Supporting Information

Comparative Investigation of Reactivities between Catalysts $[Cp^*RhCl_2]_2$ and $[Cp^*IrCl_2]_2$ in Oxidative Annulation of Isoquinolones with Alkynes: A Combined Experimental and Computational Study

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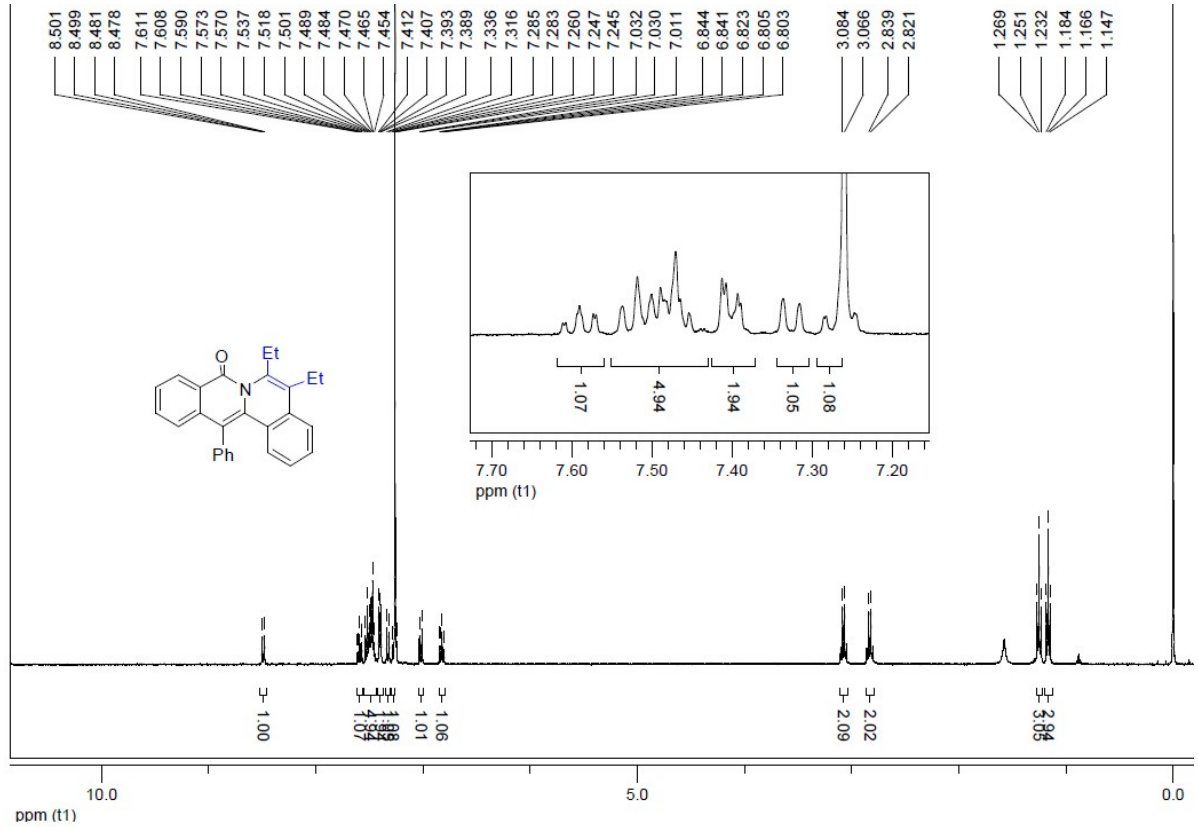
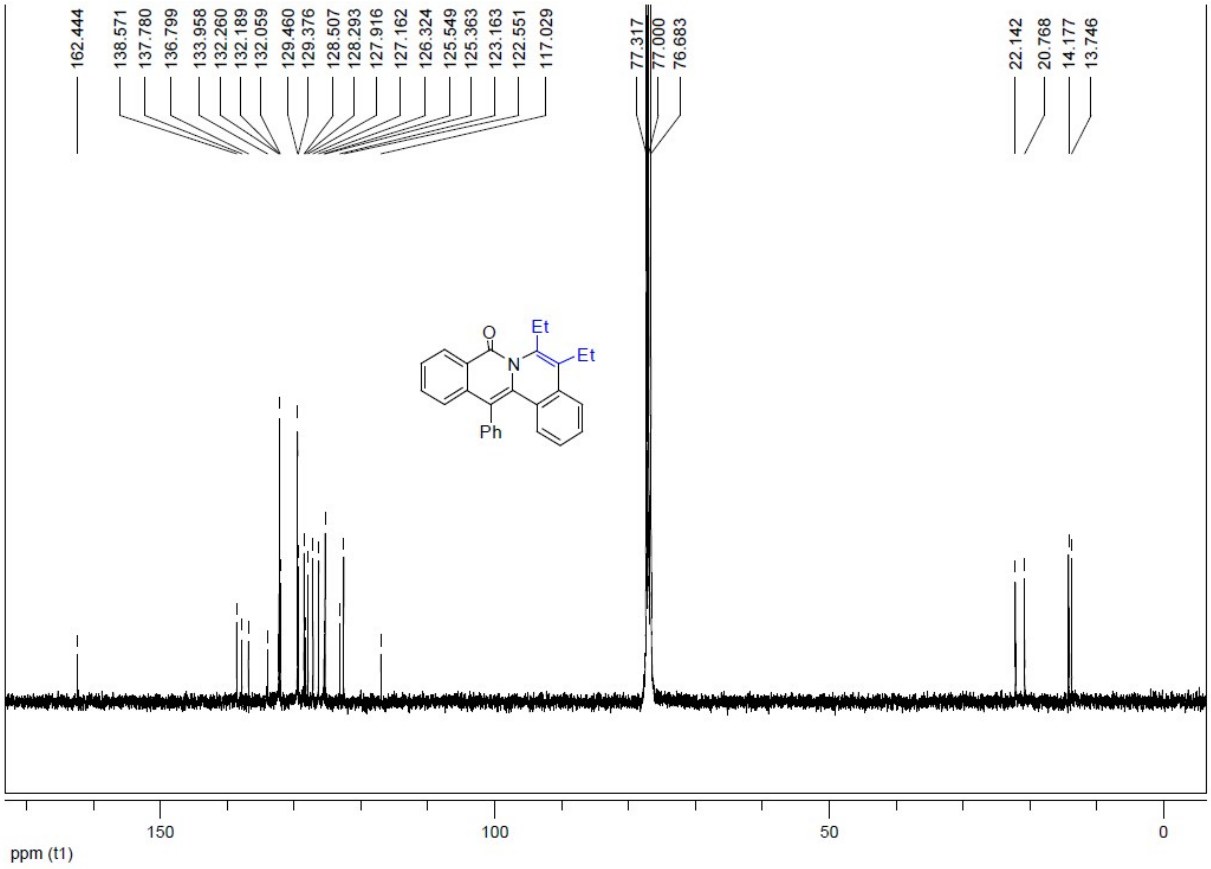
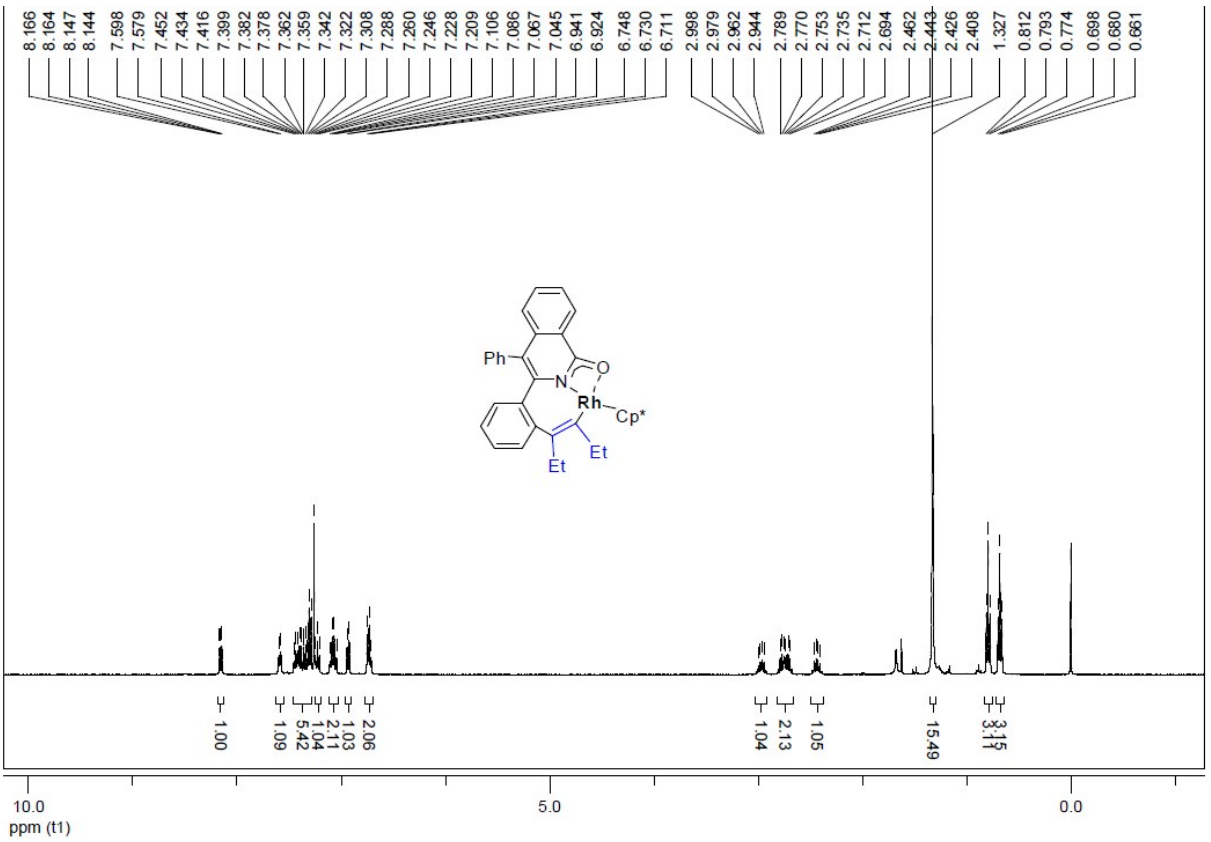
Spectral Copies of ^{1}H and ^{13}C NMR of Compounds Obtained in this Study



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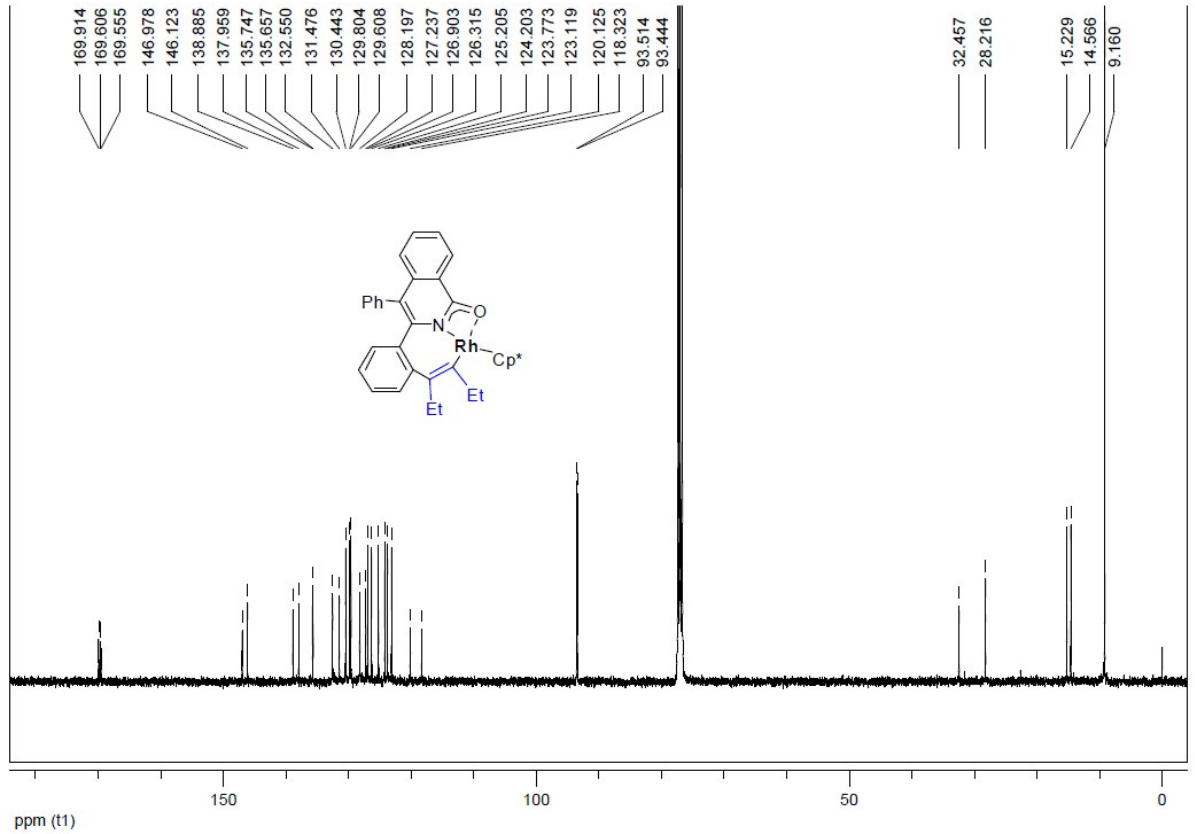
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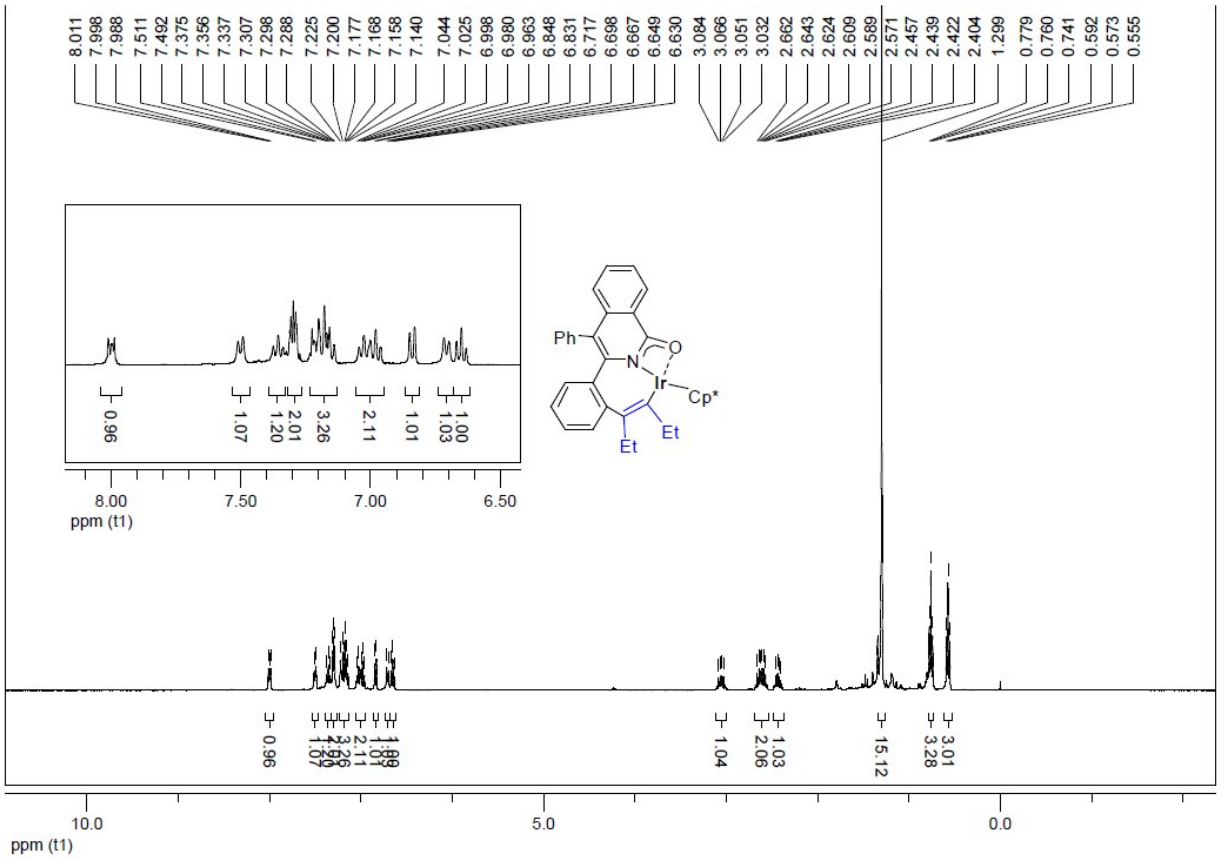
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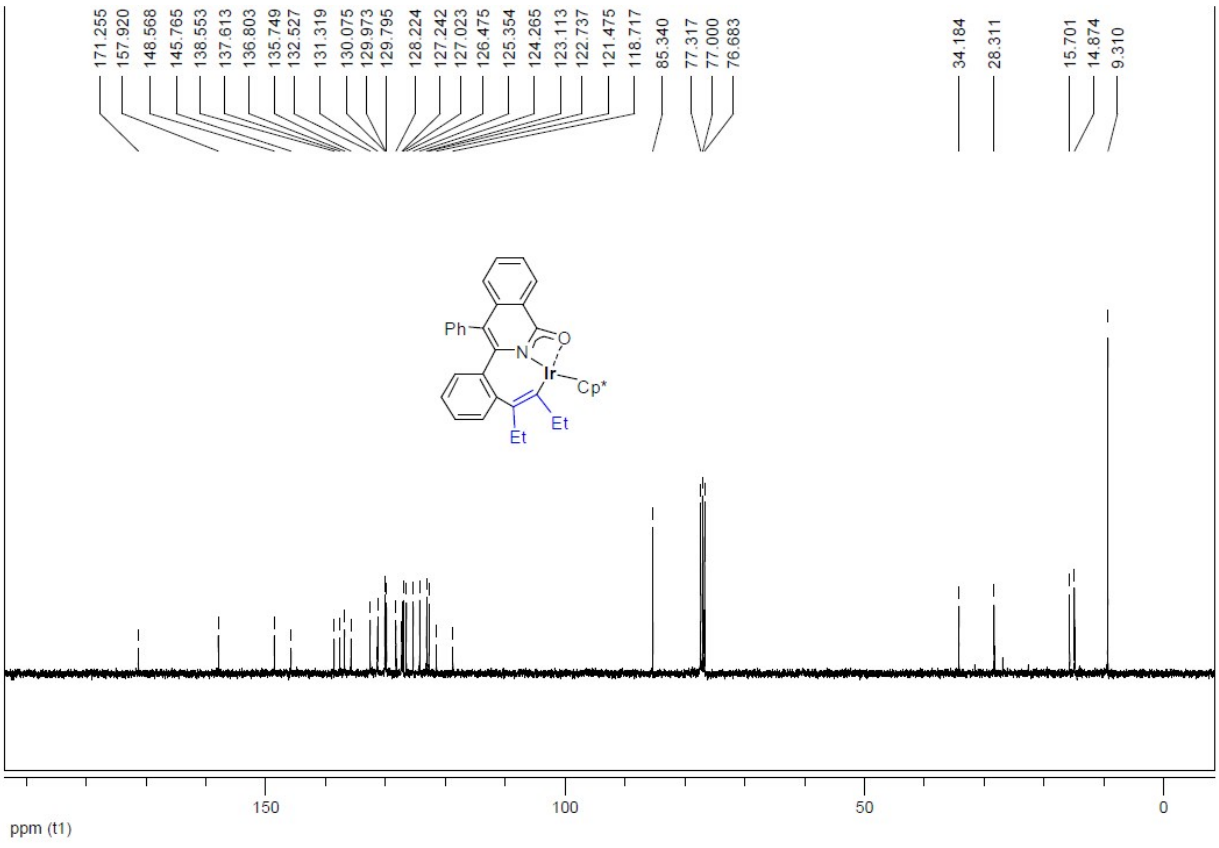
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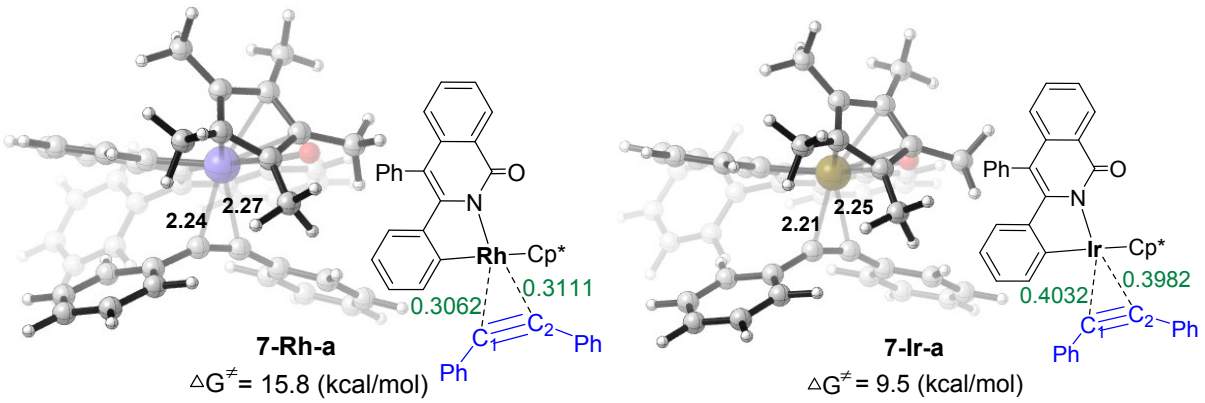

Fig. S1 Optimized geometries of the intermediates **7** with diphenyl-acetylene **a**. Numbers in black are distances (Å) between atoms, numbers in green are Wiberg bond indexes. All energies are with respect to the substrate and the active catalyst.

The binding of diphenyl-acetylene **a** to the metal center in the intermediate **7-Ir-a** is stronger than in **7-Rh-a** as demonstrated by the relative energies of the two species and the Wiberg bond indexes of M–C1 and M–C2 as shown in Fig. S1. As a result, the Ir–C2 bond will be formed more easily than the Rh–C2 bond in the alkyne insertion step.

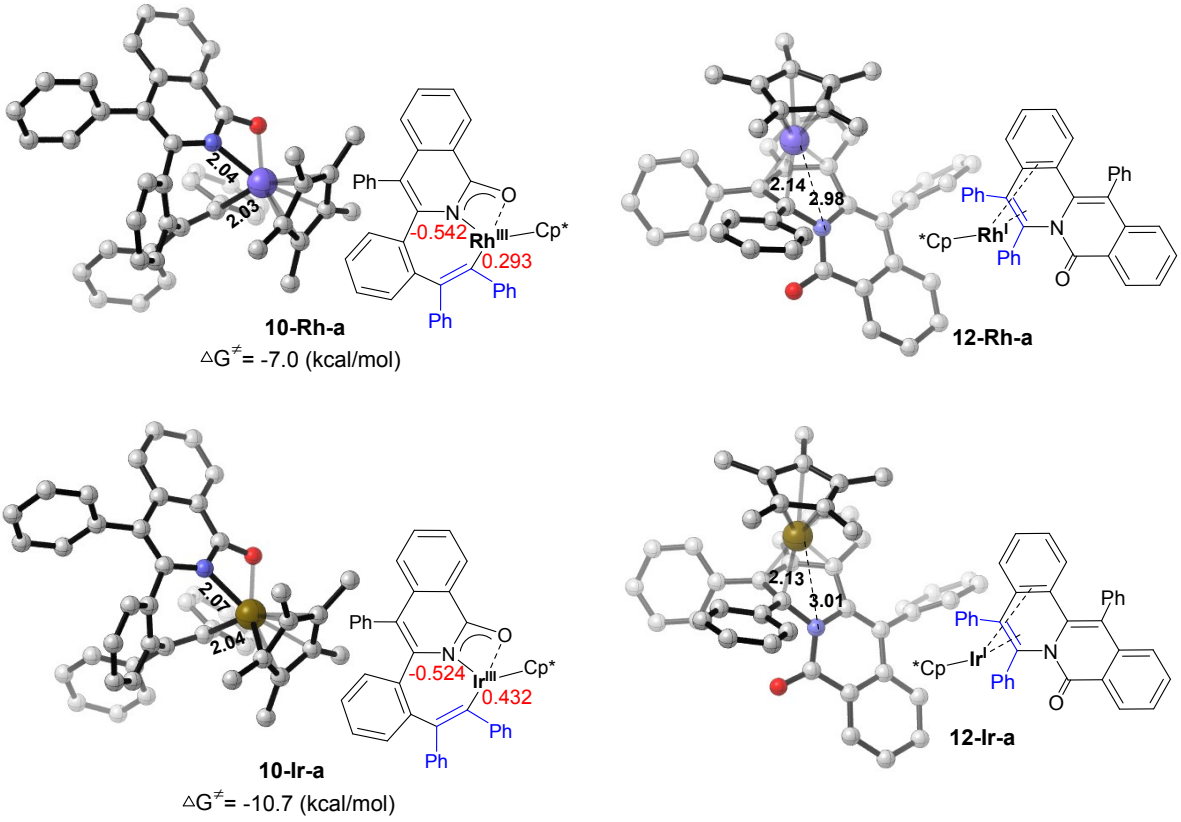

Fig. S2 Optimized geometries of the intermediates **10** and the intermediates **12** with diphenyl-acetylene **a**. Numbers in black are distances (Å) between atoms, numbers in red are NBO charges. All energies are with respect to the substrate and the active catalyst.

NBO charges (numbers in red as shown in Fig. S2) indicate that the Ir center was more positively charged than the Rh center in the **10-M-a** (M = Rh, Ir), which resulted in the

stronger electrostatic interactions between Ir and N relative to that between Rh and N. This may be one of the reasons why the intermediate **10-Ir-a** was more stable than the intermediate **10-Rh-a by** 3.7 kcal/mol. As shown in Fig. S2, obviously, the M-N bond (M = Rh, Ir) has been broken when the intermediate **10-M-a** undergoes reductive elimination to form the intermediate **12-M-a** (M = Rh, Ir). The Ir-N bond is more difficult to be broken than the Rh-N bond due to the stronger electrostatic interactions between Ir and N, which may be one of the reasons for the higher activation energy of the reductive elimination step in the reaction with $[Cp^*IrCl_2]_2$ than with $[Cp^*RhCl_2]_2$.

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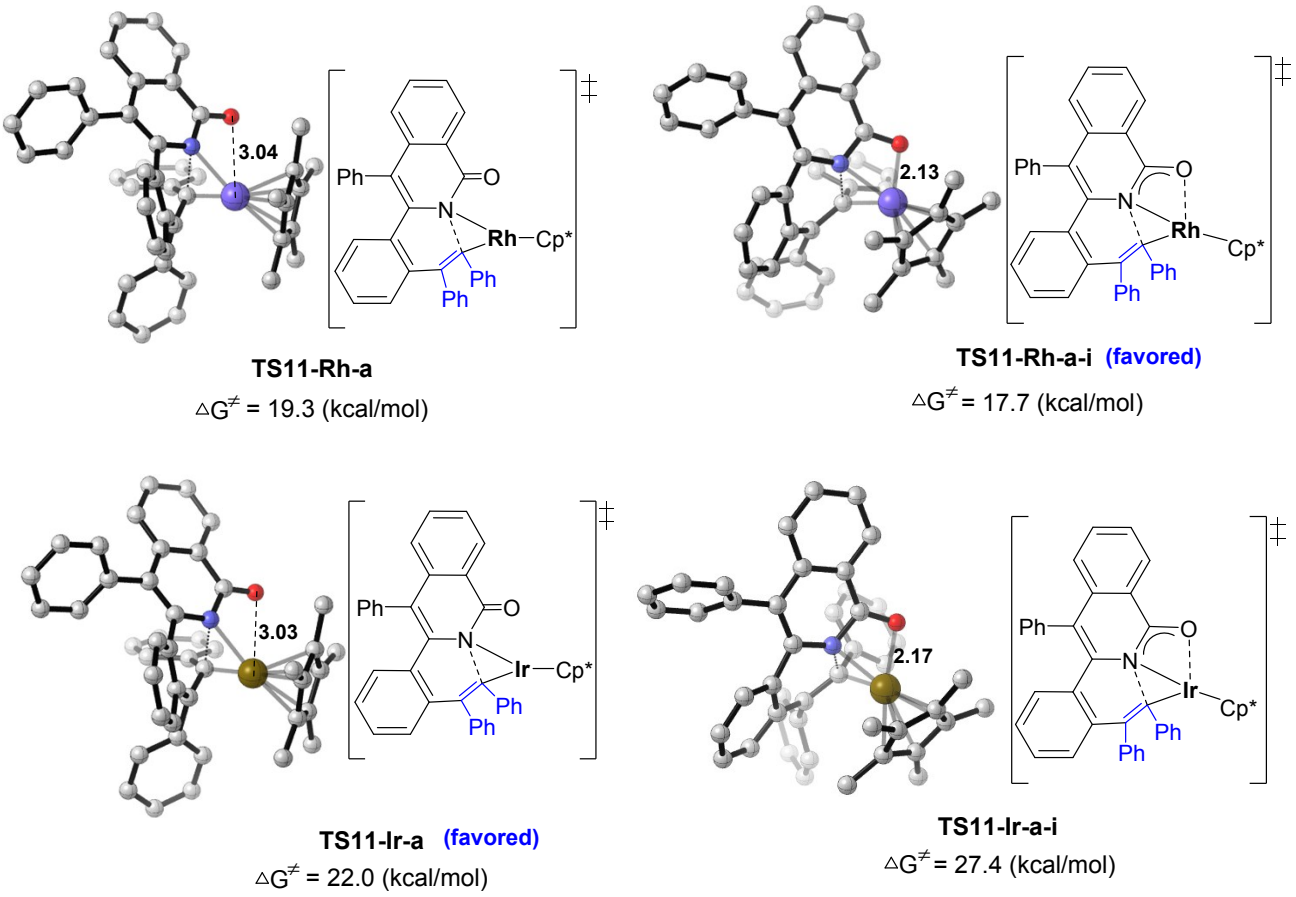
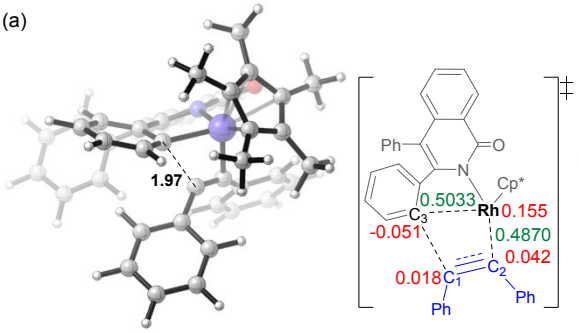


Fig. S3 Optimized geometries of isomers of the reductive elimination transition states with diphenyl-acetylene **a.** Numbers in black are distances (Å) between atoms. All energies are with respect to the substrate and the active catalyst.

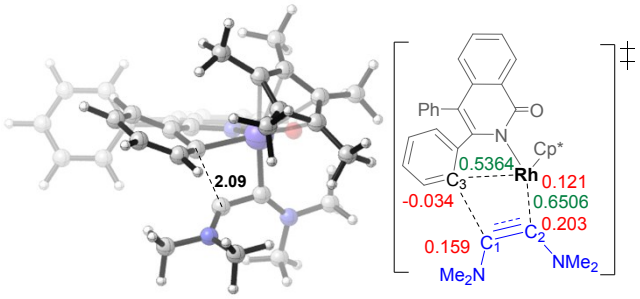
Wang's group experimentally observed two types of molecular structures for the alkyne-insertion intermediate: one contains a seven-membered metallocycle without the formation of M–O bonds (M = Rh, Ir) (intermediate **9** in Scheme 2) and the other one contains a seven-membered metallocycle with the formation of M–O bonds (M = Rh, Ir) (intermediate **10** in Scheme 2). Correspondingly, we considered two geometries of the reductive elimination transition states, **TS11-M-a** and **TS11-M-a-i** (M = Rh, Ir) as shown in Fig. S3. **TS11-M-a** contains a seven-membered metallocycle without the formation of M–O bonds (M = Rh, Ir), while **TS11-M-a-i** contains a seven-membered metallocycle with the formation of M–O bonds (M = Rh, Ir). Perhaps it is because the Rh(III) center is less electron-rich than the Ir(III)

center, the transition state **TS11-Rh-a-i** contains a seven-membered metallocycle with the formation of Rh–O bond is favored, while the transition state **TS11-Ir-a** contains a seven-membered metallocycle without the formation of Ir–O bond is favored.

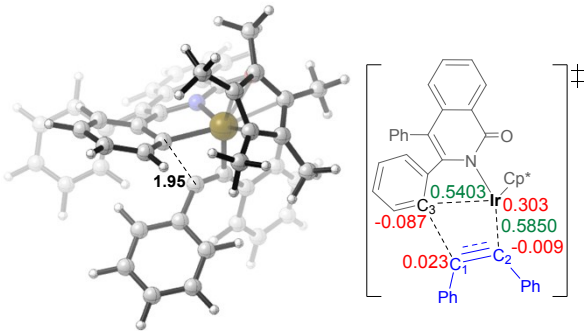
(a)



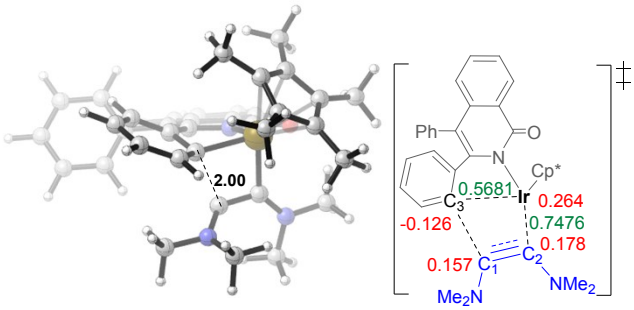
TS8-Rh-a
$\triangle G^{\neq}$ = 26.0 (kcal/mol)



TS8-Rh-b
$\triangle G^{\neq}$ = 15.7 (kcal/mol)

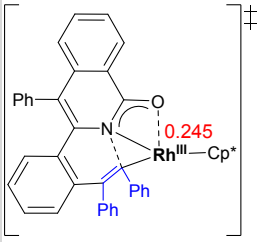


TS8-Ir-a
$\triangle G^{\neq}$ = 23.6 (kcal/mol)

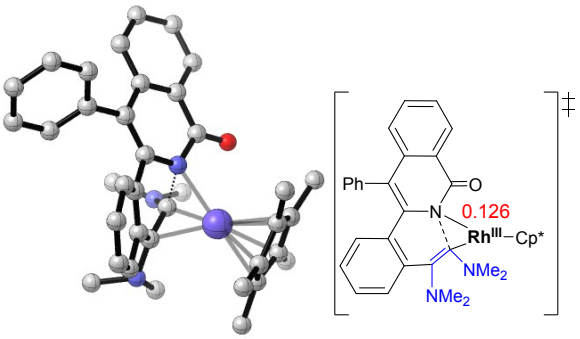


TS8-Ir-b
$\triangle G^{\neq}$ = 10.1 (kcal/mol)

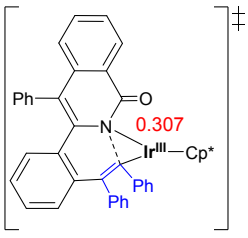
(b)



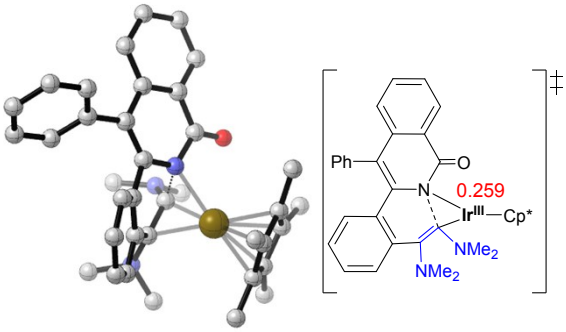
TS11-Rh-a-i
$\triangle G^{\neq}$ = 17.7 (kcal/mol)



TS11-Rh-b
$\triangle G^{\neq}$ = 4.9 (kcal/mol)



TS11-Ir-a
$\triangle G^{\neq}$ = 22.0 (kcal/mol)



TS11-Ir-b
$\triangle G^{\neq}$ = 14.9 (kcal/mol)

Fig. S4 Optimized geometries of the alkyne insertion and reductive elimination transition states with diphenyl-acetylene **a** and 2-di(dimethylamino)acetylene **b**. Numbers in red are NBO charges, numbers in green are Wiberg bond indexes. All energies are with respect to the substrate and the active catalyst.

The bonds M–C2 and M–C3 in the alkyne insertion transition states **TS8-M-b** are stronger than those in the **TS8-M-a** (M = Rh, Ir) as demonstrated by the Wiberg bond indexes of M–C2 and M–C3 as shown in Fig. S4a. Meanwhile, the electrostatic interactions between atoms C1 and C3 are greater in **TS8-M-b** than in the **TS8-M-a** as evidenced by the charge distribution (numbers in red as shown in Fig. S4a). Therefore, the alkyne insertion transition states **TS8-M-b** involving the 1,2-di(dimethylamino)acetylene **b** are more stable than the alkyne insertion transition states **TS8-M-a** involving the diphenyl-acetylene **a** and thus the electron-donating dimethylamino group NMe_2 lowers the energy barriers of the alkyne insertion.

The electron-rich 1,2-di(dimethylamino)acetylene substrate stabilizes the positive charge on the metal center M(III) (M = Rh, Ir) in the reductive elimination transition states (**TS11-M-b**) and lowers the energy barrier. As expected, the metal center in **TS11-M-b** is less positively charged than that in the transition state with the diphenyl-acetylene substrate (**TS11-M-a**) (Fig. S4b).

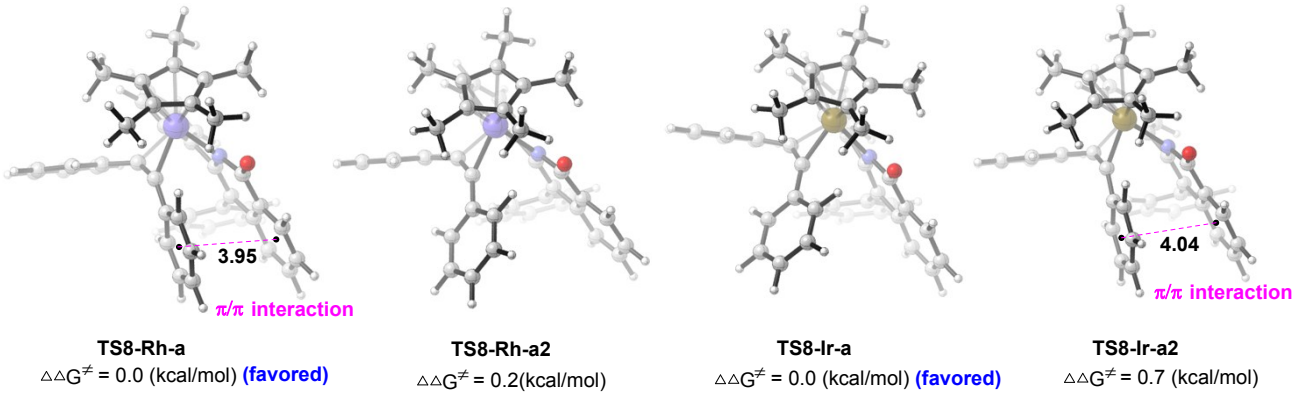


Fig. S5 Optimized geometries of the isomers of the alkyne insertion transition states with diphenyl-acetylene **a** and their relative Gibbs free energies.

Fig. S5 shows that the Gibbs free energy of **TS8-Rh-a** which has a π/π interaction between the phenyl group at the diphenylisoquinolinone and the phenyl substituent at the alkyne is only 0.2 kcal/mol lower than that of **TS8-Rh-a2** which does not have π/π interactions. On the other hand, the Gibbs free energy of **TS8-Ir-a** which does not have π/π interactions between the phenyl groups of the two substrates is 0.7 kcal/mol lower than that of **TS8-Ir-a2** which has a π/π interaction between the phenyl groups of the two substrates. These results indicate that π/π interactions has little effect on stabilizing the alkyne insertion transition states and therefor is not one of the factors for lowering the energy barriers of alkyne insertion with diphenyl-acetylene **a**.

Table of energy values

Table S1: The M11-L/SDD-6-31G(d)/SMD(*o*-xylene) computed energies, enthalpies, free energies of all stationary points discussed in the text[1].

species	E0	E0+ZPE	D3	U	H	G
$Cp^*Rh(OAc)_2$	-957.648904	-957.327903	-0.008679	-957.298427	-957.297182	-957.417845
$Cp^*Ir(OAc)_2$	-951.429230	-951.107437	-0.008786	-951.078223	-951.076978	-951.196963
a	-539.316445	-539.129726	-0.002438	-539.113087	-539.111842	-539.189390
b	-345.151630	-344.980712	-0.001617	-344.965277	-344.964032	-345.036130
c	-234.534495	-234.395216	-0.000908	-234.383372	-234.382127	-234.443314
$Cu_2(OAc)_2$	-852.095029	-851.991062	-0.001594	-851.973582	-851.972337	-852.052004
$Cu_2(OAc)_4$	-1308.917285	-1308.709663	-0.005633	-1308.681083	-1308.679838	-1308.790649
AcOH	-229.007487	-228.947208	-0.000285	-228.940299	-228.939054	-228.986273
1	-939.036373	-938.740434	-0.007822	-938.718138	-938.716893	-938.817442
2-Rh	-1896.692810	-1896.072391	-0.024504	-1896.026919	-1896.025674	-1896.214639
2-Ir	-1890.473407	-1889.852101	-0.024840	-1889.807285	-1889.806040	-1889.993187
TS3-Rh	-1896.677885	-1896.062993	-0.024993	-1896.018435	-1896.017190	-1896.206338
TS3-Ir	-1890.459299	-1889.843406	-0.024883	-1889.798926	-1889.797681	-1889.984795
4-Rh	-1667.657346	-1667.100230	-0.021828	-1667.061073	-1667.059828	-1667.228732
4-Ir	-1661.438167	-1660.880723	-0.022136	-1660.841868	-1660.840623	-1661.007129
TS5-Rh	-1667.627880	-1667.076666	-0.021493	-1667.037531	-1667.036285	-1667.202208
TS5-Ir	-1661.408304	-1660.856566	-0.021675	-1660.817597	-1660.816352	-1660.982354
6-Rh	-1667.651597	-1667.094625	-0.021989	-1667.055512	-1667.054267	-1667.220330
6-Ir	-1661.432751	-1660.876610	-0.022112	-1660.836990	-1660.835745	-1661.005406
7-Rh-a	-1977.948581	-1977.266387	-0.031494	-1977.224451	-1977.223206	-1977.413279
7-Rh-b	-1783.813308	-1783.144647	-0.028005	-1783.102567	-1783.101322	-1783.284996
7-Rh-c	-1673.170035	-1672.535517	-0.024604	-1672.493148	-1672.491903	-1672.671999
7-Ir-a	-1971.734700	-1971.051718	-0.031419	-1971.009779	-1971.008534	-1971.201726
7-Ir-b	-1777.603653	-1776.935367	-0.028226	-1776.893114	-1776.891869	-1777.078135
7-Ir-c	-1666.958501	-1666.324039	-0.024765	-1666.281786	-1666.280541	-1666.463166
TS8-Rh-a	-1977.931494	-1977.249813	-0.031791	-1977.209173	-1977.207928	-1977.397199
TS8-Rh-b	-1783.796186	-1783.128157	-0.027868	-1783.086965	-1783.085720	-1783.266286
TS8-Rh-c	-1673.150899	-1672.516717	-0.025809	-1672.476877	-1672.475632	-1672.650362
TS8-Ir-a	-1971.713405	-1971.032061	-0.030474	-1970.989915	-1970.988670	-1971.180238
TS8-Ir-b	-1777.582911	-1776.915010	-0.028099	-1776.873988	-1776.872743	-1777.053652
TS8-Ir-c	-1666.930831	-1666.296775	-0.026013	-1666.257173	-1666.255928	-1666.430535
9-Rh-a	-1977.984104	-1977.299296	-0.030260	-1977.257071	-1977.255826	-1977.446552
9-Rh-b	-1783.826473	-1783.156415	-0.028451	-1783.115757	-1783.114512	-1783.295055
9-Rh-c	-1673.199876	-1672.562951	-0.026013	-1672.523472	-1672.522227	-1672.697130
9-Ir-a	-1971.765642	-1971.081108	-0.030678	-1971.039299	-1971.038054	-1971.229310
9-Ir-b	-1777.608046	-1776.937444	-0.028807	-1776.897301	-1776.896056	-1777.075349
9-Ir-c	-1666.982026	-1666.344994	-0.026062	-1666.305616	-1666.304371	-1666.478566
10-Rh-a	-1977.990280	-1977.306570	-0.030480	-1977.264921	-1977.263676	-1977.452487

10-Rh-b	-1783.833823	-1783.163543	-0.027981	-1783.122794	-1783.121549	-1783.302732
10-Rh-c	-1673.206707	-1672.568530	-0.025522	-1672.528756	-1672.527511	-1672.703204
10-Ir-a	-1971.773499	-1971.088432	-0.030609	-1971.046851	-1971.045606	-1971.236705
10-Ir-b	-1777.616922	-1776.946119	-0.028198	-1776.905826	-1776.904581	-1777.083918
10-Ir-c	-1666.992482	-1666.354684	-0.025782	-1666.315240	-1666.313995	-1666.487896
TS11-Rh-a	-1977.948221	-1977.264685	-0.030769	-1977.223835	-1977.222590	-1977.409963
TS11-Rh-b	-1783.817253	-1783.148057	-0.028344	-1783.108141	-1783.106896	-1783.285718
TS11-Rh-c	-1673.165621	-1672.529905	-0.025874	-1672.490809	-1672.489564	-1672.663149
TS11-Ir-a	-1971.719584	-1971.036727	-0.030898	-1970.995850	-1970.994605	-1971.183859
TS11-Ir-b	-1777.578761	-1776.909661	-0.028602	-1776.869842	-1776.868597	-1777.047331
TS11-Ir-c	-1666.938138	-1666.301818	-0.025534	-1666.262671	-1666.261426	-1666.433905
TS11-Rh-a-i	-1977.949110	-1977.267002	-0.030179	-1977.225485	-1977.224240	-1977.413123
TS11-Rh-b-i	-1783.804343	-1783.135468	-0.027785	-1783.095104	-1783.093859	-1783.271691
TS11-Rh-c-i	-1673.166230	-1672.528903	-0.025169	-1672.489842	-1672.488597	-1672.659571
TS11-Ir-a-i	-1971.711711	-1971.029509	-0.030303	-1970.987913	-1970.986668	-1971.175007
TS11-Ir-b-i	-1777.571893	-1776.903543	-0.027675	-1776.862925	-1776.861680	-1777.040634
TS11-Ir-c-i	-1666.934564	-1666.297423	-0.025215	-1666.258432	-1666.257187	-1666.426784
12-Rh-a	-1977.992435	-1977.306009	-0.030470	-1977.265465	-1977.264220	-1977.448014
12-Rh-b	-1783.831928	-1783.160758	-0.028220	-1783.120987	-1783.119742	-1783.296639
12-Rh-c	-1673.208778	-1672.569467	-0.025572	-1672.530467	-1672.529222	-1672.702660
12-Ir-a	-1971.764368	-1971.078084	-0.030598	-1971.037476	-1971.036231	-1971.220834
12-Ir-b	-1777.601578	-1776.931284	-0.028274	-1776.891084	-1776.889839	-1777.069021
12-Ir-c	-1666.979361	-1666.340843	-0.025765	-1666.301896	-1666.300651	-1666.472781
product-a	-1477.191297	-1476.724757	-0.016147	-1476.692847	-1476.691602	-1476.830041
product-b	-1283.039372	-1282.588268	-0.014290	-1282.557433	-1282.556188	-1282.686851
product-c	-1172.418079	-1171.996725	-0.012486	-1171.968680	-1171.967435	-1172.087912

[1] Eo is the electronic energy calculated by using M11-L/SDD-6-31G(d)/SMD(*o*-xylene). ZPE is the Zero-point vibrational energy. D3 is the dispersion correction calculated for M06 functional with zero-damping. U, H and G are the thermal energy, enthalpy and Gibbs free energy obtained by adding the DFT-D3 dispersion corrections and the thermal corrections (at 393.15 K) from frequency calculations to Eo. All energies are in hartree.

Table S2: The M11-L/SDD-6-311+G(d,p)/SMD(*o*-xylene)//M11-L/SDD-6-31G(d)/SMD(*o*-xylene) computed energies, enthalpies, free energies of all stationary points discussed in the text[1].

species	E0	E0+ZPE	D3	U	H	G
$Cp^*Rh(OAc)_2$	-957.947103	-957.626102	-0.008679	-957.596626	-957.595381	-957.716044
$Cp^*Ir(OAc)_2$	-951.728801	-951.407008	-0.008786	-951.377794	-951.376549	-951.496534
a	-539.484458	-539.297739	-0.002438	-539.281100	-539.279855	-539.357403
b	-345.275721	-345.104803	-0.001617	-345.089368	-345.088123	-345.160221
c	-234.618900	-234.479621	-0.000908	-234.467777	-234.466532	-234.527719

$Cu_2(OAc)_2$	-852.257864	-852.153897	-0.001594	-852.136416	-852.135171	-852.214838
$Cu_2(OAc)_4$	-1309.245456	-1309.037834	-0.005633	-1309.009254	-1309.008009	-1309.118820
AcOH	-229.100861	-229.040582	-0.000285	-229.033673	-229.032428	-229.079647
1	-939.334352	-939.038413	-0.007822	-939.016117	-939.014872	-939.115421
2-Rh	-1897.288099	-1896.667680	-0.024504	-1896.622208	-1896.620963	-1896.809928
2-Ir	-1891.070145	-1890.448839	-0.024840	-1890.404023	-1890.402778	-1890.589925
TS3-Rh	-1897.274721	-1896.659829	-0.024993	-1896.615271	-1896.614026	-1896.803174
TS3-Ir	-1891.057830	-1890.441937	-0.024883	-1890.397457	-1890.396212	-1890.583326
4-Rh	-1668.165455	-1667.608339	-0.021828	-1667.569182	-1667.567937	-1667.736841
4-Ir	-1661.947807	-1661.390363	-0.022136	-1661.351508	-1661.350263	-1661.516769
TS5-Rh	-1668.139112	-1667.587898	-0.021493	-1667.548763	-1667.547517	-1667.713440
TS5-Ir	-1661.921344	-1661.369606	-0.021675	-1661.330636	-1661.329391	-1661.495393
6-Rh	-1668.163130	-1667.606158	-0.021989	-1667.567044	-1667.565799	-1667.731862
6-Ir	-1661.946007	-1661.389866	-0.022112	-1661.350246	-1661.349001	-1661.518662
7-Rh-a	-1978.539675	-1977.857481	-0.031494	-1977.815545	-1977.814300	-1978.004373
7-Rh-b	-1784.354741	-1783.686080	-0.028005	-1783.644000	-1783.642755	-1783.826429
7-Rh-c	-1673.674562	-1673.040044	-0.024604	-1672.997675	-1672.996430	-1673.176526
7-Ir-a	-1972.327826	-1971.644844	-0.031419	-1971.602906	-1971.601661	-1971.794853
7-Ir-b	-1778.146848	-1777.478562	-0.028226	-1777.436309	-1777.435064	-1777.621330
7-Ir-c	-1667.464949	-1666.830487	-0.024765	-1666.788234	-1666.786989	-1666.969614
TS8-Rh-a	-1978.522484	-1977.840803	-0.031791	-1977.800163	-1977.798918	-1977.988189
TS8-Rh-b	-1784.337257	-1783.669228	-0.027868	-1783.628036	-1783.626791	-1783.807357
TS8-Rh-c	-1673.654934	-1673.020752	-0.025809	-1672.980912	-1672.979667	-1673.154397
TS8-Ir-a	-1972.305683	-1971.624339	-0.030474	-1971.582192	-1971.580947	-1971.772515
TS8-Ir-b	-1778.126107	-1777.458206	-0.028099	-1777.417184	-1777.415939	-1777.596848
TS8-Ir-c	-1667.437215	-1666.803159	-0.026013	-1666.763556	-1666.762311	-1666.936918
9-Rh-a	-1978.573304	-1977.888496	-0.030260	-1977.846270	-1977.845025	-1978.035751
9-Rh-b	-1784.366723	-1783.696665	-0.028451	-1783.656007	-1783.654762	-1783.835305
9-Rh-c	-1673.702876	-1673.065951	-0.026013	-1673.026472	-1673.025227	-1673.200130
9-Ir-a	-1972.356942	-1971.672408	-0.030678	-1971.630599	-1971.629354	-1971.820610
9-Ir-b	-1778.150252	-1777.479650	-0.028807	-1777.439506	-1777.438261	-1777.617554
9-Ir-c	-1667.486995	-1666.849963	-0.026062	-1666.810584	-1666.809339	-1666.983534
10-Rh-a	-1978.578599	-1977.894889	-0.030480	-1977.853240	-1977.851995	-1978.040806
10-Rh-b	-1784.372222	-1783.701942	-0.027981	-1783.661193	-1783.659948	-1783.841131
10-Rh-c	-1673.708113	-1673.069936	-0.025522	-1673.030162	-1673.028917	-1673.204610
10-Ir-a	-1972.363891	-1971.678824	-0.030609	-1971.637242	-1971.635997	-1971.827096
10-Ir-b	-1778.157069	-1777.486266	-0.028198	-1777.445973	-1777.444728	-1777.624065
10-Ir-c	-1667.495301	-1666.857503	-0.025782	-1666.818059	-1666.816814	-1666.990715
TS11-Rh-a	-1978.537080	-1977.853544	-0.030769	-1977.812694	-1977.811449	-1977.998822
TS11-Rh-b	-1784.356166	-1783.686970	-0.028344	-1783.647055	-1783.645810	-1783.824632
TS11-Rh-c	-1673.668806	-1673.033090	-0.025874	-1672.993994	-1672.992749	-1673.166334
TS11-Ir-a	-1972.310804	-1971.627947	-0.030898	-1971.587070	-1971.585825	-1971.775079
TS11-Ir-b	-1778.120635	-1777.451535	-0.028602	-1777.411716	-1777.410471	-1777.589205

TS11-Ir-c	-1667.443639	-1666.807319	-0.025534	-1666.768173	-1666.766928	-1666.939407
TS11-Rh-a-i	-1978.537360	-1977.855252	-0.030179	-1977.813734	-1977.812489	-1978.001372
TS11-Rh-b-i	-1784.342454	-1783.673579	-0.027785	-1783.633215	-1783.631970	-1783.809802
TS11-Rh-c-i	-1673.667336	-1673.030009	-0.025169	-1672.990948	-1672.989703	-1673.160677
TS11-Ir-a-i	-1972.303062	-1971.620860	-0.030303	-1971.579265	-1971.578020	-1971.766359
TS11-Ir-b-i	-1778.112963	-1777.444613	-0.027675	-1777.403996	-1777.402751	-1777.581705
TS11-Ir-c-i	-1667.438567	-1666.801426	-0.025215	-1666.762436	-1666.761191	-1666.930788
12-Rh-a	-1978.582564	-1977.896138	-0.030470	-1977.855594	-1977.854349	-1978.038143
12-Rh-b	-1784.372815	-1783.701645	-0.028220	-1783.661875	-1783.660630	-1783.837527
12-Rh-c	-1673.712164	-1673.072853	-0.025572	-1673.033853	-1673.032608	-1673.206046
12-Ir-a	-1972.357690	-1971.671406	-0.030598	-1971.630799	-1971.629554	-1971.814157
12-Ir-b	-1778.145571	-1777.475277	-0.028274	-1777.435077	-1777.433832	-1777.613014
12-Ir-c	-1667.485778	-1666.847260	-0.025765	-1666.808313	-1666.807068	-1666.979198
product-a	-1477.649085	-1477.182545	-0.016147	-1477.150635	-1477.149390	-1477.287829
product-b	-1283.447410	-1282.996306	-0.014290	-1282.965471	-1282.964226	-1283.094889
product-c	-1172.788561	-1172.367207	-0.012486	-1172.339161	-1172.337916	-1172.458393

[1] Eo is the single point energy calculated by using M11-L/SDD-6-311+G(d,p)/SMD(*o*-xylene) based on geometries obtained by M11-L/SDD-6-31G(d)/SMD(*o*-xylene). ZPE is the Zero-point vibrational energy. D3 is the dispersion correction calculated for M06 functional with zero-damping. U, H, G are the results of adding corresponding corrections the same as in Table S1 to Eo. All energies are in hartree.

The Cartesian Coordinates of the stationary points discussed in the text

Cp*Rh(OAc)$_2$

Atom	X	Y	Z
Rh	0.018731	0.220695	-0.098246
C	1.299375	-1.002734	1.139199
C	0.953041	-1.581030	2.451111
C	1.178739	-1.622047	-0.130065
C	0.637424	-2.965152	-0.415168
C	1.645439	-0.704723	-1.120255
C	1.734323	-0.960891	-2.571752
C	2.139603	0.463793	-0.437002
C	2.715520	1.644541	-1.110667
C	1.912217	0.293520	0.945108
C	2.238214	1.238603	2.032099
O	-1.754466	-0.508553	-0.770197
C	-2.340333	-1.340812	0.004463
O	-1.903282	-1.746602	1.064513
C	-3.685949	-1.781921	-0.507947
H	0.257992	-2.425003	2.354329
H	0.474777	-0.835478	3.105915
H	1.865434	-1.933129	2.966198
H	0.051804	-3.359518	0.425059
H	1.466352	-3.665034	-0.623502
H	-0.012694	-2.958896	-1.305075
H	1.676940	-0.029384	-3.155915
H	0.924520	-1.621741	-2.916806
H	2.691985	-1.450829	-2.826255
H	2.123550	1.928225	-1.996334
H	3.741439	1.428835	-1.458383
H	2.764599	2.519334	-0.446223
H	3.181854	0.950570	2.529217
H	1.453974	1.249710	2.805725
H	2.357073	2.267763	1.662644
H	-4.422865	-0.982294	-0.327607
H	-3.666411	-1.958040	-1.593651
H	-4.025552	-2.686273	0.015235
C	-1.421801	2.213541	0.041576
O	-0.746731	1.969839	-0.986923
O	-1.257550	1.480230	1.041497
C	-2.409045	3.321186	0.056483
H	-3.371881	2.944372	-0.325320
H	-2.571684	3.689748	1.078359
H	-2.088466	4.141238	-0.600770

Cp*Ir(OAc)$_2$

Atom	X	Y	Z
C	1.357084	-1.003122	1.140503
C	1.044945	-1.621885	2.444115
C	1.253821	-1.611501	-0.140433
C	0.758194	-2.970762	-0.439756
C	1.688513	-0.668124	-1.122353
C	1.805868	-0.913615	-2.575033
C	2.147329	0.510216	-0.424179
C	2.712467	1.706567	-1.082176
C	1.933466	0.313740	0.959438
C	2.259250	1.247376	2.058076
O	-1.789290	-0.562243	-0.688828
C	-2.351192	-1.469172	0.021969
O	-1.892123	-1.966812	1.030447
C	-3.700774	-1.870825	-0.509602
H	0.292982	-2.416198	2.342701
H	0.645222	-0.881846	3.154775
H	1.955748	-2.055691	2.894763
H	0.182194	-3.391924	0.394350
H	1.610428	-3.640648	-0.651031
H	0.108713	-2.976480	-1.329882
H	1.720052	0.018262	-3.155052
H	1.026178	-1.602200	-2.935013
H	2.784777	-1.365207	-2.818617
H	2.136120	1.982034	-1.980281
H	3.751024	1.514159	-1.404687
H	2.726861	2.580124	-0.414088
H	3.217257	0.969131	2.532174
H	1.489178	1.230353	2.845366
H	2.350692	2.284902	1.704464
H	-4.427073	-1.066841	-0.307860
H	-3.675454	-2.006146	-1.601243

H	-4.055981	-2.790106	-0.024846
C	-1.571730	2.131581	0.056843
O	-0.912223	1.894211	-0.982798
O	-1.340084	1.420324	1.061459
C	-2.565071	3.230596	0.106492
H	-3.435710	2.936811	0.709494
H	-2.109241	4.106742	0.595796
H	-2.880724	3.525069	-0.902830
Ir	0.018487	0.190850	-0.077586

a

Atom	X	Y	Z
C	-0.606732	-0.003893	0.000041
C	0.606732	0.003891	-0.000065
C	-2.018199	-0.003404	0.000232
C	-2.730761	-1.207728	-0.000232
C	-2.726320	1.204658	0.000192
C	-4.111991	-1.198351	-0.000006
H	-2.178560	-2.154538	0.000240
C	-4.107289	1.201342	0.000224
H	-2.169921	2.149291	-0.000492
C	-4.805210	0.003242	-0.000252
H	-4.659318	-2.148445	0.000785
H	-4.650589	2.153476	-0.000376
H	-5.901312	0.005047	-0.000211
C	2.018199	0.003403	-0.000247
C	2.730761	1.207727	0.000195
C	2.726320	-1.204659	-0.000170
C	4.111990	1.198352	-0.000011
H	2.178559	2.154538	-0.000307
C	4.107290	-1.201341	-0.000183
H	2.169923	-2.149292	0.000529
C	4.805210	-0.003240	0.000274
H	4.659316	2.148447	-0.000818
H	4.650589	-2.153474	0.000448
H	5.901313	-0.005045	0.000252

b

Atom	X	Y	Z
C	-0.593721	-0.068575	0.131186
C	0.592926	-0.053634	-0.131963
N	1.914373	-0.178471	-0.238640
N	-1.915651	-0.209412	0.215408
C	-2.624833	0.872203	0.840072
H	-3.654111	0.548148	1.074180
H	-2.120245	1.150197	1.778248
H	-2.684434	1.774068	0.192070
C	-2.570236	-0.718056	-0.959266
H	-2.033049	-1.607278	-1.323692
H	-3.604997	-1.008098	-0.704062
H	-2.611071	0.030875	-1.780556
C	2.575775	-0.834980	0.855223
H	2.049526	-1.772082	1.093864
H	3.613688	-1.074819	0.563698
H	2.608114	-0.205209	1.771036
C	2.620429	0.975614	-0.722359
H	3.641519	0.680709	-1.022071
H	2.099177	1.385506	-1.601109
H	2.702793	1.777729	0.043668

c

Atom	X	Y	Z
C	0.580012	-0.362366	-0.168542
C	-0.579966	-0.361844	0.169433
C	1.983825	-0.344919	-0.524802
H	2.381906	-1.377767	-0.497323
H	2.090753	-0.020543	-1.578040
C	2.814083	0.548905	0.373386
H	3.873225	0.531257	0.070414
H	2.463523	1.592179	0.328396
H	2.753870	0.221802	1.423503
C	-1.983707	-0.343112	0.525967
H	-2.381810	-1.376049	0.502193
H	-2.090297	-0.015190	1.578137
C	-2.814227	0.547591	-0.375059
H	-3.873244	0.531066	-0.071624
H	-2.463616	1.591024	-0.333960
H	-2.754426	0.216690	-1.423995

$Cu_2(OAc)_2$

Atom	X	Y	Z
Cu	-0.001236	-1.209410	-0.010850
Cu	0.001312	1.211431	-0.010047
C	-2.394998	0.004931	-0.001848

O	-1.823234	-1.109316	-0.006623
O	-1.821800	1.117527	-0.006881
C	-3.884066	-0.003130	0.038708
H	-4.208316	-0.241038	1.065018
H	-4.301045	0.973139	-0.238999
H	-4.284388	-0.792696	-0.612571
C	2.395075	-0.001957	-0.005885
O	1.821323	-1.114694	-0.010308
O	1.823872	1.112186	-0.012385
C	3.883833	-0.004476	0.042040
H	4.297870	0.896486	-0.429660
H	4.200422	-0.002075	1.098238
H	4.292910	-0.910253	-0.424540

$Cu_2(OAc)_4$

Atom	X	Y	Z
Cu	-0.009504	-0.000835	-1.196015
Cu	-0.001699	-0.010459	1.201514
C	-1.736254	-1.716344	-0.001096
O	-1.078012	-1.571693	-1.051352
O	-1.581304	-1.068954	1.054294
C	-2.830616	-2.735414	-0.015968
H	-2.940981	-3.201799	0.971957
H	-3.775335	-2.218158	-0.249809
H	-2.656239	-3.493666	-0.789968
C	1.715686	-1.726241	-0.007999
O	1.565396	-1.066724	-1.056789
O	1.057297	-1.588411	1.042756
C	2.805323	-2.750509	-0.002152
H	2.614288	-3.528729	0.747813
H	2.932024	-3.190416	-1.000181
H	3.747408	-2.244266	0.264188
C	1.725891	1.706064	-0.000777
O	1.060608	1.571882	-1.047887
O	1.579022	1.046456	1.048271
C	2.819349	2.726148	-0.011632
H	2.933788	3.183220	0.980381
H	3.763584	2.211573	-0.253115
H	2.642303	3.491729	-0.777606
C	-1.715658	1.726445	0.015451
O	-1.060733	1.570195	1.065450
O	-1.579368	1.068451	-1.036742
C	-2.735820	2.819784	0.000792
H	-2.270087	3.715127	-0.442072
H	-3.590548	2.545576	-0.632003
H	-3.065984	3.068121	1.017227

AcOH

Atom	X	Y	Z
C	-1.354632	0.002448	-0.000015
H	-1.697682	0.560940	0.886609
H	-1.697667	0.562467	-0.885678
H	-1.819687	-0.990289	-0.000836
O	0.813791	1.013724	0.000002
H	0.210786	1.783707	-0.000058
O	0.726490	-1.161272	-0.000012
C	0.134965	-0.125189	0.000023

1

Atom	X	Y	Z
O	2.558198	-3.243960	-0.220774
C	-2.155360	-2.200361	0.774344
C	-3.512403	-2.468777	0.746456
H	-3.936467	-3.200340	1.444494
C	-4.331788	-1.808797	-0.154433
H	-5.406892	-2.022032	-0.178635
C	-3.787196	-0.880182	-1.027739
H	-4.429077	-0.362812	-1.750064
C	-2.433103	-0.604389	-0.998391
H	-2.003338	0.125117	-1.695744
C	-1.601176	-1.260645	-0.093261
C	-0.151679	-1.003615	-0.061630
C	0.429775	0.230257	0.013360
C	-0.387431	1.456807	0.087278
C	-0.276604	2.432897	-0.901838
H	0.424960	2.276420	-1.732090
C	-1.048269	3.579904	-0.856261
H	-0.949638	4.334071	-1.646407
C	-1.949277	3.771256	0.178907
H	-2.563871	4.678617	0.215367
C	-2.066357	2.810566	1.170086
H	-2.772020	2.956712	1.996600
C	-1.288527	1.666814	1.128004
H	-1.382921	0.906902	1.914837
C	1.865911	0.302719	0.042588

C	2.562449	1.514527	0.184599
H	2.003964	2.450449	0.290706
C	3.937144	1.540292	0.205025
C	4.680432	0.365822	0.090776
H	5.775368	0.401795	0.103924
C	4.023425	-0.835576	-0.021827
H	4.568088	-1.784216	-0.095048
C	2.630571	-0.879460	-0.038091
C	1.985424	-2.177359	-0.128398
H	4.453946	2.501338	0.317496
H	-1.511431	-2.711076	1.502404
N	0.621474	-2.125066	-0.103457
H	0.157655	-3.039998	-0.234766

2-Rh

Atom	X	Y	Z
Rh	-2.382292	-0.036317	0.067600
O	-0.809316	-0.969028	-1.015789
C	-4.899170	-1.485415	1.521594
H	-5.715993	-0.923904	1.051418
H	-5.238146	-1.846562	2.509200
H	-4.700235	-2.373274	0.900506
C	-3.687988	-0.659344	1.688130
C	-3.608959	0.765245	1.630648
C	-2.243742	1.137609	1.918428
C	-1.496147	-0.042726	2.090768
C	-2.378794	-1.168070	1.902410
C	-2.003829	-2.589946	2.051411
H	-0.981022	-2.784123	1.688600
H	-2.684562	-3.249328	1.490921
H	-2.038472	-2.902967	3.111276
C	-4.718692	1.727706	1.483976
H	-4.452238	2.539979	0.788142
H	-4.951928	2.192542	2.459737
H	-5.626611	1.252414	1.091862
C	-1.778756	2.531182	2.065025
H	-2.071584	2.924672	3.055695
H	-2.229462	3.188348	1.304924
H	-0.687253	2.620664	1.970246
C	-0.075696	-0.145601	2.482741
H	0.492324	0.765449	2.243567
H	0.435641	-1.001236	2.010353
H	-0.004809	-0.299307	3.575280
C	2.764851	3.931381	0.582045
H	2.259560	4.658745	1.227506
C	3.875347	4.305774	-0.154387
H	4.254672	5.332695	-0.095542
C	4.499608	3.379251	-0.975482
H	5.368323	3.672747	-1.576538
C	4.026572	2.083214	-1.048032
H	4.514975	1.358186	-1.709707
C	2.916838	1.693271	-0.301218
C	2.409229	0.313919	-0.383301
C	3.192972	-0.805313	-0.286582
C	4.630077	-0.707390	0.036604
C	5.599200	-1.188885	-0.840541
H	5.286324	-1.634161	-1.794563
C	6.943967	-1.096052	-0.526223
H	7.694616	-1.473668	-1.230953
C	7.341144	-0.522997	0.671771
H	8.406425	-0.449901	0.920235
C	6.385843	-0.044521	1.553179
H	6.691673	0.407147	2.504341
C	5.041676	-0.138786	1.238982
H	4.283279	0.241554	1.935838
C	2.568550	-2.087504	-0.423341
C	3.264367	-3.299031	-0.263625
H	4.331719	-3.281957	-0.019425
C	2.617468	-4.502984	-0.397249
C	1.252004	-4.561928	-0.687770
H	0.753189	-5.531947	-0.793077
C	0.540906	-3.396180	-0.825959
H	-0.534844	-3.399312	-1.040371
C	1.184217	-2.163238	-0.690386
C	0.408398	-0.955607	-0.774950
H	3.183399	-5.433354	-0.266624
C	-5.077913	-1.362257	-2.938665
H	-4.660497	-2.372238	-3.061112
H	-6.176260	-1.404071	-2.922265
H	-4.778520	-0.774957	-3.822633
O	-3.372793	-1.047577	-1.390047
O	-5.223368	0.154528	-1.119323
C	-4.552871	-0.674967	-1.703103
C	2.284023	2.636954	0.503928
H	1.397427	2.351429	1.084229
C	-1.896371	3.388794	-2.509098
H	-1.385774	4.334237	-2.278241

H	-1.521504	3.039936	-3.485729
H	-2.978184	3.551976	-2.612625
C	-1.583374	2.344791	-1.471146
O	-2.469513	1.457096	-1.343342
O	-0.518771	2.411406	-0.857509
H	0.479115	1.052579	-0.665363
N	1.066959	0.198822	-0.586640

2-Ir

Atom	X	Y	Z
O	-0.612555	-0.935869	-1.094314
C	-4.675224	-1.482320	1.533441
H	-5.469442	-0.931539	1.013541
H	-5.053092	-1.799186	2.521650
H	-4.465508	-2.394463	0.953000
C	-3.461602	-0.658229	1.705239
C	-3.391413	0.771142	1.657594
C	-2.021643	1.145767	1.933034
C	-1.267481	-0.036849	2.095902
C	-2.149770	-1.167308	1.922201
C	-1.772917	-2.587942	2.087495
H	-0.748682	-2.783486	1.729621
H	-2.448760	-3.254644	1.529785
H	-1.811328	-2.890852	3.149936
C	-4.522347	1.715025	1.546646
H	-4.243011	2.612987	0.973209
H	-4.843736	2.050095	2.549737
H	-5.380711	1.260021	1.034567
C	-1.552705	2.539436	2.076028
H	-1.846203	2.938511	3.063789
H	-1.994948	3.195165	1.309661
H	-0.460492	2.623092	1.983335
C	0.158682	-0.137861	2.472128
H	0.723993	0.771551	2.220547
H	0.662037	-0.993868	1.991794
H	0.245938	-0.288390	3.563519
C	2.989491	3.929356	0.568125
H	2.485679	4.661007	1.209855
C	4.110056	4.293316	-0.158184
H	4.499127	5.316337	-0.094947
C	4.732543	3.361248	-0.974396
H	5.609417	3.646557	-1.567498
C	4.247204	2.070088	-1.052507
H	4.734631	1.340688	-1.710150
C	3.126731	1.690857	-0.316205
C	2.607167	0.316364	-0.405084
C	3.379449	-0.810437	-0.301321
C	4.813414	-0.725014	0.039343
C	5.789201	-1.212588	-0.826864
H	5.484550	-1.654874	-1.784906
C	7.130772	-1.128465	-0.496868
H	7.887196	-1.509979	-1.193214
C	7.517662	-0.558859	0.706167
H	8.580491	-0.492471	0.966898
C	6.555320	-0.075644	1.577338
H	6.853042	0.372986	2.532474
C	5.214387	-0.160492	1.247258
H	4.450321	0.223730	1.935750
C	2.744908	-2.086341	-0.445584
C	3.425542	-3.304494	-0.272483
H	4.489875	-3.297711	-0.014551
C	2.766417	-4.501596	-0.407918
C	1.403432	-4.547294	-0.713159
H	0.895087	-5.512461	-0.816691
C	0.707131	-3.375032	-0.867802
H	-0.366463	-3.366963	-1.092952
C	1.363713	-2.148574	-0.732611
C	0.603407	-0.934902	-0.829512
H	3.320228	-5.437510	-0.265368
C	-4.863785	-1.341527	-2.984974
H	-4.590168	-2.407370	-2.991549
H	-5.953589	-1.231645	-3.073345
H	-4.396286	-0.888066	-3.874247
O	-3.161941	-1.006256	-1.442651
O	-5.027434	0.170939	-1.159429
C	-4.349933	-0.646766	-1.750748
C	2.496257	2.639951	0.484353
H	1.601709	2.363210	1.056352
C	-1.679364	3.414844	-2.513824
H	-1.989839	4.324018	-1.972836
H	-0.786703	3.683115	-3.098115
H	-2.495776	3.116056	-3.184533
C	-1.344140	2.345770	-1.511550
O	-2.202808	1.425165	-1.414419
O	-0.304749	2.445370	-0.861673
Ir	-2.171894	-0.030484	0.074734
H	0.686056	1.072408	-0.697724

N	1.266249	0.212664	-0.625027

TS3-Rh

Atom	X	Y	Z
Rh	-2.215471	-0.131768	0.156153
O	-0.866204	-1.141346	-1.123788
N	0.899824	0.175044	-0.750550
C	-4.832475	-1.712575	1.254168
H	-5.633532	-0.984703	1.072116
H	-5.138701	-2.379363	2.080057
H	-4.734196	-2.337175	0.351693
C	-3.556170	-1.053821	1.594149
C	-3.360183	0.317048	1.933260
C	-1.962842	0.486681	2.243887
C	-1.301574	-0.739006	2.046696
C	-2.285855	-1.699885	1.601717
C	-2.027815	-3.127868	1.333915
H	-1.048591	-3.276466	0.852923
H	-2.794398	-3.565940	0.676436
H	-2.024944	-3.708288	2.274559
C	-4.376643	1.369440	2.124240
H	-4.112261	2.284653	1.569897
H	-4.449278	1.637670	3.194352
H	-5.366646	1.054764	1.772708
C	-1.380195	1.758622	2.713526
H	-1.770101	1.998318	3.719189
H	-1.658927	2.598888	2.055793
H	-0.283155	1.718331	2.782380
C	0.125393	-1.022777	2.311948
H	0.769931	-0.152373	2.106353
H	0.502300	-1.867309	1.713084
H	0.264955	-1.295449	3.373979
C	1.971385	3.935264	0.630201
H	1.267167	4.562497	1.190200
C	3.140869	4.479854	0.124594
H	3.367657	5.541130	0.279857
C	4.016644	3.677120	-0.589179
H	4.933504	4.104834	-1.011384
C	3.737965	2.336915	-0.783895
H	4.428998	1.717821	-1.367441
C	2.570164	1.774251	-0.271119
C	2.212074	0.359610	-0.483574
C	3.100848	-0.689137	-0.394671
C	4.486383	-0.490352	0.071839
C	5.582662	-0.801427	-0.731628
H	5.411640	-1.198324	-1.741347
C	6.874242	-0.595934	-0.277572
H	7.723736	-0.840880	-0.926358
C	7.094568	-0.074610	0.987654
H	8.117668	0.089176	1.345692
C	6.013531	0.237319	1.796952
H	6.178071	0.647697	2.800509
C	4.723737	0.025426	1.344055
H	3.866042	0.275227	1.983095
C	2.610224	-2.001088	-0.682834
C	3.410184	-3.157808	-0.615661
H	4.463270	-3.070782	-0.328510
C	2.888426	-4.394118	-0.901160
C	1.545461	-4.545167	-1.258951
H	1.145895	-5.538718	-1.492658
C	0.731743	-3.441357	-1.297357
H	-0.330799	-3.526136	-1.555526
C	1.244442	-2.173703	-1.005689
C	0.375905	-1.027590	-0.962748
H	3.537021	-5.277194	-0.844039
C	-5.129830	-0.128174	-2.944922
H	-4.938055	-1.141031	-3.328620
H	-6.211452	0.060010	-2.897798
H	-4.690568	0.575500	-3.670855
O	-3.338347	-0.459909	-1.504402
O	-5.046534	0.733760	-0.731115
C	-4.489190	0.086231	-1.596064
C	1.686417	2.597568	0.425457
H	0.751438	2.169409	0.809040
C	-2.034552	3.494921	-2.261561
H	-1.256835	4.115642	-2.725788
H	-2.690919	3.114833	-3.062112
H	-2.660295	4.091977	-1.585430
C	-1.449133	2.324166	-1.547582
O	-2.101009	1.826527	-0.620734
O	-0.329069	1.926209	-1.960725
H	0.170238	1.119822	-1.305516

TS3-Ir

Atom	X	Y	Z
O	0.647856	1.086425	-0.949671

N	-1.163661	-0.168669	-0.477299
C	4.840294	1.235503	1.450764
H	5.600040	0.621797	0.950149
H	5.239605	1.570360	2.424281
H	4.681608	2.134320	0.833775
C	3.579347	0.494207	1.657411
C	3.392388	-0.915716	1.568508
C	2.005934	-1.188794	1.876184
C	1.354310	0.039049	2.127386
C	2.314864	1.102076	1.942286
C	2.051664	2.540282	2.164569
H	1.067001	2.837082	1.765503
H	2.808467	3.171143	1.674318
H	2.059044	2.785586	3.242001
C	4.422150	-1.951305	1.345282
H	4.071896	-2.713732	0.631093
H	4.666026	-2.467693	2.291267
H	5.344620	-1.525723	0.929550
C	1.427702	-2.544810	1.979110
H	1.649462	-2.979425	2.970493
H	1.852799	-3.229361	1.227068
H	0.335539	-2.544882	1.849812
C	-0.040194	0.236404	2.573979
H	-0.695749	-0.597471	2.284151
H	-0.481458	1.162211	2.169123
H	-0.069150	0.319385	3.675491
C	-3.077501	-3.832412	0.771743
H	-2.693515	-4.536283	1.520060
C	-4.085598	-4.220504	-0.094722
H	-4.501200	-5.233613	-0.037877
C	-4.563163	-3.322947	-1.035884
H	-5.353301	-3.625051	-1.733691
C	-4.045576	-2.042679	-1.100755
H	-4.424563	-1.333814	-1.847708
C	-3.038400	-1.638722	-0.228959
C	-2.503224	-0.260729	-0.297644
C	-3.333057	0.835922	-0.220784
C	-4.780435	0.697668	0.034767
C	-5.715557	1.170374	-0.884841
H	-5.362914	1.642667	-1.811765
C	-7.072684	1.037333	-0.648725
H	-7.792306	1.410009	-1.387810
C	-7.521113	0.427892	0.512070
H	-8.596402	0.321363	0.698742
C	-6.602448	-0.043916	1.435712
H	-6.948082	-0.524060	2.359223
C	-5.245947	0.093645	1.200102
H	-4.519356	-0.280717	1.933142
C	-2.742945	2.128800	-0.350455
C	-3.460089	3.332090	-0.208741
H	-4.532295	3.300159	0.012322
C	-2.827725	4.543027	-0.333319
C	-1.456709	4.617315	-0.599162
H	-0.967991	5.593520	-0.696259
C	-0.729563	3.460918	-0.726871
H	0.348584	3.481931	-0.925551
C	-1.356942	2.216354	-0.600155
C	-0.582794	1.007893	-0.676236
H	-3.407286	5.467173	-0.216477
C	4.815539	1.338146	-3.030808
H	4.642371	2.421176	-2.944879
H	5.885847	1.138247	-3.175937
H	4.273290	1.001384	-3.929324
O	3.141397	1.026339	-1.453204
O	4.918064	-0.306232	-1.317915
C	4.288543	0.600072	-1.828155
C	-2.554383	-2.553621	0.699183
H	-1.762105	-2.246864	1.394509
C	1.533745	-3.469891	-2.413118
H	1.645560	-4.325577	-1.726620
H	0.722572	-3.726212	-3.109913
H	2.477450	-3.324664	-2.952937
C	1.180317	-2.264071	-1.614765
O	2.027130	-1.376165	-1.479923
O	0.018620	-2.273020	-1.111763
H	-0.389066	-1.303166	-0.757847
Ir	2.156124	0.060150	0.072593

4-Rh

Atom	X	Y	Z
Rh	-1.920300	0.100613	0.156890
O	-0.889242	2.663255	-0.663985
N	0.072362	0.709761	-0.101183
C	-4.912449	1.235688	-0.000146
H	-5.361087	0.918014	0.952048
H	-5.731457	1.418277	-0.718013
H	-4.404780	2.200007	0.168566

C	-3.970436	0.235451	-0.538726
C	-3.730946	-1.068671	-0.059856
C	-2.679197	-1.649850	-0.865548
C	-2.299765	-0.693710	-1.842790
C	-3.058984	0.493940	-1.624287
C	-3.058050	1.699290	-2.474260
H	-3.805678	1.591210	-3.282395
H	-2.075523	1.871077	-2.935589
H	-3.306834	2.603178	-1.899698
C	-4.418673	-1.765348	1.046500
H	-5.125659	-2.517719	0.652783
H	-4.991099	-1.072068	1.679891
H	-3.706205	-2.300461	1.695521
C	-2.213551	-3.043491	-0.746177
H	-2.944105	-3.725527	-1.219437
H	-2.114984	-3.352438	0.306241
H	-1.239470	-3.204618	-1.230131
C	-1.297138	-0.861493	-2.914404
H	-0.702939	-1.776913	-2.787528
H	-0.603385	-0.005719	-2.955765
H	-1.802857	-0.918452	-3.894841
C	1.576341	-3.565306	-1.166901
H	1.940180	-4.071058	-2.069331
C	1.188105	-4.303958	-0.060288
H	1.242103	-5.399006	-0.080548
C	0.746897	-3.647139	1.076733
H	0.451702	-4.223597	1.962554
C	0.692312	-2.262616	1.115589
H	0.364716	-1.752913	2.025933
C	1.084633	-1.511806	0.013156
C	1.202923	-0.027273	0.025774
C	2.469567	0.518630	0.031873
C	3.678780	-0.326262	0.083183
C	3.949181	-1.175987	1.153855
H	3.248525	-1.211355	1.997594
C	5.082298	-1.970668	1.164205
H	5.272492	-2.633469	2.017072
C	5.979736	-1.923001	0.109500
H	6.878827	-2.550795	0.119816
C	5.732680	-1.072946	-0.956953
H	6.435251	-1.026699	-1.797957
C	4.595568	-0.286153	-0.968618
H	4.397950	0.378417	-1.820492
C	2.594455	1.936837	-0.079187
C	3.817255	2.623312	0.033389
H	4.736035	2.061561	0.236944
C	3.869120	3.989685	-0.097731
C	2.711030	4.730601	-0.343472
H	2.766287	5.820390	-0.447125
C	1.503798	4.081484	-0.441519
H	0.572152	4.630774	-0.619493
C	1.430255	2.694652	-0.302798
C	0.129644	2.045492	-0.376044
H	4.833479	4.504256	-0.001857
C	-1.272552	1.284842	3.890738
H	-0.222697	1.617979	3.933976
H	-1.905100	2.140048	4.165754
H	-1.395354	0.469229	4.616587
O	-1.371478	-0.365712	2.171152
O	-2.005088	1.613875	1.647163
C	-1.574001	0.822820	2.512434
C	1.527999	-2.182728	-1.125560
H	1.871938	-1.594780	-1.987448

4-Ir

Atom	X	Y	Z
O	-0.675864	2.674232	-0.708783
N	0.255793	0.713065	-0.119360
C	-4.781071	1.220408	0.036421
H	-5.148182	0.942363	1.034945
H	-5.656090	1.317473	-0.630088
H	-4.314892	2.216090	0.113318
C	-3.831804	0.226984	-0.505385
C	-3.590256	-1.078302	-0.023070
C	-2.551672	-1.668779	-0.841774
C	-2.188496	-0.719518	-1.836298
C	-2.938532	0.476945	-1.611735
C	-2.946573	1.676202	-2.472765
H	-3.698527	1.565035	-3.275665
H	-1.966088	1.847209	-2.939736
H	-3.189811	2.583622	-1.901144
C	-4.276119	-1.767854	1.089636
H	-5.039232	-2.468261	0.705349
H	-4.784278	-1.061108	1.762112
H	-3.571400	-2.357173	1.698140
C	-2.093693	-3.067664	-0.734570
H	-2.815228	-3.739934	-1.233897

H	-2.013787	-3.393786	0.314135
H	-1.110028	-3.221933	-1.201112
C	-1.208445	-0.904105	-2.927981
H	-0.602764	-1.810724	-2.790143
H	-0.521763	-0.044990	-3.005128
H	-1.734856	-0.991237	-3.894841
C	1.695043	-3.568172	-1.216954
H	2.030302	-4.066441	-2.134577
C	1.334764	-4.315811	-0.107190
H	1.381453	-5.410887	-0.139704
C	0.929920	-3.667962	1.048255
H	0.657379	-4.251393	1.936702
C	0.885746	-2.283638	1.103219
H	0.587786	-1.781943	2.027828
C	1.248140	-1.523656	-0.002917
C	1.379246	-0.039423	0.012123
C	2.650453	0.491300	0.009261
C	3.851575	-0.365367	0.071084
C	4.137020	-1.168758	1.172386
H	3.449727	-1.165319	2.028042
C	5.271697	-1.961472	1.200143
H	5.475910	-2.586512	2.078107
C	6.152654	-1.958923	0.130931
H	7.052971	-2.584577	0.155512
C	5.887147	-1.158780	-0.969172
H	6.575906	-1.150543	-1.822753
C	4.749932	-0.372329	-0.996571
H	4.538637	0.256055	-1.872419
C	2.796808	1.905778	-0.123619
C	4.030590	2.574912	-0.031144
H	4.942344	2.003264	0.176618
C	4.101913	3.937948	-0.188079
C	2.953590	4.691312	-0.441076
H	3.024473	5.778057	-0.565342
C	1.736281	4.058607	-0.521823
H	0.812046	4.618094	-0.706509
C	1.643468	2.675849	-0.356882
C	0.334217	2.045661	-0.415254
H	5.074483	4.439673	-0.108136
C	-0.831395	1.393722	3.831961
H	0.233553	1.676407	3.794543
H	-1.407470	2.287411	4.107900
H	-0.943732	0.613832	4.597787
O	-1.073973	-0.308589	2.175277
O	-1.722513	1.654360	1.635115
C	-1.237571	0.891169	2.498122
C	1.655254	-2.185666	-1.160035
H	1.976080	-1.590064	-2.025655
Ir	-1.753320	0.096585	0.148350

TS5-Rh

Atom	X	Y	Z
Rh	-1.719565	-0.031751	0.089136
O	-0.644881	2.834577	-0.033091
N	0.180342	0.742744	-0.070412
C	-3.737649	2.514503	-0.442377
H	-3.650387	2.657083	0.647867
H	-4.792547	2.702577	-0.713753
H	-3.112740	3.280660	-0.918851
C	-3.337227	1.149243	-0.835840
C	-3.896397	-0.052182	-0.264031
C	-3.343046	-1.163167	-0.929203
C	-2.359780	-0.674951	-1.858404
C	-2.424876	0.757956	-1.842911
C	-1.642200	1.638414	-2.733424
H	-2.043046	1.578460	-3.761297
H	-0.583978	1.332851	-2.782535
H	-1.669964	2.686048	-2.407484
C	-4.929354	-0.066598	0.791867
H	-5.910894	0.232207	0.381168
H	-4.689599	0.644850	1.599093
H	-5.047913	-1.063415	1.242986
C	-3.780950	-2.567037	-0.788719
H	-4.670649	-2.735976	-1.422832
H	-4.068481	-2.821089	0.243267
H	-3.010105	-3.281193	-1.111870
C	-1.572131	-1.493771	-2.804717
H	-1.315080	-2.477318	-2.378627
H	-0.626239	-0.997419	-3.073251
H	-2.130100	-1.672406	-3.742298
C	0.919443	-3.856754	-0.602303
H	1.444128	-4.689143	-1.087538
C	-0.255565	-4.093568	0.100777
H	-0.644677	-5.116859	0.196660
C	-0.932341	-3.026787	0.665058
H	-1.865505	-3.212619	1.217083
C	-0.455965	-1.719277	0.554717

H	-0.524084	-1.038588	1.728966
C	0.784467	-1.510771	-0.088886
C	1.232643	-0.114154	-0.126285
C	2.545622	0.306306	-0.179368
C	3.665592	-0.643925	-0.056298
C	3.785910	-1.417330	1.097715
H	3.046087	-1.287748	1.899007
C	4.800662	-2.346624	1.229753
H	4.871370	-2.950594	2.142538
C	5.729694	-2.510446	0.214346
H	6.536154	-3.246408	0.316081
C	5.635803	-1.734620	-0.930321
H	6.367595	-1.857230	-1.738222
C	4.613857	-0.809850	-1.064481
H	4.530549	-0.211438	-1.981600
C	2.789518	1.713307	-0.241636
C	4.079093	2.277437	-0.278295
H	4.957133	1.623188	-0.237491
C	4.250477	3.638139	-0.357383
C	3.151860	4.498579	-0.386941
H	3.301915	5.582305	-0.453016
C	1.884292	3.972969	-0.311286
H	0.997632	4.617454	-0.300717
C	1.688118	2.594380	-0.236343
C	0.326104	2.089374	-0.103420
H	5.266253	4.051259	-0.389908
C	-1.242900	1.112686	4.255719
H	-0.288424	1.629074	4.444625
H	-2.055448	1.849398	4.266215
H	-1.377002	0.381953	5.066835
O	-0.384644	-0.571579	2.864610
O	-1.850391	0.824217	1.995921
C	-1.162672	0.412947	2.942807
C	1.446583	-2.580370	-0.687003
H	2.375268	-2.422402	-1.246166

TS5-Ir

Atom	X	Y	Z
O	-0.443912	2.860429	-0.052421
N	0.356955	0.758062	-0.095584
C	-3.602806	2.567858	-0.490382
H	-3.611735	2.731267	0.599491
H	-4.617929	2.794779	-0.864120
H	-2.905027	3.298235	-0.920864
C	-3.225055	1.179387	-0.825640
C	-3.780128	0.004019	-0.198663
C	-3.262177	-1.137633	-0.847178
C	-2.310749	-0.695170	-1.837505
C	-2.343984	0.740099	-1.848221
C	-1.570194	1.597740	-2.769572
H	-2.096178	1.679902	-3.737203
H	-0.573001	1.176700	-2.974816
H	-1.428225	2.607370	-2.361475
C	-4.783018	0.022259	0.887193
H	-5.795493	0.198271	0.481103
H	-4.580697	0.826009	1.613077
H	-4.807561	-0.929322	1.439366
C	-3.716660	-2.528795	-0.640662
H	-4.644219	-2.699865	-1.216818
H	-3.946513	-2.745539	0.414307
H	-2.977920	-3.266906	-0.985008
C	-1.586854	-1.558106	-2.797291
H	-1.309851	-2.525468	-2.347239
H	-0.654186	-1.081804	-3.138805
H	-2.199739	-1.769664	-3.692274
C	1.096441	-3.843794	-0.673303
H	1.621096	-4.670131	-1.168720
C	-0.068939	-4.091153	0.042587
H	-0.449118	-5.117485	0.139557
C	-0.747012	-3.032533	0.617454
H	-1.669653	-3.227559	1.183132
C	-0.284224	-1.717115	0.504127
H	-0.331409	-1.084365	1.682880
C	0.956146	-1.502745	-0.140087
C	1.405407	-0.106500	-0.164644
C	2.720987	0.304528	-0.213169
C	3.834219	-0.653912	-0.088536
C	3.942386	-1.433509	1.062371
H	3.197157	-1.304602	1.858901
C	4.951973	-2.367872	1.197483
H	5.013117	-2.976718	2.107752
C	5.888316	-2.530162	0.188694
H	6.691023	-3.269886	0.293025
C	5.806718	-1.748036	-0.952442
H	6.544527	-1.869335	-1.755097
C	4.789590	-0.818476	-1.089993
H	4.715953	-0.215150	-2.004755

C	2.978265	1.709568	-0.263428
C	4.272625	2.262944	-0.292031
H	5.145061	1.601345	-0.252649
C	4.455373	3.622688	-0.360896
C	3.363834	4.492233	-0.388840
H	3.522968	5.575078	-0.446425
C	2.091859	3.976530	-0.321535
H	1.210483	4.628084	-0.309309
C	1.884298	2.598987	-0.254749
C	0.518960	2.105185	-0.125850
H	5.474545	4.027744	-0.386702
C	-0.889704	1.069934	4.272181
H	-1.667221	1.843017	4.305956
H	-1.038511	0.340138	5.081515
H	0.091093	1.541605	4.443296
O	-0.150872	-0.646821	2.849607
O	-1.551779	0.839705	2.023830
C	-0.868537	0.376387	2.954121
C	1.616389	-2.564161	-0.753138
H	2.539229	-2.397574	-1.319181
Ir	-1.571308	-0.016301	0.078030

6-Rh

Atom	X	Y	Z
Rh	-1.656302	-0.114388	-0.118491
O	-0.713719	2.692783	0.982058
N	0.134191	0.644724	0.622918
C	-3.975347	2.244079	-0.786276
H	-4.432805	1.942319	0.171103
H	-4.805673	2.491400	-1.472796
H	-3.407613	3.168295	-0.600147
C	-3.116894	1.172897	-1.335419
C	-3.470685	-0.236846	-1.346985
C	-2.440127	-0.952509	-1.992785
C	-1.370973	-0.029195	-2.233554
C	-1.853996	1.298288	-1.904371
C	-1.094312	2.540903	-2.151543
H	-1.230127	2.862430	-3.200319
H	-0.010611	2.400371	-2.002467
H	-1.413943	3.365483	-1.498866
C	-4.763490	-0.766560	-0.864186
H	-5.588789	-0.460182	-1.532426
H	-5.005511	-0.383028	0.140630
H	-4.768058	-1.865714	-0.812826
C	-2.451558	-2.382093	-2.368892
H	-2.825208	-2.499632	-3.402299
H	-3.104230	-2.981729	-1.715562
H	-1.447220	-2.831951	-2.330408
C	-0.101662	-0.324789	-2.933640
H	0.222752	-1.363875	-2.760749
H	0.712542	0.333920	-2.587744
H	-0.197914	-0.183759	-4.026157
C	-0.642485	-1.761004	0.409430
C	-1.201051	-3.008722	0.642642
H	-2.289500	-3.142275	0.556733
C	-0.404437	-4.089561	0.993022
H	-0.859302	-5.071361	1.180303
C	0.965803	-3.920985	1.120430
H	1.599151	-4.766360	1.414073
C	1.541622	-2.681790	0.902930
H	2.621060	-2.567717	1.050360
C	0.750686	-1.589588	0.540451
C	1.198549	-0.194467	0.419098
C	2.469052	0.275717	0.186450
C	3.596745	-0.623596	-0.118332
C	4.696024	-0.710248	0.735037
H	4.719068	-0.089628	1.640935
C	5.738347	-1.580248	0.464451
H	6.589437	-1.641295	1.153441
C	5.702661	-2.378783	-0.667097
H	6.525092	-3.072027	-0.879222
C	4.623682	-2.291243	-1.532606
H	4.591056	-2.913884	-2.435061
C	3.586104	-1.416138	-1.263159
H	2.726153	-1.352573	-1.943980
C	2.673637	1.694554	0.206168
C	3.908464	2.297210	-0.095982
H	4.763532	1.670335	-0.373089
C	4.054308	3.663802	-0.058224
C	2.981816	4.491979	0.273671
H	3.112521	5.579633	0.301577
C	1.759303	3.927565	0.552219
H	0.886452	4.543914	0.798375
C	1.592824	2.543869	0.521109
C	0.262049	1.990908	0.734110
H	5.028537	4.107019	-0.299470
O	-2.738103	-0.117552	1.734555

C	-2.324681	0.004328	2.874882
C	-3.223761	-0.007552	4.051054
H	-4.239840	-0.297394	3.760965
H	-2.835203	-0.691508	4.820040
H	-3.244555	0.999038	4.498357
O	-1.078681	0.166337	3.179243
H	-0.550281	0.212497	2.346902

6-Ir

Atom	X	Y	Z
O	-0.533150	2.693331	1.029943
N	0.303555	0.644628	0.644177
C	-3.842587	2.311530	-0.731681
H	-4.306888	2.003184	0.219886
H	-4.666032	2.595073	-1.412303
H	-3.250965	3.216906	-0.527327
C	-3.010896	1.230631	-1.303129
C	-3.375144	-0.177641	-1.300009
C	-2.358264	-0.902845	-1.966011
C	-1.282245	0.016553	-2.233174
C	-1.755458	1.346608	-1.894967
C	-0.981212	2.582608	-2.132621
H	-1.118565	2.919023	-3.176164
H	0.101076	2.423421	-1.991090
H	-1.284832	3.403230	-1.467408
C	-4.670963	-0.697607	-0.810692
H	-5.493117	-0.422186	-1.495803
H	-4.922742	-0.283402	0.179454
H	-4.666086	-1.794328	-0.719924
C	-2.387608	-2.331490	-2.346604
H	-2.776615	-2.442881	-3.374697
H	-3.033524	-2.926962	-1.682808
H	-1.385550	-2.787479	-2.321732
C	-0.041679	-0.283552	-2.985074
H	0.277165	-1.328488	-2.837116
H	0.792969	0.358767	-2.656322
H	-0.172729	-0.125724	-4.071358
C	-0.479731	-1.765628	0.419054
C	-1.019237	-3.025985	0.651784
H	-2.106678	-3.169984	0.572512
C	-0.212956	-4.102622	0.989042
H	-0.659697	-5.088718	1.172855
C	1.157093	-3.926862	1.108525
H	1.798939	-4.769103	1.392283
C	1.720063	-2.681650	0.893515
H	2.799581	-2.559551	1.032366
C	0.917638	-1.594841	0.542889
C	1.364414	-0.198781	0.424012
C	2.631438	0.272929	0.177289
C	3.755461	-0.621577	-0.154883
C	4.871522	-0.705718	0.676459
H	4.906345	-0.092551	1.587010
C	5.917972	-1.560965	0.377069
H	6.783403	-1.618676	1.048328
C	5.868454	-2.348945	-0.761243
H	6.694146	-3.030635	-0.996770
C	4.770724	-2.266271	-1.603471
H	4.726552	-2.881521	-2.510473
C	3.729290	-1.404745	-1.305852
H	2.854949	-1.343240	-1.968881
C	2.840103	1.691265	0.205807
C	4.071592	2.294513	-0.109807
H	4.920802	1.669257	-0.407235
C	4.221524	3.660256	-0.060453
C	3.156889	4.488225	0.296722
H	3.291018	5.575198	0.333333
C	1.937522	3.923996	0.587993
H	1.069746	4.539612	0.853032
C	1.767140	2.540880	0.544872
C	0.438450	1.991253	0.767426
H	5.192978	4.103201	-0.313043
O	-2.503866	-0.121204	1.833961
C	-2.054924	-0.014404	2.963548
C	-2.921138	-0.043521	4.162701
H	-3.947137	-0.320214	3.895396
H	-2.516275	-0.746663	4.905748
H	-2.920588	0.953356	4.631702
O	-0.801935	0.146376	3.234511
H	-0.293350	0.204450	2.391847
Ir	-1.513780	-0.112551	-0.105404

7-Rh-a

Atom	X	Y	Z
C	3.410504	-1.527594	-0.314955
C	3.578435	-0.374617	-1.141863
C	2.776276	-0.571017	-2.300788

C	2.546794	-2.444841	-0.957123
C	2.123192	-1.835719	-2.170922
C	4.597524	0.678265	-0.918766
H	5.609266	0.234374	-0.897615
H	4.593721	1.428492	-1.723395
H	4.464839	1.213852	0.037589
C	2.721384	0.278649	-3.510179
H	3.431927	-0.089152	-4.273373
H	1.718980	0.268810	-3.967006
H	2.974218	1.328211	-3.299514
C	1.262941	-2.427633	-3.216717
H	0.480728	-1.723446	-3.544736
H	1.865291	-2.675522	-4.110022
H	0.758600	-3.335895	-2.864935
C	2.277445	-3.821285	-0.488135
H	3.222709	-4.389082	-0.407337
H	1.793350	-3.847906	0.501421
H	1.611971	-4.360662	-1.174094
C	4.118880	-1.772422	0.957266
H	3.491081	-2.312818	1.684133
H	5.016320	-2.394284	0.781652
H	4.458898	-0.837013	1.427485
Rh	1.426058	-0.430761	-0.543740
C	1.389220	0.485023	1.500173
C	0.811644	-0.607290	1.633119
C	-4.530087	-3.400512	-0.358023
C	-5.311855	-2.256375	-0.183464
C	-4.756577	-1.002423	-0.268169
C	-3.384846	-0.836599	-0.541916
C	-2.601236	-1.998836	-0.682435
C	-3.182803	-3.262482	-0.591837
C	-2.746808	0.437646	-0.638224
C	-1.380572	0.462527	-0.846539
N	-0.613280	-0.663104	-0.839707
C	-1.148675	-1.906991	-0.769769
O	-0.435083	-2.902649	-0.742961
C	-3.520870	1.661837	-0.368157
C	-3.208781	2.438587	0.747085
C	-3.916470	3.590848	1.035819
C	-4.965652	3.984391	0.219697
C	-5.298529	3.215884	-0.883763
C	-4.582491	2.066651	-1.175443
C	-0.561816	1.641660	-1.120867
C	0.823662	1.444128	-1.004099
C	-1.039581	2.884044	-1.553446
C	-0.169166	3.924776	-1.808626
C	1.193034	3.749630	-1.623484
C	1.678531	2.515541	-1.222709
H	-4.985335	-4.395334	-0.289603
H	-6.383306	-2.356789	0.030222
H	-5.389527	-0.122608	-0.110194
H	-2.527401	-4.135470	-0.688357
H	-2.377634	2.123308	1.394884
H	-3.651437	4.187959	1.917016
H	-5.531053	4.895753	0.447598
H	-6.126732	3.520695	-1.535137
H	-4.839456	1.468778	-2.060198
H	-2.109500	3.042351	-1.716496
H	-0.562193	4.887621	-2.155694
H	1.889063	4.580351	-1.797713
H	2.754464	2.406191	-1.049893
C	1.912634	1.745030	1.931474
C	3.191175	1.831218	2.487252
C	1.140061	2.905814	1.828638
C	3.681534	3.045447	2.930724
H	3.794897	0.921047	2.588605
C	1.637583	4.113193	2.276605
H	0.138929	2.848600	1.382180
C	2.908237	4.190514	2.826053
H	4.683733	3.095119	3.372440
H	1.018315	5.014064	2.192943
H	3.298589	5.152784	3.177895
C	-0.007659	-1.617734	2.212418
C	-1.391667	-1.424758	2.262045
C	0.536279	-2.790028	2.743845
C	-2.210230	-2.393839	2.807619
H	-1.817385	-0.499959	1.851241
C	-0.290218	-3.747460	3.298336
H	1.622734	-2.936940	2.725611
C	-1.664476	-3.559038	3.321866
H	-3.296211	-2.237822	2.817419
H	0.146184	-4.662047	3.716676
H	-2.316079	-4.329311	3.750532

7-Rh-b

Atom	X	Y	Z
C	-3.749181	0.708103	0.041927

C	-3.635429	-0.485265	-0.748612
C	-3.020615	-0.119504	-1.983150
C	-3.182212	1.778105	-0.662456
C	-2.676609	1.250948	-1.901585
C	-4.327834	-1.756468	-0.428504
H	-5.421438	-1.603976	-0.366104
H	-4.157576	-2.525312	-1.197883
H	-4.004269	-2.172079	0.541497
C	-2.837924	-0.986034	-3.169007
H	-3.685796	-0.872188	-3.869246
H	-1.922132	-0.737172	-3.728269
H	-2.775396	-2.052887	-2.907018
C	-2.037800	2.055132	-2.967797
H	-1.462749	1.427751	-3.666078
H	-2.797087	2.594144	-3.564205
H	-1.353901	2.804128	-2.540401
C	-3.285063	3.210150	-0.301350
H	-4.320312	3.569661	-0.453087
H	-3.030543	3.406882	0.752670
H	-2.617204	3.831086	-0.912117
C	-4.433462	0.778506	1.351862
H	-4.135682	1.670973	1.925455
H	-5.530301	0.828701	1.218213
H	-4.228180	-0.111368	1.970618
C	-1.599538	-1.601016	1.981288
C	-1.244031	-0.309935	1.721811
C	3.410076	4.543304	0.482299
C	4.469143	3.636635	0.564372
C	4.268254	2.295930	0.344254
C	2.987924	1.800978	0.025955
C	1.923694	2.720761	-0.030803
C	2.149078	4.079502	0.191899
C	2.720533	0.424612	-0.238649
C	1.410550	0.049873	-0.477142
N	0.367031	0.924956	-0.379544
C	0.563187	2.258273	-0.262799
O	-0.380534	3.045417	-0.308522
C	3.861747	-0.510431	-0.260763
C	4.044499	-1.470823	0.730488
C	5.117446	-2.345213	0.686208
C	6.040917	-2.264190	-0.343966
C	5.887669	-1.296421	-1.323496
C	4.810657	-0.428470	-1.279462
C	0.944074	-1.283653	-0.866074
C	-0.444506	-1.483987	-0.747789
C	1.743546	-2.315224	-1.375204
C	1.200129	-3.546985	-1.687234
C	-0.151924	-3.777524	-1.484072
C	-0.958601	-2.748163	-1.024107
H	3.583813	5.611389	0.656350
H	5.475789	3.996663	0.810689
H	5.113150	1.602428	0.421381
H	1.290602	4.758257	0.133092
H	3.315872	-1.536106	1.550018
H	5.238127	-3.100170	1.472984
H	6.890477	-2.956273	-0.379406
H	6.616624	-1.220129	-2.139525
H	4.683385	0.331006	-2.062568
H	2.810015	-2.162725	-1.557090
H	1.843732	-4.335960	-2.093168
H	-0.588043	-4.760927	-1.706242
H	-2.026465	-2.947817	-0.872181
N	-1.028282	0.563908	2.690999
N	-0.920900	-2.683564	2.096891
C	0.522261	-2.753244	2.112931
H	0.880373	-3.390555	1.283056
H	0.942268	-1.741905	2.004235
H	0.860455	-3.198090	3.067696
C	-1.562804	-3.966606	2.180618
H	-2.652615	-3.826546	2.196222
H	-1.279407	-4.581443	1.305969
H	-1.239374	-4.496673	3.094827
C	-1.019646	0.133972	4.057886
H	-0.557540	-0.862066	4.152204
H	-0.436759	0.845732	4.665676
H	-2.051756	0.087376	4.464497
C	-1.149818	1.975874	2.512851
H	-0.265651	2.491460	2.930001
H	-1.234705	2.214349	1.446003
H	-2.045738	2.351516	3.050043
Rh	-1.559001	0.116875	-0.267218

7-Rh-c

Atom	X	Y	Z
C	-3.756359	0.263859	-0.454266
C	-3.338858	-0.828791	-1.266509
C	-2.389819	-0.320539	-2.199465

C	-3.143708	1.459364	-0.931258
C	-2.303959	1.098036	-2.005908
C	-3.960063	-2.171232	-1.285184
H	-4.927510	-2.130346	-1.818889
H	-3.335530	-2.912978	-1.804235
H	-4.172571	-2.559262	-0.275347
C	-1.728033	-1.071316	-3.289117
H	-2.300529	-1.005610	-4.232753
H	-0.718320	-0.677624	-3.490283
H	-1.617231	-2.138412	-3.040043
C	-1.507191	1.988221	-2.875729
H	-0.455503	1.662118	-2.940373
H	-1.911536	1.962858	-3.904255
H	-1.507293	3.026122	-2.520672
C	-3.426610	2.813144	-0.408324
H	-4.447402	3.138426	-0.681623
H	-3.365110	2.842337	0.693198
H	-2.713404	3.555290	-0.789833
C	-4.750641	0.211191	0.638430
H	-4.449255	0.840141	1.493267
H	-5.729378	0.588848	0.290765
H	-4.909622	-0.812690	1.010853
C	-1.805951	-0.596906	1.939129
C	-1.375193	0.567248	1.952194
C	3.395530	4.400270	-0.090458
C	4.478542	3.524159	0.010294
C	4.291162	2.164048	-0.012858
C	3.001231	1.614905	-0.149045
C	1.914762	2.508380	-0.229508
C	2.125832	3.887185	-0.199640
C	2.743726	0.211404	-0.177662
C	1.431784	-0.208925	-0.291184
N	0.385013	0.663123	-0.308655
C	0.548451	2.008219	-0.271272
O	-0.418287	2.763360	-0.252122
C	3.870563	-0.720960	0.019597
C	3.976627	-1.442044	1.207430
C	5.013519	-2.335391	1.408310
C	5.977270	-2.512474	0.428607
C	5.898865	-1.784511	-0.748149
C	4.856066	-0.895146	-0.949252
C	0.956895	-1.588611	-0.395218
C	-0.429498	-1.753560	-0.218322
C	1.739393	-2.710834	-0.691770
C	1.183712	-3.974990	-0.730696
C	-0.162431	-4.147612	-0.455354
C	-0.956670	-3.038763	-0.208031
H	3.558905	5.483718	-0.071984
H	5.494386	3.925406	0.115208
H	5.154791	1.496967	0.083235
H	1.248583	4.541694	-0.257415
H	3.208033	-1.305325	1.979544
H	5.072915	-2.900434	2.346476
H	6.800269	-3.219797	0.585130
H	6.660609	-1.915849	-1.526628
H	4.786996	-0.330137	-1.888322
H	2.803298	-2.604521	-0.916748
H	1.817271	-4.836934	-0.970191
H	-0.605377	-5.152081	-0.448897
H	-2.020779	-3.195671	-0.001780
C	-2.340023	-1.836771	2.496918
H	-3.151396	-2.229725	1.851202
H	-1.552411	-2.615224	2.475674
C	-0.899765	1.809831	2.552838
H	0.174920	1.946728	2.320294
H	-1.404029	2.676976	2.088664
C	-1.114405	1.795536	4.051648
H	-0.761842	2.738449	4.500310
H	-2.181962	1.677500	4.301480
H	-0.566296	0.966163	4.528471
C	-2.848446	-1.633534	3.907789
H	-2.046306	-1.272345	4.571946
H	-3.664222	-0.891872	3.936284
H	-3.232482	-2.579546	4.322668
Rh	-1.541785	-0.067658	-0.182464

7-Ir-a

Atom	X	Y	Z
C	3.468446	-1.114953	-0.465596
C	3.417124	0.017950	-1.330642
C	2.538451	-0.316642	-2.410300
C	2.693826	-2.166950	-1.027742
C	2.105960	-1.665114	-2.214222
C	4.319443	1.189290	-1.229055
H	5.365781	0.878260	-1.401404
H	4.086513	1.958925	-1.979533
H	4.284950	1.667402	-0.234194

C	2.267229	0.498570	-3.615287
H	2.977027	0.253270	-4.426249
H	1.251560	0.322447	-4.003815
H	2.354950	1.576934	-3.411562
C	1.282303	-2.426100	-3.177540
H	0.382823	-1.866903	-3.482826
H	1.864730	-2.623962	-4.096341
H	0.946250	-3.382186	-2.756858
C	2.618333	-3.555806	-0.522370
H	3.041446	-4.260502	-1.260525
H	3.201996	-3.672984	0.403756
H	1.583259	-3.868010	-0.319554
C	4.307627	-1.221560	0.748529
H	3.773864	-1.700075	1.586902
H	5.205022	-1.832564	0.543893
H	4.655053	-0.235153	1.090572
C	1.324758	0.521399	1.549788
C	0.831493	-0.624623	1.636780
C	-4.381480	-3.651965	-0.164837
C	-5.247489	-2.573596	0.031030
C	-4.795404	-1.279732	-0.062051
C	-3.446359	-1.007131	-0.359855
C	-2.578080	-2.101991	-0.525661
C	-3.055972	-3.408520	-0.432795
C	-2.919849	0.315926	-0.472049
C	-1.562997	0.462918	-0.681615
N	-0.709285	-0.602264	-0.692516
C	-1.145657	-1.888584	-0.668149
O	-0.355093	-2.821679	-0.728544
C	-3.850879	1.450174	-0.326392
C	-3.795551	2.291871	0.782040
C	-4.682086	3.346549	0.916816
C	-5.651129	3.570420	-0.048212
C	-5.728923	2.730448	-1.147758
C	-4.837250	1.680417	-1.282963
C	-0.838418	1.706742	-0.933794
C	0.562541	1.597832	-0.859442
C	-1.412102	2.932912	-1.291635
C	-0.625448	4.046634	-1.511514
C	0.748542	3.961408	-1.358965
C	1.327327	2.746345	-1.033853
H	-4.755075	-4.679667	-0.090766
H	-6.302582	-2.759349	0.268468
H	-5.491072	-0.450752	0.107624
H	-2.338280	-4.227468	-0.556476
H	-3.024948	2.114416	1.545464
H	-4.619560	4.001577	1.794396
H	-6.354596	4.404336	0.059795
H	-6.494543	2.898318	-1.915261
H	-4.893804	1.019237	-2.157934
H	-2.492416	3.026243	-1.424679
H	-1.096333	4.993903	-1.798053
H	1.380107	4.848477	-1.495693
H	2.409191	2.710960	-0.877411
C	1.758069	1.777384	2.094640
C	3.032137	1.900980	2.652297
C	0.912979	2.889317	2.086700
C	3.447861	3.105292	3.190551
H	3.692399	1.025884	2.683017
C	1.337633	4.088974	2.625349
H	-0.087646	2.802868	1.643774
C	2.604377	4.203994	3.175905
H	4.447567	3.182693	3.634417
H	0.662465	4.952742	2.613131
H	2.935755	5.158880	3.600703
C	0.119820	-1.719641	2.212314
C	-1.260587	-1.616590	2.403156
C	0.771162	-2.905770	2.559001
C	-1.973154	-2.688108	2.907270
H	-1.771808	-0.684370	2.129072
C	0.053399	-3.963692	3.080676
H	1.855022	-2.987257	2.408190
C	-1.321142	-3.863236	3.243769
H	-3.061239	-2.605307	3.022582
H	0.573051	-4.889878	3.352571
H	-1.889680	-4.713297	3.638564
Ir	1.339003	-0.249474	-0.522282

7-Ir-b

Atom	X	Y	Z
C	-3.661876	0.637093	0.086759
C	-3.523735	-0.526940	-0.740073
C	-2.925277	-0.103337	-1.970626
C	-3.121407	1.745702	-0.585914
C	-2.616863	1.272466	-1.848165
C	-4.186041	-1.826338	-0.469357
H	-5.286052	-1.715795	-0.450008

H	-3.955619	-2.572784	-1.245381
H	-3.882375	-2.249340	0.503681
C	-2.718264	-0.946578	-3.169016
H	-3.624062	-0.958055	-3.802390
H	-1.888696	-0.580997	-3.793313
H	-2.489912	-1.992228	-2.909579
C	-2.008070	2.133253	-2.888742
H	-1.453573	1.545305	-3.635844
H	-2.784059	2.703002	-3.432226
H	-1.310554	2.858717	-2.442682
C	-3.234524	3.161697	-0.169971
H	-4.253741	3.543561	-0.368555
H	-3.044442	3.305687	0.905970
H	-2.523528	3.800231	-0.709310
C	-4.336452	0.651324	1.404591
H	-4.033054	1.518047	2.013834
H	-5.433666	0.709137	1.280436
H	-4.127451	-0.263546	1.983838
C	-1.445206	-1.660331	2.002525
C	-1.104651	-0.350730	1.739183
C	3.514640	4.576666	0.478518
C	4.588450	3.685232	0.535071
C	4.401799	2.341744	0.319592
C	3.121889	1.828744	0.029589
C	2.043461	2.732678	-0.000105
C	2.254128	4.094593	0.218410
C	2.867468	0.450859	-0.236175
C	1.559446	0.056777	-0.455858
N	0.503677	0.916167	-0.323133
C	0.685891	2.253313	-0.203298
O	-0.268941	3.027870	-0.226757
C	4.017722	-0.472897	-0.266929
C	4.210640	-1.430865	0.724894
C	5.287009	-2.300401	0.676509
C	6.204546	-2.216540	-0.358728
C	6.042247	-1.249990	-1.337965
C	4.961496	-0.386711	-1.289840
C	1.110277	-1.278503	-0.857275
C	-0.277654	-1.495682	-0.734053
C	1.923821	-2.289362	-1.383686
C	1.400794	-3.526545	-1.706966
C	0.053875	-3.781303	-1.497190
C	-0.766414	-2.771056	-1.022527
H	3.676954	5.647082	0.649016
H	5.595403	4.059561	0.758001
H	5.258376	1.660797	0.376907
H	1.384560	4.760603	0.180721
H	3.486813	-1.497844	1.548509
H	5.415120	-3.053928	1.463479
H	7.056757	-2.905147	-0.398295
H	6.766755	-1.171391	-2.157717
H	4.826648	0.370565	-2.073805
H	2.986027	-2.117560	-1.570468
H	2.055305	-4.299801	-2.125631
H	-0.366696	-4.769821	-1.725807
H	-1.830857	-2.988803	-0.867001
N	-0.901429	0.506267	2.728922
N	-0.713131	-2.708812	2.111149
C	0.732272	-2.715102	2.121326
H	1.115205	-3.333328	1.288256
H	1.107644	-1.685903	2.015731
H	1.092834	-3.147835	3.073514
C	-1.294645	-4.020594	2.198036
H	-2.389775	-3.930719	2.209399
H	-0.979899	-4.623485	1.325915
H	-0.949109	-4.532293	3.114601
C	-0.895065	0.049635	4.086790
H	-0.430582	-0.946228	4.165582
H	-0.314944	0.751515	4.708192
H	-1.927550	-0.006045	4.490884
C	-1.042968	1.920253	2.582512
H	-0.176617	2.438186	3.032178
H	-1.111397	2.185782	1.520645
H	-1.955419	2.266549	3.111649
Ir	-1.432592	0.085025	-0.232318

7-Ir-c

Atom	X	Y	Z
C	-3.648299	0.264360	-0.410104
C	-3.224651	-0.809640	-1.245669
C	-2.303759	-0.266613	-2.197388
C	-3.066046	1.477874	-0.886410
C	-2.241111	1.148195	-1.983537
C	-3.825094	-2.161884	-1.282544
H	-4.789770	-2.130152	-1.821320
H	-3.184865	-2.886593	-1.806484
H	-4.032741	-2.564017	-0.277283

C	-1.682216	-0.994743	-3.326965
H	-2.332583	-0.984770	-4.220899
H	-0.720322	-0.543595	-3.617820
H	-1.483724	-2.048698	-3.073074
C	-1.462931	2.071702	-2.836660
H	-0.427552	1.719761	-2.978002
H	-1.920808	2.131855	-3.840801
H	-1.408937	3.081945	-2.412633
C	-3.343477	2.819404	-0.328673
H	-4.353136	3.167059	-0.614292
H	-3.306559	2.812695	0.774004
H	-2.612825	3.563464	-0.672076
C	-4.628510	0.182639	0.695247
H	-4.320389	0.795339	1.559597
H	-5.614724	0.558229	0.368402
H	-4.772519	-0.849699	1.049749
C	-1.649898	-0.615996	1.943239
C	-1.226675	0.560628	1.962885
C	3.536325	4.410692	-0.074491
C	4.623579	3.536608	-0.006090
C	4.439468	2.176348	-0.037773
C	3.147981	1.624916	-0.149549
C	2.058264	2.515994	-0.199733
C	2.266035	3.895287	-0.162536
C	2.894073	0.221562	-0.185096
C	1.582911	-0.206060	-0.273219
N	0.532274	0.665606	-0.256935
C	0.694352	2.013608	-0.222461
O	-0.274696	2.764914	-0.188426
C	4.031018	-0.704105	-0.012371
C	4.174439	-1.407820	1.181833
C	5.221772	-2.292588	1.365738
C	6.158634	-2.477864	0.361428
C	6.042767	-1.766631	-0.822631
C	4.989791	-0.885307	-1.006269
C	1.113047	-1.586237	-0.383868
C	-0.276882	-1.750408	-0.218359
C	1.901298	-2.705049	-0.678086
C	1.350577	-3.970640	-0.725658
C	0.002625	-4.147404	-0.460945
C	-0.795415	-3.042621	-0.215624
H	3.697233	5.494325	-0.048235
H	5.640436	3.939783	0.079878
H	5.306616	1.510521	0.032877
H	1.386099	4.547857	-0.196696
H	3.426324	-1.264856	1.972513
H	5.310499	-2.844631	2.309249
H	6.989810	-3.178497	0.503767
H	6.783365	-1.904330	-1.620105
H	4.891620	-0.332701	-1.950025
H	2.966156	-2.596826	-0.894367
H	1.988900	-4.829673	-0.962643
H	-0.436964	-5.153168	-0.459630
H	-1.860166	-3.202102	-0.013351
C	-2.157258	-1.855196	2.532546
H	-2.996892	-2.243065	1.919534
H	-1.374154	-2.635977	2.471756
C	-0.759816	1.782808	2.615667
H	0.301800	1.959941	2.352479
H	-1.300416	2.657919	2.208354
C	-0.917850	1.700038	4.118163
H	-0.571111	2.631081	4.595043
H	-1.971400	1.544274	4.404776
H	-0.331625	0.866184	4.538037
C	-2.601109	-1.660610	3.964848
H	-1.768364	-1.312538	4.597421
H	-3.408711	-0.912653	4.034933
H	-2.975324	-2.606466	4.388717
Ir	-1.408421	-0.068925	-0.153620

TS8-Rh-a

Atom	X	Y	Z
C	3.540884	-1.430012	0.146077
C	3.791329	-0.194525	-0.531159
C	3.371970	-0.341934	-1.889846
C	2.903774	-2.306388	-0.748209
C	2.761597	-1.607764	-2.004669
C	4.583145	0.912824	0.051261
H	5.637856	0.605304	0.176643
H	4.583712	1.812648	-0.581443
H	4.218859	1.206825	1.049457
C	3.530398	0.636788	-2.990006
H	4.269106	0.277964	-3.729066
H	2.585512	0.811656	-3.531734
H	3.880216	1.615264	-2.629226
C	2.185936	-2.176633	-3.241962
H	1.818338	-1.387510	-3.916161

H	2.945881	-2.755530	-3.798583
H	1.346481	-2.851243	-3.017735
C	2.685645	-3.754220	-0.533664
H	3.660990	-4.275056	-0.505055
H	2.163611	-3.974404	0.409719
H	2.082340	-4.197657	-1.335052
C	3.931635	-1.711558	1.544770
H	3.557769	-2.689234	1.885193
H	5.031355	-1.719102	1.655501
H	3.548800	-0.947404	2.244792
C	0.836836	0.979959	1.025502
C	0.581961	-0.243951	1.324118
C	-4.040686	-3.858833	0.090952
C	-4.915944	-2.772347	0.127293
C	-4.481977	-1.505593	-0.181027
C	-3.143201	-1.272002	-0.546506
C	-2.263385	-2.372756	-0.565103
C	-2.724174	-3.650222	-0.246265
C	-2.620688	0.024045	-0.838714
C	-1.264583	0.129462	-1.058941
N	-0.400266	-0.917339	-1.004932
C	-0.838090	-2.188991	-0.814025
O	-0.053089	-3.129309	-0.813079
C	-3.496604	1.207527	-0.791633
C	-3.284625	2.215113	0.148344
C	-4.100216	3.331626	0.192281
C	-5.153898	3.460185	-0.699555
C	-5.385621	2.461744	-1.631835
C	-4.567219	1.346274	-1.674616
C	-0.554795	1.365780	-1.369591
C	0.769842	1.428463	-0.895381
C	-1.052014	2.401827	-2.157629
C	-0.259223	3.488716	-2.474556
C	1.039857	3.566337	-1.988162
C	1.541929	2.553599	-1.194476
H	-4.398862	-4.864246	0.339327
H	-5.963983	-2.927270	0.412855
H	-5.184081	-0.665936	-0.128264
H	-2.001610	-4.474012	-0.262565
H	-2.444926	2.116847	0.852045
H	-3.915056	4.112558	0.940103
H	-5.801331	4.344526	-0.664670
H	-6.216665	2.554449	-2.341514
H	-4.747400	0.560449	-2.420525
H	-2.070018	2.338428	-2.559224
H	-0.658073	4.286012	-3.111846
H	1.669500	4.435015	-2.226439
H	2.550186	2.652207	-0.771730
C	1.186532	2.183599	1.758595
C	2.133472	2.106985	2.781917
C	0.539965	3.398373	1.526171
C	2.437833	3.220761	3.543210
H	2.629405	1.146398	2.975815
C	0.835434	4.503522	2.302316
H	-0.218689	3.463531	0.734724
C	1.790556	4.422036	3.304572
H	3.188687	3.146653	4.338909
H	0.308959	5.447970	2.121263
H	2.028120	5.304667	3.910366
C	-0.214621	-1.131261	2.101597
C	0.145564	-2.461246	2.336315
C	-1.443807	-0.669388	2.594961
C	-0.695782	-3.299869	3.040342
H	1.093312	-2.835817	1.931549
C	-2.283579	-1.517857	3.286816
H	-1.741933	0.366996	2.388330
C	-1.915345	-2.836835	3.510275
H	-0.401587	-4.342160	3.210611
H	-3.250306	-1.146793	3.647786
H	-2.590001	-3.512533	4.048583
Rh	1.588355	-0.440728	-0.493878

TS8-Rh-b

Atom	X	Y	Z
C	-3.691646	0.506077	-0.905501
C	-3.245231	-0.726053	-1.472366
C	-2.202694	-0.432142	-2.408396
C	-2.913768	1.554128	-1.442860
C	-1.967083	0.956144	-2.345815
C	-3.942075	-2.022419	-1.302358
H	-4.875302	-2.041220	-1.896753
H	-3.329477	-2.873085	-1.635664
H	-4.230444	-2.208055	-0.253059
C	-1.491739	-1.401886	-3.270808
H	-1.957217	-1.472739	-4.270920
H	-0.437483	-1.115758	-3.422183
H	-1.489617	-2.413031	-2.835727

C	-0.951074	1.709392	-3.113772
H	-0.072834	1.088102	-3.351445
H	-1.367217	2.070836	-4.071979
H	-0.598890	2.591650	-2.555736
C	-3.138104	3.011159	-1.304134
H	-3.577037	3.424995	-2.231264
H	-3.840015	3.247165	-0.488868
H	-2.201669	3.552844	-1.104204
C	-4.842538	0.622024	0.021171
H	-4.916599	1.623082	0.471486
H	-5.795258	0.427914	-0.505305
H	-4.782062	-0.109021	0.846098
Rh	-1.533868	0.090118	-0.313508
C	-0.762343	-1.019499	1.933181
C	-1.493244	0.118681	1.673913
C	3.420244	4.521407	0.543959
C	4.502145	3.639617	0.496103
C	4.309491	2.295535	0.290226
C	3.014471	1.768639	0.114126
C	1.929112	2.664334	0.193698
C	2.146558	4.026302	0.402376
C	2.748935	0.382765	-0.102636
C	1.430731	-0.010059	-0.242611
N	0.388382	0.857145	-0.130075
C	0.559607	2.178302	0.104257
O	-0.403649	2.930757	0.234615
C	3.875046	-0.567229	-0.144672
C	4.043504	-1.539856	0.837778
C	5.094323	-2.438821	0.775416
C	6.010153	-2.371491	-0.263330
C	5.868353	-1.395945	-1.236563
C	4.811192	-0.504401	-1.176548
C	0.959345	-1.375225	-0.474065
C	-0.365072	-1.613222	-0.035528
C	1.673166	-2.399279	-1.092981
C	1.123528	-3.662554	-1.238109
C	-0.149300	-3.922862	-0.750606
C	-0.883377	-2.904706	-0.170556
H	3.587685	5.592813	0.702998
H	5.522039	4.022016	0.628626
H	5.175127	1.624285	0.270416
H	1.270051	4.682307	0.454237
H	3.314071	-1.595576	1.657472
H	5.204316	-3.202822	1.554966
H	6.843309	-3.082474	-0.311388
H	6.588688	-1.332691	-2.061262
H	4.691816	0.259829	-1.956482
H	2.673870	-2.211524	-1.496767
H	1.698934	-4.450632	-1.737094
H	-0.584964	-4.926361	-0.849264
H	-1.893807	-3.120495	0.202686
N	-1.805282	1.027697	2.577349
N	-1.185350	-2.053597	2.629463
C	-2.561392	-2.297095	2.959025
H	-2.974033	-3.129264	2.349483
H	-2.657521	-2.582037	4.023868
H	-3.160089	-1.389984	2.778395
C	-0.323528	-3.172305	2.851793
H	-0.664726	-4.061077	2.284410
H	0.696508	-2.916309	2.527894
H	-0.313528	-3.436049	3.925822
C	-2.566351	2.190830	2.260006
H	-2.581484	2.316298	1.172142
H	-3.598686	2.107731	2.655135
H	-2.094468	3.084230	2.706222
C	-1.473684	0.839325	3.958482
H	-0.536029	0.263906	4.042062
H	-1.331147	1.823369	4.436567
H	-2.269784	0.301098	4.510383

TS8-Rh-c

Atom	X	Y	Z
C	-3.766071	0.505786	0.561769
C	-3.762584	-0.676624	-0.238976
C	-3.356012	-0.318945	-1.562753
C	-3.308445	1.577049	-0.225588
C	-3.020383	1.052406	-1.539635
C	-4.320417	-1.977420	0.199401
H	-5.411704	-1.893012	0.355258
H	-4.161543	-2.772453	-0.544589
H	-3.893026	-2.319058	1.158566
C	-3.308937	-1.225026	-2.731218
H	-4.306441	-1.331353	-3.195870
H	-2.625739	-0.853302	-3.510478
H	-2.969591	-2.239212	-2.462919
C	-2.558668	1.861926	-2.687645
H	-2.036249	1.250708	-3.438697

H	-3.414945	2.344162	-3.193610
H	-1.871880	2.654283	-2.357667
C	-3.339840	3.001240	0.174769
H	-4.387070	3.336997	0.291675
H	-2.826831	3.179667	1.133958
H	-2.852085	3.645676	-0.566595
C	-4.176766	0.570475	1.981682
H	-3.771441	1.464485	2.482285
H	-5.276939	0.608916	2.081066
H	-3.833991	-0.314111	2.545763
Rh	-1.667110	0.011238	-0.081124
C	-0.670195	-1.240998	1.483491
C	-0.788486	-0.006534	1.787681
C	3.292790	4.530438	-0.162088
C	4.366655	3.641904	-0.080621
C	4.167529	2.284775	-0.154383
C	2.874975	1.753308	-0.326009
C	1.793462	2.658079	-0.367249
C	2.018452	4.032615	-0.289219
C	2.592673	0.357094	-0.419580
C	1.272883	-0.021116	-0.572611
N	0.224303	0.840405	-0.516124
C	0.416044	2.174641	-0.378410
O	-0.533725	2.941279	-0.252052
C	3.656253	-0.645230	-0.242767
C	3.573905	-1.558858	0.808851
C	4.540582	-2.530620	0.987824
C	5.623445	-2.601428	0.124916
C	5.729787	-1.690505	-0.914011
C	4.756604	-0.723393	-1.095882
C	0.819453	-1.382086	-0.835714
C	-0.485966	-1.683945	-0.400359
C	1.531733	-2.323342	-1.577331
C	0.979715	-3.554096	-1.876807
C	-0.298632	-3.865620	-1.431720
C	-1.016934	-2.943425	-0.696224
H	3.465785	5.611277	-0.107723
H	5.384792	4.029463	0.049891
H	5.025233	1.608904	-0.069629
H	1.147184	4.696945	-0.320265
H	2.714744	-1.496081	1.493989
H	4.453555	-3.240465	1.819288
H	6.393152	-3.369566	0.266518
H	6.582787	-1.739970	-1.601665
H	4.833751	-0.018784	-1.934546
H	2.527387	-2.073628	-1.960028
H	1.549384	-4.276274	-2.472414
H	-0.743977	-4.842746	-1.666010
H	-2.012443	-3.216840	-0.327013
C	-0.567257	1.076960	2.750852
H	-0.953960	2.029484	2.338975
H	-1.168088	0.874205	3.663693
C	-0.573012	-2.557322	2.155090
H	-1.467035	-3.163295	1.905793
H	0.284694	-3.126332	1.740162
C	-0.452842	-2.403768	3.651034
H	-1.324130	-1.877729	4.074141
H	-0.383015	-3.387955	4.139616
H	0.447951	-1.831819	3.927007
C	0.893238	1.234644	3.120852
H	1.508162	1.463197	2.234615
H	1.024353	2.055077	3.844871
H	1.296470	0.313521	3.573980

TS8-Ir-a

Atom	X	Y	Z
C	3.512438	-0.928804	-0.001043
C	3.542009	0.110797	-0.980344
C	2.986678	-0.406586	-2.195229
C	2.919366	-2.076581	-0.585410
C	2.561906	-1.732373	-1.935876
C	4.222763	1.415813	-0.799507
H	5.312373	1.268897	-0.690339
H	4.071799	2.083410	-1.660755
H	3.877793	1.949301	0.103063
C	2.894308	0.303714	-3.489378
H	3.815117	0.163476	-4.084332
H	2.054087	-0.064324	-4.098633
H	2.752587	1.388433	-3.362158
C	1.961741	-2.658082	-2.921447
H	1.357698	-2.120615	-3.668526
H	2.752288	-3.202948	-3.468756
H	1.311436	-3.395025	-2.429395
C	2.926054	-3.436713	-0.005199
H	3.910733	-3.911172	-0.177113
H	2.761192	-3.427234	1.083938
H	2.155287	-4.077509	-0.450201

C	4.071505	-0.838077	1.366350
H	3.506309	-1.456080	2.082927
H	5.120541	-1.185408	1.388429
H	4.066778	0.197677	1.742996
C	0.626374	1.220134	0.855933
C	0.599269	0.018147	1.336320
C	-3.923981	-4.377525	0.209929
C	-4.911869	-3.391163	0.237944
C	-4.605390	-2.079496	-0.028195
C	-3.288481	-1.697120	-0.344831
C	-2.291982	-2.694991	-0.337553
C	-2.625423	-4.021904	-0.065857
C	-2.904946	-0.357512	-0.649900
C	-1.572588	-0.114828	-0.905034
N	-0.593208	-1.052514	-0.778063
C	-0.887695	-2.351917	-0.523779
O	-0.000128	-3.194628	-0.436922
C	-3.880622	0.743706	-0.577632
C	-3.684077	1.774157	0.341648
C	-4.568349	2.834360	0.423995
C	-5.677062	2.880543	-0.406108
C	-5.893674	1.858025	-1.315668
C	-5.004507	0.799735	-1.400278
C	-1.027380	1.147918	-1.382014
C	0.327656	1.371973	-1.066216
C	-1.698708	2.038869	-2.218048
C	-1.051580	3.140673	-2.743751
C	0.279793	3.378688	-2.424222
C	0.951346	2.515889	-1.584321
H	-4.182020	-5.421586	0.421917
H	-5.946524	-3.664073	0.480528
H	-5.394541	-1.320936	0.015379
H	-1.819138	-4.763881	-0.068566
H	-2.805497	1.731402	1.002016
H	-4.394269	3.633982	1.154404
H	-6.380895	3.718748	-0.341705
H	-6.767606	1.888234	-1.977995
H	-5.169140	0.001895	-2.136828
H	-2.739481	1.842960	-2.498396
H	-1.589490	3.818020	-3.416802
H	0.799534	4.256221	-2.832853
H	1.982656	2.749058	-1.292302
C	0.859854	2.560923	1.362756
C	1.904029	2.773589	2.265111
C	0.010573	3.623197	1.048642
C	2.099751	4.020009	2.832295
H	2.560756	1.931988	2.525370
C	0.202118	4.862377	1.629282
H	-0.823361	3.459474	0.352492
C	1.250020	5.067694	2.514895
H	2.927280	4.174402	3.534743
H	-0.481239	5.685079	1.388145
H	1.402313	6.055450	2.966418
C	0.294358	-0.684823	2.545318
C	0.436553	-2.071857	2.644442
C	-0.169076	0.025943	3.663320
C	0.143714	-2.722490	3.829354
H	0.744257	-2.637102	1.757178
C	-0.460959	-0.632536	4.839207
H	-0.300594	1.113542	3.592317
C	-0.300330	-2.009081	4.931116
H	0.250923	-3.812147	3.888856
H	-0.823726	-0.063120	5.703513
H	-0.536013	-2.528881	5.867134
Ir	1.401043	-0.368175	-0.537667

TS8-Ir-b

Atom	X	Y	Z
C	-3.644416	0.416324	-0.653444
C	-3.194803	-0.742694	-1.353975
C	-2.257837	-0.323832	-2.356547
C	-2.974453	1.548245	-1.185913
C	-2.094039	1.070502	-2.215615
C	-3.808369	-2.086721	-1.240700
H	-4.761011	-2.122000	-1.801863
H	-3.159839	-2.874656	-1.651440
H	-4.041469	-2.353958	-0.195948
C	-1.586835	-1.206787	-3.337387
H	-2.234362	-1.416223	-4.208361
H	-0.659439	-0.754761	-3.724242
H	-1.312132	-2.177952	-2.893596
C	-1.204719	1.941215	-3.017595
H	-0.311463	1.405320	-3.374866
H	-1.732942	2.328874	-3.907191
H	-0.864748	2.808065	-2.430436
C	-3.256264	2.975729	-0.913748
H	-3.808048	3.430771	-1.757351

H	-3.881716	3.109988	-0.017365
H	-2.332767	3.555309	-0.765352
C	-4.707411	0.407538	0.379864
H	-4.759268	1.358401	0.930933
H	-5.701037	0.237126	-0.073776
H	-4.550373	-0.394356	1.121517
C	-0.435593	-1.122980	1.863921
C	-1.206500	0.020663	1.721972
C	3.523846	4.557033	0.542977
C	4.613172	3.685890	0.477101
C	4.430992	2.343744	0.249727
C	3.140067	1.809580	0.069325
C	2.047029	2.693326	0.168403
C	2.253785	4.053616	0.397645
C	2.883133	0.425924	-0.170001
C	1.568801	0.023434	-0.305748
N	0.515157	0.876262	-0.162991
C	0.680587	2.198335	0.084975
O	-0.284925	2.943129	0.233970
C	4.010067	-0.522710	-0.219121
C	4.161019	-1.514530	0.747337
C	5.211492	-2.413585	0.686144
C	6.144783	-2.327383	-0.335399
C	6.019609	-1.334066	-1.292887
C	4.962646	-0.442013	-1.234103
C	1.115978	-1.340447	-0.560676
C	-0.185981	-1.610873	-0.062037
C	1.818544	-2.320877	-1.251570
C	1.283577	-3.587515	-1.429134
C	0.033846	-3.886571	-0.902390
C	-0.688563	-2.910472	-0.245092
H	3.682331	5.626908	0.720175
H	5.630136	4.074774	0.613308
H	5.302000	1.680083	0.216040
H	1.372255	4.701394	0.464107
H	3.419189	-1.580629	1.555585
H	5.308092	-3.191458	1.453616
H	6.978457	-3.037816	-0.382505
H	6.753725	-1.256813	-2.104182
H	4.856625	0.335468	-2.002713
H	2.797083	-2.094053	-1.688830
H	1.847527	-4.343521	-1.986907
H	-0.392701	-4.890509	-1.031306
H	-1.677938	-3.160485	0.161812
Ir	-1.430568	0.083660	-0.251839
N	-1.496525	0.851224	2.710400
N	-0.775457	-2.175110	2.588290
C	-2.119558	-2.467837	2.996710
H	-2.553751	-3.283348	2.378482
H	-2.138965	-2.800775	4.051695
H	-2.751488	-1.571117	2.896079
C	0.118633	-3.284592	2.692833
H	-0.242588	-4.152171	2.104891
H	1.111410	-2.992457	2.315852
H	0.206235	-3.600905	3.748834
C	-2.285820	2.021667	2.513829
H	-3.301470	1.893903	2.939252
H	-1.810508	2.885518	3.012685
H	-2.348684	2.232355	1.440278
C	-1.086197	0.582640	4.054790
H	-1.858471	0.032117	4.628335
H	-0.157148	-0.011077	4.054217
H	-0.895316	1.537667	4.573630

TS8-Ir-c

Atom	X	Y	Z
C	-3.671690	0.422371	0.521464
C	-3.640191	-0.687764	-0.375844
C	-3.184308	-0.223609	-1.649966
C	-3.196449	1.565157	-0.167872
C	-2.857109	1.147380	-1.504823
C	-4.207623	-2.025336	-0.083115
H	-5.311704	-1.976721	-0.065477
H	-3.929881	-2.768867	-0.845362
H	-3.891585	-2.413277	0.900331
C	-3.054273	-1.052486	-2.868707
H	-4.038015	-1.240049	-3.336552
H	-2.421675	-0.564981	-3.626097
H	-2.605094	-2.038037	-2.653598
C	-2.360288	2.037543	-2.577513
H	-1.724869	1.495627	-3.294840
H	-3.203584	2.470966	-3.144730
H	-1.767880	2.864606	-2.163467
C	-3.227871	2.947707	0.358864
H	-4.273378	3.284458	0.485373
H	-2.730331	3.029778	1.339545
H	-2.718821	3.651809	-0.310654

C	-4.140618	0.383402	1.924415
H	-3.707941	1.205909	2.516659
H	-5.239961	0.477316	1.984709
H	-3.867074	-0.563248	2.419836
C	-0.478579	-1.296699	1.480609
C	-0.640690	-0.059703	1.802395
C	3.431829	4.550484	-0.161220
C	4.516172	3.671558	-0.128743
C	4.326664	2.313075	-0.200223
C	3.033054	1.770431	-0.321498
C	1.942654	2.665267	-0.313073
C	2.157862	4.041511	-0.237267
C	2.758448	0.373175	-0.416348
C	1.438860	-0.015660	-0.541407
N	0.383837	0.837352	-0.441261
C	0.571014	2.170715	-0.270660
O	-0.377256	2.924083	-0.076504
C	3.828784	-0.625638	-0.258007
C	3.761055	-1.537705	0.796129
C	4.728803	-2.510077	0.963531
C	5.799237	-2.583518	0.085444
C	5.891439	-1.674319	-0.956322
C	4.916919	-0.706033	-1.126454
C	0.993415	-1.374738	-0.812617
C	-0.307383	-1.685863	-0.356448
C	1.700210	-2.297253	-1.580515
C	1.151608	-3.525288	-1.896740
C	-0.120232	-3.850825	-1.439733
C	-0.831669	-2.948723	-0.677031
H	3.597167	5.632582	-0.108875
H	5.535329	4.068150	-0.039775
H	5.193374	1.644927	-0.154019
H	1.279803	4.697553	-0.228066
H	2.911585	-1.473274	1.492855
H	4.652250	-3.218370	1.797310
H	6.570047	-3.352325	0.216938
H	6.734120	-1.726212	-1.656373
H	4.982687	-0.004327	-1.968470
H	2.687295	-2.033149	-1.975049
H	1.716233	-4.232975	-2.513920
H	-0.564449	-4.824772	-1.688351
H	-1.821708	-3.231146	-0.300152
C	-0.430824	0.951816	2.849031
H	-0.982069	0.657087	3.768150
H	-0.871710	1.913319	2.521206
C	-0.392850	-2.612400	2.160859
H	0.460181	-3.190532	1.748171
H	-1.292119	-3.211693	1.913948
C	-0.274342	-2.457893	3.656367
H	-0.202389	-3.442244	4.144228
H	0.624648	-1.884720	3.935446
H	-1.147467	-1.935697	4.079797
C	1.035480	1.148797	3.175330
H	1.163914	1.921807	3.950468
H	1.494740	0.216825	3.545827
H	1.606209	1.464020	2.285526
Ir	-1.537192	0.011982	-0.056953

TS8-Ir-a2

Atom	X	Y	Z
C	3.484059	-1.182875	0.358088
C	3.720542	0.009717	-0.393248
C	3.384950	-0.252985	-1.761020
C	2.939678	-2.155531	-0.511074
C	2.849190	-1.557883	-1.821357
C	4.426424	1.204585	0.126623
H	5.495999	0.978510	0.288991
H	4.379499	2.052595	-0.572956
H	4.021324	1.547281	1.093196
C	3.565552	0.679147	-2.895297
H	4.589108	0.606316	-3.305464
H	2.866292	0.463919	-3.718339
H	3.407111	1.729689	-2.603723
C	2.392253	-2.265421	-3.038017
H	2.068265	-1.567700	-3.824735
H	3.208231	-2.881117	-3.457848
H	1.549241	-2.934269	-2.810175
C	2.795786	-3.596994	-0.213359
H	3.791354	-4.079341	-0.230646
H	2.360334	-3.785757	0.780034
H	2.155560	-4.103658	-0.945108
C	3.824058	-1.376756	1.785392
H	3.209432	-2.163185	2.250418
H	4.882019	-1.676653	1.898846
H	3.688253	-0.454610	2.374465
C	0.570987	1.106452	0.987859
C	0.381514	-0.134914	1.317664

C	-3.956794	-4.043767	0.119214
C	-4.886254	-3.002428	0.133119
C	-4.514920	-1.721435	-0.196017
C	-3.187555	-1.428033	-0.560210
C	-2.253650	-2.482719	-0.557346
C	-2.651743	-3.776648	-0.220275
C	-2.729819	-0.114662	-0.879268
C	-1.379469	0.059143	-1.083519
N	-0.458841	-0.939316	-0.986250
C	-0.837867	-2.232136	-0.796837
O	-0.009365	-3.134066	-0.785108
C	-3.670138	1.019363	-0.884669
C	-3.536687	2.065266	0.026972
C	-4.412782	3.136036	0.014261
C	-5.449259	3.177583	-0.905765
C	-5.604243	2.138085	-1.808522
C	-4.725380	1.068830	-1.794984
C	-0.735209	1.325283	-1.403576
C	0.568897	1.467079	-0.878802
C	-1.264465	2.311665	-2.229706
C	-0.523082	3.433456	-2.551449
C	0.755488	3.592829	-2.029086
C	1.285832	2.631795	-1.194058
H	-4.264775	-5.060976	0.386300
H	-5.926038	-3.204829	0.418983
H	-5.257642	-0.916524	-0.162489
H	-1.889601	-4.564128	-0.220583
H	-2.711038	2.034059	0.753267
H	-4.289347	3.949810	0.739467
H	-6.143968	4.025918	-0.915660
H	-6.421935	2.161445	-2.539016
H	-4.844144	0.250066	-2.517432
H	-2.263694	2.180477	-2.660834
H	-0.944262	4.191495	-3.221198
H	1.345103	4.487180	-2.274306
H	2.275535	2.792995	-0.746059
C	0.848659	2.330650	1.723627
C	1.764567	2.301524	2.775852
C	0.162323	3.515589	1.456879
C	2.001108	3.434687	3.533206
H	2.291773	1.362466	2.993039
C	0.389885	4.640693	2.227587
H	-0.574030	3.540818	0.642099
C	1.315431	4.606970	3.259578
H	2.729825	3.400090	4.351999
H	-0.166752	5.562007	2.019212
H	1.500128	5.504994	3.861169
C	-0.386562	-0.980755	2.168794
C	-0.063118	-2.325170	2.377145
C	-1.562251	-0.477819	2.749623
C	-0.884965	-3.137707	3.132429
H	0.835498	-2.735358	1.902893
C	-2.382997	-1.299485	3.493452
H	-1.835345	0.571722	2.575797
C	-2.051737	-2.633915	3.686845
H	-0.619338	-4.191607	3.276070
H	-3.306979	-0.894431	3.922942
H	-2.713607	-3.286434	4.267944
Ir	1.508467	-0.359791	-0.415148

TS8-Rh-a2

Atom	X	Y	Z
C	3.584438	-0.998690	-0.134847
C	3.609954	0.097081	-1.052640
C	3.032151	-0.342335	-2.283256
C	2.978021	-2.101560	-0.771798
C	2.603209	-1.677307	-2.094370
C	4.312272	1.377176	-0.796910
H	5.385963	1.193433	-0.612233
H	4.244136	2.065800	-1.652127
H	3.923387	1.905388	0.091967
C	2.926938	0.430850	-3.539653
H	3.783183	0.222439	-4.206984
H	2.011762	0.178413	-4.098993
H	2.907561	1.516636	-3.360348
C	1.993163	-2.540897	-3.127178
H	1.371195	-1.961955	-3.827494
H	2.780837	-3.035812	-3.725045
H	1.361054	-3.318490	-2.676079
C	2.985079	-3.496163	-0.279487
H	3.890104	-4.015663	-0.647266
H	3.016710	-3.544289	0.820556
H	2.105972	-4.059730	-0.616097
C	4.151312	-0.970528	1.231039
H	3.610099	-1.641834	1.917199
H	5.210808	-1.286387	1.227467
H	4.120899	0.044084	1.660976

C	0.803034	1.095511	0.892812
C	0.750298	-0.123452	1.288643
C	-3.890376	-4.292830	0.065176
C	-4.846567	-3.280981	0.171638
C	-4.510934	-1.968334	-0.051736
C	-3.196326	-1.610745	-0.403932
C	-2.231450	-2.636535	-0.480218
C	-2.593407	-3.963176	-0.248031
C	-2.784393	-0.269949	-0.664332
C	-1.453906	-0.055895	-0.952657
N	-0.501306	-1.024603	-0.908807
C	-0.824996	-2.324562	-0.709835
O	0.037856	-3.196867	-0.703714
C	-3.725732	0.852803	-0.511813
C	-3.478992	1.829049	0.453640
C	-4.332071	2.906226	0.612490
C	-5.458803	3.023747	-0.185556
C	-5.725362	2.055106	-1.139994
C	-4.867591	0.979900	-1.300957
C	-0.881951	1.214061	-1.383495
C	0.481176	1.391261	-1.094633
C	-1.548090	2.168763	-2.152602
C	-0.883752	3.284712	-2.624151
C	0.456429	3.474832	-2.314863
C	1.125035	2.545674	-1.542035
H	-4.171499	-5.337198	0.244441
H	-5.879057	-3.534398	0.442988
H	-5.274546	-1.189895	0.054151
H	-1.810485	-4.726979	-0.313695
H	-2.586916	1.728915	1.089386
H	-4.118742	3.662307	1.377971
H	-6.137787	3.875480	-0.060562
H	-6.614347	2.141761	-1.776859
H	-5.072628	0.224389	-2.071194
H	-2.600036	2.015815	-2.418467
H	-1.417590	4.014060	-3.244117
H	0.987461	4.364658	-2.675421
H	2.163783	2.742434	-1.254233
C	1.049590	2.410865	1.447552
C	2.091050	2.562590	2.366765
C	0.227412	3.505118	1.171271
C	2.311714	3.779301	2.985850
H	2.724341	1.695552	2.598154
C	0.445015	4.714247	1.803822
H	-0.604452	3.391744	0.463320
C	1.490344	4.859095	2.704483
H	3.136304	3.884177	3.700858
H	-0.216460	5.562123	1.591048
H	1.662046	5.824069	3.196362
C	0.444954	-0.952152	2.413598
C	0.594129	-2.340788	2.378243
C	-0.015775	-0.350028	3.594756
C	0.305465	-3.101552	3.496727
H	0.903203	-2.816528	1.441412
C	-0.304029	-1.119138	4.702661
H	-0.147200	0.739475	3.626306
C	-0.139843	-2.497528	4.661668
H	0.418818	-4.191174	3.452815
H	-0.666034	-0.635767	5.617926
H	-0.372839	-3.104849	5.544176
Rh	1.485118	-0.380047	-0.634268

9-Rh-a

Atom	X	Y	Z
C	-2.794755	-2.298324	4.564527
C	-3.968856	-1.937793	3.900974
C	-3.931052	-1.468555	2.610838
C	-2.710213	-1.347984	1.923331
C	-1.525342	-1.690773	2.609990
C	-1.587873	-2.164034	3.921781
C	-2.604541	-0.864916	0.581419
C	-1.338699	-0.746348	0.069587
N	-0.201817	-1.058692	0.720090
C	-0.212843	-1.534996	1.987105
O	0.826228	-1.819386	2.577671
C	-3.783812	-0.509328	-0.224258
C	-3.924965	0.770670	-0.759048
C	-5.015098	1.096311	-1.546816
C	-5.995442	0.152295	-1.804843
C	-5.875577	-1.120847	-1.269706
C	-4.779752	-1.449094	-0.491992
C	-1.054499	-0.352484	-1.333680
C	-0.282213	0.793463	-1.613993
C	-1.525032	-1.143782	-2.387012
C	-1.253445	-0.812136	-3.696292
C	-0.478879	0.309064	-3.982470
C	0.005071	1.088248	-2.954824

C	1.222842	1.196396	0.142463
C	0.175356	1.710282	-0.521691
H	-2.836957	-2.673336	5.593498
H	-4.860741	-1.169942	2.113408
H	-0.645629	-2.418933	4.419852
H	-3.162333	1.528837	-0.534489
H	-5.103951	2.110377	-1.955296
H	-6.863117	0.411019	-2.423539
H	-6.645975	-1.875696	-1.469855
H	-4.680169	-2.464305	-0.084971
H	-2.130539	-2.028541	-2.149356
H	-1.644184	-1.434109	-4.510373
H	-0.255532	0.574384	-5.024980
H	0.618661	1.974048	-3.173244
C	3.230515	-1.712132	0.115394
C	3.608757	-0.744585	-0.870028
C	2.965813	-1.096091	-2.072166
C	2.450309	-2.742710	-0.548408
C	2.288624	-2.368878	-1.877226
C	1.955628	-3.967325	0.113815
H	2.757761	-4.725880	0.172063
H	1.626954	-3.762654	1.143723
H	1.113360	-4.422150	-0.429141
C	4.541281	0.382701	-0.661669
H	4.523561	0.748316	0.376611
H	5.577354	0.066879	-0.882463
H	4.312511	1.238492	-1.316645
C	3.833396	-1.855469	1.454590
H	3.118293	-2.268788	2.178029
H	4.698066	-2.543459	1.392744
H	4.205356	-0.897360	1.846714
C	3.115072	-0.418571	-3.376879
H	3.343068	0.652317	-3.261413
H	3.944061	-0.872283	-3.951320
H	2.208475	-0.505035	-3.996065
C	1.586342	-3.105976	-2.946883
H	0.974677	-2.439386	-3.577964
H	2.309762	-3.600435	-3.621294
H	0.923070	-3.888327	-2.547306
C	2.085626	1.812164	1.133309
C	2.383869	1.156478	2.331410
C	2.709578	3.037842	0.873738
C	3.260607	1.717865	3.242317
H	1.916318	0.184809	2.535613
C	3.595707	3.586769	1.781567
H	2.488043	3.559447	-0.066962
C	3.875943	2.930637	2.971866
H	3.473167	1.191996	4.181532
H	4.080219	4.544606	1.555461
H	4.581680	3.366230	3.689265
C	-0.554808	2.960221	-0.275366
C	-0.574115	3.540206	0.998992
C	-1.301886	3.583683	-1.280094
C	-1.273234	4.705717	1.242735
H	-0.043614	3.048989	1.822688
C	-2.004588	4.750556	-1.031285
H	-1.339200	3.146653	-2.285070
C	-1.987207	5.325502	0.228190
H	-1.273939	5.131103	2.253564
H	-2.577325	5.218296	-1.841543
H	-2.544565	6.248521	0.425232
H	-4.933676	-2.020994	4.416652
Rh	1.427562	-0.708698	-0.540338

9-Rh-b

Atom	X	Y	Z
C	3.472684	4.586808	0.159734
C	4.505205	3.646742	0.142171
C	4.233318	2.305569	0.026951
C	2.909002	1.843436	-0.082977
C	1.870356	2.799049	-0.039202
C	2.170228	4.158079	0.076909
C	2.570294	0.458977	-0.202557
C	1.231115	0.154663	-0.208191
N	0.238620	1.062935	-0.173887
C	0.470383	2.393416	-0.105231
O	-0.451680	3.205106	-0.107069
C	3.604968	-0.576088	-0.365994
C	3.710059	-1.657075	0.507518
C	4.668395	-2.637282	0.318478
C	5.552503	-2.554257	-0.744559
C	5.467081	-1.481597	-1.618975
C	4.504416	-0.506819	-1.432420
C	0.694306	-1.219032	-0.407017
C	-0.154772	-1.840692	0.544207
C	1.056260	-1.910282	-1.571337
C	0.622759	-3.195263	-1.802255

C	-0.216529	-3.817819	-0.879754
C	-0.601969	-3.144019	0.255143
C	-1.313699	-0.132293	1.706897
C	-0.491125	-1.187316	1.845156
H	3.701314	5.654935	0.249583
H	5.057192	1.583194	0.033728
H	1.334463	4.866704	0.103591
H	3.023408	-1.722320	1.360825
H	4.730730	-3.477224	1.021100
H	6.315151	-3.328261	-0.892162
H	6.158873	-1.406679	-2.466737
H	4.432661	0.333418	-2.136086
H	1.716983	-1.412186	-2.292564
H	0.935870	-3.724390	-2.710579
H	-0.573298	-4.840832	-1.061138
H	-1.277518	-3.627806	0.973801
C	-3.249423	1.259226	-0.924025
C	-3.761691	0.012263	-0.442513
C	-3.259263	-0.999789	-1.281202
C	-2.521063	0.992485	-2.153249
C	-2.531505	-0.378756	-2.376030
C	-1.892083	2.046583	-2.975911
H	-2.653302	2.590642	-3.564563
H	-1.379112	2.785758	-2.341482
H	-1.158193	1.634974	-3.685098
C	-4.686566	-0.195319	0.693909
H	-4.655205	0.635667	1.413022
H	-5.729515	-0.283559	0.337058
H	-4.453549	-1.118951	1.247602
C	-3.689703	2.613136	-0.525672
H	-2.845409	3.314568	-0.460906
H	-4.391556	3.007202	-1.285162
H	-4.215432	2.616835	0.438952
C	-3.590557	-2.437068	-1.196493
H	-3.706959	-2.775135	-0.154454
H	-4.546425	-2.638668	-1.715061
H	-2.824620	-3.068398	-1.671652
C	-1.944540	-1.119866	-3.511057
H	-1.405573	-2.025274	-3.184941
H	-2.732978	-1.457002	-4.208849
H	-1.238250	-0.502977	-4.087053
H	5.546758	3.980266	0.229046
N	0.123419	-1.584270	3.062290
N	-1.787669	0.635392	2.732156
C	1.062076	-0.605368	3.536413
H	1.955963	-0.492325	2.878924
H	0.569861	0.378658	3.609446
H	1.412663	-0.888639	4.545871
C	0.676462	-2.898088	3.081629
H	1.484990	-3.073279	2.331314
H	1.109847	-3.086082	4.079873
H	-0.106268	-3.657057	2.910642
C	-2.424571	-0.004004	3.837774
H	-2.371482	0.654198	4.725007
H	-3.502469	-0.206378	3.639164
H	-1.919775	-0.950750	4.078748
C	-2.235286	1.963391	2.499202
H	-1.942727	2.609785	3.349158
H	-1.778490	2.364531	1.583047
H	-3.343462	2.034144	2.415518
Rh	-1.557055	0.041446	-0.320816

9-Rh-c

Atom	X	Y	Z
C	3.801300	4.376831	0.249679
C	4.749634	3.351684	0.240466
C	4.364894	2.039424	0.107336
C	3.008523	1.696765	-0.035623
C	2.053626	2.738048	-0.004712
C	2.468059	4.063643	0.136999
C	2.549242	0.351767	-0.194290
C	1.192053	0.175296	-0.271845
N	0.279302	1.158366	-0.210673
C	0.621444	2.460488	-0.084098
O	-0.224595	3.347965	-0.038756
C	3.456495	-0.805753	-0.242986
C	3.339447	-1.815501	0.712052
C	4.152710	-2.933412	0.675747
C	5.114614	-3.059302	-0.312847
C	5.251715	-2.060089	-1.263617
C	4.429888	-0.946546	-1.231440
C	0.575409	-1.145390	-0.612757
C	-0.071621	-1.976317	0.331082
C	0.779586	-1.615949	-1.917096
C	0.395340	-2.885638	-2.290037
C	-0.184809	-3.726901	-1.344916
C	-0.414167	-3.276506	-0.063388

C	-0.976786	-0.299137	1.730143
C	-0.340201	-1.477826	1.695700
H	4.119760	5.419963	0.356927
H	5.121201	1.245892	0.119608
H	1.696208	4.841570	0.158616
H	2.596118	-1.700021	1.512646
H	4.041310	-3.713604	1.438817
H	5.764847	-3.941773	-0.342913
H	6.009184	-2.153054	-2.051653
H	4.532993	-0.165571	-1.996973
H	1.298495	-0.961529	-2.631639
H	0.580838	-3.240932	-3.312084
H	-0.463523	-4.751731	-1.620996
H	-0.884103	-3.944753	0.670252
C	-3.295627	1.391345	-0.129261
C	-3.698927	0.054355	0.206772
C	-3.391132	-0.760429	-0.895050
C	-2.908152	1.393953	-1.534394
C	-2.944774	0.083410	-1.992382
C	-2.545221	2.608280	-2.293337
H	-3.453528	3.173873	-2.571408
H	-1.906410	3.274825	-1.695847
H	-2.009648	2.369077	-3.224225
C	-4.334175	-0.410564	1.462239
H	-4.453206	0.404554	2.190948
H	-5.340922	-0.815261	1.256857
H	-3.756568	-1.213299	1.955042
C	-3.538605	2.607586	0.673568
H	-2.761366	3.366999	0.499315
H	-4.515023	3.056149	0.409003
H	-3.560226	2.390045	1.752961
C	-3.629042	-2.214604	-0.993006
H	-3.611254	-2.700538	-0.003933
H	-4.618733	-2.416244	-1.444231
H	-2.878155	-2.714343	-1.626146
C	-2.608957	-0.423954	-3.338913
H	-1.986950	-1.335082	-3.290011
H	-3.521122	-0.693867	-3.902190
H	-2.061021	0.320492	-3.935488
H	5.814315	3.593313	0.348143
C	0.037847	-2.331607	2.876650
H	0.770408	-3.096281	2.548371
H	0.569690	-1.717994	3.630462
C	-1.275272	0.485365	2.955044
H	-0.969613	-0.091079	3.854580
H	-2.369019	0.633319	3.059721
C	-1.144575	-3.011006	3.535095
H	-0.837320	-3.623769	4.399689
H	-1.878691	-2.268917	3.895095
H	-1.678691	-3.673250	2.831396
C	-0.597915	1.838346	2.979721
H	-0.942921	2.482238	2.156089
H	-0.797288	2.360862	3.929997
H	0.496955	1.736884	2.873885
Rh	-1.532591	0.180659	-0.167727

9-Ir-a

Atom	X	Y	Z
C	-2.770577	-2.803084	4.359644
C	-3.962642	-2.465211	3.716000
C	-3.949411	-1.893495	2.466666
C	-2.735406	-1.643876	1.802783
C	-1.534493	-1.967197	2.469573
C	-1.571878	-2.547505	3.738697
C	-2.654072	-1.056771	0.501925
C	-1.399140	-0.822557	0.006251
N	-0.243804	-1.112007	0.643791
C	-0.233670	-1.689045	1.870464
O	0.820232	-1.961276	2.438722
C	-3.850083	-0.713885	-0.285443
C	-4.082057	0.598932	-0.694150
C	-5.187130	0.919240	-1.463171
C	-6.090033	-0.065612	-1.830252
C	-5.878676	-1.373709	-1.421577
C	-4.770209	-1.694356	-0.658595
C	-1.141419	-0.347153	-1.376617
C	-0.458997	0.862147	-1.610232
C	-1.514275	-1.152078	-2.456112
C	-1.217724	-0.780347	-3.750092
C	-0.519332	0.399070	-3.988894
C	-0.143870	1.201616	-2.932651
C	0.932057	1.316398	0.234556
C	-0.121771	1.771528	-0.472200
H	-2.793644	-3.259785	5.355658
H	-4.894001	-1.618558	1.983698
H	-0.617591	-2.785101	4.222096
H	-3.381340	1.385591	-0.383065

H	-5.347304	1.959181	-1.772721
H	-6.967944	0.187526	-2.436758
H	-6.586831	-2.159955	-1.709685
H	-4.598722	-2.734052	-0.348697
H	-2.057084	-2.084750	-2.254349
H	-1.529030	-1.416248	-4.587547
H	-0.272676	0.694527	-5.016106
H	0.406518	2.134453	-3.115585
C	3.319333	-1.345649	0.245860
C	3.614892	-0.280175	-0.680110
C	3.086681	-0.658199	-1.931143
C	2.761580	-2.452803	-0.515133
C	2.602723	-2.028956	-1.829839
C	2.418329	-3.765096	0.071423
H	3.335748	-4.346340	0.276076
H	1.887522	-3.643637	1.028099
H	1.789930	-4.370226	-0.598919
C	4.372199	0.950908	-0.371170
H	4.282452	1.236993	0.688136
H	5.446159	0.798988	-0.582547
H	4.035005	1.808844	-0.974854
C	3.854979	-1.457752	1.616929
H	3.217900	-2.091037	2.248146
H	4.866345	-1.905031	1.581762
H	3.944777	-0.474706	2.102963
C	3.186999	0.099506	-3.196273
H	3.264944	1.183684	-3.020624
H	4.084631	-0.209849	-3.762741
H	2.316173	-0.073735	-3.848014
C	2.028443	-2.782419	-2.963160
H	1.326844	-2.166332	-3.551210
H	2.821095	-3.109547	-3.660276
H	1.483791	-3.679259	-2.631916
Ir	1.447021	-0.536970	-0.456199
C	1.635362	2.008817	1.308962
C	1.915565	1.362595	2.515604
C	2.112332	3.311015	1.130733
C	2.627745	2.004431	3.513476
H	1.562664	0.333874	2.663532
C	2.840760	3.941798	2.122643
H	1.904239	3.828646	0.184732
C	3.100914	3.293084	3.320822
H	2.825167	1.482416	4.458104
H	3.212333	4.960734	1.958013
H	3.678002	3.794464	4.106778
C	-0.980979	2.933227	-0.212141
C	-1.203763	3.380862	1.095733
C	-1.674169	3.577988	-1.240880
C	-2.048387	4.442734	1.353938
H	-0.719384	2.860730	1.930424
C	-2.522547	4.640097	-0.979081
H	-1.551612	3.242132	-2.277076
C	-2.709582	5.085694	0.318562
H	-2.206905	4.763966	2.390560
H	-3.046477	5.129189	-1.809650
H	-3.382983	5.925282	0.525963
H	-4.922171	-2.650695	4.214622

9-Ir-b

Atom	X	Y	Z
C	3.515623	4.632158	0.172094
C	4.571001	3.719383	0.130236
C	4.333814	2.373883	-0.012153
C	3.021324	1.878817	-0.121426
C	1.959578	2.807147	-0.048577
C	2.224475	4.171048	0.089389
C	2.711558	0.487324	-0.256761
C	1.380687	0.151218	-0.232169
N	0.364592	1.034767	-0.168730
C	0.568608	2.371201	-0.097647
O	-0.371155	3.161269	-0.079684
C	3.760463	-0.528788	-0.441895
C	3.844216	-1.649209	0.383548
C	4.810779	-2.617385	0.181792
C	5.728366	-2.483140	-0.847059
C	5.663590	-1.373569	-1.675361
C	4.689987	-0.411137	-1.477767
C	0.870526	-1.232940	-0.409985
C	0.072510	-1.858779	0.581100
C	1.195743	-1.923930	-1.584127
C	0.770461	-3.216492	-1.789755
C	-0.016816	-3.845401	-0.827243
C	-0.364283	-3.170192	0.320059
C	-1.095776	-0.170923	1.765332
C	-0.223800	-1.194051	1.887157
H	3.717423	5.703743	0.281833
H	5.177145	1.674458	-0.021288

H	1.370083	4.855877	0.137291
H	3.128399	-1.757223	1.207327
H	4.853427	-3.488055	0.847613
H	6.499358	-3.246727	-1.005152
H	6.380251	-1.259621	-2.497809
H	4.633896	0.455921	-2.149366
H	1.822489	-1.421859	-2.332472
H	1.052294	-3.747019	-2.707298
H	-0.362402	-4.876096	-0.985401
H	-0.996778	-3.661234	1.071843
C	-3.188961	1.224404	-0.837847
C	-3.677687	-0.045214	-0.360068
C	-3.159874	-1.038527	-1.213809
C	-2.486569	0.981656	-2.088155
C	-2.461944	-0.390794	-2.313727
C	-1.889711	2.051813	-2.914033
H	-2.670680	2.589340	-3.481792
H	-1.371982	2.790655	-2.283226
H	-1.165302	1.656144	-3.641765
C	-4.620566	-0.285868	0.755919
H	-4.699102	0.579147	1.428893
H	-5.633172	-0.491034	0.362527
H	-4.325904	-1.154679	1.366857
C	-3.645745	2.567406	-0.420573
H	-2.811547	3.282850	-0.379756
H	-4.381975	2.949674	-1.152168
H	-4.135464	2.556927	0.562529
C	-3.462346	-2.483513	-1.143293
H	-3.633997	-2.820810	-0.109042
H	-4.380100	-2.707023	-1.718306
H	-2.656343	-3.099732	-1.569823
C	-1.861117	-1.116004	-3.451986
H	-1.308419	-2.012834	-3.125992
H	-2.644766	-1.463312	-4.149820
H	-1.164400	-0.486836	-4.026235
Ir	-1.470647	0.038857	-0.251127
H	5.604203	4.077230	0.219333
N	0.455128	-1.552210	3.075515
N	-1.495547	0.614342	2.828213
C	1.420445	-0.572089	3.485334
H	2.315913	-0.518966	2.823021
H	0.950637	0.424986	3.502267
H	1.770712	-0.804136	4.508399
C	0.972731	-2.877102	3.140529
H	1.756489	-3.110752	2.379464
H	1.428971	-3.033667	4.134491
H	0.164083	-3.619618	3.024022
C	-2.070472	-0.062263	3.949935
H	-2.099858	0.621903	4.817338
H	-3.118825	-0.387575	3.746519
H	-1.471871	-0.943563	4.221230
C	-2.143509	1.851957	2.559655
H	-2.028060	2.518619	3.434032
H	-1.691726	2.342978	1.685914
H	-3.237104	1.738816	2.383225

9-Ir-c

Atom	X	Y	Z
C	3.757862	4.454374	0.325272
C	4.751738	3.474105	0.357586
C	4.432257	2.144120	0.229945
C	3.097836	1.735668	0.054725
C	2.096404	2.731211	0.052840
C	2.444308	4.077269	0.182813
C	2.708522	0.366776	-0.100683
C	1.363534	0.115385	-0.171532
N	0.403754	1.060613	-0.140276
C	0.685172	2.383703	-0.064663
O	-0.205645	3.226470	-0.086401
C	3.698022	-0.712395	-0.248090
C	3.700594	-1.828699	0.587095
C	4.625584	-2.844337	0.414477
C	5.573353	-2.762555	-0.593042
C	5.585571	-1.658156	-1.430137
C	4.656778	-0.648039	-1.260914
C	0.811287	-1.237713	-0.477203
C	0.132443	-2.027576	0.477311
C	1.060556	-1.758156	-1.752012
C	0.680374	-3.039717	-2.089165
C	0.055839	-3.838537	-1.136572
C	-0.209288	-3.337571	0.119981
C	-0.911185	-0.346685	1.781846
C	-0.180218	-1.474337	1.814394
H	4.024727	5.512649	0.424555
H	5.225338	1.389125	0.275519
H	1.636504	4.817910	0.171447
H	2.963538	-1.887359	1.400071

H	4.611026	-3.711983	1.085306
H	6.309181	-3.564688	-0.725206
H	6.327856	-1.585878	-2.234361
H	4.662176	0.219661	-1.934008
H	1.608777	-1.135918	-2.472047
H	0.897473	-3.433889	-3.088647
H	-0.227311	-4.869336	-1.384559
H	-0.712185	-3.971276	0.861880
C	-3.210349	1.344246	-0.283736
C	-3.627836	0.018324	0.110425
C	-3.257532	-0.853978	-0.929717
C	-2.779372	1.275459	-1.675546
C	-2.780335	-0.059364	-2.055517
C	-2.395642	2.450485	-2.485674
H	-3.294263	3.021839	-2.782007
H	-1.742263	3.131404	-1.920622
H	-1.871791	2.162494	-3.409521
C	-4.346939	-0.361649	1.347134
H	-4.348807	0.450135	2.089019
H	-5.401936	-0.596685	1.118556
H	-3.909839	-1.252978	1.827829
C	-3.492622	2.599850	0.441391
H	-2.725571	3.357211	0.224796
H	-4.476354	3.008171	0.142653
H	-3.512907	2.448313	1.532375
C	-3.485927	-2.313404	-0.968269
H	-3.523045	-2.747298	0.043826
H	-4.446988	-2.543871	-1.464151
H	-2.696627	-2.840235	-1.528827
C	-2.352521	-0.641587	-3.344649
H	-1.710760	-1.527822	-3.195784
H	-3.222505	-0.976441	-3.938462
H	-1.788198	0.077190	-3.956996
H	5.800359	3.766044	0.493885
C	0.265351	-2.229538	3.037295
H	1.075709	-2.929998	2.752000
H	0.724067	-1.531350	3.764881
C	-1.264070	0.449758	2.990669
H	-0.977334	-0.097446	3.912610
H	-2.363137	0.578780	3.056375
C	-0.843435	-2.999591	3.724540
H	-0.479671	-3.527936	4.622253
H	-1.658879	-2.326049	4.040421
H	-1.292343	-3.753703	3.055322
C	-0.616179	1.818381	3.006050
H	-0.955354	2.441561	2.163258
H	-0.846171	2.355591	3.941239
H	0.482938	1.738190	2.925758
Ir	-1.453586	0.133852	-0.131812

10-Rh-a

Atom	X	Y	Z
O	1.237871	-1.929889	1.344221
N	-0.199292	-1.246106	-0.116668
C	0.015741	-1.883251	1.028846
C	-1.091298	-2.399398	1.763975
C	-0.909608	-3.163155	2.921066
H	0.113607	-3.370754	3.256940
C	-1.995225	-3.640975	3.608935
H	-1.859022	-4.247779	4.510988
C	-3.283820	-3.340106	3.153517
C	-3.481592	-2.581606	2.026976
H	-4.502056	-2.346016	1.704495
C	-2.390151	-2.089967	1.284540
C	-2.545859	-1.239929	0.144221
C	-3.891304	-0.785612	-0.263604
C	-4.294353	0.527247	-0.037688
H	-3.593221	1.220388	0.446028
C	-5.559248	0.954566	-0.403943
H	-5.858655	1.993180	-0.218170
C	-6.448684	0.070469	-0.992227
H	-7.451961	0.406876	-1.278902
C	-6.064453	-1.242649	-1.214016
H	-6.762545	-1.949130	-1.679403
C	-4.796187	-1.665651	-0.852982
H	-4.490234	-2.705382	-1.031480
C	-1.405839	-0.810154	-0.500778
C	-1.365454	0.178400	-1.593824
C	-2.101288	-0.037022	-2.756148
H	-2.682310	-0.963879	-2.846682
C	-2.118355	0.894120	-3.777545
H	-2.700410	0.702916	-4.686459
C	-1.407602	2.075377	-3.629758
H	-1.420754	2.831780	-4.423572
C	-0.680733	2.300972	-2.476869
H	-0.129872	3.244184	-2.359148
C	-0.609165	1.361064	-1.445650

C	0.124322	1.724632	-0.203399
C	1.049822	0.941764	0.401711
C	1.464929	1.127973	1.791485
C	0.488821	1.149531	2.796081
H	-0.569947	1.111962	2.502358
C	0.840383	1.206579	4.132112
H	0.055778	1.213094	4.898629
C	2.174816	1.252829	4.503474
H	2.453931	1.295643	5.562810
C	3.154820	1.239316	3.521143
H	4.214418	1.283114	3.802751
C	2.803774	1.165043	2.186400
H	3.584988	1.153228	1.417582
C	2.437785	-1.855055	-2.296106
C	3.340166	-2.159160	-1.280800
C	3.924874	-0.914709	-0.810460
C	3.417775	0.137782	-1.603465
C	2.430031	-0.417515	-2.469505
C	1.770109	0.281643	-3.591159
H	1.746209	1.370693	-3.442138
H	0.732611	-0.055358	-3.744718
H	2.319348	0.086319	-4.531761
C	1.567798	-2.778375	-3.055128
H	1.944709	-2.929006	-4.082964
H	0.542909	-2.377661	-3.147058
H	1.496133	-3.767606	-2.578636
C	3.653370	-3.478914	-0.694284
H	2.971922	-4.264496	-1.053220
H	3.584206	-3.454799	0.406935
H	4.683491	-3.791503	-0.944563
C	5.001184	-0.863704	0.204498
H	5.869192	-1.463604	-0.124347
H	4.675364	-1.277516	1.174585
H	5.360053	0.160692	0.382482
C	3.794741	1.568758	-1.564721
H	4.410772	1.813371	-0.685704
H	2.906581	2.223568	-1.537240
H	4.376451	1.843622	-2.462975
H	-4.153283	-3.710581	3.710485
C	-0.205718	3.070373	0.325155
C	0.790767	3.921591	0.807037
C	-1.520744	3.542071	0.332025
C	0.482531	5.170826	1.313823
H	1.836370	3.588432	0.773541
C	-1.831487	4.789828	0.842143
H	-2.318442	2.907100	-0.075390
C	-0.831891	5.609989	1.341054
H	1.286198	5.819678	1.682555
H	-2.874762	5.128783	0.848859
H	-1.076740	6.600858	1.740842
Rh	1.764001	-0.770169	-0.429386

10-Rh-b

Atom	X	Y	Z
O	-0.977761	2.328269	0.610998
N	0.278025	0.761676	-0.188967
C	0.210818	1.956856	0.375349
C	1.404878	2.684053	0.652354
C	1.370723	3.968134	1.205835
H	0.395714	4.415219	1.434818
C	2.537246	4.645086	1.450027
H	2.516256	5.652367	1.880698
C	3.761149	4.035165	1.150068
C	3.814936	2.774726	0.611542
H	4.787928	2.315121	0.404231
C	2.635771	2.052212	0.338929
C	2.643811	0.708721	-0.148220
C	3.933905	0.030432	-0.400661
C	4.402877	-0.982980	0.429295
H	3.803804	-1.281185	1.298059
C	5.609409	-1.611862	0.172461
H	5.957720	-2.410671	0.838256
C	6.375165	-1.232215	-0.916656
H	7.330712	-1.729566	-1.120847
C	5.928471	-0.213713	-1.743966
H	6.529305	0.097325	-2.607413
C	4.720249	0.411053	-1.487229
H	4.365151	1.213254	-2.148157
C	1.426426	0.084449	-0.341758
C	1.212779	-1.335250	-0.657594
C	1.892945	-1.943416	-1.708556
H	2.611989	-1.350695	-2.287548
C	1.665455	-3.264629	-2.045416
H	2.209757	-3.720603	-2.880635
C	0.733147	-3.992172	-1.326651
H	0.522793	-5.036587	-1.588719
C	0.050544	-3.393156	-0.283252

H	-0.707197	-3.974445	0.257329
C	0.258223	-2.062190	0.094842
C	-0.437765	-1.586640	1.333015
C	-1.414556	-0.642760	1.354008
C	-2.471156	0.683428	-2.472013
C	-3.306586	1.462284	-1.682266
C	-3.903262	0.611124	-0.665350
C	-3.479251	-0.717484	-0.908962
C	-2.521501	-0.671069	-1.961787
C	-1.894195	-1.822246	-2.643251
H	-1.977050	-2.749725	-2.060523
H	-0.824129	-1.653976	-2.848075
H	-2.387019	-1.995458	-3.618463
C	-1.626125	1.097374	-3.613117
H	-2.025697	0.713027	-4.569585
H	-0.599166	0.702612	-3.520494
H	-1.553429	2.191570	-3.702909
C	-3.542449	2.918261	-1.766693
H	-2.877310	3.406438	-2.494163
H	-3.387096	3.411240	-0.791113
H	-4.583907	3.132297	-2.067699
C	-4.928410	1.051828	0.306434
H	-5.925832	1.128367	-0.165885
H	-4.694401	2.043154	0.728972
H	-5.016631	0.348072	1.149568
C	-3.923154	-1.929268	-0.185561
H	-4.210583	-1.696287	0.851828
H	-3.128306	-2.691778	-0.141203
H	-4.799801	-2.384917	-0.680496
H	4.695645	4.571757	1.355504
Rh	-1.768702	0.505966	-0.280810
N	-2.299902	-0.487090	2.385000
N	0.026814	-2.117585	2.579960
C	-2.623162	-1.545728	3.281145
H	-1.954617	-1.614919	4.163871
H	-3.659234	-1.390847	3.645456
H	-2.583332	-2.508032	2.746135
C	-2.583418	0.809469	2.900126
H	-2.478940	1.566445	2.110095
H	-3.616751	0.841778	3.296018
H	-1.899897	1.090574	3.733333
C	-0.018926	-3.533802	2.772996
H	-1.018874	-3.930379	2.528396
H	0.730824	-4.102352	2.172075
H	0.185328	-3.760342	3.837364
C	1.340664	-1.641029	2.896575
H	1.393746	-0.546238	2.761417
H	1.578026	-1.876874	3.952076
H	2.139579	-2.106656	2.268676

10-Rh-c

Atom	X	Y	Z
O	-1.022101	2.432469	0.248544
N	0.190310	0.784272	-0.443557
C	0.148151	2.044362	-0.031268
C	1.359393	2.785274	0.108585
C	1.350845	4.140360	0.452023
H	0.383586	4.639107	0.589913
C	2.530929	4.821107	0.606609
H	2.529659	5.885584	0.867353
C	3.742199	4.140824	0.439395
C	3.771343	2.807331	0.117431
H	4.735324	2.295613	0.018941
C	2.579281	2.080579	-0.069294
C	2.551413	0.673130	-0.324686
C	3.788247	-0.132750	-0.332733
C	3.997129	-1.105797	0.641953
H	3.238527	-1.245881	1.424972
C	5.133377	-1.893868	0.626799
H	5.276634	-2.657541	1.401001
C	6.088977	-1.718199	-0.360782
H	6.989569	-2.343750	-0.374871
C	5.900502	-0.746402	-1.329550
H	6.651386	-0.601254	-2.115926
C	4.759971	0.038076	-1.315881
H	4.604897	0.796233	-2.095570
C	1.321167	0.071365	-0.473198
C	1.114494	-1.379620	-0.611292
C	1.709233	-2.060765	-1.668507
H	2.290963	-1.484292	-2.399968
C	1.602121	-3.432693	-1.790599
H	2.073807	-3.952960	-2.632151
C	0.912298	-4.136272	-0.817275
H	0.828568	-5.228309	-0.879204
C	0.321703	-3.464635	0.235888
H	-0.225155	-4.048081	0.985567
C	0.367651	-2.072343	0.363840

C	-0.233945	-1.439079	1.569222
C	-1.065201	-0.375124	1.553999
C	-2.808987	-0.027304	-2.160118
C	-3.525658	0.995489	-1.553491
C	-3.977796	0.515866	-0.255476
C	-3.602499	-0.838901	-0.128005
C	-2.791441	-1.162205	-1.256579
C	-2.306968	-2.505131	-1.637600
H	-2.232822	-3.180472	-0.773756
H	-1.314995	-2.473665	-2.117610
H	-3.005092	-2.967234	-2.361433
C	-2.101443	-0.013191	-3.458395
H	-2.596770	-0.676374	-4.190543
H	-1.064050	-0.377837	-3.352430
H	-2.056676	0.993920	-3.898839
C	-3.776543	2.365610	-2.047494
H	-3.280799	2.557713	-3.010688
H	-3.419754	3.128115	-1.332875
H	-4.857840	2.543925	-2.188325
C	-4.828768	1.303529	0.662867
H	-5.867853	1.363161	0.288675
H	-4.466353	2.340039	0.765726
H	-4.869852	0.862732	1.670612
C	-3.953709	-1.749726	0.984035
H	-4.073413	-1.207146	1.935816
H	-3.182963	-2.521477	1.143634
H	-4.907160	-2.269677	0.780151
H	4.687296	4.679930	0.578763
C	0.123058	-2.124572	2.880653
H	1.065888	-2.690777	2.747964
C	-1.549660	0.277130	2.818274
H	-1.732974	-0.470584	3.616947
H	-2.534179	0.756464	2.640047
C	-0.935726	-3.054421	3.442255
H	-0.645120	-3.435512	4.436320
H	-1.908424	-2.545518	3.554209
H	-1.114056	-3.931949	2.799057
C	-0.589468	1.326806	3.345322
H	0.410669	0.898171	3.531075
H	-0.466666	2.154142	2.629863
H	-0.952332	1.754800	4.295428
H	0.354684	-1.358676	3.645489
Rh	-1.805678	0.429925	-0.152630

10-Ir-a

Atom	X	Y	Z
O	1.093641	-1.383721	1.825936
N	-0.335745	-1.144932	0.239799
C	-0.131424	-1.449346	1.514600
C	-1.236094	-1.774683	2.350584
C	-1.065234	-2.171169	3.681109
H	-0.047295	-2.228928	4.085241
C	-2.155367	-2.483543	4.450859
H	-2.027706	-2.800184	5.491875
C	-3.437421	-2.390961	3.898400
C	-3.624925	-1.992099	2.598985
H	-4.641401	-1.908921	2.198010
C	-2.529202	-1.671748	1.775180
C	-2.683020	-1.164367	0.445628
C	-4.033764	-0.915010	-0.102030
C	-4.527082	0.379340	-0.230610
H	-3.901441	1.220801	0.095192
C	-5.787211	0.609826	-0.755569
H	-6.156065	1.637887	-0.852959
C	-6.581685	-0.454020	-1.150591
H	-7.579820	-0.272368	-1.566721
C	-6.108826	-1.749525	-1.013723
H	-6.732147	-2.598101	-1.321145
C	-4.846472	-1.977129	-0.492949
H	-4.469689	-3.003697	-0.390908
C	-1.544209	-0.862880	-0.269179
C	-1.500492	-0.141245	-1.553176
C	-2.223645	-0.597808	-2.652558
H	-2.799575	-1.526994	-2.556960
C	-2.231587	0.098989	-3.846739
H	-2.803461	-0.281872	-4.700700
C	-1.522847	1.285694	-3.944398
H	-1.526895	1.857768	-4.880093
C	-0.811639	1.751722	-2.855848
H	-0.267474	2.703186	-2.929792
C	-0.753515	1.053838	-1.646947
C	-0.038869	1.697857	-0.508797
C	0.930412	1.098300	0.229629
C	1.363039	1.662977	1.516225
C	0.408493	1.915710	2.507158
H	-0.651145	1.736298	2.276144
C	0.779847	2.374856	3.757792

H	0.010590	2.556288	4.518797
C	2.114355	2.607697	4.050150
H	2.409029	2.976219	5.039551
C	3.074168	2.361238	3.080550
H	4.133830	2.543864	3.298416
C	2.703608	1.879261	1.838431
H	3.470650	1.688666	1.077632
C	2.316713	-2.309900	-1.776493
C	3.257310	-2.328911	-0.747533
C	3.809305	-0.992102	-0.611826
C	3.244010	-0.181800	-1.629271
C	2.251836	-0.960280	-2.301482
C	1.538802	-0.589667	-3.541842
H	1.545083	0.496077	-3.711908
H	0.486611	-0.914580	-3.530519
H	2.023953	-1.065614	-4.414463
C	1.466007	-3.417540	-2.262218
H	1.794859	-3.758828	-3.260379
H	0.412529	-3.102978	-2.366504
H	1.489304	-4.288192	-1.589947
C	3.631496	-3.461408	0.126204
H	2.923317	-4.299568	0.047478
H	3.670104	-3.157507	1.185963
H	4.634202	-3.847530	-0.131844
C	4.939388	-0.666541	0.287825
H	5.863227	-1.169272	-0.052868
H	4.753965	-1.000293	1.322511
H	5.150253	0.412488	0.321264
C	3.593158	1.217410	-1.962168
H	4.130102	1.715566	-1.140411
H	2.697000	1.821179	-2.184160
H	4.245133	1.253918	-2.853318
H	-4.310484	-2.633351	4.516994
C	-0.427143	3.112515	-0.293229
C	0.530294	4.105383	-0.078927
C	-1.765696	3.505676	-0.347542
C	0.164255	5.426257	0.108319
H	1.592146	3.826759	-0.069685
C	-2.135055	4.825021	-0.156294
H	-2.536166	2.749645	-0.548935
C	-1.171731	5.793282	0.076646
H	0.939146	6.185979	0.269383
H	-3.195917	5.102372	-0.191801
H	-1.462835	6.840069	0.221989
Ir	1.647812	-0.762818	-0.212734

10-Ir-b

Atom	X	Y	Z
O	-0.842229	2.265000	0.663249
N	0.421732	0.748076	-0.185514
C	0.353694	1.933617	0.397528
C	1.535950	2.680080	0.654377
C	1.494050	3.958956	1.219839
H	0.518296	4.390317	1.473985
C	2.656081	4.649857	1.444390
H	2.630374	5.653070	1.884181
C	3.882002	4.060551	1.111819
C	3.942724	2.805676	0.561084
H	4.917151	2.362710	0.326500
C	2.768453	2.068165	0.308919
C	2.785475	0.729152	-0.189893
C	4.084879	0.071081	-0.452898
C	4.596810	-0.895100	0.406229
H	4.022870	-1.176189	1.296816
C	5.819052	-1.495220	0.154900
H	6.201743	-2.257128	0.844847
C	6.557651	-1.131092	-0.957883
H	7.526237	-1.604691	-1.157624
C	6.066694	-0.159410	-1.815566
H	6.646394	0.139008	-2.697757
C	4.842717	0.436438	-1.564055
H	4.454035	1.204450	-2.246438
C	1.576236	0.086008	-0.368876
C	1.380506	-1.333871	-0.690700
C	2.042641	-1.915777	-1.767976
H	2.726961	-1.299533	-2.364332
C	1.840554	-3.240670	-2.106773
H	2.370008	-3.677454	-2.961356
C	0.952015	-3.996227	-1.362303
H	0.761302	-5.044489	-1.624058
C	0.285006	-3.421443	-0.294925
H	-0.441900	-4.025917	0.261603
C	0.467039	-2.087141	0.086849
C	-0.194678	-1.634417	1.352619
C	-1.183386	-0.697538	1.412906
C	-2.458995	0.561575	-2.428651
C	-3.283603	1.335068	-1.619363

C	-3.803886	0.498519	-0.550876
C	-3.345153	-0.826998	-0.781608
C	-2.434297	-0.780391	-1.880648
C	-1.821834	-1.935465	-2.571451
H	-1.827222	-2.840985	-1.949537
H	-0.775919	-1.742737	-2.862287
H	-2.382220	-2.161420	-3.497782
C	-1.683330	0.973053	-3.619114
H	-2.116771	0.549231	-4.543493
H	-0.640744	0.614814	-3.567168
H	-1.652205	2.066042	-3.741023
C	-3.568549	2.780722	-1.735734
H	-2.905984	3.279162	-2.458446
H	-3.451775	3.296998	-0.767310
H	-4.610009	2.951536	-2.062749
C	-4.824688	0.918900	0.435292
H	-5.841680	0.887911	0.001946
H	-4.653386	1.948477	0.789867
H	-4.824635	0.263912	1.321531
C	-3.736164	-2.035956	-0.023200
H	-3.982881	-1.794172	1.022532
H	-2.926232	-2.782944	-0.004081
H	-4.623753	-2.510823	-0.478016
H	4.812630	4.609637	1.300952
Ir	-1.643327	0.429443	-0.227921
N	0.321219	-2.187698	2.568510
N	-2.015321	-0.553632	2.497614
C	0.262840	-3.604132	2.755270
H	0.993256	-4.177719	2.135373
H	0.488074	-3.840247	3.813753
H	-0.746232	-3.988470	2.529684
C	1.652979	-1.737103	2.838980
H	2.420625	-2.219019	2.184489
H	1.723380	-0.643334	2.702417
H	1.922693	-1.978235	3.885889
C	-2.241484	-1.590869	3.445337
H	-1.514375	-1.622021	4.283007
H	-3.253036	-1.448671	3.877223
H	-2.218550	-2.568554	2.938169
C	-2.321279	0.745117	2.993527
H	-2.337457	1.475680	2.172514
H	-3.314207	0.736067	3.483145
H	-1.582588	1.099105	3.748461

10-Ir-c

Atom	X	Y	Z
O	-0.949833	2.308638	0.214542
N	0.304334	0.640469	-0.305966
C	0.237598	1.931504	-0.013719
C	1.423819	2.712589	0.046153
C	1.382310	4.087070	0.302864
H	0.405477	4.562165	0.455981
C	2.543275	4.812925	0.354276
H	2.518413	5.890975	0.548147
C	3.767425	4.160242	0.170086
C	3.827586	2.811256	-0.073355
H	4.803395	2.326840	-0.188847
C	2.654102	2.035269	-0.156100
C	2.666404	0.614409	-0.331299
C	3.949049	-0.096332	-0.510745
C	4.428145	-1.022017	0.410862
H	3.841144	-1.232147	1.313231
C	5.631574	-1.674684	0.200710
H	5.989969	-2.401546	0.939799
C	6.383381	-1.407515	-0.931665
H	7.337057	-1.922991	-1.095642
C	5.921565	-0.484056	-1.855240
H	6.506920	-0.266659	-2.756944
C	4.715648	0.161554	-1.647152
H	4.347076	0.886677	-2.385422
C	1.453883	-0.046355	-0.340749
C	1.264921	-1.505252	-0.301056
C	1.846218	-2.325992	-1.263109
H	2.432756	-1.862888	-2.067253
C	1.707691	-3.700142	-1.213608
H	2.171901	-4.328910	-1.981876
C	0.985430	-4.266294	-0.176244
H	0.868362	-5.355144	-0.112754
C	0.402505	-3.456444	0.780203
H	-0.180017	-3.923170	1.585193
C	0.494172	-2.062222	0.744003
C	-0.130487	-1.299528	1.869486
C	-1.067758	-0.336013	1.712210
C	-2.623099	-0.402542	-2.162502
C	-3.359565	0.697561	-1.737955
C	-3.897277	0.395121	-0.419377
C	-3.555467	-0.939979	-0.098635

C	-2.672291	-1.413868	-1.122091
C	-2.197172	-2.803888	-1.295598
H	-2.167270	-3.349758	-0.341372
H	-1.182379	-2.845871	-1.723815
H	-2.867614	-3.360025	-1.977757
C	-1.841903	-0.560589	-3.407691
H	-2.342652	-1.257123	-4.104314
H	-0.843643	-0.985019	-3.200811
H	-1.696237	0.392660	-3.937288
C	-3.554553	1.990707	-2.428952
H	-2.942804	2.068896	-3.340223
H	-3.294559	2.845739	-1.781033
H	-4.609785	2.127112	-2.727135
C	-4.798874	1.292906	0.336623
H	-5.823729	1.269611	-0.077243
H	-4.455438	2.339649	0.295853
H	-4.865518	1.008426	1.398245
C	-4.008550	-1.711870	1.079681
H	-4.254990	-1.056963	1.930128
H	-3.239270	-2.421636	1.423520
H	-4.915157	-2.295594	0.839005
H	4.699734	4.735194	0.231159
C	0.336000	-1.771981	3.226471
H	-0.191246	-1.224633	4.024798
H	0.069011	-2.837767	3.383872
C	-1.683817	0.368821	2.894402
H	-2.634475	0.841557	2.576964
H	-1.972480	-0.352784	3.687565
C	1.827975	-1.621198	3.426246
H	2.150031	-0.578529	3.250197
H	2.132561	-1.901072	4.448646
H	2.395431	-2.260610	2.727916
C	-0.790995	1.440593	3.486547
H	-0.519459	2.189149	2.724521
H	-1.289895	1.969580	4.316981
H	0.149838	1.016343	3.877861
Ir	-1.728251	0.272406	-0.117900

TS11-Rh-a

Atom	X	Y	Z
O	0.082393	-2.948645	-0.369378
N	-0.539363	-0.796377	-0.589630
C	-0.823662	-2.134149	-0.412208
C	-2.218277	-2.506883	-0.248550
C	-2.524810	-3.847730	-0.014577
H	-1.702966	-4.572458	-0.018288
C	-3.820059	-4.236736	0.230380
H	-4.058741	-5.289891	0.417032
C	-4.828680	-3.272365	0.256018
C	-4.547049	-1.947873	0.020555
H	-5.354346	-1.208885	0.060060
C	-3.234316	-1.529894	-0.256777
C	-2.873383	-0.168703	-0.509675
C	-3.883773	0.904253	-0.439841
C	-3.753581	1.903584	0.522557
H	-2.888796	1.872539	1.200764
C	-4.684018	2.920514	0.626111
H	-4.561663	3.696584	1.391462
C	-5.773059	2.954579	-0.230826
H	-6.513876	3.758849	-0.150676
C	-5.919902	1.965781	-1.189448
H	-6.775711	1.988399	-1.874932
C	-4.984384	0.949898	-1.293606
H	-5.098167	0.174963	-2.063707
C	-1.548531	0.127100	-0.715070
C	-1.053057	1.446152	-1.069365
C	-1.649791	2.213223	-2.063151
H	-2.543158	1.820969	-2.563966
C	-1.124751	3.433905	-2.438620
H	-1.599756	4.019170	-3.233218
C	0.024555	3.895871	-1.807719
H	0.460873	4.859803	-2.097609
C	0.632361	3.150143	-0.819903
H	1.542531	3.527428	-0.337924
C	0.114059	1.904983	-0.424395
C	0.732222	1.159873	0.665002
C	0.629423	-0.228982	0.909875
C	2.616947	-0.073604	-2.745634
C	2.357966	-1.459371	-2.496014
C	3.160976	-1.900330	-1.395742
C	3.803961	-0.760349	-0.873723
C	3.464151	0.368422	-1.710794
C	3.954916	1.749409	-1.508318
H	5.000262	1.858222	-1.851087
H	3.932229	2.040356	-0.443107
H	3.349647	2.482763	-2.064285
C	1.992803	0.769610	-3.791725

H	1.076848	0.304992	-4.190145
H	2.665409	0.945175	-4.651392
H	1.700692	1.759722	-3.398709
C	1.511011	-2.347430	-3.322576
H	1.082119	-3.161292	-2.719942
H	2.104821	-2.806940	-4.133941
H	0.678827	-1.803500	-3.796208
C	3.307854	-3.296940	-0.935060
H	3.933906	-3.889813	-1.628478
H	2.333026	-3.803594	-0.857910
H	3.788938	-3.345858	0.055205
C	4.805250	-0.742339	0.217236
H	4.527063	-1.406979	1.052645
H	4.948544	0.268621	0.630173
H	5.792970	-1.080353	-0.147970
H	-5.862151	-3.572371	0.470139
C	0.331356	-0.938378	2.126078
C	0.954203	-2.157362	2.404042
C	-0.629389	-0.438957	3.012727
C	0.634369	-2.853761	3.552901
H	1.694303	-2.543682	1.690962
C	-0.953699	-1.144404	4.153203
H	-1.118518	0.518930	2.784649
C	-0.320056	-2.350097	4.423991
H	1.129690	-3.806451	3.772861
H	-1.709776	-0.754005	4.844499
C	1.442644	1.900784	1.731407
C	0.919266	3.083197	2.258363
C	2.609382	1.388527	2.298135
C	1.548468	3.729179	3.305660
H	-0.008232	3.495458	1.839464
C	3.236454	2.032638	3.349771
H	3.023217	0.453967	1.898917
C	2.711773	3.209809	3.855175
H	1.117203	4.654069	3.707865
H	4.152737	1.608384	3.778134
Rh	1.603500	-0.348137	-0.745350
H	3.208707	3.726570	4.684712
H	-0.578646	-2.908691	5.331945

TS11-Rh-a-i

Atom	X	Y	Z
O	0.662875	-2.346623	0.845719
N	-0.450988	-0.659578	0.043009
C	-0.470882	-1.822935	0.761022
C	-1.686457	-2.299839	1.291824
C	-1.710003	-3.424873	2.128979
H	-0.762083	-3.924267	2.361777
C	-2.893723	-3.861292	2.657315
H	-2.918501	-4.731784	3.322301
C	-4.077387	-3.170810	2.358247
C	-4.076084	-2.083225	1.523138
H	-5.016831	-1.563142	1.312181
C	-2.882211	-1.619868	0.936658
C	-2.830976	-0.518294	0.031843
C	-4.080712	0.155874	-0.370776
C	-4.304662	1.491427	-0.045763
H	-3.536319	2.039057	0.516179
C	-5.469660	2.128626	-0.434159
H	-5.626636	3.181375	-0.170549
C	-6.438367	1.438543	-1.146004
H	-7.362099	1.942897	-1.452935
C	-6.233191	0.105937	-1.465295
H	-6.993447	-0.448894	-2.028366
C	-5.064642	-0.529289	-1.080672
H	-4.898247	-1.582200	-1.344957
C	-1.605561	-0.070479	-0.420188
C	-1.341483	1.038251	-1.310497
C	-2.136441	1.322816	-2.423535
H	-2.974710	0.657862	-2.661392
C	-1.865863	2.399731	-3.237143
H	-2.486710	2.588334	-4.119998
C	-0.788704	3.233080	-2.938073
H	-0.561374	4.089958	-3.584092
C	0.003610	2.973161	-1.846659
H	0.859304	3.624043	-1.628682
C	-0.226809	1.867191	-1.007860
C	0.561960	1.645732	0.173991
C	0.776305	0.353445	0.670844
C	2.008573	-0.936740	-2.819635
C	2.251074	-2.271998	-2.441548
C	3.213656	-2.224568	-1.380252
C	3.663084	-0.879925	-1.205737
C	2.882188	-0.072143	-2.061995
C	3.063514	1.383203	-2.258353
H	3.036589	1.942719	-1.307643
H	2.289660	1.813275	-2.910119

H	4.043289	1.590510	-2.726695
C	1.043402	-0.483086	-3.845157
H	0.682771	0.539473	-3.650055
H	0.160019	-1.140344	-3.897170
H	1.505588	-0.479642	-4.849422
C	1.626051	-3.491644	-2.999802
H	1.464744	-4.262318	-2.227977
H	2.250196	-3.955254	-3.787084
H	0.644845	-3.278931	-3.454653
C	3.732058	-3.402035	-0.650828
H	2.971399	-4.192413	-0.551762
H	4.073771	-3.139863	0.363053
H	4.594773	-3.843698	-1.182461
C	4.762790	-0.416537	-0.331235
H	4.905853	-1.072909	0.541911
H	4.581467	0.602835	0.048736
H	5.727808	-0.389308	-0.872861
H	-5.023685	-3.506166	2.800160
Rh	1.513165	-1.097312	-0.649219
C	0.959416	0.162842	2.130436
C	2.029461	-0.545837	2.665849
C	0.013520	0.704403	2.999007
C	2.175406	-0.674750	4.035027
H	2.757250	-0.998269	1.977228
C	0.145694	0.560671	4.368713
H	-0.835808	1.260174	2.575729
C	1.233088	-0.122597	4.890000
H	3.033601	-1.221327	4.444015
H	-0.607317	0.991701	5.039549
H	1.344300	-0.232876	5.975617
C	1.164512	2.792328	0.858882
C	0.470829	3.998765	1.014032
C	2.460468	2.724599	1.384908
C	1.040436	5.073491	1.670179
H	-0.550032	4.081082	0.618808
C	3.026919	3.796399	2.049065
H	3.036982	1.798936	1.256838
C	2.320575	4.979391	2.196872
H	0.467344	6.001736	1.784780
H	4.045263	3.710245	2.447474
H	2.769840	5.833609	2.716578

TS11-Rh-b

Atom	X	Y	Z
C	3.295392	4.523142	-0.125396
C	4.399966	3.673570	-0.069837
C	4.247315	2.306817	-0.104786
C	2.971321	1.726957	-0.198272
C	1.863940	2.594828	-0.218551
C	2.035175	3.978616	-0.195362
C	2.743398	0.310654	-0.246259
C	1.454660	-0.157434	-0.223912
N	0.360607	0.692300	-0.070508
C	0.512177	2.069942	-0.195825
O	-0.472040	2.779145	-0.220134
C	3.900041	-0.605076	-0.282333
C	4.102236	-1.550071	0.720113
C	5.182350	-2.413183	0.673770
C	6.089473	-2.340504	-0.372173
C	5.908406	-1.396334	-1.369218
C	4.823525	-0.538563	-1.325088
C	1.063721	-1.550482	-0.334400
C	-0.065572	-1.965089	0.405990
C	1.686596	-2.445972	-1.199454
C	1.243841	-3.748739	-1.322997
C	0.160297	-4.173620	-0.563102
C	-0.479256	-3.302957	0.290769
C	-0.595553	0.362321	1.293658
C	-0.758645	-1.054773	1.290496
H	3.431526	5.609875	-0.099276
H	5.132381	1.664286	-0.048025
H	1.139520	4.610409	-0.215089
H	3.381156	-1.612762	1.546209
H	5.321399	-3.153487	1.470943
H	6.946041	-3.023765	-0.408298
H	6.619181	-1.331777	-2.201827
H	4.674653	0.199312	-2.124967
H	2.530330	-2.102587	-1.808144
H	1.742011	-4.433595	-2.017375
H	-0.195830	-5.208138	-0.645659
H	-1.343510	-3.636338	0.877612
C	-3.142160	1.328896	-1.641692
C	-3.891753	0.922710	-0.532204
C	-3.852622	-0.514288	-0.491477
C	-2.665224	0.140343	-2.316058
C	-3.182595	-0.989572	-1.666467
C	-1.829281	0.160211	-3.538889

H	-2.427377	0.410769	-4.434358
H	-1.028707	0.915600	-3.470240
H	-1.347385	-0.812556	-3.724092
C	-4.610433	1.791595	0.426554
H	-4.192805	2.810888	0.446600
H	-5.682988	1.883389	0.171385
H	-4.563266	1.399134	1.456589
C	-2.931634	2.709120	-2.124993
H	-1.915143	2.857905	-2.521288
H	-3.635798	2.957942	-2.941595
H	-3.074035	3.453083	-1.326330
C	-4.608648	-1.389540	0.434620
H	-4.000177	-2.242795	0.783963
H	-4.966032	-0.850031	1.324884
H	-5.497647	-1.814195	-0.067860
C	-3.040735	-2.411499	-2.042499
H	-2.257424	-2.564213	-2.802326
H	-2.774978	-3.043915	-1.177473
H	-3.982000	-2.819106	-2.457887
H	5.408764	4.098082	0.006345
N	-1.489302	-1.657264	2.341655
N	-0.428884	1.125819	2.383426
C	-0.683684	-2.371208	3.291703
H	-1.326151	-3.051033	3.880941
H	0.079555	-2.980460	2.782435
H	-0.168484	-1.693730	4.012434
C	-2.464796	-0.864857	3.023804
H	-3.212861	-1.535119	3.488477
H	-2.037093	-0.229747	3.832294
H	-2.979255	-0.201079	2.310784
C	-1.111708	2.364720	2.572710
H	-1.454189	2.435892	3.624175
H	-0.464562	3.241022	2.365528
H	-1.984131	2.410827	1.902085
C	0.778390	0.988081	3.136974
H	1.221815	-0.005646	2.957819
H	1.526190	1.761417	2.850721
H	0.574557	1.097761	4.219938
Rh	-1.773898	0.092373	-0.262233

TS11-Rh-b-i

Atom	X	Y	Z
O	-0.899977	2.284268	0.196020
N	0.357766	0.496059	0.127889
C	0.279226	1.857121	0.193859
C	1.455267	2.629729	0.252969
C	1.389020	4.017784	0.462306
H	0.401516	4.484670	0.561961
C	2.536148	4.753385	0.564446
H	2.489986	5.833839	0.741385
C	3.780957	4.110021	0.459202
C	3.866647	2.762268	0.230447
H	4.852068	2.288226	0.158000
C	2.706619	1.970286	0.093952
C	2.733320	0.578102	-0.180601
C	4.024692	-0.106640	-0.380553
C	4.432998	-1.107254	0.498874
H	3.779895	-1.372368	1.340989
C	5.630819	-1.772317	0.310931
H	5.933197	-2.559210	1.012502
C	6.449001	-1.444430	-0.758970
H	7.397858	-1.972545	-0.909805
C	6.063561	-0.440784	-1.632605
H	6.705642	-0.172954	-2.480526
C	4.862402	0.221970	-1.444759
H	4.551664	1.007428	-2.146625
C	1.542202	-0.133248	-0.191451
C	1.354806	-1.534531	-0.466869
C	2.120974	-2.246332	-1.394418
H	2.907267	-1.723349	-1.949771
C	1.878131	-3.575308	-1.656977
H	2.475098	-4.101293	-2.410072
C	0.851745	-4.236288	-0.978448
H	0.643375	-5.292062	-1.191925
C	0.087702	-3.564224	-0.059852
H	-0.731842	-4.077973	0.457455
C	0.292978	-2.195941	0.215179
C	-0.456723	-1.538057	1.233290
C	-0.660686	-0.141981	1.250373
C	-2.714768	-0.427569	-2.216634
C	-3.080199	0.924717	-2.186677
C	-3.840157	1.126675	-0.973039
C	-4.048168	-0.124059	-0.337764
C	-3.260460	-1.071311	-1.040653
C	-3.199358	-2.525382	-0.768626
H	-3.074358	-2.746060	0.304563
H	-2.360275	-3.004111	-1.296055

H	-4.126023	-3.029084	-1.101794
C	-1.865980	-1.107862	-3.219282
H	-1.101382	-1.748127	-2.741861
H	-1.335688	-0.390383	-3.864159
H	-2.463099	-1.765881	-3.877343
C	-2.755880	1.984304	-3.167728
H	-2.496636	2.933851	-2.669695
H	-3.607904	2.199777	-3.839534
H	-1.900405	1.709308	-3.804527
C	-4.412829	2.422824	-0.548276
H	-5.288494	2.695260	-1.166187
H	-3.681157	3.241524	-0.650431
H	-4.742522	2.398587	0.502375
C	-4.946959	-0.381841	0.810008
H	-4.779392	0.310364	1.654487
H	-4.827322	-1.405620	1.197537
H	-6.008458	-0.273196	0.518659
H	4.701591	4.696786	0.562664
Rh	-1.860093	0.492016	-0.362164
N	-0.670261	0.498810	2.458915
N	-1.078764	-2.336918	2.182463
C	-1.598280	1.505838	2.830296
H	-1.994825	1.298134	3.846700
H	-1.146790	2.520917	2.850806
H	-2.440070	1.516674	2.119542
C	0.480006	0.417440	3.295744
H	1.148182	-0.386176	2.941737
H	1.056749	1.370473	3.301419
H	0.198151	0.195478	4.346419
C	-2.194460	-1.824312	2.904910
H	-2.779286	-1.146794	2.265036
H	-2.838063	-2.670367	3.217098
H	-1.912825	-1.265782	3.825321
C	-0.258417	-3.178383	3.001540
H	0.611388	-3.548731	2.438395
H	0.113529	-2.645104	3.906651
H	-0.842896	-4.051093	3.348121

TS11-Rh-c

Atom	X	Y	Z
O	-0.569926	2.877960	0.202508
N	0.237651	0.796489	-0.081990
C	0.399346	2.148880	0.041837
C	1.759915	2.661906	-0.006326
C	1.955714	4.038456	0.112213
H	1.069520	4.679442	0.183589
C	3.223970	4.564785	0.152600
H	3.375800	5.646166	0.245476
C	4.320425	3.703430	0.090884
C	4.148337	2.345803	-0.032558
H	5.026984	1.692641	-0.062858
C	2.859673	1.784135	-0.105183
C	2.610264	0.379593	-0.224818
C	3.734002	-0.572822	-0.288084
C	3.888761	-1.567586	0.674742
H	3.157953	-1.632981	1.492922
C	4.936041	-2.469408	0.604430
H	5.036389	-3.246619	1.371941
C	5.860576	-2.386910	-0.425238
H	6.691411	-3.100008	-0.479667
C	5.726379	-1.396645	-1.384511
H	6.449221	-1.325139	-2.206234
C	4.673780	-0.500880	-1.316508
H	4.561356	0.271624	-2.089285
C	1.299490	-0.043468	-0.235565
C	0.891236	-1.430970	-0.432725
C	1.460460	-2.195474	-1.444448
H	2.239469	-1.738482	-2.065527
C	1.053451	-3.491277	-1.696282
H	1.508436	-4.067577	-2.508792
C	0.060209	-4.041677	-0.900905
H	-0.272953	-5.073537	-1.067563
C	-0.525601	-3.300445	0.104159
H	-1.318694	-3.766497	0.697851
C	-0.156213	-1.966163	0.355771
C	-0.829684	-1.231189	1.424748
C	-0.885002	0.156071	1.640495
C	-4.031911	0.131573	-0.049174
C	-3.582956	-0.824143	-1.039137
C	-2.858576	-0.130744	-2.012819
C	-2.860586	1.262331	-1.639434
C	-3.662045	1.432486	-0.482247
C	-4.027972	2.719141	0.147095
H	-3.218903	3.460677	0.053650
H	-4.246119	2.605366	1.221121
H	-4.930175	3.158100	-0.319430
C	-4.904073	-0.190023	1.104685

H	-5.969451	-0.224239	0.808558
H	-4.813377	0.559247	1.907146
H	-4.663931	-1.172745	1.542646
C	-3.810418	-2.283156	-0.965338
H	-4.796678	-2.561320	-1.379416
H	-3.789153	-2.642047	0.077448
H	-3.045746	-2.850658	-1.519873
C	-2.140282	-0.696485	-3.178611
H	-1.132766	-0.257893	-3.285457
H	-2.672601	-0.508576	-4.129445
H	-2.005893	-1.787123	-3.089450
C	-2.250062	2.341532	-2.445398
H	-1.316124	2.010926	-2.927944
H	-2.015341	3.227118	-1.838438
H	-2.935453	2.652952	-3.255612
H	5.337078	4.112369	0.145064
Rh	-1.834980	0.130439	0.001789
C	-1.551114	-2.019216	2.499574
H	-2.331825	-2.649904	2.025646
H	-2.125297	-1.318633	3.136778
C	-0.577277	0.997729	2.799771
H	-1.318635	0.708521	3.578125
H	-0.810931	2.049863	2.554393
C	-0.646988	-2.866915	3.363821
H	0.063322	-2.244569	3.932054
H	-1.231351	-3.449129	4.094003
H	-0.053897	-3.578121	2.767430
C	0.831701	0.846873	3.331030
H	1.573153	1.192593	2.590883
H	0.970193	1.447441	4.243602
H	1.067138	-0.202854	3.572733

TS11-Rh-c-i

Atom	X	Y	Z
O	-1.108619	2.331971	0.363670
N	0.158464	0.571658	0.183222
C	0.076808	1.927736	0.285598
C	1.252208	2.708242	0.272762
C	1.194019	4.096125	0.472582
H	0.213182	4.563198	0.623356
C	2.344644	4.834707	0.500310
H	2.306547	5.917215	0.664499
C	3.580282	4.190817	0.338787
C	3.655193	2.839433	0.118777
H	4.635489	2.364587	0.000371
C	2.490739	2.049168	0.045536
C	2.506338	0.650716	-0.231291
C	3.786236	-0.032337	-0.501544
C	4.237510	-1.045167	0.342079
H	3.625938	-1.324364	1.211058
C	5.427423	-1.702174	0.086292
H	5.764997	-2.498288	0.760638
C	6.192474	-1.354194	-1.015603
H	7.135170	-1.875576	-1.219341
C	5.760825	-0.341262	-1.856598
H	6.359486	-0.060173	-2.731684
C	4.568190	0.313662	-1.601305
H	4.220650	1.105909	-2.277774
C	1.318404	-0.055606	-0.193146
C	1.137295	-1.469640	-0.431061
C	1.822404	-2.146970	-1.441261
H	2.458292	-1.574371	-2.126489
C	1.698594	-3.508777	-1.601297
H	2.226092	-4.017940	-2.415565
C	0.895422	-4.227357	-0.717561
H	0.796217	-5.314658	-0.825975
C	0.208322	-3.578630	0.279020
H	-0.440447	-4.162821	0.943168
C	0.266910	-2.180560	0.440445
C	-0.384363	-1.518187	1.537604
C	-0.764812	-0.184037	1.471473
C	-2.937242	-0.253187	-2.103373
C	-3.562469	0.913295	-1.680372
C	-4.093961	0.672575	-0.343758
C	-3.872261	-0.680449	-0.009575
C	-3.052052	-1.225602	-1.035384
C	-2.638131	-2.639866	-1.149258
H	-2.523058	-3.113546	-0.161778
H	-1.678406	-2.752348	-1.679608
H	-3.393645	-3.222865	-1.709532
C	-2.199994	-0.498806	-3.360962
H	-1.219542	-0.969018	-3.165256
H	-2.015724	0.429117	-3.923253
H	-2.751650	-1.187153	-4.027733
C	-3.687195	2.199761	-2.399681
H	-3.385261	3.054930	-1.771048
H	-4.732036	2.389267	-2.708518

H	-3.066938	2.226384	-3.308826
C	-4.876174	1.668079	0.422548
H	-5.919941	1.723703	0.060473
H	-4.451148	2.680857	0.326039
H	-4.911896	1.426658	1.496224
C	-4.299061	-1.390434	1.216399
H	-4.636401	-0.692549	1.998542
H	-3.477498	-1.991985	1.644310
H	-5.134377	-2.086752	1.016164
H	4.505313	4.778136	0.388861
Rh	-1.948459	0.447202	-0.145771
C	-0.621447	-2.320894	2.787974
H	-1.134396	-1.701624	3.543922
H	-1.346844	-3.135482	2.567614
C	-0.880532	0.669185	2.703829
H	-1.217003	1.680587	2.428815
H	-1.715318	0.260630	3.308131
C	0.617147	-2.940770	3.405076
H	1.365412	-2.174640	3.669268
H	0.366907	-3.495945	4.324829
H	1.112155	-3.646156	2.718482
C	0.385631	0.764576	3.528029
H	0.657650	-0.189418	4.003480
H	1.241783	1.071483	2.900568
H	0.280665	1.514495	4.328810

TS11-Ir-a

Atom	X	Y	Z
O	-0.025269	-2.911329	-0.148004
N	-0.657412	-0.765767	-0.449317
C	-0.933497	-2.106110	-0.237013
C	-2.327532	-2.487472	-0.090683
C	-2.621124	-3.826557	0.167855
H	-1.790106	-4.540165	0.200052
C	-3.916927	-4.226749	0.388505
H	-4.147586	-5.278591	0.591388
C	-4.936967	-3.275348	0.369772
C	-4.666000	-1.951904	0.113708
H	-5.482922	-1.222419	0.118600
C	-3.352880	-1.525326	-0.148596
C	-3.002277	-0.168866	-0.443108
C	-4.046378	0.872161	-0.502904
C	-4.009121	1.961767	0.364988
H	-3.189785	2.029406	1.094278
C	-4.974783	2.950601	0.308123
H	-4.924216	3.801046	0.998524
C	-6.004969	2.864868	-0.615248
H	-6.771052	3.647659	-0.661673
C	-6.061561	1.781956	-1.477948
H	-6.870327	1.708193	-2.215064
C	-5.091158	0.796059	-1.422801
H	-5.130732	-0.052036	-2.119467
C	-1.677752	0.142465	-0.628337
C	-1.196588	1.454081	-1.030783
C	-1.786321	2.168063	-2.068842
H	-2.665900	1.743593	-2.567782
C	-1.270550	3.377031	-2.490714
H	-1.741349	3.920267	-3.317148
C	-0.136552	3.879896	-1.864621
H	0.292749	4.835811	-2.189682
C	0.467757	3.182813	-0.841554
H	1.371775	3.588943	-0.371589
C	-0.042337	1.950503	-0.396395
C	0.632974	1.224126	0.671704
C	0.495787	-0.164052	1.013914
C	2.499204	-0.256289	-2.684866
C	2.283142	-1.624493	-2.299418
C	3.095481	-1.926414	-1.171098
C	3.716674	-0.707618	-0.770598
C	3.362174	0.312125	-1.727529
C	3.821250	1.718352	-1.675875
H	3.843483	2.097219	-0.639337
H	3.161527	2.385070	-2.253722
H	4.841632	1.825337	-2.086295
C	1.850933	0.437352	-3.822162
H	0.856481	0.015208	-4.040821
H	2.443577	0.359564	-4.752566
H	1.703269	1.512116	-3.619904
C	1.442754	-2.592312	-3.040937
H	1.978817	-2.976545	-3.927577
H	0.509426	-2.130175	-3.401107
H	1.163397	-3.449939	-2.412686
C	3.279518	-3.252571	-0.544372
H	4.058702	-3.842933	-1.062385
H	2.349525	-3.840963	-0.562061
H	3.590251	-3.161149	0.509154
C	4.754609	-0.573993	0.277550

H	4.517114	-1.163029	1.179125
H	4.894504	0.472007	0.591838
H	5.732189	-0.932761	-0.094713
H	-5.971178	-3.583068	0.567325
C	0.100537	-0.756020	2.268379
C	0.659833	-1.963447	2.691168
C	-0.879680	-0.137570	3.051304
C	0.259301	-2.531101	3.885227
H	1.418284	-2.441182	2.056824
C	-1.286989	-0.715129	4.236053
H	-1.316876	0.809746	2.703429
H	0.705495	-3.473454	4.222969
H	-2.058175	-0.232765	4.847595
C	1.367567	1.994579	1.703149
C	0.857463	3.197818	2.198274
C	2.538607	1.498102	2.277016
C	1.512269	3.888328	3.200530
H	-0.077374	3.595950	1.782954
C	3.190894	2.186073	3.286249
H	2.937920	0.542244	1.918045
H	1.093313	4.832213	3.569809
H	4.112235	1.773646	3.715592
Ir	1.526658	-0.355974	-0.616223
C	-0.713215	-1.908802	4.654356
H	-1.034098	-2.363648	5.599640
C	2.686742	3.390369	3.746552
H	3.205490	3.942484	4.538988

TS11-Ir-a-i

Atom	X	Y	Z
O	0.486695	-1.966478	1.401638
N	-0.590100	-0.391328	0.351375
C	-0.637826	-1.438973	1.246314
C	-1.869535	-1.820075	1.803013
C	-1.931811	-2.819191	2.788546
H	-0.997079	-3.287488	3.119592
C	-3.135165	-3.169828	3.332783
H	-3.191575	-3.939453	4.110382
C	-4.302400	-2.517691	2.901485
C	-4.263730	-1.558583	1.923523
H	-5.192286	-1.069118	1.611203
C	-3.047893	-1.191502	1.310250
C	-2.966980	-0.248456	0.246934
C	-4.202520	0.373872	-0.271058
C	-4.403488	1.747151	-0.153700
H	-3.630116	2.359230	0.328375
C	-5.549105	2.339110	-0.653634
H	-5.688469	3.422536	-0.555253
C	-6.518502	1.567808	-1.276344
H	-7.424680	2.038326	-1.675510
C	-6.335111	0.199241	-1.391628
H	-7.094931	-0.418165	-1.885433
C	-5.186514	-0.392117	-0.892861
H	-5.034768	-1.474887	-0.997655
C	-1.727349	0.115624	-0.252199
C	-1.448985	1.055562	-1.300069
C	-2.290989	1.187613	-2.411105
H	-3.097930	0.459734	-2.551183
C	-2.109242	2.185920	-3.334821
H	-2.756417	2.249061	-4.216088
C	-1.096808	3.128198	-3.124315
H	-0.966769	3.957356	-3.830733
C	-0.246983	3.017050	-2.056249
H	0.547075	3.760703	-1.925950
C	-0.338099	1.944458	-1.135802
C	0.518511	1.818497	-0.012359
C	0.674884	0.579238	0.658902
C	1.977623	-2.907737	-1.730856
C	3.052844	-2.231249	-1.022023
C	3.193577	-0.922191	-1.551834
C	2.087417	-0.712134	-2.429099
C	1.395408	-1.978286	-2.589088
C	0.223069	-2.164057	-3.469891
H	-0.514492	-1.351066	-3.343402
H	-0.294767	-3.116459	-3.280375
H	0.520699	-2.152646	-4.534336
C	1.580624	-4.312664	-1.492673
H	1.520499	-4.539882	-0.414951
H	2.310049	-5.020766	-1.927096
H	0.597620	-4.543803	-1.930815
C	3.959863	-2.898338	-0.061313
H	4.521388	-2.171761	0.545792
H	4.696416	-3.534252	-0.586039
H	3.404511	-3.549433	0.633241
C	4.292321	0.026350	-1.270613
H	4.713849	-0.110076	-0.262123
H	3.968672	1.074432	-1.352829

H	5.121926	-0.111659	-1.989500
C	1.867995	0.466291	-3.296703
H	2.187127	1.403369	-2.815068
H	0.805764	0.588036	-3.564581
H	2.436801	0.369918	-4.240547
H	-5.265887	-2.782571	3.353636
Ir	1.277710	-1.124780	-0.435329
C	1.062764	0.607239	2.097046
C	2.396369	0.491665	2.468528
C	0.101618	0.788688	3.085654
C	2.765975	0.580515	3.798543
H	3.151498	0.337930	1.684113
C	0.465293	0.837425	4.421436
H	-0.953485	0.906592	2.795180
C	1.799685	0.741841	4.779922
H	3.824320	0.508191	4.076723
H	-0.304892	0.964474	5.192102
H	2.090311	0.789538	5.836201
C	1.331020	2.968729	0.447336
C	2.457012	3.361623	-0.277061
C	1.023278	3.690217	1.601381
C	3.248319	4.422260	0.130135
H	2.709881	2.820472	-1.197856
C	1.820901	4.741997	2.020245
H	0.136882	3.414281	2.185483
C	2.937139	5.113564	1.288454
H	4.125710	4.706275	-0.464126
H	1.558888	5.286539	2.935687
H	3.565287	5.947638	1.622552

TS11-Ir-b

Atom	X	Y	Z
C	3.435814	4.565119	0.046741
C	4.548031	3.725944	0.019575
C	4.404298	2.359127	-0.051207
C	3.129780	1.772502	-0.100033
C	2.015939	2.627259	-0.034538
C	2.177517	4.010424	0.027041
C	2.907330	0.357425	-0.194133
C	1.625680	-0.123320	-0.167568
N	0.522289	0.705036	0.091969
C	0.669512	2.096946	0.068925
O	-0.300475	2.808995	0.199070
C	4.062559	-0.558220	-0.273485
C	4.255934	-1.533086	0.701767
C	5.329154	-2.402726	0.634329
C	6.238592	-2.307474	-0.407585
C	6.065947	-1.334878	-1.378370
C	4.988311	-0.468850	-1.312213
C	1.251286	-1.503276	-0.396801
C	0.137725	-1.990859	0.316209
C	1.867273	-2.303665	-1.358028
C	1.429912	-3.588901	-1.603241
C	0.354936	-4.090523	-0.875226
C	-0.277897	-3.310146	0.066414
C	-0.424743	0.278360	1.375668
C	-0.584588	-1.154724	1.252629
H	3.563452	5.651884	0.101602
H	5.296121	1.723731	-0.058438
H	1.278601	4.635003	0.079349
H	3.533282	-1.611276	1.525545
H	5.460909	-3.165572	1.411275
H	7.090041	-2.995861	-0.461752
H	6.778257	-1.253585	-2.208207
H	4.846395	0.290348	-2.093228
H	2.696251	-1.893292	-1.944748
H	1.916879	-4.199009	-2.371166
H	-0.001695	-5.111925	-1.058226
H	-1.145777	-3.706621	0.604375
C	-3.342621	1.475540	-0.893383
C	-3.845467	0.235016	-0.397319
C	-3.386127	-0.818491	-1.276804
C	-2.481146	1.168157	-1.974159
C	-2.551858	-0.243987	-2.248160
C	-1.690450	2.146046	-2.755417
H	-2.243583	2.484758	-3.650182
H	-1.442779	3.033376	-2.153957
H	-0.740564	1.710824	-3.107195
C	-4.905545	0.115408	0.632673
H	-4.669728	0.691516	1.543458
H	-5.867247	0.501036	0.246172
H	-5.081147	-0.927493	0.937388
C	-3.677024	2.821953	-0.383451
H	-2.816387	3.507191	-0.439706
H	-4.502663	3.281857	-0.958989
H	-4.000479	2.787573	0.669701
C	-3.742419	-2.252347	-1.183893

H	-2.893596	-2.903810	-1.454106
H	-4.062411	-2.535834	-0.169502
H	-4.573786	-2.501126	-1.868462
C	-1.807793	-0.959333	-3.310542
H	-1.580355	-1.999972	-3.021033
H	-2.370154	-0.999846	-4.262041
H	-0.843228	-0.471649	-3.528770
H	5.556076	4.157016	0.058742
N	-1.182546	-1.728797	2.409984
N	-0.253015	1.017707	2.496064
C	-0.378228	-2.679348	3.111475
H	-0.447523	-3.719950	2.718677
H	0.683472	-2.381168	3.078781
H	-0.689823	-2.711759	4.173234
C	-2.555875	-2.101189	2.384232
H	-2.757659	-3.086966	1.896117
H	-2.940271	-2.171416	3.420050
H	-3.132321	-1.332261	1.853731
C	-1.345073	1.803122	2.970567
H	-2.058435	1.195235	3.574016
H	-0.969822	2.622215	3.610856
H	-1.882738	2.243024	2.116515
C	0.619733	0.521318	3.511599
H	1.425130	-0.073234	3.046596
H	1.087541	1.364607	4.052691
H	0.095328	-0.115705	4.256591
Ir	-1.635160	0.122501	-0.181950

TS11-Ir-b-i

Atom	X	Y	Z
O	-0.710024	2.165772	0.119999
N	0.610399	0.425192	0.094629
C	0.488332	1.775926	0.141584
C	1.627732	2.593093	0.216034
C	1.513221	3.981500	0.409875
H	0.510278	4.418813	0.486548
C	2.633255	4.755167	0.521679
H	2.547940	5.835625	0.682830
C	3.901946	4.152239	0.449023
C	4.035255	2.805666	0.240374
H	5.036435	2.362888	0.193951
C	2.904342	1.973473	0.090712
C	2.985193	0.581360	-0.171894
C	4.305578	-0.045301	-0.372423
C	4.769533	-1.023460	0.504132
H	4.135715	-1.322967	1.349480
C	6.001607	-1.621628	0.311488
H	6.348386	-2.391204	1.011767
C	6.798229	-1.248235	-0.759802
H	7.774515	-1.723398	-0.913596
C	6.354852	-0.267851	-1.632642
H	6.978232	0.034377	-2.483078
C	5.120331	0.327485	-1.440100
H	4.763924	1.094748	-2.140250
C	1.819019	-0.173204	-0.196043
C	1.661072	-1.571029	-0.492329
C	2.478386	-2.271235	-1.385724
H	3.300272	-1.744672	-1.882304
C	2.240614	-3.589179	-1.700999
H	2.878274	-4.100850	-2.429470
C	1.160207	-4.254870	-1.114086
H	0.950061	-5.298988	-1.377921
C	0.347195	-3.601589	-0.226307
H	-0.506438	-4.122910	0.225424
C	0.551772	-2.242946	0.110521
C	-0.226623	-1.626670	1.124486
C	-0.440526	-0.213915	1.202660
C	-2.854898	-0.686854	-1.905211
C	-3.090823	0.693941	-2.127834
C	-3.726671	1.196071	-0.950434
C	-4.002491	0.102869	-0.059734
C	-3.421648	-1.061322	-0.636868
C	-3.555063	-2.461020	-0.170275
H	-3.981820	-2.520452	0.841925
H	-2.588798	-2.990893	-0.151169
H	-4.224474	-3.032008	-0.839765
C	-2.168472	-1.628768	-2.816034
H	-1.549809	-2.353279	-2.258062
H	-1.508179	-1.108693	-3.527108
H	-2.896849	-2.213306	-3.407952
C	-2.715192	1.479740	-3.325113
H	-2.436541	2.514938	-3.069262
H	-3.545513	1.541134	-4.052733
H	-1.855561	1.035498	-3.852155
C	-4.144224	2.597645	-0.726038
H	-5.179255	2.764198	-1.075664
H	-3.497821	3.308478	-1.263654

H	-4.110636	2.863489	0.342849
C	-4.835499	0.185528	1.159510
H	-4.670233	1.126267	1.709414
H	-4.635795	-0.641994	1.858271
H	-5.913172	0.145485	0.910754
H	4.800539	4.770553	0.562272
N	-0.352553	0.335272	2.462166
N	-0.852328	-2.452412	2.044735
C	-1.113251	1.460173	2.876917
H	-1.418887	1.334324	3.935545
H	-0.550804	2.418261	2.806004
H	-2.018821	1.540466	2.253827
C	0.868540	0.167523	3.178429
H	1.413630	-0.714017	2.797194
H	1.537172	1.055065	3.082309
H	0.676809	0.014883	4.259431
C	-1.939563	-1.952626	2.818446
H	-2.501398	-1.199251	2.247877
H	-2.616054	-2.792476	3.073475
H	-1.616141	-1.481160	3.773108
C	-0.047862	-3.359101	2.809306
H	0.821193	-3.705023	2.231072
H	0.323117	-2.885951	3.747536
H	-0.646249	-4.243063	3.098917
Ir	-1.794625	0.407181	-0.281300

TS11-Ir-c

Atom	X	Y	Z
O	-0.406127	2.816148	0.033457
N	0.475072	0.740898	-0.062664
C	0.588943	2.114436	-0.043487
C	1.927659	2.676493	-0.067794
C	2.062101	4.064022	-0.003376
H	1.149430	4.670737	0.001828
C	3.306088	4.642838	0.070125
H	3.410612	5.732358	0.123145
C	4.436374	3.825242	0.095080
C	4.322676	2.457446	0.024956
H	5.225822	1.839371	0.064463
C	3.061900	1.843162	-0.077575
C	2.872362	0.425945	-0.145688
C	4.045347	-0.469343	-0.157731
C	4.238596	-1.423086	0.838661
H	3.499122	-1.506658	1.646476
C	5.334108	-2.267406	0.810591
H	5.464568	-3.014472	1.603040
C	6.267991	-2.166952	-0.208822
H	7.137510	-2.834488	-0.229285
C	6.096120	-1.214678	-1.199640
H	6.827320	-1.128304	-2.012560
C	4.995146	-0.377130	-1.174982
H	4.853794	0.365425	-1.971954
C	1.586746	-0.062910	-0.170687
C	1.255770	-1.473000	-0.299294
C	1.902185	-2.295614	-1.216769
H	2.691907	-1.865154	-1.842754
C	1.553697	-3.622805	-1.370182
H	2.067314	-4.247891	-2.107684
C	0.537375	-4.142315	-0.579746
H	0.249424	-5.196620	-0.675260
C	-0.124247	-3.343652	0.328407
H	-0.933335	-3.783755	0.921630
C	0.194527	-1.981885	0.483057
C	-0.554114	-1.171855	1.430133
C	-0.617390	0.241611	1.550013
C	-2.690271	-0.457374	-2.061113
C	-2.725897	0.961772	-1.829265
C	-3.510976	1.224883	-0.674193
C	-3.837214	-0.040621	-0.099389
C	-3.367496	-1.072327	-0.995188
C	-3.557426	-2.527191	-0.801777
H	-3.665644	-2.789976	0.263818
H	-2.709885	-3.110438	-1.199489
H	-4.469041	-2.882560	-1.315497
C	-1.992436	-1.146913	-3.171553
H	-1.141577	-0.555264	-3.545865
H	-2.659088	-1.334249	-4.033672
H	-1.587834	-2.124385	-2.854706
C	-2.167933	1.986347	-2.741595
H	-1.227334	1.654118	-3.209062
H	-1.958182	2.929337	-2.215709
H	-2.875982	2.206904	-3.561113
C	-3.928397	2.555656	-0.182796
H	-4.833889	2.913012	-0.708674
H	-3.143030	3.313249	-0.334285
H	-4.166229	2.540035	0.892957
C	-4.702844	-0.265046	1.082162

H	-4.646442	0.575576	1.791851
H	-4.420941	-1.176862	1.633882
H	-5.764004	-0.376912	0.791301
H	5.432853	4.277336	0.176728
Ir	-1.640829	0.040096	-0.070037
C	-1.267916	-1.860958	2.569832
H	-2.022773	-2.561142	2.158705
H	-1.873943	-1.110900	3.117137
C	-0.463823	1.126100	2.722652
H	-0.185902	0.520367	3.609718
H	0.421866	1.766767	2.529898
C	-1.672397	1.992204	2.989067
H	-2.555282	1.378563	3.241955
H	-1.489416	2.678457	3.831009
H	-1.918001	2.587615	2.095741
C	-0.343556	-2.569881	3.531280
H	-0.905271	-3.051222	4.347540
H	0.251575	-3.348623	3.028889
H	0.369036	-1.863513	3.989464

TS11-Ir-c-i

Atom	X	Y	Z
O	-0.912911	2.259920	0.417991
N	0.370646	0.506798	0.267582
C	0.282551	1.878291	0.348926
C	1.438550	2.667304	0.322916
C	1.367439	4.058110	0.523290
H	0.383979	4.514900	0.687979
C	2.508778	4.806972	0.539072
H	2.461702	5.888350	0.707852
C	3.752004	4.175811	0.359456
C	3.839761	2.827585	0.132818
H	4.823837	2.365266	-0.003015
C	2.684235	2.021593	0.071584
C	2.712331	0.630783	-0.219553
C	4.000438	-0.030512	-0.507878
C	4.478430	-1.027764	0.339476
H	3.880749	-1.308723	1.217148
C	5.676019	-1.666858	0.076593
H	6.034508	-2.451102	0.754071
C	6.422374	-1.316194	-1.037513
H	7.371148	-1.823630	-1.248154
C	5.963901	-0.318675	-1.882538
H	6.548049	-0.035485	-2.766759
C	4.763022	0.318933	-1.619680
H	4.394372	1.099505	-2.298544
C	1.540271	-0.106033	-0.164581
C	1.368498	-1.507345	-0.409153
C	2.079517	-2.198169	-1.396051
H	2.743585	-1.636024	-2.062336
C	1.927555	-3.552052	-1.576211
H	2.468336	-4.064470	-2.379368
C	1.059857	-4.260499	-0.739269
H	0.926437	-5.340746	-0.878090
C	0.357406	-3.611476	0.241177
H	-0.339547	-4.184900	0.865055
C	0.456314	-2.213591	0.437300
C	-0.195980	-1.559071	1.515624
C	-0.494276	-0.175301	1.460852
C	-2.880797	0.081684	-2.139029
C	-3.593274	0.984873	-1.342343
C	-3.975904	0.319924	-0.109941
C	-3.509230	-1.020912	-0.180543
C	-2.743596	-1.138600	-1.379513
C	-2.108233	-2.362720	-1.913136
H	-1.952925	-3.129448	-1.141164
H	-1.121905	-2.151262	-2.361123
H	-2.736971	-2.807471	-2.706280
C	-2.281273	0.310895	-3.471232
H	-1.234640	-0.037168	-3.516049
H	-2.283783	1.376487	-3.747767
H	-2.829947	-0.233097	-4.262485
C	-3.931572	2.389937	-1.660511
H	-3.784892	3.049786	-0.789391
H	-4.991534	2.484153	-1.958089
H	-3.318521	2.788731	-2.482621
C	-4.887053	0.878337	0.914187
H	-5.947567	0.740202	0.629095
H	-4.730925	1.959199	1.059288
H	-4.745686	0.392211	1.892980
C	-3.764863	-2.086448	0.813002
H	-3.700539	-1.708025	1.846764
H	-3.042459	-2.912572	0.721215
H	-4.773905	-2.519667	0.683990
H	4.670484	4.774018	0.399570
C	-0.592504	-2.375868	2.710133
H	-1.122580	-1.745180	3.444097

H	-1.352483	-3.128698	2.406341
C	-0.533476	0.636745	2.732735
H	-0.839833	1.670355	2.509645
H	-1.360767	0.239117	3.350228
C	0.535991	-3.109726	3.409170
H	1.303083	-2.416217	3.790943
H	0.156196	-3.690822	4.266526
H	1.049981	-3.813859	2.735748
C	0.762239	0.646093	3.513934
H	1.010963	-0.339438	3.935421
H	1.609648	0.948014	2.872207
H	0.717589	1.359963	4.351914
Ir	-1.799314	0.392526	-0.104224

12-Rh-a

Atom	X	Y	Z
Rh	-1.047138	-0.929724	-0.482786
O	0.465647	3.483985	0.772856
N	0.790805	1.322756	0.183252
C	0.320474	-3.279946	-2.390569
H	0.142012	-3.924727	-3.270830
H	0.622370	-3.941797	-1.564063
H	1.181245	-2.634106	-2.631571
C	-0.893449	-2.498590	-2.064719
C	-1.931661	-2.912237	-1.164579
C	-2.966388	-1.954510	-1.228730
C	-2.558808	-0.930235	-2.133615
C	-1.285123	-1.284730	-2.676683
C	-0.573791	-0.567593	-3.758503
H	-0.917396	-0.898237	-4.757086
H	0.514128	-0.737034	-3.719471
H	-0.739045	0.521357	-3.709776
C	-1.938736	-4.156669	-0.363030
H	-2.501363	-4.037357	0.578236
H	-0.920444	-4.474943	-0.089542
H	-2.404830	-4.994423	-0.914616
C	-4.288241	-2.029044	-0.568019
H	-5.066338	-2.360252	-1.280957
H	-4.617864	-1.054380	-0.169472
H	-4.293888	-2.746138	0.267840
C	-3.415753	0.166900	-2.624075
H	-3.980239	-0.164499	-3.516271
H	-2.833311	1.054146	-2.916345
H	-4.152213	0.490212	-1.873116
C	-0.627226	1.069193	0.167438
C	-1.396220	2.052159	-0.612897
C	-0.786453	2.665487	-1.715983
H	0.255127	2.418923	-1.962347
C	-1.460959	3.578785	-2.501038
H	-0.942439	4.043485	-3.348773
C	-2.775762	3.916935	-2.216580
H	-3.307982	4.653480	-2.828742
C	-3.402839	3.297895	-1.151017
H	-4.447692	3.535115	-0.914267
C	-2.732277	2.374462	-0.366239
H	-3.280030	1.896517	0.450057
C	-1.101099	0.282635	1.279163
C	-2.237389	0.578361	2.166178
C	-2.296738	1.808073	2.821253
H	-1.506489	2.548877	2.636321
C	-3.351263	2.099047	3.668437
H	-3.388699	3.072030	4.172669
C	-4.358955	1.169797	3.876543
H	-5.196905	1.405760	4.543050
C	-4.303467	-0.059067	3.237822
H	-5.096293	-0.800125	3.397702
C	-3.249173	-0.350895	2.389869
H	-3.202330	-1.317601	1.871372
C	-0.231201	-0.827387	1.533090
C	-0.430765	-1.812812	2.541823
H	-1.147096	-1.610199	3.347968
C	0.253206	-2.987513	2.499508
H	0.089680	-3.744098	3.279004
C	1.158443	-3.254079	1.445895
H	1.642414	-4.237192	1.378071
C	1.477905	-2.283037	0.550053
H	2.228717	-2.486366	-0.220842
C	0.870221	-0.990001	0.590459
C	1.613728	0.227437	0.240698
C	2.970528	0.376270	0.139975
C	3.926423	-0.742365	0.282826
C	4.238832	-1.247306	1.541627
H	3.744116	-0.820381	2.423737
C	5.134117	-2.293887	1.680503
H	5.359197	-2.689381	2.678282
C	5.745276	-2.839913	0.563104
H	6.454142	-3.669134	0.672323

C	5.462431	-2.327584	-0.693667
H	5.947490	-2.750423	-1.581580
C	4.561275	-1.284885	-0.831380
H	4.328256	-0.882727	-1.826372
C	3.502898	1.703407	0.008290
C	4.867774	1.962681	-0.197503
H	5.567725	1.127104	-0.307265
C	5.336073	3.254707	-0.255884
C	4.474176	4.339554	-0.095256
H	4.861393	5.363433	-0.142383
C	3.138552	4.109728	0.136698
H	2.431817	4.934552	0.285956
C	2.647265	2.806451	0.183737
C	1.232081	2.605318	0.439320
H	6.405796	3.430949	-0.423187

12-Rh-b

Atom	X	Y	Z
Rh	-1.526343	-0.320154	-0.239502
O	1.203011	3.582424	0.713284
N	0.853076	1.404985	0.224584
C	-1.519105	-3.434219	-1.414870
H	-2.075295	-4.148975	-2.049485
H	-1.491462	-3.857829	-0.397747
H	-0.482651	-3.405773	-1.788918
C	-2.158826	-2.100575	-1.444202
C	-3.299865	-1.725991	-0.675340
C	-3.652465	-0.413849	-1.057997
C	-2.760291	0.001418	-2.099690
C	-1.840888	-1.045233	-2.349818
C	-0.801527	-1.091061	-3.405071
H	-1.149550	-1.626734	-4.308927
H	0.111787	-1.607052	-3.061726
H	-0.497368	-0.081031	-3.723727
C	-3.942957	-2.582537	0.347552
H	-4.668952	-2.022092	0.957756
H	-3.205110	-3.023692	1.043424
H	-4.490508	-3.428642	-0.108104
C	-4.795320	0.408304	-0.596288
H	-5.553279	0.524406	-1.393536
H	-4.476202	1.428215	-0.311837
H	-5.305124	-0.032011	0.274043
C	-2.948997	1.249864	-2.865167
H	-3.904277	1.218555	-3.421416
H	-2.147845	1.419834	-3.599536
H	-2.994089	2.132774	-2.204205
C	-0.586152	1.567540	0.248458
C	-1.228545	0.995409	1.397478
C	-0.643444	-0.269197	1.745716
C	-1.042235	-1.077701	2.849856
H	-1.603258	-0.621182	3.672032
C	-0.713697	-2.396959	2.895046
H	-1.023934	-3.009525	3.752395
C	0.017067	-2.987662	1.839280
H	0.198233	-4.070104	1.839947
C	0.545354	-2.219499	0.848814
H	1.148078	-2.697116	0.070252
C	0.326099	-0.808499	0.785731
C	1.338513	0.120626	0.272817
C	2.657238	-0.119305	0.002591
C	3.271872	-1.463177	0.063562
C	3.748715	-1.971053	1.266989
H	3.642466	-1.370443	2.179494
C	4.328779	-3.227346	1.323378
H	4.686552	-3.619939	2.283023
C	4.457307	-3.986431	0.170923
H	4.915876	-4.981464	0.214975
C	4.010366	-3.479625	-1.038912
H	4.116231	-4.071915	-1.955818
C	3.424900	-2.225299	-1.092330
H	3.062658	-1.823713	-2.048770
C	3.515423	0.998492	-0.267593
C	4.860166	0.854625	-0.645823
H	5.275959	-0.148515	-0.795982
C	5.661190	1.959758	-0.823207
C	5.164114	3.247062	-0.622821
H	5.813628	4.117277	-0.768134
C	3.854811	3.411055	-0.232988
H	3.429553	4.405645	-0.052841
C	3.029870	2.302132	-0.059572
C	1.654454	2.513227	0.353325
H	6.707556	1.822363	-1.122379
N	-1.068303	2.614661	-0.525600
N	-2.260364	1.646204	2.077716
C	-3.390044	0.904921	2.543299
H	-3.557760	0.027628	1.897426
H	-3.297649	0.552165	3.593884

H	-4.292643	1.545004	2.499680
C	-1.789457	2.596662	3.042091
H	-1.469716	2.115054	3.995855
H	-0.928329	3.154519	2.635619
H	-2.591563	3.319793	3.281692
C	-0.357629	2.829474	-1.744683
H	-1.009415	3.380811	-2.444936
H	0.573859	3.425026	-1.632468
H	-0.099258	1.859793	-2.208467
C	-1.646403	3.811158	0.013217
H	-2.413449	3.569564	0.759834
H	-0.902992	4.501349	0.458188
H	-2.150605	4.335529	-0.818641

12-Rh-c

Atom	X	Y	Z
O	-0.753876	-3.525576	-0.228916
N	-0.756649	-1.360473	0.486384
C	1.056031	0.899550	-3.281733
H	1.501416	1.082276	-4.277310
H	0.579245	1.842248	-2.967498
H	0.254457	0.155039	-3.414565
C	2.077744	0.446779	-2.310318
C	2.954404	1.313922	-1.565216
C	3.838609	0.513041	-0.821944
C	3.466595	-0.849400	-1.030411
C	2.412105	-0.886991	-2.006319
C	1.835687	-2.112736	-2.607366
H	2.506683	-2.542377	-3.375175
H	0.870727	-1.912424	-3.099450
H	1.654954	-2.904240	-1.860852
C	2.990214	2.792398	-1.638026
H	3.150921	3.251696	-0.646378
H	2.053600	3.210416	-2.038029
H	3.811056	3.145429	-2.290109
C	4.973539	1.014066	-0.015141
H	5.822652	1.308549	-0.660865
H	5.353916	0.257939	0.689220
H	4.705013	1.907956	0.574652
C	4.208188	-2.037117	-0.549658
H	5.053035	-2.272777	-1.223910
H	3.569622	-2.933553	-0.513624
H	4.633392	-1.891631	0.456997
C	0.602046	-1.341511	1.000584
C	0.988101	-0.248428	1.870780
C	0.531015	1.032611	1.459185
C	0.916683	2.295652	1.991525
H	1.465834	2.342912	2.941487
C	0.615230	3.435220	1.308243
H	0.926286	4.409606	1.709099
C	-0.074137	3.381325	0.073918
H	-0.247280	4.305724	-0.491443
C	-0.580080	2.201143	-0.379692
H	-1.199010	2.173739	-1.286187
C	-0.352144	0.986095	0.324171
C	-1.317973	-0.116964	0.278179
C	-2.656743	0.037640	0.049789
C	-3.295468	1.366804	0.076222
C	-3.200879	2.160443	1.217568
H	-2.632493	1.784811	2.079607
C	-3.792344	3.410143	1.266090
H	-3.701609	4.020528	2.172557
C	-4.502772	3.885718	0.175351
H	-4.974881	4.874579	0.212001
C	-4.618043	3.100324	-0.961622
H	-5.178647	3.468966	-1.829141
C	-4.023286	1.851943	-1.009483
H	-4.106481	1.237506	-1.915948
C	-3.453068	-1.138466	-0.147956
C	-4.848282	-1.121713	-0.290431
H	-5.393262	-0.176701	-0.192622
C	-5.541247	-2.282939	-0.545952
C	-4.874055	-3.499382	-0.673541
H	-5.434888	-4.417868	-0.880013
C	-3.506948	-3.539628	-0.521723
H	-2.951523	-4.481147	-0.597843
C	-2.794672	-2.375499	-0.240760
C	-1.359654	-2.494103	-0.018236
H	-6.632854	-2.246840	-0.647140
C	1.826605	-0.375446	3.114446
H	1.739789	-1.388316	3.539590
H	1.377333	0.289880	3.879558
C	1.224841	-2.666305	1.360364
H	2.242306	-2.427208	1.723421
H	1.370491	-3.296865	0.471488
C	0.490506	-3.454604	2.426748
H	1.112430	-4.292259	2.781374

H	0.240286	-2.835892	3.304682
H	-0.445778	-3.885265	2.047044
C	3.287924	-0.029298	2.958316
H	3.427417	0.971582	2.517876
H	3.806893	-0.047809	3.930700
H	3.796864	-0.746428	2.293215
Rh	1.648311	0.068009	-0.149012

12-Ir-a

Atom	X	Y	Z
O	0.666937	3.573520	0.524675
N	0.927878	1.373096	0.059252
C	0.182586	-3.342552	-2.256149
H	-0.038413	-4.020374	-3.100343
H	0.512600	-3.969198	-1.413051
H	1.037444	-2.714273	-2.555441
C	-1.008028	-2.533407	-1.910738
C	-2.007018	-2.891348	-0.949543
C	-3.023338	-1.907274	-0.994122
C	-2.648860	-0.926725	-1.960735
C	-1.406368	-1.329852	-2.550001
C	-0.737274	-0.676353	-3.697712
H	-1.112858	-1.070991	-4.660492
H	0.352647	-0.835715	-3.683758
H	-0.909678	0.411784	-3.706643
C	-1.999172	-4.098797	-0.092595
H	-2.519649	-3.925875	0.864081
H	-0.975863	-4.423274	0.153180
H	-2.502282	-4.950371	-0.586474
C	-4.294498	-1.918271	-0.237379
H	-5.108754	-2.359983	-0.841400
H	-4.619823	-0.903467	0.044952
H	-4.222638	-2.512835	0.687268
C	-3.509064	0.169013	-2.451691
H	-4.122374	-0.181509	-3.302779
H	-2.923538	1.032620	-2.800502
H	-4.201080	0.535606	-1.678280
C	-0.498931	1.137793	0.102974
C	-1.280905	2.117350	-0.682331
C	-0.734840	2.610795	-1.872371
H	0.275351	2.298214	-2.169436
C	-1.434183	3.485697	-2.680478
H	-0.967819	3.855220	-3.602094
C	-2.710468	3.901665	-2.328331
H	-3.262887	4.605257	-2.961201
C	-3.270273	3.408744	-1.164136
H	-4.280622	3.716277	-0.867121
C	-2.573767	2.525476	-0.355575
H	-3.063748	2.154627	0.547487
C	-0.947839	0.454628	1.305048
C	-1.974310	0.895231	2.264012
C	-1.852716	2.159598	2.837595
H	-1.021915	2.807204	2.525402
C	-2.781133	2.602290	3.761217
H	-2.676492	3.601691	4.200692
C	-3.843652	1.789878	4.127514
H	-4.582422	2.143885	4.856436
C	-3.970865	0.529850	3.565315
H	-4.810654	-0.116437	3.848324
C	-3.041830	0.085633	2.639507
H	-3.138683	-0.908475	2.182248
C	-0.101613	-0.669814	1.578708
C	-0.265030	-1.592478	2.655402
H	-0.918251	-1.318803	3.494244
C	0.377512	-2.788237	2.632068
H	0.243206	-3.497756	3.459687
C	1.212424	-3.139185	1.540748
H	1.663494	-4.139328	1.502394
C	1.512774	-2.229869	0.580277
H	2.218819	-2.494177	-0.214523
C	0.937717	-0.914069	0.572291
C	1.722456	0.263954	0.167840
C	3.082095	0.366135	0.061028
C	4.001669	-0.772290	0.271953
C	4.286389	-1.218650	1.559203
H	3.796721	-0.731189	2.412682
C	5.145606	-2.284797	1.763772
H	5.347873	-2.632701	2.783928
C	5.749057	-2.909484	0.684501
H	6.428638	-3.754349	0.846549
C	5.493413	-2.457613	-0.600897
H	5.971655	-2.943066	-1.460215
C	4.629074	-1.394351	-0.803704
H	4.419171	-1.039447	-1.821544
C	3.650442	1.667935	-0.142744
C	5.022604	1.877722	-0.355578
H	5.699124	1.017975	-0.417198

C	5.527426	3.150792	-0.479925
C	4.695251	4.266104	-0.383443
H	5.111145	5.275072	-0.482877
C	3.352432	4.085784	-0.149908
H	2.667740	4.936390	-0.051607
C	2.824228	2.801257	-0.034829
C	1.405233	2.655513	0.233926
H	6.602516	3.288102	-0.649595
Ir	-1.033309	-0.863853	-0.397598

12-Ir-b

Atom	X	Y	Z
O	1.459330	3.578876	0.652457
N	1.051929	1.408412	0.165946
C	-1.503918	-3.296165	-1.625075
H	-2.099023	-3.965085	-2.273387
H	-1.375371	-3.809787	-0.658398
H	-0.505975	-3.204890	-2.082808
C	-2.168183	-1.981516	-1.482920
C	-3.231468	-1.685416	-0.579912
C	-3.656733	-0.359402	-0.837389
C	-2.872600	0.158883	-1.912125
C	-1.953579	-0.850477	-2.326008
C	-1.043994	-0.799343	-3.494960
H	-1.501081	-1.260984	-4.390568
H	-0.098391	-1.331928	-3.302852
H	-0.778825	0.235688	-3.762903
C	-3.763799	-2.601104	0.454984
H	-4.226733	-2.049648	1.290631
H	-2.971246	-3.235262	0.887676
H	-4.534714	-3.282479	0.050041
C	-4.781091	0.373803	-0.210632
H	-5.643281	0.438033	-0.900290
H	-4.501447	1.410545	0.048250
H	-5.138862	-0.112822	0.709669
C	-3.134513	1.460116	-2.564377
H	-4.137498	1.464021	-3.028662
H	-2.404656	1.680863	-3.356763
H	-3.103644	2.294926	-1.842865
C	-0.397643	1.576453	0.241230
C	-0.985183	1.018062	1.441264
C	-0.416741	-0.272268	1.726288
C	-0.743466	-1.105371	2.841759
H	-1.207196	-0.658830	3.727375
C	-0.452131	-2.430975	2.812491
H	-0.702310	-3.065953	3.673210
C	0.170788	-3.007381	1.676089
H	0.314686	-4.094577	1.629043
C	0.653917	-2.222979	0.680111
H	1.193817	-2.683582	-0.155248
C	0.468806	-0.797993	0.673857
C	1.516657	0.120058	0.203385
C	2.833498	-0.153072	-0.040608
C	3.409832	-1.512693	0.040915
C	3.732499	-2.079919	1.270208
H	3.533109	-1.512076	2.188280
C	4.270576	-3.353705	1.341562
H	4.506189	-3.791567	2.319018
C	4.511974	-4.073612	0.182536
H	4.937300	-5.082689	0.238804
C	4.220208	-3.508816	-1.049474
H	4.415558	-4.069473	-1.971622
C	3.675187	-2.237656	-1.118055
H	3.436358	-1.791248	-2.092579
C	3.717550	0.943950	-0.312398
C	5.065069	0.775967	-0.671309
H	5.469939	-0.234562	-0.797686
C	5.882883	1.866564	-0.857945
C	5.401431	3.164050	-0.684237
H	6.064327	4.022869	-0.836682
C	4.091639	3.351650	-0.308942
H	3.679632	4.354359	-0.144436
C	3.248339	2.257225	-0.127888
C	1.877371	2.498033	0.286728
H	6.930860	1.709814	-1.141966
Ir	-1.432788	-0.248554	-0.217531
N	-0.905523	2.668771	-0.464657
N	-1.916890	1.699167	2.230222
C	-1.379953	3.877466	0.141860
H	-1.962072	4.419717	-0.626515
H	-2.066656	3.653369	0.967687
H	-0.576790	4.548898	0.501832
C	-0.280267	2.888193	-1.726565
H	0.671342	3.462068	-1.670346
H	-0.069671	1.921888	-2.220085
H	-0.966539	3.462677	-2.375010
C	-3.025120	0.983210	2.782953

H	-2.844263	0.589305	3.807203
H	-3.902493	1.655440	2.848839
H	-3.288428	0.134939	2.130535
C	-1.304681	2.578262	3.182078
H	-0.886710	2.034519	4.061885
H	-0.483565	3.141803	2.706793
H	-2.051202	3.302388	3.557684

12-Ir-c

Atom	X	Y	Z
O	-1.004430	-3.549291	-0.248020
N	-0.965328	-1.386268	0.470543
C	1.037932	0.907157	-3.285519
H	1.506704	1.077135	-4.272025
H	0.555629	1.852482	-2.989373
H	0.238546	0.161889	-3.425236
C	2.034379	0.462213	-2.284641
C	2.881136	1.326496	-1.510832
C	3.740175	0.522219	-0.735136
C	3.392630	-0.843886	-0.967242
C	2.365668	-0.877870	-1.973722
C	1.822972	-2.097948	-2.614546
H	2.485350	-2.455758	-3.424883
H	0.831063	-1.920560	-3.059450
H	1.709994	-2.928232	-1.898674
C	2.911911	2.805837	-1.576611
H	3.065913	3.264345	-0.584071
H	1.975558	3.220326	-1.980812
H	3.734003	3.162391	-2.224775
C	4.827147	1.028333	0.131596
H	5.702613	1.336054	-0.470495
H	5.179431	0.269775	0.846984
H	4.517591	1.913510	0.713564
C	4.129921	-2.028864	-0.472518
H	4.982264	-2.270187	-1.134612
H	3.488615	-2.923308	-0.435623
H	4.540115	-1.875849	0.539039
C	0.414170	-1.374580	0.956453
C	0.790036	-0.305719	1.885049
C	0.346049	0.982202	1.482222
C	0.685017	2.243367	2.058179
H	1.168185	2.280832	3.043999
C	0.406875	3.386311	1.375702
H	0.677044	4.359312	1.808232
C	-0.217827	3.343322	0.102850
H	-0.370185	4.275427	-0.455801
C	-0.696545	2.171134	-0.389249
H	-1.277485	2.154439	-1.321345
C	-0.490128	0.936186	0.301856
C	-1.497359	-0.134905	0.259731
C	-2.830246	0.054095	0.026966
C	-3.433196	1.399670	0.057277
C	-3.317533	2.180934	1.205186
H	-2.763963	1.779978	2.065443
C	-3.867870	3.448649	1.262632
H	-3.758122	4.048802	2.173745
C	-4.559428	3.955900	0.174151
H	-4.999090	4.959378	0.217072
C	-4.698312	3.182709	-0.968750
H	-5.244492	3.576056	-1.834573
C	-4.143348	1.916320	-1.025870
H	-4.243686	1.312890	-1.937957
C	-3.651892	-1.104059	-0.172007
C	-5.045102	-1.055234	-0.327301
H	-5.567875	-0.096476	-0.239984
C	-5.763236	-2.200852	-0.583262
C	-5.124244	-3.433735	-0.698032
H	-5.705038	-4.339896	-0.904034
C	-3.759634	-3.505050	-0.535726
H	-3.225588	-4.459563	-0.604194
C	-3.021970	-2.357041	-0.254662
C	-1.589206	-2.506564	-0.030988
H	-6.852845	-2.139331	-0.694667
C	1.586615	-0.460764	3.152614
H	1.514686	-1.491351	3.534345
H	1.094529	0.162322	3.927034
C	1.014871	-2.712320	1.316749
H	2.034377	-2.482151	1.680099
H	1.154526	-3.344274	0.426967
C	0.268640	-3.491681	2.382008
H	0.913762	-4.274253	2.812939
H	-0.065187	-2.848331	3.213155
H	-0.619653	-3.991437	1.974331
C	3.042561	-0.073406	3.056998
H	3.171890	0.936137	2.633144
H	3.525927	-0.091180	4.047568
H	3.593854	-0.769310	2.402633

Ir	1.508753	0.033308	-0.132038

product-a

Atom	X	Y	Z
O	0.493340	2.632113	-1.639377
N	-0.047216	0.686291	-0.609119
C	1.288118	0.352907	-0.390976
C	2.191325	1.451411	0.003668
C	1.835188	2.256923	1.081466
H	0.860069	2.111284	1.566856
C	2.705716	3.222684	1.550998
H	2.417002	3.843181	2.407882
C	3.939356	3.400028	0.946399
H	4.630853	4.164702	1.319394
C	4.293031	2.609424	-0.135166
H	5.262821	2.752109	-0.626455
C	3.425496	1.641244	-0.604902
H	3.702692	1.022432	-1.466677
C	1.669708	-0.945365	-0.331694
C	3.049227	-1.304832	0.067843
C	3.960448	-1.806423	-0.855939
H	3.649421	-1.937595	-1.900869
C	5.256077	-2.111604	-0.473773
H	5.965572	-2.497011	-1.215913
C	5.656655	-1.920521	0.838836
H	6.684208	-2.156060	1.140428
C	4.753827	-1.430891	1.767763
H	5.063902	-1.277881	2.808267
C	3.457962	-1.130351	1.386598
H	2.745319	-0.730059	2.119415
C	0.701828	-1.977863	-0.606448
C	1.071402	-3.312999	-0.798064
H	2.124885	-3.596908	-0.705338
C	0.133192	-4.269688	-1.114165
H	0.444518	-5.309550	-1.266945
C	-1.198704	-3.906183	-1.268021
H	-1.945201	-4.648318	-1.572513
C	-1.588708	-2.605717	-1.037415
H	-2.637115	-2.335736	-1.181035
C	-0.662170	-1.628967	-0.658059
C	-1.055051	-0.252134	-0.396687
C	-2.312253	0.182202	-0.052270
C	-3.350677	-0.746326	0.432396
C	-4.597894	-0.844658	-0.182018
H	-4.809630	-0.230674	-1.067483
C	-5.554101	-1.722453	0.298576
H	-6.526982	-1.793565	-0.202677
C	-5.282866	-2.513293	1.403909
H	-6.041147	-3.208901	1.782509
C	-4.050816	-2.415058	2.030557
H	-3.831292	-3.029455	2.912069
C	-3.097137	-1.535865	1.552263
H	-2.120717	-1.456953	2.047752
C	-2.598520	1.585743	-0.109069
C	-3.799516	2.150601	0.350465
H	-4.542799	1.516694	0.845274
C	-4.051134	3.493127	0.191275
C	-3.125546	4.330930	-0.432299
H	-3.341880	5.397843	-0.554942
C	-1.933209	3.807027	-0.869860
H	-1.165663	4.435157	-1.336806
C	-1.656873	2.451422	-0.695919
C	-0.341633	1.978012	-1.063075
H	-4.995530	3.909342	0.563466

product-b

Atom	X	Y	Z
O	1.014864	2.870841	-1.296406
N	0.634977	0.892201	-0.252220
C	1.974285	0.760513	0.114609
C	2.571692	-0.461221	0.041934
C	1.787622	-1.580551	-0.400285
C	2.383144	-2.816191	-0.686401
H	3.469809	-2.912913	-0.610469
C	1.633886	-3.900319	-1.076859
H	2.127062	-4.853284	-1.302201
C	0.257613	-3.771529	-1.218519
H	-0.345002	-4.613067	-1.577748
C	-0.356240	-2.575258	-0.922417
H	-1.433744	-2.493270	-1.076997
C	0.376227	-1.470162	-0.471547
C	-0.244209	-0.188551	-0.176972
C	-1.575709	0.075704	0.045733
C	-2.576407	-0.979304	0.289870
C	-3.670636	-1.120330	-0.563501
H	-3.764097	-0.448371	-1.426688

C	-4.618449	-2.103059	-0.345471
H	-5.467527	-2.203098	-1.032046
C	-4.492452	-2.962426	0.734806
H	-5.242644	-3.742832	0.909789
C	-3.415668	-2.825084	1.597309
H	-3.314562	-3.494852	2.459672
C	-2.468343	-1.840056	1.379984
H	-1.613567	-1.734688	2.060470
C	-2.026087	1.437284	-0.003147
C	-3.327303	1.832834	0.353376
H	-4.020889	1.095879	0.772797
C	-3.739438	3.133697	0.184363
C	-2.884492	4.098408	-0.350762
H	-3.229579	5.129598	-0.483279
C	-1.600626	3.743428	-0.688420
H	-0.887976	4.474673	-1.088241
C	-1.162682	2.433802	-0.498413
C	0.223539	2.128138	-0.763974
H	-4.758960	3.414366	0.476363
N	2.566833	1.864332	0.642337
N	3.881669	-0.574379	0.540642
C	4.025585	-1.367546	1.718701
H	3.235037	-1.107421	2.442500
H	3.987164	-2.468875	1.546848
H	5.002402	-1.145625	2.188436
C	4.944842	-0.760589	-0.397139
H	5.172987	-1.825396	-0.634433
H	4.707933	-0.253268	-1.346799
H	5.879029	-0.318185	0.002506
C	1.832320	2.761265	1.468095
H	2.470717	3.067995	2.319009
H	1.516794	3.682587	0.934748
H	0.938527	2.267025	1.883071
C	3.755026	2.408628	0.080964
H	4.124513	1.769158	-0.731564
H	3.548884	3.412544	-0.347408
H	4.552179	2.510364	0.842099

product-c

Atom	X	Y	Z
O	-1.061338	3.099776	-1.190153
N	-0.861133	1.035079	-0.261993
C	-2.182290	0.986043	0.208576
C	-2.804876	-0.210460	0.333010
C	-2.159782	-1.389146	-0.191734
C	-2.862689	-2.569280	-0.457989
H	-3.939048	-2.618268	-0.260960
C	-2.232224	-3.666390	-1.000460
H	-2.805699	-4.576511	-1.212195
C	-0.878979	-3.604566	-1.306869
H	-0.377761	-4.458169	-1.777057
C	-0.163929	-2.459274	-1.037691
H	0.890802	-2.415740	-1.319974
C	-0.777915	-1.346664	-0.454159
C	-0.060547	-0.105466	-0.210637
C	1.297057	0.019184	-0.046345
C	2.142744	-1.147237	0.268152
C	1.843395	-1.924574	1.384957
H	0.979282	-1.652039	2.004738
C	2.611358	-3.026938	1.708832
H	2.357985	-3.627172	2.591055
C	3.703190	-3.367517	0.926875
H	4.314505	-4.241280	1.182298
C	4.022415	-2.593943	-0.177384
H	4.885581	-2.856239	-0.801249
C	3.250434	-1.492591	-0.503825
H	3.495821	-0.892978	-1.390595
C	1.884422	1.322822	-0.116432
C	3.231749	1.586834	0.177619
H	3.873838	0.780521	0.547755
C	3.752915	2.848137	0.010569
C	2.960530	3.897337	-0.457691
H	3.389860	4.896922	-0.589707
C	1.633814	3.667622	-0.732231
H	0.971458	4.470704	-1.075501
C	1.087562	2.398177	-0.549405
C	-0.340319	2.241312	-0.736065
H	4.807426	3.029770	0.252197
C	-4.165913	-0.346163	0.948865
H	-4.248873	0.297570	1.842343
H	-4.275260	-1.372537	1.342837
C	-2.762888	2.259346	0.738919
H	-3.758267	2.026047	1.143955
H	-2.933362	2.986647	-0.068106
C	-1.928039	2.883919	1.838112
H	-2.441089	3.766130	2.252350
H	-1.761732	2.173383	2.665549

H	-0.939163	3.223470	1.489305
C	-5.297727	-0.043726	-0.009089
H	-5.257834	-0.692661	-0.900614
H	-6.280805	-0.189666	0.468490
H	-5.249837	0.997545	-0.370629