1.75219800	-1.05547900	-2.47495800
C	-0.01423300	4.46065600	-1.20419500
H	-0.63155000	5.33820900	-1.38923100
H	0.32316900	4.42198500	-0.16697900
H	0.83754000	4.42469000	-1.88583500
C	-1.37402900	-2.43043800	-2.75205000
H	-1.12228500	-2.94068000	-1.82080900
H	-2.25352800	-2.86923600	-3.22002700
H	-0.51958300	-2.44734500	-3.43192100
O	0.81705600	1.94494000	-1.08772000
O	0.21730600	-0.74846700	-1.47005600
Ni	1.71475500	0.21127700	-0.35760300
O	0.39746100	0.23447700	1.28443700
O	2.38485100	-1.67999000	0.25333400
Cl	3.87772600	-2.08016700	0.29063500
O	-0.66914900	2.43463700	1.57467900
O	4.59333300	-1.12105400	1.19319900
O	3.97859800	-3.46316500	0.76549600
O	-0.56003500	0.85046200	3.43876000
O	4.41908800	-1.94446700	-1.11267300
Cl	0.15258400	1.40148700	2.27395800
O	1.48095800	1.98048800	2.66423500
O	3.19324100	1.23005000	0.64249500
H	2.76841600	1.61354900	1.44449500
H	3.84715400	0.56995800	0.96799000
O	2.91296200	0.10737500	-2.08155300
H	3.60302200	-0.57911400	-1.89404400
H	2.38706100	-0.25345300	-2.81343100

IM6ad

C	-5.58528100	1.79658200	0.31579000
C	-4.88407300	1.94389300	-0.89011200
C	-3.99701800	0.96088300	-1.33196100
C	-3.77749800	-0.19224400	-0.56520100
C	-4.47967800	-0.35623200	0.63737500
C	-5.37157900	0.62731000	1.06398100
H	-5.04072900	2.83273400	-1.49672000
H	-3.47849500	1.09059600	-2.28029100
H	-4.33278500	-1.25720300	1.22383700
H	-5.91785400	0.48103100	1.99349700

C	-6.54495100	2.85839500	0.80019600
H	-6.16202300	3.35595200	1.70067700
H	-6.70893800	3.62853200	0.03967400
H	-7.51910700	2.42665100	1.05923400
C	-2.83330900	-1.22365100	-1.07749000
H	-2.86238200	-1.38246200	-2.15790300
O	-2.60427100	-2.41363000	-0.33344200
C	-1.49402600	-1.54988700	-0.44784800
C	-0.38833500	-1.95470000	-1.39753900
C	-1.04279600	-0.81287300	0.78960900
O	-0.62478300	-3.10089500	-1.99357600
O	-1.66925800	-1.16883500	1.87799700
C	0.39598100	-3.58640500	-2.90641200
H	0.00446600	-4.53105300	-3.28018500
H	0.54339100	-2.86858600	-3.71579600
H	1.32693900	-3.73482800	-2.35619400
C	-1.23840100	-0.53825900	3.12256200
H	-1.42936400	0.53531100	3.07131200
H	-1.84699600	-1.01257500	3.89042900
H	-0.17578600	-0.73605600	3.27107300
O	0.58684300	-1.25040700	-1.65356100
O	-0.19071200	0.08080000	0.76266700
Ni	1.39961000	0.30826400	-0.53739500
O	2.67515500	-1.02853400	0.36720200
O	2.00302400	1.94177200	0.65389300
Cl	2.91973600	3.06380100	0.11781000
O	1.01818400	-2.78999700	0.86526300
O	2.62415700	3.16651300	-1.38685800
O	2.55952200	4.31655000	0.79715900
O	3.40399500	-3.13136100	1.34873700
O	4.33354800	2.68143100	0.29666100
Cl	2.29060800	-2.16691200	1.36422200
O	2.07432400	-1.56656900	2.70169400
O	2.99032100	0.45382800	-1.87962600
H	3.24507800	1.39845200	-1.96190700
H	3.73471300	-0.00785600	-1.45235200
O	0.28609400	1.74647300	-1.62851000
H	-0.38232700	2.09966900	-1.01664900
H	0.95390900	2.46919000	-1.72252900
IM6bc			
C	5.78444000	-0.83717400	-0.43401100
C	4.80182400	-1.03013000	-1.41885300
C	3.69472000	-0.19115800	-1.50285800

C	3.53178700	0.85948000	-0.58699100
C	4.50915400	1.07013200	0.39344200
C	5.62199900	0.23029200	0.46099800
H	4.90077600	-1.85066800	-2.12551500
H	2.94613700	-0.36816000	-2.27131700
H	4.40282200	1.89633100	1.08856800
H	6.38022700	0.41215700	1.21959800
C	6.97356800	-1.76420400	-0.34029300
H	6.67722100	-2.74159200	0.06317700
H	7.41962400	-1.94394600	-1.32551400
H	7.75059800	-1.35621700	0.31461900
C	2.37432200	1.77456300	-0.75015300
H	2.13821900	2.03566800	-1.78400700
O	2.18185400	2.84054500	0.15732700
C	1.13296400	1.88238900	0.15188500
C	-0.13464900	2.32412900	-0.54027600
C	0.96903400	1.02768800	1.38265800
O	0.03370000	3.42105700	-1.25346600
O	2.01757600	1.05974800	2.17289200
C	-1.11314600	3.88525900	-2.01633900
H	-0.75303000	4.76570300	-2.54596000
H	-1.43669600	3.10656200	-2.70980600
H	-1.92816600	4.13964900	-1.33612600
C	1.99879900	0.16978400	3.32130200
H	1.86678900	-0.85815100	2.97989200
H	2.96967900	0.31007100	3.79368000
H	1.18875300	0.45678300	3.99491800
O	-1.21085500	1.73139500	-0.50060100
O	-0.04017100	0.37366800	1.65135600
Ni	-1.68535600	-0.04240500	0.44901000
O	-0.41509500	-0.99017900	-0.91344600
O	-3.27992900	-0.25147700	-0.90080700
Cl	-4.74264400	-0.43966600	-0.44721100
O	1.53811900	-1.84477200	0.32405000
O	-5.13544300	0.77995900	0.35017600
O	-5.58977200	-0.59332300	-1.63294700
O	-0.43880800	-3.27046400	0.04725000
O	-4.79285800	-1.65056900	0.44260000
Cl	0.44903900	-2.24635900	-0.60579300
O	0.97444100	-2.73805300	-1.89054700
O	-2.21061700	-1.75661200	1.48079900
H	-3.12904400	-1.96853100	1.19336200
H	-1.63479900	-2.47524100	1.12228600
O	-2.85054000	1.04468100	1.82231200

H	-3.76264000	1.11940800	1.44306600
H	-2.93693000	0.51880600	2.63521900

IM6bd

C	-5.79378800	-0.78172000	-1.24980900
C	-4.80781600	-1.77809900	-1.31460400
C	-3.74625500	-1.80161100	-0.40971700
C	-3.63640700	-0.81117300	0.57664600
C	-4.61478200	0.18975600	0.65328400
C	-5.67750400	0.19737900	-0.25017400
H	-4.87504300	-2.55017400	-2.07750100
H	-2.99713900	-2.58763500	-0.47561600
H	-4.54331400	0.95032200	1.42395900
H	-6.43407400	0.97553800	-0.17337700
C	-6.96441400	-0.77676500	-2.20526400
H	-7.17526300	0.23320900	-2.57541500
H	-6.78016200	-1.42316000	-3.06955500
H	-7.87632800	-1.13754100	-1.71111200
C	-2.51144900	-0.88496300	1.54862500
H	-2.27661700	-1.88519700	1.91849400
O	-2.35592800	0.13480000	2.52434300
C	-1.32040200	0.05867600	1.56507900
C	-0.00621300	-0.52779500	2.02512600
C	-1.22797000	1.15751100	0.53129300
O	-0.04802600	-1.00177300	3.24924300
O	-2.09116700	2.12356700	0.71887400
C	1.17564000	-1.62513100	3.74533500
H	0.90457800	-2.01406200	4.72515000
H	1.49274600	-2.41680500	3.06482500
H	1.95788800	-0.86767200	3.82063600
C	-2.06597300	3.22763600	-0.23462700
H	-2.31499200	2.85209700	-1.22911000
H	-2.82723500	3.91624900	0.12804800
H	-1.07443200	3.68110700	-0.22778300
O	0.99668400	-0.60691000	1.31858300
O	-0.43935400	1.13016700	-0.41437200
Ni	1.29939500	0.00364500	-0.61556900
O	3.38227800	-2.69301200	0.91034200
O	2.51481400	1.53740300	0.09830600
Cl	3.25559100	-2.59950200	-0.55847000
Cl	2.25337200	3.04613700	-0.13759800
O	4.46039800	-3.05373500	-1.26751600
O	3.01814100	-1.11355100	-0.95972100
O	3.50388200	3.76607500	0.14104300

O	1.84359600	3.20927800	-1.58703600
O	2.03786600	-3.37861700	-1.02486900
O	1.14526100	3.48512700	0.75215500
O	0.09648900	-1.56204800	-1.33541000
H	-0.07314100	-1.37286700	-2.27360600
H	0.70003900	-2.35408600	-1.31149900
O	1.58370200	0.67853300	-2.56416800
H	1.68843800	1.65719900	-2.43676100
H	2.46352700	0.34397700	-2.81620700

IM6cd

C	-5.36953100	-0.11104200	-1.41169100
C	-4.22834100	-0.11734300	-2.23124900
C	-3.08682900	-0.82753400	-1.86907900
C	-3.05012600	-1.54008800	-0.65983900
C	-4.18468200	-1.55212200	0.16076900
C	-5.32848100	-0.84704800	-0.21894200
H	-4.23475200	0.44081900	-3.16463000
H	-2.21653300	-0.82132600	-2.52068600
H	-4.17245000	-2.12026600	1.08511600
H	-6.20620800	-0.87389200	0.42293800
C	-6.59636700	0.67687000	-1.80591700
H	-6.42697700	1.75411900	-1.67791500
H	-6.85566100	0.51333300	-2.85846200
H	-7.46310900	0.40187000	-1.19614900
C	-1.82989400	-2.31958600	-0.32230900
H	-1.36710500	-2.85289100	-1.15485600
O	-1.75748400	-3.01456800	0.91043600
C	-0.82394600	-1.95848300	0.76837200
C	0.61513900	-2.35631800	0.53381800
C	-1.01943100	-0.72127000	1.60655100
O	0.76299700	-3.63889300	0.28934400
O	-2.11153800	-0.73316800	2.33131200
C	2.11690100	-4.10271200	-0.00292500
H	1.98295900	-5.11670800	-0.37584800
H	2.58874000	-3.45024800	-0.73864100
H	2.69706400	-4.10093300	0.92234500
C	-2.40570300	0.47839500	3.09276000
H	-2.32096100	1.35384900	2.44774800
H	-3.42176500	0.33214000	3.45488600
H	-1.70074600	0.55559600	3.92318100
O	1.55861900	-1.56518000	0.54845300
O	-0.22702000	0.22387600	1.61493300
Ni	1.40781400	0.52802600	0.36525800

O	4.68845400	-0.40833500	0.36060700
O	1.11265300	2.57945500	0.27783800
Cl	4.22114900	-0.22398800	-1.06194500
Cl	-0.25388300	3.29643100	0.13251600
O	5.23335000	0.46455200	-1.87415400
O	2.96177700	0.69576600	-1.00808200
O	0.01344000	4.67251900	-0.30867700
O	-1.04900100	2.53959800	-0.91931900
O	3.82460400	-1.52804400	-1.65208600
O	-0.97644500	3.24961000	1.42628300
O	0.26889600	0.25748000	-1.37128700
H	-0.28640400	1.08426700	-1.39721700
H	0.96476000	0.37283200	-2.04528400
O	2.76543700	0.77805900	1.91220700
H	2.56994200	0.32470500	2.74647700
H	3.60474300	0.39435000	1.55567700

IM7ab

C	1.27290300	2.70864400	0.22963300
H	0.25135100	2.29599000	0.12512600
C	1.39077600	4.15691600	-0.01416600
C	2.63365000	4.81130600	0.07018700
C	0.23228000	4.88379200	-0.33667700
C	2.71258500	6.18021400	-0.16697600
H	3.51791700	4.23179200	0.31952800
C	0.31685100	6.25766600	-0.57322100
H	-0.72768900	4.37687200	-0.40084800
C	1.55364100	6.90350500	-0.48860000
H	3.67024300	6.69044900	-0.10398500
H	-0.57905600	6.81942200	-0.82217100
H	1.61937200	7.97292700	-0.67322500
O	2.20755000	1.97036800	0.53063800
C	7.16549100	-1.82772200	-0.44326000
C	6.91811100	-1.02662700	0.68324800
C	5.61850400	-0.69828200	1.05419200
C	4.52316400	-1.16617300	0.29718000
C	4.76424400	-1.97554700	-0.83928000
C	6.06464200	-2.29305700	-1.19460900
H	7.75363200	-0.65842800	1.27270900
H	5.44150300	-0.07363300	1.92612900
H	3.92490300	-2.34207800	-1.42194100
H	6.24311100	-2.91613300	-2.06778600
C	8.57063200	-2.19199300	-0.84994900
H	8.78922400	-1.83885300	-1.86569200

H	9.31275900	-1.75806400	-0.17327300
H	8.70867600	-3.28067300	-0.85264900
C	3.20775900	-0.79521500	0.71565900
H	3.03700700	-0.18901900	1.59607000
O	2.20126100	-1.18858500	0.02634800
C	0.85096200	-0.95037700	0.19871800
C	0.26570800	-0.64206200	1.46309400
C	0.08746900	-1.18159800	-0.99374000
O	1.12661100	-0.62678900	2.50079100
O	0.80779900	-1.58577300	-2.04583700
C	0.54708400	-0.41303600	3.80870700
H	1.39114500	-0.45393500	4.49744600
H	0.05749200	0.56216300	3.84888200
H	-0.17731800	-1.19890700	4.03243800
C	0.06077400	-1.92037600	-3.23815100
H	-0.46440100	-1.03924800	-3.61427100
H	0.81425000	-2.25364000	-3.95199300
H	-0.65197400	-2.71817400	-3.01987400
O	-0.94311300	-0.42510800	1.66981400
O	-1.14202700	-1.00812800	-1.10497200
Ni	-2.49163800	-0.62419000	0.36302200
O	-2.74764300	-2.63535600	0.91468500
O	-2.30534500	1.46720500	-0.05119200
Cl	-3.51037300	2.32351400	-0.49316100
O	-1.12994000	-4.02441000	-0.32985900
O	-4.56167500	2.21505200	0.57447900
O	-3.04824000	3.71723800	-0.64720000
O	-3.16689300	-5.01806300	0.61192900
O	-4.02751100	1.77921400	-1.78747600
Cl	-2.57759400	-3.84008400	-0.05044500
O	-3.31564000	-3.51087900	-1.32450300
O	-3.88804000	-0.19398400	1.86129700
H	-4.32431400	0.64129700	1.57618100
H	-4.56321600	-0.89175600	1.81111200
O	-4.09557400	-0.89249800	-0.93418500
H	-4.14744500	-0.18774900	-1.61057200
H	-3.95186000	-1.76751200	-1.36063700
IM7ac			
C	3.29038000	2.11230800	0.34527400
H	2.23665000	2.02053200	0.03506700
C	3.92164300	3.41070100	0.04988700
C	5.25804600	3.67666200	0.39843000
C	3.15519400	4.39331700	-0.59934500

C	5.81919000	4.91423800	0.09663200
H	5.83408800	2.90569900	0.90233500
C	3.72180800	5.63307700	-0.90153400
C	5.05128400	5.89175500	-0.55424300
H	6.85141900	5.12488200	0.36394800
H	3.13086100	6.39240000	-1.40605100
H	5.49353800	6.85660800	-0.78960100
O	3.85187400	1.16719600	0.89714000
C	5.75071600	-4.02415800	-0.58064400
C	5.85291800	-2.67984100	-0.18977700
C	4.72413500	-1.94743900	0.16415600
C	3.45066500	-2.55907400	0.13281500
C	3.33780500	-3.91583400	-0.26039500
C	4.47272400	-4.62619700	-0.60950300
H	6.82915400	-2.20285600	-0.16434300
H	4.80642400	-0.90597600	0.46204900
H	2.35961600	-4.38564500	-0.28741700
H	4.38255400	-5.66669900	-0.91251800
C	6.97034000	-4.82002100	-0.96902000
H	6.90434000	-5.15173900	-2.01329600
H	7.88759800	-4.23432400	-0.85775200
H	7.06431500	-5.72238200	-0.35181900
C	2.32158900	-1.76822300	0.50367900
H	2.43960800	-0.72897300	0.79920800
O	1.15761800	-2.31325300	0.49630700
C	-0.07588300	-1.74725600	0.79004900
C	-0.23573500	-0.63229900	1.66312300
C	-1.16790800	-2.38355400	0.12956100
O	0.87029200	-0.27497000	2.33343800
O	-0.84788400	-3.47881100	-0.57206100
C	0.76996000	0.89113300	3.18344700
H	1.78706300	1.06775800	3.53233000
H	0.39807500	1.73890200	2.60515700
H	0.10098600	0.68499000	4.02259300
C	-1.91192200	-4.07768600	-1.34504800
H	-2.34299200	-3.34258500	-2.02787000
H	-1.43320100	-4.88768700	-1.89547500
H	-2.69009900	-4.46740700	-0.68435100
O	-1.31183500	-0.02526300	1.85934500
O	-2.35727900	-1.98988400	0.17495400
Ni	-2.84679600	-0.02085600	0.50802600
O	-1.71945900	0.57036300	-1.15558200
O	-4.44303200	-0.20969900	-0.89642700
Cl	-5.85672500	0.34898000	-0.67497900

O	-0.19360500	2.22602400	-0.11803600
O	-5.74644300	1.83447700	-0.46509300
O	-6.68980400	0.02969300	-1.83948600
O	0.72359900	0.29428500	-1.29750400
O	-6.40967200	-0.28954800	0.57962900
Cl	-0.37564700	1.31589300	-1.28940600
O	-0.40831100	2.06410000	-2.56162900
O	-3.39707600	1.92663600	0.98858200
H	-4.21952400	2.14729800	0.48868700
H	-3.61802600	1.99660900	1.93150300
O	-4.14597000	-0.69268300	2.04664900
H	-5.05906000	-0.66433300	1.66337500
H	-3.93052300	-1.63170200	2.17062400
H	2.12198400	4.17878200	-0.86363300

IM7ad

C	-7.34155000	-1.75091900	0.91909100
C	-7.12316200	-1.09710500	-0.30450800
C	-5.83854300	-0.75104000	-0.70928000
C	-4.72967500	-1.05104000	0.11095400
C	-4.94160300	-1.71103300	1.34568800
C	-6.22729400	-2.04899600	1.73335700
H	-7.96961600	-0.86012600	-0.94352900
H	-5.68345200	-0.24294100	-1.65770800
H	-4.09120500	-1.94837800	1.97707600
H	-6.38369600	-2.55755400	2.68168000
C	-8.72986700	-2.13572300	1.36251700
H	-8.97485700	-1.67693900	2.32873100
H	-9.48709600	-1.82419500	0.63704000
H	-8.81222000	-3.22217900	1.49376100
C	-3.43128900	-0.66866800	-0.34645300
H	-3.28162100	-0.18449000	-1.30327000
O	-2.41356200	-0.90069500	0.39780500
C	-1.07594000	-0.61578000	0.18753200
C	-0.50261300	-0.48320500	-1.11377000
C	-0.30891500	-0.61258400	1.39905100
O	-1.35611300	-0.66179200	-2.13375500
O	-1.02506800	-0.83377700	2.51198500
C	-0.77237600	-0.74333500	-3.45822800
H	-1.61725900	-0.93187900	-4.12079600
H	-0.28425500	0.20023900	-3.71093700
H	-0.05625200	-1.56555600	-3.49073200
C	-0.27576600	-0.88714400	3.74747400
H	0.21150500	0.07181800	3.93763300

H	-1.02025800	-1.10242000	4.51406100
H	0.47710500	-1.67689900	3.70033500
O	0.69623300	-0.22379000	-1.34566200
O	0.91645100	-0.40176000	1.48072200
Ni	2.25964800	-0.38145400	-0.04175500
O	2.20620800	-2.48795700	-0.06136700
O	3.79926800	-0.51730000	1.40730800
Cl	1.91290700	-3.35986500	-1.30309500
Cl	5.07854400	0.33476100	1.37483200
O	2.36690200	-4.72941600	-1.00972000
O	2.67746900	-2.77341400	-2.46836000
O	5.76807500	0.09249000	0.06231300
O	4.66352700	1.78679100	1.46005600
O	0.45114400	-3.31303100	-1.58808100
O	5.92883500	-0.03373100	2.51263800
C	-1.46172300	2.84875300	-0.31030600
H	-0.54782400	2.32145100	0.02485600
C	-1.32534600	4.31207600	-0.42232600
C	-2.40357200	5.11959200	-0.82614100
C	-0.08493500	4.89665200	-0.11683600
C	-2.23757200	6.49849700	-0.92048600
H	-3.35503900	4.64974200	-1.05795400
C	0.07799500	6.27984800	-0.21185000
H	0.74343600	4.26207000	0.19181600
C	-0.99759200	7.07834100	-0.61320600
H	-3.06756800	7.12728400	-1.23154900
H	1.03635800	6.73348700	0.02511300
H	-0.87245700	8.15558100	-0.68770400
O	-2.47977500	2.21281000	-0.56055500
O	3.59507700	-0.32037800	-1.63578600
H	3.44404400	-1.18095700	-2.09640700
H	4.50263900	-0.33882900	-1.25702600
O	2.39170000	1.74891200	-0.06299900
H	2.69823300	1.91936100	-0.97091200
H	3.16356300	1.96495500	0.52006100

IM7bc

C	-7.38310800	-0.93505500	-0.46673100
C	-6.70110000	0.29137700	-0.40213200
C	-5.31176100	0.33508200	-0.38213400
C	-4.56941300	-0.86788300	-0.42562600
C	-5.24892200	-2.10975800	-0.49616300
C	-6.63179800	-2.13179800	-0.51354200
H	-7.26806400	1.21763900	-0.36584700

H	-4.78341800	1.28324500	-0.32823900
H	-4.67773200	-3.03189400	-0.53636000
H	-7.15375300	-3.08412700	-0.56640000
C	-8.88846400	-0.98917700	-0.48997200
H	-9.27133000	-1.57706800	0.35384400
H	-9.33080600	0.00971500	-0.43743000
H	-9.24801700	-1.47402400	-1.40656700
C	-3.15173300	-0.76253900	-0.37610400
H	-2.67453700	0.21924300	-0.33539900
O	-2.42294700	-1.82105200	-0.35602700
C	-1.43462400	2.72455400	0.42564100
H	-0.85209100	2.05302700	1.07875800
C	-0.91299200	4.09367400	0.30903400
C	-1.57018500	5.06401700	-0.47029200
C	0.27305200	4.41915500	0.99010600
C	-1.04384500	6.34862700	-0.56240800
H	-2.48392100	4.79202800	-0.99092400
C	0.79778000	5.70923900	0.89216300
H	0.77386700	3.66046900	1.58668100
C	0.14058800	6.67035800	0.11846000
H	-1.54649000	7.10277200	-1.16228500
H	1.71657700	5.96198400	1.41367200
H	0.55019800	7.67448300	0.04157500
O	-2.43972400	2.30231800	-0.14759800
C	-1.01260900	-1.73632200	-0.41775500
C	-0.39459400	-0.96602900	-1.43816500
C	-0.32195100	-2.56524500	0.50815200
O	-1.24916700	-0.40516900	-2.32028400
O	-1.11891100	-3.30353200	1.29194800
C	-0.65755500	0.38852000	-3.37275000
H	-1.50480100	0.78442000	-3.93283600
H	-0.05899900	1.19688100	-2.94781400
H	-0.02851300	-0.23784400	-4.00936700
C	-0.47258400	-4.04085000	2.35160500
H	0.05549100	-3.35090700	3.01320900
H	-1.28591300	-4.53911300	2.87968700
H	0.22496300	-4.77313000	1.93805400
O	0.83535300	-0.80618600	-1.58043900
O	0.92312800	-2.63479600	0.62501800
Ni	2.23178100	-1.29054000	-0.18220100
O	1.46990100	0.29943700	1.03031600
O	3.49597300	0.16270000	-1.07550600
Cl	4.98603000	-0.06728400	-1.37661900
O	-0.19669800	-0.44252400	2.68784600

O	5.08932800	-1.23363200	-2.32825700
O	5.54466600	1.15266500	-1.97388300
O	2.19567900	-0.55128900	3.23520200
O	5.67350900	-0.41477400	-0.08503700
Cl	1.12184700	0.23173900	2.53070800
O	1.06839300	1.62484600	3.03164500
O	3.65932200	-1.80627300	1.24304800
H	4.48119500	-1.31055100	1.02378400
H	3.31471200	-1.43926100	2.08929400
O	3.03404400	-2.81510600	-1.39509500
H	3.80089800	-2.42238100	-1.87958400
H	3.40684500	-3.47699100	-0.78887400

IM7bd

C	-7.49976600	-0.32904700	-0.44607700
C	-6.96020400	0.84098200	-1.00484700
C	-5.58808100	1.06588200	-1.00201800
C	-4.71403500	0.11630300	-0.43099700
C	-5.24982200	-1.06568000	0.13499500
C	-6.61867200	-1.27401500	0.12316600
H	-7.62446700	1.58069700	-1.44363000
H	-5.18365300	1.97924500	-1.43056900
H	-4.58019800	-1.80022600	0.57116800
H	-7.02473700	-2.18444800	0.55746100
C	-8.98506100	-0.58549100	-0.45445500
H	-9.35978000	-0.76286100	0.56130600
H	-9.53862500	0.25719400	-0.87902100
H	-9.22394300	-1.47956100	-1.04476300
C	-3.31313900	0.39504100	-0.44852200
H	-2.91496700	1.28665200	-0.91732500
O	-2.50665300	-0.43624400	0.10134000
C	-1.37749600	2.79772500	1.59480300
H	-0.94177200	2.11157900	2.34903200
C	-0.43202100	3.76666100	1.01291600
C	-0.88164900	4.82358200	0.19971100
C	0.94237300	3.59755100	1.24873600
C	0.04008300	5.70085000	-0.36448000
H	-1.94823300	4.94220200	0.03077600
C	1.86666100	4.46255000	0.65944100
H	1.28455700	2.76803400	1.86324200
C	1.41342800	5.51574200	-0.14030200
H	-0.30168500	6.52617500	-0.98370000
H	2.93014300	4.30171700	0.80767200
H	2.13082300	6.19267000	-0.59703400

O	-2.56128800	2.69690000	1.29084700
C	-1.13164400	-0.42181100	0.25062500
C	-0.25645800	0.34617500	-0.57675600
C	-0.66965400	-1.39274800	1.20514900
O	-0.86279100	1.08791000	-1.52097800
O	-1.64315900	-2.06735200	1.82326900
C	0.01649600	1.77750500	-2.45112600
H	-0.65784200	2.27783300	-3.14590100
H	0.63840800	2.49681200	-1.91717300
H	0.65090900	1.05475400	-2.96692400
C	-1.22244200	-3.14577000	2.69021200
H	-0.62277300	-2.75543000	3.51577500
H	-2.15069500	-3.58089400	3.06070200
H	-0.64778800	-3.87684500	2.11839300
O	0.98550300	0.36591700	-0.48654500
O	0.52541100	-1.60846600	1.49295600
Ni	2.16314000	-0.97127700	0.46178500
O	3.75840100	1.69357500	-1.75238300
O	1.82214000	-2.33249900	-1.12118800
Cl	4.53557800	1.00739500	-0.69987100
Cl	1.28262000	-3.77163200	-0.95188000
O	5.95949300	0.86392000	-1.04780900
O	3.96598100	-0.41831500	-0.48225100
O	1.57079700	-4.51090700	-2.19224300
O	2.00462700	-4.39491900	0.22540900
O	4.38905000	1.74833000	0.62033000
O	-0.17712300	-3.71012900	-0.67056800
O	2.58384100	0.35735200	2.04946100
H	2.99360700	-0.18991500	2.74003100
H	3.30372300	0.93530200	1.68240100
O	3.40759500	-2.37467100	1.39518300
H	3.01465400	-3.23832800	1.10705800
H	4.24907200	-2.28970300	0.91112800
IM7cd			
C	-7.15821300	-1.84463800	-0.03906500
C	-6.82115400	-1.04187700	-1.14067800
C	-5.49097500	-0.80653000	-1.47210800
C	-4.45547300	-1.37590100	-0.70161000
C	-4.78668500	-2.18577400	0.41123300
C	-6.11614000	-2.40956100	0.72799500
H	-7.61061300	-0.59678800	-1.74043000
H	-5.24337200	-0.17474100	-2.32117200
H	-3.99290300	-2.62383900	1.00829500

H	-6.36481800	-3.03186000	1.58435400
C	-8.59698400	-2.10257800	0.32939400
H	-8.81883400	-1.71875900	1.33342100
H	-9.28635500	-1.62678200	-0.37430700
H	-8.81259300	-3.17831900	0.34294200
C	-3.10487600	-1.10223200	-1.08176500
H	-2.86554900	-0.48736300	-1.93774200
O	-2.15315000	-1.61484700	-0.39510200
C	-1.84675300	2.27279400	0.15836800
H	-0.85795400	1.87162900	0.44722700
C	-2.09290200	3.68051800	0.51389900
C	-3.30115900	4.31563500	0.17441000
C	-1.09074700	4.39664800	1.18834400
C	-3.49934900	5.65214300	0.50733100
H	-4.06423900	3.74739500	-0.34944400
C	-1.29090600	5.73825100	1.51829600
H	-0.15576000	3.90562000	1.45184000
C	-2.49415500	6.36370200	1.17814600
H	-4.43089100	6.14700100	0.24584400
H	-0.51450900	6.29267000	2.03775700
H	-2.65139700	7.40839800	1.43392800
O	-2.64799400	1.55864900	-0.43712200
C	-0.77446000	-1.51362700	-0.48552800
C	-0.04902800	-1.05187700	-1.63190900
C	-0.11760800	-2.05098000	0.66798700
O	-0.79654000	-0.76092100	-2.71150000
O	-0.93101800	-2.58753300	1.58346700
C	-0.07542800	-0.33196700	-3.89952200
H	-0.84894900	0.03001400	-4.57675500
H	0.64347900	0.44870000	-3.64984700
H	0.45105900	-1.18496700	-4.33411600
C	-0.29294800	-3.12264500	2.77347400
H	0.37168300	-2.38275200	3.22110900
H	-1.11971200	-3.37444200	3.43755900
H	0.28115900	-4.01560000	2.51463600
O	1.19723200	-0.95239300	-1.68893500
O	1.11491700	-2.05214900	0.84657800
Ni	2.45395900	-0.79359500	-0.05123200
O	4.32937900	-0.75098600	-2.93993900
O	3.69510400	-0.66012600	1.63013200
Cl	4.08986700	0.67162600	-2.49653500
Cl	3.27094800	-0.41637500	3.09387900
O	5.31433200	1.47940600	-2.61837400
O	3.71051700	0.61921400	-0.99029700

O	4.45507700	0.05342400	3.83107900
O	2.19420600	0.66156800	3.08217200
O	2.95892300	1.26879900	-3.25205900
O	2.71086300	-1.66262000	3.66759800
O	1.47155100	0.98539300	0.52233100
H	1.71431100	1.05604800	1.48611900
H	2.06096400	1.60141700	0.04688400
O	3.61924100	-2.34161000	-0.81536800
H	3.07619000	-3.10059100	-1.07923000
H	3.98942800	-1.95387400	-1.64667500

IM8ab

C	1.27258800	2.70849600	0.22839800
H	0.25083400	2.29631900	0.12399800
C	1.39114600	4.15676100	-0.01518500
C	2.63440100	4.81044400	0.06911400
C	0.23302600	4.88433500	-0.33743700
C	2.71408600	6.17933900	-0.16785000
H	3.51836200	4.23038000	0.31826000
C	0.31835300	6.25820700	-0.57378000
H	-0.72726200	4.37801300	-0.40164900
C	1.55550900	6.90333800	-0.48921400
H	3.67204100	6.68902700	-0.10491800
H	-0.57726400	6.82050100	-0.82255100
H	1.62182800	7.97274900	-0.67369100
O	2.20695000	1.96976400	0.52914900
C	7.16530100	-1.82882000	-0.44274100
C	6.91804800	-1.02834100	0.68423400
C	5.61850400	-0.69980000	1.05522200
C	4.52309400	-1.16691200	0.29782500
C	4.76404700	-1.97569700	-0.83907800
C	6.06438800	-2.29339800	-1.19445900
H	7.75361900	-0.66079200	1.27403000
H	5.44160500	-0.07563800	1.92752900
H	3.92465300	-2.34164100	-1.42203200
H	6.24274800	-2.91603700	-2.06797000
C	8.57039500	-2.19296800	-0.84970900
H	8.79017200	-1.83585300	-1.86382400
H	9.31241800	-1.76249900	-0.17071200
H	8.70733900	-3.28174800	-0.85678700
C	3.20775400	-0.79581300	0.71640400
H	3.03712200	-0.18989600	1.59703200
O	2.20120700	-1.18877100	0.02695500
C	0.85091900	-0.95044900	0.19909900

C	0.26556700	-0.64179900	1.46336200
C	0.08765000	-1.18165100	-0.99353300
O	1.12639200	-0.62633800	2.50111100
O	0.80821300	-1.58591600	-2.04544800
C	0.54678400	-0.41210000	3.80891800
H	1.39075800	-0.45308600	4.49775800
H	0.05749100	0.56326300	3.84879600
H	-0.17788700	-1.19768900	4.03275700
C	0.06143700	-1.92062700	-3.23788000
H	-0.46396800	-1.03963800	-3.61399800
H	0.81509300	-2.25361600	-3.95166200
H	-0.65108600	-2.71866400	-3.01973400
O	-0.94325100	-0.42468700	1.66994500
O	-1.14180400	-1.00810900	-1.10509900
Ni	-2.49134800	-0.62406000	0.36277500
O	-2.74698100	-2.63536800	0.91412400
O	-2.30491300	1.46730600	-0.05166400
Cl	-3.51006100	2.32410900	-0.49241800
O	-1.13172300	-4.02487900	-0.33304900
O	-4.56026000	2.21614000	0.57631600
O	-3.04751600	3.71763000	-0.64700200
O	-3.16767500	-5.01784800	0.61159100
O	-4.02877400	1.77997400	-1.78617300
Cl	-2.57887200	-3.83998100	-0.05142900
O	-3.31869800	-3.51023900	-1.32434700
O	-3.88694400	-0.19367000	1.86208300
H	-4.32271900	0.64203100	1.57743100
H	-4.56265900	-0.89090200	1.81163500
O	-4.09650700	-0.89158500	-0.93272400
H	-4.14921200	-0.18682800	-1.60903900
H	-3.95414800	-1.76674600	-1.35936100

IM8ac

C	1.90292500	2.16363800	0.50034400
H	1.23942600	1.66832100	1.22622400
C	1.67880100	3.60798400	0.33179500
C	2.48147200	4.38227200	-0.52592600
C	0.62789600	4.20645000	1.04843600
C	2.23368200	5.74520700	-0.65979200
H	3.28722600	3.89971300	-1.07180900
C	0.38194300	5.57371800	0.90801100
H	0.01185500	3.59527700	1.70402600
C	1.18354300	6.34003900	0.05655200
H	2.85127200	6.34988500	-1.31881200

H	-0.43208300	6.03813700	1.45742300
H	0.99226000	7.40470400	-0.05248000
O	2.75752400	1.51367400	-0.10209700
C	7.03228300	-1.33790700	-0.15245700
C	6.31191600	-1.05932000	1.02119000
C	4.92511100	-0.96962900	1.00003700
C	4.22394200	-1.16109800	-0.20812700
C	4.93944000	-1.44372000	-1.39395900
C	6.32154600	-1.52692900	-1.35740700
H	6.84657700	-0.90893800	1.95513300
H	4.37439000	-0.74362200	1.90928100
H	4.39879300	-1.59264400	-2.32312300
H	6.87101300	-1.74254100	-2.27055800
C	8.53578400	-1.44226500	-0.13628200
H	8.98494500	-0.76226500	-0.87057400
H	8.94741000	-1.20163700	0.84822500
H	8.85906500	-2.45767900	-0.39981600
C	2.80085400	-1.06019300	-0.17788500
H	2.25763000	-0.90271400	0.75240200
O	2.11381300	-1.25528400	-1.24894800
C	0.69812400	-1.35896800	-1.12157500
C	0.16833100	-2.39467500	-0.31199200
C	-0.07593600	-0.44947800	-1.87553300
O	1.08762400	-3.23934700	0.19315200
O	0.62412400	0.35955300	-2.68638200
C	0.61165600	-4.20946800	1.15166600
H	1.50044400	-4.76684000	1.44908700
H	0.16740900	-3.69725600	2.00769200
H	-0.12084300	-4.87350200	0.68722900
C	-0.12720500	1.35386500	-3.41269200
H	-0.71002100	1.97126100	-2.72568800
H	0.62601800	1.95030300	-3.92785200
H	-0.79727500	0.87618200	-4.13228400
O	-1.04964600	-2.57941800	-0.07849300
O	-1.33060400	-0.36537700	-1.82844000
Ni	-2.42791700	-1.08475700	-0.24334800
O	-1.40127400	0.19534600	1.07238600
O	-3.78120000	0.54666100	-0.50189400
Cl	-5.31001500	0.41152800	-0.44420900
O	-1.61852700	-0.82560600	3.32038800
O	-5.68461800	-0.12955500	0.90709100
O	-5.91819200	1.72564300	-0.68625900
O	0.54415100	-0.85805500	2.16420300
O	-5.72146500	-0.58040400	-1.50940600

Cl	-0.71326600	-0.07304200	2.43045300
O	-0.35984700	1.26190500	2.98378500
O	-3.63007600	-1.97685500	1.20272200
H	-4.41675000	-1.40436300	1.36263100
H	-3.96742100	-2.82511000	0.87164000
O	-3.52349300	-2.19742400	-1.68720500
H	-4.37612200	-1.70790800	-1.80489400
H	-3.02078400	-2.06864300	-2.50876200

IM8ad

C	7.27639000	-0.85153000	-0.92245600
C	7.09672800	-0.59772700	0.44708600
C	5.82622700	-0.39253300	0.97379300
C	4.69400600	-0.43201100	0.13274100
C	4.86600700	-0.68920100	-1.24866700
C	6.13819700	-0.89224600	-1.75655300
H	7.96210200	-0.56338400	1.10355900
H	5.70135800	-0.19323500	2.03509000
H	3.99565300	-0.73341000	-1.89572800
H	6.26420400	-1.09489700	-2.81744600
C	8.64920400	-1.08377800	-1.50015800
H	8.88086400	-0.34045000	-2.27355700
H	9.42613600	-1.02701600	-0.73201300
H	8.71246400	-2.07087700	-1.97535100
C	3.40943900	-0.21482600	0.71992100
H	3.28576700	-0.07373600	1.78631500
O	2.37633400	-0.19470700	-0.03743000
C	1.03391400	-0.03304800	0.24215800
C	0.45476200	-0.31159200	1.51825300
C	0.24840500	0.17934600	-0.93980700
O	1.33828700	-0.56777400	2.50050600
O	0.95337800	0.32418600	-2.06373800
C	0.78841900	-1.10107200	3.73054600
H	1.65238600	-1.25642300	4.37697500
H	0.09207000	-0.38708400	4.17446300
H	0.28132100	-2.04470500	3.52117800
C	0.18967200	0.36558100	-3.29202700
H	-0.45698300	1.24567500	-3.30858100
H	0.93909100	0.42114600	-4.08166500
H	-0.41094200	-0.54143900	-3.38471500
O	-0.76694200	-0.31978000	1.76660400
O	-0.99853900	0.27059000	-0.96304100
Ni	-2.29430500	-0.49974100	0.41375500
O	-1.94724000	-2.55335700	0.09425700

O	-3.81562100	-0.60851400	-1.08429500
Cl	-0.63015300	-3.33567000	-0.18558100
Cl	-5.26500800	-0.13948000	-0.88078100
O	-1.01069100	-4.74419700	-0.40192400
O	0.25879200	-3.18647300	1.00800000
O	-5.84410700	-0.89551900	0.28311700
O	-5.23214200	1.33386300	-0.54488800
O	0.01682500	-2.73754700	-1.38716100
O	-6.02450100	-0.37984600	-2.11324800
C	1.71042700	2.97062800	1.65157100
H	1.23304500	2.68766900	2.61282800
C	0.87355200	3.80369100	0.76577500
C	1.35786500	4.26011900	-0.47279400
C	-0.42875700	4.13591300	1.17467900
C	0.54259200	5.03814200	-1.29091100
H	2.36761600	3.99525900	-0.77266000
C	-1.24517700	4.91473000	0.35153800
H	-0.80000400	3.78039200	2.13383900
C	-0.75828500	5.36435000	-0.88070500
H	0.91362600	5.39346200	-2.24850500
H	-2.25170500	5.17278800	0.66919500
H	-1.39170100	5.97070800	-1.52289000
O	2.84638700	2.59173200	1.39975700
O	-3.58546700	-1.32789700	1.83351200
H	-3.33188800	-2.26707600	1.75829000
H	-4.50134200	-1.26967000	1.47190900
O	-2.86830100	1.49789500	0.81232100
H	-3.75993500	1.62141200	0.40011200
H	-2.25806900	2.02632500	0.26968900

IM8bc

C	-2.13280200	2.23760900	0.04752400
H	-1.47090000	1.77535400	0.80102100
C	-2.08925000	3.70839500	-0.02118700
C	-2.94192500	4.42402800	-0.88192500
C	-1.17029400	4.39487800	0.79082300
C	-2.87623300	5.81334100	-0.92421100
H	-3.64537400	3.87575900	-1.50201400
C	-1.10557700	5.78908900	0.74128400
H	-0.50400900	3.83675800	1.44456300
C	-1.95714600	6.49596200	-0.11255800
H	-3.53473000	6.37081700	-1.58528200
H	-0.39101100	6.31996500	1.36400900
H	-1.90693800	7.58136400	-0.14981200

O	-2.84042200	1.52622900	-0.66382800
C	-7.10915700	-2.00478500	-0.11648900
C	-6.75559000	-1.19326500	-1.20640200
C	-5.42066800	-0.94449300	-1.50823300
C	-4.39772500	-1.50871600	-0.71832200
C	-4.74503400	-2.32674700	0.38272000
C	-6.07918800	-2.56496200	0.66931000
H	-7.53600000	-0.75002500	-1.81929300
H	-5.15956400	-0.30202100	-2.34487900
H	-3.95989400	-2.75879000	0.99534900
H	-6.34036800	-3.19392300	1.51711900
C	-8.55365500	-2.27404400	0.22138100
H	-9.23109200	-1.81337100	-0.50376200
H	-8.75914400	-3.35159500	0.24298000
H	-8.80294200	-1.88000000	1.21503800
C	-3.04021600	-1.22025100	-1.06615100
H	-2.78592300	-0.60928400	-1.92155800
O	-2.10120700	-1.72278400	-0.35294200
C	-0.72337500	-1.59880900	-0.40358800
C	-0.01135500	-1.02409900	-1.49904200
C	-0.07831700	-2.14060100	0.75798800
O	-0.76919300	-0.70697900	-2.56863800
O	-0.90538200	-2.71301400	1.63962600
C	-0.07498300	-0.10672300	-3.68897500
H	-0.85601300	0.10436000	-4.41947400
H	0.42521700	0.81090200	-3.37366600
H	0.65950600	-0.80595000	-4.09380900
C	-0.31243200	-3.14018300	2.88667400
H	0.14366400	-2.28584100	3.39059700
H	-1.14516100	-3.53620600	3.46825800
H	0.43576200	-3.91569200	2.70675000
O	1.21710900	-0.82470500	-1.54026800
O	1.15165800	-2.12100500	0.97370300
Ni	2.53402800	-0.97490300	0.00592900
O	1.73428600	0.82184000	0.83148000
O	3.85143400	0.25918100	-1.09138800
Cl	5.35536500	-0.02661700	-1.24987800
O	2.22273400	0.34279900	3.20548900
O	5.49923600	-1.36435000	-1.93348900
O	5.95962500	1.04383500	-2.05241200
O	1.19043200	2.47231800	2.54041900
O	5.96159900	-0.09989700	0.12371400
Cl	1.24701300	1.01765800	2.27920900
O	-0.10377600	0.39966100	2.41800300

O	3.86320200	-1.19426700	1.59292700
H	4.69823200	-0.74125400	1.33495300
H	3.46292800	-0.67884800	2.33061600
O	3.38736500	-2.72284500	-0.80818500
H	4.17872900	-2.43763600	-1.32795100
H	3.73173200	-3.22712200	-0.05180800

IM8bd

C	1.26279800	2.85155400	-0.30190000
H	0.30710400	2.30450000	-0.41466700
C	1.22292000	4.26348600	-0.72331900
C	2.36522700	5.08061800	-0.65280600
C	0.01075600	4.79019800	-1.19879500
C	2.29045500	6.41064100	-1.05661500
H	3.29343700	4.65595600	-0.28153100
C	-0.06136000	6.12451200	-1.60226400
H	-0.86754200	4.15015500	-1.24699000
C	1.07759800	6.93251300	-1.53077300
H	3.17030200	7.04638800	-1.00414700
H	-0.99938200	6.53386100	-1.96684100
H	1.02305600	7.97215500	-1.84359100
O	2.25036000	2.27850900	0.14600700
C	7.27473200	-1.64327900	0.61744700
C	6.84726500	-0.69702100	1.56307000
C	5.50883100	-0.32968500	1.65034500
C	4.55594300	-0.90393900	0.78169700
C	4.97859500	-1.86062800	-0.17296300
C	6.31521200	-2.21520300	-0.24600700
H	7.57230500	-0.24651300	2.23569000
H	5.19207200	0.40689200	2.38444800
H	4.24821500	-2.30949900	-0.83883500
H	6.63339100	-2.95153600	-0.98019900
C	8.72254200	-2.05118900	0.51934000
H	9.12011200	-1.84959000	-0.48338500
H	9.34343100	-1.51660700	1.24429000
H	8.83960000	-3.12729900	0.69989600
C	3.19554800	-0.48421000	0.90208800
H	2.88228100	0.23343700	1.65019700
O	2.32091400	-0.96692300	0.09868300
C	0.96653800	-0.70592900	-0.00238000
C	0.17734400	-0.24409600	1.09323000
C	0.41980900	-1.07662000	-1.27677700
O	0.83257300	-0.09441200	2.25795700
O	1.31224900	-1.57581600	-2.13784000

C	0.01423900	0.25228400	3.40729900
H	0.71748700	0.31017500	4.23797400
H	-0.48291500	1.20915000	3.24124700
H	-0.73623000	-0.52140300	3.57813900
C	0.78253500	-2.08579000	-3.38327100
H	0.30893900	-1.28134400	-3.95096700
H	1.65193500	-2.47225900	-3.91546700
H	0.06186600	-2.88013000	-3.18054000
O	-1.04350700	0.00255600	1.04511200
O	-0.77245500	-0.93470300	-1.61874700
Ni	-2.34801300	-0.51293000	-0.40168000
O	-3.60928800	0.96994800	2.86869800
O	-2.41818800	-2.49034900	0.34407900
Cl	-4.37968900	1.10745700	1.61601600
Cl	-2.13667900	-3.75970000	-0.49243000
O	-5.83401900	1.15341200	1.84655800
O	-4.09582200	-0.11217100	0.69853300
O	-2.68430800	-4.91357000	0.24050700
O	-2.83554700	-3.59181200	-1.82702800
O	-3.92695500	2.34310900	0.85710000
O	-0.67005800	-3.88492800	-0.70651700
O	-2.37820800	1.46731700	-1.15977700
H	-2.88970000	1.39961300	-1.98361000
H	-2.96160900	1.93678700	-0.50553200
O	-3.74155500	-1.02553000	-1.87936300
H	-3.53215400	-1.98093800	-2.04468600
H	-4.58802700	-1.01818900	-1.39639500

IM8cd

C	-1.93429800	1.75921400	-1.12340500
H	-0.90159200	1.47757700	-0.85125100
C	-2.16668200	3.19885600	-1.31375900
C	-3.42453500	3.68719600	-1.71466300
C	-1.10405900	4.09034800	-1.08318900
C	-3.61234400	5.05508100	-1.88570600
H	-4.23245800	2.98223000	-1.88814700
C	-1.29958800	5.46253200	-1.25341800
H	-0.13217600	3.71508800	-0.76929100
C	-2.54961600	5.94249500	-1.65465400
H	-4.58023800	5.43789900	-2.19850500
H	-0.47887300	6.15113100	-1.07410700
H	-2.70047500	7.01064700	-1.78961400
O	-2.79032300	0.88465900	-1.24905800
C	-7.07544400	-2.10592300	0.24889800

C	-6.43491200	-2.11281800	-1.00148700
C	-5.05962200	-1.93736800	-1.09786700
C	-4.28614000	-1.74864300	0.06734900
C	-4.92334000	-1.74044100	1.33160200
C	-6.29427500	-1.91574300	1.41005000
H	-7.02316500	-2.25403300	-1.90401800
H	-4.57522700	-1.93065200	-2.07055900
H	-4.33051300	-1.59796700	2.22951800
H	-6.78096400	-1.90935200	2.38226700
C	-8.56577200	-2.29755300	0.36237400
H	-9.03487000	-1.43542400	0.85312700
H	-9.03342200	-2.42642500	-0.61799100
H	-8.80180500	-3.17964500	0.97103200
C	-2.88133100	-1.56147200	-0.08394400
H	-2.40899600	-1.61942900	-1.05739100
O	-2.14734500	-1.35348300	0.94759400
C	-0.74595200	-1.23220500	0.89193100
C	0.04870900	-2.16292000	0.16636500
C	-0.19562800	-0.27084100	1.78888000
O	-0.63757000	-3.12969300	-0.47579500
O	-1.09204600	0.37584500	2.54470500
C	0.15594300	-4.14671800	-1.14349000
H	-0.56200200	-4.71420800	-1.73584300
H	0.92279700	-3.68705600	-1.76776800
H	0.63178800	-4.78837300	-0.39780100
C	-0.56606200	1.37304200	3.45830900
H	0.11266500	2.05120100	2.93942100
H	-1.44695300	1.89418200	3.83336400
H	-0.03423200	0.87941900	4.27604300
O	1.29693600	-2.15324100	0.12966300
O	1.02464800	-0.01222900	1.89103500
Ni	2.43938900	-0.46783900	0.47802200
O	4.53642400	-3.10914400	-0.16587300
O	3.51619500	1.31484000	0.85356600
Cl	4.32115600	-2.34150700	-1.44730700
Cl	2.99178200	2.76008200	0.87925200
O	5.58483100	-2.17325900	-2.18325100
O	3.81698800	-0.92428600	-1.05128000
O	4.14558800	3.66677500	0.77303200
O	2.07562600	2.93361500	-0.33099300
O	3.28144100	-2.99903200	-2.27955000
O	2.20831200	2.99584800	2.11653400
O	1.46424500	0.46295400	-1.14494200
H	1.68797200	1.42352600	-1.01818500

H	2.04141600	0.14389800	-1.86394000
O	3.63412600	-1.47437700	1.84494700
H	3.10652400	-1.93717700	2.51415700
H	4.07700000	-2.16639300	1.29407700
TS1ab			
O	-0.87666200	-1.20702300	-1.37416300
O	2.56790300	-1.02119000	1.63957500
O	0.47428200	-1.71491500	2.13470500
O	-0.40587800	0.47474200	0.67221900
C	0.64856900	-0.29735400	0.27327100
C	1.42200200	0.80839900	-0.42690000
C	0.18167300	-1.35232600	-0.77404900
C	1.36445100	-1.04678000	1.42577000
C	0.93184100	-2.47857600	3.27088800
H	0.02661900	-2.92217700	3.68143200
H	1.40978300	-1.81440400	3.99563600
H	1.64187400	-3.24307300	2.94405700
O	0.98696800	-2.38336000	-0.95388400
C	0.51770700	-3.42165700	-1.85695000
H	0.42044200	-3.01705200	-2.86666800
H	1.28188700	-4.19659000	-1.81447900
H	-0.44732400	-3.79639600	-1.51048000
C	3.98297800	-0.04993300	-0.55788400
H	4.05863700	0.53393300	0.36564900
O	2.92378600	-0.01476300	-1.21303800
C	5.14534200	-0.81275200	-0.97331900
C	5.14587600	-1.57455200	-2.15974100
C	6.29173400	-0.77464100	-0.15663800
C	6.28505300	-2.28543000	-2.51870000
H	4.25483000	-1.59463500	-2.77930600
C	7.42939000	-1.49206600	-0.52076700
H	6.27881200	-0.19165200	0.76095100
C	7.42439100	-2.24450200	-1.70027500
H	6.29418400	-2.87364000	-3.43172900
H	8.31388000	-1.46836300	0.10882000
H	8.31120200	-2.80417400	-1.98561700
H	0.99509600	1.00774800	-1.40487200
C	1.93058200	2.01119200	0.24285200
C	2.24512900	3.11586300	-0.57428300
C	2.11374800	2.13823300	1.63379300
C	2.73980300	4.29621900	-0.02657700
H	2.09545400	3.04387600	-1.64924800
C	2.59490900	3.32690800	2.17374400

H	1.85462000	1.32434300	2.29758400
C	2.91886400	4.42609100	1.35979200
H	2.97489700	5.13277400	-0.68013300
H	2.71247600	3.40761900	3.25189300
C	3.40948600	5.71734000	1.96741100
H	4.11880400	5.53206300	2.78195600
H	3.89937800	6.35280700	1.22276300
H	2.57274400	6.28871700	2.39124100
Ni	-2.13444700	0.15537500	-0.32041200
Cl	-4.74030800	0.79933100	-2.13602200
Cl	-3.20301800	-1.69653100	2.18909700
O	-5.32624400	1.53891800	-0.96827300
O	-3.77675600	-0.26798500	-1.59165300
O	-4.62193500	-2.08355200	2.04937700
O	-2.57919800	-1.58304700	0.77844900
O	-3.93179800	1.76024900	-2.98046300
O	-5.77662500	0.14358500	-2.94229600
O	-3.08570600	-0.34675400	2.86051700
O	-2.42602500	-2.70857400	2.94398700
O	-3.19865300	1.48696800	0.85015400
H	-3.27051500	1.00685200	1.71229400
H	-4.10405300	1.55890800	0.47326900
O	-1.60121700	1.81205800	-1.56381500
H	-1.65172600	2.55446700	-0.93719200
H	-2.35203500	1.93903500	-2.19837400
TS1ac			
O	-1.05548400	-2.00903700	-0.08118400
O	2.62731400	-0.35480700	2.09883900
O	0.68159600	-1.01538800	3.03301900
O	-0.51875800	0.39728500	0.92722300
C	0.56223400	-0.41503100	0.75160500
C	1.20032600	0.31563300	-0.42426700
C	0.08993200	-1.83466600	0.31556100
C	1.43166000	-0.58187000	2.02308700
C	1.33829000	-1.20285300	4.30334600
H	0.56082100	-1.56851600	4.97329800
H	1.74023900	-0.25153600	4.66093300
H	2.14714500	-1.93188200	4.20659400
O	0.97781300	-2.80849100	0.41701300
C	0.51724900	-4.14022400	0.05400500
H	0.20652300	-4.15176800	-0.99241100
H	1.37588100	-4.78920200	0.22142400
H	-0.32419900	-4.42342200	0.68918600

C	3.83097500	-0.34262500	-0.46595900
H	3.90197400	0.60394100	0.08288400
O	2.72629900	-0.70226200	-0.91063700
C	5.04973200	-1.10895700	-0.65734200
C	5.05339800	-2.32437200	-1.37183500
C	6.24597400	-0.60501400	-0.11229400
C	6.24520800	-3.02061600	-1.53616700
H	4.12321200	-2.69922000	-1.78724700
C	7.43687400	-1.30957400	-0.27790700
H	6.23190000	0.32977400	0.44275100
C	7.43441000	-2.51412800	-0.98954900
H	6.25730800	-3.95630700	-2.08760700
H	8.36106900	-0.92561200	0.14365300
H	8.36270600	-3.06383700	-1.12069300
H	0.70732900	0.04376500	-1.35249900
C	1.62913900	1.71238100	-0.38883600
C	1.75757900	2.37200700	-1.62971000
C	1.88354000	2.44791400	0.78613600
C	2.13939200	3.70702200	-1.69601500
H	1.53835900	1.82975200	-2.54662600
C	2.25179400	3.78632300	0.71032400
H	1.75788100	1.99101000	1.75833500
C	2.38381300	4.44267800	-0.52507600
H	2.22030800	4.19445200	-2.66442600
H	2.41732100	4.34200800	1.63012000
C	2.72629300	5.91013300	-0.58606700
H	3.39984600	6.20022700	0.22771900
H	3.19823700	6.17585900	-1.53777800
H	1.81628700	6.51753100	-0.48861600
Ni	-2.22612700	-0.23767200	0.07674100
Cl	-4.48738600	-2.42245300	-0.91234600
O	-3.32248100	1.51721300	0.38376600
O	-3.85879200	-1.00572300	-1.03399400
O	-4.64990200	-2.70289100	0.56327400
O	-2.12861800	2.94579300	-1.23456100
O	-1.91292200	3.39593400	1.17124200
O	-5.79651200	-2.38572600	-1.58798500
O	-3.56907300	-3.40938700	-1.52860500
O	-1.65418500	0.36095500	-1.88000200
H	-2.39264500	-0.01725600	-2.39259000
H	-1.81924200	1.33912700	-1.83016600
Cl	-2.84185300	2.96797200	0.10367800
O	-4.04241400	3.82068000	0.03351500
O	-3.09749100	-0.86561700	1.86727100

H	-3.57842700	-0.07590600	2.17145400
H	-3.77919600	-1.52520300	1.58713100
TS1ad			
O	-1.05584000	-2.00937100	-0.08215700
O	2.62813100	-0.35574700	2.09689100
O	0.68288200	-1.01964300	3.02969800
O	-0.51786300	0.39669800	0.92636000
C	0.56302900	-0.41542100	0.74939500
C	1.20066400	0.31665700	-0.42591000
C	0.09055400	-1.83469500	0.31217000
C	1.43267500	-0.58374000	2.02058300
C	1.33950500	-1.20845600	4.29991100
H	0.56234500	-1.57639100	4.96899000
H	1.74001600	-0.25717500	4.65928300
H	2.14941800	-1.93617800	4.20211700
O	0.97943500	-2.80806500	0.41031200
C	0.51846600	-4.13981400	0.04744200
H	0.20117900	-4.14994700	-0.99721300
H	1.37907100	-4.78781100	0.20860100
H	-0.31873600	-4.42553400	0.68741900
C	3.83158200	-0.34112400	-0.46719700
H	3.90228100	0.60535300	0.08182300
O	2.72730700	-0.70038100	-0.91305600
C	5.05036500	-1.10778100	-0.65727900
C	5.05439400	-2.32342600	-1.37139700
C	6.24621600	-0.60406100	-0.11105200
C	6.24617100	-3.02013100	-1.53417000
H	4.12449200	-2.69812400	-1.78768300
C	7.43709600	-1.30905800	-0.27512900
H	6.23185900	0.33089900	0.44372000
C	7.43498900	-2.51386000	-0.98638000
H	6.25853900	-3.95604400	-2.08525500
H	8.36099300	-0.92526200	0.14735400
H	8.36325700	-3.06394400	-1.11627100
H	0.70770500	0.04537400	-1.35435300
C	1.62882900	1.71354500	-0.38938800
C	1.75456800	2.37490000	-1.62962800
C	1.88509800	2.44768600	0.78611300
C	2.13530400	3.71031600	-1.69487900
H	1.53393000	1.83374100	-2.54686500
C	2.25242900	3.78640600	0.71137200
H	1.76184100	1.98929300	1.75793200
C	2.38152400	4.44455300	-0.52344300

H	2.21395700	4.19912700	-2.66279300
H	2.41954300	4.34094700	1.63159000
C	2.72297300	5.91233200	-0.58299000
H	3.40180900	6.20064600	0.22709200
H	3.18850200	6.18067100	-1.53712400
H	1.81339700	6.51911800	-0.47790400
Ni	-2.22609300	-0.23804900	0.07735600
Cl	-4.48826500	-2.42252000	-0.91023800
O	-3.32192200	1.51702200	0.38522700
O	-3.85964100	-1.00582600	-1.03229400
O	-4.64969900	-2.70303500	0.56547700
O	-2.12952300	2.94519700	-1.23452100
O	-1.91164100	3.39590400	1.17097000
O	-5.79788700	-2.38565600	-1.58490900
O	-3.57047600	-3.40947300	-1.52726100
O	-1.65548200	0.36043100	-1.87985100
H	-2.39428100	-0.01791100	-2.39185600
H	-1.82061500	1.33858700	-1.83001400
Cl	-2.84155300	2.96770700	0.10435500
O	-4.04216300	3.82041700	0.03507600
O	-3.09638900	-0.86593500	1.86842100
H	-3.77836400	-1.52536800	1.58864100
H	-3.57705100	-0.07617400	2.17291100
TS1bc			
O	-1.12716400	-1.10865800	-1.43399600
O	2.12828800	-1.65841400	1.53299600
O	0.06919500	-1.92252300	2.42194600
O	-0.92129200	0.08178100	0.95968800
C	0.20418100	-0.54860500	0.50284500
C	0.94610300	0.70488800	0.05463000
C	-0.14698600	-1.40482500	-0.75442200
C	0.92478700	-1.43893400	1.54365600
C	0.55552900	-2.88672700	3.37546400
H	-0.33059100	-3.20632100	3.92211600
H	1.28608900	-2.42192100	4.04408500
H	1.01505600	-3.72875900	2.85199100
O	0.66504300	-2.39997300	-1.03108400
C	0.26953800	-3.27947200	-2.11737700
H	0.21558300	-2.71479600	-3.05083600
H	1.05018300	-4.03802400	-2.16050800
H	-0.69913200	-3.72029100	-1.87636000
C	3.52583600	-0.12615300	-0.38435600
H	3.64404400	0.16612800	0.66535500

O	2.44932100	0.09896000	-0.96254000
C	4.66577400	-0.74023000	-1.04491200
C	4.61631500	-1.11210100	-2.40357700
C	5.83728200	-0.95465400	-0.29494400
C	5.73195400	-1.69002200	-2.99846400
H	3.70624700	-0.93807700	-2.96928700
C	6.95108500	-1.53803100	-0.89603900
H	5.86335100	-0.67164400	0.75454800
C	6.89687000	-1.90326700	-2.24554900
H	5.70264200	-1.97696100	-4.04572400
H	7.85544100	-1.70896700	-0.31936300
H	7.76518700	-2.35717900	-2.71582000
H	0.49759500	1.10092900	-0.84892000
C	1.45336400	1.74461600	0.94895200
C	1.48403100	3.06007300	0.43765900
C	1.90777100	1.53008500	2.26595000
C	1.95212400	4.11652100	1.21148200
H	1.11327700	3.25137900	-0.56605900
C	2.37195800	2.59534700	3.03289200
H	1.89628000	0.53854500	2.70108100
C	2.40206000	3.90512700	2.52515000
H	1.95458500	5.12141500	0.79644600
H	2.71190800	2.40832000	4.04892300
C	2.86788300	5.05814300	3.37983900
H	3.59430300	4.73412300	4.13315000
H	3.32688100	5.84713800	2.77416600
H	2.02030500	5.50898800	3.91442800
Ni	-2.47223900	0.09415000	-0.30278200
Cl	-2.35498600	3.01168600	-1.86813800
Cl	-3.12995200	-2.92118500	0.94924300
O	-3.19623100	3.56456000	-0.75430100
O	-1.57156800	1.80991000	-1.30560400
O	-4.13724100	-3.94291000	0.58412600
O	-3.54949200	-1.61567700	0.21682000
O	-1.38022200	4.00943300	-2.35106300
O	-3.22630600	2.51642200	-2.98227000
O	-3.10465900	-2.66200500	2.40782600
O	-1.77056800	-3.31576500	0.45464400
O	-3.45845200	1.36346600	1.02579700
H	-2.84644900	1.41769600	1.78007000
H	-3.47435500	2.25211500	0.60605700
O	-4.06878600	0.21591300	-1.63799700
H	-4.37313700	-0.66190600	-1.91820000
H	-3.93235200	0.79650900	-2.41539700

TS1bd

O	-1.54776500	-1.51544200	-0.14644200
O	2.24991000	-1.26480600	2.22435100
O	0.13255800	-1.64013300	2.91497800
O	-0.58517000	0.49889600	1.29192200
C	0.34563300	-0.42083600	0.89675400
C	1.17840500	0.50564500	0.02793400
C	-0.34579500	-1.55846900	0.07716900
C	1.05026800	-1.13860000	2.07439700
C	0.63481000	-2.37393000	4.05500900
H	-0.25071100	-2.74395500	4.57095600
H	1.20968600	-1.70791100	4.70307000
H	1.26627200	-3.20055600	3.72115100
O	0.42278700	-2.56811100	-0.28703900
C	-0.23479500	-3.63701800	-1.02824500
H	-0.63134100	-3.24017700	-1.96461200
H	0.54639700	-4.37492000	-1.20638900
H	-1.04951100	-4.05239400	-0.43243200
C	3.66368300	-0.68245700	-0.34701800
H	3.90626100	-0.05824800	0.52378000
O	2.52606600	-0.62517800	-0.83542600
C	4.71805600	-1.53367200	-0.87766300
C	4.51112700	-2.33492800	-2.01854600
C	5.96616600	-1.53740400	-0.22726300
C	5.54717800	-3.12933600	-2.49663300
H	3.54469400	-2.31490200	-2.51261300
C	6.99942400	-2.33924300	-0.70897800
H	6.11590200	-0.91739200	0.65346300
C	6.78848100	-3.13219100	-1.84218000
H	5.39726300	-3.74628100	-3.37790900
H	7.96300100	-2.34708100	-0.20805900
H	7.59419400	-3.75569300	-2.22062600
H	0.70311600	0.65062700	-0.93655500
C	1.91346000	1.67298500	0.50091600
C	2.11095700	2.71376600	-0.43464400
C	2.42865100	1.83960800	1.80458800
C	2.80212100	3.86755100	-0.08061200
H	1.68549600	2.62209400	-1.43006000
C	3.11216900	3.00136500	2.14762200
H	2.29271200	1.07080200	2.55327100
C	3.31274800	4.03589600	1.21648200
H	2.93028600	4.65728800	-0.81684000
H	3.49410600	3.11295900	3.15990100

C	4.02012100	5.30834400	1.61209000
H	4.72700800	5.13923300	2.43141200
H	4.56583400	5.74358300	0.76799800
H	3.29602800	6.06092600	1.95352800
Ni	-2.42493500	0.32966000	0.40186100
Cl	-1.53332700	2.21741100	-2.26704600
Cl	-5.03016900	-1.46516800	-0.23666500
O	-1.69904700	3.33013400	-1.25754800
O	-1.65262100	0.87302300	-1.51971800
O	-4.31627300	-0.09559800	-0.34282300
O	-4.88690100	-1.93532900	1.20277300
O	-0.15563200	2.26120000	-2.83597900
O	-2.56347700	2.29664500	-3.31392400
O	-6.44979000	-1.24953600	-0.56494200
O	-4.38282500	-2.43735000	-1.14620500
O	-3.00370900	2.25579500	0.88424200
H	-2.60308200	2.48399200	1.73817400
H	-2.58855600	2.83668700	0.20057600
O	-3.05112500	-0.30397900	2.29889500
H	-2.30040900	-0.78008900	2.69101700
H	-3.77012900	-0.96152200	2.10479300
TS1cd			
O	-0.86361600	-2.29419600	0.68771900
O	2.14723300	0.64896800	2.41955900
O	0.26390900	-0.18445500	3.34811100
O	-0.92036000	0.35110500	0.89124300
C	0.32628800	-0.20729600	0.98882000
C	0.89347600	0.35431300	-0.30003700
C	0.21551200	-1.76212300	0.92294200
C	1.04537200	0.14736000	2.31207900
C	0.78609900	0.08575800	4.66739700
H	0.03080400	-0.29113000	5.35640800
H	0.92790600	1.16130200	4.79905300
H	1.73772400	-0.43247700	4.80860700
O	1.32586400	-2.43067800	1.15862600
C	1.24856400	-3.87769300	1.03058000
H	0.96831700	-4.13175200	0.00622500
H	2.24992800	-4.23370900	1.27008000
H	0.51108900	-4.27121600	1.73357000
C	3.71024400	0.32897100	-0.05980600
H	3.50783500	1.36032800	0.26349800
O	2.77089000	-0.39061800	-0.41795100
C	5.10041800	-0.11292400	-0.05251500

C	5.46091800	-1.39963700	-0.49849400
C	6.08727300	0.77887400	0.40489300
C	6.79763100	-1.78314000	-0.48245200
H	4.68703600	-2.07201700	-0.85595200
C	7.42528900	0.38732900	0.42274900
H	5.79959300	1.76964600	0.74879200
C	7.77789700	-0.89152600	-0.02132600
H	7.08371200	-2.77205700	-0.82908600
H	8.18943600	1.07238500	0.77835000
H	8.82091000	-1.19691700	-0.01078300
H	0.64682400	-0.27527700	-1.14758200
C	1.03670000	1.76044800	-0.61835100
C	1.10027000	2.09405600	-1.99082800
C	1.08295900	2.80743700	0.32727300
C	1.21418800	3.41692100	-2.39917700
H	1.04099800	1.30246900	-2.73336600
C	1.18679400	4.12788600	-0.09265200
H	1.01217000	2.59373500	1.38538000
C	1.25134600	4.45961000	-1.45784100
H	1.25132000	3.64881000	-3.46064700
H	1.20182800	4.92172000	0.65012800
C	1.31179800	5.89954900	-1.90118700
H	1.79113500	6.53375200	-1.14805800
H	1.85722600	6.00792100	-2.84463300
H	0.29840700	6.29175100	-2.06251800
Ni	-2.38596200	-0.88208200	0.24254000
Cl	-1.22130600	-1.99174600	-2.65260000
Cl	-4.63425300	1.46618600	0.51684600
O	-1.29874200	-1.61132900	-4.07503400
O	-1.72735000	-0.80406200	-1.80818400
O	-3.89405600	0.43079100	-0.37701600
O	-5.15874500	0.71059300	1.71975800
O	0.19124900	-2.27131300	-2.24377300
O	-2.09335700	-3.18299400	-2.35916100
O	-3.67133000	2.50555500	0.94562100
O	-5.74874700	2.01224900	-0.27697400
O	-3.77354000	-2.33703600	-0.30920000
H	-4.51335200	-1.81325500	-0.66582500
H	-3.36486600	-2.80069000	-1.07654400
O	-2.99449800	-0.87497300	2.25251600
H	-2.32563000	-0.26478700	2.61451000
H	-3.85158800	-0.38160700	2.27781700

TS5ab

C	6.65460500	0.34689400	-0.81553500
C	6.07571700	1.54504800	-0.35420700
C	4.86131500	1.53427000	0.31495400
C	4.18626200	0.30950300	0.54276500
C	4.75568200	-0.89884800	0.06423700
C	5.97368400	-0.86998900	-0.59207300
H	6.58843000	2.48730300	-0.52644100
H	4.42299400	2.46383900	0.66975100
H	4.22087600	-1.82992600	0.21481400
H	6.41196800	-1.79739900	-0.95229200
C	7.97525300	0.35207000	-1.53879700
H	7.87714300	-0.09654700	-2.53537800
H	8.36970200	1.36506300	-1.65792100
H	8.71940500	-0.24248400	-0.99342600
C	2.98221500	0.32161900	1.28880900
H	2.58917200	1.25356600	1.69154400
O	2.35963600	-0.80045100	1.64655900
C	1.06895300	-0.44328000	1.16106000
C	0.08045900	-0.09660900	2.14951100
C	0.76582800	-0.67951600	-0.22575400
O	0.58856700	-0.00130600	3.38635400
O	1.76370400	-1.21803500	-0.93613800
C	-0.35275200	0.31357700	4.43858100
H	0.24490800	0.33668100	5.34909100
H	-0.81887800	1.28294500	4.24907300
H	-1.12289100	-0.45877000	4.49571700
C	1.44840900	-1.57455200	-2.30498700
H	1.19460600	-0.67990400	-2.87859600
H	2.35996800	-2.03362900	-2.68790200
H	0.61667100	-2.28078700	-2.31843300
O	-1.12167000	0.12635500	1.93660200
O	-0.32706500	-0.42768400	-0.76145500
Ni	-2.08568300	0.11692300	0.12724700
O	-2.73228000	-1.85569800	0.41735000
O	-1.48759500	2.14145400	-0.05502100
Cl	-2.31743800	3.17781700	-0.84345800
O	-0.91517800	-3.40005300	-0.22592000
O	-3.69198400	3.21058100	-0.23340900
O	-1.64804800	4.48419200	-0.73493300
O	-3.24762100	-4.16245800	-0.17837700
O	-2.39889300	2.72275000	-2.26976700
Cl	-2.33494200	-3.04897000	-0.49323300
O	-2.49724300	-2.60430400	-1.92580500
O	-3.87577400	0.70732600	1.02822700

H	-4.05171600	1.61014600	0.67456700
H	-4.57103400	0.12859000	0.67223500
O	-3.10446000	0.08195700	-1.68330500
H	-2.82697200	0.81615700	-2.26904900
H	-2.90131500	-0.78719200	-2.09562600

TS5ac

C	-5.85825800	-1.66102600	0.52854500
C	-5.05551200	-1.11665100	1.54837500
C	-4.02445900	-0.23762100	1.25073400
C	-3.77151800	0.11968600	-0.09846900
C	-4.56279700	-0.44196700	-1.13378300
C	-5.59490100	-1.30599300	-0.81373600
H	-5.24280000	-1.39329200	2.58227700
H	-3.38819700	0.15937200	2.03755300
H	-4.34960500	-0.18056600	-2.16448500
H	-6.21226100	-1.72527100	-1.60448300
C	-6.96394300	-2.63094000	0.85212300
H	-6.64248300	-3.66068600	0.64285400
H	-7.24902400	-2.58184600	1.90718200
H	-7.85344600	-2.44078600	0.24106400
C	-2.75655300	1.07197200	-0.35779600
H	-2.24255900	1.57582800	0.46113900
O	-2.46102300	1.47717400	-1.60353900
C	-1.07848700	1.14640300	-1.49515800
C	-0.16123200	2.21145800	-1.17751100
C	-0.65372000	-0.18852100	-1.78879600
O	-0.74119600	3.40660100	-1.09002300
O	-1.61565900	-1.00631500	-2.23869300
C	0.08975300	4.49434400	-0.62126400
H	-0.57674500	5.35555600	-0.58230500
H	0.48012400	4.25285500	0.36935300
H	0.90989000	4.66966400	-1.32135300
C	-1.23534800	-2.38608300	-2.44760700
H	-0.82456000	-2.80934100	-1.52850700
H	-2.15909600	-2.88984100	-2.73228700
H	-0.49556800	-2.45667200	-3.24813800
O	1.06396000	2.06851200	-0.98828600
O	0.52436000	-0.59839300	-1.68539400
Ni	1.87637000	0.27407100	-0.39127000
O	0.46863600	-0.07310200	1.10791900
O	2.64176800	-1.65028500	0.08224900
Cl	4.13926900	-1.95074400	0.26490400
O	-0.48900600	2.10481700	1.75731900

O	4.66140900	-1.07883900	1.37055400
O	4.30732700	-3.37540600	0.57211900
O	-1.10944000	0.06024600	2.94367800
O	4.83639900	-1.58912400	-1.02846700
Cl	0.01448200	0.79891800	2.30640600
O	1.14502400	1.00406500	3.23057000
O	3.26726300	1.25559200	0.79402400
H	3.82762300	0.58123400	1.24554500
H	3.86479000	1.78720500	0.24296700
O	3.25928700	0.41185800	-1.99056200
H	3.91409400	-0.31742100	-1.84299100
H	2.77666200	0.19149400	-2.80380400

TS5ad

C	6.85748100	-1.37589600	0.22319500
C	6.47897200	-1.35986600	-1.13326600
C	5.30868200	-0.73350500	-1.53560200
C	4.47624800	-0.10059700	-0.58066700
C	4.84368500	-0.12768400	0.78912800
C	6.02074100	-0.74798500	1.17121300
H	7.11434500	-1.84204800	-1.87114400
H	5.02915000	-0.71928600	-2.58641200
H	4.19011000	0.33592000	1.51975500
H	6.30400200	-0.76113200	2.22087800
C	8.12941200	-2.04967300	0.66612700
H	7.92064700	-2.83011500	1.40827200
H	8.65945100	-2.50956500	-0.17247600
H	8.80552400	-1.32905400	1.14328700
C	3.32398000	0.59721800	-1.02598300
H	3.09382600	0.66559100	-2.08783200
O	2.58160800	1.32888800	-0.19810800
C	1.33181700	0.74608600	-0.54657600
C	0.43261100	1.57307300	-1.31815600
C	0.90982300	-0.43937500	0.14845500
O	1.02920900	2.65308800	-1.82694500
O	1.81751500	-0.97927100	0.96436500
C	0.16427600	3.61345600	-2.47803600
H	0.82851100	4.41869600	-2.79086100
H	-0.33030800	3.15499400	-3.33742800
H	-0.57970000	3.97389500	-1.76461900
C	1.34771000	-2.04779600	1.82260900
H	1.02342500	-2.90195300	1.22438700
H	2.21008700	-2.30935500	2.43578200
H	0.52306600	-1.68489600	2.43850600

O	-0.76247500	1.32632000	-1.55066700
O	-0.21571900	-0.96427500	0.01867200
Ni	-1.94307600	-0.02551800	-0.55480300
O	-2.24574000	1.18598100	1.10598300
O	-2.98642500	-1.61856500	0.41831800
Cl	-4.41444000	-2.05835400	0.04540400
O	-0.60167800	3.02877400	1.02689700
O	-4.59961500	-1.69410300	-1.43509900
O	-4.51390600	-3.51654100	0.22674900
O	-1.96019300	2.63928600	3.03633000
O	-5.39793100	-1.30370200	0.84719300
Cl	-1.21200700	2.01124400	1.93205800
O	-0.16721700	1.06892500	2.42714300
O	-3.69149200	0.94056200	-1.17829900
H	-4.38134400	0.26142400	-1.33858200
H	-3.96234900	1.44731500	-0.39067700
O	-2.00752500	-1.28012700	-2.26657900
H	-1.44046800	-2.03793300	-2.04561500
H	-2.93219500	-1.62378900	-2.22985700

TS5bc

C	6.43033900	-0.56455500	-0.13048200
C	5.59504600	-0.93540000	-1.20057400
C	4.36075700	-0.32915400	-1.38136400
C	3.92756500	0.67708300	-0.48364000
C	4.75479200	1.03926800	0.61045000
C	5.98761800	0.43133000	0.76844300
H	5.91945800	-1.71062000	-1.88913500
H	3.71313800	-0.63298300	-2.19854700
H	4.40766600	1.79199700	1.30944600
H	6.62649900	0.71738200	1.60055000
C	7.77412000	-1.21557300	0.06653500
H	7.82253900	-1.72486500	1.03757600
H	7.98704700	-1.95155500	-0.71392500
H	8.57568600	-0.46595600	0.05872000
C	2.69939600	1.33327800	-0.74026800
H	2.14125300	1.11953700	-1.64931800
O	2.25427600	2.33809300	0.02558900
C	0.99238300	1.72548200	0.27834700
C	-0.13521600	2.21641200	-0.47145300
C	0.87838600	0.78318900	1.35653900
O	0.18819500	3.17086100	-1.35153500
O	1.99278200	0.61871600	2.07816900
C	-0.89736200	3.69660800	-2.15185400

H	-0.42573000	4.41575400	-2.82099400
H	-1.37802200	2.89134700	-2.71105800
H	-1.63210900	4.18587400	-1.50871100
C	1.95403400	-0.41803900	3.08566500
H	1.72273000	-1.37994700	2.62262800
H	2.95478900	-0.42412000	3.51791800
H	1.20699800	-0.17743800	3.84568500
O	-1.30826300	1.81739900	-0.36642200
O	-0.16428900	0.16722200	1.65515800
Ni	-1.85140200	0.04397200	0.49241400
O	-0.75947100	-0.89093300	-1.08337200
O	-3.53866100	0.03168400	-0.78290700
Cl	-4.96927700	-0.26791400	-0.29874100
O	1.50772300	-1.60849000	-0.44132300
O	-5.33420700	0.77319000	0.73091600
O	-5.88071500	-0.21695400	-1.44733200
O	-0.40099600	-3.09463700	-0.02416000
O	-4.96318300	-1.62600400	0.34703500
Cl	0.19877700	-2.09447000	-0.97549800
O	0.35962900	-2.66940000	-2.32402800
O	-2.37945900	-1.76109200	1.36948800
H	-3.28101500	-1.98344200	1.04117400
H	-1.75853100	-2.42435300	0.98773500
O	-2.92380200	1.01716600	2.01562500
H	-3.86361900	1.08383300	1.71342700
H	-2.92865700	0.42470400	2.78601700

TS5bd

C	-7.03282500	-0.04540100	-0.70687000
C	-6.33061300	-1.15991600	-1.20544300
C	-5.06344500	-1.46788900	-0.73469800
C	-4.45617600	-0.65716200	0.25647300
C	-5.15336600	0.47494300	0.75275600
C	-6.42298800	0.75901400	0.28123900
H	-6.78919800	-1.78311500	-1.96822000
H	-4.52922300	-2.33152300	-1.12351700
H	-4.67554200	1.10663900	1.49324400
H	-6.95932200	1.62220000	0.66738000
C	-8.40635500	0.29807900	-1.21890500
H	-8.40667700	1.28595600	-1.69804300
H	-8.76275300	-0.43359600	-1.94951300
H	-9.13077700	0.34288500	-0.39577700
C	-3.18083500	-1.02555500	0.74942500
H	-2.68810800	-1.92693900	0.38940100

O	-2.58575600	-0.36960200	1.74341700
C	-1.33045400	-0.16518400	1.09985600
C	-0.22839500	-0.97527300	1.55143400
C	-1.19027400	0.96203700	0.21757200
O	-0.56515300	-1.86861700	2.48438800
O	-2.28993700	1.73017500	0.11946500
C	0.51981900	-2.68778400	2.99927700
H	0.04171400	-3.36113000	3.70985400
H	1.00090200	-3.23437100	2.18625300
H	1.25768700	-2.05252700	3.49378500
C	-2.17302600	2.89688500	-0.72832900
H	-1.98471100	2.59637700	-1.76197800
H	-3.13530400	3.40168000	-0.64147500
H	-1.36163200	3.53863200	-0.37923700
O	0.93659300	-0.90304400	1.12802000
O	-0.15673300	1.27326300	-0.39834000
Ni	1.59155200	0.15412600	-0.47796000
O	3.43283900	-2.92816600	0.78706000
O	2.46791400	1.49682000	0.84948700
Cl	3.47559100	-2.53892300	-0.63712200
Cl	3.12904900	2.84820000	0.48095700
O	4.74002600	-2.91380400	-1.29176000
O	3.32988100	-0.99925100	-0.76025400
O	4.56738900	2.62204800	0.22165200
O	2.45252000	3.35476900	-0.78288500
O	2.29710800	-3.15427200	-1.37627600
O	2.88552000	3.78243700	1.59492300
O	0.53467400	-1.16701900	-1.76411500
H	0.66561700	-0.78749400	-2.64920700
H	1.08831300	-1.99337700	-1.73515400
O	2.28362300	1.09538200	-2.20924200
H	2.39025800	2.04021000	-1.91681600
H	3.18595700	0.74651800	-2.33035400
TS5cd			
C	-6.40985100	-0.19388600	-0.93312900
C	-5.48152000	-0.26979900	-1.99181400
C	-4.20705900	-0.76834600	-1.78134800
C	-3.82125600	-1.21350900	-0.49054800
C	-4.74713600	-1.12831000	0.58082000
C	-6.02062900	-0.63690800	0.34914800
H	-5.77118200	0.07091700	-2.98208800
H	-3.49591000	-0.82138600	-2.60183000
H	-4.43985700	-1.44451200	1.57138900

H	-6.73224300	-0.57957900	1.16873500
C	-7.78159500	0.38244900	-1.15965000
H	-7.76543800	1.47107800	-1.00343400
H	-8.12859700	0.20601600	-2.18347400
H	-8.51531900	-0.03698500	-0.46301400
C	-2.52827500	-1.75991700	-0.32009200
H	-1.84578200	-1.84455400	-1.16459900
O	-2.12096200	-2.27960200	0.83896700
C	-0.91404900	-1.53101000	0.94789600
C	0.32367600	-2.20874300	0.66605400
C	-0.96655800	-0.19984800	1.48238700
O	0.17290500	-3.49195900	0.33198500
O	-2.16341300	0.18873300	1.93496400
C	1.39095000	-4.23283300	0.05026800
H	1.04771300	-5.18132000	-0.36146700
H	2.01809100	-3.68535400	-0.65451200
H	1.94181000	-4.39244600	0.98052500
C	-2.24420600	1.54371600	2.45737900
H	-1.82155800	2.25619600	1.74771500
H	-3.30915000	1.71430700	2.61514600
H	-1.70016500	1.60218800	3.40308000
O	1.44869000	-1.67584800	0.71229000
O	0.02448800	0.55398000	1.57321400
Ni	1.68614800	0.36702800	0.37347200
O	4.80538600	-1.03821700	0.56392100
O	1.79718200	2.43524000	0.01352900
Cl	4.40844500	-0.92467100	-0.88674100
Cl	0.62921700	3.39287300	-0.29809600
O	5.52934800	-0.44450200	-1.71002200
O	3.28012500	0.14609700	-0.96572400
O	1.18426300	4.57018200	-0.98534400
O	-0.33656400	2.64938700	-1.21400300
O	3.87026300	-2.21637100	-1.38330700
O	-0.07290100	3.75636800	0.95586100
O	0.57789200	0.14743900	-1.41918600
H	0.20496000	1.06118500	-1.54536300
H	1.32809200	0.06882600	-2.03814100
O	3.01567500	0.51513000	1.95816700
H	2.68288300	0.08201800	2.75973000
H	3.79528000	-0.00960500	1.64987000
TS6ab			
C	1.60803700	1.80615700	-1.19898700
H	0.92868700	1.50001100	-2.00351800

C	1.18219700	2.92097500	-0.35580500
C	2.11442200	3.65443000	0.40806900
C	-0.17263600	3.30751400	-0.35988200
C	1.69197000	4.74597800	1.16149900
H	3.16629500	3.38771700	0.36568700
C	-0.59015700	4.39757600	0.40179600
H	-0.90068500	2.74478800	-0.93696000
C	0.33915100	5.11576800	1.16274500
H	2.41336500	5.32101800	1.73636900
H	-1.63792500	4.68361600	0.39683900
H	0.01389800	5.97162300	1.74873300
O	2.80127200	1.35517900	-1.23633600
C	7.28277100	-0.90659200	-0.46930200
C	6.97879800	0.21353500	0.31859600
C	5.65605500	0.59517800	0.53811600
C	4.60574100	-0.14080800	-0.02850900
C	4.89750500	-1.26387600	-0.82358600
C	6.21934500	-1.63605100	-1.03428000
H	7.78487800	0.79047200	0.76385600
H	5.43922200	1.46630500	1.15196000
H	4.08478300	-1.83181500	-1.26566300
H	6.43732700	-2.50672700	-1.64884400
C	8.71150300	-1.33315300	-0.70460400
H	8.92474700	-1.42838800	-1.77634600
H	9.42129900	-0.61624900	-0.28024800
H	8.90916000	-2.31195300	-0.24875000
C	3.23007500	0.29426300	0.19509100
H	3.04741000	1.05048700	0.95150800
O	2.29990200	-0.63643000	0.03543500
C	0.94852500	-0.31658600	0.03483200
C	0.31786600	0.19912100	1.22345600
C	0.19074800	-1.03541500	-0.96908000
O	1.17880700	0.54818200	2.19336500
O	0.94284800	-1.67661300	-1.86130700
C	0.59607800	1.02772700	3.42809800
H	1.44609600	1.20395700	4.08721300
H	0.04205900	1.95140500	3.24877100
H	-0.06998200	0.27025300	3.84608300
C	0.23845300	-2.48267600	-2.83550800
H	-0.39582900	-1.84989500	-3.46085400
H	1.02507500	-2.94808500	-3.42904400
H	-0.36538900	-3.23532500	-2.32519200
O	-0.90280600	0.36917100	1.38417100
O	-1.05073500	-1.03667700	-1.06979100

Ni	-2.43047500	-0.50153700	0.32997500
O	-2.23359300	-2.24712800	1.48246300
O	-2.73826300	1.31983700	-0.71540100
Cl	-4.11908400	1.75711300	-1.25778600
O	-0.37927600	-3.60777600	0.59166900
O	-5.07452900	1.77356000	-0.09764400
O	-3.96552500	3.09886600	-1.84726600
O	-2.14943500	-4.64001900	1.94486000
O	-4.55918300	0.75478000	-2.27727000
Cl	-1.82991500	-3.63618500	0.91491300
O	-2.63503200	-3.86924200	-0.33898400
O	-3.83644500	0.07934500	1.76219900
H	-4.46090900	0.67525000	1.28790600
H	-4.33624300	-0.72194900	1.99365000
O	-3.96739200	-1.47614300	-0.67635000
H	-4.20586200	-1.03738200	-1.51769200
H	-3.64880300	-2.39138700	-0.84298800
TS6ac			
C	-2.21926500	1.37340700	1.10305200
H	-1.39552400	1.17078800	1.79340900
C	-2.19342300	2.61344900	0.34591000
C	-3.35162500	3.13381900	-0.27844800
C	-0.98636600	3.34183200	0.29581700
C	-3.29259300	4.35839400	-0.93592900
H	-4.29381600	2.59885000	-0.19751900
C	-0.93379200	4.56058900	-0.37725500
C	-2.08318500	5.07082000	-0.98853500
H	-4.18553100	4.77515600	-1.39433200
H	0.00431400	5.10696000	-0.41157400
H	-2.04463400	6.03157000	-1.49597700
O	-3.19145800	0.54939100	1.08777700
C	-7.05405900	-2.46478400	0.13674000
C	-7.02158500	-1.22471500	-0.51805700
C	-5.81667000	-0.55071200	-0.71575000
C	-4.61563400	-1.10883400	-0.26019000
C	-4.63522500	-2.34732300	0.40568000
C	-5.84057100	-3.01179700	0.59382800
H	-7.94801100	-0.78255200	-0.87538000
H	-5.81104300	0.41121600	-1.22338500
H	-3.70602500	-2.77173400	0.77143100
H	-5.84732100	-3.97003300	1.10857600
C	-8.35119500	-3.20740100	0.34637000
H	-8.49844900	-3.45496900	1.40474800

H	-9.21130500	-2.61865800	0.01308500
H	-8.35523500	-4.15389200	-0.20940500
C	-3.36101300	-0.37161100	-0.43007500
H	-3.34511000	0.48363000	-1.09992400
O	-2.27544700	-1.13446400	-0.39752800
C	-0.96823000	-0.66935400	-0.30541000
C	-0.39145000	0.21410500	-1.26601500
C	-0.14895900	-1.47838000	0.56763100
O	-1.25700800	0.66399300	-2.19836600
O	-0.84023200	-2.23575300	1.42428000
C	-0.72408900	1.55843800	-3.19948300
H	-1.57523900	1.80817100	-3.83321000
H	-0.31327300	2.45401300	-2.72984200
H	0.05139500	1.05305400	-3.78010400
C	-0.05910300	-3.02813500	2.35052200
H	0.58309300	-2.37884000	2.94894100
H	-0.79729700	-3.53170700	2.97442400
H	0.55323300	-3.75282500	1.80884700
O	0.79621800	0.60420400	-1.27202300
O	1.09692100	-1.53270600	0.55398900
Ni	2.43609000	-0.31830500	-0.39033900
O	2.84191500	0.62916300	1.41436300
O	4.03702300	-1.54912500	0.31551000
Cl	5.31323700	-1.86169300	-0.47666800
O	2.12265700	2.96027900	1.02443100
O	5.97743500	-0.56124200	-0.83362700
O	6.19069900	-2.71364700	0.33228300
O	0.76207600	1.48885100	2.42907200
O	4.89638400	-2.56913800	-1.75087200
Cl	2.16342200	1.86774700	2.03854600
O	2.95702300	2.24251200	3.22256000
O	3.72921200	0.94872500	-1.40446500
H	4.65310700	0.64524400	-1.23265200
H	3.59701100	0.90114400	-2.36497100
O	2.39987100	-1.59022500	-2.13219600
H	3.27410300	-2.06144400	-2.12766100
H	1.73319500	-2.27945000	-1.98021500
H	-0.09347400	2.94857700	0.76635500
TS6ad			
C	7.23920100	-1.63140000	-0.60650200
C	7.06363400	-0.53284600	0.24809300
C	5.79918600	0.01496400	0.45690700
C	4.67841400	-0.52920200	-0.18795200

C	4.84236900	-1.62804900	-1.05148600
C	6.10682600	-2.16767300	-1.24958100
H	7.92457700	-0.10510200	0.75547900
H	5.68132700	0.86553700	1.12438100
H	3.97635900	-2.04770500	-1.55293800
H	6.22573100	-3.01988300	-1.91474800
C	8.60353600	-2.23574500	-0.83339400
H	8.86075000	-2.24078100	-1.89989900
H	9.38310900	-1.68293800	-0.30017700
H	8.63390400	-3.27764600	-0.49000600
C	3.37299800	0.07804100	0.03320700
H	3.27085200	0.80445400	0.83178400
O	2.32216400	-0.68152000	-0.23332800
C	1.04073600	-0.15161800	-0.26020600
C	0.44053700	0.36696100	0.95231000
C	0.22219700	-0.69652500	-1.32941300
O	1.30909100	0.56931200	1.94419100
O	0.90618800	-1.39924100	-2.23327800
C	0.75684400	0.95787900	3.22747900
H	1.62044900	1.03400200	3.88787900
H	0.24742500	1.91944200	3.13926000
H	0.06798800	0.18572600	3.57259700
C	0.12931200	-1.99361300	-3.30170600
H	-0.35043100	-1.21501300	-3.89871000
H	0.85529700	-2.54824900	-3.89546000
H	-0.63025600	-2.65924300	-2.88677500
O	-0.75854200	0.66973300	1.08625400
O	-0.99630300	-0.49811400	-1.47638000
Ni	-2.33905200	-0.07277900	-0.00168100
O	-2.03346600	-2.03327300	0.70570200
O	-3.85069200	-0.87226900	-1.24340300
Cl	-1.67308400	-2.42374600	2.15841600
Cl	-5.22202000	-0.20533500	-1.45161200
O	-1.96542800	-3.85572600	2.32672700
O	-2.52000700	-1.58301400	3.08580900
O	-5.86865700	-0.04216900	-0.10536200
O	-4.97938100	1.15837000	-2.05761100
O	-0.23159900	-2.12164700	2.38390000
O	-6.02842500	-1.04171300	-2.34678500
C	1.98081800	1.84217200	-1.34296900
H	1.33851000	1.63770700	-2.20791600
C	1.59909200	2.97600700	-0.49310700
C	2.53844300	3.59363600	0.35558000
C	0.29329400	3.49554000	-0.57863900

C	2.17296400	4.70504500	1.11179700
H	3.55718100	3.21835500	0.38312900
C	-0.06657100	4.60758000	0.18107500
H	-0.44125700	3.01682900	-1.22095400
C	0.86985700	5.21260100	1.02705600
H	2.90358200	5.18739300	1.75562700
H	-1.07489500	5.00626000	0.11062300
H	0.58881000	6.08413500	1.61252000
O	3.14271000	1.31419000	-1.33520700
O	-3.65742400	0.37773300	1.53867500
H	-3.42148100	-0.26686600	2.24892000
H	-4.56034800	0.15000100	1.22003600
O	-2.72626300	1.89195400	-0.70216500
H	-3.04285900	2.34633000	0.09796100
H	-3.51796600	1.81606600	-1.29441300

TS6bc

C	-7.45317600	-0.71043700	-0.85188700
C	-7.01157800	0.62041000	-0.83483200
C	-5.65558700	0.92265600	-0.71114600
C	-4.70981200	-0.10637100	-0.60714700
C	-5.13945800	-1.44480800	-0.62181200
C	-6.49331300	-1.73456700	-0.74357300
H	-7.73525900	1.42702700	-0.92132400
H	-5.33212100	1.96118900	-0.70397200
H	-4.40768600	-2.24166100	-0.53652300
H	-6.81828100	-2.77253100	-0.75398600
C	-8.91931800	-1.04714200	-0.98051800
H	-9.27911000	-1.58453500	-0.09399700
H	-9.53048500	-0.14700800	-1.09853000
H	-9.10172400	-1.69571900	-1.84623000
C	-3.29291800	0.23523700	-0.46171600
H	-3.00659600	1.27428000	-0.59170500
O	-2.44357900	-0.68000900	-0.91405700
C	-1.79474800	0.55422700	1.64860900
H	-1.11774300	-0.15171000	2.14239500
C	-1.41582000	1.96049000	1.59396200
C	-2.38912400	2.96622700	1.39805200
C	-0.06945400	2.32542300	1.80566700
C	-2.01716700	4.30649400	1.39919400
H	-3.43364500	2.68527200	1.29832100
C	0.29635500	3.67065400	1.79109100
H	0.68591600	1.55944100	1.95074100
C	-0.67256800	4.65918300	1.58798600

H	-2.76940600	5.07990500	1.26930500
H	1.33652400	3.94445200	1.94190100
H	-0.38489100	5.70741400	1.58970700
O	-2.94088000	0.11808000	1.29954700
C	-1.06658800	-0.57031400	-0.73087400
C	-0.33121300	0.54698700	-1.23939200
C	-0.42783800	-1.82179100	-0.40517400
O	-1.08734100	1.49551400	-1.82472900
O	-1.27683300	-2.80477700	-0.09742100
C	-0.38293000	2.64222400	-2.35550000
H	-1.16072200	3.26933300	-2.79152000
H	0.14121200	3.16847700	-1.55531400
H	0.33183100	2.32510900	-3.11779100
C	-0.68680300	-4.05444300	0.32884600
H	-0.07185300	-3.89007300	1.21559000
H	-1.53683100	-4.69798600	0.55559300
H	-0.08201400	-4.48149100	-0.47460000
O	0.90168000	0.70897800	-1.15009400
O	0.80318900	-2.03153900	-0.39634800
Ni	2.29415700	-0.65795000	-0.54835700
O	2.06794200	-0.16181700	1.51444600
O	3.71589800	0.90184500	-0.63950600
Cl	5.05139000	0.79282400	-1.39694500
O	0.49795700	-1.63635000	2.71312300
O	4.73613600	0.52897900	-2.84884200
O	5.79026400	2.05147800	-1.23753000
O	2.84978100	-2.30133600	2.48338600
O	5.81086600	-0.37379600	-0.83054200
Cl	1.90890000	-1.14869200	2.69716500
O	2.23536000	-0.41187300	3.93171200
O	3.73640300	-2.09739000	-0.11677700
H	4.61210100	-1.65291000	-0.18137300
H	3.59441400	-2.33261300	0.82933300
O	2.60356900	-1.19227900	-2.57192500
H	3.33668400	-0.61777800	-2.90371300
H	2.96338600	-2.09524300	-2.54663500

TS6bd

C	-7.31681800	-0.61726900	-0.62346600
C	-6.83299400	0.60929700	-1.10231500
C	-5.48599000	0.94472800	-0.97517900
C	-4.59097100	0.05363600	-0.36513700
C	-5.06463100	-1.17785200	0.12319100
C	-6.40899800	-1.50189700	-0.00993600

H	-7.51649500	1.30524800	-1.58214400
H	-5.12753500	1.89847500	-1.35578600
H	-4.37272200	-1.86784800	0.59524300
H	-6.76743300	-2.45777700	0.36530400
C	-8.77328300	-0.99021700	-0.75807400
H	-9.23486500	-1.13630300	0.22675800
H	-9.34049200	-0.21619500	-1.28415100
H	-8.89019200	-1.93047000	-1.31110900
C	-3.18930200	0.43620800	-0.23649000
H	-2.84506200	1.30989100	-0.77994400
O	-2.32848000	-0.56075800	-0.08871500
C	-1.81051900	1.54098300	1.69489300
H	-1.31027500	1.04432200	2.53462300
C	-1.18608700	2.75504800	1.16848700
C	-1.93544500	3.69496000	0.43101000
C	0.17409200	3.00644900	1.43681200
C	-1.32788800	4.85691900	-0.03764700
H	-2.99517300	3.52133000	0.26777900
C	0.78073600	4.16349500	0.95082000
H	0.75810600	2.28043600	1.99629900
C	0.03150400	5.08819900	0.21452400
H	-1.90997800	5.58780200	-0.59282600
H	1.83742900	4.33641500	1.13220100
H	0.50535900	5.99167900	-0.16006800
O	-3.01003200	1.18910100	1.43570800
C	-0.99901500	-0.31603200	0.22412400
C	-0.14926900	0.40314800	-0.69344500
C	-0.45059500	-1.26419500	1.17658100
O	-0.78624800	0.95773100	-1.73023100
O	-1.36892700	-2.02083200	1.77190000
C	0.05145500	1.63561200	-2.70591100
H	-0.64344000	1.98433000	-3.46938300
H	0.57815200	2.46741500	-2.23610600
H	0.77503000	0.93306000	-3.12285800
C	-0.87843600	-3.05686500	2.65522300
H	-0.33854700	-2.61293800	3.49486100
H	-1.77458600	-3.57172400	3.00092200
H	-0.22630800	-3.73360100	2.10045900
O	1.07413400	0.57331200	-0.55193400
O	0.75184400	-1.35936000	1.49212900
Ni	2.35373900	-0.62928500	0.45373700
O	3.67913300	2.06016900	-1.88923200
O	2.14423800	-2.04517000	-1.09812500
Cl	4.49725000	1.53629300	-0.77700800

Cl	1.72289500	-3.52068700	-0.89752700
O	5.93891900	1.55053800	-1.07625900
O	4.09903200	0.06265700	-0.49136100
O	2.07138700	-4.25925400	-2.12168600
O	2.49264100	-4.05697500	0.29242800
O	4.21419200	2.32265700	0.49317500
O	0.26349100	-3.56852100	-0.61459200
O	2.67286600	0.74637400	2.02691400
H	3.18609300	0.25295000	2.68870100
H	3.29528600	1.40713900	1.62134800
O	3.71072200	-1.90009900	1.41781900
H	3.39236100	-2.80110100	1.15151700
H	4.54154200	-1.75650900	0.92891400

TS6cd

C	-7.47710000	-1.08865800	-0.59663200
C	-7.12963100	0.26660500	-0.49942900
C	-5.79627900	0.65615700	-0.37491600
C	-4.77907800	-0.30799300	-0.35082400
C	-5.11410100	-1.67033100	-0.44521000
C	-6.44619800	-2.04725300	-0.56634800
H	-7.90954300	1.02350400	-0.52276500
H	-5.54661000	1.71245200	-0.30384900
H	-4.32724900	-2.41740700	-0.41949900
H	-6.69804700	-3.10297100	-0.63696100
C	-8.91699100	-1.51934300	-0.73883500
H	-9.18974300	-2.24940900	0.03290800
H	-9.60174000	-0.66948300	-0.65805700
H	-9.08942600	-1.99869100	-1.71108100
C	-3.38811700	0.12276600	-0.20090400
H	-3.17874000	1.18679800	-0.25484900
O	-2.48375200	-0.69045600	-0.73880500
C	-1.83624000	0.34423000	1.86251500
H	-1.11666200	-0.36948900	2.27791300
C	-1.51286500	1.76194900	1.92880200
C	-2.52684200	2.74262800	1.84822800
C	-0.17301100	2.15717900	2.12074300
C	-2.19768400	4.09084000	1.94227600
H	-3.56420300	2.43320100	1.76024000
C	0.15105300	3.51065400	2.18996300
H	0.60266900	1.39938500	2.17818500
C	-0.85838900	4.47582300	2.10274100
H	-2.97894400	4.84497300	1.90070200
H	1.18796000	3.81265400	2.29985800

H	-0.60370000	5.53044300	2.16587700
O	-2.98302500	-0.10787500	1.53308200
C	-1.11844600	-0.50413100	-0.54924700
C	-0.44893500	0.68689300	-0.99302400
C	-0.38912300	-1.74114100	-0.37316500
O	-1.26136100	1.65027700	-1.45719200
O	-1.15628200	-2.80916800	-0.15395400
C	-0.61843400	2.87121500	-1.91126400
H	-1.44181900	3.54536000	-2.14664800
H	0.02350700	3.27811100	-1.12935600
H	-0.01944400	2.66606900	-2.80113700
C	-0.45917600	-4.06781600	0.04806900
H	0.23157200	-3.98899900	0.88854200
H	-1.25114000	-4.78901800	0.24812200
H	0.10085800	-4.33535700	-0.84968100
O	0.78069700	0.87632000	-0.94570000
O	0.85185600	-1.85770500	-0.40741800
Ni	2.30836600	-0.43002800	-0.42333900
O	3.42421600	2.14773400	-2.39968100
O	3.83532800	-1.80360200	-0.01779800
Cl	3.74149700	2.45267500	-0.95606000
Cl	3.72982100	-3.05999600	0.87774900
O	5.08809400	3.03027300	-0.81706400
O	3.73488400	1.09549000	-0.19673200
O	5.09807700	-3.45217600	1.25429900
O	2.93189800	-2.66375300	2.11330400
O	2.69922400	3.33428800	-0.36979400
O	3.01859100	-4.13550100	0.15059400
O	2.14457400	-0.13996300	1.66446500
H	2.42621400	-1.03044700	2.01241000
H	2.91537000	0.44673800	1.78318300
O	2.82646300	-0.54658900	-2.44507500
H	2.11935400	-0.80753900	-3.05430800
H	3.08052100	0.38198800	-2.66846700
TS7ab			
C	1.85786200	2.10550900	0.32074600
H	1.36728400	1.84587600	1.26694300
C	1.25759500	3.15137800	-0.47255900
C	1.84978600	3.59428800	-1.67709100
C	0.05523200	3.72993000	-0.01605500
C	1.24232300	4.60994600	-2.40269900
H	2.77186000	3.13406000	-2.01792200
C	-0.55271700	4.74051000	-0.75727100

H	-0.41623300	3.37122100	0.89404100
C	0.04283500	5.18084900	-1.94349800
H	1.69067100	4.96073300	-3.32802400
H	-1.49055700	5.16483800	-0.41371700
H	-0.43053300	5.96993000	-2.52214400
O	2.92775500	1.52388500	-0.00100600
C	7.34202400	-0.91365800	0.16467600
C	6.87843600	-0.21885800	1.29170100
C	5.51816800	0.02959100	1.46859000
C	4.59081400	-0.41573600	0.51648500
C	5.04178300	-1.10935400	-0.61983400
C	6.40056700	-1.35155400	-0.78565100
H	7.58840000	0.12644700	2.03887100
H	5.17617500	0.56817800	2.34954700
H	4.32384200	-1.45765200	-1.35530800
H	6.74259500	-1.89259200	-1.66488900
C	8.81188400	-1.19962800	-0.02797800
H	9.16455200	-0.82456200	-0.99655400
H	9.41901800	-0.73625500	0.75619000
H	9.00716800	-2.27973000	-0.01055700
C	3.16783100	-0.14202200	0.72848300
H	2.85461100	0.15929300	1.72605400
O	2.32770700	-0.88518500	0.03581200
C	0.93465300	-0.72515700	0.22571300
C	0.35648600	-1.08359900	1.47460300
C	0.17358000	-0.54647100	-0.96726800
O	1.25669300	-1.41105400	2.43285700
O	0.90418100	-0.46548100	-2.08898500
C	0.71084900	-1.87202500	3.68804600
H	1.58112300	-2.09903400	4.30462500
H	0.09747900	-1.09391600	4.14823800
H	0.10519000	-2.76709800	3.52967100
C	0.16287300	-0.41319400	-3.32820500
H	-0.43658700	0.49943700	-3.37611300
H	0.92595300	-0.41347100	-4.10719400
H	-0.48341400	-1.28908900	-3.41411500
O	-0.86044200	-1.10028000	1.75305400
O	-1.07169200	-0.43813500	-1.02436700
Ni	-2.39955600	-0.74464400	0.47734400
O	-2.67940600	-2.79096500	0.09826800
O	-2.23513000	1.33023200	1.02000600
Cl	-3.43972900	2.29001300	1.02464500
O	-1.09090100	-3.50476200	-1.65366300
O	-4.47950600	1.72378800	1.94486500

O	-2.96325400	3.60871400	1.49929900
O	-3.12659100	-4.80115400	-1.20539900
O	-3.97394200	2.38577400	-0.37050400
Cl	-2.53124400	-3.45495600	-1.29755700
O	-3.28499800	-2.60160500	-2.28923000
O	-3.79338500	-1.02664600	2.02240100
H	-4.24723500	-0.16247600	2.13825600
H	-4.45535100	-1.64612700	1.67111600
O	-4.01650200	-0.40843600	-0.79461100
H	-4.06416100	0.51793800	-1.10164400
H	-3.87960400	-1.01583500	-1.55747600

TS7ac

C	1.86257900	1.74620800	0.47766400
H	1.28830200	1.14684400	1.19187600
C	1.58104300	3.15897800	0.37995600
C	2.30991000	3.99969800	-0.49132500
C	0.53863100	3.68153400	1.17511300
C	1.99649600	5.35017800	-0.55759100
H	3.10585600	3.57773100	-1.09714100
C	0.23064500	5.03903800	1.09467300
H	-0.01655200	3.02156700	1.83741200
C	0.95633400	5.86763500	0.23366500
H	2.55128200	6.00705400	-1.22146900
H	-0.57448000	5.44689200	1.69836000
H	0.71369500	6.92556000	0.17354100
O	2.74252000	1.18361600	-0.22191800
C	7.12266000	-1.17901000	-0.22381600
C	6.43049600	-0.99676400	0.98257400
C	5.04823600	-0.81200400	0.99452300
C	4.32809900	-0.80763400	-0.20778400
C	5.00788100	-0.98870600	-1.42277600
C	6.38741000	-1.17047500	-1.42313300
H	6.97808600	-1.00221600	1.92182500
H	4.52743600	-0.67629600	1.93982900
H	4.45105500	-0.99085300	-2.35445300
H	6.90708300	-1.31019400	-2.36842900
C	8.61629700	-1.40158200	-0.24057600
H	9.10090300	-0.79861000	-1.01732900
H	9.07146500	-1.14674600	0.72177700
H	8.85313200	-2.45276800	-0.45239000
C	2.87138600	-0.60775800	-0.16346100
H	2.37138400	-0.73369500	0.79601500
O	2.19800200	-1.01506800	-1.22922500

C	0.78981200	-1.13242100	-1.08661300
C	0.28421600	-2.21778700	-0.32582500
C	-0.02415000	-0.23503900	-1.80668700
O	1.22947300	-3.03943800	0.16596700
O	0.63605800	0.64280600	-2.59058100
C	0.77823200	-4.07499500	1.06345000
H	1.68533200	-4.60429000	1.35719400
H	0.28848000	-3.62931000	1.93205200
H	0.08940500	-4.75032400	0.55031400
C	-0.17427800	1.58167600	-3.32361400
H	-0.81147700	2.15588700	-2.64693900
H	0.54014000	2.23115400	-3.83093500
H	-0.80005300	1.06110300	-4.05353100
O	-0.92871100	-2.45690000	-0.09935800
O	-1.28511000	-0.20374100	-1.77257700
Ni	-2.38006000	-1.04643300	-0.26455200
O	-1.48924600	0.23870400	1.16215600
O	-3.81656400	0.52234200	-0.50362100
Cl	-5.33513900	0.30291500	-0.55158400
O	-1.72158300	-0.91221800	3.34901800
O	-5.75707800	-0.35014800	0.73550300
O	-6.00224100	1.59741300	-0.74204700
O	0.47930800	-0.74053400	2.27070200
O	-5.62759400	-0.63154200	-1.70350000
Cl	-0.83997700	-0.06154300	2.53070300
O	-0.58868600	1.26546000	3.16329300
O	-3.58797200	-2.04509400	1.10631500
H	-4.43100400	-1.54511300	1.21400900
H	-3.82469000	-2.91921400	0.75602900
O	-3.36195700	-2.16913600	-1.78314300
H	-4.22498700	-1.70980700	-1.93767800
H	-2.82170600	-2.00434300	-2.57388900
TS7ad			
C	7.33487000	-0.65557000	-0.70083800
C	7.09615200	-0.38294500	0.65493300
C	5.79992900	-0.18612700	1.12635400
C	4.71071200	-0.25401600	0.24422800
C	4.93678500	-0.52109600	-1.11858700
C	6.23364100	-0.72018100	-1.57575000
H	7.93297300	-0.32855400	1.34657900
H	5.63192300	0.02378500	2.18021900
H	4.09422200	-0.58006700	-1.79997100
H	6.40150100	-0.93281400	-2.62896800

C	8.73403900	-0.89386000	-1.21414600
H	8.93614700	-0.29487500	-2.11002200
H	9.48774500	-0.64498100	-0.46063300
H	8.87383500	-1.94677900	-1.49211000
C	3.36889500	-0.03020100	0.76542700
H	3.21915600	-0.07427600	1.83980100
O	2.37163400	-0.41038500	-0.00812700
C	1.04201700	-0.12529600	0.30980300
C	0.44073100	-0.66933300	1.49839300
C	0.24963200	0.25742300	-0.82922900
O	1.32086700	-1.17281800	2.37999200
O	0.95124700	0.50342800	-1.93447000
C	0.76189000	-1.92092000	3.48777400
H	1.62631100	-2.26084700	4.05827600
H	0.11977600	-1.27864300	4.09401100
H	0.19344300	-2.76789400	3.09955500
C	0.18272000	0.73238600	-3.13993400
H	-0.41907500	1.63850000	-3.04160900
H	0.92940300	0.84489300	-3.92602400
H	-0.46216700	-0.12712600	-3.33236600
O	-0.77367600	-0.64836900	1.77079400
O	-0.98931200	0.42765900	-0.81613800
Ni	-2.33312200	-0.45597300	0.44610600
O	-2.17911900	-2.43907300	-0.21561700
O	-3.88230900	-0.16110500	-1.00324400
Cl	-0.93274700	-3.25192300	-0.68201500
Cl	-5.29696300	0.33778400	-0.66944200
O	-1.42882900	-4.56603000	-1.13118600
O	-0.00783700	-3.38264100	0.48414300
O	-5.91007700	-0.61242100	0.32168300
O	-5.16711400	1.70123300	-0.02886100
O	-0.27345900	-2.49327000	-1.78115400
O	-6.08387000	0.41156200	-1.90581400
C	1.97048400	2.14448500	1.17732000
H	1.67344800	1.74281900	2.15567100
C	1.14097700	3.20774000	0.62051400
C	1.47549700	3.83311800	-0.59641300
C	0.00048600	3.62516800	1.33391200
C	0.67209600	4.85722700	-1.09024300
H	2.35785500	3.50269000	-1.13511400
C	-0.79847500	4.65323700	0.83455700
H	-0.25631300	3.14250800	2.27429400
C	-0.46373500	5.26740700	-0.37825700
H	0.92638100	5.34006600	-2.02970000

H	-1.67651100	4.97582800	1.38697800
H	-1.08772000	6.06661000	-0.76899900
O	3.09354600	1.82809200	0.69143700
O	-3.67073000	-1.39130000	1.75228100
H	-3.47609100	-2.32415600	1.54221800
H	-4.58371100	-1.22947700	1.41444600
O	-2.71799800	1.49873700	1.16095500
H	-3.63569800	1.72506100	0.86640500
H	-2.13413200	2.03705700	0.59854400

TS7bc

C	-2.61642900	1.56231000	-0.30339500
H	-1.66514100	1.37649100	-0.81795200
C	-3.01978800	2.93223000	-0.09999700
C	-4.22796800	3.26039800	0.55652400
C	-2.16632900	3.94978100	-0.57988000
C	-4.57201700	4.59422000	0.72655100
H	-4.87124400	2.46529000	0.92056800
C	-2.52326200	5.28539200	-0.40120000
H	-1.24299100	3.67843600	-1.08488800
C	-3.71987700	5.60458300	0.24838500
H	-5.49808900	4.85852400	1.22893300
H	-1.87155100	6.07311500	-0.76713700
H	-3.99621700	6.64689200	0.38555700
O	-3.32836900	0.59514900	0.07648600
C	-6.36374500	-3.27585300	-0.49507400
C	-5.76778200	-2.65489000	-1.60244100
C	-4.58700400	-1.92485200	-1.46522400
C	-3.97590100	-1.80274800	-0.21097300
C	-4.56032500	-2.41938800	0.90572400
C	-5.73959600	-3.14374100	0.75838300
H	-6.22875300	-2.74750000	-2.58273100
H	-4.13798800	-1.45543900	-2.33800500
H	-4.08209700	-2.33687700	1.87645400
H	-6.18385700	-3.62144300	1.62883900
C	-7.63144000	-4.08406600	-0.63961100
H	-8.38508600	-3.77708800	0.09555400
H	-8.06702800	-3.97392500	-1.63773300
H	-7.43724700	-5.15207300	-0.47600000
C	-2.72204000	-1.03002400	-0.09293400
H	-2.14713800	-0.88258600	-1.00902100
O	-2.00059800	-1.26271300	0.99763400
C	-0.60709100	-0.98812000	0.92500200
C	0.21528200	-1.98072500	0.32811900

C	-0.10609600	0.13147300	1.62053100
O	-0.46607800	-3.02433300	-0.19133300
O	-1.04738500	0.88615200	2.24048200
C	0.32795200	-4.04877700	-0.82644700
H	-0.39689500	-4.77534000	-1.19510400
H	0.91122600	-3.62600000	-1.64777900
H	1.00302800	-4.51019100	-0.10181800
C	-0.56173000	2.00334200	3.00898000
H	-0.00323500	2.69753100	2.37605900
H	-1.45797500	2.47881400	3.40983900
H	0.08119500	1.65656600	3.82228900
O	1.46437400	-1.96037000	0.24538300
O	1.09925700	0.48030400	1.69453600
Ni	2.59183000	-0.31227700	0.55448100
O	1.64876000	0.37884800	-1.26858600
O	4.10825800	-1.16839700	-0.66023900
Cl	5.60585900	-1.13809200	-0.31474200
O	1.89224600	2.78739300	-0.77357100
O	5.79032600	-1.84425500	1.00629000
O	6.35664900	-1.81122600	-1.38175300
O	2.18909900	1.95812200	-3.07035900
O	6.02107700	0.30149300	-0.17171300
Cl	1.43975800	1.79141400	-1.81356500
O	-0.03441900	1.96666300	-2.04159900
O	3.69852200	1.42952200	0.84306000
H	4.58320800	1.29376100	0.43171600
H	3.22718100	2.11622300	0.32006700
O	3.48623400	-1.07466900	2.30016000
H	4.35526900	-1.46358500	2.03364700
H	3.69219400	-0.30703700	2.85921400

TS7bd

C	2.02287300	2.13337000	0.82152300
H	1.43103200	1.91747000	1.72045200
C	1.54579800	3.19390100	-0.04987700
C	2.30741700	3.62212600	-1.15739700
C	0.31315200	3.81052300	0.23916100
C	1.83995200	4.66132700	-1.95389400
H	3.25316500	3.13403500	-1.37035800
C	-0.14941500	4.84940000	-0.56590500
H	-0.28730300	3.45880500	1.07347300
C	0.61390300	5.27643600	-1.65759800
H	2.42439600	4.99848500	-2.80543700
H	-1.10275500	5.32095700	-0.34624300

H	0.25331800	6.08858000	-2.28358600
O	3.14215200	1.57179800	0.66198500
C	7.19294100	-1.48155100	0.71266600
C	6.69390100	-0.97411100	1.92213600
C	5.36217400	-0.57993000	2.03641400
C	4.49857900	-0.68586800	0.93586700
C	4.98719800	-1.18837800	-0.28387200
C	6.31661100	-1.58012700	-0.38491400
H	7.35416800	-0.88946600	2.78154900
H	4.99207400	-0.18735600	2.98080200
H	4.31910800	-1.27207500	-1.13498900
H	6.68715800	-1.97138800	-1.32956300
C	8.62865300	-1.93005600	0.58747400
H	9.09953300	-1.50993200	-0.30917600
H	9.22203400	-1.62935900	1.45646900
H	8.69037300	-3.02286600	0.50211900
C	3.11440400	-0.24965500	1.08079600
H	2.72835600	-0.08683700	2.08293500
O	2.26953500	-0.68012700	0.16446400
C	0.93314100	-0.25568700	0.14848900
C	0.06891700	-0.54698000	1.25142200
C	0.43633500	0.08398800	-1.15623400
O	0.68647700	-1.05613500	2.33474400
O	1.37654300	0.13544500	-2.10355000
C	-0.18065800	-1.47636000	3.42202200
H	0.49798100	-1.86790600	4.17971600
H	-0.75534500	-0.62976200	3.80092800
H	-0.86637800	-2.24976100	3.07173900
C	0.91209200	0.33617500	-3.45825200
H	0.42154300	1.30808300	-3.55185400
H	1.81535000	0.29938700	-4.06795300
H	0.22281000	-0.46445000	-3.73248700
O	-1.15817200	-0.33378100	1.29277000
O	-0.75035500	0.36714900	-1.42720200
Ni	-2.38514500	-0.06715900	-0.28833000
O	-3.82441000	-0.72907500	3.16809500
O	-2.27315800	-2.13104600	-0.74292000
Cl	-4.60377200	-0.00168600	2.14547300
Cl	-1.87849700	-2.72299100	-2.11492900
O	-6.05395700	-0.22933500	2.26989700
O	-4.17973600	-0.48564700	0.73250800
O	-2.31921100	-4.12756300	-2.14474600
O	-2.58899400	-1.91551100	-3.18352000
O	-4.29540900	1.48401900	2.21220000

O	-0.40666000	-2.59982300	-2.29000600
O	-2.63541900	1.98664100	0.15068400
H	-3.13935200	2.32764300	-0.60729600
H	-3.26455900	1.97402300	0.92032900
O	-3.71284100	0.20029100	-1.89053300
H	-3.41699000	-0.49396400	-2.53421300
H	-4.55600700	-0.12205500	-1.52245000

TS7cd

C	-1.94512700	1.53227900	-0.76298400
H	-1.02152900	0.98833300	-0.99859300
C	-1.95447000	2.96599100	-0.87163200
C	-3.13456400	3.71277800	-0.63795900
C	-0.75031200	3.62208900	-1.20968100
C	-3.10186000	5.09406300	-0.75280800
H	-4.05087900	3.19436100	-0.37403900
C	-0.72911400	5.01153700	-1.31239000
H	0.16762800	3.06139800	-1.36248900
C	-1.89954400	5.74217600	-1.08904900
H	-4.00198500	5.67671500	-0.57977100
H	0.20033200	5.51675500	-1.55535500
H	-1.88092600	6.82586400	-1.17080600
O	-2.96990800	0.88515700	-0.40705700
C	-6.96832900	-2.05497900	-0.29276900
C	-6.18226300	-1.97324500	-1.45133000
C	-4.84825600	-1.57035600	-1.38510100
C	-4.27245700	-1.24102200	-0.15194500
C	-5.04738600	-1.31654100	1.01577000
C	-6.37728000	-1.71845400	0.93856200
H	-6.61596100	-2.23241500	-2.41394600
H	-4.25422300	-1.51878400	-2.29508600
H	-4.60090000	-1.06988900	1.97371800
H	-6.96986800	-1.77719400	1.84879100
C	-8.40731000	-2.50909600	-0.35376400
H	-9.06806200	-1.80871600	0.17098800
H	-8.75794300	-2.59699200	-1.38684000
H	-8.53016400	-3.48910600	0.12532000
C	-2.85763900	-0.82094000	-0.10546300
H	-2.24406200	-1.08009600	-0.96899100
O	-2.26458400	-0.95063200	1.07846000
C	-0.84625400	-0.89629000	1.08594200
C	-0.12965300	-2.03085100	0.62722000
C	-0.22206800	0.18935300	1.74411300
O	-0.90031300	-3.05160100	0.20268800

O	-1.05950100	1.07872200	2.31282100
C	-0.20543300	-4.24613600	-0.23252900
H	-0.98265500	-4.87753400	-0.66398700
H	0.56834700	-4.00374900	-0.96229000
H	0.25379700	-4.73986500	0.62779600
C	-0.43977900	2.17558800	3.02617400
H	0.27942500	2.69494900	2.39074700
H	-1.26870200	2.82608600	3.30746000
H	0.06793100	1.79942100	3.91838900
O	1.12115300	-2.13611600	0.59035700
O	1.02100700	0.36848200	1.82150500
Ni	2.32892600	-0.48478900	0.50853600
O	4.30447400	-3.28869300	0.36970600
O	3.51154900	1.29056100	0.43326500
Cl	4.05163000	-2.81153900	-1.03789300
Cl	3.11694600	2.69452000	-0.03033600
O	5.28292900	-2.85987000	-1.84397800
O	3.61176600	-1.32132100	-0.94350000
O	4.34203500	3.48402700	-0.22574100
O	2.37468000	2.54649800	-1.36092100
O	2.95086000	-3.58608700	-1.66588000
O	2.19737100	3.32391600	0.95360400
O	1.32063900	0.09531000	-1.30052100
H	1.72640300	0.98489800	-1.48714500
H	1.79722100	-0.52954400	-1.88041000
O	3.54216500	-1.22065500	2.02337800
H	2.99428100	-1.52194500	2.76533700
H	3.94076500	-2.02876600	1.61634000

Other metal test

IM1-Cu(ClO₄)₂

O	-1.04250200	-1.50735500	-0.46273500
O	1.88540400	-0.34960300	2.58988100
O	-0.08604800	0.53983500	3.26695800
O	-0.84209100	0.96104300	0.62459200
C	0.14369000	-0.01145800	0.97954500
C	0.44228400	1.06116300	-0.02972400
C	-0.19523300	-1.37600300	0.42689200
C	0.75886600	0.03986400	2.36680100
C	0.40236300	0.61875600	4.62548700
H	-0.42244900	1.04147200	5.19784900
H	1.28275200	1.26466200	4.66845400
H	0.65777600	-0.37967900	4.98833100
O	0.45310200	-2.37615500	0.96081200

C	0.12757800	-3.71009900	0.47026100
H	0.39352900	-3.77743100	-0.58616200
H	0.73774100	-4.37908100	1.07471700
H	-0.93759500	-3.89623200	0.61624400
C	3.50776200	-1.39417000	-0.37461700
H	3.42306300	-1.25281800	0.72013500
O	2.53742900	-1.18002600	-1.09197800
C	4.82810300	-1.83851900	-0.86392300
C	5.05694800	-2.06080100	-2.23364700
C	5.86516000	-2.04092600	0.06081000
C	6.31160600	-2.48051800	-2.66753500
H	4.24299900	-1.90018100	-2.93478400
C	7.12250200	-2.46162400	-0.37611800
H	5.68105400	-1.86655900	1.11903600
C	7.34400000	-2.68093700	-1.73952000
H	6.49204100	-2.65371100	-3.72506000
H	7.92496000	-2.61808200	0.33952500
H	8.32203400	-3.00890200	-2.08236100
H	0.43237600	0.72554200	-1.06491000
C	1.27382500	2.25904400	0.25926500
C	2.41373300	2.49272700	-0.52377300
C	0.93960900	3.17003000	1.26934000
C	3.21419000	3.60813400	-0.28330200
H	2.67274400	1.79868600	-1.31957200
C	1.74451200	4.28751500	1.49650700
H	0.04130300	3.01503200	1.85898700
C	2.89436600	4.52626500	0.72971800
H	4.09682600	3.77322000	-0.89743700
H	1.46772800	4.99159900	2.27815300
C	3.74693700	5.75245200	0.95990500
H	3.57454400	6.17982900	1.95325700
H	4.81453200	5.52118000	0.86996600
H	3.52038700	6.53332100	0.22149200
Cu	-2.58324900	-0.14063100	-0.56648800
Cl	-3.23248900	1.63924800	-2.45767400
Cl	-4.05669200	-2.05360500	0.96278200
O	-3.92150700	1.36306600	-1.09577400
O	-2.08817900	0.55981000	-2.37632900
O	-4.11140600	-2.19448600	-0.52943600
O	-3.28606300	-0.67590700	1.17888100
O	-2.65191900	2.98470600	-2.49782000
O	-4.12676800	1.35311700	-3.57960200
O	-5.38384200	-1.92849800	1.57755800
O	-3.24121900	-3.11890300	1.58889900

IM1-Cu(OTf)₂

O	-0.54246800	0.48403600	2.27397900
O	1.10199000	4.43383200	1.27568800
O	-0.77071000	4.07629900	0.04548900
O	-0.13064400	1.40557200	-0.22237400
C	0.37945100	2.18504200	0.87044600
C	1.31267500	1.40015800	-0.00116200
C	0.03451200	1.56162900	2.21097000
C	0.29413400	3.69847900	0.75692600
C	-0.94884300	5.50175400	-0.11708600
H	-1.85748900	5.60766100	-0.70856900
H	-0.08845000	5.92818800	-0.63865100
H	-1.06085600	5.97824500	0.85982800
Cu	-1.41416400	-0.22068700	0.30973600
O	0.41829200	2.27852100	3.24351900
C	0.20272900	1.69392600	4.55425000
H	0.76348300	0.76027000	4.62475500
H	0.58150300	2.43676100	5.25458500
H	-0.86320500	1.51283200	4.70814600
O	-1.10971900	-1.21478200	-2.24164700
O	-2.97815900	1.05519600	0.50878900
S	-0.14046500	-2.05062700	-1.51056800
S	-3.98585700	-0.04102800	0.84853200
O	1.20151900	-2.26755500	-2.04921600
O	-4.85499400	0.18198000	1.99094700
O	-0.10422700	-1.61041800	-0.03150300
O	-3.15953700	-1.30731600	0.79938800
C	-0.90580400	-3.76412100	-1.39851700
C	-5.11205500	-0.11858400	-0.65685700
F	-0.99468600	-4.28954400	-2.62873800
F	-2.12834500	-3.70209300	-0.86254000
F	-0.13791900	-4.56255100	-0.64223700
F	-5.97916300	-1.12464900	-0.50810700
F	-4.39298900	-0.31164300	-1.76366200
F	-5.78479200	1.03379600	-0.76138800
C	3.64290700	-0.90767500	2.85022800
H	4.23944100	-0.76538900	3.77621800
O	2.70846500	-0.15210400	2.61435600
C	4.08366700	-2.02027800	1.99170900
C	3.35822000	-2.38816900	0.84369000
C	5.25996900	-2.71220800	2.32864800
C	3.81781600	-3.42432900	0.03501600
H	2.43382600	-1.87483400	0.60130600

C	5.71805100	-3.75096200	1.51791600
H	5.81332400	-2.42870400	3.22202700
C	4.99716600	-4.10334000	0.37114300
H	3.25537100	-3.69694500	-0.85282700
H	6.62916700	-4.28381400	1.77611300
H	5.35304700	-4.91213300	-0.26212900
H	1.67620000	0.47894200	0.44894200
C	2.16137200	2.00124200	-1.06088100
C	1.62188200	2.72322800	-2.13335900
C	3.55009900	1.82916800	-0.97885000
C	2.46616100	3.26977300	-3.10000000
H	0.54570100	2.83514000	-2.22266600
C	4.38462300	2.38913500	-1.94475200
H	3.97697200	1.26011600	-0.15653300
C	3.85866500	3.11623500	-3.02365600
H	2.03359300	3.81858000	-3.93367800
H	5.46052000	2.25168900	-1.86391500
C	4.76464200	3.68368400	-4.09145700
H	5.73335500	3.98413300	-3.67720600
H	4.96104900	2.93944700	-4.87509900
H	4.31570700	4.55751700	-4.57587800

IM1-Hg(ClO₄)₂

O	-0.56784700	-1.55932200	-0.70027300
O	2.33031900	-0.84639800	2.53285900
O	0.30833200	-0.23978600	3.35849400
O	-0.45353200	0.69250500	0.85311600
C	0.55871500	-0.31267800	1.00904200
C	0.82758700	0.92391600	0.20613100
C	0.23743600	-1.57163900	0.22914100
C	1.18019400	-0.49390600	2.38369800
C	0.79310100	-0.41191900	4.71014500
H	-0.05639500	-0.17037700	5.34775700
H	1.62977100	0.26596400	4.89583500
H	1.11354300	-1.44544000	4.86136500
O	0.86451000	-2.64419000	0.64843500
C	0.57200300	-3.88761800	-0.05053700
H	0.88718500	-3.79751700	-1.09178200
H	1.15663200	-4.64147600	0.47419300
H	-0.49750500	-4.09644100	0.01326600
C	3.93844900	-1.35036200	-0.53158100
H	3.87164300	-1.37564100	0.57299200
O	2.94361900	-1.07762900	-1.19374800
C	5.26537100	-1.65639900	-1.10171700

C	5.47299500	-1.66665800	-2.49256000
C	6.33077600	-1.94231300	-0.23287300
C	6.73472800	-1.96049700	-3.00277600
H	4.63750600	-1.44374800	-3.14995400
C	7.59525100	-2.23610100	-0.74626300
H	6.16293200	-1.93208300	0.84224800
C	7.79544100	-2.24509300	-2.13036300
H	6.89883800	-1.96984600	-4.07695300
H	8.41963500	-2.45680500	-0.07376700
H	8.77895300	-2.47397800	-2.53280000
H	0.80041800	0.77804300	-0.87165100
C	1.64411600	2.06811500	0.68691000
C	2.75405600	2.46140200	-0.07345800
C	1.33237200	2.77152300	1.85766300
C	3.54800900	3.52900900	0.34348400
H	2.99583600	1.93059100	-0.99091100
C	2.12876500	3.84369800	2.26058000
H	0.45590200	2.49653900	2.43674200
C	3.24901300	4.24128100	1.51500300
H	4.40695500	3.82010000	-0.25705800
H	1.86785500	4.38798700	3.16559500
C	4.08306300	5.42848100	1.93675400
H	4.05507300	5.57379300	3.02209500
H	5.12981000	5.31121900	1.63548800
H	3.71125700	6.35228600	1.47313800
Hg	-2.46171200	-0.02245900	-0.51239500
Cl	-2.51972300	2.60696400	-2.03488500
Cl	-3.80873800	-2.41814200	0.81891700
O	-3.32917900	2.18174500	-0.77526500
O	-1.73147700	1.32047200	-2.39247500
O	-3.94420600	-1.90057400	-0.63858700
O	-2.96692600	-1.32342200	1.51001700
O	-1.58143300	3.68699000	-1.68498100
O	-3.43819300	2.96543200	-3.12458900
O	-5.13540300	-2.52369000	1.44153400
O	-3.06779600	-3.69711400	0.82905000
IM1-Hg(OTf) ₂			
O	0.00905300	-1.27958800	-1.03652100
O	3.05356400	-1.66702900	2.11594500
O	1.07841300	-1.39164700	3.19281600
O	0.20756600	0.32248100	1.17974300
C	1.21394300	-0.67317400	0.94391500
C	1.45902900	0.76014500	0.58461900

C	0.84023600	-1.60498900	-0.19149600
C	1.89969500	-1.29656600	2.14773800
C	1.62844400	-2.00065100	4.38317900
H	0.81358500	-1.99452800	5.10610700
H	2.47815500	-1.41579800	4.74378300
H	1.94873400	-3.02212200	4.16447400
Hg	-1.87171100	0.11215300	-0.27249400
O	1.45084000	-2.76567800	-0.16210500
C	1.09842400	-3.71816000	-1.20680700
H	1.35055700	-3.29454500	-2.18072200
H	1.70390800	-4.59699100	-0.99087200
H	0.03196200	-3.94466800	-1.14651300
O	-2.91976600	2.20092500	0.22888400
O	-2.32952400	-1.87763000	1.10755100
S	-2.05272800	3.06246200	-0.66936300
S	-3.04892600	-2.61878100	0.00671900
O	-1.42743100	4.23185100	-0.06452600
O	-2.49907900	-3.91930800	-0.37475500
O	-1.15936200	2.12615700	-1.45245900
O	-3.31508700	-1.63465900	-1.11028100
C	-3.25732000	3.71886000	-1.95211800
C	-4.75120000	-2.96607200	0.71820000
F	-4.17236400	4.49636700	-1.36361400
F	-3.87882100	2.69911600	-2.56276500
F	-2.59756600	4.43679900	-2.86858800
F	-5.51984400	-3.55500500	-0.20454400
F	-5.33081100	-1.82182400	1.10419400
F	-4.64163800	-3.77785500	1.77750000
C	4.50723400	-1.17425700	-1.01345900
H	4.50101700	-1.56600700	0.02179700
O	3.48913900	-0.67775200	-1.48112600
C	5.78781100	-1.29680900	-1.73867600
C	5.91873500	-0.84165400	-3.06274500
C	6.88626900	-1.88060500	-1.08748400
C	7.13777600	-0.97164500	-3.72287500
H	5.05830800	-0.39335500	-3.55120100
C	8.10769300	-2.01025900	-1.75087100
H	6.77783100	-2.22964100	-0.06252900
C	8.23172800	-1.55577800	-3.06766300
H	7.24276300	-0.62130000	-4.74618400
H	8.95760800	-2.46191200	-1.24664100
H	9.18155600	-1.65557300	-3.58683600
H	1.37737800	0.98229000	-0.47721000
C	2.31143800	1.68178800	1.37987400

C	3.39165100	2.30958000	0.74461100
C	2.06045000	1.95369500	2.73109300
C	4.21586100	3.18008400	1.45687300
H	3.58703500	2.11421900	-0.30689900
C	2.88646300	2.83278400	3.43173600
H	1.20741000	1.49787900	3.22469400
C	3.97763500	3.45979100	2.81115700
H	5.05125400	3.65726700	0.94931900
H	2.67247700	3.04319500	4.47737900
C	4.84446100	4.43993900	3.56680400
H	4.87044100	4.21003100	4.63754300
H	5.87411800	4.43685500	3.19256300
H	4.46125400	5.46394500	3.46117500

IM1-Mn(ClO₄)₂

O	-0.98873600	-1.62572500	-0.62825100
O	1.75952500	-0.55595300	2.61841200
O	-0.28151100	0.19100700	3.26367000
O	-0.96182700	0.73719200	0.62631100
C	0.07260300	-0.20477000	0.95967600
C	0.35076600	0.93988600	0.03265900
C	-0.19758000	-1.54477200	0.31218600
C	0.62436600	-0.20777300	2.37333600
C	0.14522400	0.20703600	4.64548200
H	-0.72504300	0.54684800	5.20553900
H	0.98526600	0.89498700	4.76802700
H	0.44117200	-0.79797300	4.95541400
O	0.42411000	-2.56442000	0.84719400
C	0.14860800	-3.87244600	0.26817000
H	0.47721200	-3.88147500	-0.77268300
H	0.72934900	-4.56775900	0.87194200
H	-0.92074200	-4.08072300	0.33642000
C	3.51031400	-1.39359200	-0.33344900
H	3.41497400	-1.36638100	0.76929600
O	2.53362600	-1.15176800	-1.03324400
C	4.85044300	-1.72746800	-0.85426300
C	5.09206800	-1.80350100	-2.23765600
C	5.89315800	-1.97471000	0.05312700
C	6.36496200	-2.12353500	-2.70223100
H	4.27357400	-1.61049800	-2.92518800
C	7.16875900	-2.29531500	-0.41462500
H	5.69912600	-1.91418700	1.12218100
C	7.40287200	-2.36939200	-1.79146100
H	6.55533000	-2.18352200	-3.77040900

H	7.97556200	-2.48651900	0.28754900
H	8.39514300	-2.61928500	-2.15829200
H	0.39288100	0.67122100	-1.02071200
C	1.10024500	2.15969800	0.43044300
C	2.26739200	2.48726200	-0.27553400
C	0.66943100	2.99573400	1.46716500
C	3.00065100	3.62039600	0.06962900
H	2.59902300	1.85389400	-1.09454400
C	1.40783700	4.13370300	1.79818800
H	-0.25230200	2.77161800	1.99517500
C	2.58492300	4.46439000	1.11257400
H	3.90435200	3.85979800	-0.48683000
H	1.05448500	4.78160700	2.59705800
C	3.37614200	5.70314400	1.46331100
H	2.98517900	6.18620300	2.36464700
H	4.43251900	5.46535000	1.63853100
H	3.34079600	6.43856400	0.64915200
Mn	-2.67276400	-0.17701400	-0.64163800
Cl	-2.84742500	2.00188600	-2.43555900
Cl	-4.20517500	-2.13609300	0.72717500
O	-3.57933700	1.75692700	-1.08886600
O	-2.02274200	0.69149900	-2.56016700
O	-4.11938600	-1.81852800	-0.78591100
O	-3.33871300	-0.99995300	1.32494300
O	-1.94532100	3.15840700	-2.32579400
O	-3.81081500	2.11833900	-3.53513200
O	-5.58981000	-2.04508300	1.20111000
O	-3.58451800	-3.44428700	1.01207900
IM1-Mn(OTf) ₂			
O	-0.46550700	0.95456000	-1.24950200
O	2.12105500	-2.60033300	-1.42696100
O	0.02925300	-3.29970200	-0.89454300
O	-0.43059500	-1.01206200	0.56612800
C	0.56464000	-1.04804100	-0.46779100
C	0.91360800	-0.58738800	0.91702100
C	0.31723500	0.03716500	-1.49220100
C	1.00989900	-2.40638900	-0.98164300
C	0.31530700	-4.63057700	-1.38169300
H	-0.61214400	-5.18426500	-1.24266900
H	1.13066800	-5.07124500	-0.80262400
H	0.59159900	-4.58833900	-2.43794800
Mn	-2.13569100	0.47772600	0.16016400
O	0.97443200	-0.09890700	-2.61825200

C	0.77332500	0.93489600	-3.61953600
H	1.12533900	1.89106500	-3.22774300
H	1.36962700	0.61421500	-4.47222700
H	-0.28586800	0.99549400	-3.87652400
O	-3.01241500	2.47130700	0.32861300
O	-3.66813700	-1.01805700	0.67407600
S	-2.29779300	2.84433500	1.61141100
S	-3.74802600	-1.63411100	-0.70518700
O	-3.08978700	3.41272000	2.69035800
O	-3.68987500	-3.08621000	-0.80608800
O	-1.40922000	1.66188300	1.92866100
O	-2.79177500	-0.83102400	-1.55983900
C	-1.10505400	4.19990300	1.09006200
C	-5.44688500	-1.13842400	-1.33477800
F	-1.78842300	5.26945100	0.66745400
F	-0.31234300	3.77101400	0.09599500
F	-0.33795600	4.55368900	2.12989500
F	-5.59091300	-1.53956800	-2.60533300
F	-5.58627800	0.19236500	-1.28046400
F	-6.39708200	-1.70912100	-0.58623400
C	4.11022100	0.32464800	-1.18848500
H	3.90372500	-0.72109900	-1.48766700
O	3.22337600	0.99662600	-0.67466900
C	5.47985000	0.80832600	-1.45338900
C	5.86191600	2.12164600	-1.12614200
C	6.40791500	-0.06384700	-2.04465600
C	7.15943700	2.55191200	-1.39054400
H	5.13106100	2.78283600	-0.66942500
C	7.70844000	0.36929300	-2.30871900
H	6.10551500	-1.07883600	-2.29460000
C	8.08237100	1.67664100	-1.98157300
H	7.45836500	3.56605700	-1.13937300
H	8.42638700	-0.30590300	-2.76611400
H	9.09423000	2.01692100	-2.18651300
H	1.00719300	0.49024800	1.02928800
C	1.65252600	-1.41759500	1.90336000
C	2.84515000	-0.91696300	2.44219000
C	1.18469400	-2.67145300	2.32065200
C	3.56705300	-1.66962400	3.36891500
H	3.20917700	0.05989300	2.13385400
C	1.91023900	-3.41064100	3.25417400
H	0.24544300	-3.05412800	1.93300200
C	3.11323600	-2.92731800	3.79290600
H	4.49288300	-1.26832100	3.77492600

H	1.52994600	-4.37761300	3.57656000
C	3.87288500	-3.72362200	4.82829600
H	3.83088300	-4.79828200	4.61795700
H	4.92599800	-3.42609800	4.87032000
H	3.44779600	-3.57151200	5.82961100

IM1-Zn(ClO₄)₂

O	-0.98039700	-1.66851900	-0.54527500
O	1.78311600	-0.50147200	2.65146500
O	-0.25303500	0.28927900	3.26041100
O	-0.92585400	0.73498600	0.60629600
C	0.10614800	-0.19460900	0.97482400
C	0.38929600	0.91931600	0.01048000
C	-0.16308700	-1.55399100	0.36985100
C	0.65218700	-0.15160400	2.39024500
C	0.16795400	0.35655400	4.64260100
H	-0.70212200	0.72493500	5.18451100
H	1.01272700	1.04251700	4.74135100
H	0.45471600	-0.63762200	4.99332700
O	0.48936000	-2.55230900	0.90498400
C	0.21740000	-3.87607900	0.36021600
H	0.54046600	-3.90809900	-0.68189900
H	0.80603700	-4.55278000	0.97724500
H	-0.85030200	-4.08879500	0.43906000
C	3.55134500	-1.39766300	-0.29326900
H	3.45005500	-1.34535900	0.80810600
O	2.57641100	-1.18035900	-1.00360600
C	4.89675900	-1.73303100	-0.79866300
C	5.14679900	-1.83973300	-2.17857700
C	5.93614400	-1.95074400	0.12010600
C	6.42469700	-2.16077500	-2.62841900
H	4.33081100	-1.66931100	-2.87499400
C	7.21674700	-2.27240600	-0.33293400
H	5.73561000	-1.86653800	1.18635300
C	7.45920200	-2.37714100	-1.70634800
H	6.62162000	-2.24442100	-3.69380500
H	8.02099400	-2.44077400	0.37795400
H	8.45540600	-2.62797000	-2.06168400
H	0.43553900	0.61660000	-1.03325100
C	1.13374100	2.15310700	0.37116400
C	2.29894400	2.46481500	-0.34385700
C	0.69922700	3.01708800	1.38417300
C	3.02677000	3.61194100	-0.03239700
H	2.63430200	1.80872300	-1.14317400

C	1.43130900	4.16749300	1.68078600
H	-0.22082900	2.80367200	1.91928200
C	2.60614800	4.48483400	0.98347000
H	3.92996200	3.83842000	-0.59477700
H	1.07554400	4.83618000	2.46140000
C	3.37666700	5.74883700	1.28634000
H	3.14866500	6.12715900	2.28838000
H	4.45830400	5.58438400	1.22218100
H	3.12519800	6.54242200	0.56989700
Zn	-2.56331600	-0.21319500	-0.60078100
Cl	-2.78652700	1.87648200	-2.40996000
Cl	-4.20452100	-2.02333400	0.73120100
O	-3.47815500	1.67690000	-1.03636400
O	-1.96810900	0.55728300	-2.51416700
O	-4.05449700	-1.74417300	-0.78510500
O	-3.30893700	-0.90942900	1.33048100
O	-1.87523400	3.03083400	-2.36471600
O	-3.77677300	1.96336800	-3.48790900
O	-5.59877300	-1.86570700	1.15709300
O	-3.64934600	-3.34921200	1.06617300
IM1-Zn(OTf) ₂			
O	-0.57963700	0.89495300	-1.41890900
O	1.99903300	-2.64224500	-1.75481500
O	-0.10524400	-3.29990500	-1.21568300
O	-0.46444600	-1.07369200	0.36654400
C	0.51670800	-1.09090000	-0.68497000
C	0.91073100	-0.70189400	0.70771500
C	0.27126400	0.03823800	-1.66191900
C	0.90536100	-2.43637800	-1.27573700
C	0.13124300	-4.61479400	-1.77151700
H	-0.81321100	-5.14349600	-1.65113900
H	0.93499300	-5.11035600	-1.22151400
H	0.40150800	-4.52944000	-2.82662000
Zn	-2.07728500	0.36891600	0.03669200
O	0.99822900	0.00755000	-2.74905500
C	0.81359400	1.09873300	-3.69252200
H	1.10007900	2.03805200	-3.21607800
H	1.47469600	0.85958600	-4.52372200
H	-0.22939100	1.13570300	-4.01245500
O	-2.54239300	2.09860600	0.86883000
O	-3.52893000	-1.08246900	0.75513600
S	-1.51081100	2.72147900	1.82051400
S	-3.97354100	-1.46667000	-0.63623500

O	-2.07899000	3.19345900	3.07610300
O	-4.05941600	-2.88202200	-0.96816400
O	-0.29346700	1.88184500	1.84172900
O	-3.16400400	-0.57768100	-1.56407700
C	-1.02250200	4.26774500	0.87272000
C	-5.72249400	-0.79734200	-0.77564500
F	-2.07609700	5.07648500	0.70610000
F	-0.53616200	3.94170300	-0.33817000
F	-0.07200600	4.92825100	1.54942100
F	-6.18467500	-1.00000800	-2.01593500
F	-5.73334800	0.51553800	-0.51481200
F	-6.51913700	-1.42498000	0.09567100
C	4.13569300	0.26014800	-1.21247000
H	3.96275500	-0.75121900	-1.63027500
O	3.19876800	0.88930400	-0.73684000
C	5.52658600	0.75104700	-1.27777100
C	5.86586000	2.02584400	-0.79029900
C	6.51758500	-0.07227400	-1.83579500
C	7.18444600	2.46704400	-0.86317700
H	5.08565700	2.64865200	-0.36215600
C	7.83919500	0.37163400	-1.90722900
H	6.24811200	-1.05828200	-2.20924200
C	8.17061500	1.64055100	-1.42118200
H	7.45053300	3.45145500	-0.48777500
H	8.60663600	-0.26544100	-2.33816900
H	9.19901300	1.98843000	-1.47613600
H	1.02965000	0.36452000	0.87591400
C	1.62901700	-1.59972800	1.64778500
C	2.81250900	-1.13269500	2.23748300
C	1.15401200	-2.87521100	1.98062400
C	3.51992100	-1.94144500	3.12543300
H	3.17457100	-0.13558000	2.00132500
C	1.86564800	-3.67158500	2.87854200
H	0.21780100	-3.23114200	1.56172200
C	3.05959400	-3.22374100	3.46336700
H	4.43743200	-1.56584000	3.57301400
H	1.47975000	-4.65514100	3.13709000
C	3.80800700	-4.07724900	4.46060200
H	3.56370600	-5.13841500	4.34400800
H	4.89250300	-3.96329100	4.35175300
H	3.55262900	-3.79220300	5.49014200
IM5-Cu(ClO ₄) ₂			
C	5.44108700	-0.97380900	0.30970800

C	4.50182600	-1.37429100	-0.65545500
C	3.46784100	-0.52863800	-1.04894700
C	3.33566400	0.74149300	-0.46668100
C	4.26285000	1.15387700	0.49808800
C	5.30456100	0.30239100	0.87406200
H	4.57647900	-2.36275000	-1.10260400
H	2.74885600	-0.86911000	-1.78893200
H	4.17199400	2.13960300	0.94347400
H	6.02468200	0.63877800	1.61677200
C	6.56420900	-1.89826400	0.71870800
H	7.20111200	-1.44182400	1.48333300
H	6.17422700	-2.84081100	1.12296600
H	7.19955500	-2.15427900	-0.13851800
C	2.24887600	1.64654900	-0.93368500
H	2.12995400	1.73175200	-2.01532900
O	2.01454900	2.85833000	-0.23489800
C	0.95736300	1.91637200	-0.17262200
C	-0.28294600	2.25147800	-0.97374500
C	0.72870100	1.20687400	1.13752500
O	-0.04949400	3.17972000	-1.88724200
O	1.52525800	1.61374400	2.09987100
C	-1.16699600	3.53828500	-2.74168600
H	-0.76963900	4.29718500	-3.41391800
H	-1.50879800	2.65958800	-3.29261500
H	-1.98219100	3.93706500	-2.13470500
C	1.42318600	0.92098600	3.37420400
H	1.65496500	-0.13655200	3.23491800
H	2.16069100	1.40673700	4.01074800
H	0.41471600	1.03622300	3.77580600
O	-1.37373400	1.72003300	-0.81272600
O	-0.10092400	0.31065400	1.30194100
Cu	-1.70283200	-0.30367500	0.13682800
O	-3.00208300	0.25373000	1.55904200
O	-1.03364300	-2.71432800	0.40686100
Cl	-4.30613700	-0.11714200	0.76091500
Cl	-0.39472600	-2.59575100	-0.94701200
O	-5.06580400	-1.14308900	1.47687300
O	-3.65459400	-0.68306000	-0.52540200
O	-0.64534900	-1.06757800	-1.33107500
O	1.06603600	-2.80019100	-0.89582900
O	-5.08532700	1.09182800	0.47476900
O	-1.04703400	-3.43675200	-1.96001200

IM5-Cu(OTf)₂

C	6.11536600	-0.26963400	-1.01790900
C	5.23069700	0.80997600	-0.85565200
C	4.13856100	0.72630800	0.00505000
C	3.89070100	-0.46069600	0.71428700
C	4.76389500	-1.54466000	0.56277700
C	5.86397200	-1.44272800	-0.29246900
H	5.39864600	1.73182700	-1.40793700
H	3.47156400	1.57704200	0.11283900
H	4.58547100	-2.45893100	1.12005900
H	6.54034600	-2.28900400	-0.39222100
C	7.30996500	-0.15457800	-1.93625100
H	7.83191000	-1.11179100	-2.03771600
H	7.01177400	0.17637600	-2.93856200
H	8.03151900	0.58017600	-1.55608800
C	2.73803100	-0.51433600	1.65663600
H	2.60950100	0.34931300	2.30760500
O	2.39672300	-1.75384300	2.26095700
C	1.42442800	-1.22794300	1.37168300
C	0.16613500	-0.66944700	1.99978500
C	1.25402800	-1.91179000	0.04366200
O	0.34845100	-0.33827000	3.26227100
O	2.01900600	-2.96764100	-0.11150000
C	-0.76002700	0.32086400	3.92668000
H	-0.40463500	0.50900800	4.93872200
H	-0.98852800	1.25311600	3.40671700
H	-1.63263800	-0.33525900	3.93182900
C	1.96911200	-3.63756000	-1.39997200
H	2.28651400	-2.94760300	-2.18406900
H	2.66364800	-4.47034500	-1.30396400
H	0.95365700	-3.98847500	-1.59331400
O	-0.90327600	-0.54502500	1.41153000
O	0.49914700	-1.51040400	-0.84788100
Cu	-1.15097300	-0.29150600	-0.76912600
O	-2.39772600	-1.91943300	-0.98961800
O	1.49835200	3.11267700	-1.12482900
O	-4.45505000	-1.43182100	-2.41097400
O	-3.07056200	0.35087700	-1.21985000
O	-0.25590400	1.36833400	-1.21395500
O	0.80789600	1.91296000	0.98096500
S	0.46472600	2.41547200	-0.36247700
S	-3.62048000	-1.06224000	-1.28244900
C	-4.70815000	-1.23294700	0.24291800
C	-0.89611500	3.67736600	-0.07286600
F	-1.92028200	3.10923100	0.58722400

F	-0.41934800	4.68822300	0.66869500
F	-1.34664900	4.16389700	-1.23314100
F	-4.03063600	-0.87588100	1.33897400
F	-5.10127700	-2.50555600	0.36504300
F	-5.78053200	-0.44769000	0.11237000

IM5-Hg(ClO₄)₂

C	5.17248900	-1.44744000	-1.72275100
C	4.28634100	-0.46866800	-2.19633900
C	3.51935600	0.29882100	-1.31871500
C	3.61442900	0.09013200	0.06431800
C	4.49645600	-0.88491900	0.55284400
C	5.26388300	-1.63911500	-0.33434100
H	4.19464500	-0.30081500	-3.26673200
H	2.83250400	1.04498900	-1.70932300
H	4.58516500	-1.03821300	1.62380700
H	5.95188200	-2.38489100	0.05896200
C	6.01901700	-2.26428200	-2.67133700
H	5.88998100	-3.33951300	-2.49663600
H	5.76108700	-2.05989700	-3.71526200
H	7.08593300	-2.04152900	-2.54097700
C	2.80892600	0.94195400	0.98363600
H	2.75942600	2.00310800	0.73680200
O	2.84593600	0.67493000	2.38066100
C	1.60036600	0.43988100	1.75253000
C	0.49313800	1.42623300	2.05158400
C	1.16349800	-0.99283200	1.55665300
O	0.93682500	2.51861500	2.63273900
O	1.86524500	-1.85658700	2.25923600
C	-0.02860000	3.58581300	2.85367300
H	0.54424300	4.37703300	3.33442900
H	-0.42979100	3.91096600	1.89223900
H	-0.82857500	3.22730200	3.50408600
C	1.53113400	-3.26205700	2.09074100
H	1.69714600	-3.55644000	1.05276400
H	2.20636500	-3.78841700	2.76321500
H	0.48791100	-3.42911900	2.36520000
O	-0.69109600	1.23868400	1.77080900
O	0.25171900	-1.32218800	0.80023400
Hg	-1.52330700	0.02984100	-0.19029000
O	-2.50968500	-1.82099700	-1.34580500
O	0.20901100	1.29631500	-1.38666600
Cl	-3.56754600	-2.20574100	-0.27514300
Cl	-0.58365200	2.61552800	-1.56509000

O	-4.91691600	-2.15234100	-0.85429800
O	-3.39893600	-1.09491600	0.79767400
O	-2.00452500	2.24939600	-1.09858300
O	-0.00454200	3.64667100	-0.67195600
O	-3.23841700	-3.51821600	0.30756900
O	-0.58781600	3.02571500	-2.97541200

IM5-Hg(OTf)₂

C	4.75567000	-2.42634600	-2.30472700
C	4.22781700	-1.12666900	-2.33395600
C	3.71367800	-0.52839500	-1.18309300
C	3.70753500	-1.23052800	0.03055300
C	4.23376500	-2.52939900	0.07616400
C	4.75268900	-3.11295400	-1.07989500
H	4.22178500	-0.57152200	-3.26899700
H	3.30213200	0.47633900	-1.22832600
H	4.24662700	-3.06905000	1.01799200
H	5.17139900	-4.11600100	-1.02773000
C	5.30443000	-3.07630600	-3.55386600
H	4.61417400	-3.83900200	-3.93849600
H	5.46201400	-2.34261600	-4.35097800
H	6.26100700	-3.57489000	-3.35806800
C	3.19116200	-0.55710400	1.25553900
H	3.50623900	0.47604300	1.40562300
O	3.07978200	-1.30758800	2.45893000
C	1.85394200	-0.88150000	1.89380400
C	1.12755200	0.23523700	2.61057500
C	0.97700100	-1.92124100	1.23835100
O	1.89433400	0.85202900	3.48280400
O	1.33850900	-3.15781100	1.51306200
C	1.34033500	2.03209200	4.13243000
H	2.11639500	2.35035600	4.82659700
H	1.14467800	2.79595500	3.37764800
H	0.42352600	1.76456800	4.66082500
C	0.57981900	-4.21859000	0.87272300
H	0.68487900	-4.14085600	-0.21118100
H	1.02322700	-5.14012600	1.24634900
H	-0.47232800	-4.14306400	1.15330700
O	-0.04243100	0.54815700	2.39016700
O	0.03120800	-1.64387400	0.50407300
Hg	-1.16373300	0.46948200	0.19542400
O	-2.63371200	-0.34762400	-1.53018000
O	0.99333800	1.49322800	-0.51061000
O	-5.10047900	0.02353700	-1.05927000

O	-3.38288500	-0.27773100	0.78618400
O	-0.87897800	2.89592300	0.18445300
O	1.46703400	3.53015800	0.89874400
S	0.60110100	2.89273700	-0.09569000
S	-3.83487800	-0.55590400	-0.63183300
C	-4.09235300	-2.41663800	-0.65868100
C	0.78105500	3.90446000	-1.66678800
F	0.42484400	5.17191100	-1.43801300
F	2.05780200	3.87600700	-2.07558500
F	0.00509200	3.39620600	-2.63132100
F	-2.97055800	-3.04807100	-0.26647200
F	-4.40034100	-2.82114500	-1.89581300
F	-5.08539400	-2.75467900	0.17167500

IM5-Mn(ClO₄)₂

C	-5.49232200	0.73662500	0.40131000
C	-4.56635600	1.26615900	-0.51315700
C	-3.49663000	0.50468400	-0.97689300
C	-3.31476400	-0.80866300	-0.51652200
C	-4.22561300	-1.34843600	0.39981500
C	-5.30283500	-0.57970200	0.84629500
H	-4.67991800	2.28913100	-0.86384600
H	-2.78881000	0.94184500	-1.67636200
H	-4.09353100	-2.36640100	0.75288800
H	-6.00908100	-1.01313900	1.55098800
C	-6.66580300	1.56311000	0.87313400
H	-7.17355500	1.09260600	1.72145900
H	-6.34856700	2.56652100	1.18056200
H	-7.40568500	1.68961100	0.07176300
C	-2.18611100	-1.61474300	-1.05677500
H	-2.05950100	-1.59225600	-2.14096600
O	-1.88522300	-2.87239300	-0.47260400
C	-0.88656500	-1.88358800	-0.30876000
C	0.36748700	-2.04597200	-1.13504500
C	-0.69390700	-1.28517300	1.06237500
O	0.25135000	-2.97709900	-2.05884400
O	-1.44963900	-1.83353400	1.98636600
C	1.39508700	-3.17196500	-2.93693000
H	1.09077200	-3.97056300	-3.61126100
H	1.60295200	-2.24865500	-3.48119800
H	2.26588200	-3.46183500	-2.34607200
C	-1.36354600	-1.26549000	3.32269300
H	-1.65724800	-0.21458500	3.29295800
H	-2.06006800	-1.85396300	3.91726300

H	-0.34263400	-1.36142200	3.69701800
O	1.38321400	-1.36970600	-0.98775700
O	0.08350300	-0.35907200	1.28769600
Mn	1.73381700	0.51877600	0.11509500
O	3.13545900	-0.23844800	1.64927000
O	1.10882100	2.59747700	0.47973000
Cl	4.42220000	-0.07116300	0.79804300
Cl	0.25733600	2.78830500	-0.79642300
O	5.36453200	0.84107900	1.45652000
O	3.84316200	0.57103300	-0.48825000
O	0.42380300	1.40766000	-1.48136500
O	-1.15718300	3.00687000	-0.44541000
O	5.00779700	-1.38724200	0.49563200
O	0.80949600	3.85602800	-1.63840200

IM5-Mn(OTf)₂

C	5.65677900	-1.61244400	-1.40265800
C	5.03429400	-0.35548700	-1.38277800
C	4.07924200	-0.03583400	-0.41678600
C	3.71172900	-0.98547600	0.54765000
C	4.32588000	-2.24648800	0.54109000
C	5.28864800	-2.54808000	-0.42159200
H	5.30035500	0.38898800	-2.12913600
H	3.61224000	0.94504400	-0.41988100
H	4.05660200	-2.97824700	1.29634000
H	5.76890200	-3.52453200	-0.40615600
C	6.69192100	-1.95748400	-2.44820100
H	6.30479800	-2.69878500	-3.15980000
H	6.99167900	-1.07418100	-3.02101600
H	7.59214500	-2.38681400	-1.99221400
C	2.72734500	-0.60487800	1.59744200
H	2.87180700	0.37004700	2.06102400
O	2.23291000	-1.60100300	2.48097800
C	1.26701800	-1.04238600	1.60657000
C	0.26086000	-0.10143800	2.22363000
C	0.76050000	-1.88763400	0.47187700
O	0.66824000	0.39637700	3.36651400
O	1.25996300	-3.10032900	0.44314500
C	-0.18091100	1.39915500	3.98933800
H	0.33767100	1.66611800	4.90853000
H	-0.27273000	2.25708100	3.32082000
H	-1.16314400	0.97180000	4.19883400
C	0.87958700	-3.94454400	-0.67828600
H	1.20050500	-3.47844300	-1.61158900

H	1.40292300	-4.88326400	-0.50564100
H	-0.20241100	-4.08825100	-0.68071000
O	-0.83331500	0.17057400	1.72205000
O	-0.03166400	-1.46790200	-0.37704600
Mn	-1.43520000	0.19885200	-0.35827600
O	-2.80424400	-0.84924800	-1.73967500
O	-0.52894400	1.85134300	-1.11658400
O	-5.20912100	-0.00915300	-1.73523200
O	-3.57136400	0.37984500	0.17663200
O	1.32609300	1.98421000	0.53105000
O	1.70560400	2.69518600	-1.85376700
S	0.78385900	2.52880400	-0.73275300
S	-4.05666600	-0.46826200	-0.97897600
C	-4.57678800	-2.07470100	-0.15612500
C	0.17799500	4.24970600	-0.29222200
F	1.21308600	5.00283900	0.10737300
F	-0.40404800	4.83274900	-1.34432800
F	-0.71352100	4.18179400	0.71379200
F	-3.54649700	-2.57312100	0.55681400
F	-4.93191500	-2.97538300	-1.07860200
F	-5.60536000	-1.86195100	0.67016400

IM5-Zn(ClO₄)₂

C	-5.51429400	0.77850900	0.20874100
C	-4.55169700	1.24648600	-0.69734800
C	-3.46881700	0.45170500	-1.07421300
C	-3.31521500	-0.83038400	-0.53037100
C	-4.26618000	-1.31030500	0.38199300
C	-5.35240200	-0.51258000	0.73871800
H	-4.64378400	2.24696700	-1.11199700
H	-2.73176400	0.84216000	-1.77102900
H	-4.15465800	-2.30608500	0.79957600
H	-6.08926900	-0.89973700	1.43964500
C	-6.70098600	1.62865800	0.59941500
H	-6.79819700	1.70172200	1.68947200
H	-6.61459500	2.64405700	0.20018400
H	-7.63689700	1.19859800	0.21946900
C	-2.17850000	-1.67916500	-0.98108100
H	-2.02379600	-1.73497500	-2.06056500
O	-1.90322600	-2.89395800	-0.30202200
C	-0.89837600	-1.90549500	-0.18487700
C	0.37027900	-2.13372400	-0.97135900
C	-0.72708700	-1.21815600	1.14602900
O	0.28840000	-3.16045800	-1.78995000

O	-1.54868100	-1.65356800	2.07242600
C	1.45171500	-3.42522400	-2.62433900
H	1.17532100	-4.29999700	-3.21032100
H	1.64941400	-2.56291900	-3.26394400
H	2.31784900	-3.62744100	-1.99177100
C	-1.49423800	-0.98422000	3.36336100
H	-1.72392600	0.07511100	3.23533100
H	-2.25207900	-1.48406000	3.96394900
H	-0.49999200	-1.10529600	3.79732500
O	1.37109800	-1.42404700	-0.88743100
O	0.09228600	-0.32056600	1.34198700
Zn	1.66504000	0.44724100	0.11440300
O	3.10725600	-0.13291600	1.58973500
O	1.13628200	2.51068800	0.46618400
Cl	4.35227400	0.01961200	0.66985100
Cl	0.24236900	2.69144200	-0.78085500
O	5.29373600	0.99639700	1.22871400
O	3.69448100	0.55790900	-0.62329200
O	0.35007800	1.28633800	-1.43112500
O	-1.15252100	2.95533000	-0.38419200
O	4.96668500	-1.29638200	0.42729500
O	0.78425800	3.72149600	-1.67437700

IM5-Zn(OTf)₂

C	5.51449400	-1.83151800	-1.46797200
C	4.92210300	-0.56299000	-1.55663300
C	4.03420000	-0.10861400	-0.58058200
C	3.70520100	-0.93237600	0.50595900
C	4.29190600	-2.20209400	0.61017800
C	5.18772900	-2.63833900	-0.36536600
H	5.15924300	0.08369800	-2.39783600
H	3.58732500	0.87800000	-0.66645700
H	4.05396000	-2.83517400	1.45930700
H	5.64687200	-3.61992500	-0.26539600
C	6.47469800	-2.32381700	-2.52594400
H	6.03302800	-3.14068800	-3.11180400
H	6.74583900	-1.52504500	-3.22352700
H	7.39823000	-2.71009000	-2.07803200
C	2.78937000	-0.41020500	1.55678900
H	2.97653200	0.60766100	1.89600600
O	2.32643200	-1.28602200	2.57449700
C	1.32392200	-0.80783800	1.69432300
C	0.37100900	0.22376200	2.24793600
C	0.73849500	-1.76954500	0.69993500

O	0.82896900	0.80637100	3.33003800
O	1.22260700	-2.98456000	0.78109600
C	0.03003800	1.88734900	3.88601500
H	0.59184600	2.22441700	4.75542600
H	-0.06992300	2.68124000	3.14391800
H	-0.95254600	1.50816900	4.17258900
C	0.75214900	-3.95203100	-0.19905300
H	0.99411000	-3.60274900	-1.20423000
H	1.28830200	-4.86833400	0.04120000
H	-0.32629100	-4.08410900	-0.09489200
O	-0.72565400	0.49405600	1.75232400
O	-0.10505500	-1.44350700	-0.14264300
Zn	-1.39425200	0.21331600	-0.23598400
O	-2.67693400	-0.79546700	-1.68527500
O	-0.63530900	1.79858400	-1.15285500
O	-5.12381100	-0.10484400	-1.48385500
O	-3.42432200	0.12388500	0.39998300
O	1.42445300	2.01448400	0.22696400
O	1.43271400	2.74067200	-2.18500900
S	0.68812000	2.53076400	-0.94737300
S	-3.91477700	-0.59491900	-0.84387400
C	-4.32880300	-2.31765500	-0.22190300
C	0.07613600	4.22406400	-0.41669400
F	1.12277900	5.02906300	-0.18361200
F	-0.69389800	4.77277000	-1.36006500
F	-0.64147500	4.12033600	0.71994800
F	-3.25833400	-2.85207600	0.39999200
F	-4.66517000	-3.10945600	-1.24558400
F	-5.34402300	-2.26599600	0.64589500

IM7-Cu(ClO₄)₂

C	-5.61235100	-3.42282800	-0.17262100
C	-5.05138400	-2.74169900	-1.26637600
C	-3.80193800	-2.14280900	-1.16500600
C	-3.07809100	-2.22048200	0.04354300
C	-3.63287900	-2.90701900	1.14877900
C	-4.88170500	-3.49331200	1.03390500
H	-5.60370500	-2.68036600	-2.20007900
H	-3.37751800	-1.60618100	-2.00911600
H	-3.07348400	-2.96972400	2.07663300
H	-5.30839800	-4.02104800	1.88334100
C	-6.96926600	-4.07042100	-0.27248500
H	-7.67308900	-3.61000300	0.43284500
H	-7.38894400	-3.97897700	-1.27841100

H	-6.91474200	-5.13665600	-0.01989900
C	-1.79641300	-1.60351100	0.09140800
H	-1.34692900	-1.12745300	-0.78234600
O	-1.08368500	-1.66637400	1.16607500
C	0.29553100	-1.32485800	1.05233900
C	1.10926700	-2.14834700	0.24674500
C	0.75350100	-0.20688900	1.78156400
O	0.48705500	-3.19480600	-0.31701600
O	-0.15622000	0.38665700	2.55570000
C	1.25319200	-3.97049500	-1.26849800
H	0.56120100	-4.73432600	-1.62322100
H	1.58335900	-3.33006300	-2.08906800
H	2.11542000	-4.42687200	-0.77799900
C	0.25502600	1.59641000	3.23183900
H	0.59477900	2.33523800	2.50294800
H	-0.63985500	1.94047200	3.75023200
H	1.05567700	1.38034700	3.94298000
O	2.34410100	-1.98413300	0.04669600
O	1.93434000	0.24021700	1.74654000
Cu	3.23502900	-0.27484100	0.37192100
O	4.62353300	1.14138000	0.85824600
O	2.38595200	0.60835500	-1.53179100
Cl	5.80132500	0.45737300	0.09530500
Cl	0.94802200	0.96147500	-1.87298400
O	6.29496300	1.31105900	-0.98683900
O	5.04976800	-0.78609600	-0.46391500
O	0.17759500	-0.31840600	-2.09192100
O	0.34851000	1.69684900	-0.70721800
O	6.85283300	0.04841000	1.03537800
O	0.92344300	1.79333100	-3.09494300
C	-2.78634200	1.86897600	-0.08991500
H	-1.76772900	2.03864400	-0.47645900
C	-3.65806200	3.05678300	-0.01215200
C	-4.96636300	2.97655500	0.49713200
C	-3.15417800	4.28905300	-0.46012200
C	-5.75838000	4.11996400	0.55578000
H	-5.33836000	2.01549900	0.84062500
C	-3.95156600	5.43377100	-0.40275600
H	-2.14099100	4.34174900	-0.85288100
C	-5.25141200	5.34811900	0.10533900
H	-6.76964900	4.06326200	0.95005500
H	-3.56268700	6.38645200	-0.75143300
H	-5.87347500	6.23845000	0.15201200
O	-3.13003000	0.73727800	0.24668400

IM7-Cu(OTf)₂

C	6.96853900	-2.22566100	0.46360700
C	6.15772300	-1.70752200	1.48755300
C	4.81912700	-1.41475200	1.25487600
C	4.25847600	-1.64077500	-0.01910500
C	5.06493400	-2.16575800	-1.05457400
C	6.39805400	-2.44908700	-0.80822500
H	6.58373300	-1.53188800	2.47160500
H	4.19858900	-1.00694700	2.04850500
H	4.63172400	-2.34312100	-2.03367900
H	7.01787900	-2.85254800	-1.60526100
C	8.42286100	-2.53884500	0.70498200
H	9.06577700	-1.91644700	0.06929100
H	8.70743200	-2.36515400	1.74681900
H	8.64568200	-3.58455100	0.45921800
C	2.87819000	-1.33171700	-0.20572300
H	2.24558100	-0.98792500	0.61346200
O	2.31186700	-1.56858100	-1.34110600
C	0.89297500	-1.47201200	-1.39557700
C	0.13501300	-2.35946000	-0.59892500
C	0.34344700	-0.54767800	-2.30781100
O	0.84923000	-3.25488800	0.09602600
O	1.22423500	0.08251800	-3.09218600
C	0.12333900	-4.06642200	1.04930600
H	0.88242600	-4.70049300	1.50747000
H	-0.35050800	-3.42287300	1.79321900
H	-0.62875500	-4.67031000	0.53771300
C	0.69824600	1.07856400	-3.99630700
H	0.16303000	1.85220600	-3.44121500
H	1.57633500	1.49321500	-4.49114500
H	0.02585100	0.61582800	-4.72259700
O	-1.12345200	-2.38346500	-0.53118000
O	-0.88806700	-0.29069600	-2.41865300
O	-3.76585900	0.26870900	-1.85196300
O	-1.62281500	0.39491600	0.62145800
O	-4.06878600	-1.60320000	-0.40340700
O	0.44799700	-0.51524600	1.69089900
O	-0.15257400	1.89558200	1.96363300
O	-5.97580000	-0.98820100	-1.97668200
C	2.63737100	2.05292500	0.10623600
H	1.81408100	1.78318200	0.78621500
C	2.83970600	3.49750200	-0.08727900
C	3.87987100	3.99649000	-0.89259200

C	1.95777700	4.38219000	0.55828400
C	4.03570700	5.37096700	-1.04574300
H	4.54927800	3.29567400	-1.38340700
C	2.11771900	5.76018600	0.39857600
H	1.15364400	3.98046100	1.17072200
C	3.15450600	6.25216400	-0.40016700
H	4.83843400	5.76347900	-1.66451800
H	1.43651400	6.44680000	0.89348200
H	3.27942000	7.32513600	-0.52326300
O	3.31253000	1.17501000	-0.43375800
S	-0.62132700	0.51856000	1.72154300
S	-4.84738300	-0.55254900	-1.16903400
C	-1.61472000	0.07658700	3.25224600
C	-5.57229300	0.58663500	0.14059700
F	-0.83126300	0.12211500	4.34521200
F	-2.63365300	0.93024700	3.42456900
F	-2.11509600	-1.16868400	3.14611400
F	-4.61893300	1.05626400	0.94211700
F	-6.46719100	-0.09508600	0.86779200
F	-6.18888000	1.61185800	-0.46257200
Cu	-2.22790000	-0.87058900	-1.09144600

IM7-Hg(ClO₄)₂

C	-7.10079900	-2.68839200	0.40108100
C	-6.77916900	-2.24398100	-0.89152600
C	-5.46441400	-1.95287500	-1.23952500
C	-4.43007900	-2.10116700	-0.29231200
C	-4.74547500	-2.54711800	1.01312000
C	-6.05983500	-2.83273900	1.34365300
H	-7.56884900	-2.12299400	-1.62825000
H	-5.22965900	-1.59736600	-2.23933600
H	-3.95208400	-2.65969700	1.74539200
H	-6.29697300	-3.17480900	2.34827800
C	-8.52272800	-3.00846000	0.78600900
H	-8.84579300	-2.39752800	1.63830300
H	-9.21569800	-2.82966100	-0.04141100
H	-8.62014300	-4.05868200	1.08936300
C	-3.09538500	-1.78611000	-0.69822800
H	-2.86815900	-1.47151000	-1.70768400
O	-2.14269600	-1.91758500	0.14825600
C	-0.77947000	-1.66318800	0.04204500
C	-0.08388400	-1.61995900	-1.20523200
C	-0.14362400	-1.56006100	1.32567600
O	-0.85190500	-1.89898100	-2.28355100

O	-0.97672400	-1.72367400	2.36699500
C	-0.18206800	-1.89237100	-3.56587100
H	-0.96194100	-2.13069500	-4.28938000
H	0.24384400	-0.90644800	-3.76306500
H	0.60797600	-2.64590000	-3.58362900
C	-0.39590000	-1.54821700	3.67907000
H	0.01736000	-0.54181000	3.77588300
H	-1.22529800	-1.69506500	4.37115900
H	0.38780200	-2.28952800	3.85118500
O	1.12982700	-1.38703300	-1.35859200
O	1.06809600	-1.34214000	1.52293100
Hg	2.60938400	-0.23724900	0.11556500
O	4.60368300	-1.56925300	0.49560100
O	2.51706600	1.67458200	1.70024300
Cl	5.44414800	-1.02621200	-0.68508100
Cl	1.34984900	2.44167900	1.07083100
O	6.67435200	-0.39020500	-0.18633400
O	4.51504300	0.04030500	-1.32319000
O	1.08008100	1.71075900	-0.25517900
O	0.14309700	2.33482800	1.93525100
O	5.70971100	-2.10476100	-1.65466500
O	1.72014500	3.84604600	0.82274500
C	-2.65493100	1.87142500	-0.39633900
H	-1.81361600	1.70110900	0.29779100
C	-3.07871200	3.27458200	-0.53866800
C	-4.13787700	3.63429600	-1.39222400
C	-2.40275300	4.26199000	0.19830500
C	-4.51315800	4.96950400	-1.50500800
H	-4.64756900	2.85758200	-1.95499200
C	-2.78227800	5.60054200	0.08153400
H	-1.58307900	3.97700400	0.85315600
C	-3.83504800	5.95258600	-0.76808500
H	-5.32943700	5.25289800	-2.16429400
H	-2.25590000	6.36448700	0.64667400
H	-4.12950400	6.99496500	-0.86103400
O	-3.16933200	0.92322300	-0.98700000
IM7-Hg(OTf) ₂			
C	7.39678300	-2.31111100	0.27175000
C	6.67965600	-1.65409100	1.28602700
C	5.33091000	-1.35980900	1.12665900
C	4.66381200	-1.72624700	-0.06041400
C	5.37527100	-2.39243600	-1.08434900
C	6.72050100	-2.67417300	-0.91293800

H	7.18746200	-1.37064300	2.20387700
H	4.78474900	-0.84243400	1.91095600
H	4.85997500	-2.67840600	-1.99563300
H	7.26667700	-3.18643700	-1.70123600
C	8.86344600	-2.61924300	0.43058000
H	9.46258000	-2.01988100	-0.26760900
H	9.21490900	-2.40548200	1.44420800
H	9.07214100	-3.67276600	0.20911500
C	3.27743300	-1.40950500	-0.17626500
H	2.72556800	-0.94285900	0.63808100
O	2.62103400	-1.75463400	-1.22742100
C	1.19876600	-1.62957500	-1.19864700
C	0.49651600	-2.38961400	-0.22983900
C	0.63205900	-0.80431600	-2.20048500
O	1.28797000	-3.17318900	0.53477300
O	1.51850600	-0.33423700	-3.09579800
C	0.63999300	-3.90053200	1.59932500
H	1.44078500	-4.46155000	2.08197100
H	0.17744700	-3.20363500	2.30193200
H	-0.11510400	-4.57777400	1.19427800
C	1.00253300	0.53960700	-4.11965300
H	0.54899800	1.42782400	-3.67306000
H	1.87269300	0.81159800	-4.71740300
H	0.26085400	0.01863400	-4.72996100
O	-0.74642300	-2.41305400	-0.06396000
O	-0.58258400	-0.49467000	-2.29757600
Hg	-2.12257300	-0.58101900	-0.52300000
O	-3.98538700	0.59587100	-1.53503200
O	-1.40705800	0.81942700	1.21191700
O	-4.36726500	-1.45695800	-0.28045500
O	0.87621500	-0.08973400	1.68687700
O	0.39790000	2.35082000	1.99601500
O	-5.92849800	-0.89359600	-2.19870800
C	3.12211800	2.06449500	-0.16462200
H	2.31603900	1.88022500	0.56380800
C	3.36496600	3.47984000	-0.48762500
C	4.37799000	3.86601200	-1.38441300
C	2.55456300	4.45183600	0.12497600
C	4.57742500	5.21521200	-1.66158400
H	4.99186200	3.09896400	-1.84791100
C	2.75861100	5.80396400	-0.15804300
H	1.77176500	4.13865800	0.81206600
C	3.76769200	6.18359600	-1.04826200
H	5.35879900	5.52048300	-2.35260800

H	2.13300200	6.55754000	0.31218000
H	3.92640500	7.23639100	-1.26826300
O	3.74738400	1.11986900	-0.64564700
S	-0.11400700	0.97324300	1.97582500
S	-5.04136100	-0.41371900	-1.14529100
C	-0.66540100	0.62576400	3.73622400
C	-6.13648900	0.52300400	0.05863000
F	0.38996400	0.69352100	4.56582600
F	-1.58263400	1.51374600	4.13560800
F	-1.19348300	-0.60847500	3.82387700
F	-7.08549900	-0.28960200	0.54131900
F	-6.72333300	1.55431900	-0.56235800
F	-5.40669900	0.99175200	1.08135000

IM7-Mn(ClO₄)₂

C	-6.31085400	-3.12565400	-0.04249900
C	-5.90574700	-2.30727300	-1.11097400
C	-4.60753800	-1.81799800	-1.18003600
C	-3.67655100	-2.14008800	-0.16949400
C	-4.07583000	-2.96258300	0.91102800
C	-5.37375300	-3.44117500	0.96547500
H	-6.61944000	-2.05029400	-1.88889900
H	-4.30711100	-1.16900900	-1.99762500
H	-3.35907400	-3.21468800	1.68598700
H	-5.67868400	-4.07356600	1.79554100
C	-7.71301900	-3.67236100	0.02927400
H	-8.15684500	-3.49312100	1.01576000
H	-8.36243200	-3.22203400	-0.72701800
H	-7.71346600	-4.75888100	-0.13013300
C	-2.35720400	-1.61498200	-0.27852300
H	-2.03973700	-1.05886400	-1.15398600
O	-1.49879200	-1.83298200	0.65221400
C	-0.13976600	-1.46591400	0.49071100
C	0.58967100	-1.93421600	-0.63194000
C	0.42668300	-0.74730700	1.57371900
O	-0.12576300	-2.66731000	-1.50946400
O	-0.41864200	-0.49669400	2.58411100
C	0.59022300	-3.16399300	-2.66397800
H	-0.15841700	-3.70130600	-3.24640200
H	1.00576000	-2.33132200	-3.23530300
H	1.39276400	-3.83519100	-2.35058900
C	0.11800400	0.23632300	3.70663800
H	0.46146500	1.22303300	3.38740500
H	-0.71487200	0.32442700	4.40426700

H	0.94770900	-0.31197400	4.15880200
O	1.80874100	-1.74122300	-0.82514400
O	1.61226800	-0.34635500	1.62539200
Mn	3.04970200	-0.28372200	0.08292600
O	4.77716300	0.04720000	1.41916700
O	2.87882900	1.49349500	-1.00647600
Cl	5.75637600	-0.91702500	0.70370700
Cl	1.61089600	1.95070600	-1.78523400
O	6.92706400	-0.18798200	0.19674000
O	4.87440000	-1.42335200	-0.46282500
O	0.51622200	0.98258900	-1.43437900
O	1.26526100	3.31383900	-1.31648700
O	6.11879300	-2.03211800	1.59472900
O	1.91696900	1.91356800	-3.22780500
C	-2.39397900	1.98207600	-0.21098200
H	-1.36043200	1.89856700	-0.58550700
C	-2.82897600	3.33422100	0.16870700
C	-4.13486300	3.58336800	0.63031800
C	-1.90714400	4.38978500	0.05416500
C	-4.51151800	4.87826500	0.97294800
H	-4.83191300	2.75422500	0.71135600
C	-2.29036500	5.68708300	0.40016500
H	-0.89962300	4.18919700	-0.30380100
C	-3.58910700	5.92984500	0.85764100
H	-5.51888100	5.07736400	1.32907400
H	-1.57974900	6.50406100	0.31205400
H	-3.88776800	6.94035600	1.12525400
O	-3.09696400	0.98544300	-0.14322400

IM7-Mn(OTf)₂

C	6.99386600	-2.52636200	0.36184200
C	6.28254800	-1.87490800	1.38376700
C	4.94675600	-1.53225300	1.21310200
C	4.28706600	-1.84238300	0.00596200
C	4.99287600	-2.50180300	-1.02642000
C	6.32513100	-2.83280100	-0.84303400
H	6.78475300	-1.63403200	2.31669800
H	4.40567800	-1.01855400	2.00326700
H	4.48329000	-2.74467400	-1.95329100
H	6.86678500	-3.34024100	-1.63754700
C	8.44636400	-2.88929400	0.53423800
H	9.07515200	-2.30849200	-0.15333700
H	8.79422200	-2.69592500	1.55316300
H	8.61788300	-3.94854300	0.30769000

C	2.91486000	-1.47536000	-0.12239000
H	2.36215200	-1.02307600	0.69921200
O	2.26614700	-1.75949300	-1.19777700
C	0.85151600	-1.59351500	-1.18107100
C	0.10017600	-2.35904000	-0.25475400
C	0.29850500	-0.72981200	-2.15393700
O	0.83118300	-3.19556500	0.50779300
O	1.17719900	-0.22854300	-3.03488400
C	0.11361800	-3.93108600	1.52280400
H	0.86831900	-4.55507200	2.00214100
H	-0.33089400	-3.23795800	2.24059900
H	-0.66524600	-4.54626200	1.06743900
C	0.65169300	0.67725900	-4.02783000
H	0.19176000	1.54495100	-3.54904800
H	1.51833500	0.97589800	-4.61774300
H	-0.08730000	0.17056800	-4.65303700
O	-1.14657900	-2.32223400	-0.13474500
O	-0.91872200	-0.41584000	-2.22053700
O	-4.03824800	0.41432700	-1.69770300
O	-1.83787000	0.54792600	0.92216300
O	-4.30427300	-1.72560700	-0.63080800
O	0.43841500	-0.10582300	1.72875100
O	-0.20262700	2.31146200	1.57701700
O	-5.93388500	-1.09140700	-2.47560900
C	2.78511600	1.98952600	-0.13086100
H	1.88097200	1.82562700	0.47687900
C	3.07974700	3.39501600	-0.45319200
C	4.20950200	3.75403000	-1.21106200
C	2.19936300	4.38553600	0.01660400
C	4.45454600	5.09466300	-1.49294800
H	4.87615300	2.97309900	-1.56565300
C	2.45012300	5.72904200	-0.27002000
H	1.32804800	4.09315000	0.59807400
C	3.57474600	6.08156600	-1.02228500
H	5.32564700	5.37896700	-2.07742100
H	1.77140700	6.49698200	0.09053200
H	3.76960000	7.12766100	-1.24521700
O	3.47068200	1.03244000	-0.49068800
S	-0.63091100	0.91662600	1.75228300
S	-5.05709100	-0.65813500	-1.39635100
C	-1.33896300	0.82384700	3.48730800
C	-6.18064300	0.11758000	-0.10672400
F	-0.38186800	1.11995100	4.38312000
F	-2.34891400	1.68860400	3.63594400

F	-1.79010400	-0.41592700	3.74223900
F	-5.46201900	0.52994700	0.94723300
F	-7.08479500	-0.77904700	0.31005500
F	-6.82204400	1.16953200	-0.63208800
Mn	-2.35453700	-0.67749100	-0.69100800

IM7-Zn(ClO₄)₂

C	-6.14221200	-3.41497200	0.01939400
C	-5.76766100	-2.66537700	-1.10864900
C	-4.49963800	-2.10505600	-1.20204900
C	-3.56825800	-2.28692700	-0.15817400
C	-3.93610700	-3.04083600	0.98147400
C	-5.20430600	-3.59063100	1.06023400
H	-6.48069200	-2.51917000	-1.91534700
H	-4.22427500	-1.51138800	-2.06916200
H	-3.21857200	-3.18600000	1.78265300
H	-5.48397000	-4.17136200	1.93578200
C	-7.51685800	-4.02205600	0.12955900
H	-8.06460900	-3.59329900	0.97866600
H	-8.10827300	-3.85297800	-0.77490600
H	-7.45572900	-5.10376100	0.30157200
C	-2.27892900	-1.69524000	-0.29415600
H	-1.98114500	-1.19032300	-1.20686100
O	-1.41522800	-1.81132600	0.65042100
C	-0.07285300	-1.39305500	0.46785100
C	0.68195900	-1.90847800	-0.61364700
C	0.46014000	-0.58327600	1.50580500
O	0.00791600	-2.74091600	-1.43416100
O	-0.40499900	-0.27918700	2.48269000
C	0.75533000	-3.30200100	-2.53826700
H	0.04244000	-3.94002300	-3.06087400
H	1.11783800	-2.50492700	-3.19086700
H	1.59929100	-3.88656900	-2.16627600
C	0.09520800	0.57310600	3.53854500
H	0.43401400	1.52548900	3.12511100
H	-0.75575100	0.71680400	4.20439800
H	0.91997500	0.08395100	4.06192600
O	1.89334900	-1.67014600	-0.83200100
O	1.63650500	-0.15354600	1.54584900
Zn	3.03816600	-0.20725500	0.03660600
O	4.65252500	-0.43315600	1.42299100
O	2.85645500	1.60778500	-0.87696400
Cl	5.71182100	-0.92400900	0.39690800
Cl	1.48126900	2.26737700	-1.18654200

O	6.83980700	0.01542100	0.32745900
O	4.88507700	-0.89741100	-0.90677700
O	0.53970800	1.17246100	-1.58057400
O	0.99269100	2.93271200	0.05438700
O	6.13333200	-2.29807000	0.71829200
O	1.69773800	3.23106800	-2.27854300
C	-2.52627400	1.82548000	-0.12116800
H	-1.42544600	1.79107900	-0.15101700
C	-3.11592100	3.16379800	0.03872500
C	-4.50961700	3.34708700	0.10486500
C	-2.25343900	4.27109000	0.12188800
C	-5.03199700	4.62804300	0.25429900
H	-5.15910100	2.47896900	0.03861000
C	-2.78350500	5.55445900	0.26994600
H	-1.17791800	4.11875700	0.06720200
C	-4.16862900	5.73151300	0.33625400
H	-6.10744600	4.77609800	0.30646600
H	-2.11899600	6.41171600	0.33115700
H	-4.58098200	6.73086000	0.45118500
O	-3.17697200	0.78511400	-0.22809400

IM7-Zn(OTf)₂

C	7.07331500	-2.41594200	0.36528700
C	6.35965500	-1.77074200	1.38958200
C	5.01636600	-1.45339800	1.22918000
C	4.35114700	-1.78345800	0.03032800
C	5.05940900	-2.43700700	-1.00427200
C	6.39904500	-2.74265000	-0.83114600
H	6.86601400	-1.51456700	2.31617100
H	4.47369200	-0.94428700	2.02122700
H	4.54589300	-2.69504800	-1.92485000
H	6.94239100	-3.24546600	-1.62742900
C	8.53399000	-2.75011200	0.52597300
H	9.14583800	-2.15264100	-0.16269200
H	8.88486900	-2.55471100	1.54347200
H	8.72579600	-3.80428400	0.29244500
C	2.97197700	-1.44038900	-0.08923100
H	2.41976000	-0.98989100	0.73309400
O	2.32012600	-1.74404300	-1.15678100
C	0.90585700	-1.58474300	-1.14403100
C	0.15448400	-2.31556900	-0.18916600
C	0.35129700	-0.76173100	-2.15079000
O	0.88179000	-3.13484200	0.59290900
O	1.22584900	-0.30094100	-3.05606300

C	0.16592200	-3.82375700	1.64219100
H	0.91974300	-4.43455100	2.13954900
H	-0.26687000	-3.09809200	2.33425500
H	-0.62131800	-4.44978000	1.21721600
C	0.69936200	0.57177700	-4.07840700
H	0.25398700	1.46201000	-3.62822000
H	1.56334100	0.83770900	-4.68754300
H	-0.05158000	0.04979900	-4.67595000
O	-1.09147500	-2.26733800	-0.06338800
O	-0.86593400	-0.44748300	-2.23057900
O	-3.85099800	0.41365000	-1.71101900
O	-1.78344400	0.65751800	0.78297300
O	-4.09172700	-1.69960800	-0.59816000
O	0.41284000	-0.08201300	1.73486400
O	-0.23526800	2.33809600	1.76373200
O	-5.71488900	-1.14222800	-2.47490400
C	2.75070500	2.01780600	-0.06748400
H	1.87268200	1.81821100	0.56751200
C	2.99502400	3.43561000	-0.37495600
C	4.09082700	3.83915200	-1.16002700
C	2.10157600	4.39235800	0.13852500
C	4.28940500	5.19075100	-1.42522700
H	4.76806100	3.08358900	-1.54791600
C	2.30594600	5.74702700	-0.13176700
H	1.25597500	4.06537300	0.73925800
C	3.39697800	6.14402500	-0.91074600
H	5.13399000	5.50976200	-2.03032700
H	1.61687500	6.48899100	0.26194800
H	3.55567100	7.19886200	-1.12081800
O	3.44881500	1.08494500	-0.46527100
S	-0.66344900	0.93325600	1.75921400
S	-4.85810900	-0.66447700	-1.39808800
C	-1.52738000	0.66953500	3.40404900
C	-6.01349000	0.11835500	-0.14229800
F	-0.65869200	0.86949100	4.40945200
F	-2.55182600	1.51760100	3.54539900
F	-1.99290100	-0.58881000	3.48938400
F	-5.32162200	0.56112400	0.91589700
F	-6.91264900	-0.78360800	0.27429900
F	-6.66077900	1.15012900	-0.69991000
Zn	-2.22025500	-0.66506300	-0.70163400
TS1-Cu(ClO ₄) ₂			
O	-1.21469900	-2.06096900	-0.85305900

O	2.09667500	-1.26843800	2.10148900
O	0.05807700	-2.13713000	2.53652300
O	-0.95995700	-0.08236400	0.98640300
C	0.19033700	-0.74169100	0.63390700
C	0.88265400	0.43104600	-0.03972200
C	-0.11466600	-1.91173200	-0.35860200
C	0.91381400	-1.39252100	1.84076200
C	0.58139600	-2.82899400	3.68940800
H	-0.26503000	-3.38063600	4.09694100
H	0.96008600	-2.10818400	4.41847400
H	1.38488100	-3.50687500	3.38975900
O	0.91512600	-2.72943000	-0.56218300
C	0.67242500	-3.85219900	-1.44571000
H	0.41238700	-3.48987700	-2.44286300
H	1.60935700	-4.40810100	-1.46198400
H	-0.14148400	-4.46557900	-1.05271600
C	3.59782000	-0.21494000	-0.22253000
H	3.60333400	0.32867000	0.73196900
O	2.53726300	-0.32073800	-0.85320400
C	4.86326600	-0.76792100	-0.68686200
C	4.96184700	-1.44305300	-1.91976600
C	6.00225400	-0.60623500	0.12320800
C	6.19049700	-1.94792500	-2.33080400
H	4.07500200	-1.55422000	-2.53601800
C	7.23056200	-1.11823000	-0.29221300
H	5.91629800	-0.08596000	1.07418400
C	7.32266500	-1.78650000	-1.51779200
H	6.27517600	-2.46568900	-3.28192700
H	8.11106600	-0.99754500	0.33201000
H	8.28023800	-2.18355300	-1.84427300
H	0.49536600	0.58427300	-1.04174600
C	1.31699200	1.65117000	0.62027500
C	1.50455400	2.78324600	-0.20596300
C	1.53960300	1.79482800	2.00764500
C	1.91403300	3.99841300	0.32936200
H	1.29194000	2.70759800	-1.26758200
C	1.93446500	3.01917400	2.53318300
H	1.38735800	0.96206800	2.68007100
C	2.12964600	4.14237800	1.70951700
H	2.04045900	4.85484400	-0.32812900
H	2.08495700	3.11160400	3.60621400
C	2.51435400	5.47566600	2.29973300
H	3.11555300	5.35652800	3.20752200
H	3.08007100	6.08351700	1.58590600

H	1.61624500	6.04569500	2.57433300
Cu	-2.53945300	-0.24068800	-0.13244700
Cl	-2.13908000	2.09515500	-2.06310100
Cl	-5.00027400	-1.12459500	0.51342000
O	-2.66375700	2.62977500	-0.77763200
O	-1.79821600	0.57144600	-1.80026700
O	-4.45465700	-0.53218700	-0.81774800
O	-3.71369000	-1.03189500	1.38451200
O	-0.84974600	2.73047400	-2.44709400
O	-3.12736200	2.16404100	-3.15302700
O	-6.06884900	-0.28411100	1.06513500
O	-5.40761100	-2.52497300	0.33305300
TS1-Cu(OTf) ₂			
O	-0.41398600	-1.74975800	-1.58884100
O	2.91753900	-2.17210300	1.40614700
O	0.95327100	-3.28552400	1.39360500
O	-0.25149300	-0.83507400	0.95830100
C	0.93468800	-1.16379500	0.35196900
C	1.52060400	0.23816100	0.30765500
C	0.68676900	-1.76035200	-1.07354900
C	1.73596100	-2.24491300	1.12116900
C	1.55936200	-4.39573500	2.08759700
H	0.76336100	-5.13156700	2.19427100
H	1.92083900	-4.07296900	3.06687800
H	2.39040700	-4.79822700	1.50267000
Cu	-1.83371400	-0.55944200	-0.13559500
O	1.76585700	-2.30993600	-1.62532000
C	1.57784200	-2.91188600	-2.92954500
H	1.27071800	-2.14892100	-3.64861200
H	2.54904300	-3.33033500	-3.19173900
H	0.81609300	-3.69246500	-2.87250900
O	-2.46594500	2.57263700	0.35070600
O	-2.97448600	-2.06097700	0.80793800
S	-1.56067800	2.47669900	-0.79904800
S	-4.19132700	-1.75316600	-0.03985500
O	-0.38696600	3.36199100	-0.86256600
O	-4.90316600	-2.86487100	-0.65130900
O	-1.17133200	1.03213600	-1.12868500
O	-3.73555300	-0.61903200	-0.93759000
C	-2.58387700	2.94438900	-2.30426000
C	-5.41330700	-0.95948500	1.14791300
F	-2.97463800	4.22530700	-2.20093000
F	-3.66956400	2.16965900	-2.40176000

F	-1.85687700	2.81085900	-3.42711600
F	-6.48452400	-0.52935700	0.47165000
F	-4.84773900	0.07386800	1.77907800
F	-5.80376600	-1.86546600	2.05580200
C	4.26715900	-0.02421300	-0.16603200
H	4.27768000	0.00616400	0.93222000
O	3.18959200	0.08994000	-0.76494300
C	5.54601400	-0.18769100	-0.84551700
C	5.63506300	-0.19133500	-2.25197600
C	6.70619400	-0.33663100	-0.06349800
C	6.87544200	-0.34401900	-2.86196600
H	4.73123700	-0.06804600	-2.84075000
C	7.94655800	-0.49331200	-0.68064400
H	6.62757800	-0.33483600	1.02130200
C	8.02898300	-0.49594700	-2.07742000
H	6.95259800	-0.34343200	-3.94570900
H	8.84371400	-0.61141100	-0.07988900
H	8.99557200	-0.61535500	-2.56006000
H	1.08167100	0.80696200	-0.50513900
C	1.88772400	1.04612700	1.45960600
C	1.87823000	2.44836200	1.27169400
C	2.22933700	0.54618200	2.73626600
C	2.20709800	3.30914600	2.31248500
H	1.56613800	2.85797200	0.31532300
C	2.54843000	1.41863300	3.77043100
H	2.23748000	-0.51786100	2.92806700
C	2.54445500	2.81249300	3.58202200
H	2.17674000	4.38271700	2.14351800
H	2.79798900	1.01295800	4.74820900
C	2.84896400	3.74887700	4.72478400
H	3.49807100	3.27727600	5.47169000
H	3.33294300	4.66815200	4.37483500
H	1.92108200	4.04292000	5.23494100
TS1-Hg(ClO ₄) ₂			
O	-0.81482700	-1.89036300	-0.87126000
O	2.60244100	-1.46564100	2.09876200
O	0.56481700	-2.35946700	2.48483800
O	-0.42314600	-0.09937900	1.19362300
C	0.66879800	-0.78033300	0.73187200
C	1.38978700	0.40447900	0.10219200
C	0.28575600	-1.84949000	-0.34938000
C	1.41454700	-1.55704400	1.84645700
C	1.10141600	-3.15707200	3.56140000

H	0.25805100	-3.73955900	3.93054500
H	1.49607900	-2.50794900	4.34701500
H	1.89547400	-3.80889100	3.18795300
O	1.25680000	-2.71420900	-0.61545100
C	0.95632300	-3.74342100	-1.59289800
H	0.73015200	-3.28227800	-2.55675500
H	1.85845000	-4.35147400	-1.64931000
H	0.10288300	-4.33619800	-1.25673900
C	4.05408000	-0.30032300	-0.22470800
H	4.11929700	0.18272200	0.75921600
O	2.96052600	-0.33983000	-0.80792800
C	5.27794000	-0.85235600	-0.78596000
C	5.29950100	-1.44726900	-2.06364300
C	6.45891400	-0.76906500	-0.02493400
C	6.49353100	-1.95152000	-2.56651900
H	4.38200900	-1.49714600	-2.64182300
C	7.65210700	-1.27971300	-0.53317500
H	6.43244900	-0.31061800	0.96070000
C	7.66749700	-1.86839600	-1.80218200
H	6.51929000	-2.40700100	-3.55225000
H	8.56467100	-1.21927000	0.05245100
H	8.59779400	-2.26393000	-2.20120500
H	0.96563200	0.63564100	-0.87107900
C	1.87873800	1.57607700	0.81602000
C	1.99772700	2.76635300	0.06436900
C	2.21942200	1.61591100	2.18689800
C	2.44716200	3.94290500	0.65456800
H	1.69999900	2.77212700	-0.97970100
C	2.65849600	2.79948600	2.76684500
H	2.13005400	0.73106000	2.80167900
C	2.78069500	3.98411700	2.01684000
H	2.51450400	4.84698000	0.05506900
H	2.90307100	2.81136600	3.82658600
C	3.22034500	5.26812100	2.67466500
H	4.05476100	5.09994600	3.36529900
H	3.52880600	6.01425500	1.93581000
H	2.39828600	5.70182000	3.25985800
Hg	-2.30386500	-0.00436000	-0.09786100
Cl	-1.61269900	2.30240300	-2.14816600
Cl	-5.06941600	-1.16135900	0.54612000
O	-2.54039000	2.28868500	-0.91785000
O	-0.99791200	0.89806300	-2.17429500
O	-4.26883900	-1.21297100	-0.78165800
O	-4.17888500	-0.30630400	1.47016000

O	-0.53950200	3.30888800	-1.95220600
O	-2.39206200	2.55392200	-3.37208000
O	-6.36814100	-0.50260200	0.32730500
O	-5.20878900	-2.52494700	1.09529300
TS1-Hg(OTf) ₂			
O	-0.28089800	-0.84105100	-1.88163600
O	3.11949600	-2.75069500	0.49296600
O	1.10142900	-3.60442500	-0.05443600
O	0.13539000	-1.12659000	0.82939600
C	1.22471800	-1.24953200	0.00897600
C	1.94084900	0.01208300	0.46636700
C	0.83693800	-1.15147200	-1.50539800
C	1.95072300	-2.60534700	0.18528100
C	1.60932600	-4.94684800	0.09830700
H	0.77359000	-5.59750900	-0.15671800
H	1.92469000	-5.11059500	1.13175100
H	2.45411300	-5.10941300	-0.57593100
Hg	-1.82882800	-0.30929900	0.00923000
O	1.82713300	-1.46286000	-2.32956800
C	1.53666300	-1.38777800	-3.74903100
H	1.25502200	-0.36622300	-4.01292900
H	2.46253500	-1.68123900	-4.24232500
H	0.72433100	-2.07419100	-3.99765900
O	-1.99265300	2.00512600	0.19244700
O	-3.66642800	-1.26208700	1.34121000
S	-0.82703900	2.91418300	-0.15330700
S	-4.42037700	-1.82142200	0.16030300
O	-0.36383700	3.74876900	0.95993700
O	-4.80366200	-3.22915600	0.21413400
O	0.21320200	2.20821400	-0.93960200
O	-3.71987000	-1.35062700	-1.09532800
C	-1.61881200	4.09703000	-1.37745400
C	-6.03194600	-0.85803200	0.15677400
F	-2.62545400	4.76992000	-0.80575400
F	-2.09693600	3.42452300	-2.43713100
F	-0.70344400	4.97981000	-1.81102600
F	-6.79292300	-1.23852500	-0.87882400
F	-5.78919400	0.45668700	0.05404100
F	-6.70445400	-1.08547600	1.29328800
C	4.66012800	-0.25643000	-0.20674600
H	4.68859300	-0.67618400	0.80848100
O	3.58595700	0.15461200	-0.66343500
C	5.91563400	-0.20415000	-0.94583300

C	5.98655400	0.37144100	-2.23000200
C	7.07153900	-0.73436500	-0.34406700
C	7.20495400	0.41186600	-2.89892300
H	5.08665700	0.78332100	-2.67629000
C	8.28938700	-0.69506200	-1.02154700
H	7.00727000	-1.17761200	0.64686600
C	8.35408000	-0.12181900	-2.29603400
H	7.26847600	0.85870200	-3.88694500
H	9.18322800	-1.10567600	-0.56112700
H	9.30358800	-0.08757900	-2.82371000
H	1.55013400	0.88193600	-0.05568800
C	2.39479700	0.30019400	1.81629900
C	2.41388500	1.66528400	2.18716800
C	2.78628700	-0.65938500	2.77642300
C	2.80770200	2.05274700	3.46263700
H	2.08363400	2.41875400	1.47723500
C	3.17722200	-0.25829000	4.04870600
H	2.77964100	-1.71329600	2.53204700
C	3.19273600	1.09886800	4.41876700
H	2.79647100	3.10737200	3.72583000
H	3.46746500	-1.01241600	4.77663900
C	3.57119600	1.51460400	5.81818600
H	4.26563000	0.80274100	6.27690000
H	4.03262500	2.50767700	5.83190300
H	2.67940300	1.56125300	6.45816800

TS1-Mn(ClO₄)₂

O	-1.27936300	-1.75428000	-0.87671000
O	2.17281400	-1.23107200	2.04180600
O	0.11197700	-2.00047300	2.55171800
O	-0.85971200	0.09550000	1.00156600
C	0.23917300	-0.62541300	0.63797300
C	0.97912300	0.48276400	-0.10024200
C	-0.17829600	-1.76482900	-0.34757200
C	0.97634600	-1.30373100	1.81880000
C	0.63844300	-2.70420300	3.69583800
H	-0.21910300	-3.21303700	4.13455600
H	1.07118100	-1.99416600	4.40510100
H	1.40105900	-3.42065900	3.37951600
O	0.71698400	-2.72442300	-0.52683500
C	0.32280400	-3.82071600	-1.39420200
H	0.13687000	-3.44540900	-2.40279500
H	1.16647100	-4.50968200	-1.37900900
H	-0.58054500	-4.29351000	-1.00332500

C	3.59860200	-0.29306800	-0.30541600
H	3.67188500	0.31115000	0.60731400
O	2.51081400	-0.35925400	-0.90175700
C	4.80059700	-0.96606600	-0.76859200
C	4.80564700	-1.73785400	-1.94818500
C	5.97899500	-0.82321700	-0.01184900
C	5.98075300	-2.35608800	-2.35956600
H	3.88999600	-1.83531900	-2.52302900
C	7.15305800	-1.44837400	-0.42793300
H	5.96477300	-0.22908300	0.89865100
C	7.15212600	-2.21182800	-1.60029700
H	5.99362500	-2.94982900	-3.26898700
H	8.06338400	-1.34246500	0.15467100
H	8.06761900	-2.69783900	-1.92705700
H	0.54668800	0.63390200	-1.08503100
C	1.47198300	1.71287100	0.51031400
C	1.64730200	2.82099500	-0.34759200
C	1.76291100	1.87847900	1.88066600
C	2.10909200	4.03744800	0.14032000
H	1.39104400	2.72846300	-1.39883000
C	2.21240700	3.10388200	2.36056400
H	1.62274400	1.06171800	2.57546000
C	2.39321200	4.20474200	1.50540200
H	2.22276100	4.87713700	-0.54069300
H	2.41669600	3.21403100	3.42294700
C	2.83618500	5.54126000	2.04620100
H	3.43631400	5.42979000	2.95546800
H	3.42358800	6.09883400	1.30892700
H	1.96429100	6.15864400	2.30199100
Mn	-2.59610600	-0.01685700	-0.11235500
Cl	-2.39829700	2.35929900	-1.77332800
Cl	-4.97500300	-1.50468500	0.44741300
O	-3.12657500	2.12736200	-0.43643100
O	-1.78759100	0.97389100	-2.05899300
O	-4.36445600	-1.13399400	-0.91943900
O	-3.98960600	-0.81619700	1.42291700
O	-1.31755400	3.35648100	-1.60323500
O	-3.34942600	2.74351100	-2.82653300
O	-6.32650100	-0.94193300	0.58951800
O	-4.94747700	-2.96661600	0.64563100
TS1-Mn(OTf) ₂			
O	-0.70479500	-0.27228300	-1.89232500
O	2.71635600	-2.72596100	-0.10986100

O	0.69184800	-3.37450200	-0.87570800
O	-0.24595600	-1.14764700	0.57382100
C	0.85762000	-1.11318500	-0.23981200
C	1.58420200	-0.01044800	0.50295100
C	0.43836100	-0.64680700	-1.66952100
C	1.55628400	-2.48467700	-0.38823700
C	1.16786800	-4.72581600	-1.05109500
H	0.32148300	-5.27343300	-1.46395700
H	1.46506000	-5.14456000	-0.08647300
H	2.01807300	-4.73902400	-1.73790700
Mn	-2.03109000	-0.36052100	-0.04704500
O	1.38423000	-0.71802400	-2.58862400
C	1.01941500	-0.29291800	-3.92850700
H	0.72979300	0.75975500	-3.91240900
H	1.91680000	-0.44612200	-4.52658800
H	0.19146600	-0.90262300	-4.29630500
O	-2.26478400	1.66352600	0.25626200
O	-3.55793900	-1.41293800	1.20543900
S	-1.30417400	2.83785100	0.33951300
S	-4.28824600	-2.00429200	0.02401600
O	-1.28897200	3.49664300	1.64630800
O	-4.60399600	-3.42681200	0.06085000
O	0.00418900	2.54349700	-0.28804600
O	-3.57778000	-1.47673300	-1.20272200
C	-2.12474400	4.04669500	-0.83817700
C	-5.94375500	-1.11777600	0.01104600
F	-3.35569500	4.36057700	-0.41489300
F	-2.21601200	3.51473000	-2.06924800
F	-1.39618300	5.17270700	-0.91546300
F	-6.66365800	-1.51268100	-1.04852500
F	-5.76235300	0.20795000	-0.05902900
F	-6.62397800	-1.40433100	1.12897800
C	4.33390500	-0.17552500	-0.23326600
H	4.34681700	-0.80102200	0.67135700
O	3.27351200	0.34501600	-0.59656100
C	5.59898900	0.00043900	-0.93963800
C	5.69179900	0.81992300	-2.08165500
C	6.73982300	-0.66076500	-0.45015400
C	6.91687300	0.97014800	-2.72248500
H	4.80286500	1.32871500	-2.44176100
C	7.96484400	-0.50926900	-1.09860200
H	6.65858100	-1.29256300	0.43127000
C	8.05131700	0.30593900	-2.23206900
H	6.99696800	1.60373600	-3.60120100

H	8.84708000	-1.02042700	-0.72445600
H	9.00609600	0.42753000	-2.73688300
H	1.23319500	0.96910300	0.18894300
C	2.04993700	-0.05358500	1.87341800
C	2.16449200	1.19566400	2.52887000
C	2.35841200	-1.22367500	2.60261500
C	2.57418000	1.27091600	3.85421200
H	1.90306000	2.10302700	1.99063900
C	2.76101300	-1.13504900	3.92971200
H	2.27287000	-2.19648000	2.13735500
C	2.87415800	0.10677300	4.58150000
H	2.64196900	2.24163500	4.33878400
H	2.98347100	-2.04691100	4.47890800
C	3.26563800	0.18261100	6.03570400
H	3.89774100	-0.66261400	6.32780500
H	3.80082200	1.11113500	6.26078600
H	2.37159200	0.15872400	6.67382000

TS1-Zn(ClO₄)₂

O	-1.28473200	-1.78388900	-0.81797700
O	2.17781900	-1.20649600	2.06553100
O	0.11607600	-1.98914800	2.55265600
O	-0.83776200	0.11887900	1.00419000
C	0.25491900	-0.61241300	0.64220600
C	1.00087500	0.48704800	-0.10253400
C	-0.16626300	-1.76385000	-0.32766400
C	0.98444700	-1.28634100	1.83054000
C	0.63115900	-2.68567800	3.70645800
H	-0.22838800	-3.20197300	4.13231200
H	1.04502700	-1.96971700	4.42097400
H	1.40592400	-3.39500700	3.40397000
O	0.74641300	-2.69935000	-0.53606700
C	0.35177800	-3.80679400	-1.38947300
H	0.12306800	-3.43740100	-2.39138100
H	1.21299800	-4.47368800	-1.40192100
H	-0.52554500	-4.30192400	-0.96825000
C	3.62718800	-0.29056500	-0.29181800
H	3.69263700	0.31450000	0.62117900
O	2.54296500	-0.36403900	-0.89276900
C	4.83632100	-0.95638000	-0.74800400
C	4.85367000	-1.72646800	-1.92851400
C	6.00881100	-0.80765900	0.01664900
C	6.03507400	-2.33737100	-2.33291400
H	3.94242900	-1.82815300	-2.50963800

C	7.18924200	-1.42548800	-0.39240900
H	5.98521300	-0.21444900	0.92756800
C	7.20053900	-2.18737900	-1.56572700
H	6.05746100	-2.92967200	-3.24309400
H	8.09508500	-1.31496400	0.19630800
H	8.12102700	-2.66752800	-1.88708500
H	0.57538300	0.62927500	-1.09162500
C	1.49502200	1.72119200	0.49770200
C	1.66202800	2.82402000	-0.36885900
C	1.79536200	1.89672300	1.86500000
C	2.12357200	4.04498500	0.10779500
H	1.39791400	2.72393600	-1.41736500
C	2.24468300	3.12655100	2.33348400
H	1.66356600	1.08393500	2.56599700
C	2.41657500	4.22218700	1.46975200
H	2.23036100	4.88037400	-0.57959600
H	2.45615100	3.24434000	3.39364100
C	2.85818900	5.56383200	1.99879300
H	3.46555500	5.46045500	2.90421400
H	3.43828800	6.11879900	1.25380100
H	1.98578800	6.17945700	2.25702000
Zn	-2.51619400	-0.04826100	-0.09923800
Cl	-2.35118200	2.23727400	-1.81060400
Cl	-4.89671300	-1.40967200	0.46892400
O	-3.06253500	2.01668000	-0.46034200
O	-1.71776200	0.86064300	-2.07267200
O	-4.26369100	-1.07820500	-0.89995000
O	-3.88484400	-0.74984000	1.43720400
O	-1.28965600	3.25978300	-1.66762800
O	-3.32006600	2.58672500	-2.85932800
O	-6.22526000	-0.79292900	0.59929900
O	-4.92934400	-2.86918100	0.68234300
TS1-Zn(OTf) ₂			
O	-0.69439600	0.41755300	-1.79962600
O	2.75096900	-2.48727300	-1.06768000
O	0.71899400	-2.85721900	-1.98445100
O	-0.22625100	-1.32131200	0.17128700
C	0.87006000	-0.97508800	-0.57702300
C	1.58683000	-0.21515200	0.51976700
C	0.44696400	-0.01733600	-1.73557300
C	1.58136600	-2.18703900	-1.22130000
C	1.20853500	-4.04471100	-2.64303700
H	0.36079900	-4.42269900	-3.21325400

H	1.53066300	-4.77716200	-1.89877300
H	2.04458300	-3.79297900	-3.30057200
Zn	-1.94306400	-0.33353400	-0.13073600
O	1.38896900	0.25138500	-2.62008300
C	1.02304300	1.14679000	-3.70403300
H	0.73570000	2.11735700	-3.29466800
H	1.91918500	1.22622800	-4.31804100
H	0.19311700	0.71943500	-4.27059300
O	-2.25348400	1.38243600	0.86624900
O	-3.40997200	-1.72127300	0.74274300
S	-1.36325300	2.56159900	1.22130100
S	-4.17937500	-1.83957400	-0.54835700
O	-1.48514700	2.98288200	2.61576000
O	-4.51741600	-3.17315500	-1.03009400
O	0.00120100	2.43323800	0.66012700
O	-3.48588400	-0.90286000	-1.51711600
C	-2.15092500	3.92987500	0.20560500
C	-5.82104500	-1.00064400	-0.19517300
F	-3.42434600	4.12261300	0.57048800
F	-2.12182800	3.61936200	-1.10310100
F	-1.47395500	5.07647900	0.38317200
F	-6.55890800	-0.95220900	-1.31358500
F	-5.62238500	0.24687700	0.24726300
F	-6.49249000	-1.69133800	0.73608400
C	4.32176100	-0.03869000	-0.24608100
H	4.35886300	-0.96566400	0.34438600
O	3.24757600	0.56084400	-0.36871000
C	5.57163100	0.42434900	-0.83993900
C	5.63374300	1.62854800	-1.56849300
C	6.72969700	-0.35391700	-0.66162300
C	6.84555800	2.04249500	-2.11077100
H	4.73213100	2.22108500	-1.68993300
C	7.94107400	0.06387900	-1.21119300
H	6.67255000	-1.28232100	-0.09822400
C	7.99709300	1.26080000	-1.93318600
H	6.90195100	2.97210000	-2.66988400
H	8.83646400	-0.53615200	-1.07762200
H	8.94139700	1.58936500	-2.35926700
H	1.20923000	0.80109400	0.59567900
C	2.07196900	-0.75487400	1.77457200
C	2.17893400	0.16541000	2.84415400
C	2.41002300	-2.10462500	2.01598100
C	2.61119600	-0.24599400	4.09875300
H	1.89756100	1.20269100	2.68134700

C	2.83425500	-2.50501900	3.27767300
H	2.33055700	-2.83833100	1.22505600
C	2.94120900	-1.59022000	4.34091500
H	2.67522600	0.47846400	4.90675700
H	3.07934200	-3.55066700	3.44808300
C	3.35848900	-2.04826200	5.71575200
H	4.00844000	-2.92833000	5.66788400
H	3.88425000	-1.25740100	6.26110700
H	2.47712600	-2.32397300	6.31090400

TS5-Cu(ClO₄)₂

C	6.01968700	-0.59994400	0.23076400
C	5.27651400	-0.87705900	-0.93077100
C	4.09981000	-0.20058200	-1.19751100
C	3.61729900	0.77650800	-0.27674800
C	4.35394400	1.04932100	0.89586600
C	5.53877500	0.37583900	1.13496700
H	5.62788200	-1.64283300	-1.62176400
H	3.51436100	-0.44123100	-2.08327300
H	3.96961800	1.77583800	1.60368200
H	6.10441500	0.58522900	2.03522700
C	7.30869900	-1.32923200	0.50247400
H	7.57428400	-1.30417000	1.56660600
H	7.25160000	-2.38063700	0.18208600
H	8.13480700	-0.86669800	-0.05423900
C	2.40728000	1.44946200	-0.58099800
H	1.90344400	1.28697000	-1.53550700
O	1.89394400	2.37043900	0.22990300
C	0.61460300	1.74861800	0.34986200
C	-0.48054100	2.32262300	-0.40018400
C	0.47013000	0.67243800	1.27733800
O	-0.09848000	3.34419200	-1.18170200
O	1.53287800	0.42248700	2.04399400
C	-1.14249500	3.96725000	-1.96147900
H	-0.63277800	4.74056200	-2.54290700
H	-1.61852700	3.22863400	-2.61553200
H	-1.89303100	4.40961900	-1.29982000
C	1.47726800	-0.75964100	2.87587000
H	1.28630200	-1.64256300	2.25358800
H	2.45184900	-0.82326500	3.33693400
H	0.68602600	-0.65242600	3.63015400
O	-1.65465800	1.92677800	-0.36446300
O	-0.57575700	-0.01753100	1.43012000
Cu	-2.05790000	-0.20103700	0.13698400

O	-3.55475600	-0.04879000	1.54219100
O	-0.73300800	-2.87358200	-0.23911200
Cl	-4.70055600	-0.39077000	0.54236000
Cl	-0.05734200	-2.03149700	-1.25773800
O	-5.38388700	-1.62664100	0.93358700
O	-3.84684000	-0.61169900	-0.74590800
O	-0.92146000	-0.72256100	-1.42223300
O	1.29497300	-1.59937700	-0.79132100
O	-5.60992600	0.74773500	0.37773600
O	0.01163800	-2.66620500	-2.58567400

TS5-Cu(OTf)₂

C	6.43254500	-0.62561800	-0.48773000
C	5.77471500	0.24669400	0.39805100
C	4.51110100	-0.05426100	0.88466300
C	3.86927700	-1.25334800	0.48829000
C	4.51869800	-2.12889300	-0.41900000
C	5.78402700	-1.81693400	-0.88311400
H	6.25977400	1.17160600	0.69640200
H	3.99113400	0.62992400	1.54872000
H	4.01290400	-3.03448800	-0.73454900
H	6.28886100	-2.49258700	-1.56893900
C	7.80114100	-0.29850500	-1.02485400
H	7.76409700	-0.14379700	-2.11126700
H	8.21000700	0.60774600	-0.56905200
H	8.50227900	-1.12237100	-0.84292200
C	2.60673700	-1.55361000	1.05414800
H	2.19084600	-0.91452700	1.83034100
O	1.93696600	-2.67743000	0.75392800
C	0.76530100	-1.97593900	0.34369400
C	-0.32451800	-1.88710500	1.29334900
C	0.67732200	-1.51753800	-1.00808600
O	-0.03365400	-2.45732800	2.47115900
O	1.69009600	-1.87383400	-1.79931400
C	-1.05721000	-2.37265100	3.48954800
H	-0.63078500	-2.87489400	4.35791900
H	-1.27920400	-1.32608800	3.71248700
H	-1.96554500	-2.87954700	3.15326000
C	1.71454300	-1.28179900	-3.12223900
H	1.73908900	-0.19344600	-3.03696600
H	2.62948300	-1.66138400	-3.57716100
H	0.83861300	-1.59950200	-3.69163700
O	-1.41180300	-1.33333400	1.08426600
O	-0.27454100	-0.85024700	-1.48529400

Cu	-1.65794500	0.14702400	-0.51701200
O	-3.27244200	-0.66519100	-1.61144100
O	1.78388000	1.48032400	-0.77401500
O	-5.18521500	1.00459800	-1.84384900
O	-3.39075700	1.12154000	-0.03898800
O	-0.53366600	1.63902800	0.17987400
O	1.42806000	1.34556900	1.70292700
S	0.95533200	1.83227600	0.39157400
S	-4.25616500	0.29740800	-0.97917900
C	-5.32359000	-0.76090600	0.15101400
C	1.02758500	3.70420700	0.51521400
F	0.28256700	4.14528000	1.53569800
F	2.30300900	4.08155600	0.72039700
F	0.59307900	4.27057500	-0.61825200
F	-4.56312300	-1.45618600	1.00288500
F	-6.04269700	-1.61365700	-0.58896300
F	-6.15275100	0.02603100	0.84564400
TS5-Hg(ClO ₄) ₂			
C	-6.24849800	-1.10921700	0.96447300
C	-5.46357900	-0.19177500	1.68821000
C	-4.38028600	0.43884600	1.09450200
C	-4.05398400	0.16018000	-0.25706000
C	-4.83257000	-0.77396000	-0.98844700
C	-5.91517800	-1.38456700	-0.38116900
H	-5.70833300	0.02058500	2.72516500
H	-3.76872500	1.14019800	1.65623000
H	-4.56468200	-0.99677300	-2.01531500
H	-6.51872900	-2.09386900	-0.94231200
C	-7.42173200	-1.80095700	1.60660700
H	-7.25589900	-2.88529600	1.65071400
H	-7.59615400	-1.44353300	2.62526700
H	-8.33752100	-1.64159400	1.02388000
C	-2.97277800	0.86460000	-0.83790300
H	-2.44772000	1.62515400	-0.26157800
O	-2.62208100	0.70975900	-2.11998400
C	-1.25499800	0.40134700	-1.83934200
C	-0.30746600	1.47911200	-1.95096400
C	-0.90451400	-0.96488700	-1.56674300
O	-0.86660900	2.63008500	-2.34217000
O	-1.91763300	-1.83484900	-1.71931800
C	0.00665300	3.78145000	-2.40986000
H	-0.63871300	4.60074100	-2.72526000
H	0.44033600	3.98077900	-1.42739200

H	0.80130500	3.60856600	-3.13898700
C	-1.62307900	-3.21643300	-1.41361600
H	-1.29851100	-3.31541700	-0.37521100
H	-2.56194800	-3.74519300	-1.57851500
H	-0.84452900	-3.59319600	-2.08031600
O	0.91167300	1.40700600	-1.69750300
O	0.23253800	-1.36721200	-1.24951600
Hg	1.76326500	-0.02894700	-0.00430600
O	3.22538600	-1.61797600	1.03406300
O	-0.27370800	-0.02360600	1.51472500
Cl	4.54429500	-1.21941500	0.31568900
Cl	-0.11351600	1.39112400	2.08549200
O	5.53518900	-0.75715100	1.30015000
O	4.10604600	-0.04545400	-0.59683400
O	1.22973000	1.87697300	1.53523900
O	-1.21408000	2.25145000	1.55523400
O	5.02818000	-2.34388700	-0.50359700
O	-0.10620500	1.36900800	3.55650500
TS5-Hg(OTf) ₂			
C	6.46758100	-0.65035300	-1.74431000
C	5.84507800	0.52350100	-1.27970500
C	4.81452500	0.46278600	-0.35310200
C	4.37813900	-0.79534700	0.13465500
C	4.99010200	-1.98378500	-0.34111100
C	6.02401000	-1.90039900	-1.25658400
H	6.17524700	1.48824200	-1.65492200
H	4.32327800	1.36660800	-0.00190600
H	4.63748800	-2.94274400	0.02210600
H	6.50233000	-2.80908100	-1.61406200
C	7.57797800	-0.58793800	-2.75965300
H	7.24054200	-0.98852600	-3.72504200
H	7.92060400	0.43770700	-2.92340500
H	8.43598300	-1.19367400	-2.44440000
C	3.36479600	-0.80879100	1.12301100
H	2.98418600	0.13104200	1.52075400
O	2.92102600	-1.94367800	1.67707500
C	1.54529800	-1.70178600	1.37694500
C	0.72845000	-1.16854400	2.43680400
C	1.03856600	-2.11837100	0.09722500
O	1.40482000	-0.98235600	3.57736000
O	1.92792200	-2.79072800	-0.65475700
C	0.67094100	-0.38166800	4.66950400
H	1.39599700	-0.29887000	5.47871200

H	0.29849000	0.60200700	4.37499800
H	-0.16435100	-1.02309300	4.95939400
C	1.48128800	-3.17818000	-1.97308200
H	1.19050300	-2.29730400	-2.55009500
H	2.34129000	-3.67208000	-2.42576200
H	0.63574800	-3.86555700	-1.89906300
O	-0.47796600	-0.86895500	2.34415100
O	-0.12296400	-1.92934900	-0.31180100
Hg	-1.39865600	0.00039000	0.31885600
O	-2.98955100	0.30639700	-1.48215600
O	0.63488700	1.11246900	-0.72285300
O	-5.25991600	1.16995300	-0.74292800
O	-3.76550300	-0.21935700	0.76638400
O	-0.44220100	2.16867700	1.20231900
O	2.08047700	2.19599000	1.02719500
S	0.78037800	2.16953500	0.33323800
S	-4.22806100	0.14729700	-0.62747100
C	-5.00734900	-1.43675600	-1.26721700
C	0.69750600	3.79387200	-0.60193200
F	0.78667200	4.82111000	0.25208000
F	1.71864200	3.86713900	-1.47211000
F	-0.45295900	3.88338600	-1.27588600
F	-4.12565000	-2.44885300	-1.19988900
F	-5.38533500	-1.28130500	-2.54228400
F	-6.08043900	-1.75226700	-0.53153600

TS5-Mn(ClO₄)₂

C	6.11439000	-0.69688500	0.19947000
C	5.29634000	-1.14956300	-0.85281300
C	4.09394900	-0.52069100	-1.13777700
C	3.67458400	0.59044300	-0.36417800
C	4.48478000	1.03854700	0.71180900
C	5.68784100	0.40740600	0.97144000
H	5.60860500	-2.00649300	-1.44296900
H	3.45756400	-0.88707500	-1.93807900
H	4.14678900	1.87224400	1.31730000
H	6.31414300	0.75747500	1.78839000
C	7.41918300	-1.37866300	0.51507700
H	7.39196400	-1.82280400	1.51867700
H	7.64515800	-2.17366500	-0.20090800
H	8.24860600	-0.66057300	0.50621000
C	2.46919800	1.24193700	-0.71551300
H	1.91280700	0.93540700	-1.59922000
O	2.02020200	2.31774200	-0.05643300

C	0.73342600	1.77306400	0.21565900
C	-0.36926900	2.23466200	-0.58745100
C	0.56972000	0.88582200	1.33404700
O	-0.01837500	3.14381400	-1.50240400
O	1.64560600	0.76397500	2.12267400
C	-1.07854200	3.63560900	-2.35659600
H	-0.58919300	4.33796700	-3.03064400
H	-1.52948300	2.80853200	-2.90926200
H	-1.84121400	4.13685200	-1.75665300
C	1.53163300	-0.18304700	3.21166200
H	1.31860700	-1.18095200	2.82217300
H	2.50240100	-0.15617300	3.70645900
H	0.73836500	0.12523900	3.89572600
O	-1.54493800	1.83670100	-0.48290300
O	-0.48790700	0.27992000	1.59573900
Mn	-2.04319700	-0.16645100	0.17298500
O	-3.70596500	-0.23702700	1.61872300
O	-1.21614400	-2.28716100	0.07107200
Cl	-4.85272000	-0.30200400	0.57646100
Cl	-0.30242500	-2.10288500	-1.14567600
O	-5.61053800	-1.55283500	0.71780100
O	-4.04985700	-0.29306500	-0.74741400
O	-0.65371800	-0.67760000	-1.61173700
O	1.12467700	-2.13860300	-0.73110400
O	-5.70133400	0.89635200	0.67313000
O	-0.59809900	-3.09139300	-2.19141400

TS5-Mn(OTf)₂

C	6.33075100	-1.26079000	-1.17043700
C	5.76443500	0.01540100	-0.99589000
C	4.63815500	0.19241500	-0.20558700
C	4.04347200	-0.92356100	0.43514700
C	4.59686600	-2.21683400	0.24634000
C	5.72871100	-2.36988500	-0.53411800
H	6.21210300	0.87214000	-1.49182600
H	4.18689800	1.17402800	-0.09676200
H	4.12502200	-3.06923900	0.72251800
H	6.16200800	-3.35817000	-0.66778400
C	7.54741000	-1.45610400	-2.03614900
H	7.28514400	-2.00198500	-2.95245200
H	7.99276100	-0.50157200	-2.33055900
H	8.31024600	-2.04920800	-1.51768400
C	2.93612400	-0.69749500	1.28904200
H	2.60677500	0.31559400	1.52011900

O	2.32728600	-1.70320400	1.94159400
C	1.04557900	-1.39077200	1.40611100
C	0.14137100	-0.64249200	2.24552100
C	0.66660900	-1.92682700	0.13043500
O	0.66215500	-0.31193500	3.42309600
O	1.54089500	-2.78632200	-0.40600400
C	-0.13807500	0.55452100	4.26325700
H	0.46083700	0.69890800	5.16183400
H	-0.30898200	1.50199100	3.74814100
H	-1.09006400	0.07502900	4.50027800
C	1.22029700	-3.28895900	-1.72436400
H	1.13523600	-2.46296500	-2.43401300
H	2.05462600	-3.94029500	-1.98398800
H	0.28386100	-3.84979900	-1.69598300
O	-1.01886300	-0.31163000	1.92597100
O	-0.40030400	-1.65217700	-0.46222900
Mn	-1.70745300	-0.01103100	-0.06761900
O	-3.18322200	-0.49376600	-1.65631800
O	-0.55729200	1.64111200	-0.55677800
O	-5.38524200	0.77359900	-1.49659800
O	-3.81101300	0.42830200	0.47413900
O	1.13476600	2.06748300	1.23244200
O	1.86592000	1.78605300	-1.14444500
S	0.80992100	2.19150900	-0.20437400
S	-4.37929900	-0.04949500	-0.84397200
C	-5.23733200	-1.65930000	-0.39761600
C	0.53933500	4.02501300	-0.49586100
F	1.67756100	4.69038200	-0.23572500
F	0.19012400	4.25195000	-1.76784400
F	-0.42402600	4.49152200	0.30996200
F	-4.36854400	-2.48734700	0.21041700
F	-5.70090300	-2.25896000	-1.50082000
F	-6.25899500	-1.42388200	0.43381300
TS5-Zn(ClO ₄) ₂			
C	6.12742400	-0.64699600	0.12703300
C	5.30961700	-1.06835700	-0.93848300
C	4.10127600	-0.43974000	-1.19666900
C	3.67548700	0.63968700	-0.38240700
C	4.48598000	1.05598600	0.70619800
C	5.69483000	0.42578300	0.93924200
H	5.62664700	-1.90111500	-1.55981000
H	3.46587500	-0.78206500	-2.00843600
H	4.14314500	1.86425800	1.34267000

H	6.32099600	0.75127900	1.76637000
C	7.43829700	-1.32935100	0.41429100
H	7.41735400	-1.80914100	1.40150200
H	7.66832000	-2.09656900	-0.33016300
H	8.26205900	-0.60487400	0.42892100
C	2.46048800	1.28779100	-0.70275100
H	1.89937500	1.00078400	-1.59016300
O	2.00043700	2.33282700	-0.00386700
C	0.72085200	1.76577200	0.25692600
C	-0.39165100	2.23366500	-0.52773800
C	0.57644000	0.83276900	1.33866500
O	-0.06895200	3.20039000	-1.39139200
O	1.65456700	0.69624500	2.11967100
C	-1.14259100	3.70134500	-2.22397400
H	-0.67496200	4.45638400	-2.85506500
H	-1.56187900	2.89068400	-2.82383000
H	-1.92490000	4.14137500	-1.60188200
C	1.56369100	-0.30688100	3.16054500
H	1.37013800	-1.28739700	2.72027900
H	2.53563300	-0.28418600	3.65323900
H	0.76692200	-0.04969600	3.86128200
O	-1.55512900	1.79355400	-0.45225900
O	-0.47145900	0.20065600	1.58231500
Zn	-1.96392400	-0.17725200	0.17273600
O	-3.59033800	-0.18896500	1.57436400
O	-1.23944300	-2.27861600	0.07149600
Cl	-4.71805200	-0.29008000	0.51223100
Cl	-0.26747700	-2.10921900	-1.10216900
O	-5.48923500	-1.52779100	0.68966900
O	-3.88523600	-0.34110900	-0.79295900
O	-0.57184800	-0.67631300	-1.57430200
O	1.13874900	-2.17411600	-0.62333300
O	-5.56019100	0.91644800	0.54137400
O	-0.53240200	-3.08982300	-2.16369400
TS5-Zn(OTf) ₂			
C	6.28830800	-1.32262600	-1.19995900
C	5.74043000	-0.03510200	-1.05087300
C	4.62918400	0.17684500	-0.24814700
C	4.03192300	-0.91406800	0.43216600
C	4.56641400	-2.21884400	0.26955200
C	5.68324600	-2.40681300	-0.52469700
H	6.19041800	0.80229000	-1.57682900
H	4.19052400	1.16609800	-0.15880500

H	4.09194500	-3.05228500	0.77576800
H	6.10218500	-3.40367200	-0.63894000
C	7.48818700	-1.55629800	-2.07938100
H	7.20428400	-2.12318500	-2.97627800
H	7.94029300	-0.61571900	-2.40654100
H	8.25206200	-2.14495800	-1.55738800
C	2.94041600	-0.65129400	1.29520800
H	2.62458100	0.37159400	1.50047400
O	2.32957400	-1.63046000	1.98436700
C	1.04214700	-1.31895800	1.46230500
C	0.15886300	-0.53869100	2.29459700
C	0.63757200	-1.88540900	0.20857500
O	0.69010800	-0.20121000	3.46459000
O	1.48835800	-2.77470000	-0.31446000
C	-0.08794100	0.69865700	4.29118600
H	0.52107000	0.85229300	5.18139000
H	-0.24653600	1.63656000	3.75521600
H	-1.04618400	0.24155800	4.54638300
C	1.14192700	-3.30728900	-1.61509800
H	1.05697200	-2.49859300	-2.34425800
H	1.96412900	-3.97612100	-1.86880100
H	0.19882600	-3.85447600	-1.55834000
O	-0.99580100	-0.18811100	1.97592800
O	-0.43372300	-1.61364300	-0.37987600
Zn	-1.65164100	0.01491600	0.01606400
O	-3.02863300	-0.43993200	-1.61761600
O	-0.60213900	1.64929200	-0.54449500
O	-5.25794200	0.77603100	-1.39587800
O	-3.69878800	0.30368800	0.56221700
O	1.11985400	2.12089400	1.21044700
O	1.82081200	1.71820200	-1.15580800
S	0.77974900	2.18492600	-0.22686000
S	-4.24552400	-0.08056600	-0.79841600
C	-5.09090100	-1.72782300	-0.48861400
C	0.53855600	4.00702400	-0.60141800
F	1.69209500	4.66019500	-0.37928900
F	0.18501700	4.18310200	-1.87984500
F	-0.40850300	4.52862600	0.18926800
F	-4.22777800	-2.59015200	0.07616700
F	-5.52292900	-2.24796700	-1.64398800
F	-6.13416600	-1.56434900	0.33343100
TS7-Cu(ClO ₄) ₂			
C	5.99451600	-2.99131700	0.29913500

C	5.32719300	-2.43361300	1.40197900
C	4.10611200	-1.78052800	1.24331900
C	3.52083300	-1.68107600	-0.02945400
C	4.17331200	-2.24292900	-1.14073100
C	5.39471500	-2.88644700	-0.97094700
H	5.76547600	-2.51540500	2.39451900
H	3.59846200	-1.35840900	2.10892100
H	3.71611700	-2.17794800	-2.12399800
H	5.89364100	-3.32202200	-1.83490500
C	7.33114500	-3.67447800	0.46191700
H	8.14577600	-3.02724700	0.10688900
H	7.53447500	-3.91619200	1.51069400
H	7.37910600	-4.60296800	-0.11958200
C	2.23091100	-1.00091000	-0.15204200
H	1.66089000	-0.78612600	0.75394000
O	1.52065800	-1.23269200	-1.24167300
C	0.11455800	-1.07769300	-1.12422000
C	-0.59273300	-2.13196100	-0.50971500
C	-0.50481900	0.04889900	-1.70098100
O	0.16698200	-3.15722200	-0.09749700
O	0.30426700	0.90477800	-2.33678800
C	-0.50315000	-4.23525600	0.59613200
H	0.29603100	-4.92535400	0.87389000
H	-1.01912600	-3.85672000	1.48549500
H	-1.21904000	-4.72210400	-0.06850600
C	-0.31461600	2.09462600	-2.87626200
H	-0.81271300	2.65252400	-2.07849100
H	0.50941400	2.66483600	-3.30137500
H	-1.03938700	1.82801000	-3.64900300
O	-1.84322000	-2.18487400	-0.32629300
O	-1.74649600	0.29632300	-1.66527900
Cu	-2.97599600	-0.60593300	-0.45704900
O	-4.56896100	0.64662700	-0.77427300
O	-2.21967100	0.16490600	1.57359000
Cl	-5.61763900	-0.29747800	-0.11031700
Cl	-1.03489900	0.95428300	2.08196500
O	-6.21829800	0.32620200	1.07040100
O	-4.67820300	-1.47520700	0.29068400
O	0.15601500	0.02657200	2.18559600
O	-0.69603800	2.03560100	1.08930200
O	-6.60966500	-0.74114300	-1.09811000
O	-1.35116400	1.53267300	3.40448900
C	2.30485000	1.69460300	0.22308200
H	1.50109700	1.48443100	0.94295900

C	2.70241900	3.07744100	0.03887700
C	3.75662200	3.43459000	-0.82640500
C	1.99611100	4.06824900	0.75109300
C	4.09721300	4.77245800	-0.97364000
H	4.28918900	2.65687100	-1.36525600
C	2.34490900	5.40877800	0.59429400
H	1.17036900	3.77815400	1.39820700
C	3.39106100	5.75801100	-0.26433800
H	4.90794300	5.05777200	-1.63618000
H	1.80069100	6.17781000	1.13508200
H	3.66031800	6.80333700	-0.38658000
O	2.83770800	0.75550900	-0.40625900

TS7-Cu(OTf)₂

C	6.75476100	-2.63537300	0.71356100
C	5.98962700	-2.00311200	1.70486800
C	4.74298300	-1.45398800	1.40661300
C	4.23442200	-1.53059100	0.10242700
C	4.98804100	-2.16362300	-0.89905300
C	6.23219900	-2.70436700	-0.59094400
H	6.37170800	-1.94288300	2.72093400
H	4.16004000	-0.97245800	2.18849300
H	4.59180300	-2.23249900	-1.90715300
H	6.81033400	-3.19299200	-1.37209500
C	8.09662700	-3.24885800	1.03511600
H	8.85150600	-2.96859300	0.29105600
H	8.45692600	-2.93515100	2.01998400
H	8.03599900	-4.34524600	1.03651300
C	2.91570400	-0.94630700	-0.17862600
H	2.25854700	-0.71744100	0.66166300
O	2.31392200	-1.35755600	-1.28725400
C	0.89868500	-1.27629000	-1.30908500
C	0.18504100	-2.27489800	-0.60648900
C	0.28130200	-0.29173800	-2.10226000
O	0.94830500	-3.17966100	0.02081900
O	1.11190700	0.50943700	-2.79182400
C	0.26381900	-4.14651600	0.84793000
H	1.05933900	-4.75534300	1.27776300
H	-0.30260100	-3.63582100	1.62974200
H	-0.40748000	-4.75873800	0.24161400
C	0.49608400	1.52215400	-3.61660100
H	-0.12311000	2.18698700	-3.00993000
H	1.33197100	2.06432700	-4.05947700
H	-0.11711900	1.05942200	-4.39359700

O	-1.07147300	-2.37747000	-0.53355200
O	-0.96717100	-0.10785700	-2.20622600
O	-3.91670300	0.13170400	-1.71391000
O	-1.87106400	0.19290700	0.88481100
O	-4.06023900	-1.86530900	-0.41407500
O	0.42247500	-0.19512400	1.82283000
O	-0.23097400	2.07430000	1.03971900
O	-5.99946900	-1.30953400	-1.96903400
C	2.68252600	1.72069200	-0.16533400
H	1.76972000	1.52692800	0.41000800
C	3.00579800	3.10089200	-0.46017500
C	4.16929800	3.45568700	-1.17713200
C	2.11482600	4.09528300	-0.00403300
C	4.43465200	4.79512500	-1.43042900
H	4.84267800	2.67628900	-1.52045200
C	2.39176000	5.43680400	-0.26606600
H	1.21980600	3.80012400	0.53729300
C	3.54618000	5.78364300	-0.97495300
H	5.32758400	5.07975200	-1.97970000
H	1.71003700	6.20815300	0.07988900
H	3.75989400	6.83012200	-1.17718500
O	3.40496100	0.76870200	-0.54625600
S	-0.68193600	0.76552700	1.57209900
S	-4.92318900	-0.83416300	-1.11354400
C	-1.34741900	1.15998100	3.28126700
C	-5.76563900	0.12631000	0.26719100
F	-0.37285500	1.69635600	4.04093900
F	-2.35687200	2.03987600	3.20735100
F	-1.79090700	0.04769600	3.88728700
F	-4.87034300	0.62373200	1.11819300
F	-6.59601800	-0.69227800	0.92713100
F	-6.47485600	1.13084500	-0.26545200
Cu	-2.28663500	-0.92740000	-1.00574000
TS7-Hg(ClO ₄) ₂			
C	-7.02677600	-2.66644400	-0.26269500
C	-6.39710600	-2.22833100	-1.43638700
C	-5.09900700	-1.71700000	-1.40487600
C	-4.40224800	-1.63632200	-0.19332700
C	-5.01969300	-2.07162200	0.98932000
C	-6.31543100	-2.57751200	0.94760800
H	-6.92490900	-2.29157700	-2.38478500
H	-4.62684800	-1.38848100	-2.32859900
H	-4.47859000	-2.01824800	1.92863100

H	-6.78574300	-2.91439200	1.86873100
C	-8.42429000	-3.23840100	-0.29060800
H	-9.06335900	-2.76486400	0.46425200
H	-8.89603300	-3.10083500	-1.26868000
H	-8.41211100	-4.31450700	-0.07395100
C	-3.02732300	-1.08719000	-0.18080100
H	-2.52084700	-1.04403400	-1.14631800
O	-2.27711600	-1.48789500	0.84027200
C	-0.87270700	-1.28518700	0.74748600
C	-0.15101900	-2.09996600	-0.15951100
C	-0.29052200	-0.43055000	1.71926600
O	-0.93044800	-2.95420400	-0.87130400
O	-1.18119900	0.16402700	2.53855700
C	-0.24683200	-3.82826400	-1.79212100
H	-1.03595800	-4.42971700	-2.24489500
H	0.28521900	-3.25022200	-2.55183600
H	0.46323000	-4.46461900	-1.25887100
C	-0.63746100	1.06753700	3.52397700
H	-0.11313000	1.89211600	3.03529700
H	-1.50532400	1.43106500	4.07573600
H	0.04651100	0.53835600	4.19195600
O	1.08740400	-2.09101900	-0.36847600
O	0.93698300	-0.20709100	1.87681400
Hg	2.52195500	-0.32264800	0.17525500
O	4.66324500	-1.07348300	1.04905500
O	2.69699200	2.10497100	0.02172200
Cl	5.36269200	-1.34354300	-0.30469800
Cl	1.33885500	2.57245700	-0.50877400
O	6.56816200	-0.50719800	-0.43083900
O	4.30317000	-0.91273600	-1.34937000
O	0.63222900	1.30709200	-0.99297500
O	0.55252400	3.19072900	0.58938900
O	5.65047200	-2.78312900	-0.44576000
O	1.52652900	3.51375300	-1.63501000
C	-2.60644200	1.42439300	-0.60012200
H	-1.80265500	1.07051700	-1.25559800
C	-2.83323800	2.83853400	-0.49766000
C	-3.83043900	3.36799600	0.35512700
C	-2.03850700	3.69951400	-1.28493500
C	-4.02133800	4.74043800	0.41062200
H	-4.43071600	2.69367700	0.95759700
C	-2.24003100	5.07529800	-1.22245700
H	-1.26148600	3.28990900	-1.92316500
C	-3.22663900	5.59168100	-0.37707000

H	-4.78080400	5.15909800	1.06435500
H	-1.61961200	5.74007600	-1.81506100
H	-3.37817300	6.66655000	-0.32245300
O	-3.30382900	0.58478200	0.03433000
TS7-Hg(OTf) ₂			
C	7.52174600	-2.32408400	0.49601700
C	6.83413700	-1.63311600	1.50410400
C	5.53050300	-1.17979900	1.30104700
C	4.88529500	-1.41434600	0.08004500
C	5.56100300	-2.10614100	-0.93765100
C	6.86217800	-2.55079000	-0.72593700
H	7.32123000	-1.45117100	2.45882600
H	5.01192600	-0.65074900	2.09782200
H	5.05982800	-2.29736400	-1.88113600
H	7.37772800	-3.08802400	-1.51893800
C	8.92858900	-2.82884600	0.71211200
H	9.60295300	-2.47513500	-0.07733800
H	9.33153400	-2.49789000	1.67442500
H	8.95988900	-3.92586600	0.69505200
C	3.50562300	-0.92854400	-0.10695600
H	2.94577800	-0.65968900	0.78874100
O	2.81165000	-1.52530800	-1.06543400
C	1.39555800	-1.39964000	-1.01280500
C	0.72022000	-2.16343800	-0.02715000
C	0.77876300	-0.61913700	-2.01632300
O	1.54744300	-2.88154800	0.76492600
O	1.63731000	-0.08780900	-2.91677200
C	0.92752200	-3.65702400	1.80967300
H	1.75529400	-4.15312500	2.31754100
H	0.38580800	-3.00462200	2.49878400
H	0.24104300	-4.39288900	1.38424500
C	1.05114200	0.67637300	-3.98709900
H	0.50670400	1.53989000	-3.59607700
H	1.89689400	0.99831800	-4.59597300
H	0.36969400	0.05607700	-4.57472000
O	-0.52060700	-2.23494200	0.16092100
O	-0.45383800	-0.38561100	-2.13750800
Hg	-2.05861100	-0.60921000	-0.45325500
O	-4.03182200	0.04940700	-1.71085700
O	-1.68569600	1.09355900	1.13485400
O	-4.19395500	-1.65772200	0.01978900
O	0.71823700	0.58602600	1.58775700
O	-0.11562200	2.93958800	1.74397800

O	-5.76121800	-1.78732400	-1.96988400
C	3.06293000	1.65455000	-0.26875200
H	2.29200800	1.43481800	0.48252300
C	3.20949600	3.01174400	-0.73751500
C	4.19302000	3.36440000	-1.68978100
C	2.33788700	3.99011800	-0.21157600
C	4.30025900	4.68459500	-2.10385300
H	4.85294800	2.59777800	-2.08381000
C	2.45545700	5.31241400	-0.63848500
H	1.57489500	3.70944600	0.51191600
C	3.43186000	5.65688400	-1.57800100
H	5.05340300	4.96774200	-2.83355900
H	1.78569100	6.06894300	-0.24082100
H	3.52118600	6.68872800	-1.90805100
O	3.78744700	0.71807900	-0.69476500
S	-0.42041300	1.50367000	1.84159400
S	-4.96607100	-0.95441600	-1.07431000
C	-0.85910200	1.21278800	3.64325800
C	-6.19970300	0.10885800	-0.13962400
F	0.19573600	1.51158000	4.42115500
F	-1.89394000	1.97584000	4.01159100
F	-1.18021600	-0.07683200	3.84079900
F	-7.04739400	-0.66887600	0.54663400
F	-6.90083300	0.85991100	-0.99956300
F	-5.56165800	0.91675500	0.71937100

TS7-Mn(ClO₄)₂

C	6.75007600	-2.00492300	-0.03553600
C	6.13300300	-1.52980400	1.13119700
C	4.78916200	-1.15770400	1.12953200
C	4.03238700	-1.25628300	-0.04590700
C	4.63739900	-1.72956800	-1.22164800
C	5.97902400	-2.09674100	-1.20883200
H	6.70862400	-1.45404700	2.05028400
H	4.32702600	-0.79534000	2.04525700
H	4.05158900	-1.81236700	-2.13148800
H	6.44020000	-2.46444700	-2.12269700
C	8.20017800	-2.42575600	-0.03671800
H	8.74882100	-1.95932800	-0.86367400
H	8.69891400	-2.15312700	0.89854700
H	8.29295700	-3.51263800	-0.16049600
C	2.61746300	-0.85800400	-0.01880500
H	2.13673600	-0.77772400	0.95558600
O	1.86617300	-1.32372900	-1.00348100

C	0.45909600	-1.20737000	-0.85279300
C	-0.18822200	-2.05953300	0.07735400
C	-0.22533800	-0.35131800	-1.74331300
O	0.63930300	-2.86625400	0.76633100
O	0.54757700	0.25528500	-2.66518100
C	0.02839000	-3.70948200	1.76788500
H	0.85537900	-4.27499500	2.19794800
H	-0.46179700	-3.09637600	2.52751300
H	-0.69942500	-4.38047200	1.30642200
C	-0.13086500	1.10392900	-3.61282600
H	-0.64556700	1.92142000	-3.10183300
H	0.65942900	1.48832300	-4.25842100
H	-0.85510400	0.52705200	-4.19311100
O	-1.42714500	-2.10933100	0.28546100
O	-1.46581100	-0.12368100	-1.72444500
Mn	-2.80639100	-0.61144600	-0.18242500
O	-4.58535700	0.29007600	-1.17124400
O	-2.51487600	0.77071800	1.40302200
Cl	-5.55995800	-0.86840200	-0.85463400
Cl	-1.49161800	0.84608100	2.56175500
O	-6.66267500	-0.40533400	-0.00074800
O	-4.63018200	-1.83315500	-0.07237900
O	-0.22595800	0.17555400	2.09771800
O	-1.22951000	2.28634400	2.81638500
O	-6.02636400	-1.50446900	-2.09738800
O	-2.05086200	0.15917900	3.73942400
C	1.89777900	1.67080100	0.24952100
H	1.19347100	1.24819600	0.97898800
C	1.83377000	3.08823800	-0.01825600
C	2.70773400	3.71018100	-0.93850600
C	0.86323300	3.84636200	0.67184300
C	2.60743900	5.07689300	-1.15875800
H	3.44675100	3.11058300	-1.46088600
C	0.77154900	5.21801800	0.43949800
H	0.19142100	3.36185900	1.37717000
C	1.63970600	5.82886100	-0.47049700
H	3.27440600	5.56608200	-1.86282200
H	0.02479800	5.80569500	0.96478900
H	1.56617000	6.89847400	-0.64949500
O	2.72368500	0.91354400	-0.32155200
TS7-Mn(OTf) ₂			
C	7.20481800	-2.36149500	0.48708200
C	6.51609800	-1.70411200	1.51708800

C	5.21218900	-1.24676900	1.32877400
C	4.56768600	-1.44250100	0.09997600
C	5.24508500	-2.09911100	-0.94007600
C	6.54656100	-2.54876000	-0.74226300
H	7.00326800	-1.55193800	2.47693400
H	4.69274900	-0.74333000	2.14129000
H	4.74507400	-2.25917400	-1.88991300
H	7.06354400	-3.05846900	-1.55222600
C	8.61049700	-2.87467300	0.68928800
H	9.27633700	-2.53723600	-0.11408200
H	9.02950700	-2.53586400	1.64194200
H	8.63168300	-3.97223800	0.68600600
C	3.18972500	-0.95576400	-0.06881000
H	2.62254700	-0.72270700	0.83178900
O	2.50345700	-1.49021000	-1.06573500
C	1.09037600	-1.35252900	-1.02144500
C	0.37892600	-2.14170700	-0.08361900
C	0.47083500	-0.54116100	-1.99486600
O	1.15850400	-2.90633200	0.70678900
O	1.30820800	0.03125100	-2.88384800
C	0.47960900	-3.70310700	1.69987300
H	1.27366200	-4.24693200	2.21240200
H	-0.06246700	-3.05917600	2.39642000
H	-0.21655900	-4.39593700	1.22179700
C	0.69693600	0.82739900	-3.91849200
H	0.14402800	1.66554600	-3.48688500
H	1.53023800	1.18523400	-4.52414500
H	0.01806200	0.21796700	-4.52000800
O	-0.86949200	-2.17604200	0.05031700
O	-0.76830400	-0.32027100	-2.07713700
O	-3.99537500	-0.05913700	-1.85833800
O	-2.05446500	0.68589300	0.89502200
O	-4.07423100	-1.97825400	-0.40812300
O	0.31709900	0.52813800	1.66773500
O	-0.79947300	2.75894600	1.49490600
O	-5.68622300	-1.88663700	-2.37087800
C	2.67919900	1.64155700	-0.17677700
H	1.86422300	1.36956800	0.50857500
C	2.79799100	3.01853600	-0.59751500
C	3.84400800	3.44494000	-1.44705400
C	1.83315700	3.93796800	-0.13239500
C	3.92091100	4.77985100	-1.81905600
H	4.57553000	2.72263300	-1.79585800
C	1.92042000	5.27570400	-0.51697500

H	1.02139900	3.60120000	0.50939100
C	2.95932300	5.69353900	-1.35399600
H	4.72202700	5.11942100	-2.46932900
H	1.17836800	5.98677900	-0.16653600
H	3.02499600	6.73715300	-1.65099700
O	3.47718100	0.75129900	-0.56579400
S	-0.94221500	1.30963900	1.69816500
S	-4.90428600	-1.16441900	-1.37615600
C	-1.58184700	1.10699900	3.45028500
C	-6.15603300	-0.29114800	-0.28175800
F	-0.68399400	1.60283200	4.31889500
F	-2.73982200	1.75682900	3.61054100
F	-1.77120700	-0.19254300	3.72947700
F	-5.52996900	0.40622000	0.67622500
F	-6.96447900	-1.19043500	0.29565600
F	-6.89716300	0.54991500	-1.01582700
Mn	-2.24033700	-0.74129900	-0.63545500

TS7-Zn(ClO₄)₂

C	6.33995100	-2.88392800	0.13399700
C	5.78873200	-2.30443700	1.28615400
C	4.54023300	-1.68323700	1.24877200
C	3.81430900	-1.63302200	0.05183700
C	4.35303700	-2.20956900	-1.10891200
C	5.60074700	-2.82370400	-1.06134000
H	6.33966500	-2.34256400	2.22260100
H	4.12851200	-1.24298000	2.15441100
H	3.78835500	-2.18084700	-2.03527300
H	6.01006800	-3.26987900	-1.96494900
C	7.68269000	-3.57404500	0.17043600
H	8.33519900	-3.21711700	-0.63536600
H	8.19628900	-3.40606200	1.12229600
H	7.57039900	-4.65806700	0.03824900
C	2.49526300	-0.97319200	0.03852000
H	2.00209100	-0.82932100	0.99997300
O	1.69815300	-1.29807100	-0.97257000
C	0.30473500	-1.10086600	-0.78649300
C	-0.38579900	-2.03066300	0.02796600
C	-0.32995900	-0.06672600	-1.50655200
O	0.39508400	-2.98173400	0.57623300
O	0.48255300	0.67059400	-2.29180300
C	-0.26209200	-3.94139500	1.43128200
H	0.53246700	-4.61238600	1.75868000
H	-0.72279300	-3.43804600	2.28452500

H	-1.02501400	-4.48889300	0.87329600
C	-0.15405100	1.69812000	-3.08133000
H	-0.65249000	2.42559000	-2.43639700
H	0.65895800	2.16395300	-3.63925600
H	-0.88430000	1.25613700	-3.76329300
O	-1.62087700	-2.03013000	0.26900700
O	-1.55855400	0.20912500	-1.46163500
Zn	-2.89052500	-0.47259300	-0.06753200
O	-4.57592600	0.01642400	-1.31118600
O	-2.74293000	0.75737400	1.58819900
Cl	-5.57413400	-0.96760100	-0.64554800
Cl	-1.50048100	1.54849800	2.05099600
O	-6.69872000	-0.23929800	-0.04122000
O	-4.67387400	-1.59929200	0.44254400
O	-0.31405900	0.62716100	1.99262900
O	-1.28585900	2.68368700	1.10571200
O	-6.00977300	-1.98809600	-1.61329700
O	-1.75739800	2.01311800	3.42336900
C	2.20234600	1.63744100	0.15171200
H	1.28632200	1.39547600	0.70644500
C	2.51857600	3.02272400	-0.09991700
C	3.70848600	3.39849600	-0.76462200
C	1.60758700	4.00481100	0.34541600
C	3.97877500	4.74351500	-0.97386900
H	4.39748900	2.63018100	-1.10124300
C	1.89025700	5.35236300	0.12697500
H	0.68631200	3.70390900	0.83789600
C	3.07037700	5.71872400	-0.52756200
H	4.89087700	5.04365500	-1.48152400
H	1.19197300	6.11235400	0.46439200
H	3.28878800	6.77029100	-0.69498900
O	2.95966200	0.70647600	-0.22997800

TS7-Zn(OTf)₂

C	7.25547300	-2.28855600	0.43142400
C	6.57119500	-1.65575800	1.47969800
C	5.25922800	-1.21299600	1.31444900
C	4.60206600	-1.39869600	0.09074000
C	5.27514300	-2.03022700	-0.96762100
C	6.58459500	-2.46577200	-0.79258300
H	7.06839100	-1.51167800	2.43563400
H	4.74350400	-0.72868600	2.14083600
H	4.76550500	-2.18214600	-1.91365700
H	7.09807500	-2.95624400	-1.61651300

C	8.66993800	-2.78648600	0.60874900
H	9.32144100	-2.42848300	-0.19745700
H	9.09623300	-2.45669600	1.56131100
H	8.70495000	-3.88351900	0.58850100
C	3.21613300	-0.92853000	-0.05386100
H	2.65614800	-0.71786700	0.85657200
O	2.52705300	-1.45370700	-1.05297800
C	1.11437300	-1.31442500	-1.00490600
C	0.40259700	-2.10104100	-0.06456800
C	0.49595800	-0.50778600	-1.98299900
O	1.18022500	-2.87395200	0.71822900
O	1.33102400	0.04763500	-2.88283000
C	0.50172500	-3.66166000	1.71943800
H	1.29531100	-4.21020800	2.22763800
H	-0.02959300	-3.01017300	2.41711400
H	-0.20372000	-4.35009000	1.24883300
C	0.72083500	0.84683400	-3.91646900
H	0.18817500	1.69752000	-3.48407400
H	1.55333400	1.18524600	-4.53424800
H	0.02394100	0.24520900	-4.50482600
O	-0.84510200	-2.12924900	0.07769400
O	-0.74232900	-0.27625000	-2.06499600
O	-3.82838300	0.07785400	-1.81118100
O	-2.04456700	0.70699300	0.85229400
O	-3.88561500	-1.93521400	-0.50387200
O	0.29818400	0.49866700	1.70427700
O	-0.82945300	2.73034700	1.65564800
O	-5.45735900	-1.75375300	-2.49425500
C	2.66421600	1.66432500	-0.10465600
H	1.86575000	1.36695000	0.58974600
C	2.74916400	3.04993700	-0.50486500
C	3.76845900	3.50926700	-1.36963300
C	1.77805800	3.94389400	-0.00447300
C	3.81260100	4.85102500	-1.72179900
H	4.50509100	2.80629500	-1.74611600
C	1.83204200	5.28879900	-0.36953500
H	0.98597300	3.58297100	0.64865500
C	2.84460900	5.73917300	-1.22179500
H	4.59288800	5.21554300	-2.38379700
H	1.08430400	5.97987700	0.00774000
H	2.88427900	6.78824700	-1.50375700
O	3.47078400	0.79527500	-0.52276500
S	-0.96720200	1.26976300	1.74422100
S	-4.71967800	-1.07837300	-1.43465900

C	-1.67457300	0.93422200	3.44920400
C	-6.02449500	-0.32486800	-0.31477100
F	-0.81441800	1.36344300	4.38821200
F	-2.84062900	1.56828300	3.61141000
F	-1.86943500	-0.38323600	3.62091300
F	-5.44859300	0.30655700	0.71647000
F	-6.82850300	-1.28623300	0.16032000
F	-6.76337400	0.55506300	-1.00444200
Zn	-2.13456900	-0.69968000	-0.62747400