

# Supporting Information

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### Teaching cyclopentadienyl how to leave: a case study of $[\text{CpIr}(\text{COD})\text{Br}]^+$ complex

Aleksandr A. Chamkin

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## Computational Methods

The computations for **the non-anionic systems** were performed as follows:

1. Geometry optimizations were carried out without symmetry constraints using M06-L density functional<sup>1</sup> and tight convergence criteria as implemented in the Gaussian 09 E.01 package.<sup>2</sup> The def2-TZVPP<sup>3</sup> all-electron triple-zeta basis set of the Karlsruhe group was used together with the corresponding fitting basis set<sup>4</sup> and effective core potentials. The D3 version of Grimme's dispersion correction with the original D3 damping function was applied.<sup>5</sup> A pruned (99, 590) integration grid (UltraFine) was used. Frequency calculations were performed to confirm the nature of the stationary points to yield one imaginary frequency for the transition states and none for the minima. Gas-phase thermochemical parameters at 298.15 K (E, H, and  $G_{\text{uncorr.}}$ ) were obtained from the frequency calculations.
2. The Gibbs free energies ( $G_{\text{uncorr.}}$ ) were corrected using the quasi-harmonic approximation<sup>6</sup> and to a solution-phase standard state as implemented in the GoodVibes 3.0.1 program<sup>7</sup> (corrected values were reported as G).
3. The solvent corrections were considered using the SMD solvation model<sup>8</sup> and acetone as a solvent. The corresponding calculations were performed on the gas-phase geometries, and the solvation energies were evaluated as the difference between the SMD ( $E_{\text{solv}}$ ) and gas-phase electronic energies; then, the obtained earlier thermochemical parameters were corrected using the solvation energies ( $H_{\text{solv}} = H + E_{\text{solv}} - E$ ;  $G_{\text{solv}} = G + E_{\text{solv}} - E$ ).<sup>9</sup>
4. The gas-phase domain-based local pair natural orbital coupled-cluster theory with single-, double-, and perturbative triple excitations (DLPNO-CCSD(T))<sup>10</sup> electronic energies ( $E_{\text{CC}}$ ) were obtained using "TightPNO" default convergence thresholds, and tight SCF convergence criteria as implemented in the ORCA 4.2.1 code.<sup>11</sup> The def2-TZVPP orbital basis set was used together with the corresponding auxiliary basis set for correlated methods (def2-TZVPP/C<sup>12</sup>). Additionally, the iterative full LMP2 guess was requested.
5. Finally, the solvent-corrected DLPNO-CCSD(T) Gibbs free energies were evaluated as  $G_{\text{CC}} = E_{\text{CC}} + G_{\text{solv}} - E$ . These values were used for the analysis and production of energy diagrams.

The corresponding computations for **the anionic systems** and for all **the systems involved in a reaction step together with an anionic system** (i.e., when the corresponding energies are subtracted; such cases are denoted with the quotation mark (') after an identifier) were performed using the abovementioned methods with the following differences:

1. Geometry optimizations were performed using the ORCA 4.2.1 code. The minimally augmented def2-TZVPP basis set (ma-def2-TZVPP<sup>13</sup>) was used. The other options were chosen similarly to the case of the non-anionic systems: M06-L density functional, tight geometry and SCF convergence criteria, Lebedev

590 points grid, D3 version of Grimme's dispersion correction, and SMD solvation model for acetone as a solvent. Additionally, the RI-J approximation with an automatically generated auxiliary basis set<sup>14</sup> was invoked.

2. The obtained gas-phase Gibbs free energies were not corrected manually using the quasi-harmonic approximation because ORCA performs this correction by default. The resulted values were corrected to a solution-phase standard state by adding  $+0.00301640938 \text{ Eh}$  (which is equal to  $R \times T \times \ln(24.46)$ , where 24.46 stands for the molar volume at 1 atm and 298.15 K). The corrected values were reported as G.

3. The DLPNO-CCSD(T) computations were performed using the ma-def2-TZVPP basis set and an automatically generated auxiliary basis set for correlated methods.

With the mean absolute deviations for the bond distances and angles of 0.021 Å and 1.73 ° (Table S2), respectively, the used approach provides the structures of the quality comparable to those from the classical hybrid<sup>15</sup> or recently developed functionals, such as r<sup>2</sup>SCAN-3c.<sup>16</sup>

The nuclei movements corresponding to the single imaginary frequencies were visualized and analyzed for all found transition states. In difficult cases (TS\_1\_IM8, TS\_IM1\_IM2, TS\_3\_IM13, TS\_IM9\_IM10), the reaction path was traced from the transition state to the product and back to the reactant by using the Intrinsic Reaction Coordinate method.<sup>17</sup> In the case of a barrierless step, the corresponding transition state cannot be localized (TS\_IM2\_IM3, TS\_IM7\_2, TS\_IM6\_IM7', TS\_IM13\_IM14, TS\_IM14\_IM15, TS\_IM15\_4), and the relaxed potential energy surface scan was performed to ensure that the surface was smooth (the single key geometrical parameter was varied with a step of 0.04 Å).

Supplementary Data for Discussion

Table S1. Changes in solvent-corrected DLPNO-CCSD(T) Gibbs free energies ( $\Delta G_{CC}$ ) given for reactions of complexes bearing different halogens, in kcal mol<sup>-1</sup>.

<b>Reaction step</b>	<b>X = Cl</b>	<b>X = Br</b>	<b>X = I</b>
<b>1:X + PO → IM1:X</b>	-5.25	-6.12	-4.21
<b>TS( 1:X + PO → IM1:X )</b>	17.23	16.11	17.25
<b>IM1:X → IM2:X</b>	3.83	8.83	7.35
<b>TS( IM1:X → IM2:X )</b>	18.51	21.79	14.87
<b>1:X → IM8:X</b>	18.76	23.16	16.82
<b>TS( 1:X → IM8:X )</b>	20.59	26.99	20.29
<b>IM6:X' → IM7' + X'</b>	7.14	12.41	7.16

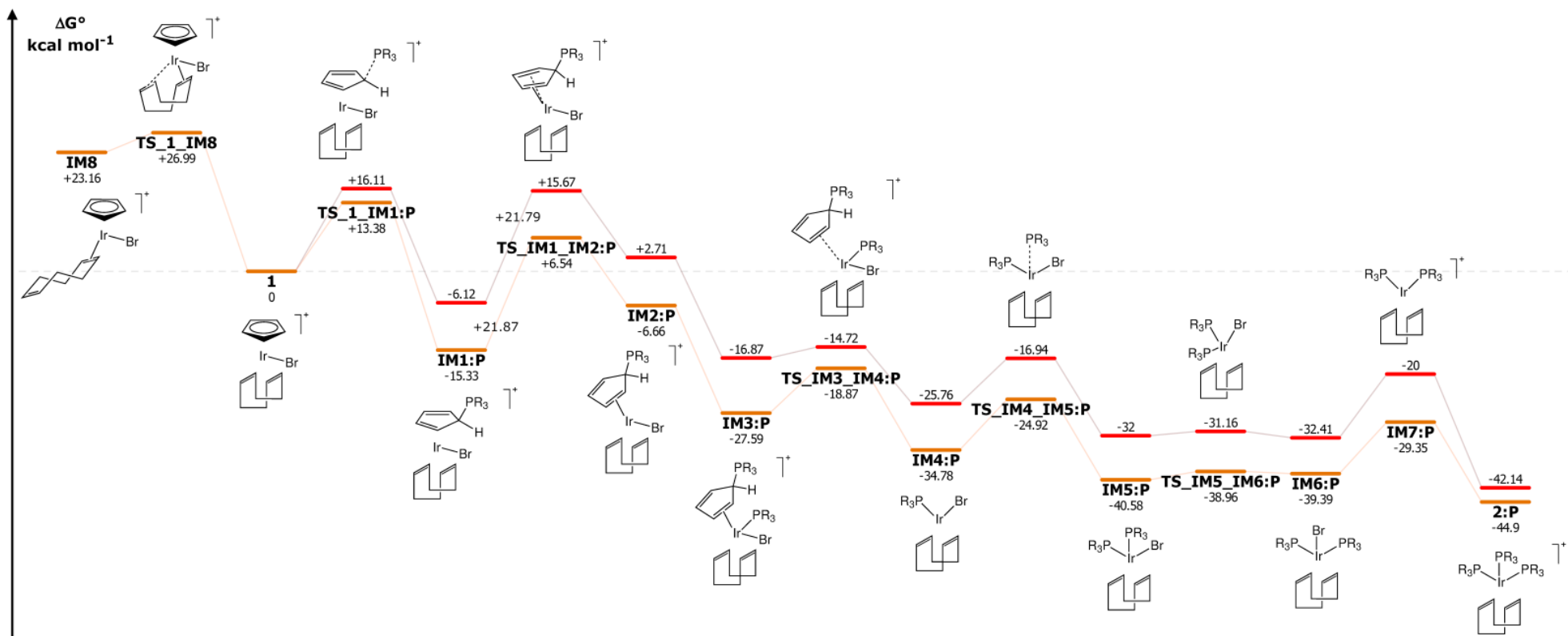


Figure S1. Energy diagram for reaction of **1** with phosphine ( $\text{PR}_3 = \text{PMe}_3$ ) leading to **2:P** (shown in orange). Corresponding levels for reaction with phosphite ( $\text{PR}_3 = \text{P(OMe)}_3$ ) are given in red for comparison.

*Comparison of Optimized and XRD Geometries*

Table S2. Selected bond lengths (d, Å) and angles ( $\omega$ , °) obtained from XRD and optimized structures. CCDC deposition numbers and references are provided for each compound. Cp and C=C stand for the centroids of Cp ring and carbon–carbon double bond, respectively. The mean absolute deviations for d and  $\omega$  are equal to 0.021 Å and 1.73 °, respectively.

Parameter	XRD value(s)	Calculated value(s)	Deviation(s)
		<b>1</b> (CCDC 871722; <sup>18</sup> )	
d(Ir–Br)	2.539	2.584	0.045
d(Ir–Cp)	1.857	1.852	–0.005
d(Ir–C=C)	2.139; 2.149	2.130; 2.157	–0.009; 0.008
$\omega$ (C=C–Ir–C=C)	86.03	82.26	–3.77
$\omega$ (Cp–Ir–Br)	112.88	112.14	–0.74
		<b>1:I</b> (CCDC 871723; <sup>18</sup> )	
d(Ir–I)	2.720	2.800	0.080
d(Ir–Cp)	2.225	2.207	–0.018
d(Ir–C=C)	2.151; 2.120	2.147; 2.120	–0.004; 0
$\omega$ (C=C–Ir–C=C)	83.42	82.42	–1
$\omega$ (Cp–Ir–I)	114.80	110.71	–4.09
		<b>2</b> (CCDC 1536381; <sup>19</sup> )	
d(Ir–P)	2.318; 2.248; 2.269	2.332; 2.261; 2.300	0.014; 0.013; 0.031
d(Ir–C=C)	2.075; 2.192	2.078; 2.198;	0.003; 0.006
$\omega$ (C=C–Ir–C=C)	82.08	81.95	–0.13
		<b>4</b> (CCDC 1845090; <sup>20</sup> )	
d(Ir–P)	2.233; 2.238	2.263; 2.272	0.030; 0.034
d(Ir–Br)	2.529	2.583	0.054
d(Ir–Cp)	1.876	1.869	–0.007
$\omega$ (Cp–Ir–Br)	119.30	121.41	2.11
$\omega$ (P–Ir–P)	93.63	93.35	–0.28

*Thermochemical Data*

Table S3. Electronic energies (E), enthalpies (H), and Gibbs free energies (G) obtained without using (no subscript) and using SMD solvation model (“solv” subscript), gas-phase DLPNO-CCSD(T) electronic energies (E<sub>CC</sub>), and solvent-corrected DLPNO-CCSD(T) Gibbs free energies (G<sub>CC</sub>), in Hartree.

Compound	E	H	G	E <sub>solv</sub>	H <sub>solv</sub>	G <sub>solv</sub>	E <sub>CC</sub>	G <sub>CC</sub>
<b>PO</b>	-686.892593	-686.753083	-686.796436	-686.898686	-686.759176	-686.802529	-685.849233	-685.759169
<b>1</b>	-3184.050377	-3183.764932	-3183.817888	-3184.140672	-3183.855227	-3183.908183	-3181.271342	-3181.129148
<b>TS_1_IM1</b>	-3870.953513	-3870.527556	-3870.604928	-3871.033670	-3870.607713	-3870.685085	-3867.131078	-3866.862650
<b>IM1</b>	-3870.976034	-3870.548333	-3870.624435	-3871.062493	-3870.634792	-3870.710894	-3867.163211	-3866.898071
<b>TS_IM1_IM2</b>	-3870.947170	-3870.521069	-3870.596704	-3871.030331	-3870.604230	-3870.679865	-3867.130657	-3866.863352
<b>IM2</b>	-3870.967050	-3870.539815	-3870.616755	-3871.052675	-3870.625440	-3870.702380	-3867.148669	-3866.883999
<b>IM3</b>	-4557.917223	-4557.347139	-4557.444730	-4557.993770	-4557.423686	-4557.521277	-4553.070310	-4552.674364
<b>TS_IM3_IM4</b>	-4557.913857	-4557.345285	-4557.443066	-4557.993351	-4557.424779	-4557.522560	-4553.062245	-4552.670948
<b>diene</b>	-880.241955	-880.011578	-880.064553	-880.319425	-880.089048	-880.142023	-878.796285	-878.696353
<b>IM4</b>	-3677.660125	-3677.322730	-3677.390950	-3677.675686	-3677.338291	-3677.406511	-3674.245798	-3673.992184
<b>TS_IM4_IM5</b>	-4364.570573	-4364.092775	-4364.182059	-4364.586714	-4364.108916	-4364.198200	-4360.109676	-4359.737303
<b>IM5</b>	-4364.583877	-4364.104775	-4364.194192	-4364.598528	-4364.119426	-4364.208843	-4360.136330	-4359.761296
<b>TS_IM5_IM6</b>	-4364.583281	-4364.105036	-4364.192773	-4364.597953	-4364.119708	-4364.207445	-4360.135796	-4359.759960
<b>IM6</b>	-4364.589668	-4364.109938	-4364.198639	-4364.605218	-4364.125488	-4364.214189	-4360.137433	-4359.761954
<b>IM6'</b>	-4364.594876	-4364.115274	-4364.203677	-4364.611050	-4364.131447	-4364.219850	-4360.142613	-4359.767588
<b>Br'</b>	-2574.137668	-2574.132475	-2574.148012	-2574.222655	-2574.217462	-2574.232999	-2572.783445	-2572.878776
<b>IM7</b>	-1790.294347	-1789.817111	-1789.902770	-1790.365612	-1789.888376	-1789.974035	-1787.190636	-1786.870324
<b>IM7'</b>	-1790.297921	-1789.820918	-1789.908029	-1790.363231	-1789.886229	-1789.973339	-1787.193619	-1786.869038
<b>2</b>	-2477.249511	-2476.629843	-2476.736108	-2477.310826	-2476.691158	-2476.797423	-2473.116858	-2472.664770
<b>TS_1_IM8</b>	-3184.012515	-3183.729431	-3183.784176	-3184.108917	-3183.825833	-3183.880578	-3181.218066	-3181.086129
<b>IM8</b>	-3184.022140	-3183.737497	-3183.793595	-3184.114117	-3183.829474	-3183.885572	-3181.228805	-3181.092237
<b>IM1'</b>	-3870.980065	-3870.552624	-3870.628631	-3871.064479	-3870.637038	-3870.713045	-3867.165628	-3866.898609
<b>IMs'</b>	-1296.554205	-1296.130180	-1296.204362	-1296.787462	-1296.363438	-1296.437620	-1294.080944	-1293.964359
<b>3</b>	-3380.717548	-3380.284519	-3380.352685	-3380.801319	-3380.368290	-3380.436456	-3377.523532	-3377.242440
<b>TS_3_IM9</b>	-4067.599771	-4067.027198	-4067.118697	-4067.680233	-4067.107660	-4067.199159	-4063.368087	-4062.967475
<b>IM9</b>	-4067.608848	-4067.034313	-4067.124595	-4067.694370	-4067.119835	-4067.210117	-4063.384417	-4062.985686
<b>TS_IM9_IM10</b>	-4067.579841	-4067.006593	-4067.096000	-4067.665949	-4067.092701	-4067.182108	-4063.351381	-4062.953648
<b>IM10</b>	-4067.597476	-4067.022660	-4067.115951	-4067.691369	-4067.116553	-4067.209844	-4063.359365	-4062.971733
<b>IM11</b>	-2990.686508	-2990.491655	-2990.536240	-2990.711780	-2990.516927	-2990.561512	-2988.308048	-2988.183052

Compound	E	H	G	E <sub>solv</sub>	H <sub>solv</sub>	G <sub>solv</sub>	E <sub>CC</sub>	G <sub>CC</sub>
<b>IM12</b>	-1076.888988	-1076.511141	-1076.580273	-1076.961553	-1076.583706	-1076.652838	-1075.028237	-1074.792087
<b>TS_3_IM13</b>	-3380.687102	-3380.256571	-3380.327069	-3380.777034	-3380.346503	-3380.417001	-3377.478339	-3377.208238
<b>IM13</b>	-3380.695954	-3380.263965	-3380.336657	-3380.782678	-3380.350689	-3380.423381	-3377.488113	-3377.215540
<b>IM14</b>	-4067.664730	-4067.089660	-4067.182458	-4067.741938	-4067.166868	-4067.259666	-4063.429186	-4063.024122
<b>COD</b>	-312.098811	-311.909388	-311.945921	-312.107963	-311.918540	-311.955073	-311.447878	-311.304140
<b>IM15</b>	-3755.532408	-3755.149168	-3755.227236	-3755.610499	-3755.227259	-3755.305327	-3751.933096	-3751.706015
<b>4</b>	-4442.510873	-4441.984718	-4442.082183	-4442.579736	-4442.053581	-4442.151046	-4437.881997	-4437.522170
<b>P</b>	-461.134409	-461.013864	-461.047678	-461.137980	-461.017435	-461.051249	-460.427146	-460.343986
<b>TS_1_IM1:P</b>	-3645.196025	-3644.789200	-3644.858441	-3645.279014	-3644.872189	-3644.941430	-3641.706408	-3641.451813
<b>IM1:P</b>	-3645.223419	-3644.815303	-3644.883202	-3645.316927	-3644.908811	-3644.976710	-3641.744270	-3641.497561
<b>TS_IM1_IM2:P</b>	-3645.191285	-3644.784928	-3644.852979	-3645.284893	-3644.878536	-3644.946587	-3641.707407	-3641.462709
<b>IM2:P</b>	-3645.211152	-3644.803751	-3644.872859	-3645.307514	-3644.900113	-3644.969221	-3641.725677	-3641.483746
<b>IM3:P</b>	-4106.399766	-4105.868684	-4105.950993	-4106.487859	-4105.956777	-4106.039086	-4102.221776	-4101.861096
<b>TS_IM3_IM4:P</b>	-4106.385788	-4105.856244	-4105.939162	-4106.481904	-4105.952360	-4106.035278	-4102.197698	-4101.847188
<b>diene:P</b>	-654.486002	-654.275397	-654.320060	-654.573790	-654.363185	-654.407848	-653.373703	-653.295549
<b>IM4:P</b>	-3451.894604	-3451.576627	-3451.636936	-3451.912018	-3451.594041	-3451.654350	-3448.817252	-3448.576998
<b>TS_IM4_IM5:P</b>	-3913.038174	-3912.598952	-3912.673952	-3913.055738	-3912.616516	-3912.691516	-3909.251921	-3908.905263
<b>IM5:P</b>	-3913.054411	-3912.613574	-3912.687299	-3913.071035	-3912.630198	-3912.703923	-3909.280715	-3908.930227
<b>TS_IM5_IM6:P</b>	-3913.052480	-3912.612495	-3912.684994	-3913.068219	-3912.628234	-3912.700733	-3909.279399	-3908.927652
<b>IM6:P</b>	-3913.055246	-3912.613866	-3912.687608	-3913.073517	-3912.632137	-3912.705879	-3909.277697	-3908.928330
<b>IM6:P'</b>	-3913.059905	-3912.618858	-3912.692972	-3913.077020	-3912.635972	-3912.710086	-3909.280365	-3908.930546
<b>IM7:P</b>	-1338.766901	-1338.327476	-1338.397124	-1338.843552	-1338.404127	-1338.473775	-1336.334793	-1336.041667
<b>IM7:P'</b>	-1338.770715	-1338.331284	-1338.400935	-1338.840215	-1338.400784	-1338.470435	-1336.336045	-1336.035765
<b>2:P</b>	-1799.942927	-1799.380052	-1799.462426	-1800.014555	-1799.451680	-1799.534054	-1796.819309	-1796.410436
<b>1:Cl</b>	-1070.191223	-1069.905643	-1069.957744	-1070.285167	-1069.999587	-1070.051688	-1068.284401	-1068.144866
<b>TS_1_IM1:Cl</b>	-1757.095516	-1756.669415	-1756.745857	-1757.177556	-1756.751455	-1756.827897	-1754.144202	-1753.876583
<b>IM1:Cl</b>	-1757.118728	-1756.690969	-1756.766158	-1757.207023	-1756.779264	-1756.854453	-1754.176674	-1753.912399
<b>TS_IM1_IM2:Cl</b>	-1757.089967	-1756.663634	-1756.738028	-1757.180423	-1756.754090	-1756.828484	-1754.144385	-1753.882902
<b>IM2:Cl</b>	-1757.112243	-1756.684818	-1756.760752	-1757.204344	-1756.776919	-1756.852853	-1754.165688	-1753.906298
<b>TS_1_IM8:Cl</b>	-1070.155108	-1069.871957	-1069.926577	-1070.262685	-1069.979534	-1070.034154	-1068.233002	-1068.112048
<b>IM8:Cl</b>	-1070.165108	-1069.880308	-1069.935400	-1070.265295	-1069.980495	-1070.035587	-1068.244489	-1068.114968
<b>IM6:Cl'</b>	-2250.735465	-2250.255747	-2250.343222	-2250.753933	-2250.274214	-2250.361689	-2247.156407	-2246.782630
<b>Cl'</b>	-460.270137	-460.264944	-460.279330	-460.373898	-460.368705	-460.383091	-459.789261	-459.902215



<b>Compound</b>	<b>E</b>	<b>H</b>	<b>G</b>	<b>E<sub>solv</sub></b>	<b>H<sub>solv</sub></b>	<b>G<sub>solv</sub></b>	<b>E<sub>CC</sub></b>	<b>G<sub>CC</sub></b>
<b>I:I</b>	-907.868297	-907.583049	-907.636786	-907.961426	-907.676178	-907.729915	-905.708722	-905.570340
<b>TS_1_IM1:I</b>	-1594.769568	-1594.343588	-1594.421443	-1594.852505	-1594.426525	-1594.504380	-1591.567202	-1591.302014
<b>IM1:I</b>	-1594.791025	-1594.363602	-1594.440758	-1594.879079	-1594.451656	-1594.528812	-1591.598433	-1591.336220
<b>TS_IM1_IM2:I</b>	-1594.762878	-1594.336954	-1594.413364	-1594.859252	-1594.433328	-1594.509738	-1591.565670	-1591.312530
<b>IM2:I</b>	-1594.779667	-1594.352698	-1594.430574	-1594.873467	-1594.446498	-1594.524374	-1591.579798	-1591.324505
<b>TS_1_IM8:I</b>	-907.830066	-907.546983	-907.602304	-907.941985	-907.658902	-907.714223	-905.653848	-905.538005
<b>IM8:I</b>	-907.839207	-907.554857	-907.611840	-907.946440	-907.662090	-907.719073	-905.663676	-905.543542
<b>IM6:I'</b>	-2088.411441	-2087.932088	-2088.021334	-2088.429261	-2087.949909	-2088.039155	-2084.576775	-2084.204490
<b>I'</b>	-297.964611	-297.959417	-297.975610	-298.052069	-298.046876	-298.063068	-297.225576	-297.324034
<b>bipy</b>	-495.496995	-495.329389	-495.369744	-495.509605	-495.341999	-495.382354	-494.489891	-494.375250
<b>TS_1_IM1:bipy</b>	-3679.557409	-3679.103314	-3679.176108	-3679.641999	-3679.187904	-3679.260698	-3675.776655	-3675.479944
<b>IM1:bipy</b>	-3679.562014	-3679.106149	-3679.178476	-3679.649831	-3679.193966	-3679.266293	-3675.788115	-3675.492394
<b>TS_IM1_IM2:bipy</b>	-3679.518726	-3679.064304	-3679.135876	-3679.607674	-3679.153252	-3679.224824	-3675.741507	-3675.447605
<b>IM2:bipy</b>	-3679.542711	-3679.087266	-3679.160451	-3679.634687	-3679.179242	-3679.252427	-3675.763064	-3675.472780

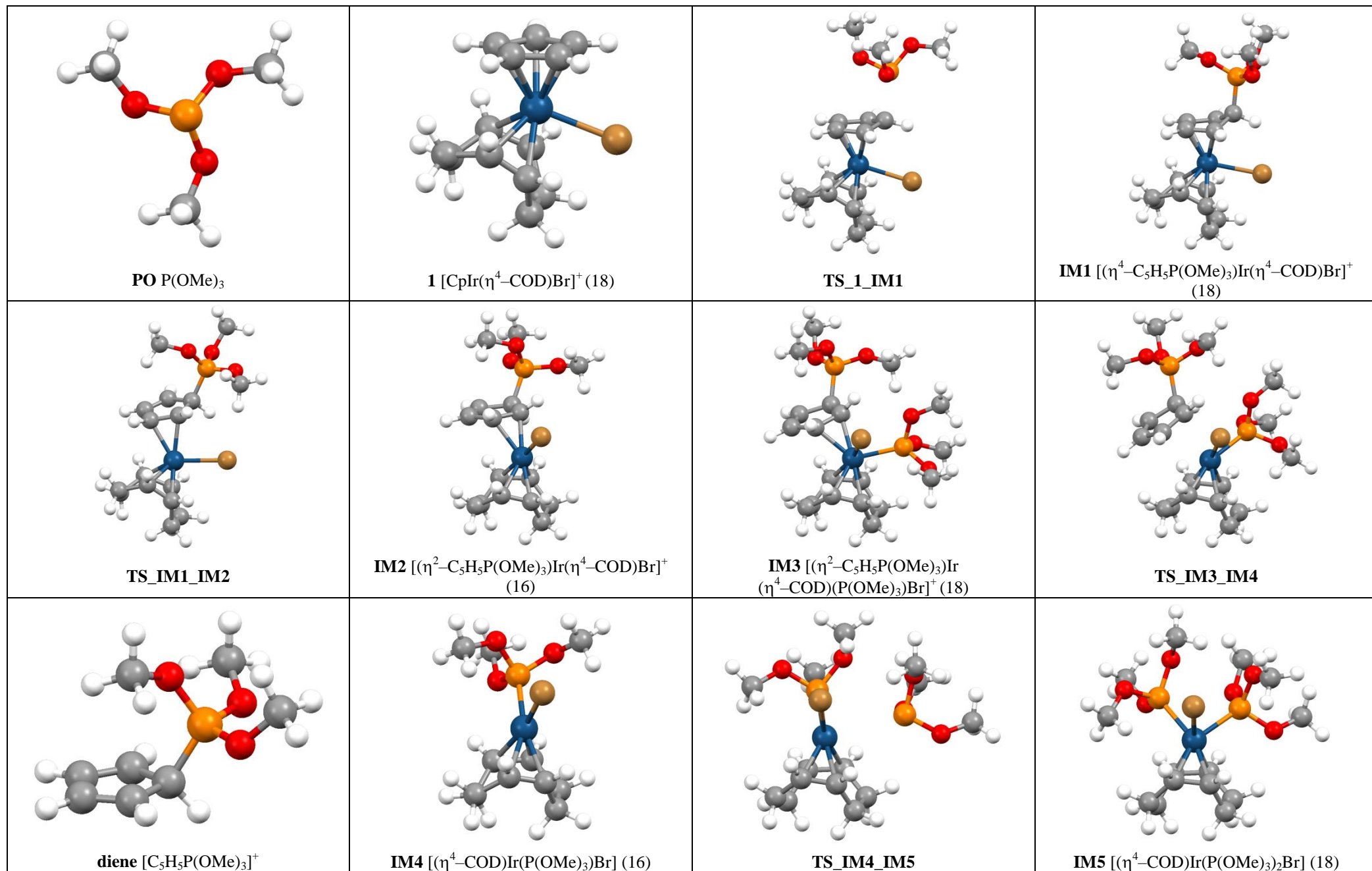
Table S4. Changes in electronic energies (E), enthalpies (H), and Gibbs free energies (G) obtained without using (no subscript) and using SMD solvation model (“solv” subscript), changes in gas-phase DLPNO-CCSD(T) electronic energies ( $E_{CC}$ ) and solvent-corrected DLPNO-CCSD(T) Gibbs free energies ( $G_{CC}$ ), in kcal mol<sup>-1</sup>.

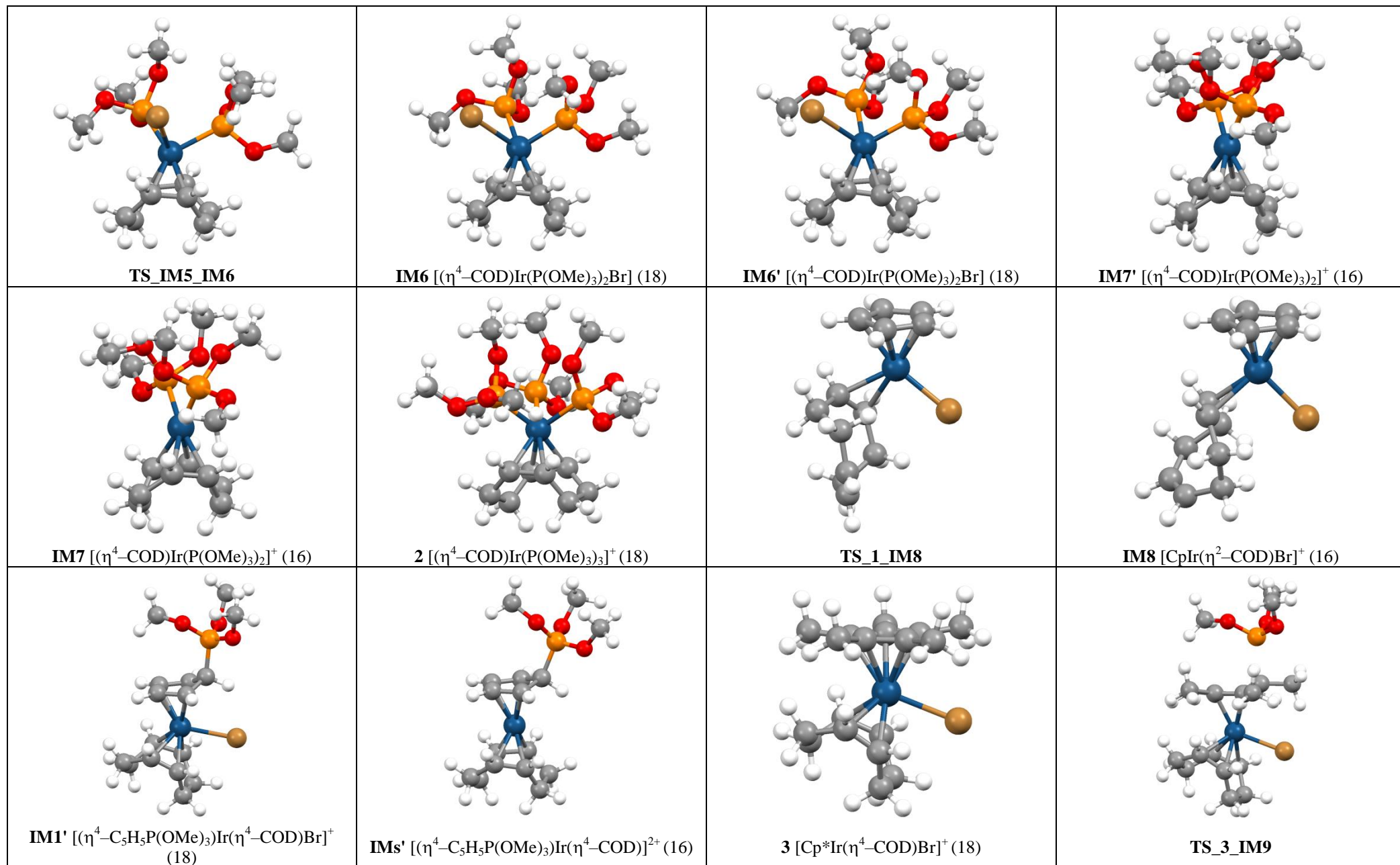
Reaction step	$\Delta E$	$\Delta H$	$\Delta G$	$\Delta E_{solv}$	$\Delta H_{solv}$	$\Delta G_{solv}$	$\Delta E_{CC}$	$\Delta G_{CC}$
<b>1 + PO =&gt; IM1</b>	-20.75	-19.02	-6.34	-14.52	-12.79	-0.11	-26.75	-6.12
<b>TS( 1 + PO =&gt; IM1 )</b>	-6.62	-5.99	5.90	3.57	4.20	16.08	-6.59	16.11
<b>1 =&gt; IM8</b>	17.72	17.22	15.24	16.66	16.16	14.19	26.69	23.16
<b>TS( 1 =&gt; IM8 )</b>	23.76	22.28	21.15	19.93	18.45	17.32	33.43	26.99
<b>IM1 =&gt; IM2</b>	5.64	5.35	4.82	6.16	5.87	5.34	9.12	8.83
<b>TS( IM1 =&gt; IM2 )</b>	18.11	17.11	17.40	20.18	19.18	19.47	20.43	21.79
<b>IM2 + PO =&gt; IM3</b>	-36.13	-34.04	-19.79	-26.61	-24.52	-10.27	-45.44	-19.58
<b>IM3 =&gt; IM4 + diene</b>	9.50	8.05	-6.76	-0.84	-2.29	-17.10	17.71	-8.89
<b>TS( IM3 =&gt; IM4 + diene )</b>	2.11	1.16	1.04	0.26	-0.69	-0.81	5.06	2.14
<b>IM4 + PO =&gt; IM5</b>	-19.55	-18.17	-4.27	-15.16	-13.78	0.12	-25.92	-6.24
<b>TS( IM4 + PO =&gt; IM5 )</b>	-11.20	-10.64	3.34	-7.74	-7.18	6.80	-9.19	8.82
<b>IM5 =&gt; IM6</b>	-3.63	-3.24	-2.79	-4.20	-3.80	-3.35	-0.69	-0.41
<b>TS( IM5 =&gt; IM6 )</b>	0.37	-0.16	0.89	0.36	-0.18	0.88	0.34	0.84
<b>IM6' =&gt; IM7' + Br'</b>	99.95	101.58	92.64	15.79	17.42	8.48	103.88	12.41
<b>IM7 + PO =&gt; 2</b>	-39.26	-37.43	-23.16	-29.20	-27.36	-13.09	-48.31	-22.14
<b>IM1' =&gt; IMs' + Br'</b>	180.84	181.96	173.35	34.11	35.23	26.62	189.03	34.81
<b>total from 1 to 2</b>	-4.24	3.07	34.35	-68.57	-61.26	-29.99	-16.39	-42.14
<b>3 + PO =&gt; IM9</b>	0.81	2.06	15.39	3.54	4.79	18.11	-7.31	9.99
<b>TS( 3 + PO =&gt; IM9 )</b>	6.51	6.53	19.09	12.41	12.43	24.99	2.94	21.42
<b>IM9 =&gt; IM10</b>	7.14	7.31	5.42	1.88	2.06	0.17	15.72	8.76
<b>TS( IM9 =&gt; IM10 )</b>	18.20	17.39	17.94	17.83	17.03	17.58	20.73	20.10
<b>IM9 =&gt; IM11 + IM12</b>	20.93	19.78	5.07	13.20	12.05	-2.66	30.20	6.62
<b>IM10 =&gt; IM11 + IM12</b>	13.79	12.46	-0.35	11.32	9.99	-2.83	14.48	-2.14
<b>3 =&gt; IM13</b>	13.55	12.90	10.06	11.70	11.04	8.20	22.23	16.88
<b>TS( 3 =&gt; IM13 )</b>	19.11	17.54	16.07	15.24	13.67	12.21	28.36	21.46
<b>IM13 + PO =&gt; IM14</b>	-47.81	-45.56	-30.98	-38.01	-35.77	-21.18	-57.63	-31.01
<b>IM14 =&gt; IM15 + COD</b>	21.03	19.52	5.84	14.73	13.22	-0.46	30.25	8.76
<b>IM15 + PO =&gt; 4</b>	-53.89	-51.75	-36.72	-44.27	-42.13	-27.10	-62.54	-35.76
<b>total from 3 to 4</b>	-67.11	-64.90	-51.80	-55.85	-53.64	-40.54	-67.69	-41.12

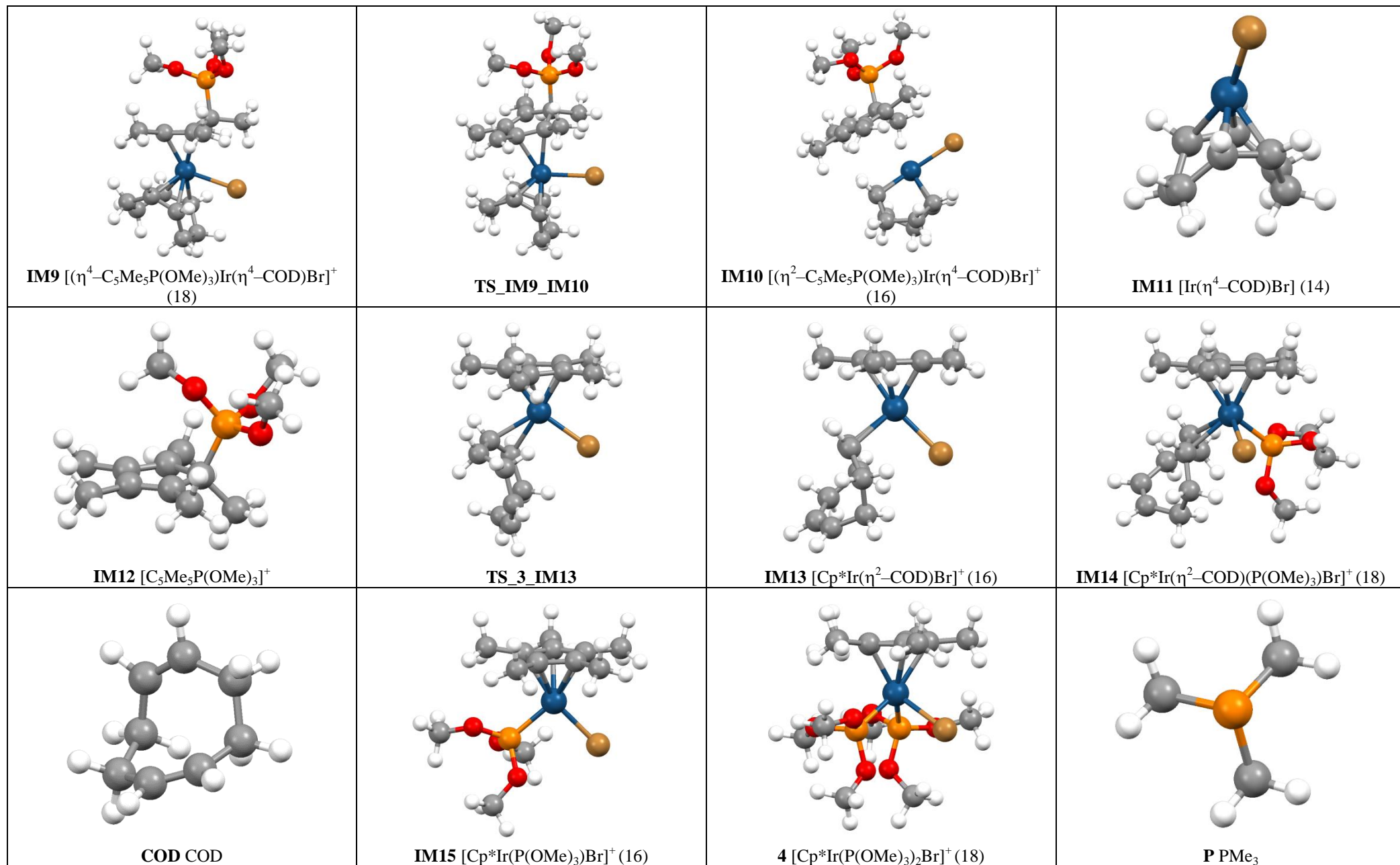
Reaction step	$\Delta E$	$\Delta H$	$\Delta G$	$\Delta E_{\text{solv}}$	$\Delta H_{\text{solv}}$	$\Delta G_{\text{solv}}$	$\Delta E_{\text{CC}}$	$\Delta G_{\text{CC}}$
<b>1 + P =&gt; IM1:P</b>	-24.24	-22.91	-11.07	-24.02	-22.68	-10.84	-28.73	-15.33
<b>TS( 1 + P =&gt; IM1:P )</b>	-7.05	-6.53	4.47	-0.23	0.30	11.30	-4.97	13.38
<b>IM1:P =&gt; IM2:P</b>	7.70	7.25	6.49	5.91	5.46	4.70	11.67	8.67
<b>TS( IM1:P =&gt; IM2:P )</b>	20.16	19.06	18.97	20.10	19.00	18.90	23.13	21.87
<b>IM2:P + P =&gt; IM3:P</b>	-34.01	-32.05	-19.11	-26.58	-24.62	-11.68	-43.27	-20.94
<b>IM3:P =&gt; IM4:P + diene:P</b>	12.02	10.45	-3.77	1.29	-0.28	-14.50	19.34	-7.19
<b>TS( IM3:P =&gt; IM4:P + diene:P )</b>	8.77	7.81	7.42	3.74	2.77	2.39	15.11	8.73
<b>IM4:P + P =&gt; IM5:P</b>	-15.94	-14.48	-1.68	-13.20	-11.75	1.05	-22.79	-5.80
<b>TS( IM4:P + P =&gt; IM5:P )</b>	-5.75	-5.31	6.69	-3.60	-3.16	8.84	-4.72	9.87
<b>IM5:P =&gt; IM6:P</b>	-0.52	-0.18	-0.19	-1.56	-1.22	-1.23	1.89	1.19
<b>TS( IM5:P =&gt; IM6:P )</b>	1.21	0.68	1.45	1.77	1.23	2.00	0.83	1.62
<b>IM6:P' =&gt; IM7:P' + Br'</b>	95.08	97.33	90.38	8.88	11.12	4.17	100.95	10.04
<b>IM7:P + P =&gt; 2:P</b>	-26.12	-24.29	-11.06	-20.72	-18.90	-5.67	-36.00	-15.55
<b>total from 1 to 2:P</b>	13.97	21.11	49.98	-70.01	-62.86	-34.00	3.07	-44.90
<b>1:Cl + PO =&gt; IM1:Cl</b>	-21.91	-20.23	-7.52	-14.54	-12.86	-0.15	-27.01	-5.25
<b>TS( 1:Cl + PO =&gt; IM1:Cl )</b>	-7.34	-6.71	5.22	3.95	4.59	16.52	-6.63	17.23
<b>1:Cl =&gt; IM8:Cl</b>	16.39	15.90	14.02	12.47	11.98	10.10	25.05	18.76
<b>TS( 1:Cl =&gt; IM8:Cl )</b>	22.66	21.14	19.56	14.11	12.58	11.00	32.25	20.59
<b>IM1:Cl =&gt; IM2:Cl</b>	4.07	3.86	3.39	1.68	1.47	1.00	6.89	3.83
<b>TS( IM1:Cl =&gt; IM2:Cl )</b>	18.05	17.15	17.65	16.69	15.80	16.30	20.26	18.51
<b>IM6:Cl' =&gt; IM7' + Cl'</b>	105.05	106.60	97.80	10.54	12.10	3.30	108.89	7.14
<b>1:I + PO =&gt; IM1:I</b>	-18.91	-17.24	-4.73	-11.90	-10.23	2.28	-25.40	-4.21
<b>TS( 1:I + PO =&gt; IM1:I )</b>	-5.45	-4.68	7.39	4.77	5.54	17.61	-5.80	17.25
<b>1:I =&gt; IM8:I</b>	18.25	17.69	15.65	9.40	8.84	6.80	28.27	16.82
<b>TS( 1:I =&gt; IM8:I )</b>	23.99	22.63	21.64	12.20	10.84	9.85	34.43	20.29
<b>IM1:I =&gt; IM2:I</b>	7.13	6.84	6.39	3.52	3.24	2.78	11.69	7.35
<b>TS( IM1:I =&gt; IM2:I )</b>	17.66	16.72	17.19	12.44	11.50	11.97	20.56	14.87
<b>IM6:I' =&gt; IM7' + I'</b>	93.44	95.23	86.41	8.76	10.54	1.72	98.88	7.16
<b>1 + bipy =&gt; IM1:bipy</b>	-9.19	-7.42	5.75	0.28	2.05	15.21	-16.87	7.53
<b>TS( 1 + bipy =&gt; IM1:bipy )</b>	-6.30	-5.64	7.23	5.19	5.85	18.72	-9.68	15.35
<b>IM1:bipy =&gt; IM2:bipy</b>	12.11	11.85	11.31	9.50	9.24	8.70	15.72	12.31
<b>TS( IM1:bipy =&gt; IM2:bipy )</b>	27.16	26.26	26.73	26.45	25.55	26.02	29.25	28.11

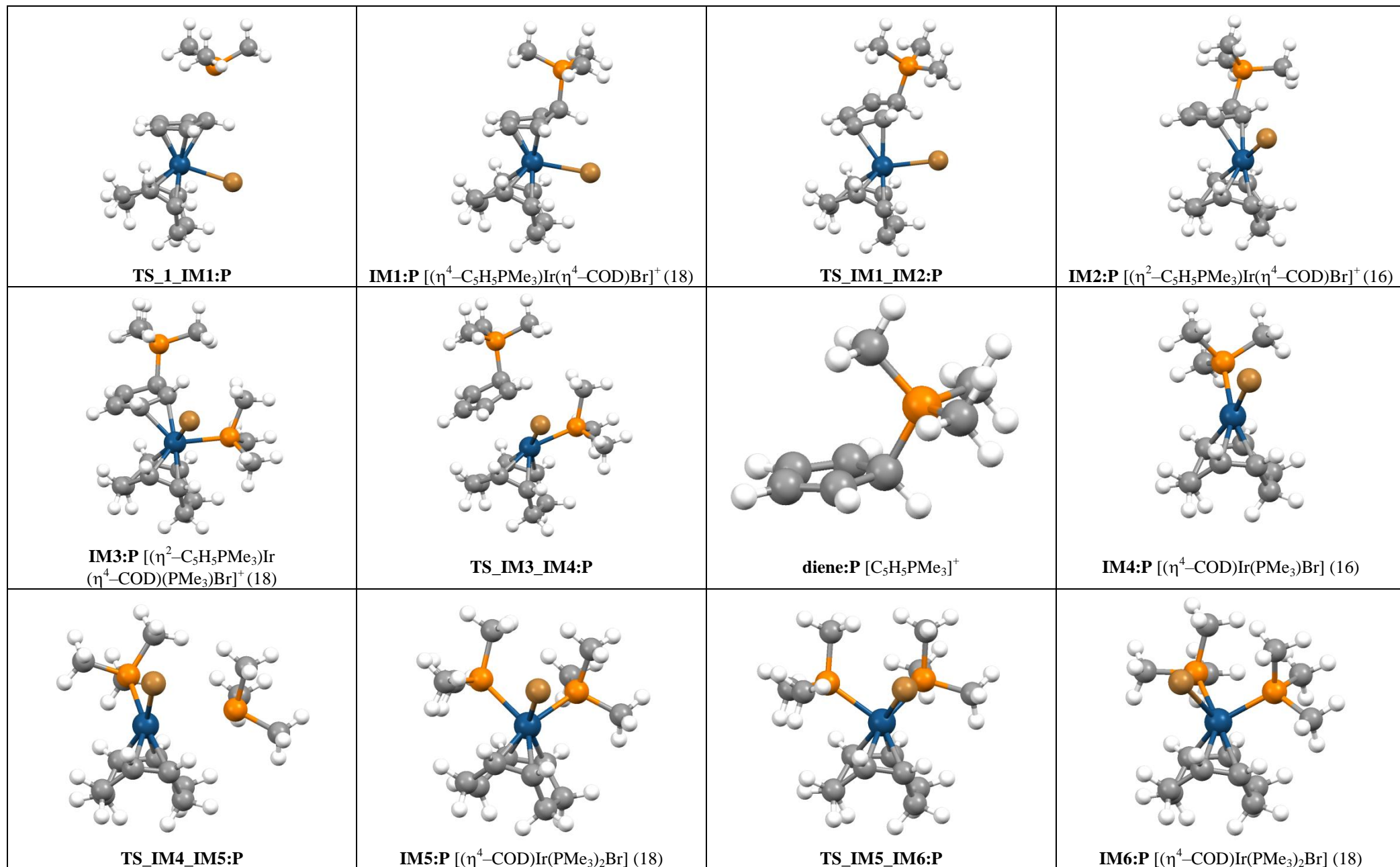
### Identifiers and Visual Representations of Optimized Structures

- Visual representations of the compounds are given after this note. The labels contain the **identifiers**, text formulas, and numbers of valence electrons of iridium in brackets. The cartesian coordinates of atoms are provided as a supplementary material.
- The quotation mark (') after an identifier implies that the associated computations were performed using a diffuse basis set (ma-def2-TZVPP) instead of def2-TZVPP (see the “computational methods” Section of this document).
- The compounds bearing –Br and/or –P(OMe)<sub>3</sub> fragments are abbreviated without any transcript after the colon. On the contrary, the variation of the halogen (:Cl, :I) and/or nucleophile (:P, :bipy) is given after the colon.
- In this way, the reactants and products are abbreviated with the following identifiers: [CpIr(COD)Br]<sup>+</sup> (**1**), [CpIr(COD)Cl]<sup>+</sup> (**1:Cl**), [CpIr(COD)I]<sup>+</sup> (**1:I**), [(COD)Ir(P(OMe)<sub>3</sub>)<sub>3</sub>]<sup>+</sup> (**2**), [(COD)Ir(PMe<sub>3</sub>)<sub>3</sub>]<sup>+</sup> (**2:P**), [Cp\*Ir(COD)Br]<sup>+</sup> (**3**), [Cp\*Ir(P(OMe)<sub>3</sub>)<sub>2</sub>Br]<sup>+</sup> (**4**), P(OMe)<sub>3</sub> (**PO**), [C<sub>5</sub>H<sub>5</sub>P(OMe)<sub>3</sub>]<sup>+</sup> (**diene**), PMe<sub>3</sub> (**P**), [C<sub>5</sub>H<sub>5</sub>PMe<sub>3</sub>]<sup>+</sup> (**diene:P**), COD (**COD**), bipy (**bipy**), Cl<sup>–</sup> (**Cl'**), Br<sup>–</sup> (**Br'**), and I<sup>–</sup> (**I'**).
- The intermediates are abbreviated following the same principles. For instance, the intermediates **IM1–15**, **IM1'**, **IMs'**, **IM6'**, and **IM7'** have –Br and/or –P(OMe)<sub>3</sub> fragments in the structure. On the contrary, the intermediates **IM1:Cl**, **IM1:I**, and **IM6:Cl'**, **IM6:I'** are the full analogues of **IM1** and **IM6'**, respectively, but with a halogen other than bromine. Similarly, the intermediates **IM1:bipy** and **IM1:P** have the attached nucleophile other than the P(OMe)<sub>3</sub>.
- The transition states are abbreviated with **TS\_<reactant>\_<product>** identifiers, where the <reactant> and <product> indicate the initial and final intermediates, respectively, which are connected via this transition state. For instance, the transition state for the addition of **PO** to **1** with the formation of **IM1** is abbreviated as **TS\_1\_IM1**. For the addition of **bipy** to **1** and the addition of **PO** to **1:Cl**, the corresponding identifiers are **TS\_1\_IM1:bipy** and **TS\_1\_IM1:Cl**, respectively.

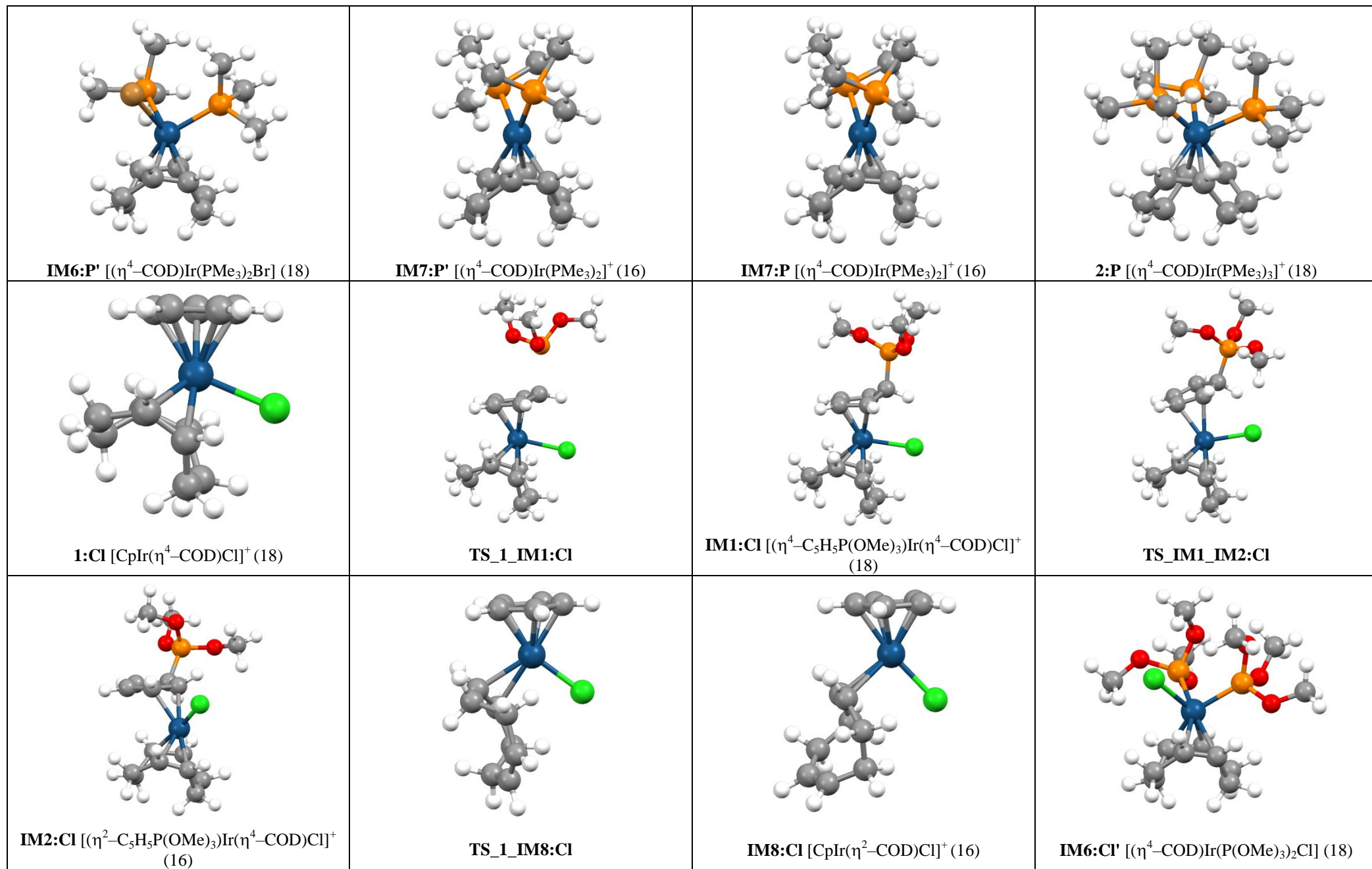


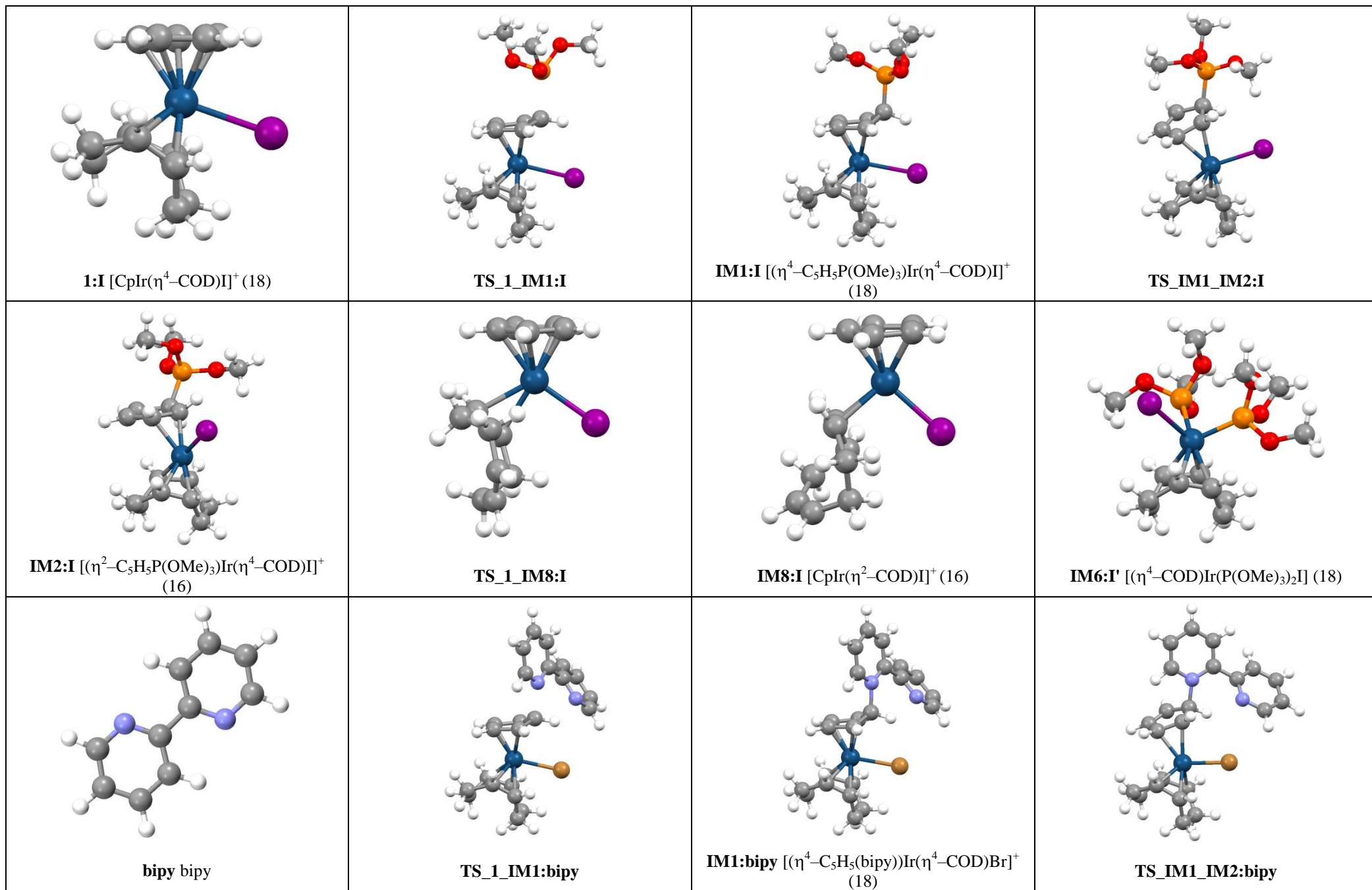


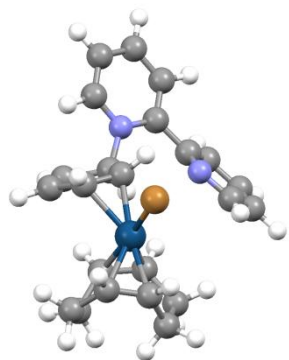








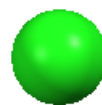




**IM2:bipy**  $[(\eta^2\text{-C}_5\text{H}_5(\text{bipy}))\text{Ir}(\eta^4\text{-COD})\text{Br}]^+$   
(16)



**Br'** Br<sup>-</sup>



**Cl'** Cl<sup>-</sup>



**I'** I<sup>-</sup>

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## Cartesian Coordinates of Optimized Structures

Multiple XYZ-file format is used.

16

structure of PO

P	-1.503022000	-0.506683000	-0.325613000
O	-0.857889000	0.517981000	0.764769000
O	-0.563335000	-1.794613000	0.010860000
O	-0.678713000	0.022499000	-1.627868000
C	-0.810483000	-2.993409000	-0.704606000
H	-0.315286000	-2.971572000	-1.675888000
H	-0.409729000	-3.817439000	-0.120700000
H	-1.879165000	-3.160185000	-0.860785000
C	-1.184498000	1.158375000	-2.309018000
H	-0.866788000	2.077199000	-1.815148000
H	-0.786951000	1.143610000	-3.320102000
H	-2.276074000	1.148488000	-2.360219000
C	-1.340088000	0.449628000	2.096308000
H	-1.127064000	1.400971000	2.576012000
H	-2.418007000	0.272795000	2.129203000
H	-0.839010000	-0.346809000	2.647398000

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structure of 1

Ir	1.140982000	12.505657000	4.348966000
C	1.444450000	10.859588000	7.044832000
H	2.377542000	10.319084000	7.192032000
H	0.723420000	10.396087000	7.714415000
C	1.606965000	12.330652000	7.403054000
H	0.643982000	12.746727000	7.700589000
H	2.257582000	12.460983000	8.272253000
C	2.148432000	13.144720000	6.267145000
H	1.969608000	14.211118000	6.342701000
C	3.152535000	12.762041000	5.378571000
H	3.613239000	13.566158000	4.822034000
C	3.955001000	11.486316000	5.455667000
H	4.126303000	11.251001000	6.505857000
H	4.935445000	11.685516000	5.031569000
C	3.335346000	10.287862000	4.722099000
H	3.785592000	10.190712000	3.739519000
H	3.560682000	9.360405000	5.254835000
C	1.850357000	10.385341000	4.555694000
H	1.438682000	9.874748000	3.693643000

C	0.984383000	10.668296000	5.618297000
H	-0.048797000	10.366662000	5.494429000
C	-0.298136000	14.166666000	4.810007000
C	-0.950288000	12.905453000	4.910664000
C	0.196769000	14.316021000	3.492637000
H	-0.156788000	14.862510000	5.620547000
C	-0.923255000	12.289399000	3.611725000
H	-1.431450000	12.511721000	5.790512000
C	-0.223920000	13.157899000	2.746496000
H	0.748462000	15.153364000	3.101386000
H	-1.358541000	11.340848000	3.345033000
H	0.015396000	12.963046000	1.714772000
Br	2.800317000	12.457430000	2.368191000

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structure of TS\_1\_IM1

Ir	1.343200000	12.541641000	4.551125000
C	1.609721000	11.492838000	7.522200000
H	2.156164000	10.561783000	7.663221000
H	1.003279000	11.617329000	8.416871000
C	2.568252000	12.667661000	7.382610000
H	2.075022000	13.581921000	7.715255000
H	3.437441000	12.552188000	8.036455000
C	3.033211000	12.865447000	5.968658000
H	3.417882000	13.856256000	5.751120000
C	3.407347000	11.856536000	5.075205000
H	4.012275000	12.173077000	4.236620000
C	3.489319000	10.384724000	5.411137000
H	3.841942000	10.281332000	6.437484000
H	4.262014000	9.942652000	4.787338000
C	2.181804000	9.608128000	5.202397000
H	2.203263000	9.119305000	4.233208000
H	2.090551000	8.811524000	5.945827000
C	0.953260000	10.468065000	5.265398000
H	0.106038000	10.113648000	4.691192000
C	0.699336000	11.352805000	6.321653000
H	-0.335430000	11.627891000	6.484543000
C	1.392346000	14.507949000	3.573561000
C	0.894959000	14.645880000	4.910400000
C	0.337729000	13.918997000	2.765926000
H	2.271935000	14.989601000	3.181113000
C	-0.307286000	13.895825000	5.004917000
H	1.353994000	15.205452000	5.708234000
C	-0.552644000	13.297968000	3.730371000

H	-0.915940000	13.788403000	5.886981000
H	-1.406701000	12.690056000	3.483036000
Br	1.992581000	11.248825000	2.370123000
H	0.556372000	13.448768000	1.822114000
P	-0.801839000	15.814184000	1.859745000
O	-1.709034000	16.253537000	3.084608000
O	-1.809592000	16.124921000	0.645187000
O	0.400886000	16.848638000	1.700415000
C	-2.789178000	17.203745000	3.029339000
H	-3.164075000	17.297720000	4.042157000
H	-2.441546000	18.172281000	2.678401000
H	-3.575581000	16.841266000	2.374255000
C	-1.402558000	15.883146000	-0.709670000
H	-1.225744000	14.822706000	-0.877754000
H	-2.218811000	16.214221000	-1.341335000
H	-0.503031000	16.446085000	-0.953483000
C	0.222191000	18.262387000	1.511992000
H	0.051410000	18.742485000	2.473111000
H	1.138532000	18.644297000	1.075563000
H	-0.611950000	18.467070000	0.842867000

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structure of IM1

Ir	1.481636000	12.826946000	4.552645000
C	0.792676000	10.379353000	6.426870000
H	1.604661000	9.685718000	6.638775000
H	-0.123295000	9.831738000	6.640152000
C	0.879888000	11.606199000	7.324860000
H	-0.118100000	12.024518000	7.465368000
H	1.228360000	11.342444000	8.327952000
C	1.764982000	12.675915000	6.749156000
H	1.597183000	13.669117000	7.153353000
C	3.003063000	12.469341000	6.125793000
H	3.652077000	13.333360000	6.074578000
C	3.700014000	11.131350000	6.004077000
H	3.485876000	10.538741000	6.893533000
H	4.772832000	11.308173000	6.020604000
C	3.343013000	10.358206000	4.729568000
H	4.081459000	10.572802000	3.961629000
H	3.389669000	9.280277000	4.907918000
C	1.990496000	10.711386000	4.177215000
H	1.873309000	10.552902000	3.111663000
C	0.823273000	10.744554000	4.957283000
H	-0.113119000	10.615955000	4.427544000

C	0.976278000	14.948192000	4.440042000
C	-0.117454000	14.213044000	5.006302000
C	0.857422000	14.883947000	2.929787000
H	1.496567000	15.742103000	4.953803000
C	-0.559490000	13.292700000	4.015337000
H	-0.508508000	14.302034000	6.006726000
C	0.263461000	13.487857000	2.860620000
H	-1.341777000	12.560372000	4.134282000
H	0.147733000	12.942795000	1.936112000
Br	3.634319000	13.288492000	3.125086000
H	1.834639000	14.933732000	2.438122000
P	-0.129808000	16.183929000	2.194080000
O	0.581733000	17.533629000	2.469073000
O	-1.572199000	16.391408000	2.771233000
O	-0.215535000	15.821982000	0.678851000
C	-0.043207000	18.832081000	2.596101000
H	0.761421000	19.527405000	2.800099000
H	-0.543497000	19.106613000	1.671801000
H	-0.751424000	18.821371000	3.418214000
C	-2.679647000	15.498204000	2.525516000
H	-2.853859000	14.907668000	3.419104000
H	-3.546149000	16.116359000	2.316633000
H	-2.478645000	14.843767000	1.680034000
C	-0.794349000	16.680669000	-0.327973000
H	-0.112653000	17.499089000	-0.542470000
H	-0.922726000	16.070547000	-1.213591000
H	-1.759282000	17.064129000	-0.001792000

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structure of TS\_IM1\_IM2

Ir	1.000004000	-0.606047000	0.951724000
C	0.276263000	-3.340258000	2.277784000
H	1.072493000	-4.063475000	2.449831000
H	-0.644307000	-3.919558000	2.262033000
C	0.219709000	-2.294080000	3.384268000
H	-0.815768000	-2.001472000	3.558185000
H	0.579902000	-2.683844000	4.340652000
C	1.001167000	-1.068483000	2.999425000
H	0.716303000	-0.167129000	3.537916000
C	2.352669000	-1.111855000	2.501748000
H	2.943689000	-0.221935000	2.682109000
C	3.158982000	-2.387300000	2.356481000
H	2.804479000	-3.142095000	3.057274000
H	4.193566000	-2.194308000	2.629398000



C	3.071684000	-2.864504000	0.915750000
H	3.860907000	-2.397504000	0.328781000
H	3.214522000	-3.944422000	0.813870000
C	1.753036000	-2.466255000	0.316180000
H	1.751339000	-2.421469000	-0.770966000
C	0.470561000	-2.671948000	0.930061000
H	-0.342135000	-2.824500000	0.230360000
C	-0.386028000	0.867637000	0.066487000
C	-1.187658000	-0.144923000	0.649162000
C	-0.505370000	0.762044000	-1.444457000
H	-0.155938000	1.808851000	0.547145000
C	-1.784988000	-0.911249000	-0.446643000
H	-1.639474000	-0.086983000	1.629594000
C	-1.423759000	-0.416535000	-1.638007000
H	-2.418888000	-1.774078000	-0.305299000
H	-1.669756000	-0.811785000	-2.610321000
Br	2.776566000	0.899403000	-0.144988000
H	0.468495000	0.620101000	-1.933167000
P	-1.107574000	2.276730000	-2.167414000
O	-0.025335000	3.372726000	-2.292622000
O	-2.256806000	2.943249000	-1.349467000
O	-1.543970000	1.916359000	-3.610681000
C	0.651638000	4.015383000	-1.177525000
H	1.196071000	4.847225000	-1.606492000
H	-0.081047000	4.379463000	-0.462361000
H	1.342021000	3.306855000	-0.722091000
C	-3.479767000	2.260703000	-0.985284000
H	-3.287059000	1.591564000	-0.151820000
H	-4.179324000	3.034193000	-0.692026000
H	-3.874410000	1.703831000	-1.831975000
C	-1.942978000	2.913652000	-4.586262000
H	-1.087573000	3.527272000	-4.850129000
H	-2.291557000	2.361292000	-5.449524000
H	-2.744596000	3.529462000	-4.186696000

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structure of IM2

Ir	0.172792000	12.941365000	5.349522000
C	1.457332000	10.349278000	6.409941000
H	2.499269000	10.139636000	6.177478000
H	1.028475000	9.395586000	6.709577000
C	1.338848000	11.340122000	7.569732000
H	0.411086000	11.151166000	8.110984000
H	2.138924000	11.189711000	8.300796000

C	1.334854000	12.776998000	7.118793000
H	0.960325000	13.468301000	7.870345000
C	2.172201000	13.318863000	6.118247000
H	2.346993000	14.383779000	6.189551000
C	3.262952000	12.557262000	5.394216000
H	3.665466000	11.779108000	6.039871000
H	4.095756000	13.231031000	5.200638000
C	2.771010000	11.972656000	4.069684000
H	2.870577000	12.719624000	3.281597000
H	3.396317000	11.131554000	3.755776000
C	1.337574000	11.543526000	4.122127000
H	0.823667000	11.515500000	3.167096000
C	0.730702000	10.844545000	5.179855000
H	-0.188111000	10.325895000	4.928526000
C	-0.631403000	14.922902000	5.688180000
C	0.041499000	14.967405000	4.431496000
H	-1.707853000	14.805136000	5.733881000
H	-0.430169000	14.736216000	3.487184000
Br	-1.940931000	12.456900000	4.117378000
C	1.159813000	15.887713000	4.527470000
C	1.188880000	16.472081000	5.734103000
C	0.070382000	15.934741000	6.587910000
H	1.931193000	17.160224000	6.109151000
P	-1.090472000	17.190285000	7.086614000
O	-0.248360000	18.292651000	7.778870000
O	-1.960635000	17.741905000	5.921379000
O	-2.118075000	16.688372000	8.131573000
C	-0.838851000	19.453213000	8.419719000
C	-1.452597000	18.315174000	4.692453000
C	-3.273022000	15.855064000	7.854923000
H	-0.009537000	20.081870000	8.717668000
H	-1.406609000	19.139624000	9.289999000
H	-1.477742000	19.983586000	7.718438000
H	-1.252221000	17.517438000	3.984545000
H	-0.549032000	18.890019000	4.880685000
H	-2.235814000	18.963143000	4.317181000
H	-3.729976000	16.143410000	6.912970000
H	-3.963674000	16.021236000	8.672408000
H	-2.966387000	14.813528000	7.831672000
H	0.450524000	15.528444000	7.533316000
H	1.875353000	16.060190000	3.736987000

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structure of IM3

Ir	0.148568000	13.055659000	5.614549000
C	1.795534000	10.505449000	6.385593000
H	2.788603000	10.355465000	5.961873000
H	1.470740000	9.518731000	6.711477000
C	1.859648000	11.435838000	7.597583000
H	1.108440000	11.129892000	8.327071000
H	2.820146000	11.348506000	8.114844000
C	1.619004000	12.881034000	7.251859000
H	1.293176000	13.493100000	8.083367000
C	2.218480000	13.546435000	6.172638000
H	2.282831000	14.620622000	6.270665000
C	3.270112000	12.925896000	5.276158000
H	3.828760000	12.182894000	5.845262000
H	3.995240000	13.693262000	5.008840000
C	2.674768000	12.314126000	4.013040000
H	2.651545000	13.064199000	3.222760000
H	3.308322000	11.506376000	3.633827000
C	1.271433000	11.817239000	4.219944000
H	0.681014000	11.729821000	3.315257000
C	0.854402000	11.008558000	5.307968000
H	-0.001702000	10.378069000	5.100993000
C	-0.580987000	15.089051000	5.662575000
C	0.129711000	14.922599000	4.410341000
H	-1.665547000	15.072885000	5.677986000
H	-0.369670000	14.644468000	3.492849000
Br	-1.898640000	12.538411000	4.116882000
C	1.239246000	15.862471000	4.392646000
C	1.272325000	16.615959000	5.499736000
C	0.144430000	16.210388000	6.421984000
H	2.021501000	17.340174000	5.779603000
P	-0.958267000	17.570369000	6.742356000
O	-0.078229000	18.807715000	7.064439000
O	-1.957709000	17.853712000	5.582441000
O	-1.868906000	17.357907000	7.985554000
C	-0.637513000	20.086598000	7.451867000
C	-1.576422000	18.028739000	4.195405000
C	-2.741552000	16.213669000	8.125996000
H	0.191677000	20.782553000	7.467968000
H	-1.082322000	20.007226000	8.438995000
H	-1.380480000	20.407647000	6.726232000
H	-2.425019000	18.496381000	3.710788000
H	-1.376907000	17.057055000	3.753419000
H	-0.700362000	18.667997000	4.117778000

H	-3.400119000	16.129717000	7.264562000
H	-3.322789000	16.390785000	9.023013000
H	-2.147286000	15.308132000	8.233196000
H	0.513632000	15.918320000	7.413414000
H	1.961603000	15.924795000	3.590714000
P	-1.309249000	12.435365000	7.393185000
O	-0.872706000	12.963186000	8.846468000
O	-1.550678000	10.895082000	7.773368000
O	-2.773668000	13.045559000	7.163265000
C	-1.135125000	12.279302000	10.078784000
C	-2.087324000	9.958843000	6.823573000
C	-3.867763000	12.775133000	8.037710000
H	-0.859222000	12.963907000	10.874350000
H	-2.183901000	12.009029000	10.177509000
H	-0.532616000	11.376910000	10.148089000
H	-3.039295000	9.595164000	7.203146000
H	-2.234844000	10.418212000	5.846710000
H	-1.394985000	9.125769000	6.740399000
H	-3.794533000	13.376702000	8.944856000
H	-4.775109000	13.038707000	7.503041000
H	-3.909057000	11.722356000	8.312349000

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structure of TS\_IM3\_IM4

Ir	0.134933000	12.585549000	5.684980000
C	1.926806000	10.026969000	5.672853000
H	2.891823000	10.108039000	5.171481000
H	1.706489000	8.961675000	5.710461000
C	2.002753000	10.588674000	7.084609000
H	1.289946000	10.067538000	7.725560000
H	2.984186000	10.415427000	7.537643000
C	1.675384000	12.054488000	7.140884000
H	1.413814000	12.399115000	8.133998000
C	2.160924000	13.051679000	6.266179000
H	2.187830000	14.055373000	6.680874000
C	3.190517000	12.777653000	5.183513000
H	3.870824000	12.001072000	5.535443000
H	3.810535000	13.664669000	5.058739000
C	2.573940000	12.386276000	3.836551000
H	2.506128000	13.268847000	3.199164000
H	3.232032000	11.693807000	3.302507000
C	1.190216000	11.808389000	3.971002000
H	0.557447000	11.908049000	3.095235000
C	0.869296000	10.734829000	4.850469000

H	0.007852000	10.138909000	4.571528000
C	-0.726230000	14.890549000	5.564258000
C	0.096206000	14.806974000	4.453325000
H	-1.767913000	14.614899000	5.573783000
H	-0.182598000	14.346227000	3.519105000
Br	-2.050222000	12.160664000	4.384251000
C	1.250406000	15.658829000	4.657309000
C	1.155969000	16.310669000	5.830394000
C	-0.123641000	15.906621000	6.505728000
H	1.881461000	16.969191000	6.280473000
P	-1.275184000	17.254498000	6.622985000
O	-0.616029000	18.282241000	7.583500000
O	-1.662168000	17.886806000	5.254875000
O	-2.628315000	16.837691000	7.253142000
C	-1.285837000	19.493792000	8.010264000
C	-0.762532000	18.563701000	4.346496000
C	-3.767835000	16.284284000	6.540566000
H	-0.561503000	20.044938000	8.596475000
H	-2.148570000	19.241069000	8.618952000
H	-1.590000000	20.080565000	7.147030000
H	-1.334878000	19.363422000	3.889735000
H	-0.430416000	17.857904000	3.593163000
H	0.093393000	18.971155000	4.879222000
H	-3.896580000	16.794038000	5.591301000
H	-4.625371000	16.458058000	7.179662000
H	-3.615719000	15.218776000	6.392095000
H	0.013732000	15.548208000	7.531752000
H	2.077584000	15.737669000	3.967452000
P	-1.108699000	12.656862000	7.619555000
O	-0.500417000	13.545947000	8.824745000
O	-1.326521000	11.283364000	8.432357000
O	-2.600903000	13.249145000	7.450445000
C	-0.487192000	13.155634000	10.202098000
C	-1.801216000	10.135649000	7.714944000
C	-3.512705000	13.278275000	8.547544000
H	-0.069318000	13.990154000	10.756358000
H	-1.488367000	12.940334000	10.568960000
H	0.134987000	12.274809000	10.345868000
H	-1.706535000	9.287697000	8.384656000
H	-2.843195000	10.266779000	7.426257000
H	-1.207702000	9.972862000	6.814802000
H	-3.285255000	14.112384000	9.213059000
H	-4.509324000	13.406797000	8.135121000

H	-3.483615000	12.348447000	9.113500000
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structure of diene

C	-0.576788000	14.898577000	5.712901000
C	0.064161000	14.755876000	4.540336000
H	-1.391670000	14.311223000	6.103031000
H	-0.153789000	14.009654000	3.791861000
C	1.124119000	15.740684000	4.435752000
C	1.150517000	16.499589000	5.544615000
C	0.059729000	16.032674000	6.459218000
H	1.847624000	17.283835000	5.789885000
P	-1.117282000	17.341192000	6.731415000
O	-0.493525000	18.556083000	7.461918000
O	-1.718850000	17.931964000	5.426486000
O	-2.185999000	16.716230000	7.664139000
C	0.051471000	19.736886000	6.818737000
C	-2.565010000	17.227159000	4.484326000
C	-3.278316000	17.479430000	8.240592000
H	0.616137000	20.255413000	7.583269000
H	-0.762197000	20.357874000	6.459280000
H	0.701116000	19.456811000	5.994337000
H	-3.276003000	17.955013000	4.110345000
H	-3.087077000	16.407521000	4.972026000
H	-1.948124000	16.849920000	3.676348000
H	-2.881449000	18.240370000	8.905246000
H	-3.874928000	16.768309000	8.797360000
H	-3.875054000	17.932301000	7.453016000
H	0.420681000	15.744407000	7.451210000
H	1.803418000	15.823437000	3.601642000

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structure of IM4

Ir	1.021286000	13.023348000	5.322988000
C	1.801630000	11.148092000	7.703841000
H	2.652770000	10.481934000	7.570446000
H	1.251125000	10.754172000	8.556998000
C	2.273388000	12.570881000	8.019853000
H	1.517635000	13.068637000	8.628957000
H	3.178457000	12.543791000	8.636356000
C	2.493443000	13.412747000	6.792932000
H	2.556625000	14.475315000	7.007704000
C	3.134324000	12.977195000	5.598655000
H	3.601137000	13.756669000	5.008643000
C	3.753461000	11.603133000	5.425232000

H	4.120770000	11.237545000	6.384262000
H	4.636137000	11.686715000	4.792597000
C	2.786174000	10.597456000	4.795561000
H	2.835320000	10.684635000	3.710162000
H	3.092764000	9.571240000	5.023832000
C	1.358566000	10.809648000	5.203472000
H	0.608934000	10.495344000	4.486521000
C	0.917418000	11.090567000	6.485446000
H	-0.148751000	10.999545000	6.660058000
P	0.971385000	15.170619000	4.686071000
O	0.102071000	16.234717000	5.510356000
O	0.441410000	15.528191000	3.208130000
O	2.402697000	15.884848000	4.785560000
C	-1.304313000	16.044407000	5.672445000
C	0.802644000	14.701098000	2.104480000
C	2.557132000	17.265405000	4.458337000
H	-1.664159000	16.884561000	6.258147000
H	-1.805174000	16.025339000	4.706052000
H	-1.511661000	15.110520000	6.193193000
H	0.215265000	15.036703000	1.255618000
H	1.863854000	14.806137000	1.873424000
H	0.573121000	13.655897000	2.312835000
H	2.149074000	17.891857000	5.248707000
H	3.622367000	17.449720000	4.358998000
H	2.056747000	17.502025000	3.520160000
Br	-1.295913000	12.651976000	4.371321000

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structure of TS\_IM4\_IM5

Ir	0.876144000	12.738378000	5.344933000
C	1.868293000	10.192461000	6.830857000
H	2.714353000	9.628085000	6.438060000
H	1.356519000	9.515289000	7.513096000
C	2.356660000	11.419142000	7.614340000
H	1.670423000	11.609066000	8.440975000
H	3.327993000	11.214123000	8.077876000
C	2.429658000	12.671916000	6.782496000
H	2.430971000	13.588543000	7.362642000
C	3.009729000	12.738046000	5.485519000
H	3.405755000	13.703424000	5.195564000
C	3.682737000	11.557730000	4.812311000
H	4.088581000	10.884312000	5.567422000
H	4.543698000	11.909447000	4.244798000
C	2.729633000	10.814853000	3.879508000

H	2.725514000	11.304419000	2.904593000
H	3.075824000	9.791376000	3.698685000
C	1.318424000	10.801293000	4.387534000
H	0.553016000	10.695483000	3.627597000
C	0.928189000	10.547517000	5.704044000
H	-0.115778000	10.292137000	5.849393000
P	0.827817000	14.983825000	5.170347000
O	-0.270309000	15.924952000	5.873464000
O	0.713852000	15.590594000	3.676965000
O	2.141203000	15.667674000	5.791417000
C	-1.608861000	16.031176000	5.390116000
C	1.222609000	14.859851000	2.563797000
C	2.297743000	17.083996000	5.798559000
H	-2.164125000	16.587037000	6.140734000
H	-1.624317000	16.568078000	4.443103000
H	-2.057223000	15.048970000	5.252539000
H	1.002963000	15.449938000	1.678989000
H	2.301905000	14.719729000	2.643576000
H	0.737613000	13.886212000	2.489934000
H	1.692886000	17.529073000	6.586512000
H	3.347926000	17.286805000	5.986520000
H	2.010226000	17.516429000	4.840836000
Br	-1.426730000	12.592120000	4.195976000
P	-0.733266000	13.301734000	8.115217000
O	-1.040675000	12.440728000	9.465253000
O	-2.044831000	14.287012000	8.030981000
O	0.323732000	14.430358000	8.600538000
C	-1.392710000	13.049880000	10.699837000
C	-3.250623000	13.692626000	7.560307000
C	-0.001116000	15.717849000	9.108859000
H	-1.746389000	12.267291000	11.365670000
H	-0.525219000	13.532271000	11.151778000
H	-2.183814000	13.789536000	10.566262000
H	-3.074085000	13.091064000	6.665784000
H	-3.703231000	13.065789000	8.330627000
H	-3.935784000	14.499777000	7.315002000
H	-0.675283000	15.664671000	9.963009000
H	0.935057000	16.174052000	9.421704000
H	-0.460424000	16.328195000	8.333450000
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structure of IM5			
Ir	0.651647000	12.856552000	5.854399000
C	1.594241000	10.020477000	6.703520000



H	2.416240000	9.534529000	6.172560000
H	1.049123000	9.210480000	7.186457000
C	2.125291000	10.972915000	7.775130000
H	1.455263000	10.956546000	8.632397000
H	3.104103000	10.651990000	8.150603000
C	2.223389000	12.402141000	7.305822000
H	2.245441000	13.138388000	8.102843000
C	2.827915000	12.785739000	6.087074000
H	3.211130000	13.795382000	6.050709000
C	3.540645000	11.791522000	5.188688000
H	3.928638000	10.977949000	5.803562000
H	4.417583000	12.276651000	4.760435000
C	2.639063000	11.255545000	4.084960000
H	2.760061000	11.869433000	3.191157000
H	2.938295000	10.243037000	3.788424000
C	1.188805000	11.299034000	4.487264000
H	0.500267000	11.272999000	3.648549000
C	0.681782000	10.724733000	5.713336000
H	-0.324335000	10.324116000	5.650812000
P	0.847379000	15.070673000	5.174200000
O	-0.175028000	16.214534000	5.681885000
O	0.757849000	15.427821000	3.593687000
O	2.210630000	15.775526000	5.658856000
C	-1.514284000	16.325686000	5.208829000
C	1.215790000	14.483659000	2.633701000
C	2.451876000	17.157066000	5.405610000
H	-1.843223000	17.335840000	5.442512000
H	-1.564943000	16.164100000	4.134067000
H	-2.156754000	15.602729000	5.708126000
H	0.947545000	14.873788000	1.656258000
H	2.300151000	14.366212000	2.685535000
H	0.737829000	13.514988000	2.785084000
H	1.885105000	17.774981000	6.099564000
H	3.514849000	17.326061000	5.551235000
H	2.178015000	17.423289000	4.385344000
Br	-1.584557000	12.887890000	4.524309000
P	-0.411352000	13.608218000	7.803758000
O	-0.409648000	12.519928000	9.005382000
O	-1.937720000	14.155064000	7.821069000
O	0.296337000	14.893629000	8.473103000
C	-0.785100000	12.896706000	10.324410000
C	-3.006717000	13.227875000	7.626089000
C	-0.383343000	16.014282000	9.023669000

H	-0.832185000	11.989196000	10.919085000
H	-0.046278000	13.571212000	10.757759000
H	-1.761991000	13.382694000	10.338809000
H	-3.702217000	13.655944000	6.909844000
H	-2.652717000	12.277286000	7.229924000
H	-3.510828000	13.060905000	8.578240000
H	-1.089063000	15.723042000	9.800902000
H	0.380244000	16.656972000	9.453428000
H	-0.917381000	16.558372000	8.246927000

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structure of TS\_IM5\_IM6

Ir	0.046349000	-0.577597000	-0.553416000
C	1.019766000	-3.233456000	0.709488000
H	1.735879000	-3.904309000	0.228777000
H	0.490950000	-3.850416000	1.434579000
C	1.753816000	-2.110392000	1.456758000
H	1.263299000	-1.938248000	2.413292000
H	2.780575000	-2.408443000	1.697665000
C	1.776562000	-0.801727000	0.704709000
H	1.922725000	0.078148000	1.322057000
C	2.226720000	-0.714239000	-0.643300000
H	2.641479000	0.240102000	-0.935956000
C	2.804476000	-1.911504000	-1.375262000
H	3.203237000	-2.619535000	-0.647148000
H	3.660603000	-1.589158000	-1.968197000
C	1.760090000	-2.567518000	-2.257285000
H	1.759978000	-2.085981000	-3.236344000
H	1.990617000	-3.623297000	-2.445826000
C	0.384017000	-2.418697000	-1.669390000
H	-0.416270000	-2.519360000	-2.393550000
C	0.022250000	-2.730711000	-0.321631000
H	-0.993615000	-3.085393000	-0.186889000
P	0.250693000	1.606421000	-1.170647000
O	-0.763355000	2.746733000	-0.650508000
O	0.218726000	2.005539000	-2.740796000
O	1.609841000	2.266961000	-0.619305000
C	-2.099354000	2.877377000	-1.127583000
C	0.673177000	1.072262000	-3.715054000
C	1.896709000	3.644426000	-0.842871000
H	-2.423073000	3.883484000	-0.870990000
H	-2.145522000	2.740356000	-2.205993000
H	-2.748254000	2.146155000	-0.649116000
H	0.431716000	1.492641000	-4.686833000

H	1.753190000	0.927043000	-3.646023000
H	0.169459000	0.112347000	-3.594123000
H	1.310172000	4.268934000	-0.171650000
H	2.954497000	3.785597000	-0.640920000
H	1.682373000	3.928581000	-1.872563000
Br	-2.186481000	-0.508130000	-1.969207000
P	-1.115520000	0.027286000	1.400728000
O	-1.159014000	-1.183623000	2.475832000
O	-2.635804000	0.595728000	1.443872000
O	-0.405720000	1.230172000	2.202671000
C	-1.569556000	-0.946162000	3.817448000
C	-3.715000000	-0.280187000	1.112933000
C	-1.081519000	2.314087000	2.828119000
H	-1.659190000	-1.912630000	4.304355000
H	-0.828042000	-0.346110000	4.345430000
H	-2.533432000	-0.436596000	3.856103000
H	-4.330271000	0.198949000	0.356586000
H	-3.361301000	-1.228378000	0.710365000
H	-4.305398000	-0.464013000	2.010579000
H	-1.806901000	1.971808000	3.565196000
H	-0.318183000	2.908119000	3.322881000
H	-1.593165000	2.926562000	2.087951000

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structure of IM6

Ir	0.137465000	-0.519879000	-0.469191000
C	1.533250000	-3.045510000	0.937493000
H	2.104190000	-3.728862000	0.309558000
H	1.347243000	-3.581345000	1.867680000
C	2.338137000	-1.780904000	1.226076000
H	2.033632000	-1.380131000	2.194866000
H	3.403925000	-2.017946000	1.322420000
C	2.125414000	-0.697675000	0.202734000
H	2.517640000	0.256844000	0.535038000
C	2.125786000	-0.893358000	-1.233882000
H	2.564446000	-0.069120000	-1.785808000
C	2.334842000	-2.241399000	-1.904738000
H	3.014848000	-2.858945000	-1.314162000
H	2.841733000	-2.095421000	-2.858656000
C	1.013040000	-2.958277000	-2.158780000
H	0.575750000	-2.577534000	-3.083035000
H	1.158690000	-4.033519000	-2.314501000
C	-0.009337000	-2.748224000	-1.080971000
H	-1.038762000	-2.810732000	-1.411386000

C	0.210401000	-2.757065000	0.278564000
H	-0.661550000	-2.838481000	0.910474000
P	0.330105000	1.670282000	-0.910818000
O	-0.796295000	2.709853000	-0.445224000
O	0.468005000	2.162769000	-2.431025000
O	1.590208000	2.312491000	-0.164828000
C	-2.067934000	2.800261000	-1.091300000
C	1.056718000	1.400710000	-3.479248000
C	1.854758000	3.710818000	-0.251232000
H	-2.538402000	3.703556000	-0.711691000
H	-1.948396000	2.865352000	-2.170405000
H	-2.679462000	1.932124000	-0.855785000
H	0.660464000	1.793457000	-4.410873000
H	2.140889000	1.518544000	-3.466709000
H	0.787970000	0.348550000	-3.394026000
H	1.169510000	4.264946000	0.387693000
H	2.874410000	3.860785000	0.090197000
H	1.757484000	4.067880000	-1.275747000
Br	-1.767936000	-0.397910000	-2.509423000
P	-1.176596000	-0.026412000	1.326685000
O	-1.241916000	-1.217673000	2.432486000
O	-2.720790000	0.499934000	1.307436000
O	-0.560079000	1.208380000	2.162585000
C	-1.779824000	-0.967269000	3.723523000
C	-3.694796000	-0.346940000	0.697066000
C	-1.309890000	2.263717000	2.747191000
H	-1.854944000	-1.922981000	4.234268000
H	-1.122528000	-0.309619000	4.292963000
H	-2.770930000	-0.515148000	3.662267000
H	-3.345439000	-0.713728000	-0.269983000
H	-3.932496000	-1.189755000	1.348319000
H	-4.589842000	0.250891000	0.550013000
H	-2.060988000	1.895359000	3.445155000
H	-0.597811000	2.887684000	3.281195000
H	-1.804008000	2.856572000	1.979477000

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structure of IM6'

Ir	0.117321000	-0.596752000	-0.529399000
C	1.565751000	-2.995357000	1.023550000
H	2.195645000	-3.681310000	0.458671000
H	1.358373000	-3.491650000	1.970943000
C	2.301274000	-1.683260000	1.287030000
H	1.935445000	-1.252840000	2.221425000

H	3.370503000	-1.865725000	1.443309000
C	2.090048000	-0.652481000	0.210786000
H	2.419318000	0.329170000	0.527700000
C	2.154767000	-0.896888000	-1.214971000
H	2.563450000	-0.070580000	-1.786953000
C	2.452688000	-2.259904000	-1.816163000
H	3.122026000	-2.822469000	-1.162514000
H	3.004773000	-2.133492000	-2.746953000
C	1.174478000	-3.038433000	-2.105123000
H	0.758922000	-2.694761000	-3.053359000
H	1.372117000	-4.108982000	-2.231665000
C	0.100911000	-2.853210000	-1.073371000
H	-0.909950000	-2.977629000	-1.440104000
C	0.261950000	-2.802872000	0.292106000
H	-0.633207000	-2.903745000	0.887118000
P	0.232786000	1.594818000	-0.938719000
O	-0.879740000	2.598439000	-0.360367000
O	0.224614000	2.131214000	-2.451895000
O	1.531199000	2.252759000	-0.265099000
C	-2.161065000	2.707178000	-0.993023000
C	0.859641000	1.430078000	-3.519833000
C	1.714851000	3.668693000	-0.298316000
H	-2.857657000	3.050469000	-0.233281000
H	-2.106655000	3.430929000	-1.803973000
H	-2.488458000	1.747505000	-1.393279000
H	0.375208000	1.750635000	-4.436729000
H	1.918988000	1.687068000	-3.554270000
H	0.731372000	0.354139000	-3.408177000
H	1.062295000	4.151203000	0.427077000
H	2.752163000	3.859106000	-0.040808000
H	1.505580000	4.071495000	-1.288675000
Br	-1.768006000	-0.656272000	-2.598362000
P	-1.166367000	-0.086496000	1.260009000
O	-1.434405000	-1.314618000	2.296604000
O	-2.597450000	0.702154000	1.282654000
O	-0.353329000	0.979665000	2.173350000
C	-1.945708000	-1.039131000	3.596009000
C	-3.690512000	0.089036000	0.596228000
C	-0.919476000	2.123473000	2.802058000
H	-2.188574000	-1.991276000	4.058443000
H	-1.198553000	-0.526978000	4.202846000
H	-2.845461000	-0.424056000	3.547049000
H	-3.385751000	-0.276251000	-0.386987000

H	-4.09520000	-0.737928000	1.181829000
H	-4.459323000	0.848191000	0.479585000
H	-1.721383000	1.859823000	3.491242000
H	-0.114181000	2.600027000	3.355744000
H	-1.308042000	2.818081000	2.059003000

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structure of IM7'

Ir	0.958082000	12.747752000	5.395876000
C	1.995516000	11.030547000	7.806384000
H	2.908449000	10.452052000	7.692064000
H	1.489746000	10.615148000	8.675392000
C	2.313904000	12.503526000	8.086097000
H	1.477397000	12.959451000	8.615730000
H	3.168044000	12.582495000	8.764523000
C	2.567463000	13.317091000	6.856190000
H	2.448051000	14.387413000	6.989529000
C	3.202894000	12.899834000	5.696352000
H	3.481505000	13.682024000	5.001435000
C	3.871158000	11.565125000	5.488051000
H	4.258122000	11.190832000	6.432304000
H	4.740907000	11.713277000	4.851560000
C	2.954889000	10.530960000	4.825782000
H	2.940331000	10.699712000	3.748998000
H	3.361473000	9.524368000	4.958809000
C	1.538894000	10.573282000	5.309015000
H	0.821430000	10.128320000	4.626854000
C	1.109457000	10.833682000	6.601559000
H	0.072774000	10.608873000	6.825707000
P	-1.157929000	12.438287000	4.699630000
O	-2.086033000	13.695053000	5.026117000
O	-2.131913000	11.288008000	5.272868000
O	-1.166369000	12.210083000	3.109431000
C	-3.510764000	13.642179000	5.204127000
C	-1.999672000	9.915445000	4.898152000
C	-2.364045000	12.254051000	2.323065000
H	-3.872476000	14.658878000	5.087380000
H	-3.988609000	13.001766000	4.467117000
H	-3.749566000	13.277845000	6.199190000
H	-2.987530000	9.469320000	4.963991000
H	-1.630173000	9.814434000	3.878072000
H	-1.330486000	9.394419000	5.580418000
H	-2.770645000	13.264549000	2.308915000
H	-2.091250000	11.963071000	1.313934000

H	-3.116893000	11.563716000	2.703256000
P	0.717410000	14.909175000	4.799302000
O	-0.015536000	15.773508000	5.913162000
O	-0.140272000	15.332597000	3.504908000
O	2.149779000	15.593595000	4.570937000
C	-1.024731000	16.762517000	5.662269000
C	0.287935000	14.902347000	2.206662000
C	2.247000000	17.001978000	4.305413000
H	-1.364777000	17.103500000	6.633920000
H	-0.622057000	17.602723000	5.100482000
H	-1.852154000	16.327453000	5.109334000
H	-0.551533000	15.048655000	1.534316000
H	1.130438000	15.500618000	1.863776000
H	0.565447000	13.848729000	2.213840000
H	2.060975000	17.568838000	5.215432000
H	3.256771000	17.191666000	3.959241000
H	1.537090000	17.305839000	3.536949000

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structure of IM7

Ir	0.926292000	12.801597000	5.416560000
C	1.984787000	10.992388000	7.762772000
H	2.882296000	10.396317000	7.615297000
H	1.483117000	10.557662000	8.624832000
C	2.341932000	12.446883000	8.086212000
H	1.540127000	12.893659000	8.673365000
H	3.228459000	12.483713000	8.726118000
C	2.557876000	13.303312000	6.877785000
H	2.445362000	14.369072000	7.046309000
C	3.178989000	12.920087000	5.697910000
H	3.460558000	13.721043000	5.026253000
C	3.841568000	11.589570000	5.451555000
H	4.235687000	11.192748000	6.384213000
H	4.707330000	11.747744000	4.811789000
C	2.914529000	10.574763000	4.777309000
H	2.907642000	10.750549000	3.701654000
H	3.304587000	9.560626000	4.905482000
C	1.498516000	10.634765000	5.258419000
H	0.777075000	10.210611000	4.568111000
C	1.079881000	10.857385000	6.564082000
H	0.044393000	10.629795000	6.791724000
P	-1.207942000	12.468168000	4.742886000
O	-2.170296000	13.658083000	5.176757000
O	-2.085416000	11.234455000	5.289320000

O	-1.289864000	12.336822000	3.149867000
C	-3.556480000	13.526762000	5.521181000
C	-1.913996000	9.893343000	4.829870000
C	-2.530746000	12.421411000	2.440131000
H	-3.934502000	14.536242000	5.645180000
H	-4.118300000	13.020970000	4.739485000
H	-3.664152000	12.977996000	6.452228000
H	-2.883486000	9.407618000	4.888078000
H	-1.563514000	9.867081000	3.798510000
H	-1.212493000	9.358663000	5.467797000
H	-2.925541000	13.435178000	2.496662000
H	-2.321666000	12.173234000	1.405024000
H	-3.264250000	11.719008000	2.835876000
P	0.715042000	14.970223000	4.773963000
O	-0.177658000	15.881123000	5.712152000
O	0.045320000	15.279277000	3.347003000
O	2.148655000	15.678877000	4.723127000
C	-1.173285000	16.813107000	5.276924000
C	0.625452000	14.695300000	2.174797000
C	2.272490000	17.081107000	4.449309000
H	-1.645953000	17.193747000	6.176000000
H	-0.725078000	17.636217000	4.724381000
H	-1.910430000	16.318322000	4.650262000
H	-0.107495000	14.786579000	1.380018000
H	1.533356000	15.227475000	1.895261000
H	0.852566000	13.641084000	2.337988000
H	1.896609000	17.662233000	5.288985000
H	3.328747000	17.284618000	4.313310000
H	1.731219000	17.351942000	3.543708000

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structure of 2

Ir	0.639164000	12.937726000	5.795897000
C	2.210657000	10.736872000	7.505806000
H	2.893292000	10.046980000	7.010711000
H	1.960997000	10.268470000	8.456005000
C	2.884941000	12.080400000	7.757175000
H	2.492258000	12.504186000	8.682752000
H	3.958863000	11.950794000	7.925974000
C	2.644433000	13.074570000	6.652735000
H	2.892052000	14.092467000	6.926138000
C	2.777879000	12.780416000	5.256298000
H	3.100433000	13.622635000	4.656411000
C	3.237122000	11.434371000	4.722710000



H	3.905001000	10.967642000	5.447151000
H	3.845616000	11.591113000	3.833398000
C	2.072430000	10.522603000	4.379706000
H	1.730442000	10.737959000	3.367408000
H	2.367311000	9.467302000	4.372959000
C	0.899016000	10.691454000	5.297822000
H	-0.036699000	10.327576000	4.888884000
C	0.945277000	10.842555000	6.684269000
H	0.034007000	10.608891000	7.217198000
P	-1.139086000	12.633715000	4.369135000
O	-2.088810000	13.924845000	4.212445000
O	-2.184645000	11.427955000	4.592425000
O	-0.694423000	12.293839000	2.872723000
C	-3.513583000	13.867635000	4.186575000
C	-2.644849000	10.972718000	5.860031000
C	-1.636713000	12.233793000	1.796370000
H	-3.863698000	14.886806000	4.049771000
H	-3.880516000	13.249672000	3.369207000
H	-3.901344000	13.482607000	5.127852000
H	-3.553628000	11.497259000	6.150009000
H	-2.854289000	9.911413000	5.762740000
H	-1.894457000	11.124854000	6.636292000
H	-2.073926000	13.216421000	1.622632000
H	-1.085689000	11.926524000	0.913968000
H	-2.420449000	11.507336000	2.002939000
P	0.701155000	15.056262000	5.008962000
O	-0.454382000	16.027987000	5.506616000
O	0.588831000	15.304151000	3.426407000
O	2.073405000	15.770838000	5.424916000
C	-1.153847000	16.963459000	4.678696000
C	1.492854000	14.651417000	2.531216000
C	2.304245000	17.150033000	5.117766000
H	-1.869328000	17.464139000	5.323262000
H	-0.476802000	17.699515000	4.250753000
H	-1.671652000	16.442666000	3.878032000
H	1.114853000	14.820094000	1.528241000
H	2.492205000	15.077526000	2.619566000
H	1.526965000	13.580333000	2.732939000
H	1.671106000	17.784385000	5.736397000
H	3.345923000	17.353124000	5.341024000
H	2.112490000	17.356160000	4.065354000
P	-0.685153000	13.520570000	7.624905000
O	-2.249045000	13.742888000	7.326336000

O	-0.429733000	14.898153000	8.422702000
O	-0.644646000	12.398382000	8.777843000
C	-3.040840000	14.818269000	7.839433000
C	0.885671000	15.276160000	8.815376000
C	-1.438158000	12.526664000	9.962664000
H	-4.067103000	14.608476000	7.553099000
H	-2.975702000	14.887991000	8.922582000
H	-2.722115000	15.763052000	7.404423000
H	0.790751000	16.189399000	9.393794000
H	1.351963000	14.508800000	9.434541000
H	1.509272000	15.463252000	7.940880000
H	-2.496228000	12.428548000	9.723455000
H	-1.145535000	11.722682000	10.629196000
H	-1.260802000	13.484393000	10.450212000

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structure of TS\_1\_IM8

Ir	-0.926284000	0.509211000	-1.234856000
C	-2.542649000	0.912840000	-2.544704000
C	-2.337522000	2.052356000	-1.723697000
C	-2.887841000	-0.205341000	-1.695350000
H	-2.424038000	0.871939000	-3.615331000
C	-2.518490000	1.631774000	-0.362606000
H	-2.036249000	3.032488000	-2.052443000
C	-2.913528000	0.259742000	-0.355662000
H	-2.382132000	2.250769000	0.510048000
H	-3.126312000	-0.328917000	0.520558000
Br	0.970656000	1.553670000	-2.306129000
H	-3.100489000	-1.207197000	-2.030770000
C	0.581872000	-1.257696000	-0.729423000
C	-0.345143000	-1.151020000	0.294632000
H	0.230879000	-1.844290000	-1.575502000
C	2.076707000	-1.133490000	-0.662802000
C	-0.150977000	-0.604426000	1.677467000
H	-1.231837000	-1.764362000	0.179593000
H	2.427127000	-0.186747000	-1.070524000
H	2.450002000	-1.882469000	-1.361173000
C	2.721824000	-1.371808000	0.709983000
C	0.566892000	0.739552000	1.820461000
H	0.351272000	-1.362165000	2.284122000
H	-1.140931000	-0.508302000	2.124457000
H	2.158187000	-2.126068000	1.262523000
H	3.689649000	-1.832824000	0.528259000
C	2.945140000	-0.135479000	1.529289000

H	0.271417000	1.400519000	0.987907000
H	0.155461000	1.234119000	2.700945000
C	2.051852000	0.753799000	1.951508000
H	3.979870000	0.077058000	1.767222000
H	2.435615000	1.622767000	2.471997000

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structure of IM8

Ir	0.940989000	12.690584000	4.361801000
C	1.457323000	14.783873000	4.275835000
C	0.118003000	14.659138000	4.692795000
C	1.575540000	14.163054000	2.973812000
H	2.265396000	15.210901000	4.846844000
C	-0.604751000	13.957532000	3.653854000
H	-0.285871000	14.972216000	5.641607000
C	0.286454000	13.713330000	2.570519000
H	-1.648028000	13.688216000	3.688897000
H	0.044487000	13.216647000	1.645396000
Br	1.663441000	11.921012000	6.517249000
H	2.484545000	14.078073000	2.400581000
C	1.517021000	10.704601000	3.244959000
C	0.208631000	10.541063000	3.665206000
H	1.626685000	11.132858000	2.251338000
C	2.759910000	10.044021000	3.753502000
C	-0.355151000	9.644865000	4.726963000
H	-0.538747000	10.917130000	2.972711000
H	2.742708000	9.913072000	4.827484000
H	3.612340000	10.688706000	3.538811000
C	2.976783000	8.701242000	3.047243000
C	0.546488000	8.524340000	5.240354000
H	-1.248047000	9.200825000	4.278722000
H	-0.739387000	10.236371000	5.560194000
H	3.077062000	8.871672000	1.972155000
H	3.953050000	8.315948000	3.352795000
C	1.938860000	7.650309000	3.263888000
H	1.396021000	8.936876000	5.777981000
H	-0.022597000	7.977973000	5.990606000
C	0.954773000	7.565834000	4.156212000
H	2.030142000	6.816319000	2.577047000
H	0.333773000	6.680108000	4.089219000

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structure of IM1'

Ir	1.496825000	12.852628000	4.583479000
C	0.787593000	10.228493000	6.184438000

H	1.615108000	9.567770000	6.436288000
H	-0.109242000	9.615992000	6.255182000
C	0.696124000	11.387013000	7.170379000
H	-0.336809000	11.736391000	7.219771000
H	0.942143000	11.066297000	8.186901000
C	1.566980000	12.549936000	6.780283000
H	1.286602000	13.493862000	7.236790000
C	2.873441000	12.474193000	6.280751000
H	3.461807000	13.378000000	6.365011000
C	3.666860000	11.192685000	6.135641000
H	3.392301000	10.514860000	6.943573000
H	4.717060000	11.426604000	6.291480000
C	3.505256000	10.513147000	4.770699000
H	4.294143000	10.853429000	4.105677000
H	3.624926000	9.430386000	4.863952000
C	2.189976000	10.811958000	4.107882000
H	2.192337000	10.738930000	3.026767000
C	0.950335000	10.706741000	4.756136000
H	0.085118000	10.566579000	4.118736000
C	0.875325000	14.951120000	4.531571000
C	-0.212460000	14.132531000	4.974346000
C	0.885065000	14.938949000	3.013466000
H	1.308067000	15.746657000	5.118353000
C	-0.525909000	13.234986000	3.916051000
H	-0.681084000	14.150907000	5.945251000
C	0.371540000	13.522034000	2.838112000
H	-1.277152000	12.462051000	3.944564000
H	0.347128000	13.022377000	1.882344000
Br	3.749485000	13.557315000	3.404980000
H	1.896339000	15.058491000	2.609594000
P	-0.090713000	16.213813000	2.226845000
O	0.756254000	17.516189000	2.232428000
O	-1.431481000	16.651077000	2.919017000
O	-0.392264000	15.649624000	0.800018000
C	0.225998000	18.864757000	2.167900000
H	1.087251000	19.520513000	2.157762000
H	-0.355802000	19.003304000	1.260650000
H	-0.389423000	19.059035000	3.040464000
C	-2.630237000	15.844552000	2.965076000
H	-2.715961000	15.402344000	3.952576000
H	-3.467403000	16.510633000	2.784940000
H	-2.609667000	15.063036000	2.208261000
C	-1.094095000	16.371398000	-0.238030000

H	-0.418273000	17.079419000	-0.709034000
H	-1.413715000	15.632433000	-0.962984000
H	-1.962380000	16.887677000	0.167331000

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structure of IMs'

Ir	0.946972000	12.737320000	4.840718000
C	1.383892000	9.940100000	6.243962000
H	2.408728000	9.590056000	6.331047000
H	0.753833000	9.065912000	6.388879000
C	1.059964000	10.966572000	7.335901000
H	-0.008638000	10.957811000	7.547781000
H	1.542553000	10.682244000	8.275270000
C	1.456321000	12.363239000	6.985979000
H	0.934197000	13.138826000	7.537305000
C	2.602967000	12.751115000	6.286354000
H	2.866198000	13.801704000	6.370566000
C	3.724995000	11.828605000	5.861152000
H	3.816430000	11.007331000	6.566546000
H	4.661129000	12.377487000	5.927474000
C	3.552921000	11.315112000	4.426993000
H	3.960447000	12.045764000	3.728030000
H	4.143226000	10.409520000	4.266047000
C	2.121947000	11.053717000	4.042685000
H	1.922545000	11.048258000	2.974894000
C	1.151556000	10.473926000	4.857221000
H	0.243584000	10.141658000	4.366013000
C	0.204900000	14.793129000	4.817204000
C	-0.837102000	13.932202000	5.207657000
C	0.422911000	14.677562000	3.322337000
H	0.600574000	15.597750000	5.418064000
C	-1.104151000	13.022248000	4.124986000
H	-1.330913000	13.929251000	6.166804000
C	-0.228355000	13.334019000	3.073940000
H	-1.831353000	12.225759000	4.133889000
H	-0.199054000	12.831432000	2.119944000
H	1.493862000	14.659742000	3.070960000
P	-0.178060000	16.071627000	2.325997000
O	0.979849000	17.090641000	2.371561000
O	-1.417765000	16.814802000	2.893641000
O	-0.464648000	15.430273000	0.942252000
C	0.900327000	18.516146000	2.035919000
H	1.748182000	18.979459000	2.523383000
H	0.978266000	18.628609000	0.959483000

H	-0.029441000	18.932074000	2.410354000
C	-2.817940000	16.448433000	2.714608000
H	-3.340375000	17.348556000	2.410807000
H	-2.922769000	15.676646000	1.956501000
H	-3.197372000	16.102210000	3.669514000
C	-0.829447000	16.167043000	-0.270494000
H	0.080588000	16.440208000	-0.794141000
H	-1.420072000	15.486077000	-0.870793000
H	-1.413568000	17.050310000	-0.023148000

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structure of 3

Ir	1.213437000	12.465093000	4.373651000
C	1.492710000	10.886995000	7.108863000
H	2.400161000	10.310149000	7.280051000
H	0.747574000	10.471376000	7.784436000
C	1.718395000	12.357973000	7.436570000
H	0.781353000	12.812996000	7.759965000
H	2.400888000	12.475347000	8.282936000
C	2.246221000	13.137003000	6.269471000
H	2.077872000	14.205973000	6.315958000
C	3.248238000	12.719849000	5.399940000
H	3.719778000	13.497903000	4.816654000
C	4.021064000	11.430058000	5.511088000
H	4.172121000	11.209083000	6.567792000
H	5.011879000	11.597411000	5.096866000
C	3.382671000	10.231361000	4.793175000
H	3.829849000	10.118132000	3.810589000
H	3.599294000	9.308418000	5.337534000
C	1.898764000	10.349971000	4.627021000
H	1.478671000	9.813425000	3.784326000
C	1.036432000	10.674930000	5.682170000
H	0.004498000	10.369309000	5.566694000
C	-0.228310000	14.171638000	4.780882000
C	-0.882772000	12.903109000	4.926230000
C	0.278339000	14.266174000	3.452753000
C	-0.857255000	12.238332000	3.638679000
C	-0.180508000	13.092064000	2.728578000
Br	2.919350000	12.385620000	2.411741000
C	-1.680965000	12.472401000	6.101119000
H	-1.268526000	12.834251000	7.039241000
H	-2.691805000	12.874856000	6.020191000
H	-1.777238000	11.391814000	6.164732000
C	-1.552978000	10.973547000	3.294715000

H	-1.585870000	10.277909000	4.130009000
H	-2.586468000	11.179428000	3.013811000
H	-1.082940000	10.471405000	2.453505000
C	-0.074984000	12.878859000	1.268788000
H	0.098451000	11.836632000	1.015814000
H	-1.020203000	13.177774000	0.810814000
H	0.719810000	13.466873000	0.823776000
C	0.981360000	15.423902000	2.848962000
H	1.715956000	15.095290000	2.117381000
H	0.273240000	16.079258000	2.340914000
H	1.498793000	16.017440000	3.598341000
C	-0.169688000	15.226797000	5.817848000
H	0.667616000	15.904008000	5.673313000
H	-1.078754000	15.827683000	5.763353000
H	-0.121778000	14.819041000	6.825216000

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structure of TS\_3\_IM9

Ir	1.697112000	12.771369000	4.613190000
C	0.709648000	10.151014000	6.079193000
H	1.464527000	9.435468000	6.403390000
H	-0.223335000	9.592065000	6.030611000
C	0.577045000	11.284659000	7.088328000
H	-0.438375000	11.684941000	7.054858000
H	0.707714000	10.919974000	8.111533000
C	1.535633000	12.411987000	6.831630000
H	1.245461000	13.359033000	7.269465000
C	2.882168000	12.285309000	6.505382000
H	3.494787000	13.160478000	6.671053000
C	3.628137000	10.975584000	6.413635000
H	3.247844000	10.306706000	7.186743000
H	4.668296000	11.161978000	6.668957000
C	3.571010000	10.296499000	5.038113000
H	4.468478000	10.541054000	4.478312000
H	3.567195000	9.208896000	5.153839000
C	2.382332000	10.697697000	4.215097000
H	2.523154000	10.644956000	3.141552000
C	1.066763000	10.648186000	4.694789000
H	0.289251000	10.551720000	3.948106000
C	1.230269000	14.924290000	4.337676000
C	0.094889000	14.268594000	4.915457000
C	1.177843000	14.663776000	2.872636000
C	-0.323714000	13.247507000	3.999379000
C	0.544092000	13.339964000	2.835727000

Br	4.196528000	13.296558000	3.948452000
P	-0.286496000	16.219071000	2.165050000
O	0.464674000	17.605506000	2.119355000
O	-1.595270000	16.628261000	3.003821000
O	-0.788010000	15.824154000	0.710613000
C	-0.126022000	18.907842000	2.304146000
H	0.647354000	19.626334000	2.058863000
H	-0.981734000	19.048270000	1.649186000
H	-0.435239000	19.030786000	3.338147000
C	-2.734394000	15.764988000	3.084568000
H	-2.716758000	15.221185000	4.026521000
H	-3.620470000	16.391270000	3.050020000
H	-2.761653000	15.058635000	2.254732000
C	-1.517559000	16.722183000	-0.149310000
H	-0.862078000	17.518662000	-0.493069000
H	-1.854602000	16.138236000	-0.997782000
H	-2.377597000	17.142560000	0.369596000
C	0.368177000	12.547414000	1.587481000
H	1.297313000	12.482041000	1.025301000
H	0.044299000	11.530390000	1.798531000
H	-0.380221000	12.997265000	0.929768000
C	-1.541551000	12.404138000	4.134381000
H	-1.723741000	12.106432000	5.164930000
H	-2.423605000	12.949120000	3.795690000
H	-1.485947000	11.503872000	3.528861000
C	-0.593178000	14.652286000	6.172205000
H	-1.072904000	13.808340000	6.663408000
H	0.077764000	15.129684000	6.881257000
H	-1.373019000	15.382592000	5.947046000
C	1.972638000	16.059253000	4.947062000
H	2.020470000	15.968495000	6.029994000
H	2.995614000	16.094426000	4.577947000
H	1.499465000	17.017846000	4.717366000
C	2.256599000	15.031901000	1.900426000
H	3.089661000	14.338175000	1.989441000
H	1.884515000	14.984205000	0.878731000
H	2.640691000	16.031831000	2.084296000

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structure of IM9

Ir	1.627440000	12.836868000	4.572215000
C	0.685788000	10.198982000	6.044879000
H	1.447862000	9.484099000	6.353857000
H	-0.244832000	9.635044000	6.004069000



C	0.559114000	11.321459000	7.067686000
H	-0.459141000	11.715883000	7.048627000
H	0.700790000	10.943579000	8.084871000
C	1.508909000	12.458113000	6.816554000
H	1.213048000	13.400364000	7.260514000
C	2.847135000	12.345512000	6.472065000
H	3.455236000	13.226033000	6.624006000
C	3.602136000	11.043487000	6.354213000
H	3.232705000	10.358259000	7.118300000
H	4.642714000	11.233584000	6.605781000
C	3.540829000	10.387771000	4.968534000
H	4.425312000	10.662417000	4.401757000
H	3.562056000	9.298168000	5.064301000
C	2.334135000	10.780132000	4.167171000
H	2.461363000	10.733064000	3.091287000
C	1.023111000	10.708046000	4.659100000
H	0.242572000	10.592739000	3.918319000
C	1.179885000	14.982293000	4.306946000
C	0.045824000	14.328648000	4.894580000
C	1.031082000	14.843991000	2.783155000
C	-0.380528000	13.311732000	3.976246000
C	0.494652000	13.414871000	2.814729000
Br	4.143908000	13.424237000	3.913354000
P	-0.177789000	16.100425000	2.220637000
O	0.556049000	17.473069000	2.163583000
O	-1.414772000	16.393407000	3.146184000
O	-0.692200000	15.645232000	0.813262000
C	-0.022459000	18.768603000	2.437347000
H	0.773671000	19.486262000	2.281613000
H	-0.844628000	18.974714000	1.757629000
H	-0.369789000	18.809074000	3.465073000
C	-2.643467000	15.644208000	3.135071000
H	-2.761205000	15.166861000	4.102559000
H	-3.455416000	16.346298000	2.972072000
H	-2.640790000	14.892112000	2.348342000
C	-1.413709000	16.512521000	-0.088174000
H	-0.747260000	17.283313000	-0.466093000
H	-1.753817000	15.889338000	-0.906175000
H	-2.270187000	16.963449000	0.409559000
C	0.321422000	12.600241000	1.576957000
H	1.225999000	12.605343000	0.971908000
H	0.103940000	11.561060000	1.816703000
H	-0.494640000	12.963086000	0.946170000

C	-1.580261000	12.442159000	4.126251000
H	-1.739543000	12.138962000	5.159167000
H	-2.484601000	12.955949000	3.798837000
H	-1.506734000	11.542555000	3.521612000
C	-0.624443000	14.700924000	6.165052000
H	-1.099846000	13.852931000	6.653796000
H	0.059016000	15.166221000	6.870258000
H	-1.402711000	15.439777000	5.961711000
C	1.938436000	16.093340000	4.944504000
H	2.052100000	15.929466000	6.014124000
H	2.940043000	16.166288000	4.524855000
H	1.444094000	17.060648000	4.813323000
C	2.221480000	15.076584000	1.854510000
H	2.888239000	14.223521000	1.892666000
H	1.892258000	15.204697000	0.823436000
H	2.792354000	15.955824000	2.140221000

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structure of TS\_IM9\_IM10

Ir	1.428953000	-0.921688000	0.928767000
C	0.270213000	-3.589319000	2.049576000
H	0.966158000	-4.376234000	2.341222000
H	-0.673147000	-4.096554000	1.854168000
C	0.098883000	-2.561928000	3.162072000
H	-0.935916000	-2.217483000	3.188337000
H	0.285303000	-2.991169000	4.150980000
C	0.989464000	-1.366468000	2.941383000
H	0.666088000	-0.470388000	3.461204000
C	2.404766000	-1.482310000	2.712533000
H	3.004943000	-0.624713000	2.993999000
C	3.141333000	-2.807219000	2.733238000
H	2.608253000	-3.507294000	3.377696000
H	4.118983000	-2.666845000	3.187971000
C	3.283517000	-3.343240000	1.317648000
H	4.217297000	-2.985483000	0.887712000
H	3.328855000	-4.435301000	1.289114000
C	2.163508000	-2.833882000	0.452742000
H	2.399394000	-2.812005000	-0.607963000
C	0.764796000	-2.922574000	0.778612000
H	0.092085000	-2.995582000	-0.072945000
C	0.417077000	1.002003000	0.171216000
C	-0.569213000	0.210138000	0.820909000
C	0.187728000	0.843489000	-1.344174000
C	-1.245437000	-0.613225000	-0.188152000

C	-0.788033000	-0.327184000	-1.430019000
Br	3.650603000	0.107468000	0.113370000
P	-0.790546000	2.283495000	-1.830871000
O	0.097131000	3.555381000	-1.834877000
O	-1.983177000	2.619875000	-0.874665000
O	-1.337256000	2.003205000	-3.271051000
C	-0.236804000	4.893157000	-1.406690000
H	0.638167000	5.283561000	-0.899616000
H	-0.457493000	5.495319000	-2.282830000
H	-1.086355000	4.878049000	-0.731094000
C	-3.258016000	1.941597000	-0.896887000
H	-3.351188000	1.360536000	0.014619000
H	-4.028120000	2.705823000	-0.932275000
H	-3.337457000	1.284144000	-1.759885000
C	-1.935799000	3.044235000	-4.073898000
H	-1.166205000	3.731350000	-4.414857000
H	-2.391307000	2.551319000	-4.924029000
H	-2.697486000	3.579248000	-3.509095000
C	-1.056555000	-1.053992000	-2.696432000
H	-0.133099000	-1.440643000	-3.131806000
H	-1.715401000	-1.902167000	-2.532097000
H	-1.512744000	-0.426637000	-3.461963000
C	-2.264780000	-1.623945000	0.189873000
H	-1.930715000	-2.222921000	1.036564000
H	-3.192111000	-1.142623000	0.507771000
H	-2.512611000	-2.297550000	-0.625723000
C	-1.235897000	0.588499000	2.102498000
H	-1.647765000	-0.266123000	2.635029000
H	-0.565474000	1.113259000	2.777632000
H	-2.065562000	1.272809000	1.902708000
C	0.992308000	2.258857000	0.755842000
H	1.301802000	2.102869000	1.786859000
H	1.879363000	2.579814000	0.213529000
H	0.270962000	3.082741000	0.769437000
C	1.379147000	0.764426000	-2.294216000
H	1.896561000	-0.178788000	-2.136677000
H	1.059734000	0.809883000	-3.334424000
H	2.098291000	1.556923000	-2.107616000
63			
structure of IM10			
Ir	0.487107000	12.447899000	5.670702000
C	2.741923000	10.793134000	6.858247000
H	3.341974000	10.184521000	6.182450000

H	2.875804000	10.355750000	7.845177000
C	3.225930000	12.243358000	6.865097000
H	3.068226000	12.670453000	7.856720000
H	4.303685000	12.297125000	6.686836000
C	2.475621000	13.096454000	5.874398000
H	2.493240000	14.159438000	6.107698000
C	2.248210000	12.746912000	4.515972000
H	2.098565000	13.567521000	3.821432000
C	2.783057000	11.477915000	3.884081000
H	3.697927000	11.171143000	4.389758000
H	3.072320000	11.675125000	2.853630000
C	1.736441000	10.364909000	3.921826000
H	1.111965000	10.417756000	3.030308000
H	2.203945000	9.375973000	3.897188000
C	0.837542000	10.475349000	5.117809000
H	-0.118721000	9.971579000	5.014481000
C	1.282971000	10.698277000	6.462686000
H	0.612530000	10.343831000	7.239155000
C	-0.937852000	15.208870000	5.427716000
C	0.020829000	15.376537000	4.475695000
Br	-1.787352000	11.830021000	6.470931000
C	1.171098000	16.083417000	5.038870000
C	0.951502000	16.357963000	6.345830000
C	-0.429326000	15.839979000	6.714594000
P	-1.460096000	17.281747000	6.971638000
O	-0.794534000	18.111347000	8.114965000
O	-1.674753000	18.166040000	5.703785000
O	-2.882209000	16.848111000	7.402469000
C	-1.477682000	19.214173000	8.753688000
C	-0.663737000	18.999233000	5.093180000
C	-4.161008000	17.333645000	6.937002000
H	-0.751327000	19.685998000	9.403695000
H	-2.310874000	18.838233000	9.341043000
H	-1.827487000	19.929313000	8.011590000
H	-0.287412000	18.494351000	4.209197000
H	0.153313000	19.192357000	5.784807000
H	-1.149959000	19.928644000	4.816536000
H	-4.073022000	17.741421000	5.935327000
H	-4.519543000	18.092624000	7.625910000
H	-4.830523000	16.481469000	6.938994000
C	2.381794000	16.408093000	4.243528000
H	2.901338000	15.507242000	3.915824000
H	2.118960000	16.954454000	3.336518000

H	3.092293000	17.012136000	4.799847000
C	1.923282000	16.869346000	7.344597000
H	1.590694000	17.772656000	7.853706000
H	2.103793000	16.127967000	8.126261000
H	2.882764000	17.083157000	6.882430000
C	-0.462200000	14.943097000	7.956052000
H	-1.440646000	14.490606000	8.097132000
H	0.248848000	14.126541000	7.808961000
H	-0.178650000	15.487030000	8.855303000
C	-0.115420000	15.045903000	3.033794000
H	0.828020000	14.731331000	2.592724000
H	-0.847600000	14.261009000	2.863627000
H	-0.443446000	15.922859000	2.470165000
C	-2.355862000	14.827120000	5.190712000
H	-2.843602000	14.452107000	6.085804000
H	-2.928713000	15.680043000	4.811229000
H	-2.431160000	14.039209000	4.445964000

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structure of IM11

Ir	0.478110000	12.391262000	5.698383000
C	2.769915000	10.776792000	6.855886000
H	3.362540000	10.172313000	6.168612000
H	2.921546000	10.338107000	7.840256000
C	3.243978000	12.231663000	6.856105000
H	3.118066000	12.650403000	7.854207000
H	4.314578000	12.293142000	6.638839000
C	2.447836000	13.080766000	5.896488000
H	2.424237000	14.139951000	6.147204000
C	2.211231000	12.743229000	4.535998000
H	2.015261000	13.567894000	3.855900000
C	2.771991000	11.493288000	3.888281000
H	3.700826000	11.205912000	4.381279000
H	3.042927000	11.704136000	2.855332000
C	1.754632000	10.350972000	3.933687000
H	1.128273000	10.383833000	3.042389000
H	2.248992000	9.374375000	3.914110000
C	0.848836000	10.450869000	5.129379000
H	-0.092704000	9.918518000	5.024296000
C	1.303742000	10.675359000	6.479941000
H	0.652953000	10.301142000	7.265093000
Br	-1.874856000	12.120516000	6.304916000

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structure of IM12

C	-0.968389000	15.266780000	5.371334000
C	-0.018082000	15.446440000	4.428729000
C	1.142409000	16.123919000	5.009043000
C	0.925825000	16.384790000	6.317762000
C	-0.458583000	15.864010000	6.670153000
P	-1.485652000	17.294445000	6.968452000
O	-0.843922000	18.061226000	8.168616000
O	-1.681634000	18.248520000	5.750242000
O	-2.926341000	16.833766000	7.326244000
C	-1.492493000	19.174759000	8.821317000
C	-0.648335000	19.070953000	5.163010000
C	-4.160365000	17.472516000	6.927355000
H	-0.765612000	19.590961000	9.507892000
H	-2.360143000	18.822944000	9.373071000
H	-1.784136000	19.928997000	8.092981000
H	-0.274106000	18.573945000	4.273794000
H	0.164969000	19.237158000	5.865841000
H	-1.114485000	20.014020000	4.898791000
H	-4.196849000	17.572227000	5.847148000
H	-4.249266000	18.448663000	7.395750000
H	-4.954782000	16.822360000	7.272762000
C	2.362548000	16.422844000	4.219838000
H	2.782231000	15.517335000	3.782029000
H	2.137149000	17.084541000	3.381818000
H	3.138132000	16.896626000	4.813613000
C	1.870475000	16.958463000	7.310386000
H	1.626162000	17.979542000	7.606313000
H	1.891879000	16.374245000	8.230687000
H	2.882400000	16.973332000	6.915745000
C	-0.490445000	14.912197000	7.868221000
H	-1.494916000	14.546519000	8.066746000
H	0.145870000	14.059511000	7.644503000
H	-0.116359000	15.389165000	8.770914000
C	-0.064390000	15.017303000	3.009294000
H	0.777956000	14.371508000	2.762261000
H	-0.977942000	14.482976000	2.767510000
H	0.002736000	15.873265000	2.336210000
C	-2.287524000	14.598145000	5.236728000
H	-2.543324000	14.015681000	6.121111000
H	-3.108565000	15.300992000	5.078589000
H	-2.294214000	13.919787000	4.387905000

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structure of TS\_3\_IM13

Ir	-0.928621000	0.359926000	-1.195261000
C	-2.497388000	0.792810000	-2.587099000
C	-2.278755000	1.940348000	-1.771332000
C	-2.887752000	-0.312707000	-1.717922000
C	-2.532580000	1.546561000	-0.395852000
C	-2.980919000	0.184390000	-0.380573000
Br	0.967125000	1.188821000	-2.490777000
C	0.516999000	-1.356809000	-0.478514000
C	-0.324924000	-1.006678000	0.566654000
H	0.076882000	-2.073365000	-1.168957000
C	2.017848000	-1.317409000	-0.535027000
C	0.013396000	-0.233474000	1.808563000
H	-1.234598000	-1.588915000	0.646596000
H	2.383234000	-0.478777000	-1.125344000
H	2.300797000	-2.199004000	-1.110228000
C	2.751543000	-1.353209000	0.813906000
C	0.809522000	1.064972000	1.657923000
H	0.521373000	-0.899822000	2.510486000
H	-0.931833000	0.006076000	2.298364000
H	2.187091000	-1.953779000	1.529809000
H	3.675170000	-1.906146000	0.659803000
C	3.106838000	-0.008243000	1.375260000
H	0.488363000	1.588229000	0.743021000
H	0.495410000	1.731557000	2.462690000
C	2.299629000	1.000200000	1.686791000
H	4.167527000	0.174689000	1.494119000
H	2.770301000	1.920324000	2.011580000
C	-3.232395000	-1.678211000	-2.175112000
H	-3.073771000	-2.419700000	-1.396121000
H	-4.285105000	-1.723245000	-2.458911000
H	-2.651256000	-1.968913000	-3.046244000
C	-3.510732000	-0.543862000	0.795979000
H	-2.994580000	-0.280011000	1.716098000
H	-4.561127000	-0.285886000	0.935617000
H	-3.462815000	-1.622286000	0.672107000
C	-2.452917000	2.447768000	0.775074000
H	-1.669930000	3.192545000	0.660290000
H	-3.396384000	2.985277000	0.887003000
H	-2.278283000	1.902310000	1.698824000
C	-1.900014000	3.300170000	-2.220026000
H	-1.402524000	3.281429000	-3.184777000
H	-2.790031000	3.923485000	-2.310717000
H	-1.229702000	3.782853000	-1.513262000

C	-2.369011000	0.710593000	-4.059607000
H	-3.354587000	0.809407000	-4.516955000
H	-1.733114000	1.496540000	-4.454426000
H	-1.958520000	-0.244907000	-4.376006000

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structure of IM13

Ir	0.934363000	12.640348000	4.361034000
C	1.464119000	14.739731000	4.311947000
C	0.111449000	14.613328000	4.717054000
C	1.590694000	14.126219000	2.992053000
C	-0.609776000	13.920026000	3.653197000
C	0.293785000	13.685884000	2.565386000
Br	1.686679000	11.897047000	6.548570000
C	1.480595000	10.666165000	3.231862000
C	0.190161000	10.495266000	3.697398000
H	1.552328000	11.070014000	2.225295000
C	2.750542000	10.037779000	3.718058000
C	-0.330462000	9.608212000	4.790451000
H	-0.582891000	10.845390000	3.019985000
H	2.766368000	9.938522000	4.795808000
H	3.583306000	10.695226000	3.463858000
C	2.977521000	8.682422000	3.042082000
C	0.604676000	8.509473000	5.292783000
H	-1.229995000	9.142444000	4.378878000
H	-0.691324000	10.207419000	5.628633000
H	3.056206000	8.829280000	1.961481000
H	3.964186000	8.316667000	3.338702000
C	1.958417000	7.621001000	3.297721000
H	1.463225000	8.946356000	5.795227000
H	0.069303000	7.966442000	6.070070000
C	0.995523000	7.539807000	4.213350000
H	2.044144000	6.777501000	2.621746000
H	0.382292000	6.646824000	4.172803000
C	-2.058271000	13.612709000	3.672144000
H	-2.396170000	13.318812000	4.662970000
H	-2.629357000	14.497780000	3.386834000
H	-2.316358000	12.822089000	2.973105000
C	-0.056325000	13.117849000	1.240127000
H	-0.435685000	13.903275000	0.586141000
H	0.803397000	12.677558000	0.742233000
H	-0.833543000	12.360059000	1.307658000
C	2.842809000	14.067297000	2.203701000
H	2.989879000	15.006034000	1.667127000



H	3.712342000	13.920943000	2.839709000
H	2.821925000	13.271435000	1.464065000
C	2.566915000	15.376868000	5.066762000
H	2.709367000	16.401207000	4.719925000
H	2.361426000	15.410929000	6.132172000
H	3.507916000	14.851981000	4.923355000
C	-0.488196000	15.085418000	5.985559000
H	0.256624000	15.206182000	6.766020000
H	-0.969215000	16.051973000	5.829108000
H	-1.249447000	14.400416000	6.350122000

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structure of IM14

Ir	0.978164000	12.566173000	4.588067000
C	1.973510000	14.409841000	3.825819000
C	0.728038000	14.748157000	4.440109000
C	1.702001000	13.522354000	2.734850000
C	-0.336713000	14.152949000	3.645488000
C	0.257789000	13.400717000	2.610195000
Br	-0.676982000	12.483346000	6.566906000
C	1.414914000	10.577897000	3.547441000
C	0.229509000	10.408728000	4.268879000
H	1.280758000	10.893804000	2.519274000
C	2.713687000	9.857845000	3.742298000
C	-0.006597000	9.449482000	5.409803000
H	-0.671314000	10.664967000	3.721178000
H	2.888869000	9.627910000	4.788148000
H	3.536870000	10.503242000	3.435706000
C	2.749823000	8.593192000	2.873515000
C	0.784836000	8.134006000	5.343535000
H	-1.072338000	9.223651000	5.407946000
H	0.175957000	9.920593000	6.371789000
H	2.828896000	8.903853000	1.828484000
H	3.685672000	8.062326000	3.069955000
C	1.590951000	7.649825000	2.985144000
H	1.808657000	8.299117000	5.673834000
H	0.350775000	7.466083000	6.087000000
C	0.761106000	7.458016000	4.007594000
H	1.427005000	7.044240000	2.101294000
H	-0.030359000	6.731203000	3.864352000
C	-1.784573000	14.364128000	3.869745000
H	-2.014782000	14.465536000	4.926868000
H	-2.103064000	15.279067000	3.368090000
H	-2.382233000	13.546767000	3.475252000

C	-0.459182000	12.689092000	1.523254000
H	-0.537974000	13.334037000	0.647404000
H	0.055953000	11.787343000	1.199537000
H	-1.469548000	12.415085000	1.813999000
C	2.707096000	13.029000000	1.759677000
H	2.901213000	13.792167000	1.004907000
H	3.655223000	12.796911000	2.239318000
H	2.370263000	12.140593000	1.231140000
C	3.304092000	14.944986000	4.204658000
H	3.446035000	15.921734000	3.740681000
H	3.397927000	15.080766000	5.279874000
H	4.110896000	14.301328000	3.867373000
C	0.531210000	15.703932000	5.557577000
H	1.427092000	15.795423000	6.166859000
H	0.294840000	16.695471000	5.169619000
H	-0.288872000	15.394954000	6.202175000
P	2.578408000	12.155416000	6.125795000
O	2.873760000	13.275937000	7.226560000
O	4.016715000	12.111841000	5.442395000
O	2.362612000	10.807077000	6.938730000
C	2.065621000	13.497050000	8.393285000
C	5.245786000	12.466981000	6.095431000
C	3.337125000	10.255484000	7.831979000
H	1.264940000	14.195352000	8.167724000
H	1.627613000	12.567491000	8.749322000
H	2.725568000	13.913717000	9.148171000
H	6.044683000	12.135821000	5.440387000
H	5.301480000	13.543757000	6.232419000
H	5.345329000	11.980966000	7.062328000
H	3.711908000	11.008556000	8.524151000
H	2.839234000	9.470332000	8.391103000
H	4.163722000	9.827417000	7.266345000

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structure of COD

C	1.402632000	10.631816000	3.185624000
C	0.170422000	10.437232000	3.649778000
H	1.491883000	11.306680000	2.340759000
C	2.696318000	10.022829000	3.640253000
C	-0.322215000	9.570981000	4.762639000
H	-0.619126000	10.990859000	3.151709000
H	2.755997000	9.975846000	4.724411000
H	3.512626000	10.679233000	3.337756000
C	2.963341000	8.641653000	3.039715000

C	0.625904000	8.495861000	5.296888000
H	-1.241587000	9.085736000	4.422410000
H	-0.643610000	10.209280000	5.592344000
H	3.023455000	8.741157000	1.952053000
H	3.963270000	8.308753000	3.337117000
C	1.983303000	7.555076000	3.340915000
H	1.493722000	8.959987000	5.757999000
H	0.114963000	7.977234000	6.108485000
C	1.026445000	7.484441000	4.263554000
H	2.084253000	6.690701000	2.692362000
H	0.428343000	6.579195000	4.260086000

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structure of IM15

Ir	0.991523000	12.948447000	4.791162000
C	2.024678000	14.559795000	3.755452000
C	0.774993000	15.006720000	4.313627000
C	1.722137000	13.498036000	2.849874000
C	-0.315895000	14.312913000	3.639552000
C	0.265408000	13.380208000	2.756023000
Br	-0.626372000	11.571021000	5.963241000
C	-1.759284000	14.547534000	3.879961000
H	-1.960884000	14.774809000	4.923754000
H	-2.107527000	15.394093000	3.287649000
H	-2.359166000	13.683683000	3.609640000
C	-0.442761000	12.410372000	1.891561000
H	-0.482442000	12.786215000	0.868053000
H	0.070292000	11.452084000	1.860110000
H	-1.462142000	12.238544000	2.223124000
C	2.693205000	12.730428000	2.036296000
H	2.826977000	13.205199000	1.062951000
H	3.666175000	12.680275000	2.517121000
H	2.352529000	11.714333000	1.855567000
C	3.356943000	15.146610000	4.040412000
H	3.494836000	16.048590000	3.443456000
H	3.460029000	15.432231000	5.085272000
H	4.161771000	14.460430000	3.797742000
C	0.613285000	16.079506000	5.320051000
H	1.478119000	16.150380000	5.975129000
H	0.501995000	17.044105000	4.821002000
H	-0.271947000	15.928221000	5.932376000
P	2.700474000	12.279267000	6.164219000
O	2.881759000	13.087010000	7.534260000
O	4.127563000	12.518814000	5.516405000

O	2.583140000	10.749665000	6.548645000
C	1.811207000	13.123426000	8.491422000
C	5.320813000	12.852610000	6.246093000
C	3.581706000	10.052199000	7.307796000
H	0.942597000	13.632723000	8.074755000
H	1.523369000	12.117207000	8.790624000
H	2.182968000	13.671484000	9.349544000
H	6.125937000	12.864402000	5.519531000
H	5.220631000	13.831693000	6.706613000
H	5.536094000	12.114912000	7.014712000
H	3.852849000	10.610331000	8.202923000
H	3.146871000	9.100998000	7.592687000
H	4.463605000	9.877621000	6.694978000

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structure of 4

Ir	0.994304000	12.792091000	4.709340000
C	1.886743000	14.759495000	4.088940000
C	0.582168000	15.008172000	4.586967000
C	1.773077000	13.850628000	2.966255000
C	-0.367488000	14.289105000	3.754851000
C	0.365993000	13.632679000	2.729677000
Br	-0.477866000	12.492729000	6.811122000
C	-1.841162000	14.339586000	3.917168000
H	-2.120139000	14.313159000	4.968595000
H	-2.243732000	15.258447000	3.489505000
H	-2.327603000	13.500669000	3.426976000
C	-0.195818000	12.903475000	1.565838000
H	-0.153124000	13.546703000	0.686247000
H	0.367702000	12.002181000	1.333482000
H	-1.233548000	12.627559000	1.723310000
C	2.875184000	13.457556000	2.051456000
H	3.048159000	14.236167000	1.306825000
H	3.805833000	13.301406000	2.590027000
H	2.639986000	12.542722000	1.512452000
C	3.154051000	15.375268000	4.558721000
H	3.392975000	16.240493000	3.939427000
H	3.087185000	15.720452000	5.586906000
H	3.990451000	14.684374000	4.484375000
C	0.194333000	15.910825000	5.698066000
H	1.058046000	16.307952000	6.223935000
H	-0.368707000	16.758466000	5.306875000
H	-0.445561000	15.402168000	6.419157000
P	2.838393000	12.091460000	5.836934000

O	3.346398000	12.990174000	7.055559000
O	4.091635000	12.131413000	4.856043000
O	2.979932000	10.608305000	6.399009000
C	2.563585000	13.885982000	7.844823000
C	5.423713000	11.890244000	5.344506000
C	2.402555000	10.220484000	7.654482000
H	1.794319000	14.367877000	7.243734000
H	2.080601000	13.350179000	8.658403000
H	3.247295000	14.629098000	8.244249000
H	6.067311000	11.846540000	4.472803000
H	5.737349000	12.702583000	5.995746000
H	5.467867000	10.947171000	5.883431000
H	2.915853000	10.725598000	8.470529000
H	1.338320000	10.447056000	7.681223000
H	2.553768000	9.149962000	7.743002000
P	0.369359000	10.687919000	4.157454000
O	1.108393000	9.979841000	2.917701000
O	-1.113032000	10.718444000	3.600101000
O	0.464433000	9.636628000	5.339530000
C	2.501738000	9.665039000	3.017049000
C	-1.717340000	9.741273000	2.739898000
C	0.011266000	8.283779000	5.221654000
H	3.090218000	10.568170000	3.179100000
H	2.685511000	8.969940000	3.835689000
H	2.785827000	9.204839000	2.076939000
H	-2.575756000	10.223404000	2.283565000
H	-1.022653000	9.418981000	1.968886000
H	-2.057509000	8.885136000	3.316988000
H	0.201474000	7.883706000	4.226209000
H	0.561504000	7.700557000	5.953188000
H	-1.051480000	8.231427000	5.447697000

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structure of P

P	-1.477582000	-0.505533000	-0.338766000
C	-0.804268000	0.651517000	0.921982000
H	-1.193324000	1.653174000	0.752807000
H	-1.121011000	0.343611000	1.916054000
H	0.285253000	0.696917000	0.905357000
C	-0.447658000	-1.979722000	0.045432000
H	-0.748156000	-2.404490000	1.000722000
H	-0.597741000	-2.745688000	-0.712250000
H	0.616065000	-1.743589000	0.091803000
C	-0.561614000	0.108776000	-1.810180000

H	-0.715337000	-0.563658000	-2.651310000
H	-0.939812000	1.086002000	-2.102252000
H	0.510210000	0.193755000	-1.627429000

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structure of TS\_1\_IM1:P

Ir	1.377945000	12.492860000	4.610559000
C	1.735872000	11.435722000	7.568697000
H	2.237916000	10.476442000	7.682928000
H	1.183879000	11.592610000	8.492923000
C	2.747571000	12.556620000	7.375606000
H	2.321582000	13.497489000	7.726645000
H	3.641138000	12.397192000	7.985744000
C	3.151658000	12.723141000	5.939458000
H	3.581177000	13.689645000	5.697775000
C	3.423885000	11.693202000	5.032285000
H	4.003695000	11.975421000	4.164292000
C	3.441591000	10.219366000	5.367600000
H	3.847425000	10.096812000	6.371954000
H	4.150470000	9.734790000	4.701225000
C	2.082871000	9.516402000	5.238097000
H	2.025370000	9.015825000	4.276614000
H	1.985573000	8.735322000	5.996964000
C	0.909614000	10.444700000	5.354302000
H	0.016676000	10.138164000	4.823533000
C	0.759559000	11.345847000	6.416560000
H	-0.248223000	11.681332000	6.628441000
C	1.475860000	14.456093000	3.608958000
C	1.080245000	14.632240000	4.973828000
C	0.362056000	13.879785000	2.897206000
H	2.359470000	14.870573000	3.152919000
C	-0.155123000	13.954817000	5.159244000
H	1.626507000	15.166348000	5.733460000
C	-0.526542000	13.368003000	3.908949000
H	-0.706710000	13.891521000	6.082406000
H	-1.427674000	12.807887000	3.723447000
Br	1.850828000	11.148346000	2.416187000
H	0.458930000	13.433299000	1.924456000
P	-0.863866000	15.941334000	1.838842000
C	-1.669633000	15.972246000	0.210158000
H	-0.941322000	15.770046000	-0.570590000
H	-2.438373000	15.205979000	0.157514000
H	-2.128871000	16.940712000	0.016459000
C	-2.176026000	16.458124000	2.986098000

H	-2.953628000	15.699541000	3.034833000
H	-1.768273000	16.587185000	3.986260000
H	-2.630416000	17.398459000	2.677879000
C	0.251925000	17.376086000	1.803439000
H	0.709809000	17.516941000	2.779990000
H	1.046697000	17.216249000	1.078999000
H	-0.278846000	18.289172000	1.538290000

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structure of IM1:P

Ir	1.485714000	12.814050000	4.575950000
C	0.789955000	10.369101000	6.451249000
H	1.598905000	9.671240000	6.660782000
H	-0.128319000	9.826392000	6.666817000
C	0.885757000	11.595355000	7.349177000
H	-0.109681000	12.018540000	7.492679000
H	1.235769000	11.329683000	8.351171000
C	1.774841000	12.660701000	6.771772000
H	1.612760000	13.654648000	7.176601000
C	3.010148000	12.448380000	6.145075000
H	3.663440000	13.309138000	6.092667000
C	3.699891000	11.106964000	6.020814000
H	3.485088000	10.515323000	6.910693000
H	4.773631000	11.278225000	6.034452000
C	3.335446000	10.335817000	4.747177000
H	4.073101000	10.546184000	3.977336000
H	3.376762000	9.257727000	4.925550000
C	1.983213000	10.695734000	4.198520000
H	1.862202000	10.537725000	3.133287000
C	0.818373000	10.734138000	4.981732000
H	-0.120169000	10.611056000	4.454637000
C	0.984143000	14.935979000	4.464145000
C	-0.108533000	14.200428000	5.034240000
C	0.864092000	14.872500000	2.954846000
H	1.513259000	15.720019000	4.985577000
C	-0.557828000	13.286001000	4.041167000
H	-0.498388000	14.288365000	6.035389000
C	0.264314000	13.481931000	2.887274000
H	-1.343835000	12.558057000	4.159899000
H	0.148815000	12.926924000	1.968178000
Br	3.644496000	13.264186000	3.142425000
H	1.846219000	14.908829000	2.472487000
P	-0.110419000	16.202406000	2.171943000
C	-0.218637000	15.889081000	0.414118000

H	0.780633000	15.813187000	-0.007955000
H	-0.741334000	14.952308000	0.237580000
H	-0.754651000	16.689275000	-0.089705000
C	-1.763733000	16.296635000	2.849091000
H	-2.284896000	15.356019000	2.689525000
H	-1.716722000	16.493638000	3.917171000
H	-2.325181000	17.094610000	2.369430000
C	0.717953000	17.764514000	2.442422000
H	1.730362000	17.716912000	2.048515000
H	0.185899000	18.575269000	1.951458000
H	0.770306000	17.974555000	3.507826000

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structure of TS\_IM1\_IM2:P

Ir	1.025099000	-0.617111000	0.918215000
C	0.271293000	-3.278159000	2.368234000
H	1.050770000	-4.022166000	2.527924000
H	-0.667411000	-3.825842000	2.414696000
C	0.301312000	-2.195174000	3.439637000
H	-0.714571000	-1.860363000	3.649276000
H	0.691594000	-2.566005000	4.391752000
C	1.104810000	-1.010877000	2.978024000
H	0.875770000	-0.083086000	3.497947000
C	2.429822000	-1.117450000	2.421234000
H	3.058323000	-0.243577000	2.544259000
C	3.184811000	-2.424941000	2.283537000
H	2.838552000	-3.142845000	3.026020000
H	4.237148000	-2.259839000	2.501358000
C	3.013389000	-2.947221000	0.866208000
H	3.790501000	-2.530209000	0.227663000
H	3.112906000	-4.034599000	0.797058000
C	1.682997000	-2.520953000	0.312970000
H	1.632779000	-2.512782000	-0.773981000
C	0.423723000	-2.660693000	0.991142000
H	-0.426051000	-2.806783000	0.335290000
C	-0.339842000	0.877918000	0.040710000
C	-1.164684000	-0.073829000	0.684586000
C	-0.508208000	0.726350000	-1.457073000
H	-0.034935000	1.818699000	0.479111000
C	-1.824842000	-0.853125000	-0.363891000
H	-1.577030000	0.031192000	1.677759000
C	-1.465776000	-0.424232000	-1.582731000
H	-2.492163000	-1.680411000	-0.172604000
H	-1.747133000	-0.865086000	-2.526405000



Br	2.785662000	0.797950000	-0.320510000
H	0.449279000	0.552163000	-1.966296000
P	-1.119301000	2.259360000	-2.197668000
C	-1.425405000	2.006644000	-3.941080000
H	-0.521037000	1.650514000	-4.428495000
H	-2.213450000	1.271128000	-4.079722000
H	-1.730615000	2.938406000	-4.410591000
C	-2.633484000	2.769597000	-1.399634000
H	-3.375452000	1.979385000	-1.485629000
H	-2.449871000	2.963453000	-0.346134000
H	-3.020746000	3.673308000	-1.862830000
C	0.137829000	3.511944000	-2.000487000
H	1.075398000	3.154406000	-2.421416000
H	-0.156101000	4.432204000	-2.498636000
H	0.302707000	3.716218000	-0.945726000

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structure of IM2:P

Ir	0.168737000	12.909434000	5.404503000
C	1.512565000	10.318545000	6.386083000
H	2.545189000	10.117211000	6.108790000
H	1.101558000	9.359918000	6.694775000
C	1.437227000	11.298522000	7.558992000
H	0.534212000	11.098886000	8.136939000
H	2.268567000	11.146095000	8.253897000
C	1.405619000	12.739258000	7.121359000
H	1.059308000	13.422827000	7.893181000
C	2.197255000	13.293779000	6.090947000
H	2.367941000	14.359242000	6.162866000
C	3.261333000	12.544250000	5.316700000
H	3.692405000	11.761644000	5.937949000
H	4.082999000	13.223455000	5.096311000
C	2.718422000	11.970472000	4.007611000
H	2.780579000	12.726121000	3.224024000
H	3.334798000	11.136424000	3.659119000
C	1.291273000	11.531959000	4.115630000
H	0.738236000	11.509286000	3.182613000
C	0.732803000	10.819767000	5.191204000
H	-0.191875000	10.296555000	4.972991000
C	-0.643792000	14.878867000	5.815031000
C	-0.048513000	14.948577000	4.522048000
H	-1.710539000	14.723693000	5.932989000
H	-0.568598000	14.726005000	3.601994000
Br	-1.982479000	12.417652000	4.243577000

C	1.073157000	15.867714000	4.572030000
C	1.173036000	16.421099000	5.790378000
C	0.081053000	15.898187000	6.680936000
H	1.950356000	17.088276000	6.132828000
P	-1.076190000	17.227189000	7.115048000
H	0.463154000	15.517451000	7.635142000
H	1.744839000	16.053109000	3.746847000
C	-0.212327000	18.546262000	7.959565000
H	0.295382000	18.160701000	8.840293000
H	0.523778000	18.993310000	7.296582000
H	-0.913704000	19.316354000	8.271168000
C	-1.829479000	17.873761000	5.631489000
H	-1.057111000	18.218486000	4.948384000
H	-2.412080000	17.098879000	5.140150000
H	-2.482880000	18.706349000	5.879310000
C	-2.344992000	16.582356000	8.196617000
H	-1.897606000	16.195677000	9.108893000
H	-3.050678000	17.366849000	8.458353000
H	-2.884263000	15.777937000	7.702951000

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structure of IM3:P

Ir	0.180335000	13.060552000	5.751264000
C	1.892809000	10.476977000	6.246621000
H	2.841972000	10.378753000	5.719874000
H	1.623490000	9.463216000	6.538160000
C	2.055490000	11.338339000	7.496824000
H	1.389003000	10.965894000	8.275698000
H	3.062270000	11.248860000	7.917017000
C	1.752284000	12.794328000	7.253346000
H	1.518589000	13.363771000	8.146340000
C	2.266382000	13.530433000	6.170230000
H	2.347303000	14.595053000	6.338377000
C	3.247004000	12.969099000	5.159052000
H	3.875129000	12.224024000	5.648166000
H	3.926160000	13.764434000	4.854992000
C	2.556757000	12.383301000	3.929349000
H	2.480837000	13.149461000	3.157997000
H	3.158704000	11.582353000	3.489229000
C	1.167687000	11.886649000	4.223364000
H	0.506874000	11.845468000	3.365102000
C	0.840831000	11.027959000	5.305014000
H	-0.036642000	10.408158000	5.159032000
C	-0.573202000	15.095978000	5.846287000

C	0.081100000	14.922249000	4.562171000
H	-1.657138000	15.060480000	5.900093000
H	-0.454034000	14.653726000	3.662201000
Br	-2.004345000	12.548557000	4.451777000
C	1.205264000	15.842086000	4.509573000
C	1.285843000	16.591611000	5.619728000
C	0.136533000	16.259622000	6.537233000
H	2.073001000	17.284095000	5.878748000
P	-0.985926000	17.684237000	6.576267000
H	0.441099000	16.077895000	7.574497000
H	1.910460000	15.884099000	3.691000000
P	-1.232862000	12.373531000	7.623214000
C	-1.583251000	18.018548000	4.927334000
H	-0.740345000	18.198358000	4.265147000
H	-2.142030000	17.163090000	4.556345000
H	-2.228937000	18.892812000	4.934305000
C	-2.390268000	17.347994000	7.635927000
H	-2.965215000	16.518863000	7.230940000
H	-2.054085000	17.090034000	8.637493000
H	-3.036577000	18.219931000	7.698183000
C	-0.139814000	19.133614000	7.198654000
H	-0.821031000	19.979243000	7.249438000
H	0.253313000	18.941601000	8.193934000
H	0.685527000	19.388783000	6.539223000
C	-2.820573000	13.255164000	7.728194000
H	-2.632852000	14.285071000	8.025328000
H	-3.328604000	13.245483000	6.768617000
H	-3.456495000	12.795398000	8.482293000
C	-1.709451000	10.626741000	7.579645000
H	-2.174853000	10.414646000	6.619707000
H	-0.827886000	9.997746000	7.679707000
H	-2.406365000	10.386679000	8.380224000
C	-0.660292000	12.616319000	9.338521000
H	-1.442648000	12.319783000	10.034735000
H	0.231595000	12.040259000	9.562988000
H	-0.435898000	13.668604000	9.505506000

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structure of TS\_IM3\_IM4:P

Ir	0.190807000	12.456586000	5.885113000
C	2.166434000	10.096544000	5.783676000
H	3.087444000	10.243778000	5.218733000
H	2.036674000	9.018556000	5.855099000
C	2.293240000	10.695321000	7.180855000

H	1.676172000	10.124909000	7.878186000
H	3.316669000	10.608936000	7.558896000
C	1.838912000	12.128378000	7.233776000
H	1.625530000	12.481756000	8.233723000
C	2.179356000	13.128350000	6.294475000
H	2.128499000	14.148628000	6.667131000
C	3.168868000	12.916674000	5.161757000
H	3.926604000	12.201286000	5.483598000
H	3.709485000	13.847327000	4.990132000
C	2.503634000	12.453764000	3.862765000
H	2.330482000	13.313628000	3.213809000
H	3.176151000	11.799347000	3.299297000
C	1.177185000	11.783118000	4.104455000
H	0.487438000	11.809816000	3.266977000
C	1.004736000	10.699399000	5.019421000
H	0.180428000	10.024662000	4.812603000
C	-0.799144000	15.059236000	5.660790000
C	-0.048470000	14.856605000	4.538761000
H	-1.786525000	14.663729000	5.836786000
H	-0.338124000	14.241617000	3.701709000
Br	-2.038681000	12.066078000	4.652805000
C	1.127796000	15.702627000	4.593365000
C	1.110255000	16.448967000	5.712133000
C	-0.149437000	16.146077000	6.468318000
H	1.867081000	17.136672000	6.054227000
P	-1.233509000	17.602238000	6.411944000
H	0.009432000	15.912811000	7.525737000
H	1.910454000	15.708529000	3.849851000
P	-1.176186000	12.283907000	7.840498000
C	-0.491775000	12.488723000	9.522177000
H	0.265450000	11.735207000	9.722802000
H	-0.032466000	13.467954000	9.644569000
H	-1.279617000	12.380013000	10.265383000
C	-2.677193000	13.315905000	7.971513000
H	-2.396189000	14.346039000	8.186605000
H	-3.224471000	13.279797000	7.031250000
H	-3.325364000	12.966750000	8.773308000
C	-1.861634000	10.602999000	7.938097000
H	-1.048303000	9.881990000	7.977998000
H	-2.490176000	10.478087000	8.818406000
H	-2.443706000	10.405315000	7.041773000
C	-1.609435000	18.018966000	4.717814000
H	-0.688176000	18.147341000	4.155797000

H	-2.193948000	17.225958000	4.259964000
H	-2.177983000	18.945140000	4.688294000
C	-0.434739000	18.995949000	7.200795000
H	-0.148659000	18.740639000	8.218149000
H	0.456044000	19.276872000	6.645306000
H	-1.110088000	19.847480000	7.232473000
C	-2.760040000	17.258527000	7.278766000
H	-2.559075000	17.026095000	8.321652000
H	-3.416051000	18.124691000	7.236082000
H	-3.266650000	16.413066000	6.819446000

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structure of diene:P

C	-0.523089000	14.886578000	5.693510000
C	0.089542000	14.779639000	4.503116000
H	-1.315651000	14.267142000	6.080997000
H	-0.136906000	14.049149000	3.742076000
C	1.135654000	15.781356000	4.399263000
C	1.175261000	16.512901000	5.524876000
C	0.107166000	16.015580000	6.450874000
H	1.860954000	17.309074000	5.765579000
P	-1.109333000	17.319117000	6.769652000
H	0.496795000	15.710040000	7.427100000
H	1.791836000	15.896120000	3.550544000
C	-2.414694000	16.682828000	7.812183000
H	-2.945838000	15.883151000	7.302944000
H	-2.001916000	16.296318000	8.740768000
H	-3.121277000	17.474785000	8.048661000
C	-0.321050000	18.686623000	7.608941000
H	-1.057140000	19.450580000	7.847496000
H	0.140198000	18.347353000	8.533158000
H	0.443637000	19.126294000	6.974228000
C	-1.805344000	17.890593000	5.229114000
H	-2.535339000	18.671994000	5.425051000
H	-1.021038000	18.289178000	4.591387000
H	-2.294803000	17.068631000	4.713849000

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structure of IM4:P

Ir	1.058030000	13.028783000	5.365354000
C	1.786518000	11.121857000	7.710126000
H	2.594226000	10.407567000	7.553204000
H	1.230825000	10.750921000	8.570104000
C	2.348834000	12.509842000	8.030257000
H	1.646522000	13.037004000	8.677471000

H	3.277141000	12.426192000	8.606015000
C	2.557274000	13.356801000	6.802769000
H	2.661416000	14.413834000	7.037700000
C	3.164516000	12.909599000	5.592236000
H	3.668732000	13.668378000	5.002719000
C	3.731703000	11.513856000	5.409158000
H	4.096525000	11.133452000	6.363694000
H	4.608672000	11.562198000	4.764853000
C	2.710489000	10.552779000	4.795088000
H	2.759933000	10.624486000	3.708551000
H	2.962794000	9.514578000	5.035660000
C	1.297815000	10.852786000	5.206789000
H	0.530992000	10.551771000	4.501541000
C	0.878802000	11.137550000	6.505220000
H	-0.184583000	11.056483000	6.699257000
P	1.022941000	15.228523000	4.665272000
Br	-1.322226000	12.830550000	4.524056000
C	0.519015000	15.482755000	2.939473000
H	1.218174000	14.984879000	2.272709000
H	-0.462047000	15.038499000	2.793639000
H	0.485704000	16.543204000	2.693878000
C	2.563528000	16.199382000	4.758264000
H	2.968082000	16.190224000	5.767516000
H	3.311940000	15.776620000	4.092346000
H	2.386878000	17.232740000	4.465579000
C	-0.154026000	16.255572000	5.594318000
H	-0.183190000	17.275541000	5.213906000
H	-1.141183000	15.806593000	5.512726000
H	0.123037000	16.276160000	6.645692000

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structure of TS\_IM4\_IM5:P

Ir	0.930404000	12.921484000	5.330743000
C	1.782935000	10.396243000	6.922503000
H	2.493087000	9.681305000	6.503945000
H	1.262354000	9.861043000	7.716460000
C	2.527972000	11.593950000	7.531738000
H	2.016205000	11.900818000	8.444743000
H	3.536921000	11.298183000	7.840921000
C	2.588729000	12.789817000	6.615230000
H	2.762166000	13.725158000	7.142458000
C	3.036726000	12.716997000	5.261653000
H	3.512417000	13.603608000	4.852535000
C	3.523964000	11.421105000	4.639945000

H	3.930496000	10.772244000	5.416998000
H	4.357199000	11.626901000	3.968995000
C	2.411461000	10.711462000	3.871623000
H	2.365490000	11.106494000	2.856709000
H	2.630248000	9.643121000	3.767672000
C	1.061695000	10.906029000	4.500178000
H	0.219637000	10.822451000	3.822773000
C	0.777828000	10.787852000	5.864758000
H	-0.265136000	10.649235000	6.124637000
P	1.032215000	15.211548000	5.043134000
Br	-1.469636000	13.037906000	4.432014000
P	-0.667658000	13.093072000	8.341474000
C	1.149983000	15.631231000	3.278298000
H	2.042521000	15.179957000	2.852167000
H	0.284331000	15.213018000	2.769872000
H	1.180839000	16.708927000	3.121184000
C	-0.371890000	16.234044000	5.586413000
H	-0.235780000	17.273562000	5.291797000
H	-1.283467000	15.841533000	5.142204000
H	-0.473429000	16.189323000	6.668402000
C	2.438199000	16.119070000	5.771515000
H	3.383565000	15.660576000	5.491142000
H	2.444446000	17.156745000	5.442839000
H	2.367770000	16.102655000	6.857063000
C	0.194992000	14.472086000	9.201409000
H	1.153856000	14.124288000	9.582832000
H	0.401431000	15.279201000	8.500152000
H	-0.379915000	14.878225000	10.034372000
C	-1.037910000	12.037588000	9.803073000
H	-1.685694000	11.215003000	9.507575000
H	-0.116892000	11.605195000	10.190527000
H	-1.525432000	12.589183000	10.607990000
C	-2.314970000	13.847246000	8.075364000
H	-2.252567000	14.603466000	7.296030000
H	-3.002772000	13.087312000	7.711295000
H	-2.724494000	14.294212000	8.981719000

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structure of IM5:P

Ir	0.631380000	12.876883000	6.105576000
C	1.662834000	9.923058000	6.279028000
H	2.557406000	9.691283000	5.697395000
H	1.179292000	8.963505000	6.458788000
C	2.030775000	10.574419000	7.602155000

H	1.278875000	10.311842000	8.348561000
H	2.984161000	10.202637000	7.998280000
C	2.065470000	12.078683000	7.500575000
H	2.031548000	12.562448000	8.472890000
C	2.738283000	12.817738000	6.485136000
H	3.117001000	13.785665000	6.797015000
C	3.552983000	12.145113000	5.390406000
H	4.015084000	11.243635000	5.797533000
H	4.386339000	12.794141000	5.120335000
C	2.725173000	11.816281000	4.145871000
H	2.853415000	12.617252000	3.414160000
H	3.109993000	10.914967000	3.654433000
C	1.251075000	11.691940000	4.447867000
H	0.602245000	11.841135000	3.589530000
C	0.741403000	10.825797000	5.479653000
H	-0.259469000	10.442630000	5.317191000
P	0.835417000	15.048493000	5.058499000
Br	-1.761080000	12.895929000	5.030906000
P	-0.351962000	13.649897000	8.107857000
C	0.704416000	14.924092000	3.246649000
H	1.497375000	14.287603000	2.861074000
H	-0.248808000	14.458263000	3.003799000
H	0.766844000	15.900156000	2.767031000
C	2.413736000	15.948377000	5.249031000
H	2.591235000	16.187882000	6.295803000
H	3.236332000	15.323766000	4.906727000
H	2.418583000	16.873814000	4.674575000
C	-0.380389000	16.370218000	5.384318000
H	-1.376927000	15.969985000	5.206221000
H	-0.319802000	16.703077000	6.418484000
H	-0.221371000	17.229926000	4.734082000
C	0.616524000	14.899659000	9.032489000
H	1.635353000	14.551983000	9.191875000
H	0.669494000	15.817552000	8.449732000
H	0.173211000	15.129604000	10.000661000
C	-0.647663000	12.401674000	9.410079000
H	-1.303003000	11.628743000	9.014749000
H	0.284788000	11.929355000	9.708707000
H	-1.111944000	12.842747000	10.291518000
C	-1.988816000	14.444331000	8.059139000
H	-2.269484000	14.796534000	9.051040000
H	-1.992614000	15.280208000	7.366137000
H	-2.724487000	13.729531000	7.701977000



## structure of TS\_IM5\_IM6:P

Ir	-0.267935000	-0.385354000	-0.201358000
C	0.828458000	-3.303436000	0.118230000
H	1.678907000	-3.583610000	-0.507010000
H	0.364994000	-4.245108000	0.410343000
C	1.290755000	-2.548417000	1.355221000
H	0.620395000	-2.776300000	2.185836000
H	2.286358000	-2.867604000	1.687964000
C	1.275555000	-1.054335000	1.148671000
H	1.288936000	-0.498156000	2.077496000
C	1.864720000	-0.385325000	0.040406000
H	2.238087000	0.610549000	0.250671000
C	2.621301000	-1.128635000	-1.049730000
H	3.113622000	-1.997352000	-0.608049000
H	3.431932000	-0.496753000	-1.413395000
C	1.722377000	-1.547614000	-2.213497000
H	1.786914000	-0.792688000	-3.000626000
H	2.088251000	-2.473677000	-2.672259000
C	0.275050000	-1.668041000	-1.803258000
H	-0.429186000	-1.590340000	-2.626916000
C	-0.155622000	-2.469580000	-0.682152000
H	-1.153748000	-2.885734000	-0.764325000
P	-0.139143000	1.734610000	-1.344770000
Br	-2.711030000	-0.488077000	-1.147871000
P	-1.340153000	0.315449000	1.813147000
C	-0.407353000	1.520519000	-3.134630000
H	0.343385000	0.846725000	-3.541145000
H	-1.383448000	1.065164000	-3.288304000
H	-0.359481000	2.469379000	-3.667624000
C	1.454494000	2.628301000	-1.335254000
H	1.724153000	2.917829000	-0.321478000
H	2.241765000	1.982932000	-1.719310000
H	1.409414000	3.524426000	-1.952762000
C	-1.306820000	3.093001000	-0.995444000
H	-2.320789000	2.698427000	-1.010181000
H	-1.111211000	3.511136000	-0.010207000
H	-1.224271000	3.890639000	-1.733132000
C	-0.378634000	1.109280000	3.157530000
H	0.352912000	0.428355000	3.583514000
H	0.154116000	1.976087000	2.769522000
H	-1.038661000	1.437295000	3.959181000
C	-2.109945000	-1.082219000	2.696979000

H	-2.826216000	-1.556123000	2.028794000
H	-1.350902000	-1.819007000	2.950307000
H	-2.619848000	-0.768336000	3.607547000
C	-2.742010000	1.481763000	1.737484000
H	-3.251026000	1.518070000	2.699594000
H	-2.387375000	2.480605000	1.499451000
H	-3.442047000	1.171282000	0.966797000

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structure of IM6:P

Ir	0.156126000	-0.512662000	-0.363497000
C	1.554981000	-3.068864000	0.851709000
H	2.095949000	-3.749651000	0.193872000
H	1.362382000	-3.638628000	1.760803000
C	2.410863000	-1.845788000	1.181983000
H	2.188658000	-1.521261000	2.201665000
H	3.475579000	-2.106652000	1.184448000
C	2.141543000	-0.679029000	0.263774000
H	2.551673000	0.244593000	0.665834000
C	2.119130000	-0.780876000	-1.186765000
H	2.523838000	0.083660000	-1.706698000
C	2.375554000	-2.086750000	-1.922238000
H	3.041506000	-2.726948000	-1.339949000
H	2.910916000	-1.889353000	-2.850694000
C	1.062477000	-2.788440000	-2.233217000
H	0.649042000	-2.379873000	-3.155873000
H	1.201330000	-3.861309000	-2.413996000
C	0.028856000	-2.591392000	-1.161089000
H	-0.994795000	-2.682066000	-1.502426000
C	0.234351000	-2.701859000	0.213665000
H	-0.645846000	-2.927991000	0.797673000
P	0.368747000	1.714511000	-0.956005000
Br	-2.104095000	-0.247122000	-1.977725000
P	-1.215448000	-0.113934000	1.533514000
C	-0.447649000	1.077578000	2.695163000
H	0.547100000	0.727800000	2.965397000
H	-0.336313000	2.052371000	2.225732000
H	-1.036238000	1.200198000	3.603876000
C	-1.515020000	-1.496862000	2.693529000
H	-2.141513000	-2.253113000	2.226478000
H	-0.575352000	-1.964778000	2.979432000
H	-2.018786000	-1.143433000	3.592208000
C	-2.910955000	0.543406000	1.393228000
H	-3.356988000	0.706214000	2.373947000

H	-2.913952000	1.475946000	0.836614000
H	-3.515071000	-0.159688000	0.825195000
C	-0.981882000	2.882614000	-0.610418000
H	-1.892286000	2.495850000	-1.063175000
H	-1.138896000	2.995519000	0.459461000
H	-0.754435000	3.861021000	-1.030537000
C	1.811797000	2.600566000	-0.275456000
H	1.846373000	3.622483000	-0.648929000
H	1.769206000	2.625194000	0.811177000
H	2.731447000	2.096990000	-0.564899000
C	0.594905000	1.952459000	-2.743524000
H	-0.276974000	1.550624000	-3.253684000
H	0.710925000	3.008661000	-2.982794000
H	1.472901000	1.410491000	-3.083588000

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structure of IM6:P'

Ir	0.132068000	-0.520518000	-0.377632000
C	1.526071000	-3.072446000	0.848622000
H	2.086680000	-3.743455000	0.197776000
H	1.322768000	-3.649692000	1.750533000
C	2.364643000	-1.843477000	1.203619000
H	2.115721000	-1.523594000	2.218690000
H	3.430822000	-2.096721000	1.232386000
C	2.109693000	-0.675213000	0.283202000
H	2.503865000	0.249660000	0.697867000
C	2.117941000	-0.772058000	-1.166011000
H	2.525427000	0.097202000	-1.675626000
C	2.396150000	-2.074207000	-1.899285000
H	3.052341000	-2.712391000	-1.304192000
H	2.951071000	-1.871350000	-2.814875000
C	1.092604000	-2.779810000	-2.241595000
H	0.697167000	-2.365099000	-3.169037000
H	1.241353000	-3.850234000	-2.428626000
C	0.034139000	-2.597682000	-1.189971000
H	-0.981721000	-2.692838000	-1.552557000
C	0.212887000	-2.715072000	0.187074000
H	-0.676055000	-2.949060000	0.754683000
P	0.350615000	1.704168000	-0.963598000
Br	-2.125157000	-0.254851000	-1.990666000
P	-1.207463000	-0.118381000	1.524501000
C	-0.411241000	1.072078000	2.672085000
H	0.580138000	0.708864000	2.936924000
H	-0.288026000	2.041898000	2.195513000

H	-0.989626000	1.209438000	3.585227000
C	-1.484016000	-1.496463000	2.697788000
H	-2.118836000	-2.256629000	2.249404000
H	-0.535700000	-1.959706000	2.962512000
H	-1.965790000	-1.139588000	3.607114000
C	-2.900301000	0.553017000	1.410175000
H	-3.331091000	0.720227000	2.396930000
H	-2.898734000	1.486422000	0.854727000
H	-3.518658000	-0.143026000	0.849300000
C	-0.988524000	2.886569000	-0.610093000
H	-1.907953000	2.511234000	-1.052933000
H	-1.133306000	3.005235000	0.460891000
H	-0.752290000	3.861127000	-1.034208000
C	1.801006000	2.583868000	-0.282992000
H	1.841535000	3.604064000	-0.660406000
H	1.756449000	2.614285000	0.803375000
H	2.718827000	2.074586000	-0.567627000
C	0.574161000	1.946466000	-2.752227000
H	-0.303571000	1.556487000	-3.261053000
H	0.702661000	3.002169000	-2.987226000
H	1.444918000	1.394925000	-3.095284000

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structure of IM7:P'

Ir	0.923954000	12.816080000	5.464336000
C	1.953153000	10.994853000	7.807059000
H	2.820050000	10.361381000	7.635582000
H	1.457312000	10.580862000	8.682391000
C	2.376553000	12.433244000	8.110482000
H	1.613293000	12.913255000	8.723053000
H	3.288471000	12.446078000	8.714357000
C	2.568254000	13.265775000	6.879878000
H	2.530926000	14.335566000	7.062474000
C	3.149690000	12.846376000	5.684070000
H	3.489873000	13.623622000	5.012658000
C	3.769556000	11.491563000	5.441521000
H	4.173197000	11.095637000	6.370255000
H	4.624470000	11.613689000	4.779938000
C	2.787962000	10.505034000	4.805850000
H	2.770208000	10.657535000	3.726623000
H	3.129210000	9.476034000	4.951233000
C	1.386358000	10.654198000	5.313414000
H	0.633716000	10.224462000	4.659201000
C	1.010381000	10.908164000	6.631633000

H	-0.016771000	10.690384000	6.892830000
P	-1.253334000	12.400806000	4.733614000
P	0.845294000	15.059666000	4.827513000
C	-0.040732000	16.127207000	6.007456000
H	-1.067608000	15.798777000	6.135015000
H	0.446079000	16.080886000	6.978499000
H	-0.040898000	17.160869000	5.666452000
C	2.443196000	15.922382000	4.673613000
H	2.272076000	16.978050000	4.473182000
H	3.032896000	15.838994000	5.582497000
H	3.019651000	15.508309000	3.850403000
C	0.099100000	15.484508000	3.220353000
H	0.629767000	14.972987000	2.421099000
H	-0.946852000	15.197264000	3.172005000
H	0.166029000	16.557052000	3.047711000
C	-2.549761000	13.635420000	5.073522000
H	-2.633753000	13.797119000	6.145399000
H	-2.333334000	14.589005000	4.601576000
H	-3.509778000	13.282091000	4.701964000
C	-1.376543000	12.135873000	2.935881000
H	-0.758589000	11.288763000	2.648427000
H	-2.405568000	11.931553000	2.645894000
H	-1.023149000	13.004746000	2.389075000
C	-2.060984000	10.904127000	5.387964000
H	-3.024673000	10.765349000	4.902217000
H	-1.459811000	10.015904000	5.213572000
H	-2.228705000	11.001720000	6.457420000

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structure of IM7:P

Ir	0.920091000	12.817353000	5.456159000
C	1.944211000	11.014144000	7.810513000
H	2.804157000	10.369605000	7.642715000
H	1.445723000	10.611877000	8.689917000
C	2.384597000	12.449369000	8.101748000
H	1.636256000	12.938135000	8.725751000
H	3.307000000	12.456273000	8.689877000
C	2.563434000	13.274689000	6.864422000
H	2.532374000	14.345600000	7.041524000
C	3.140212000	12.844550000	5.667960000
H	3.481718000	13.616029000	4.990110000
C	3.762187000	11.488186000	5.442260000
H	4.168603000	11.106926000	6.376361000
H	4.616332000	11.602079000	4.778076000

C	2.781947000	10.490233000	4.824474000
H	2.772795000	10.614494000	3.741558000
H	3.117656000	9.463784000	4.999111000
C	1.378050000	10.657777000	5.319749000
H	0.626955000	10.220574000	4.668649000
C	0.999933000	10.927151000	6.636458000
H	-0.027589000	10.711481000	6.899167000
P	-1.259418000	12.391099000	4.721647000
P	0.846574000	15.069332000	4.826561000
C	-0.018591000	16.122273000	6.031170000
H	-1.045718000	15.797342000	6.166449000
H	0.479799000	16.055603000	6.995361000
H	-0.016744000	17.161967000	5.708967000
C	2.446910000	15.922451000	4.664578000
H	2.281491000	16.980604000	4.472496000
H	3.044192000	15.829420000	5.567703000
H	3.014029000	15.509772000	3.834094000
C	0.086595000	15.508411000	3.232612000
H	0.617145000	15.010331000	2.424586000
H	-0.956824000	15.211890000	3.186582000
H	0.143866000	16.583283000	3.071119000
C	-2.555841000	13.619786000	5.068070000
H	-2.646618000	13.763391000	6.142149000
H	-2.333343000	14.581079000	4.614969000
H	-3.514285000	13.274895000	4.684520000
C	-1.369932000	12.129823000	2.924962000
H	-0.748594000	11.283303000	2.642312000
H	-2.395968000	11.924664000	2.625048000
H	-1.011301000	12.999173000	2.382193000
C	-2.059372000	10.889531000	5.369868000
H	-3.019477000	10.743546000	4.879059000
H	-1.451398000	10.005118000	5.198979000
H	-2.233986000	10.984820000	6.438546000

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structure of 2:P

Ir	0.597481000	12.930079000	5.706627000
C	2.041035000	10.713390000	7.423497000
H	2.774776000	10.037502000	6.983958000
H	1.697924000	10.206221000	8.324369000
C	2.688185000	12.046323000	7.796742000
H	2.253205000	12.406645000	8.731797000
H	3.752929000	11.913830000	8.013404000
C	2.491436000	13.114605000	6.750068000

H	2.658356000	14.116686000	7.130167000
C	2.773944000	12.906823000	5.362090000
H	3.098368000	13.778836000	4.807520000
C	3.376023000	11.614448000	4.841983000
H	3.947281000	11.134645000	5.636684000
H	4.101024000	11.839240000	4.061926000
C	2.303217000	10.691199000	4.303855000
H	2.103707000	10.940153000	3.260573000
H	2.621680000	9.642642000	4.301184000
C	1.015223000	10.819578000	5.064769000
H	0.173677000	10.396123000	4.529881000
C	0.871621000	10.856197000	6.467025000
H	-0.073192000	10.479065000	6.840134000
P	-1.243398000	12.505523000	4.287295000
P	0.730143000	15.152995000	4.975278000
P	-0.681658000	13.445914000	7.685035000
C	0.120571000	14.685196000	8.755036000
H	1.124293000	14.357067000	9.014832000
H	0.206386000	15.637985000	8.237196000
H	-0.443517000	14.843120000	9.672732000
C	-2.384066000	14.105835000	7.608402000
H	-2.419797000	15.029882000	7.037609000
H	-3.048471000	13.387829000	7.132650000
H	-2.764705000	14.306428000	8.608964000
C	-0.923335000	12.074497000	8.858972000
H	0.033472000	11.637212000	9.132986000
H	-1.419200000	12.424083000	9.762856000
H	-1.533850000	11.293327000	8.411712000
C	0.966615000	15.359266000	3.181965000
H	1.821503000	14.771608000	2.856139000
H	0.092592000	15.000973000	2.643126000
H	1.129985000	16.402895000	2.918233000
C	-0.619827000	16.330454000	5.321406000
H	-1.577402000	15.986338000	4.948171000
H	-0.707525000	16.485394000	6.394378000
H	-0.396992000	17.292107000	4.862498000
C	2.111883000	16.135287000	5.647685000
H	2.110574000	17.119094000	5.182770000
H	1.993110000	16.264841000	6.720744000
H	3.076980000	15.672707000	5.466607000
C	-2.495457000	13.784584000	3.933258000
H	-2.909709000	14.194652000	4.850081000
H	-2.070179000	14.596643000	3.349049000

H	-3.308039000	13.349386000	3.354320000
C	-0.880700000	11.964382000	2.582234000
H	-0.334647000	12.744624000	2.057247000
H	-0.263688000	11.070823000	2.575984000
H	-1.799136000	11.754871000	2.036395000
C	-2.334545000	11.174205000	4.897023000
H	-3.112430000	10.942523000	4.171926000
H	-1.778887000	10.264254000	5.106296000
H	-2.811317000	11.491335000	5.822298000

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structure of 1:Cl

Ir	1.139281000	12.502556000	4.339463000
C	1.450852000	10.876260000	7.056422000
H	2.383603000	10.336335000	7.206560000
H	0.731647000	10.421156000	7.733732000
C	1.615765000	12.351036000	7.400225000
H	0.653166000	12.771088000	7.693677000
H	2.265416000	12.487388000	8.269182000
C	2.159751000	13.155458000	6.259043000
H	1.979330000	14.222382000	6.322521000
C	3.154959000	12.761652000	5.368831000
H	3.602808000	13.553528000	4.784681000
C	3.951158000	11.483616000	5.446249000
H	4.119595000	11.244938000	6.495914000
H	4.932907000	11.679020000	5.023641000
C	3.328453000	10.289660000	4.707866000
H	3.758969000	10.211491000	3.715252000
H	3.574205000	9.357944000	5.223758000
C	1.841232000	10.373134000	4.570486000
H	1.419594000	9.867918000	3.710097000
C	0.984989000	10.667025000	5.634540000
H	-0.050404000	10.370294000	5.517509000
C	-0.301349000	14.138735000	4.824850000
C	-0.953395000	12.875424000	4.887999000
C	0.206551000	14.322732000	3.514108000
H	-0.171529000	14.814946000	5.653801000
C	-0.911471000	12.289992000	3.574329000
H	-1.442643000	12.461152000	5.753852000
C	-0.203561000	13.181511000	2.739347000
H	0.758992000	15.170883000	3.148212000
H	-1.340519000	11.346737000	3.280306000
H	0.065968000	13.001517000	1.712011000
Cl	2.715975000	12.396520000	2.501703000



structure of TS\_1\_IM1:Cl

Ir	1.334935000	12.550393000	4.566166000
C	1.637223000	11.479036000	7.530776000
H	2.182607000	10.545738000	7.658369000
H	1.042185000	11.598599000	8.433756000
C	2.596653000	12.653233000	7.388842000
H	2.109063000	13.565976000	7.733630000
H	3.472645000	12.531241000	8.032258000
C	3.046587000	12.860875000	5.971706000
H	3.426537000	13.853574000	5.754719000
C	3.402876000	11.858337000	5.066404000
H	3.981707000	12.177838000	4.210656000
C	3.477952000	10.383376000	5.384546000
H	3.824831000	10.263757000	6.410752000
H	4.250792000	9.945210000	4.758273000
C	2.167002000	9.618603000	5.156908000
H	2.175088000	9.178546000	4.164525000
H	2.084865000	8.787694000	5.862716000
C	0.941666000	10.475756000	5.272906000
H	0.083484000	10.138891000	4.704303000
C	0.710245000	11.350037000	6.341749000
H	-0.320436000	11.630121000	6.521323000
C	1.386678000	14.518425000	3.601553000
C	0.894495000	14.649146000	4.941784000
C	0.336446000	13.921017000	2.796930000
H	2.266879000	14.998286000	3.208448000
C	-0.309425000	13.901217000	5.036639000
H	1.355790000	15.206092000	5.740224000
C	-0.561025000	13.310199000	3.760019000
H	-0.915938000	13.791732000	5.919982000
H	-1.414982000	12.702167000	3.512981000
H	0.561788000	13.438056000	1.860858000
P	-0.803316000	15.809574000	1.851264000
O	-1.725493000	16.251176000	3.064704000
O	-1.798421000	16.116543000	0.624795000
O	0.398241000	16.847839000	1.702602000
C	-2.807097000	17.198357000	2.993882000
H	-3.190817000	17.298465000	4.002829000
H	-2.459143000	18.165384000	2.639109000
H	-3.587261000	16.829639000	2.334794000
C	-1.375996000	15.871630000	-0.724593000
H	-1.196526000	14.810909000	-0.888070000

H	-2.18520000	16.200544000	-1.366408000
H	-0.474102000	16.434512000	-0.959788000
C	0.217190000	18.260078000	1.506571000
H	0.033041000	18.743499000	2.463577000
H	1.137483000	18.643556000	1.079875000
H	-0.609354000	18.459437000	0.826479000
Cl	1.930875000	11.328856000	2.515368000

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structure of IM1:Cl

Ir	1.454526000	12.825495000	4.564511000
C	0.815988000	10.365317000	6.441379000
H	1.636801000	9.678247000	6.639177000
H	-0.091899000	9.808181000	6.664385000
C	0.902775000	11.589184000	7.344004000
H	-0.097721000	11.994815000	7.502488000
H	1.270429000	11.324891000	8.340030000
C	1.765281000	12.672318000	6.759321000
H	1.588699000	13.662918000	7.166086000
C	2.995252000	12.482138000	6.116499000
H	3.629998000	13.355312000	6.043223000
C	3.704942000	11.153708000	5.974866000
H	3.499577000	10.544252000	6.854647000
H	4.776097000	11.340198000	5.990468000
C	3.350024000	10.401675000	4.687973000
H	4.062676000	10.667090000	3.911621000
H	3.440849000	9.321969000	4.835090000
C	1.975970000	10.722373000	4.171768000
H	1.840287000	10.571037000	3.107225000
C	0.822225000	10.736852000	4.972806000
H	-0.120639000	10.598519000	4.456953000
C	0.942536000	14.942931000	4.459324000
C	-0.147374000	14.204881000	5.026977000
C	0.837902000	14.869266000	2.948549000
H	1.465164000	15.735164000	4.973211000
C	-0.590221000	13.283700000	4.037141000
H	-0.537028000	14.293867000	6.027989000
C	0.227910000	13.480127000	2.880366000
H	-1.371840000	12.550843000	4.157408000
H	0.114644000	12.931446000	1.957750000
H	1.823756000	14.896966000	2.471601000
P	-0.122367000	16.176362000	2.193701000
O	0.598731000	17.520629000	2.469859000
O	-1.568338000	16.398897000	2.755684000

O	-0.195523000	15.809035000	0.679213000
C	-0.016221000	18.824483000	2.590725000
H	0.793163000	19.513778000	2.796365000
H	-0.510372000	19.100533000	1.663585000
H	-0.728037000	18.821650000	3.409790000
C	-2.679841000	15.512063000	2.504934000
H	-2.860830000	14.921132000	3.396924000
H	-3.541912000	16.135491000	2.293561000
H	-2.479282000	14.857793000	1.659223000
C	-0.753941000	16.670657000	-0.336672000
H	-0.062980000	17.483283000	-0.543441000
H	-0.875364000	16.059993000	-1.222881000
H	-1.720054000	17.062218000	-0.023871000
Cl	3.468899000	13.279437000	3.200136000

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structure of TS\_IM1\_IM2:Cl

Ir	0.964039000	-0.614840000	0.935535000
C	0.300713000	-3.330624000	2.326760000
H	1.109402000	-4.040968000	2.493931000
H	-0.612688000	-3.921090000	2.342081000
C	0.255663000	-2.264601000	3.414725000
H	-0.779125000	-1.981521000	3.607459000
H	0.643576000	-2.630621000	4.369633000
C	1.011401000	-1.037101000	2.987167000
H	0.728378000	-0.128805000	3.514981000
C	2.352486000	-1.075602000	2.457537000
H	2.935667000	-0.172660000	2.596036000
C	3.170786000	-2.344304000	2.321782000
H	2.836723000	-3.090551000	3.041276000
H	4.207830000	-2.135521000	2.572790000
C	3.060841000	-2.845600000	0.890937000
H	3.830210000	-2.375967000	0.280118000
H	3.217909000	-3.924648000	0.802037000
C	1.723201000	-2.474084000	0.315926000
H	1.695132000	-2.447504000	-0.771835000
C	0.456451000	-2.683046000	0.963402000
H	-0.368808000	-2.862040000	0.284951000
C	-0.449026000	0.850901000	0.081111000
C	-1.239305000	-0.187117000	0.625725000
C	-0.521696000	0.769284000	-1.433085000
H	-0.227409000	1.779942000	0.588673000
C	-1.792165000	-0.946493000	-0.498308000
H	-1.705514000	-0.165883000	1.600463000

C	-1.412999000	-0.421237000	-1.671262000
H	-2.410972000	-1.824603000	-0.388741000
H	-1.629537000	-0.801529000	-2.656379000
Cl	2.583278000	0.859673000	-0.133291000
H	0.473011000	0.646925000	-1.885469000
P	-1.110536000	2.288294000	-2.157056000
O	-0.020312000	3.377953000	-2.261328000
O	-2.267927000	2.953209000	-1.348903000
O	-1.534491000	1.940225000	-3.606961000
C	0.708400000	3.939270000	-1.133350000
H	1.294525000	4.752846000	-1.541665000
H	0.005981000	4.320848000	-0.397084000
H	1.361507000	3.176192000	-0.711475000
C	-3.494954000	2.264618000	-1.010149000
H	-3.310718000	1.576273000	-0.190273000
H	-4.195715000	3.032268000	-0.704904000
H	-3.883622000	1.728138000	-1.872696000
C	-1.918854000	2.946929000	-4.578958000
H	-1.057498000	3.557318000	-4.830707000
H	-2.262954000	2.402815000	-5.449216000
H	-2.720285000	3.564636000	-4.181940000

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structure of IM2:Cl

Ir	0.187029000	12.944577000	5.352109000
C	1.451518000	10.346071000	6.408242000
H	2.489901000	10.126857000	6.168847000
H	1.016124000	9.396715000	6.712260000
C	1.350592000	11.340366000	7.567497000
H	0.426809000	11.158152000	8.117826000
H	2.156459000	11.185187000	8.291033000
C	1.350477000	12.777305000	7.113949000
H	0.988413000	13.471567000	7.868957000
C	2.184312000	13.312072000	6.105534000
H	2.367726000	14.376209000	6.173779000
C	3.268071000	12.539839000	5.380402000
H	3.667887000	11.762547000	6.028833000
H	4.104681000	13.206966000	5.180424000
C	2.768022000	11.950770000	4.060475000
H	2.872364000	12.691180000	3.266924000
H	3.385207000	11.101997000	3.751420000
C	1.330698000	11.535817000	4.119732000
H	0.806661000	11.519448000	3.169948000
C	0.722090000	10.846311000	5.182012000

H	-0.209882000	10.346421000	4.939984000
C	-0.630613000	14.918851000	5.695859000
C	0.038280000	14.971232000	4.438674000
H	-1.704510000	14.780129000	5.746460000
H	-0.431911000	14.727006000	3.496867000
Cl	-1.784649000	12.519284000	4.146427000
C	1.152247000	15.896440000	4.535189000
C	1.181854000	16.474886000	5.744690000
C	0.064256000	15.932967000	6.596782000
H	1.922110000	17.164035000	6.121753000
P	-1.099131000	17.189548000	7.087828000
O	-0.258840000	18.293772000	7.779420000
O	-1.965101000	17.737374000	5.917823000
O	-2.130443000	16.691377000	8.130871000
C	-0.851283000	19.455525000	8.416336000
C	-1.454704000	18.319732000	4.694128000
C	-3.290396000	15.865986000	7.852393000
H	-0.022854000	20.084575000	8.715909000
H	-1.421958000	19.143565000	9.285290000
H	-1.487766000	19.984807000	7.712028000
H	-1.252820000	17.527132000	3.980981000
H	-0.551484000	18.893124000	4.888308000
H	-2.237211000	18.970393000	4.321965000
H	-3.741958000	16.155214000	6.908172000
H	-3.982688000	16.038982000	8.667084000
H	-2.990967000	14.822411000	7.832958000
H	0.442596000	15.529142000	7.543767000
H	1.866078000	16.074112000	3.744355000

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structure of TS\_1\_IM8:Cl

Ir	-0.940521000	0.569494000	-1.180844000
C	-2.525915000	0.783086000	-2.550639000
C	-2.380461000	2.018217000	-1.853210000
C	-2.870897000	-0.244823000	-1.596799000
H	-2.380185000	0.631522000	-3.608220000
C	-2.579159000	1.741374000	-0.466272000
H	-2.094635000	2.964349000	-2.280408000
C	-2.919483000	0.357788000	-0.314560000
H	-2.472477000	2.451973000	0.338090000
H	-3.127746000	-0.139057000	0.618022000
H	-3.050471000	-1.282014000	-1.827582000
C	0.567198000	-1.221530000	-0.744581000
C	-0.350783000	-1.154992000	0.289374000

H	0.216367000	-1.780598000	-1.609038000
C	2.056553000	-1.055833000	-0.687496000
C	-0.138631000	-0.645424000	1.681681000
H	-1.242679000	-1.758797000	0.162956000
H	2.364025000	-0.066458000	-1.023158000
H	2.446995000	-1.732781000	-1.446623000
C	2.729029000	-1.377338000	0.656561000
C	0.587017000	0.694301000	1.835509000
H	0.375337000	-1.417193000	2.260643000
H	-1.120223000	-0.560862000	2.147886000
H	2.184638000	-2.174894000	1.167162000
H	3.698506000	-1.813429000	0.428247000
C	2.955031000	-0.201521000	1.559719000
H	0.324371000	1.353055000	0.988399000
H	0.156310000	1.202843000	2.697858000
C	2.067638000	0.680577000	2.010785000
H	3.986053000	-0.030901000	1.842952000
H	2.451664000	1.508984000	2.593024000
Cl	0.897222000	1.629130000	-2.015847000

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structure of IM8:Cl

Ir	0.927332000	12.679854000	4.344556000
C	1.467787000	14.767487000	4.291456000
C	0.128033000	14.652374000	4.705854000
C	1.579965000	14.159528000	2.981558000
H	2.281180000	15.175313000	4.869127000
C	-0.600752000	13.969021000	3.657513000
H	-0.272978000	14.954920000	5.659374000
C	0.287038000	13.729322000	2.570486000
H	-1.645933000	13.706434000	3.690588000
H	0.040083000	13.247056000	1.639181000
H	2.489432000	14.068384000	2.409804000
C	1.502089000	10.698489000	3.217600000
C	0.195990000	10.530651000	3.641433000
H	1.607690000	11.122288000	2.221629000
C	2.750896000	10.059088000	3.737438000
C	-0.358677000	9.649430000	4.719068000
H	-0.555087000	10.899993000	2.949035000
H	2.733983000	9.947675000	4.813481000
H	3.597370000	10.707507000	3.510395000
C	2.980871000	8.706035000	3.053854000
C	0.550831000	8.541918000	5.246443000
H	-1.252778000	9.196121000	4.282523000

H	-0.739959000	10.253117000	5.545274000
H	3.084748000	8.859907000	1.976709000
H	3.958677000	8.333973000	3.370578000
C	1.949548000	7.651156000	3.282801000
H	1.397616000	8.968075000	5.777087000
H	-0.013845000	8.002048000	6.004619000
C	0.964741000	7.571964000	4.174764000
H	2.047565000	6.809029000	2.606892000
H	0.349380000	6.681574000	4.118490000
Cl	1.589847000	11.867082000	6.352229000

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structure of IM6:Cl'

Ir	0.124160000	-0.585735000	-0.516432000
C	1.557611000	-3.007539000	1.008451000
H	2.185095000	-3.688882000	0.435316000
H	1.348768000	-3.514154000	1.950021000
C	2.298943000	-1.700877000	1.287674000
H	1.935992000	-1.281849000	2.228434000
H	3.367504000	-1.890179000	1.440123000
C	2.088709000	-0.654189000	0.225716000
H	2.424838000	0.321406000	0.555513000
C	2.158047000	-0.881113000	-1.204714000
H	2.573773000	-0.050124000	-1.764965000
C	2.452396000	-2.238282000	-1.820900000
H	3.116860000	-2.812473000	-1.172366000
H	3.007530000	-2.104306000	-2.748915000
C	1.169361000	-3.004250000	-2.121256000
H	0.757708000	-2.644288000	-3.064967000
H	1.358698000	-4.074428000	-2.262966000
C	0.095974000	-2.823399000	-1.087508000
H	-0.916569000	-2.919843000	-1.459381000
C	0.254985000	-2.800519000	0.279074000
H	-0.641323000	-2.901546000	0.872470000
P	0.248402000	1.603757000	-0.927324000
O	-0.870669000	2.609462000	-0.365305000
O	0.246800000	2.118633000	-2.446895000
O	1.540701000	2.267326000	-0.250551000
C	-2.149569000	2.687879000	-1.010518000
C	0.814219000	1.367380000	-3.520251000
C	1.722427000	3.683625000	-0.286043000
H	-2.863812000	3.002291000	-0.254757000
H	-2.106089000	3.423698000	-1.811173000
H	-2.442512000	1.723254000	-1.425892000

H	0.33972000	1.719934000	-4.430713000
H	1.888112000	1.548095000	-3.574356000
H	0.608618000	0.305128000	-3.398699000
H	1.066748000	4.166513000	0.436284000
H	2.758592000	3.875912000	-0.025302000
H	1.516389000	4.084149000	-1.277870000
Cl	-1.698281000	-0.598314000	-2.431340000
P	-1.159572000	-0.081165000	1.274939000
O	-1.418418000	-1.309721000	2.313196000
O	-2.597221000	0.694665000	1.286374000
O	-0.357772000	0.991632000	2.190001000
C	-1.940847000	-1.036415000	3.608626000
C	-3.667778000	0.076682000	0.566827000
C	-0.931748000	2.140456000	2.802064000
H	-2.168003000	-1.990222000	4.075474000
H	-1.206395000	-0.506796000	4.216029000
H	-2.851731000	-0.438690000	3.551146000
H	-3.332644000	-0.279983000	-0.409674000
H	-4.080819000	-0.755952000	1.138406000
H	-4.439301000	0.830563000	0.435131000
H	-1.738070000	1.881359000	3.487839000
H	-0.132080000	2.625024000	3.356960000
H	-1.316453000	2.826410000	2.048940000

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structure of 1:I

Ir	1.140140000	12.506731000	4.360392000
C	1.440546000	10.848350000	7.037968000
H	2.373979000	10.307045000	7.181825000
H	0.719237000	10.379585000	7.703522000
C	1.603205000	12.316755000	7.404381000
H	0.640836000	12.730689000	7.706686000
H	2.257037000	12.443590000	8.271709000
C	2.139590000	13.135726000	6.268845000
H	1.964814000	14.202047000	6.354733000
C	3.152236000	12.761396000	5.381799000
H	3.628516000	13.576699000	4.855515000
C	3.959881000	11.487317000	5.461631000
H	4.141341000	11.262909000	6.512865000
H	4.936238000	11.686560000	5.027593000
C	3.338118000	10.278930000	4.746330000
H	3.808832000	10.148060000	3.776902000
H	3.538378000	9.361661000	5.306322000
C	1.856551000	10.392958000	4.548190000



H	1.453896000	9.873089000	3.687479000
C	0.982460000	10.670416000	5.608845000
H	-0.048876000	10.364243000	5.480928000
C	-0.303112000	14.181981000	4.806126000
C	-0.955486000	12.922985000	4.924390000
C	0.184722000	14.314690000	3.485478000
H	-0.156813000	14.887818000	5.606980000
C	-0.932482000	12.290813000	3.634639000
H	-1.431605000	12.538250000	5.810971000
C	-0.241914000	13.149920000	2.752447000
H	0.730339000	15.149885000	3.081179000
H	-1.371957000	11.340522000	3.381382000
H	-0.034592000	12.955706000	1.714014000
I	2.906241000	12.516702000	2.188105000

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structure of TS\_1\_IM1:I

Ir	1.356742000	12.532996000	4.534831000
C	1.570448000	11.503929000	7.509587000
H	2.117161000	10.575635000	7.668649000
H	0.946321000	11.633482000	8.391266000
C	2.528603000	12.679753000	7.378570000
H	2.027633000	13.595165000	7.696408000
H	3.386836000	12.570836000	8.047934000
C	3.016879000	12.868692000	5.970915000
H	3.408596000	13.857485000	5.756542000
C	3.415714000	11.853830000	5.091857000
H	4.054437000	12.168652000	4.278118000
C	3.502873000	10.385556000	5.447081000
H	3.852110000	10.298692000	6.476446000
H	4.281404000	9.939622000	4.832918000
C	2.200893000	9.597875000	5.245876000
H	2.242792000	9.064848000	4.300392000
H	2.094266000	8.834112000	6.021255000
C	0.969689000	10.458270000	5.248436000
H	0.136342000	10.083752000	4.666857000
C	0.685526000	11.352041000	6.291365000
H	-0.354874000	11.618281000	6.431617000
C	1.401818000	14.498543000	3.541385000
C	0.901873000	14.645063000	4.875224000
C	0.337893000	13.922666000	2.732283000
H	2.279784000	14.982350000	3.147673000
C	-0.298167000	13.892764000	4.972572000
H	1.361065000	15.206684000	5.671462000

C	-0.540103000	13.287514000	3.700533000
H	-0.907146000	13.788153000	5.854711000
H	-1.396485000	12.681819000	3.455210000
H	0.545086000	13.468856000	1.777864000
P	-0.800801000	15.824339000	1.877857000
O	-1.688073000	16.268248000	3.114662000
O	-1.825568000	16.130015000	0.677083000
O	0.402416000	16.853304000	1.696590000
C	-2.766819000	17.221288000	3.073265000
H	-3.130162000	17.313872000	4.090362000
H	-2.420158000	18.189566000	2.720675000
H	-3.561004000	16.861921000	2.425942000
C	-1.439165000	15.880276000	-0.682617000
H	-1.263950000	14.818937000	-0.846814000
H	-2.265457000	16.206684000	-1.303517000
H	-0.544097000	16.442571000	-0.943532000
C	0.226202000	18.267459000	1.506954000
H	0.071504000	18.750493000	2.469272000
H	1.137484000	18.644441000	1.055983000
H	-0.616997000	18.473357000	0.849686000
I	2.091950000	11.158472000	2.174004000

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structure of IM1:I

Ir	1.516771000	12.829181000	4.537496000
C	0.762044000	10.395535000	6.401270000
H	1.562749000	9.694537000	6.632512000
H	-0.163799000	9.858578000	6.598326000
C	0.845636000	11.625034000	7.295270000
H	-0.149494000	12.057826000	7.410376000
H	1.166805000	11.361459000	8.307548000
C	1.759318000	12.679183000	6.735501000
H	1.600683000	13.674706000	7.137761000
C	3.009482000	12.453816000	6.141071000
H	3.674580000	13.306682000	6.122381000
C	3.691424000	11.105004000	6.044727000
H	3.464760000	10.532252000	6.944418000
H	4.766082000	11.270602000	6.065471000
C	3.335039000	10.307745000	4.784175000
H	4.105918000	10.458540000	4.032687000
H	3.325125000	9.235232000	4.998421000
C	2.014048000	10.699868000	4.182065000
H	1.923265000	10.530868000	3.115717000
C	0.827830000	10.754599000	4.931564000

H	-0.097665000	10.636348000	4.380917000
C	1.017893000	14.955829000	4.415155000
C	-0.080661000	14.223674000	4.978407000
C	0.882555000	14.902531000	2.905701000
H	1.533859000	15.752517000	4.929069000
C	-0.519958000	13.303828000	3.985957000
H	-0.474353000	14.312522000	5.977770000
C	0.309794000	13.497722000	2.834223000
H	-1.302836000	12.571809000	4.102810000
H	0.190690000	12.957989000	1.906970000
H	1.849476000	14.979899000	2.397454000
P	-0.138257000	16.192572000	2.194136000
O	0.564546000	17.548548000	2.461744000
O	-1.573816000	16.386394000	2.793635000
O	-0.245159000	15.833516000	0.679341000
C	-0.070263000	18.841271000	2.596694000
H	0.730330000	19.543436000	2.793014000
H	-0.582518000	19.112393000	1.677946000
H	-0.769737000	18.823688000	3.426148000
C	-2.677297000	15.484208000	2.564140000
H	-2.833082000	14.891906000	3.460024000
H	-3.551942000	16.095271000	2.368709000
H	-2.483753000	14.831676000	1.715428000
C	-0.852113000	16.686683000	-0.315363000
H	-0.182857000	17.511872000	-0.542733000
H	-0.991913000	16.075724000	-1.198694000
H	-1.814169000	17.060647000	0.029804000
I	3.858259000	13.307389000	3.034510000

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structure of TS\_IM1\_IM2:I

Ir	1.064919000	-0.595165000	0.961103000
C	0.239916000	-3.344323000	2.193864000
H	1.015216000	-4.085814000	2.383666000
H	-0.689687000	-3.905593000	2.127965000
C	0.156258000	-2.320996000	3.319978000
H	-0.879902000	-2.009603000	3.452973000
H	0.462730000	-2.741007000	4.282324000
C	0.979838000	-1.103619000	3.001762000
H	0.689464000	-0.210189000	3.550093000
C	2.348689000	-1.161309000	2.562205000
H	2.948595000	-0.292299000	2.802530000
C	3.135023000	-2.449820000	2.420123000
H	2.741529000	-3.208343000	3.096087000

H	4.162763000	-2.281445000	2.732623000
C	3.092941000	-2.906437000	0.970545000
H	3.921726000	-2.460513000	0.422874000
H	3.205140000	-3.989491000	0.862545000
C	1.814327000	-2.463138000	0.318302000
H	1.863993000	-2.402012000	-0.766165000
C	0.503646000	-2.655161000	0.869447000
H	-0.282249000	-2.771453000	0.133100000
C	-0.287837000	0.894617000	0.038790000
C	-1.101008000	-0.082212000	0.673903000
C	-0.474978000	0.758753000	-1.464468000
H	-0.046097000	1.850998000	0.481986000
C	-1.758309000	-0.856629000	-0.379857000
H	-1.527955000	0.023051000	1.662044000
C	-1.424833000	-0.404004000	-1.595459000
H	-2.408895000	-1.698540000	-0.193438000
H	-1.711306000	-0.819407000	-2.548200000
I	3.055444000	0.946460000	-0.141596000
H	0.467457000	0.595933000	-2.003426000
P	-1.108723000	2.266061000	-2.177168000
O	-0.043269000	3.375198000	-2.335253000
O	-2.243015000	2.927037000	-1.334914000
O	-1.575496000	1.892498000	-3.607889000
C	0.589128000	4.099918000	-1.246455000
H	1.070668000	4.955547000	-1.703271000
H	-0.162806000	4.430720000	-0.535287000
H	1.331448000	3.457294000	-0.775262000
C	-3.462135000	2.252126000	-0.945364000
H	-3.272061000	1.647094000	-0.064111000
H	-4.179039000	3.032290000	-0.718449000
H	-3.832836000	1.628929000	-1.755847000
C	-2.015883000	2.878674000	-4.576515000
H	-1.178470000	3.506682000	-4.863335000
H	-2.375406000	2.317154000	-5.429338000
H	-2.818661000	3.481488000	-4.159762000

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structure of IM2:I

Ir	0.148042000	12.941225000	5.346217000
C	1.456761000	10.353368000	6.406675000
H	2.504142000	10.158163000	6.186176000
H	1.036441000	9.392493000	6.695180000
C	1.310676000	11.334303000	7.570746000
H	0.376084000	11.133761000	8.095787000

H	2.100566000	11.187193000	8.313697000
C	1.302534000	12.772891000	7.129288000
H	0.907937000	13.457117000	7.877049000
C	2.148873000	13.328760000	6.145553000
H	2.311405000	14.394370000	6.225864000
C	3.251019000	12.585030000	5.422962000
H	3.655222000	11.802198000	6.061798000
H	4.079313000	13.268401000	5.244020000
C	2.773409000	12.014011000	4.087869000
H	2.867991000	12.774682000	3.312203000
H	3.410686000	11.185600000	3.764046000
C	1.345223000	11.565362000	4.124996000
H	0.849240000	11.524903000	3.160816000
C	0.738204000	10.846832000	5.170788000
H	-0.158380000	10.300694000	4.899924000
C	-0.630344000	14.935273000	5.673663000
C	0.052729000	14.962132000	4.419429000
H	-1.710505000	14.855774000	5.707724000
H	-0.419742000	14.747407000	3.471438000
I	-2.166968000	12.373649000	4.112632000
C	1.178121000	15.874126000	4.514841000
C	1.204244000	16.471070000	5.715461000
C	0.082680000	15.943329000	6.571458000
H	1.950279000	17.157051000	6.087354000
P	-1.075130000	17.195573000	7.083115000
O	-0.232932000	18.298496000	7.774101000
O	-1.955359000	17.749939000	5.926378000
O	-2.093835000	16.685837000	8.133352000
C	-0.823122000	19.457145000	8.418583000
C	-1.453447000	18.301381000	4.685086000
C	-3.226935000	15.820519000	7.863225000
H	0.005852000	20.089794000	8.708948000
H	-1.382178000	19.141866000	9.293868000
H	-1.470264000	19.983881000	7.722171000
H	-1.254006000	17.491258000	3.990886000
H	-0.550625000	18.881879000	4.859090000
H	-2.239687000	18.940465000	4.301152000
H	-3.705034000	16.104525000	6.930287000
H	-3.910939000	15.958478000	8.691416000
H	-2.890644000	14.788294000	7.824351000
H	0.464952000	15.532124000	7.514321000
H	1.898746000	16.035356000	3.726518000

structure of TS\_1\_IM8:I

Ir	-0.929823000	0.480360000	-1.263373000
C	-2.581700000	0.925984000	-2.530133000
C	-2.346367000	2.041676000	-1.686349000
C	-2.917515000	-0.207912000	-1.700174000
H	-2.494382000	0.912096000	-3.604127000
C	-2.505142000	1.592961000	-0.330409000
H	-2.051723000	3.029169000	-1.998220000
C	-2.915902000	0.227571000	-0.349921000
H	-2.354322000	2.192936000	0.552779000
H	-3.118698000	-0.380356000	0.515490000
H	-3.148933000	-1.199335000	-2.053444000
C	0.592408000	-1.251593000	-0.734466000
C	-0.341660000	-1.136786000	0.285372000
H	0.249442000	-1.860690000	-1.567522000
C	2.090518000	-1.145789000	-0.650346000
C	-0.161423000	-0.586587000	1.669770000
H	-1.218499000	-1.764905000	0.174475000
H	2.464955000	-0.207676000	-1.056846000
H	2.463560000	-1.905247000	-1.337477000
C	2.710860000	-1.380489000	0.734267000
C	0.562638000	0.750591000	1.832985000
H	0.323313000	-1.349892000	2.283877000
H	-1.157695000	-0.482967000	2.101518000
H	2.125510000	-2.118028000	1.286194000
H	3.674094000	-1.858802000	0.573927000
C	2.939218000	-0.134238000	1.537333000
H	0.261562000	1.428701000	1.018343000
H	0.161089000	1.225707000	2.728965000
C	2.048947000	0.760699000	1.953020000
H	3.975694000	0.081895000	1.764512000
H	2.437263000	1.634653000	2.462047000
I	1.032403000	1.614546000	-2.538476000

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structure of IM8:I

Ir	0.975630000	12.703041000	4.361869000
C	1.403254000	14.818837000	4.259238000
C	0.065821000	14.642080000	4.669071000
C	1.553797000	14.197886000	2.962637000
H	2.187438000	15.287873000	4.830139000
C	-0.624165000	13.911693000	3.630740000
H	-0.356612000	14.949392000	5.611573000
C	0.284142000	13.695150000	2.556396000

H	-1.658117000	13.608482000	3.658581000
H	0.068199000	13.184861000	1.632095000
H	2.466678000	14.150817000	2.391475000
C	1.557741000	10.713607000	3.264038000
C	0.241426000	10.566480000	3.670881000
H	1.681113000	11.143022000	2.272466000
C	2.782967000	10.010898000	3.761011000
C	-0.346634000	9.668406000	4.720111000
H	-0.493920000	10.945746000	2.968003000
H	2.763330000	9.859276000	4.832504000
H	3.651713000	10.637263000	3.559145000
C	2.964052000	8.675785000	3.033033000
C	0.531168000	8.527613000	5.229732000
H	-1.242783000	9.241829000	4.261729000
H	-0.729300000	10.257840000	5.555596000
H	3.056181000	8.859623000	1.959245000
H	3.935158000	8.264440000	3.320819000
C	1.908350000	7.642226000	3.246215000
H	1.387006000	8.919031000	5.774504000
H	-0.051298000	7.986835000	5.973843000
C	0.925074000	7.568687000	4.140477000
H	1.983228000	6.810607000	2.554505000
H	0.289808000	6.693411000	4.069874000
I	1.862239000	12.024078000	6.690297000

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structure of IM6:I'

Ir	0.082088000	-0.612068000	-0.576816000
C	1.504841000	-2.975851000	1.045007000
H	2.161747000	-3.668860000	0.520420000
H	1.260857000	-3.455608000	1.992218000
C	2.222061000	-1.655442000	1.314699000
H	1.822660000	-1.214564000	2.230553000
H	3.287078000	-1.826861000	1.508749000
C	2.040575000	-0.638597000	0.220637000
H	2.340123000	0.350776000	0.540475000
C	2.151521000	-0.894155000	-1.197341000
H	2.561043000	-0.066041000	-1.765762000
C	2.498826000	-2.258812000	-1.765994000
H	3.148536000	-2.797384000	-1.073310000
H	3.090000000	-2.136030000	-2.672875000
C	1.250291000	-3.066714000	-2.095370000
H	0.872224000	-2.752525000	-3.069321000
H	1.473989000	-4.135733000	-2.188460000

C	0.129594000	-2.883220000	-1.115354000
H	-0.860378000	-3.050360000	-1.518955000
C	0.230276000	-2.807863000	0.255750000
H	-0.687544000	-2.927804000	0.811432000
P	0.194172000	1.580197000	-0.984822000
O	-0.895706000	2.589467000	-0.375128000
O	0.175547000	2.141554000	-2.491262000
O	1.512457000	2.220972000	-0.328907000
C	-2.188460000	2.736278000	-0.971122000
C	0.910974000	1.500724000	-3.531077000
C	1.713594000	3.633902000	-0.356268000
H	-2.842017000	3.140792000	-0.203253000
H	-2.129839000	3.423234000	-1.813163000
H	-2.575565000	1.779213000	-1.320810000
H	0.494563000	1.848104000	-4.471061000
H	1.964315000	1.779110000	-3.469862000
H	0.803038000	0.417082000	-3.471488000
H	1.069853000	4.121864000	0.373504000
H	2.754117000	3.809827000	-0.100885000
H	1.506385000	4.044155000	-1.344097000
I	-1.933100000	-0.726218000	-2.811593000
P	-1.183786000	-0.098401000	1.227497000
O	-1.436901000	-1.330972000	2.262340000
O	-2.601415000	0.711536000	1.302925000
O	-0.330521000	0.952890000	2.122697000
C	-1.884081000	-1.060461000	3.586115000
C	-3.738244000	0.112138000	0.681591000
C	-0.865778000	2.086356000	2.795121000
H	-2.136173000	-2.011979000	4.044989000
H	-1.096076000	-0.580638000	4.167414000
H	-2.765827000	-0.417937000	3.585449000
H	-3.492450000	-0.270821000	-0.311304000
H	-4.127815000	-0.701346000	1.295464000
H	-4.497729000	0.884217000	0.592788000
H	-1.641055000	1.813216000	3.510521000
H	-0.036757000	2.548656000	3.325457000
H	-1.280124000	2.797005000	2.081845000
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structure of bipy			
C	-4.453921000	-0.479214000	-0.084857000
C	-3.356990000	-0.289554000	0.755667000
C	-2.685736000	0.917327000	0.713534000
C	-3.122810000	1.899676000	-0.160950000



C	-4.222886000	1.620707000	-0.958380000
N	-4.878817000	0.467808000	-0.930698000
H	-1.831810000	1.090724000	1.354635000
H	-3.060494000	-1.089779000	1.417082000
H	-2.627266000	2.857723000	-0.226274000
H	-4.595573000	2.363930000	-1.655644000
C	-5.203405000	-1.753730000	-0.075559000
C	-6.300331000	-1.943393000	-0.916089000
N	-4.778515000	-2.700748000	0.770288000
C	-6.971585000	-3.150274000	-0.873956000
H	-6.596823000	-1.143170000	-1.577509000
C	-5.434445000	-3.853647000	0.797971000
C	-6.534516000	-4.132619000	0.000535000
H	-7.825506000	-3.323673000	-1.515062000
H	-5.061762000	-4.596867000	1.495239000
H	-7.030061000	-5.090666000	0.065859000

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structure of TS\_1\_IM1:bipy

Ir	1.652128000	12.771455000	4.688258000
C	0.815496000	10.446683000	6.663162000
H	1.596845000	9.738034000	6.933016000
H	-0.125592000	9.942920000	6.873929000
C	0.921312000	11.713102000	7.501673000
H	-0.062351000	12.175836000	7.589929000
H	1.229017000	11.487030000	8.526696000
C	1.869281000	12.714948000	6.907619000
H	1.724113000	13.735881000	7.245235000
C	3.115276000	12.428674000	6.340388000
H	3.797890000	13.263761000	6.260986000
C	3.760604000	11.061601000	6.301698000
H	3.514090000	10.533377000	7.222912000
H	4.838472000	11.201282000	6.320869000
C	3.394211000	10.216322000	5.073089000
H	4.173488000	10.313772000	4.323421000
H	3.355600000	9.156613000	5.340114000
C	2.087710000	10.603494000	4.442726000
H	2.002616000	10.399290000	3.382450000
C	0.902760000	10.734152000	5.179743000
H	-0.024087000	10.629859000	4.629744000
C	1.135266000	14.899126000	4.564252000
C	0.017897000	14.138846000	5.060658000
C	1.237165000	14.681300000	3.133929000
H	1.649100000	15.673456000	5.110232000

C	-0.371596000	13.237907000	4.030503000
H	-0.449248000	14.235034000	6.026832000
C	0.517337000	13.426367000	2.931129000
H	-1.168679000	12.515986000	4.092554000
H	0.478609000	12.885584000	1.999263000
Br	3.904478000	12.971555000	3.368084000
H	2.149720000	14.873455000	2.597677000
N	0.225808000	16.049512000	2.184596000
C	-0.014618000	16.011236000	0.860012000
C	-0.372610000	16.957138000	2.950949000
C	-0.908301000	16.920508000	0.298687000
C	-1.252501000	17.894043000	2.447924000
H	-0.132806000	16.917510000	4.006124000
C	-1.529179000	17.866593000	1.091214000
H	-1.080169000	16.895559000	-0.767251000
H	-1.704641000	18.619812000	3.106183000
H	-2.211573000	18.581007000	0.653351000
C	0.691634000	15.027378000	0.013858000
C	0.054865000	14.445688000	-1.080267000
N	1.957608000	14.751511000	0.341529000
C	0.763291000	13.543985000	-1.856592000
H	-0.976831000	14.676107000	-1.306498000
C	2.626694000	13.888142000	-0.413236000
C	2.075767000	13.259548000	-1.522301000
H	0.294017000	13.070277000	-2.707229000
H	3.649026000	13.690708000	-0.113958000
H	2.663662000	12.564315000	-2.103183000

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structure of IM1:bipy

Ir	1.610022000	12.832905000	4.654930000
C	0.781505000	10.454936000	6.568785000
H	1.564353000	9.742767000	6.824602000
H	-0.157843000	9.942315000	6.766682000
C	0.879635000	11.701839000	7.437783000
H	-0.107409000	12.156726000	7.532868000
H	1.184221000	11.452151000	8.458518000
C	1.821807000	12.725073000	6.869083000
H	1.672959000	13.734782000	7.238040000
C	3.069656000	12.459561000	6.293815000
H	3.749301000	13.299274000	6.238354000
C	3.721733000	11.095959000	6.224208000
H	3.464980000	10.536861000	7.124047000
H	4.799113000	11.237378000	6.263602000

C	3.373313000	10.293859000	4.963401000
H	4.146436000	10.448028000	4.215820000
H	3.366834000	9.222544000	5.182959000
C	2.056134000	10.679551000	4.351833000
H	1.969567000	10.498419000	3.287138000
C	0.869536000	10.777475000	5.091994000
H	-0.055674000	10.674517000	4.538317000
C	1.143731000	14.949672000	4.524478000
C	0.010075000	14.220961000	5.033488000
C	1.130159000	14.866508000	3.033396000
H	1.667707000	15.713353000	5.079225000
C	-0.395270000	13.323157000	4.005787000
H	-0.443914000	14.315649000	6.006492000
C	0.503059000	13.505828000	2.909722000
H	-1.197680000	12.607018000	4.072210000
H	0.448682000	12.950878000	1.985410000
Br	3.840665000	13.134698000	3.305944000
H	2.105932000	14.947719000	2.572430000
N	0.263830000	15.969657000	2.309687000
C	0.046789000	15.916528000	0.967844000
C	-0.330173000	16.911806000	3.059296000
C	-0.835100000	16.825291000	0.398094000
C	-1.185753000	17.843941000	2.522189000
H	-0.097672000	16.880977000	4.112165000
C	-1.456413000	17.791483000	1.165136000
H	-0.993627000	16.778250000	-0.668814000
H	-1.630315000	18.587706000	3.164627000
H	-2.129906000	18.501963000	0.707978000
C	0.751005000	14.933661000	0.118952000
C	0.059258000	14.246834000	-0.874954000
N	2.059355000	14.784779000	0.334696000
C	0.763394000	13.348752000	-1.660775000
H	-1.003088000	14.393105000	-1.014325000
C	2.722922000	13.927734000	-0.430227000
C	2.118760000	13.183324000	-1.436525000
H	0.257754000	12.787205000	-2.433388000
H	3.781731000	13.830498000	-0.224339000
H	2.701996000	12.491428000	-2.025994000

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structure of TS\_IM1\_IM2:bipy

Ir	0.990821000	-0.660512000	1.437592000
C	-0.307047000	-2.618753000	3.478770000
H	0.178803000	-3.568884000	3.699678000

H	-1.353780000	-2.758756000	3.741604000
C	0.290393000	-1.479622000	4.297926000
H	-0.495699000	-0.771241000	4.560877000
H	0.701812000	-1.828784000	5.249045000
C	1.343679000	-0.742737000	3.515104000
H	1.531501000	0.270248000	3.861966000
C	2.426721000	-1.397588000	2.836857000
H	3.314794000	-0.798440000	2.676120000
C	2.668593000	-2.891801000	2.897585000
H	2.233209000	-3.306917000	3.806039000
H	3.736670000	-3.083570000	2.965998000
C	2.090415000	-3.533575000	1.649209000
H	2.835281000	-3.522184000	0.855240000
H	1.813196000	-4.582003000	1.794653000
C	0.899832000	-2.751258000	1.172263000
H	0.666144000	-2.899071000	0.121271000
C	-0.199895000	-2.324077000	1.994575000
H	-1.150003000	-2.259837000	1.476601000
C	-0.065193000	1.056714000	0.517254000
C	-0.741571000	0.661230000	1.710641000
C	-0.970141000	0.752053000	-0.655433000
H	0.628818000	1.881750000	0.438898000
C	-2.010458000	0.044010000	1.303198000
H	-0.635850000	1.148269000	2.671294000
C	-2.152480000	0.071575000	-0.026885000
H	-2.705887000	-0.409894000	1.995201000
H	-2.956618000	-0.359954000	-0.602609000
Br	2.815702000	-0.413943000	-0.309678000
H	-0.499072000	0.180569000	-1.446878000
N	-1.433241000	2.054978000	-1.325006000
C	-1.213044000	2.355035000	-2.630743000
C	-2.159503000	2.878572000	-0.540706000
C	-1.820596000	3.491321000	-3.158953000
C	-2.734060000	4.023940000	-1.023485000
H	-2.266376000	2.552338000	0.483020000
C	-2.581224000	4.326412000	-2.370094000
H	-1.638454000	3.723160000	-4.197253000
H	-3.299855000	4.655381000	-0.356901000
H	-3.032552000	5.213312000	-2.791024000
C	-0.291631000	1.563758000	-3.464612000
C	-0.599070000	1.282603000	-4.792358000
N	0.866955000	1.229363000	-2.890298000
C	0.348402000	0.617627000	-5.553666000

H	-1.556436000	1.558393000	-5.212565000
C	1.769248000	0.603779000	-3.635541000
C	1.556427000	0.278993000	-4.970322000
H	0.143075000	0.370385000	-6.585418000
H	2.695831000	0.349887000	-3.134826000
H	2.323418000	-0.232255000	-5.533225000

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structure of IM2:bipy

Ir	0.354569000	13.033477000	5.961423000
C	2.484066000	11.069040000	7.024046000
H	3.323950000	10.799587000	6.386906000
H	2.443133000	10.299428000	7.791833000
C	2.711611000	12.429882000	7.685775000
H	2.199408000	12.449594000	8.649259000
H	3.770558000	12.584938000	7.914931000
C	2.201831000	13.580571000	6.857800000
H	2.078098000	14.502201000	7.422579000
C	2.363922000	13.706488000	5.460261000
H	2.334518000	14.718688000	5.081367000
C	3.138494000	12.740602000	4.587955000
H	3.938858000	12.278192000	5.162748000
H	3.636611000	13.299321000	3.797471000
C	2.230382000	11.682996000	3.960735000
H	1.806977000	12.069451000	3.033249000
H	2.801448000	10.794871000	3.673843000
C	1.097819000	11.287705000	4.856403000
H	0.225133000	10.884714000	4.353684000
C	1.193011000	11.041658000	6.237087000
H	0.389222000	10.449621000	6.660961000
C	-0.596092000	14.983399000	5.985231000
C	-0.597519000	14.551205000	4.632946000
H	-1.449908000	14.895676000	6.642112000
H	-1.387695000	13.974937000	4.174739000
Br	-1.924092000	12.058969000	6.170798000
C	0.247164000	15.452879000	3.859118000
C	0.699792000	16.450230000	4.631086000
C	0.246949000	16.241611000	6.046851000
H	1.382769000	17.235156000	4.340102000
H	1.099995000	16.172324000	6.720975000
H	0.487909000	15.314313000	2.815084000
N	-0.556580000	17.411772000	6.571772000
C	-0.450759000	17.841059000	7.858053000
C	-1.377863000	18.035664000	5.701704000

C	-1.127235000	18.995749000	8.229306000
C	0.290097000	17.055382000	8.863536000
C	-2.093458000	19.150271000	6.055451000
H	-1.403765000	17.606384000	4.711140000
C	-1.945201000	19.659147000	7.337329000
H	-1.030654000	19.332502000	9.250442000
C	1.130643000	17.677321000	9.781098000
N	0.020614000	15.745949000	8.883681000
H	-2.741576000	19.614198000	5.328771000
H	-2.477870000	20.548102000	7.642897000
C	1.724672000	16.894465000	10.758066000
H	1.327796000	18.738868000	9.722645000
C	0.579498000	15.014880000	9.839870000
C	1.440156000	15.540449000	10.795799000
H	2.394736000	17.338870000	11.479977000
H	0.321645000	13.961777000	9.840932000
H	1.872589000	14.900313000	11.550639000