Supplementary Material (ESI) for Dalton Transactions
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Supporting Information for:

# Alkene-Alkyl Interconversion: An Experimental and Computational Study of the Olefin Insertion and β-Hydride Elimination Processes

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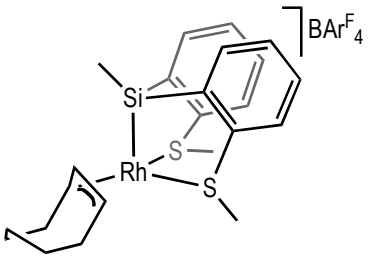
## 1. Characterisation of new compounds

**{Rh(η³-cyclooctenyl)[SiMe(*o*-$C_6H_4SMe)_2$]}[$BAr^F_4$] (1)**



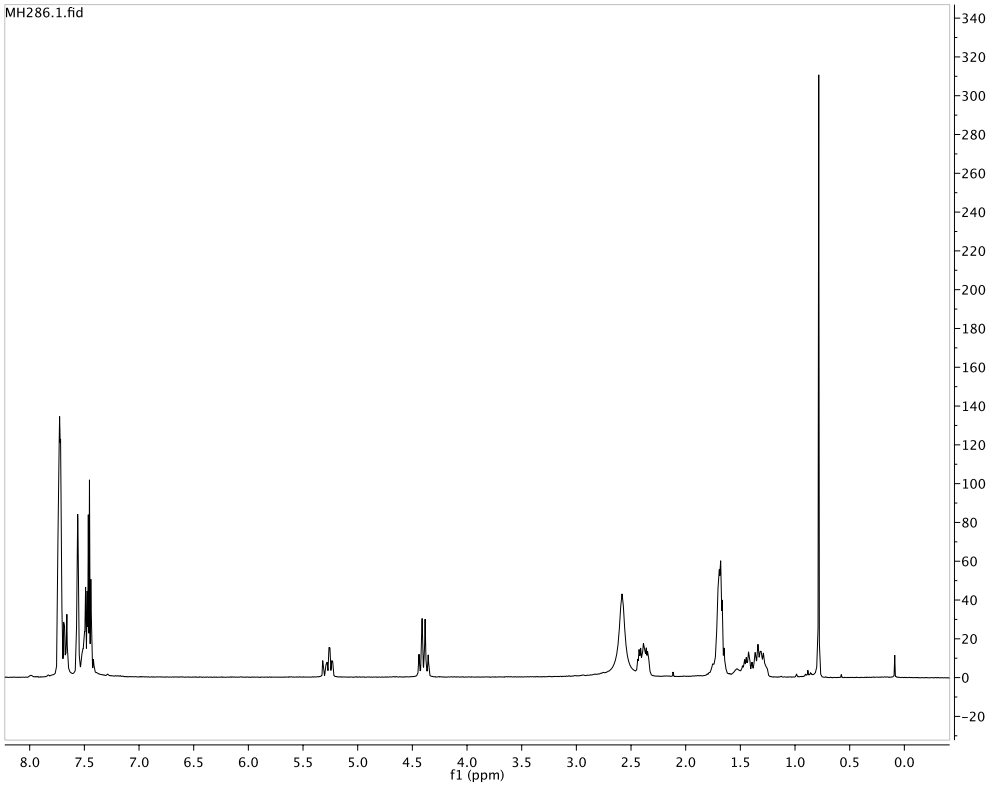




**Figure S.1.** $^1H$ NMR ($CD_2Cl_2$) spectrum of **1**

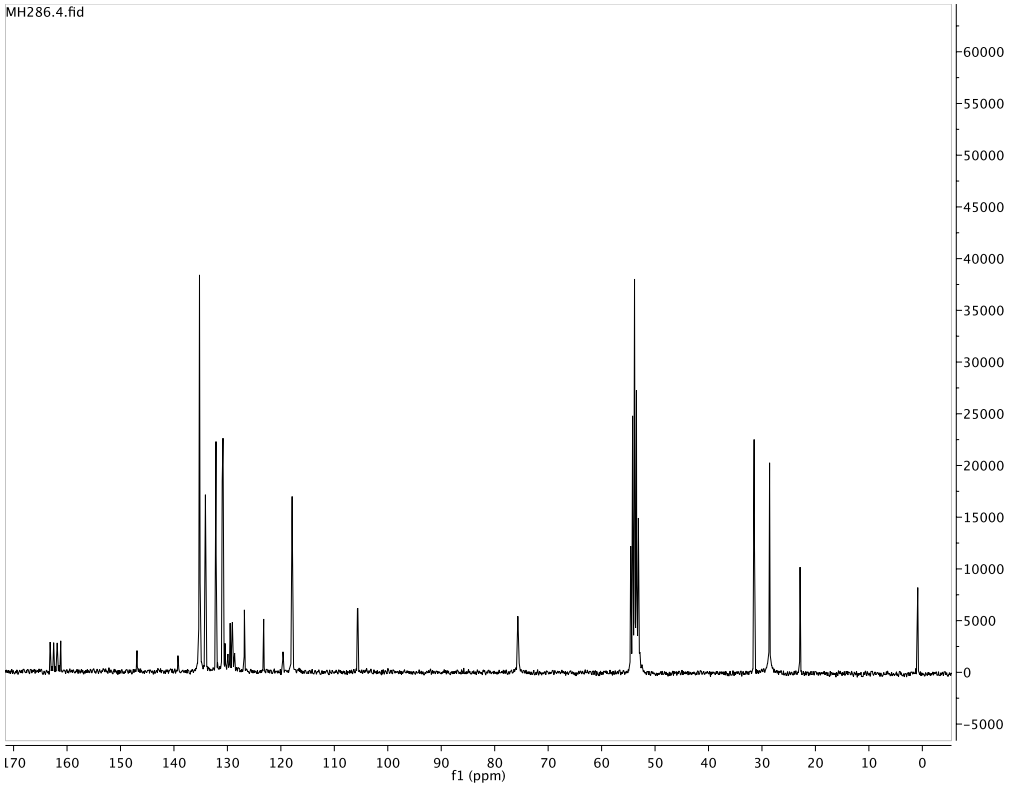



**Figure S.2.** $^{13}C$ NMR ($CD_2Cl_2$) spectrum of **1**

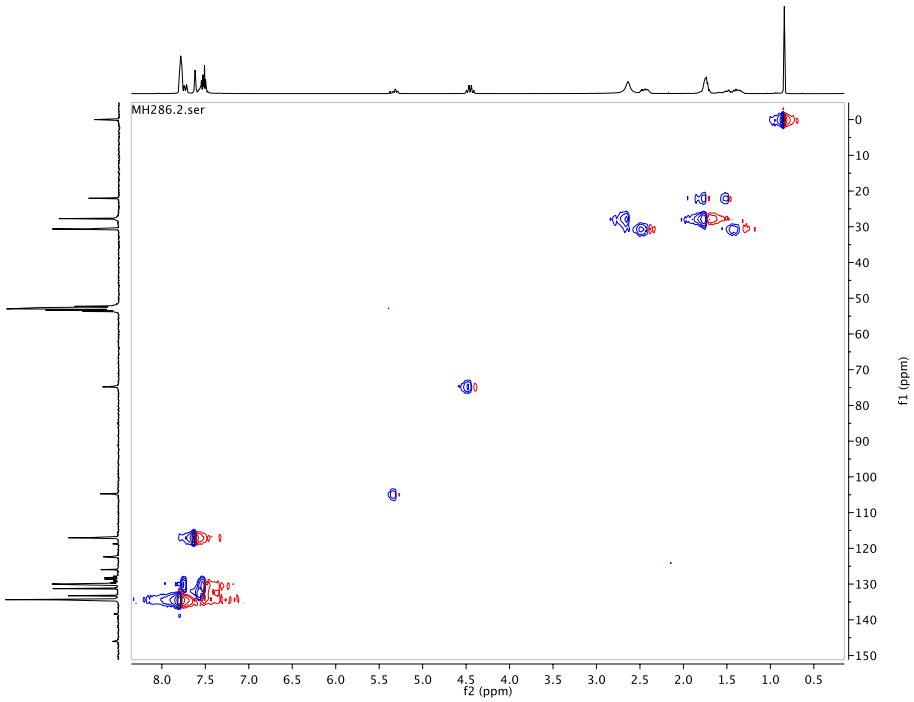



**Figure S.3.** $^{1}H$-$^{13}C$ HSQC ($CD_2Cl_2$) spectrum of **1**

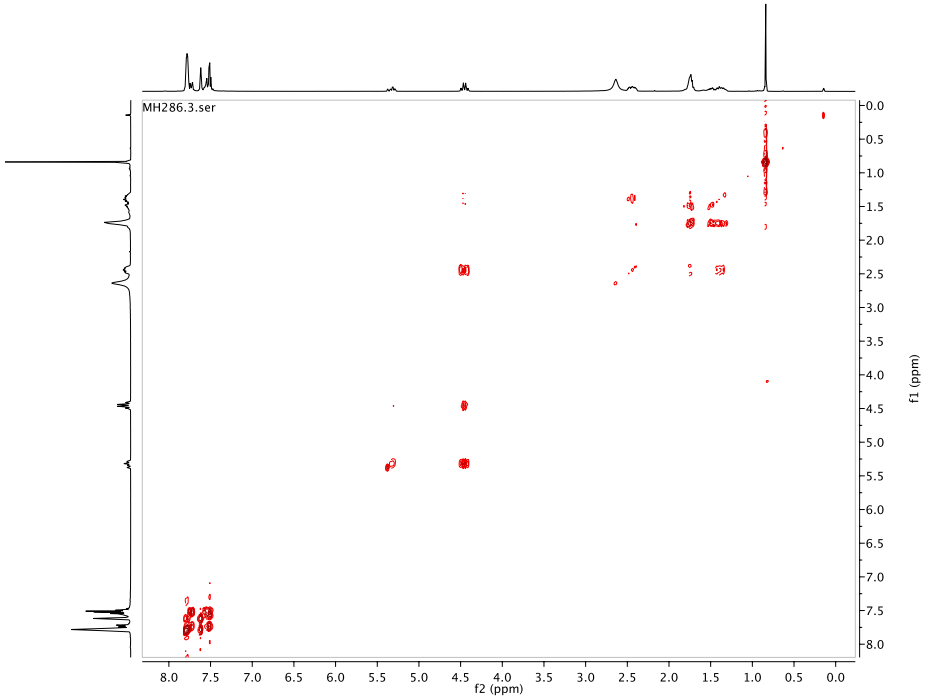



**Figure S.4.** COSY ($CD_2Cl_2$) spectrum of **1**

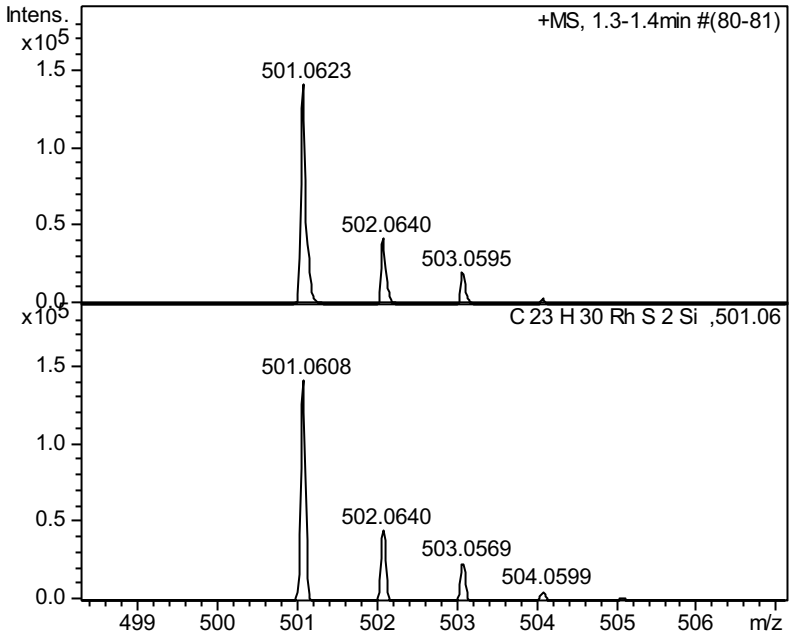
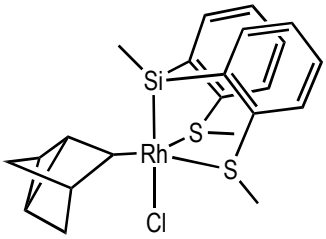



**Figure S.5.** ESI-MS for **1**. Found (top) and calculated (bottom)

**{Rh(ntyl)[SiMe(*o*-$C_6H_4SMe)_2$]Cl} (2)**



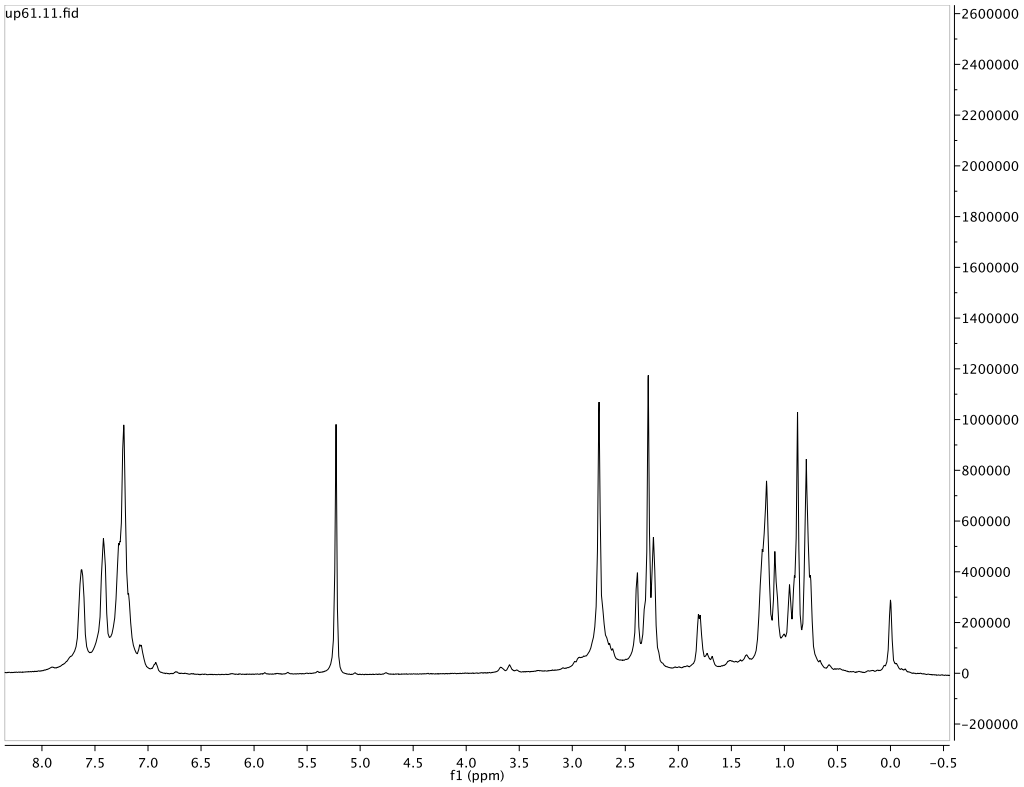




**Figure S.6.** $^1H$ NMR ($CD_2Cl_2$) spectrum of **2**

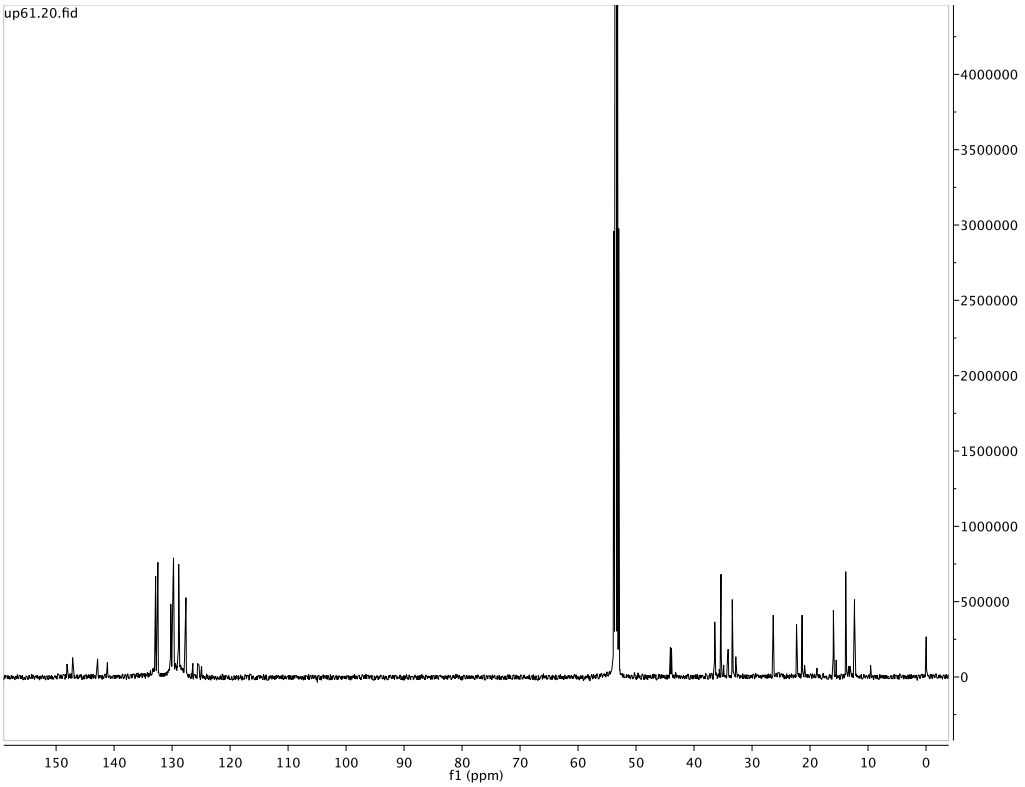



**Figure S.7.** $^{13}C$ NMR ($CD_2Cl_2$) spectrum of **2**

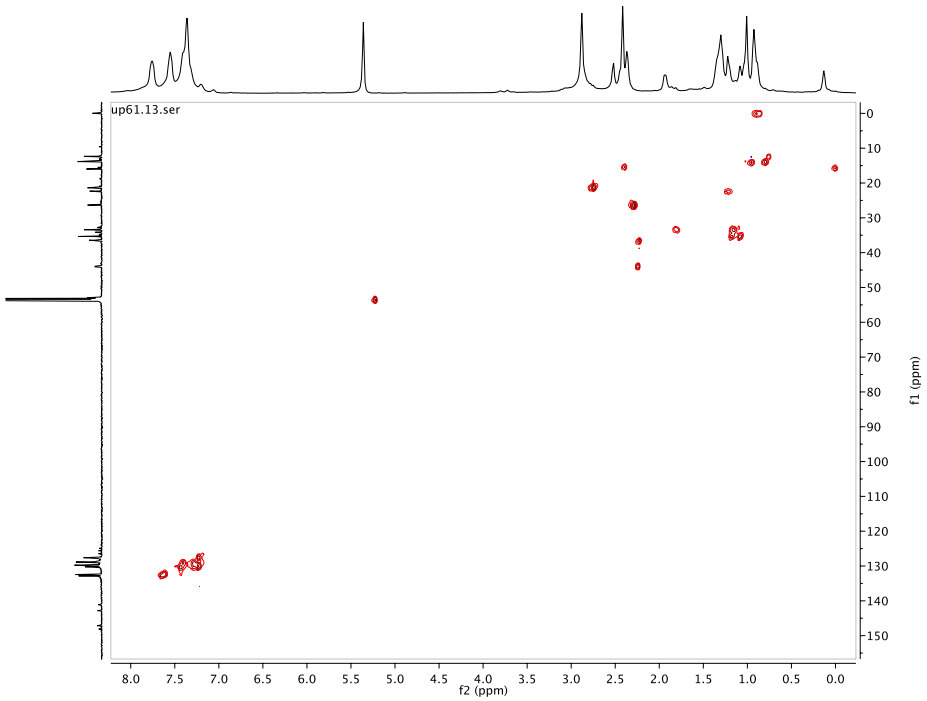



**Figure S.8.** $^{1}H$-$^{13}C$ HSQC ($CD_2Cl_2$) spectrum of **2**

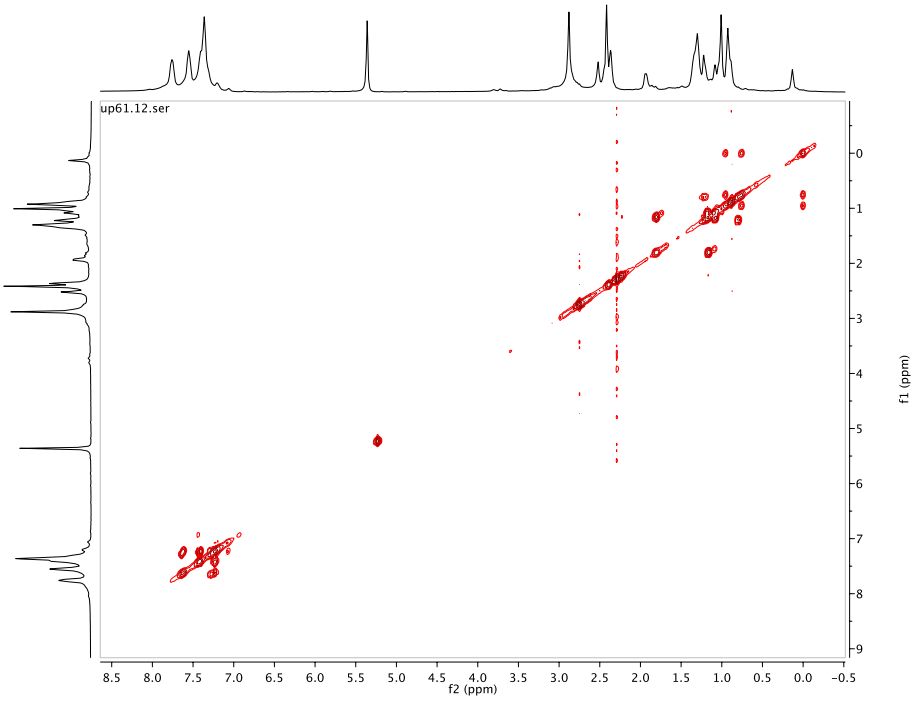



**Figure S.9.** COSY ($CD_2Cl_2$) spectrum of **2**

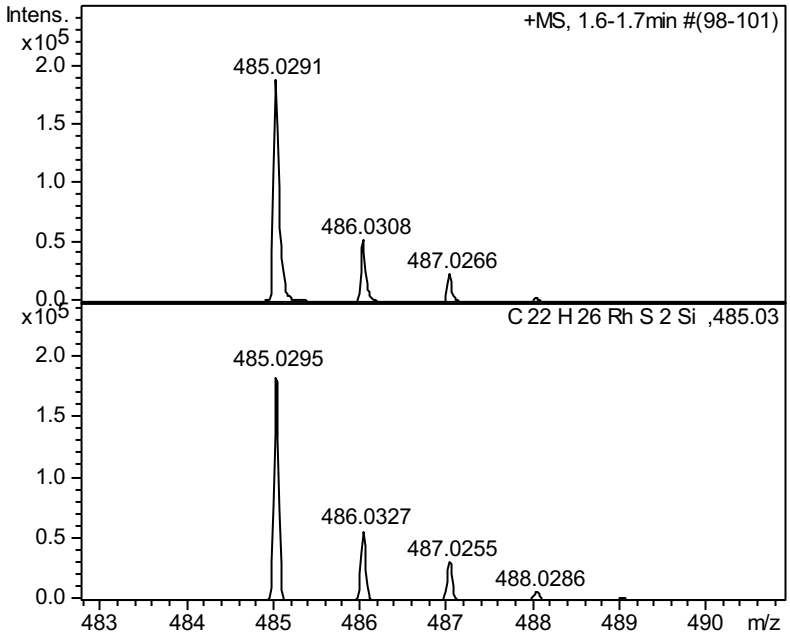
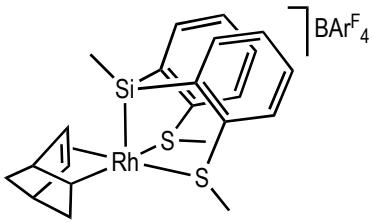



**Figure S.10.** ESI-MS for **2**. Found (top) and calculated (bottom)

**{Rh[SiMe(*o*-$C_6H_4SMe)_2$](nbyl)}[$BAr^F_4$] (3)**.



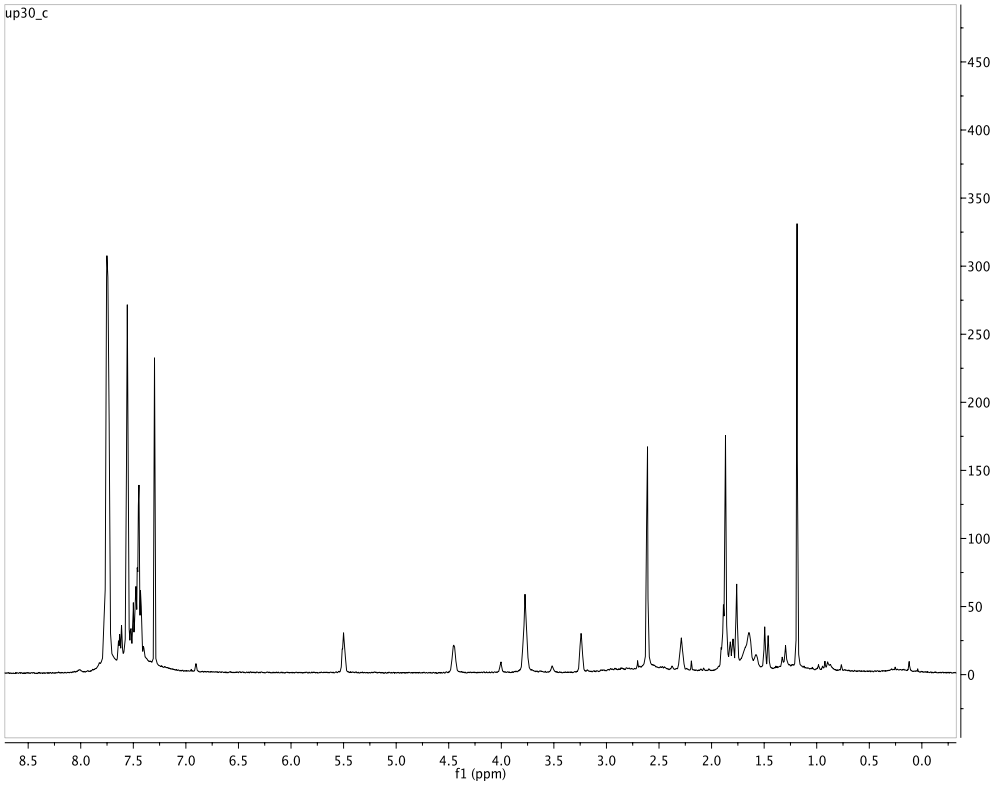




**Figure S.11.** $^1H$ NMR ($CDCl_3$) spectrum of **3**

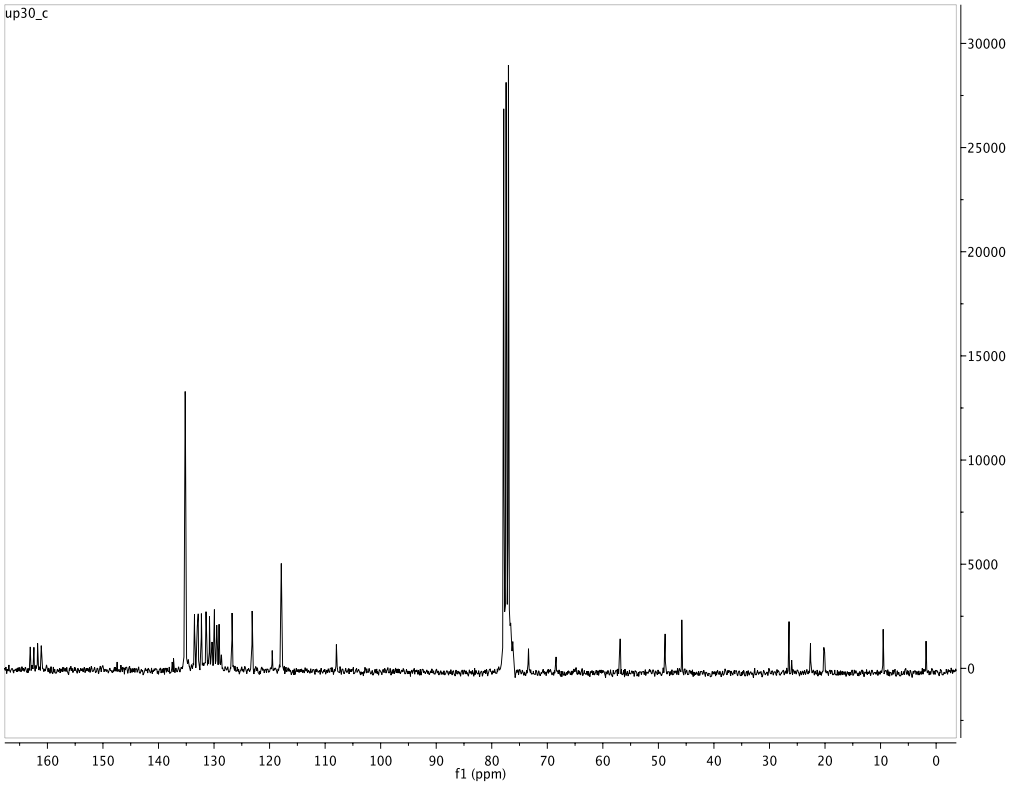



**Figure S.12.** $^{13}C$ NMR ($CDCl_3$) spectrum of **3**

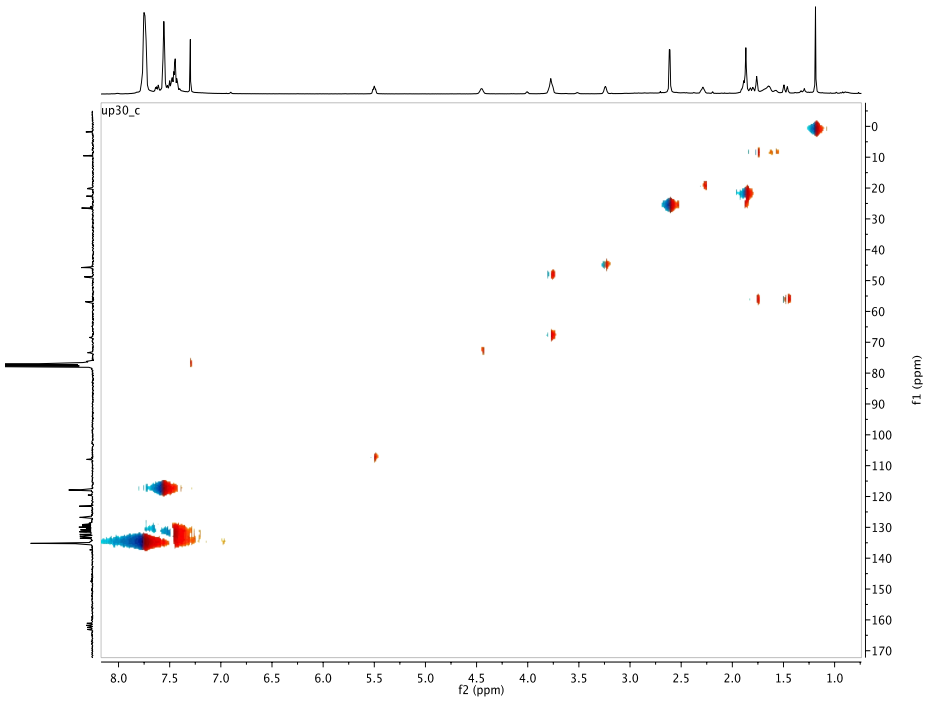



**Figure S.13.** $^{1}H$-$^{13}C$ HSQC ($CDCl_3$) spectrum of **3**

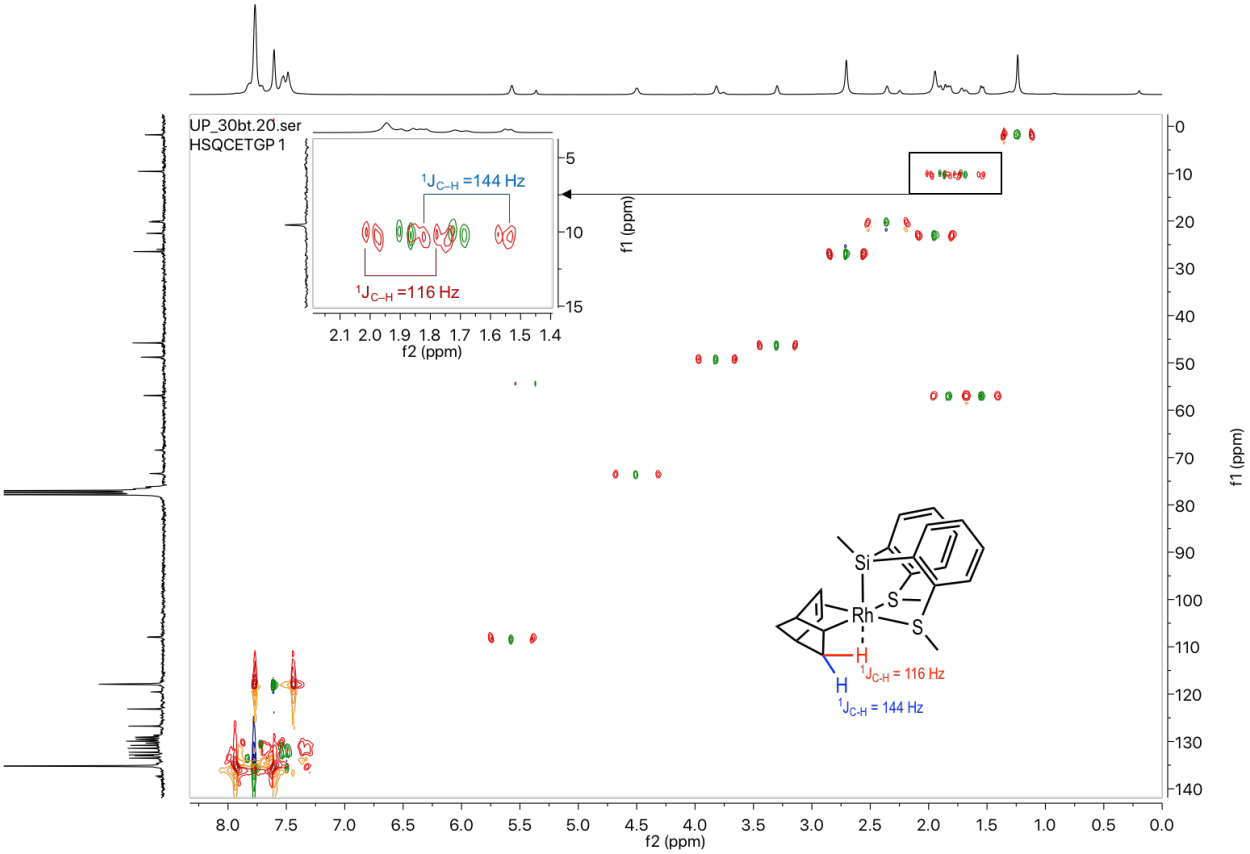



**Figure S.14.** Overlapped $^1$H-$^{13}$C HSQC (green) and $^1$H-$^{13}$C HSQC_coupled (red) ($CD_2Cl_2$) spectra of **3**

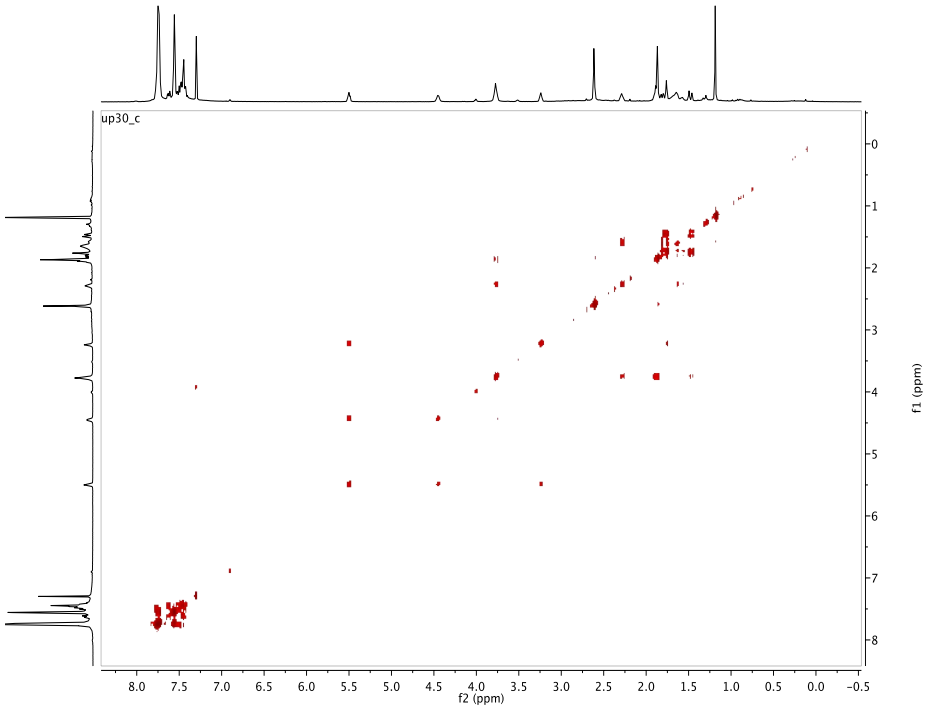



**Figure S.15.** COSY ($CDCl_3$) spectrum of **3**

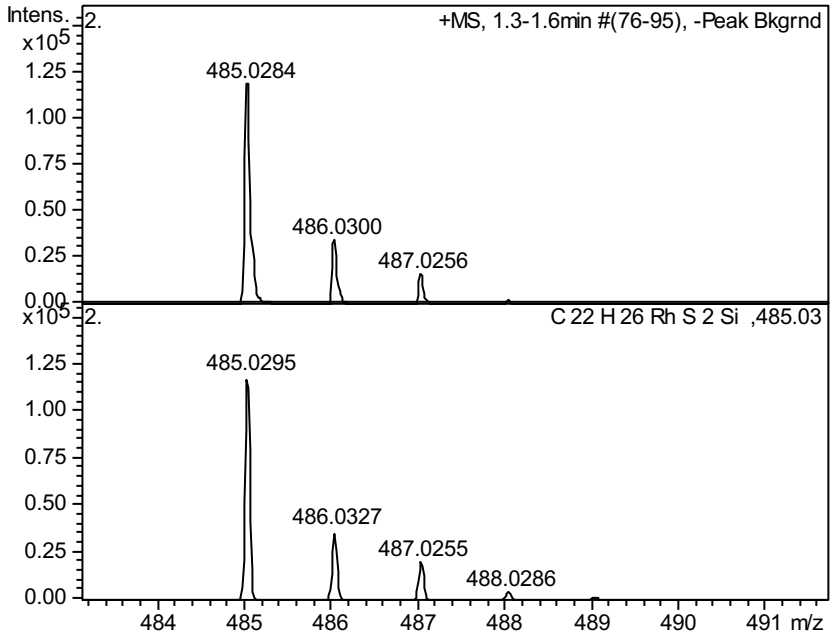
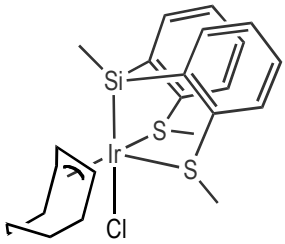



**Figure S.16.** ESI-MS for **3**. Found (top) and calculated (bottom)

**{Ir(η³-cyclooctenyl)[SiMe(*o*-$C_6H_4SMe)_2$]Cl} (4)**.



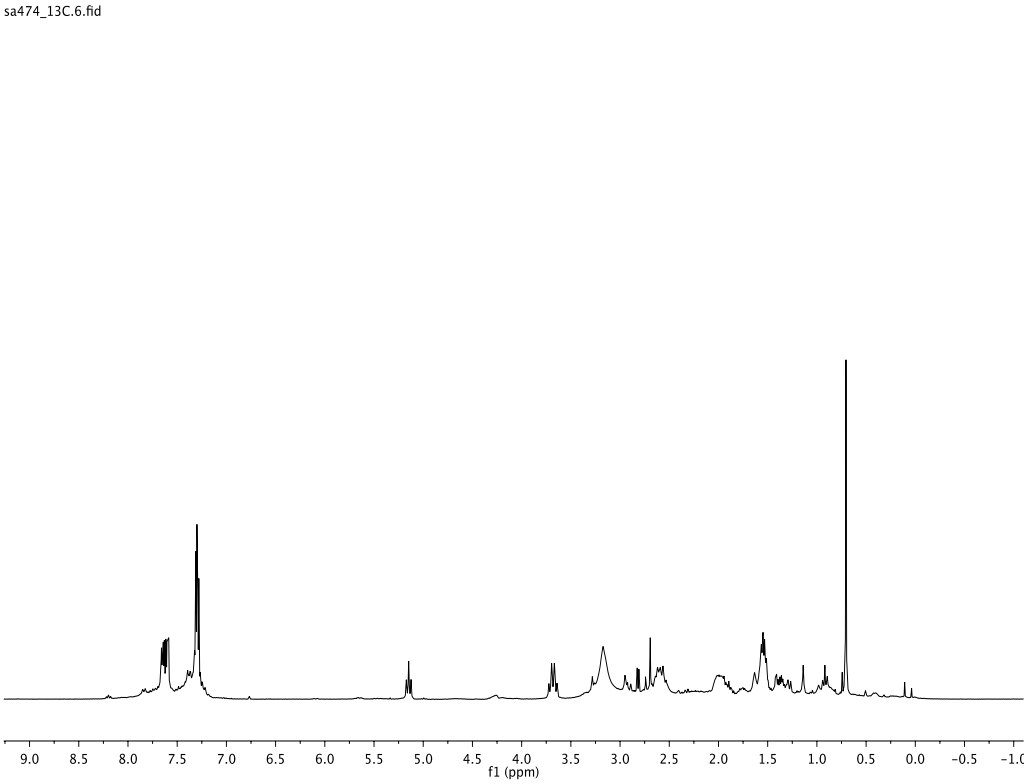




**Figure S.17.** $^1$H NMR ($CDCl_3$) spectrum of **4**

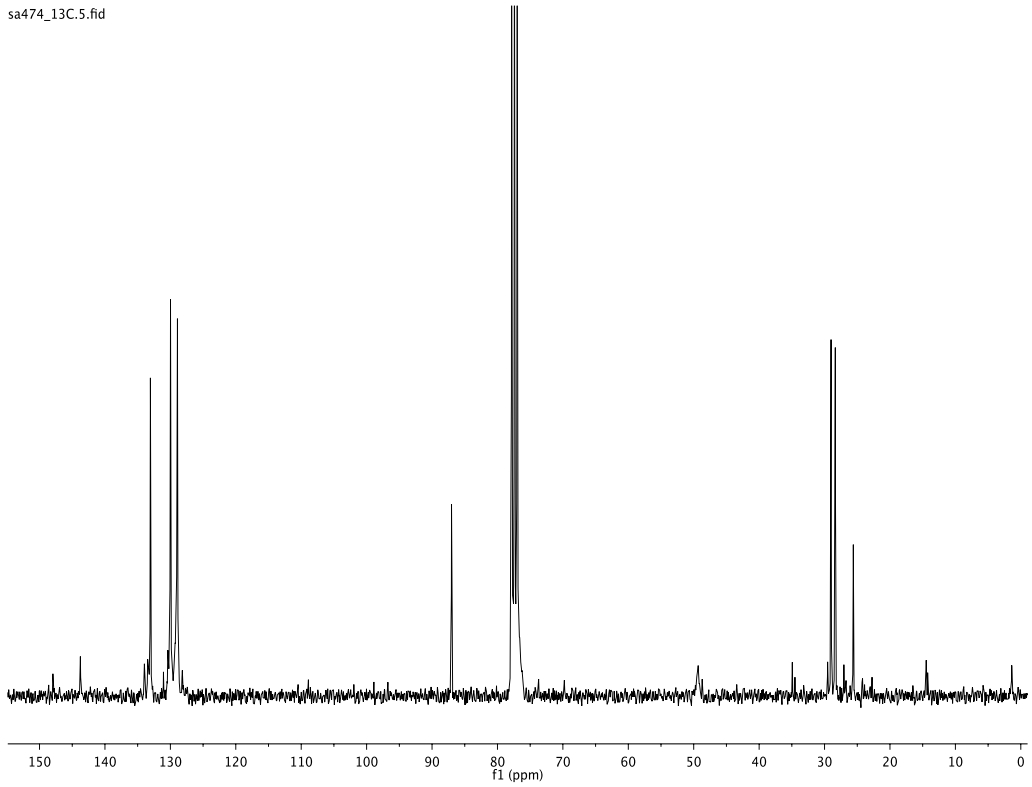



**Figure S.18.** $^{13}C$ NMR ($CDCl_3$) spectrum of **4**

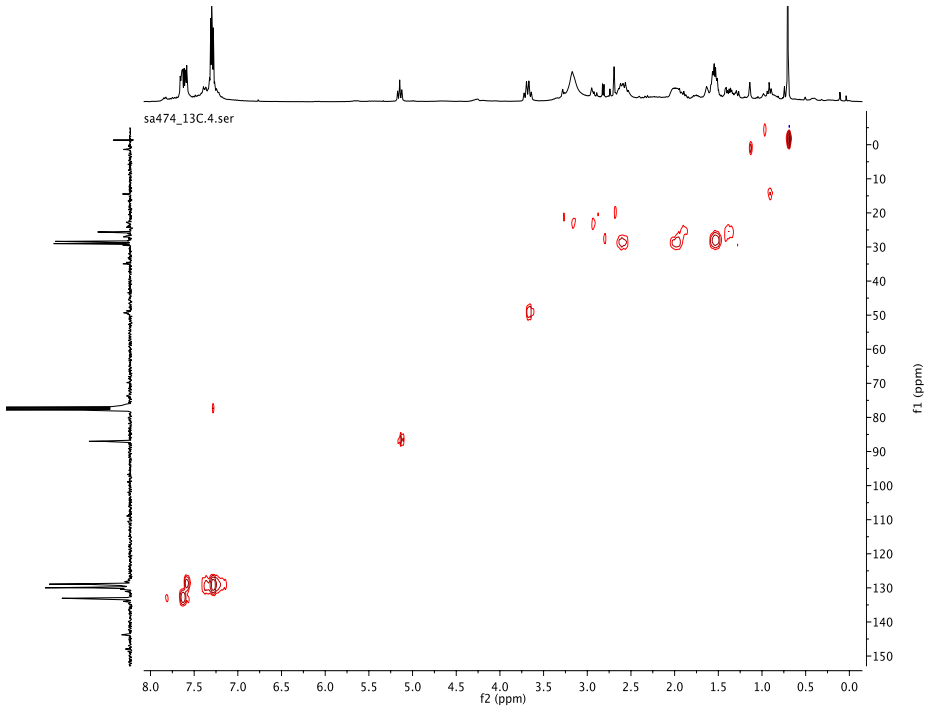



**Figure S.19.** $^{1}H$-$^{13}C$ HSQC ($CDCl_3$) spectrum of **4**

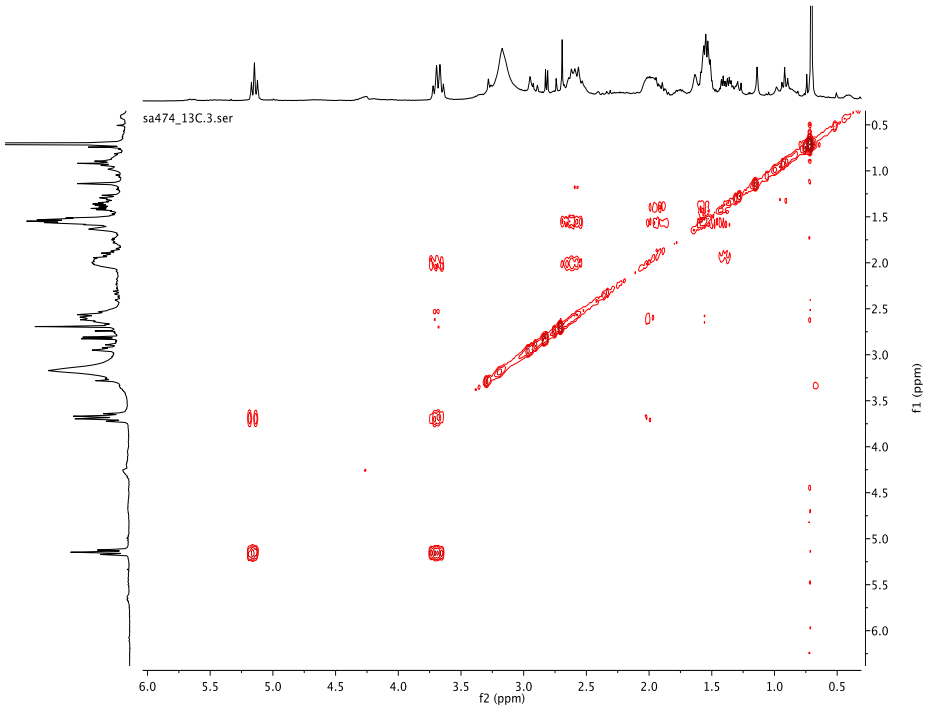



**Figure S.20.** COSY ($CDCl_3$) spectrum of **4**

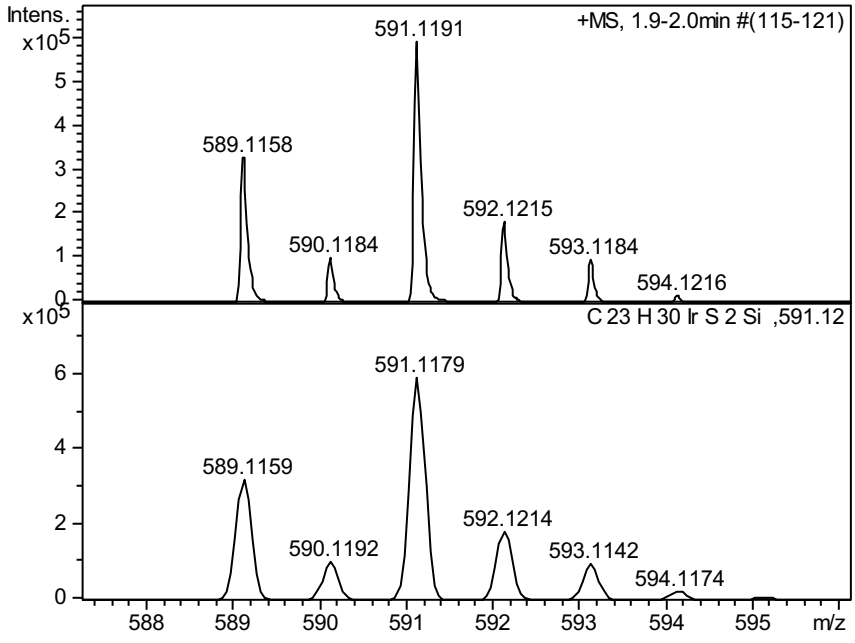
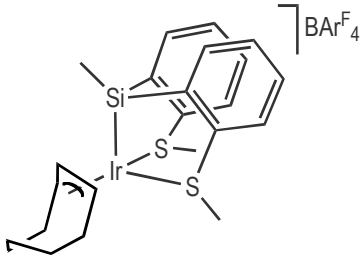



**Figure S.21.** ESI-MS for **4**. Found (top) and calculated (bottom)

**{Ir(η$^3$-cyclooctenyl)[SiMe(*o*-C$_6$H$_4$SMe)$_2$]}[BAr$^F_4$] (5)**.



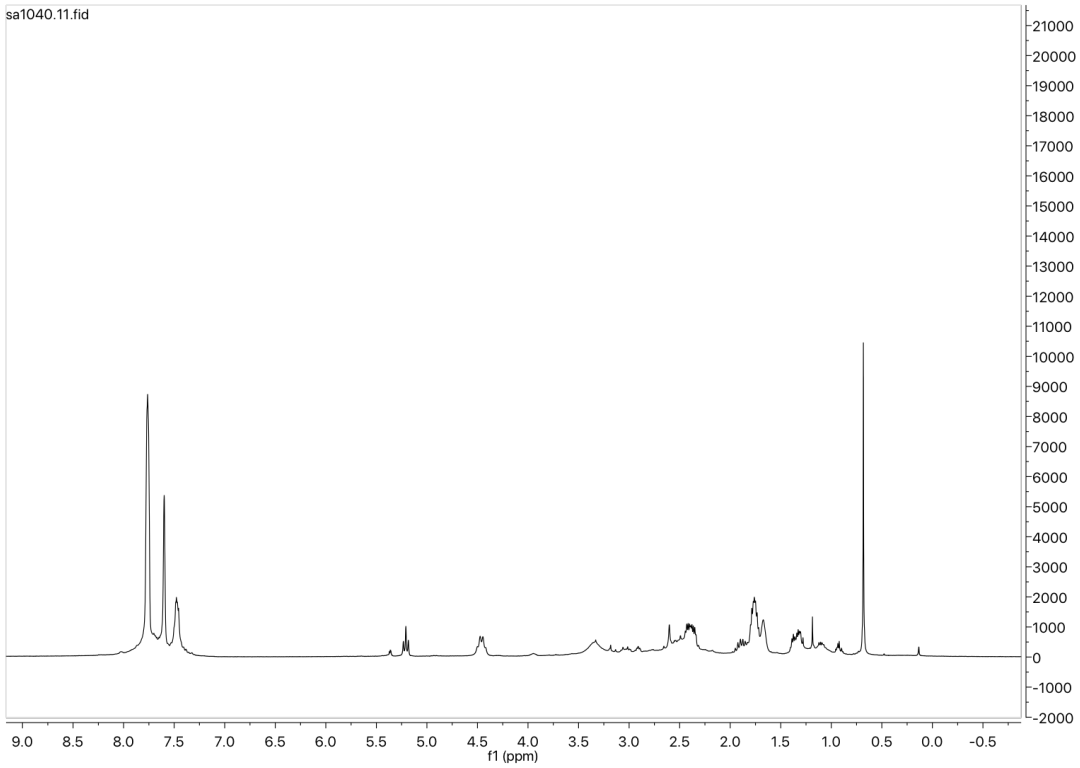




**Figure S.22.** $^1$H NMR ($CD_2Cl_2$) spectrum of **5**

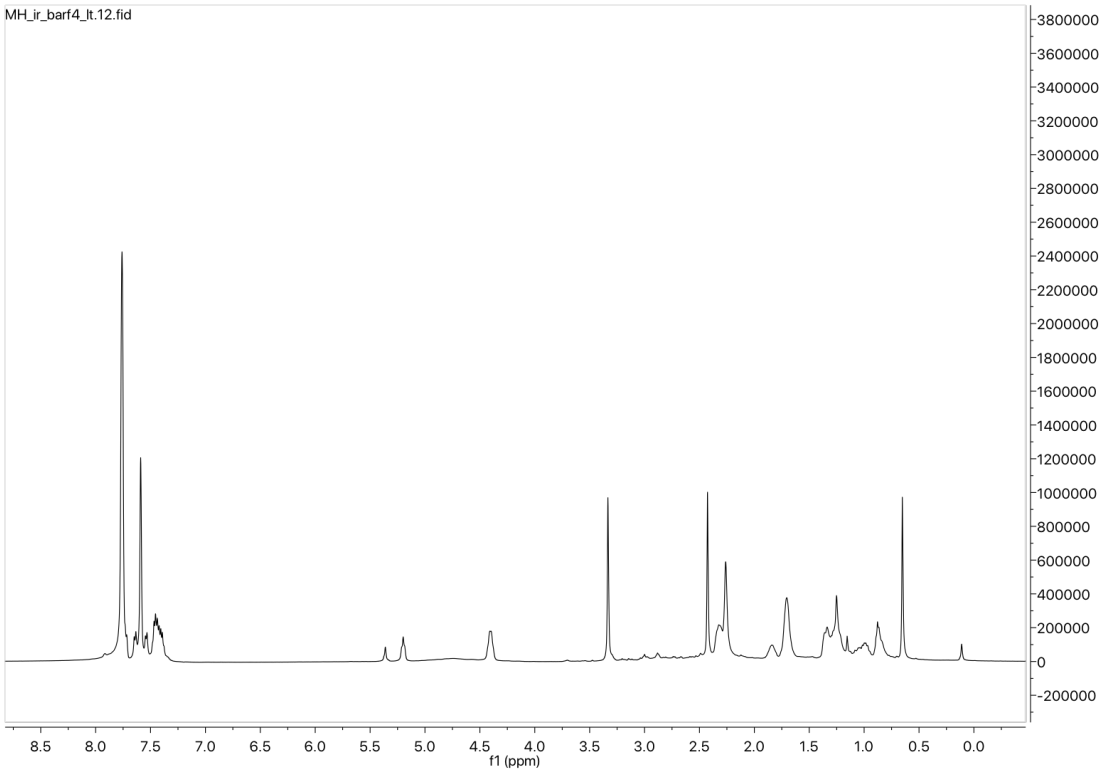



**Figure S.23.** $^{1}H$ NMR ($CD_2Cl_2$, -25 ºC) spectrum of **5**

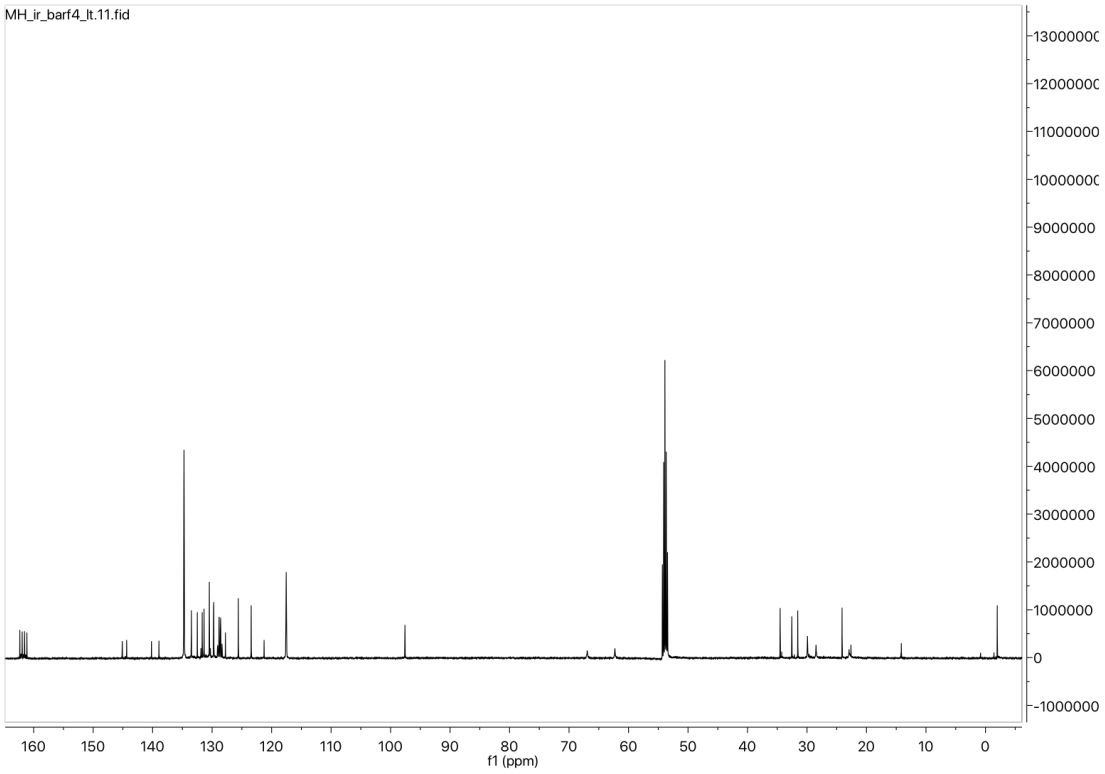



**Figure S.24.** $^{13}C\{^{1}H\}$ NMR ($CD_2Cl_2$, -25 ºC) spectrum of **5**

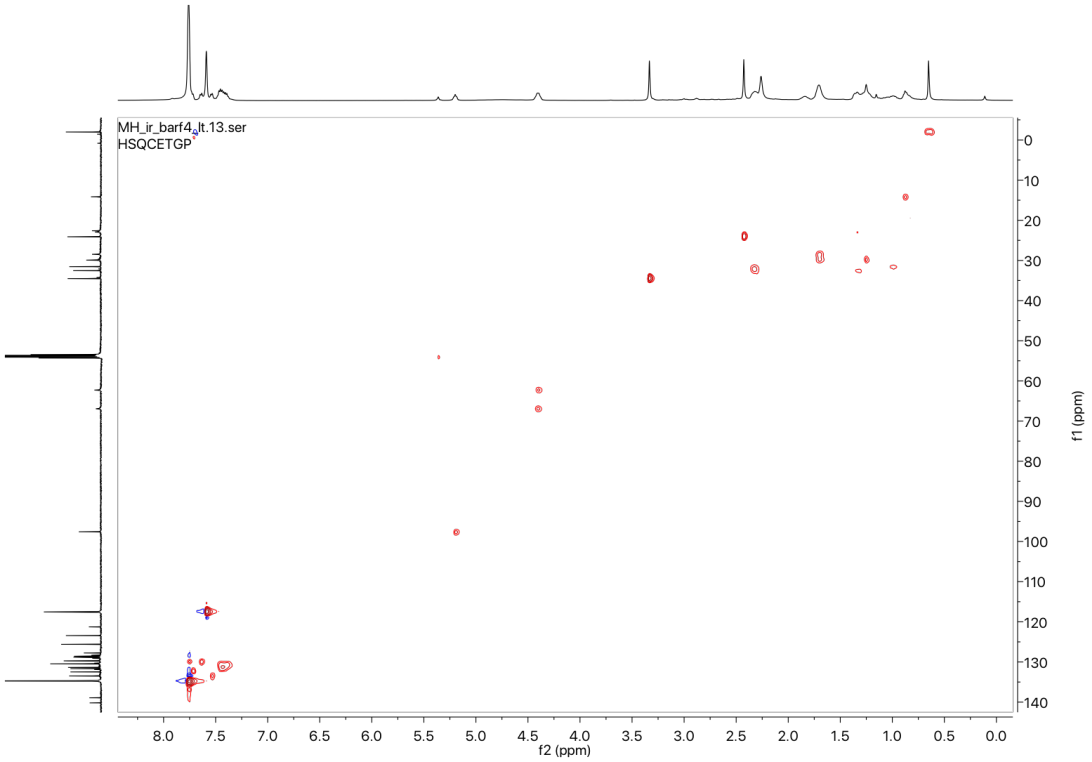
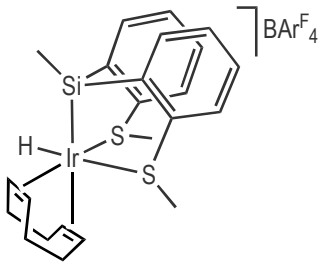



**Figure S.25.** $^{1}H$-$^{13}C$ HSQC ($CD_2Cl_2$, -25 ºC) spectrum of **5**

**{Ir(H)[SiMe(*o*-$C_6H_4SMe)_2$](cod)}[$BAr^F_4$] (6)**.



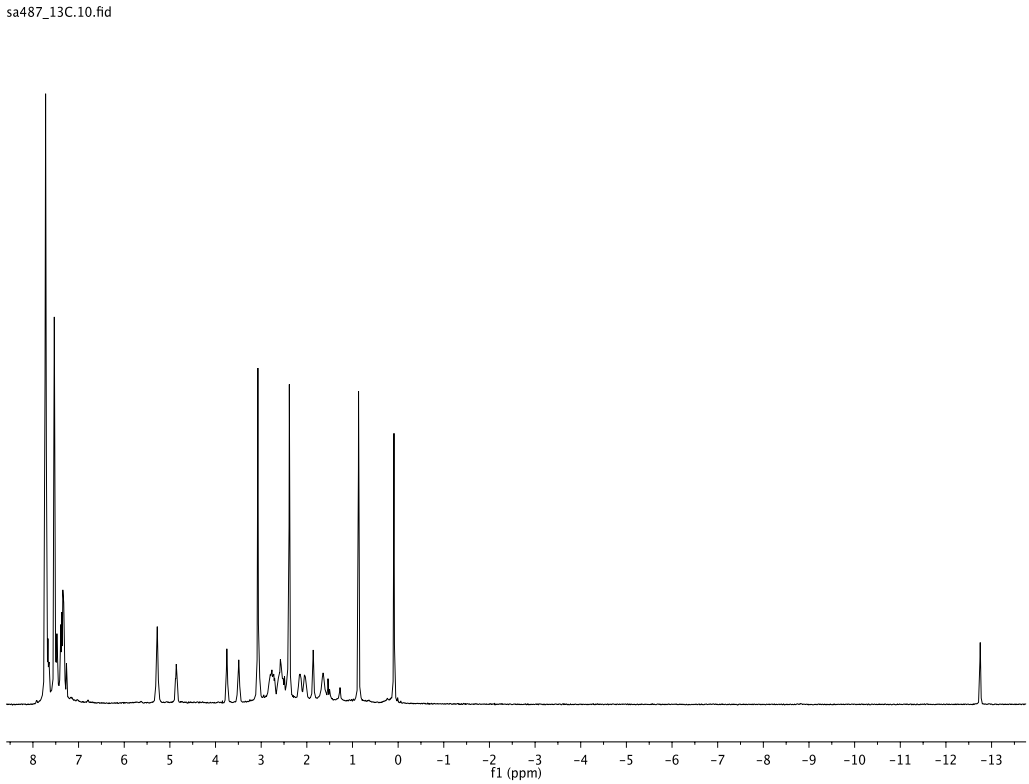




**Figure S.26.** $^1H$ NMR ($CDCl_3$) spectrum of **6**

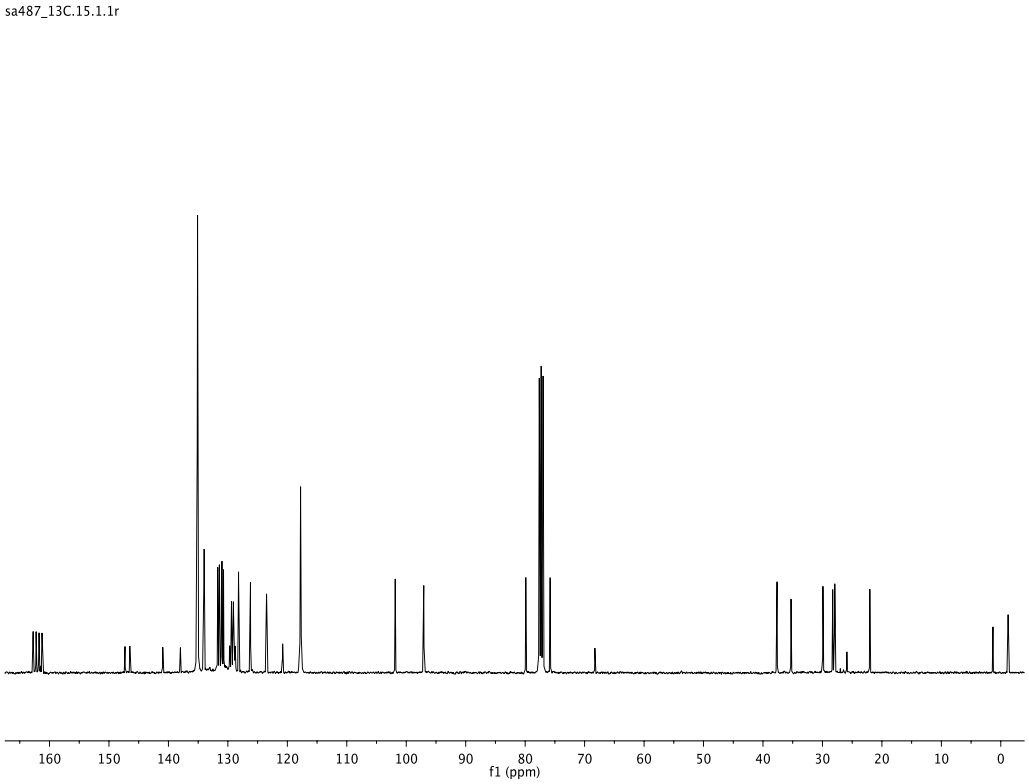



**Figure S.27.** $^{13}C$ NMR ($CDCl_3$) spectrum of **6**

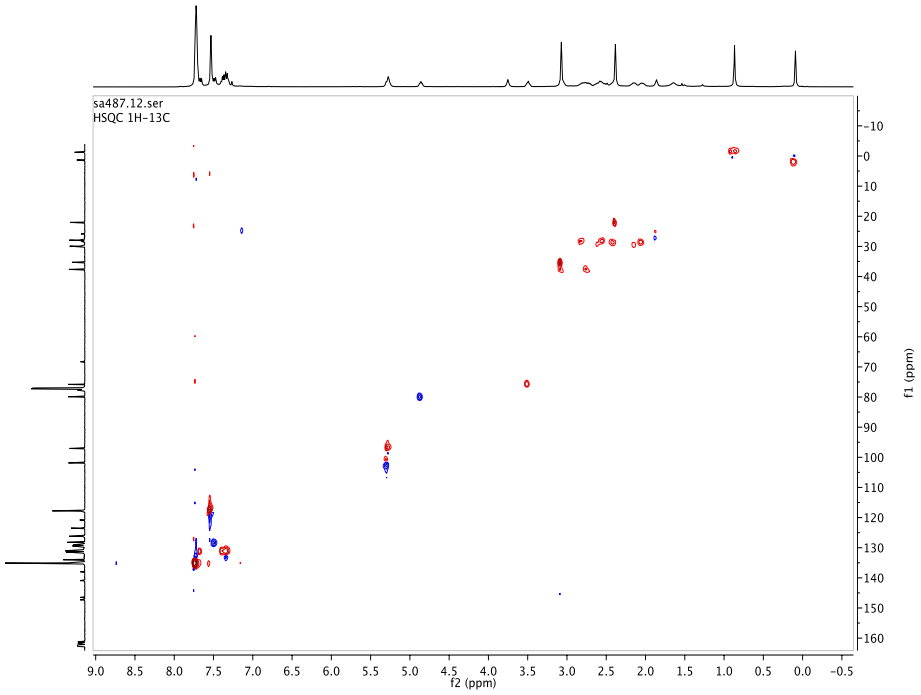



**Figure S.28.** $^{1}H$-$^{13}C$ HSQC ($CDCl_3$) spectrum of **6**

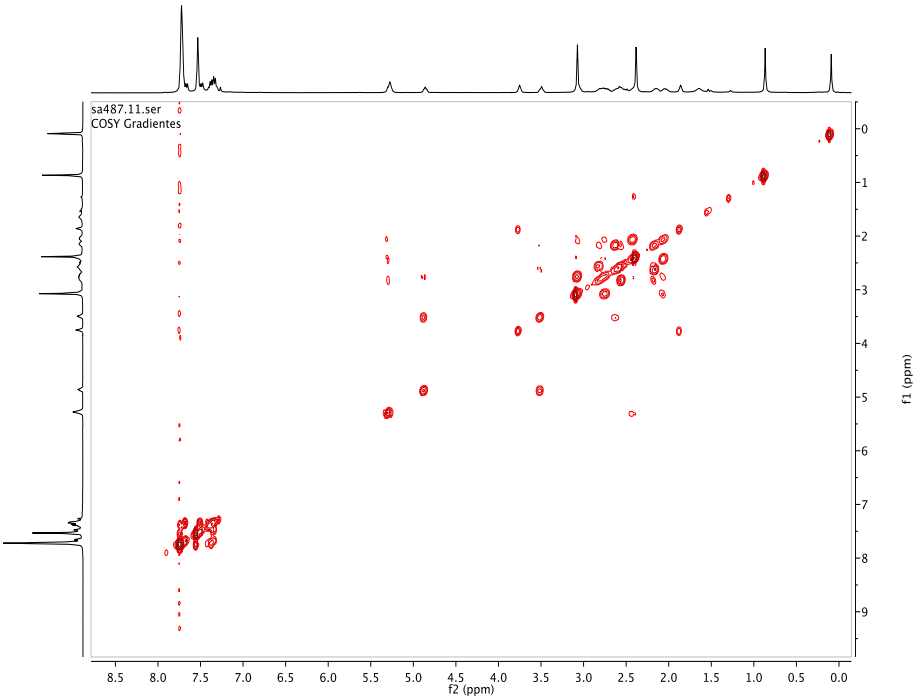



**Figure S.29.** COSY ($CDCl_3$) spectrum of **6**

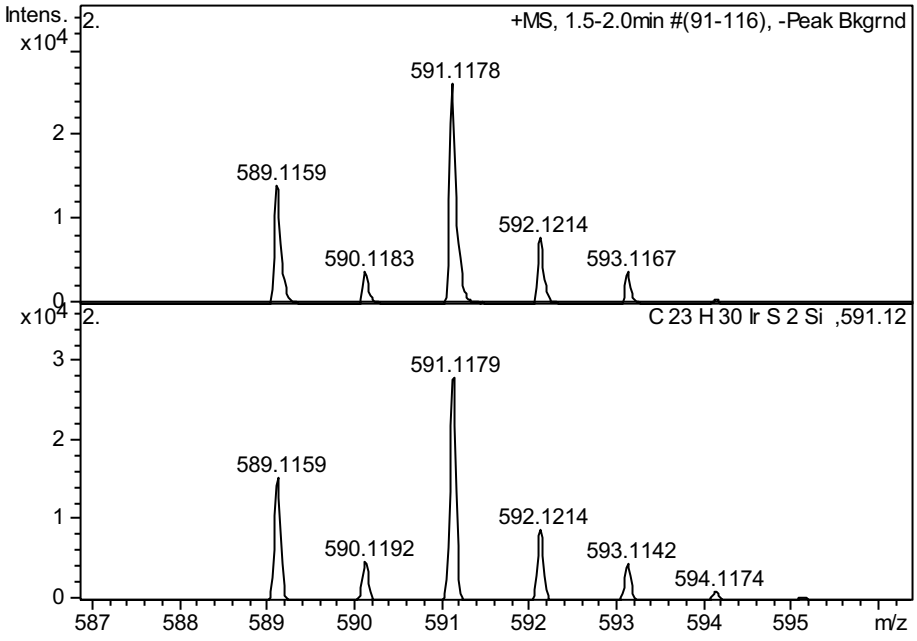



**Figure S.30.** ESI-MS for **6**. Found (top) and calculated (bottom)

## Transformation of 5 into 6

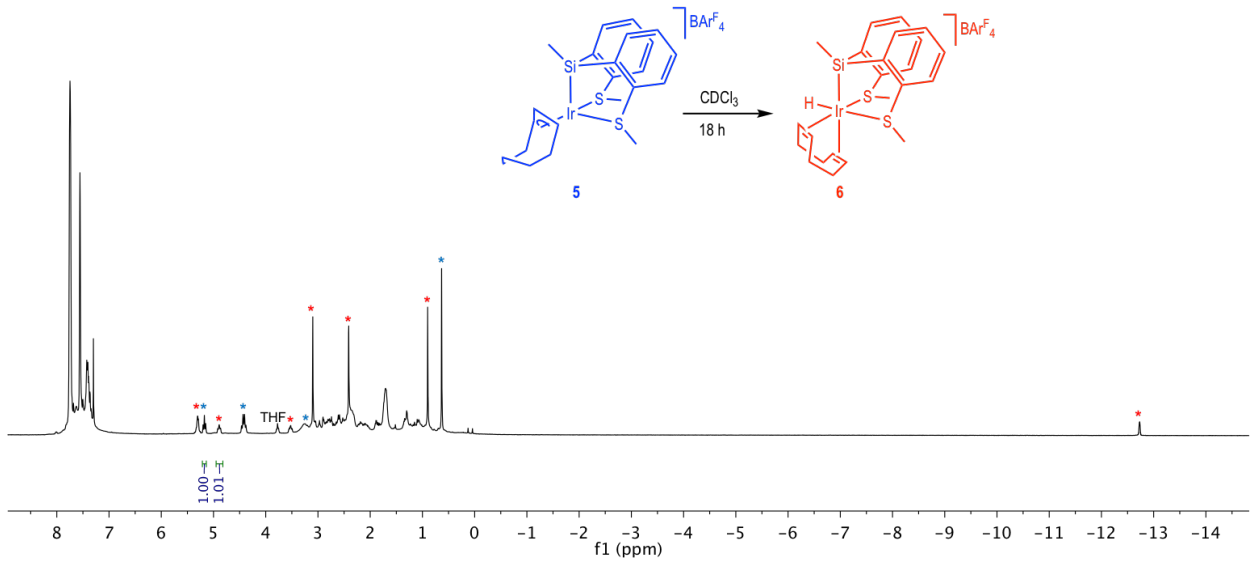



**Figure S.31.** $^{1}H$ NMR of compound **5** in $CDCl_3$ after 18 hours stored in the NMR tube at room temperature. Slow formation of compound **6**.

## 2. Crystallography

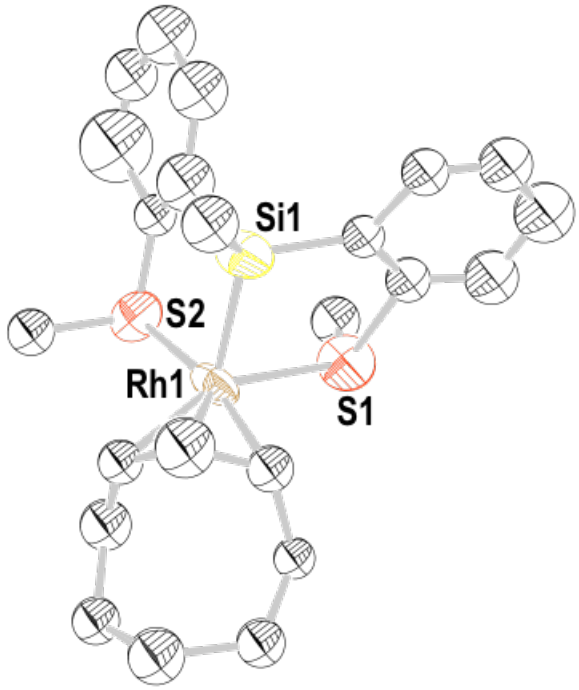



**Figure S.32.** Molecular structure of **1**. The anion and hydrogen atoms are omitted for clarity.

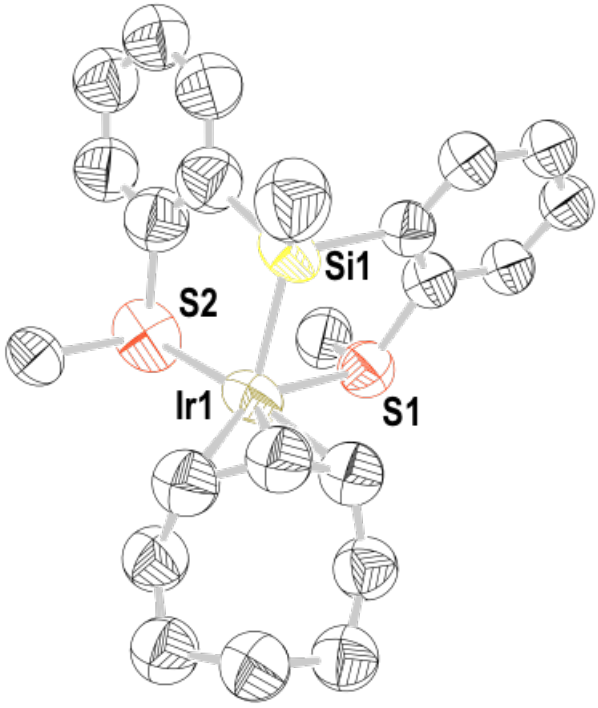



**Figure S.33.** Molecular structure of **5**. The anion and hydrogen atoms are omitted for clarity.

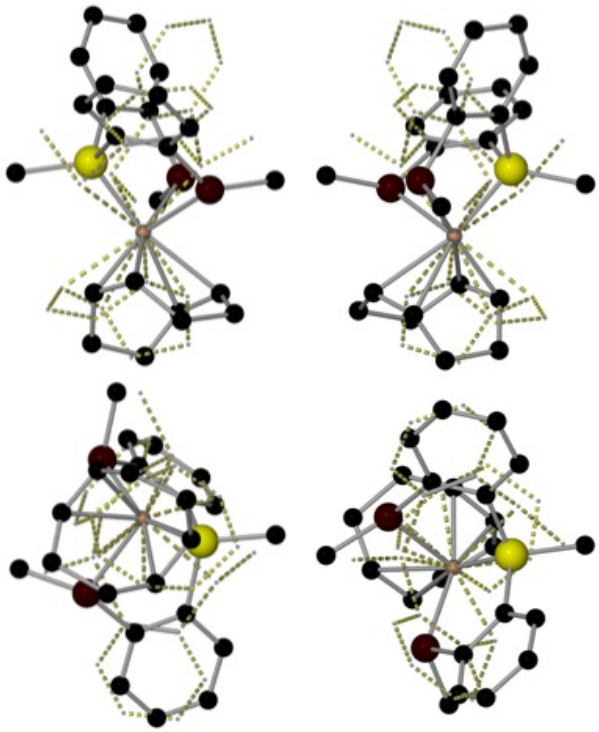


**Figure S34.** Picture of **6** showing the disorder presents in all structure.

**Table S1.** Crystallographic data and structure refinement details of all compounds.

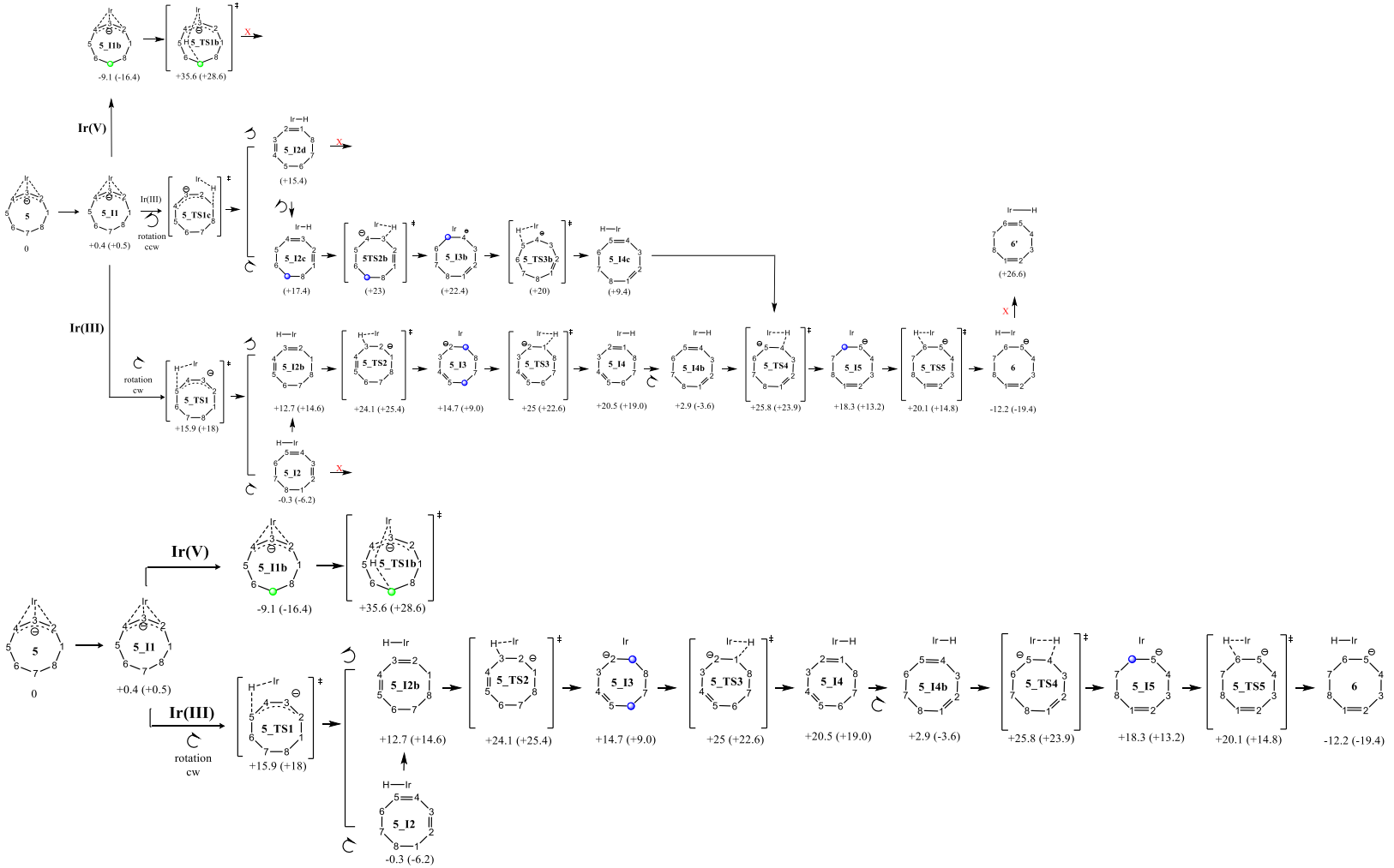
| Compound | 1 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|
| Chem. form. | $C_{55}H_{42}BF_{24}S_2SiRh$ | $C_{54}H_{38}BF_{24}S_2SiRh$ | $C_{24}H_{31}Cl_4S_2SiIr$ | $C_{55}H_{42}BF_{24}S_2SiIr$ | $C_{55}H_{41}BF_{24}S_2SiIr$ |
| CCDC | *Support.Inf.* | 1565673 | 1565674 | *Support.Inf.* | 1565675 |
| Form. weight | 1364.81 | 1348.77 | 745.70 | 1454.10 | 1453.10 |
| Cryst. system | Triclinic | Triclinic | Triclinic | Triclinic | Triclinic |
| Space group | *P*-1 | *P*-1 | *P*-1 | *P*-1 | *P*-1 |
| *a* (Å) | 12.212(3) | 12.2532(6) | 10.3166(6) | 12.316(3) | 12.2683(5) |
| *b* (Å) | 12.428(3) | 12.7478(7) | 11.3775(7) | 12.382(4) | 12.4775(5) |
| *c* (Å) | 18.878(5) | 19.0546(11) | 13.4886(8) | 19.003(4) | 19.1517(9) |
| $\alpha$ (º) | 84.071(6) | 73.523(2) | 66.355(2) | 83.660(7) | 73.970(2) |
| $\beta$ (º) | 83.693(6) | 89.902(2) | 70.426(2) | 83.383(7) | 89.285(2) |
| $\gamma$ (º) | 80.925(6) | 79.469(2) | 84.189(2) | 80.909(7) | 81.529(2) |
| V (Å$^3$) | 2801.2(12) | 2802.1(3) | 1365.51(14) | 2829.7(12) | 2785.7(2) |
| Z | 2 | 2 | 2 | 2 | 2 |
| GOF [a] | 1.093 | 1.031 | 1.054 | 2.426 | 1.043 |
| $R_{int}$ | 0.1549 | 0.1208 | 0.0502 | 0.1748 | 0.0456 |
| $R_1$ [b] / $wR^2$ [c] [I>2σ(I)] | 0.2598 / 0.5568 | 0.0827 / 0.2043 | 0.0299 / 0.0696 | 0.2557 / 0.6122 | 0.0893 / 0.2322 |
| $R_1$ [b] / $wR^2$ [c] (all data) | 0.3182 / 0.5891 | 0.1377 / 0.2415 | 0.0324 / 0.0710 | 0.3266 / 0.6363 | 0.1023 / 0.2469 |

[a] $S = [\sum w(F_0^2 - F_c^2)^2 / (N_{obs} - N_{param})]^{1/2}$ [b] $R_1 = \sum||F_0|-|F_c|| / \sum|F_0|$ [c] $wR_2 = [\sum w(F_0^2 - F_c^2)^2 / \sum wF_0^2]^{1/2}$; $w = 1/[\sigma^2(F_0^2) + (aP)^2 + bP]$ where $P = (\max(F_0^2,0) + 2Fc^2)/3$

## 3. DFT Calculations

**Table S2.** Calculated electronic enthalpies in vacuum ($\varepsilon^\circ$, Hartree), zero point vibrational energies (ZPVE, Hartree/particle), the sum of electronic and zero point energies ($\varepsilon^\circ$+ZPVE, Hartree), the sum of electronic and thermal energies ($\varepsilon^\circ+E_{tot}$, Hartree), the sum of electronic and thermal enthalpies ($\varepsilon^\circ + H_{corr}$, Hartree), the sum of electronic and thermal free energies ($\varepsilon^\circ + G_{corr}$, Hartree), enthropies (S, cal/mol·K) and ΔG of solvation (ΔGsolv, kcal/mol) for **5** and **6**, as well as for the intermediate species and transition state structures. Also, enthalpy difference (ΔH, kcal/mol), Gibss free energy difference in vaccumm ($\Delta G_v$, kcal/mol) and Gibss free energy difference with solvent effects ($\Delta G_s$, kcal/mol, dichlorlomethane) of each species with respect to **5**.

| | $\varepsilon^\circ$ | ZPVE | $\varepsilon^\circ$+ZPVE | $\varepsilon^\circ+E_{tot}$ | $\varepsilon^\circ + H_{corr}$ | $\varepsilon^\circ + G_{corr}$ | S | $\Delta G_{solv}$ | ΔH | $\Delta G_v$ | $\Delta G_s$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **5** | -2083,558571 | 0,451672 | -2083,106899 | -2083,078343 | -2083,0774 | -2083,161295 | 176,6 | -55,6 | 0,0 | 0,0 | 0,0 |
| **6** | -2083,5925 | 0,4580042 | -2083,134496 | -2083,105273 | -2083,10433 | -2083,192246 | 185,0 | -48,4 | -16,9 | -19,4 | -12,2 |
| | | | | | **Ir(III)** | | | | | | |
| **5_I1** | -2083,557488 | 0,4514836 | -2083,106004 | -2083,077364 | -2083,07642 | -2083,160525 | 177,0 | -55,7 | 0,6 | 0,5 | 0,4 |
| **5_I2** | -2083,567504 | 0,4558444 | -2083,111659 | -2083,081799 | -2083,08086 | -2083,171224 | 190,2 | -49,7 | -2,2 | -6,2 | -0,3 |
| **5_I2b** | -2083,530447 | 0,4480371 | -2083,08241 | -2083,053277 | -2083,05233 | -2083,138061 | 180,4 | -57,4 | 15,7 | 14,6 | 12,7 |
| **5_I3** | -2083,54272 | 0,4554525 | -2083,087267 | -2083,057457 | -2083,05651 | -2083,14692 | 190,3 | -50,0 | 13,1 | 9,0 | 14,7 |
| **5_I4** | -2083,523388 | 0,4473809 | -2083,076007 | -2083,047105 | -2083,04616 | -2083,130972 | 178,5 | -54,1 | 19,6 | 19,0 | 20,5 |
| **5_I4b** | -2083,566292 | 0,45763 | -2083,108662 | -2083,079263 | -2083,07832 | -2083,16697 | 186,6 | -49,1 | -0,6 | -3,6 | 2,9 |
| **5_I5** | -2083,533808 | 0,4484882 | -2083,085319 | -2083,05658 | -2083,05564 | -2083,140334 | 178,3 | -50,5 | 13,7 | 13,2 | 18,3 |
| **5_TS1** | -2083,523921 | 0,446068 | -2083,077853 | -2083,049242 | -2083,0483 | -2083,132581 | 177,4 | -57,7 | 18,3 | 18,0 | 15,9 |
| **5_TS2** | -2083,510975 | 0,4453547 | -2083,06562 | -2083,03665 | -2083,03571 | -2083,120778 | 179,0 | -56,9 | 26,2 | 25,4 | 24,1 |
| **5_TS3** | -2083,516627 | 0,4456761 | -2083,070951 | -2083,042538 | -2083,04159 | -2083,12528 | 176,1 | -53,2 | 22,5 | 22,6 | 25,0 |
| **5_TS4** | -2083,515592 | 0,4468351 | -2083,068757 | -2083,040342 | -2083,0394 | -2083,123277 | 176,5 | -53,7 | 23,8 | 23,9 | 25,8 |
| **5_TS5** | -2083,530231 | 0,44795 | -2083,082281 | -2083,053278 | -2083,05233 | -2083,13778 | 179,8 | -50,3 | 15,7 | 14,8 | 20,1 |
| | | | | | **Ir(V)** | | | | | | |
| **5_I1b** | -2083,588116 | 0,459175 | -2083,128941 | -2083,099494 | -2083,09855 | -2083,187370 | 186,9 | -48,4 | -13,3 | -16,4 | -9,1 |
| **5_TS1b** | -2083,509985 | 0,447476 | -2083,062509 | -2083,034598 | -2083,03365 | -2083,115708 | 172,7 | -48,6 | 27,5 | 28,6 | 35,6 |




**Scheme S1**. Simplified representation of the different species involved in either alternative Ir(III)- or an Ir(V)-intermediate mediated mechanisms to trigger transformation of **5** into **6**. Blue spheres represent agostic interactions. Solvent corrected (dichloromethane) and gas phase free (in parenthesis) energy values, in kcal/mol, are indicated below each calculated structure. A red cross indicates either that i) subsequent steps/species were not identified or that ii) high kinetic barriers discouraged a deeper analysis of the particular mechanism. ↻ cw: clockwise rotation of COD; ccw: ↺counterclockwise rotation of COD.

**Table S3.** Calculated electronic enthalpies in vacuum ($\varepsilon^\circ$, Hartree), zero point vibrational energies (ZPVE, Hartree/particle), the sum of electronic and zero point energies ($\varepsilon^\circ$+ZPVE, Hartree), the sum of electronic and thermal energies ($\varepsilon^\circ$+$E_{tot}$, Hartree), the sum of electronic and thermal enthalpies ($\varepsilon^\circ$ + $H_{corr}$, Hartree), the sum of electronic and thermal free energies ($\varepsilon^\circ$ + $G_{corr}$, Hartree), enthropies (S, cal/mol·K) and ΔG of solvation (ΔGsolv, kcal/mol) for **2[BAr$^F_4$]**. and **3**, as well as for the intermediate species and transition state structures. Also, enthalpy difference (ΔH, kcal/mol), Gibss free energy difference in vaccumm ($\Delta G_v$, kcal/mol) and Gibss free energy difference with solvent effects ($\Delta G_s$, kcal/mol, dichlorlomethane) of each species with respect to **2[BAr$^F_4$]**.

| | $\varepsilon^\circ$ | ZPVE | $\varepsilon^\circ$+ZPVE | $\varepsilon^\circ$ +$E_{tot}$ | $\varepsilon^\circ$ + $H_{corr}$ | $\varepsilon^\circ$ + $G_{corr}$ | S | $\Delta G_{solv}$ | ΔH | $\Delta G_v$ | $\Delta G_s$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **2[BAr]** | -2047,848104 | 0,408127 | 2047,439978 | 2047,412314 | -2047,41137 | -2047,498499 | 183,4 | -50,2 | 0,0 | 0,0 | 0,0 |
| **3** | -2047,869437 | 0,408363 | -2047,461074 | -2047,433718 | -2047,432774 | -2047,51729 | 177,9 | -49,9 | -13,2 | -11,8 | -11,5 |
| **2b** | -2047,865691 | 0,408463 | -2047,457227 | -2047,429971 | -2047,429027 | -2047,513526 | 177,8 | -50,2 | -10,8 | -9,4 | -9,4 |
| **I_23** | -2047,83908 | 0,405483 | -2047,433597 | -2047,406895 | -2047,405951 | -2047,488867 | 174,5 | -49,9 | 4,0 | 6,0 | 6,4 |
| **TS2** | -2047,833848 | 0,404096 | -2047,429752 | -2047,403057 | -2047,402113 | -2047,484806 | 174,0 | -49,6 | 6,4 | 8,6 | 9,2 |
| **TS3** | -2047,79846 | 0,395529 | -2047,402931 | -2047,376772 | -2047,375828 | -2047,45469 | 166,0 | -49,6 | 23,2 | 27,5 | 28,1 |

## XYZ coordinates of all the calculates structures

### 2[BAr$^F_4$].xyz

52

| | | | |
|---|---|---|---|
| Rh | -0.922832 | -0.130358 | -0.509891 |
| Si | 0.731268 | -0.119160 | 1.100360 |
| S | 0.883472 | -1.245450 | -1.901063 |
| S | -0.434962 | 2.059067 | -0.856992 |
| C | -2.853155 | -1.264881 | 0.976689 |
| C | -2.579715 | 0.182677 | 0.669466 |
| C | -3.889420 | 0.488677 | -0.104822 |
| H | -4.006952 | 1.503939 | -0.501026 |
| C | -4.403913 | -1.384262 | 1.131481 |
| H | -4.808381 | -2.099634 | 1.848045 |
| C | -4.955231 | 0.025492 | 0.925018 |
| H | -5.977236 | 0.026483 | 0.509607 |
| H | -4.944358 | 0.628403 | 1.846916 |
| C | -3.753652 | -1.815225 | -0.152314 |
| C | -3.944165 | -0.665389 | -1.139602 |
| C | 1.195538 | 2.407628 | -0.117971 |
| C | 1.850752 | 3.596730 | -0.463381 |
| H | 1.402547 | 4.307609 | -1.162471 |
| C | 3.104056 | 3.855062 | 0.104647 |
| H | 3.633210 | 4.775787 | -0.152675 |
| C | 3.680635 | 2.932756 | 0.990060 |

| | | | |
|---|---|---|---|
| H | 4.661225 | 3.138316 | 1.426814 |
| C | 3.008983 | 1.746814 | 1.311432 |
| H | 3.477201 | 1.034910 | 1.998004 |
| C | 1.743942 | 1.461827 | 0.758594 |
| C | 1.945418 | -2.030356 | -0.658849 |
| C | 2.794741 | -3.074832 | -1.048609 |
| H | 2.852883 | -3.382794 | -2.095698 |
| C | 3.556765 | -3.733097 | -0.075057 |
| H | 4.220532 | -4.549748 | -0.369263 |
| C | 3.450111 | -3.359935 | 1.271304 |
| H | 4.033028 | -3.886420 | 2.031368 |
| C | 2.592641 | -2.317899 | 1.647551 |
| H | 2.520049 | -2.040532 | 2.703215 |
| C | 1.831650 | -1.621435 | 0.686013 |
| C | 0.208435 | -0.176872 | 2.911683 |
| H | -0.421127 | 0.688965 | 3.168689 |
| H | -0.347976 | -1.097886 | 3.145088 |
| H | 1.104103 | -0.143526 | 3.556251 |
| C | 2.050892 | -0.099881 | -2.732176 |
| H | 1.464122 | 0.457676 | -3.475832 |
| H | 2.501899 | 0.588828 | -2.007113 |
| H | 2.823919 | -0.688890 | -3.243513 |
| C | -1.439770 | 3.210568 | 0.161496 |
| H | -2.478717 | 3.133488 | -0.182040 |
| H | -1.356123 | 2.961829 | 1.226553 |
| H | -1.060667 | 4.223749 | -0.032616 |
| H | -3.130465 | -0.605032 | -1.886253 |
| H | -3.694439 | -2.862025 | -0.449419 |
| H | -4.909590 | -0.713376 | -1.668834 |
| H | -2.215932 | -1.906563 | 1.584595 |
| H | -2.402461 | 0.837924 | 1.534614 |

**2b.xyz**

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| | | | |
|---|---|---|---|
| Rh | 1.107250 | -0.311472 | -0.338017 |
| Si | -0.647803 | 0.226004 | 1.127089 |
| S | -0.094277 | 1.141566 | -1.811097 |
| S | -0.187377 | -2.376782 | -0.868485 |
| C | 2.384101 | -0.470883 | 1.479091 |
| C | 2.939879 | -1.353840 | 0.547881 |
| C | 4.109421 | -0.619710 | -0.144523 |
| H | 4.867498 | -1.273572 | -0.591490 |
| C | 3.128970 | 0.855254 | 1.271512 |
| H | 2.993452 | 1.623211 | 2.040685 |
| C | 4.557282 | 0.338587 | 0.991488 |

| | | | |
|---|---|---|---|
| H | 5.257121 | 1.114320 | 0.643100 |
| H | 4.988808 | -0.183910 | 1.859421 |
| C | 2.554969 | 1.176620 | -0.136750 |
| C | 3.459759 | 0.407517 | -1.114757 |
| C | -1.831651 | -2.096880 | -0.162180 |
| C | -2.862622 | -2.983784 | -0.508675 |
| H | -2.665289 | -3.830404 | -1.171032 |
| C | -4.150302 | -2.765001 | -0.010051 |
| H | -4.957064 | -3.452686 | -0.272544 |
| C | -4.404658 | -1.656084 | 0.807352 |
| H | -5.412891 | -1.478009 | 1.187938 |
| C | -3.370655 | -0.771175 | 1.129870 |
| H | -3.593682 | 0.096650 | 1.758195 |
| C | -2.056858 | -0.976236 | 0.657856 |
| C | -0.945323 | 2.333390 | -0.744690 |
| C | -1.323183 | 3.572386 | -1.273142 |
| H | -1.123441 | 3.822527 | -2.317834 |
| C | -1.941605 | 4.500933 | -0.426253 |
| H | -2.237771 | 5.475978 | -0.818680 |
| C | -2.156488 | 4.188433 | 0.921275 |
| H | -2.624472 | 4.922493 | 1.581018 |
| C | -1.765023 | 2.943332 | 1.430646 |
| H | -1.933215 | 2.724405 | 2.488751 |
| C | -1.157739 | 1.982380 | 0.600245 |
| C | -0.458981 | 0.176502 | 3.007771 |
| H | -0.231606 | -0.836034 | 3.374135 |
| H | 0.307663 | 0.873047 | 3.378608 |
| H | -1.422994 | 0.465583 | 3.460086 |
| C | -1.514175 | 0.386299 | -2.699217 |
| H | -1.104167 | -0.404596 | -3.341167 |
| H | -2.241108 | -0.024317 | -1.988777 |
| H | -1.971488 | 1.166512 | -3.321680 |
| C | 0.371430 | -3.815690 | 0.124731 |
| H | 1.325038 | -4.151257 | -0.303898 |
| H | 0.495309 | -3.539775 | 1.179714 |
| H | -0.367774 | -4.620435 | 0.024412 |
| H | 2.918305 | -0.079566 | -1.957302 |
| H | 2.275447 | 2.210367 | -0.362973 |
| H | 4.213255 | 1.053125 | -1.600631 |
| H | 1.780669 | -0.735742 | 2.345055 |
| H | 2.814576 | -2.436393 | 0.534859 |

**I2_3.xyz**

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| | | | |
|---|---|---|---|
| Rh | 1.221639 | 0.241655 | -0.423210 |
| Si | -0.641086 | -0.046721 | 1.169028 |
| S | -0.089155 | 2.040405 | -1.321168 |
| S | 0.070489 | -1.469756 | -1.657348 |
| C | 2.301931 | -0.920802 | 1.122467 |
| C | 3.126242 | -0.770091 | -0.023956 |
| C | 3.986881 | 0.484151 | 0.224448 |
| H | 4.860839 | 0.606239 | -0.422871 |
| C | 2.675683 | 0.248099 | 2.059419 |
| H | 2.355331 | 0.159319 | 3.100748 |
| C | 4.183256 | 0.416652 | 1.757317 |
| H | 4.603603 | 1.344262 | 2.178722 |
| H | 4.783082 | -0.451396 | 2.076003 |
| C | 2.070967 | 1.417148 | 1.252647 |
| C | 2.894330 | 1.563979 | 0.105938 |
| C | -1.112954 | -2.310288 | -0.559211 |
| C | -1.731770 | -3.485081 | -1.013234 |
| H | -1.489764 | -3.911926 | -1.989374 |
| C | -2.669728 | -4.117282 | -0.190006 |
| H | -3.147508 | -5.039936 | -0.528206 |
| C | -2.993483 | -3.566604 | 1.057257 |
| H | -3.723567 | -4.063135 | 1.701431 |
| C | -2.385691 | -2.377910 | 1.477157 |
| H | -2.656920 | -1.958658 | 2.450347 |
| C | -1.430763 | -1.717874 | 0.673109 |
| C | -1.672302 | 2.147428 | -0.432671 |
| C | -2.583602 | 3.138266 | -0.831443 |
| H | -2.368909 | 3.793011 | -1.679640 |
| C | -3.776139 | 3.288872 | -0.117027 |
| H | -4.493936 | 4.054345 | -0.421436 |
| C | -4.036877 | 2.471977 | 0.991854 |
| H | -4.965379 | 2.594749 | 1.555153 |
| C | -3.105899 | 1.503547 | 1.382494 |
| H | -3.326026 | 0.877809 | 2.252522 |
| C | -1.899295 | 1.313585 | 0.672950 |
| C | -0.516204 | -0.016441 | 3.056817 |
| H | 0.108368 | -0.839278 | 3.437431 |

| | | | |
|---|---|---|---|
| H | -0.100356 | 0.936850 | 3.418055 |
| H | -1.521229 | -0.127521 | 3.498432 |
| C | -0.657270 | 1.671996 | -3.021262 |
| H | 0.246940 | 1.554147 | -3.632667 |
| H | -1.261534 | 0.757333 | -3.043208 |
| H | -1.238657 | 2.531032 | -3.380923 |
| C | 1.264411 | -2.815939 | -1.980069 |
| H | 2.044371 | -2.392736 | -2.626583 |
| H | 1.691121 | -3.192223 | -1.041814 |
| H | 0.741733 | -3.618323 | -2.516667 |
| H | 2.037892 | 0.390775 | -1.849149 |
| H | 2.958432 | 2.438238 | -0.540421 |
| H | 1.403207 | 2.172444 | 1.666549 |
| H | 1.803431 | -1.835932 | 1.442179 |
| H | 3.365202 | -1.534586 | -0.760287 |

**3.xyz**

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| | | | |
|---|---|---|---|
| Rh | -1.114323 | 0.303530 | -0.357797 |
| Si | 0.624659 | -0.198930 | 1.123668 |
| S | 0.285688 | -1.137951 | -1.899936 |
| S | 0.032175 | 2.334739 | -0.762916 |
| C | -2.751044 | 1.088371 | 0.648426 |
| C | -3.604070 | 0.966358 | -0.631072 |
| C | -4.013042 | -0.531644 | -0.548145 |
| H | -4.692337 | -0.876427 | -1.336513 |
| C | -3.169715 | -0.132255 | 1.518770 |
| H | -3.099635 | -0.003907 | 2.604169 |
| C | -4.519123 | -0.584102 | 0.917995 |
| H | -4.801446 | -1.596345 | 1.246733 |
| H | -5.353281 | 0.110053 | 1.106554 |
| C | -2.220313 | -1.156696 | 0.880605 |
| C | -2.698861 | -1.335871 | -0.423925 |
| C | 1.710852 | 2.163726 | -0.109234 |
| C | 2.677864 | 3.114519 | -0.464734 |
| H | 2.426625 | 3.954297 | -1.117265 |
| C | 3.980808 | 2.961046 | 0.020212 |
| H | 4.746053 | 3.693623 | -0.244752 |

| | | | |
|---|---|---|---|
| C | 4.304645 | 1.862367 | 0.827584 |
| H | 5.325585 | 1.740789 | 1.196303 |
| C | 3.327647 | 0.915931 | 1.156048 |
| H | 3.604341 | 0.057131 | 1.774984 |
| C | 2.001762 | 1.053117 | 0.697720 |
| C | 1.110588 | -2.279798 | -0.757948 |
| C | 1.560185 | -3.514866 | -1.241004 |
| H | 1.439685 | -3.774977 | -2.295408 |
| C | 2.150753 | -4.420395 | -0.350903 |
| H | 2.505435 | -5.385818 | -0.718120 |
| C | 2.266769 | -4.096990 | 1.005989 |
| H | 2.714712 | -4.811642 | 1.700088 |
| C | 1.799887 | -2.863761 | 1.478451 |
| H | 1.889705 | -2.633270 | 2.544069 |
| C | 1.220292 | -1.925066 | 0.602649 |
| C | 0.290905 | -0.114957 | 2.980800 |
| H | -0.128540 | 0.864372 | 3.256212 |
| H | -0.399516 | -0.897168 | 3.328490 |
| H | 1.240362 | -0.228330 | 3.530860 |
| C | 1.718194 | -0.329935 | -2.718600 |
| H | 1.302501 | 0.415630 | -3.409814 |
| H | 2.370377 | 0.151466 | -1.980243 |
| H | 2.268035 | -1.089400 | -3.288757 |
| C | -0.597458 | 3.720595 | 0.262205 |
| H | -1.631673 | 3.911486 | -0.051868 |
| H | -0.553349 | 3.464149 | 1.327337 |
| H | 0.016547 | 4.604980 | 0.049295 |
| H | -3.062786 | 1.209266 | -1.572264 |
| H | -2.408191 | -2.129247 | -1.114112 |
| H | -1.543349 | -1.826663 | 1.412640 |
| H | -2.662729 | 2.061454 | 1.140196 |
| H | -4.484755 | 1.633891 | -0.624995 |

**TS2.xyz**

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| | | | |
|---|---|---|---|
| C | -2.162832 | 0.940769 | 0.714724 |
| C | -1.967316 | 2.021526 | -0.156877 |
| C | -2.992945 | 2.921759 | -0.482920 |
| C | -4.268364 | 2.713839 | 0.048767 |
| C | -4.502423 | 1.634664 | 0.910904 |

| | | | |
|---|---|---|---|
| C | -3.458441 | 0.767898 | 1.245983 |
| S | -0.294151 | 2.337342 | -0.783921 |
| C | -0.588237 | 2.381237 | -2.592555 |
| Si | -0.715461 | -0.214189 | 1.184908 |
| C | -0.608871 | -0.216832 | 3.075196 |
| Rh | 1.126660 | 0.458024 | -0.292986 |
| C | 2.278412 | 1.583482 | 1.134643 |
| C | 2.789352 | 0.425754 | 2.020491 |
| C | 2.186026 | -0.763888 | 1.246658 |
| C | 2.896736 | -0.821543 | 0.027607 |
| C | 3.965475 | 0.295450 | 0.085174 |
| C | 3.057522 | 1.533113 | -0.080032 |
| C | 4.277344 | 0.341099 | 1.600230 |
| S | -0.076996 | -1.014406 | -1.810969 |
| C | 1.065613 | -1.959500 | -2.885689 |
| C | -1.115977 | -1.968373 | 0.558900 |
| C | -0.805527 | -2.313258 | -0.771632 |
| C | -1.115798 | -3.568862 | -1.309307 |
| C | -1.723175 | -4.527370 | -0.489467 |
| C | -2.029799 | -4.223569 | 0.841086 |
| C | -1.733332 | -2.954996 | 1.353203 |
| H | 4.796409 | 0.206300 | -0.622370 |
| H | 2.550850 | 0.490034 | 3.086611 |
| H | 4.860582 | 1.227803 | 1.895249 |
| H | 4.776332 | -0.571397 | 1.963231 |
| H | -0.892853 | -3.815686 | -2.348882 |
| H | -1.956214 | -5.512971 | -0.898007 |
| H | -2.498939 | -4.975222 | 1.479584 |
| H | -1.978011 | -2.733185 | 2.395886 |
| H | -2.808063 | 3.781353 | -1.131059 |
| H | -5.076741 | 3.403225 | -0.203767 |
| H | -5.499988 | 1.473945 | 1.325471 |
| H | -3.659570 | -0.067153 | 1.923578 |
| H | 0.112833 | -0.949471 | 3.466024 |
| H | -0.326392 | 0.780343 | 3.445983 |
| H | -1.593556 | -0.452594 | 3.511540 |
| H | 0.388194 | 2.553624 | -3.062623 |
| H | -1.022900 | 1.433476 | -2.932236 |
| H | -1.256645 | 3.221585 | -2.818146 |
| H | 1.689753 | -1.214930 | -3.394783 |
| H | 1.685822 | -2.644810 | -2.294894 |
| H | 0.482820 | -2.516132 | -3.630407 |

| | | | |
|---|---|---|---|
| H | 2.144118 | 1.007700 | -1.497919 |
| H | 1.794917 | 2.477468 | 1.528365 |
| H | 3.330206 | 2.407471 | -0.671015 |
| H | 1.610745 | -1.577954 | 1.685418 |
| H | 2.940760 | -1.666617 | -0.657431 |

**TS3.xyz**

52

| | | | |
|---|---|---|---|
| Rh | -1.268120 | 0.157879 | -0.398801 |
| Si | 0.710231 | -0.157319 | 1.179603 |
| S | 0.139964 | -1.456609 | -1.919562 |
| S | -0.002160 | 2.242269 | -1.093972 |
| C | -2.823589 | 1.026259 | 0.938370 |
| C | -3.479939 | 0.836061 | -0.356301 |
| C | -4.170607 | -0.578009 | -0.265327 |
| H | -4.905526 | -0.811610 | -1.057730 |
| C | -3.194284 | -0.238791 | 1.806685 |
| H | -3.058532 | -0.136841 | 2.898916 |
| C | -4.643122 | -0.587338 | 1.251626 |
| H | -5.013069 | -1.581295 | 1.588802 |
| H | -5.402854 | 0.193220 | 1.479838 |
| C | -2.328261 | -1.341420 | 1.090527 |
| C | -2.910496 | -1.524673 | -0.190184 |
| C | 1.637531 | 2.315035 | -0.185761 |
| C | 2.543166 | 3.356730 | -0.546498 |
| H | 2.277720 | 4.102277 | -1.314855 |
| C | 3.808518 | 3.420291 | 0.094683 |
| H | 4.515432 | 4.224516 | -0.169732 |
| C | 4.160455 | 2.439518 | 1.063705 |
| H | 5.144766 | 2.483183 | 1.560135 |
| C | 3.250847 | 1.397602 | 1.386723 |
| H | 3.557600 | 0.642445 | 2.131235 |
| C | 1.957085 | 1.305648 | 0.767335 |
| C | 1.325528 | -2.325868 | -0.748655 |
| C | 1.919226 | -3.531906 | -1.220844 |
| H | 1.703309 | -3.905839 | -2.235893 |
| C | 2.783403 | -4.265484 | -0.362937 |
| H | 3.246862 | -5.199592 | -0.722323 |
| C | 3.026200 | -3.800849 | 0.957762 |
| H | 3.685050 | -4.373411 | 1.632706 |

| | | | |
|---|---|---|---|
| C | 2.410610 | -2.603948 | 1.417145 |
| H | 2.609085 | -2.275375 | 2.452008 |
| C | 1.546292 | -1.825316 | 0.574866 |
| C | 0.514112 | -0.199341 | 3.115588 |
| H | 0.004295 | 0.724725 | 3.470814 |
| H | -0.076443 | -1.076021 | 3.463562 |
| H | 1.505063 | -0.240535 | 3.623841 |
| C | 1.329180 | -0.561462 | -3.107688 |
| H | 0.692247 | 0.027373 | -3.797638 |
| H | 2.023670 | 0.094235 | -2.548871 |
| H | 1.886203 | -1.336794 | -3.669744 |
| C | -0.880085 | 3.784766 | -0.408557 |
| H | -1.897359 | 3.796581 | -0.848205 |
| H | -0.916423 | 3.751441 | 0.697237 |
| H | -0.314467 | 4.671607 | -0.755643 |
| H | -2.273347 | 0.473982 | -1.737581 |
| H | -2.705983 | -2.334174 | -0.905654 |
| H | -1.620027 | -2.016791 | 1.586610 |

**5.xyz**

57

| | | | |
|---|---|---|---|
| C | 2.095463 | 2.226895 | -0.305812 |
| C | 2.459262 | 1.224072 | 0.641558 |
| C | 3.809569 | 1.253013 | 1.126094 |
| C | 4.733646 | 2.237674 | 0.686658 |
| C | 4.336751 | 3.215105 | -0.266786 |
| C | 3.012087 | 3.208815 | -0.778655 |
| Si | 1.180338 | -0.148673 | 1.197358 |
| Ir | -0.765652 | 0.171676 | -0.166497 |
| S | 0.354887 | 2.229257 | -1.012560 |
| C | -0.363439 | 3.777614 | -0.162019 |
| C | 0.967990 | -0.063813 | 3.120449 |
| C | 1.881882 | -1.891259 | 0.671027 |
| C | 1.565007 | -2.406535 | -0.625110 |
| C | 2.043580 | -3.661380 | -1.091657 |
| C | 2.887940 | -4.432144 | -0.246650 |
| C | 3.223017 | -3.954138 | 1.048732 |
| C | 2.720605 | -2.703927 | 1.502478 |
| S | 0.393615 | -1.441417 | -1.729139 |
| C | 1.606887 | -0.656111 | -2.979750 |
| C | -2.238759 | -0.365915 | 1.369334 |
| C | -2.295197 | -1.422781 | 0.372391 |
| C | -3.356855 | -1.533063 | -0.768809 |
| C | -4.875863 | -1.534786 | -0.272440 |

| | | | |
|---|---|---|---|
| C | -5.298378 | -0.463336 | 0.805135 |
| C | -5.083408 | 1.065088 | 0.479203 |
| C | -3.610613 | 1.552103 | 0.097113 |
| C | -2.470371 | 1.037838 | 1.040391 |
| H | -1.814076 | -0.605122 | 2.359371 |
| H | -2.227535 | 1.735562 | 1.863442 |
| H | -1.911369 | -2.398489 | 0.723754 |
| H | -3.417549 | 1.286248 | -0.966091 |
| H | -3.602440 | 2.664830 | 0.127901 |
| H | -3.166319 | -2.480093 | -1.320648 |
| H | -3.235445 | -0.726108 | -1.525859 |
| H | -5.423841 | 1.647028 | 1.367266 |
| H | -5.748687 | 1.366437 | -0.364045 |
| H | -5.512192 | -1.426943 | -1.182176 |
| H | -5.104256 | -2.541026 | 0.149703 |
| H | -4.808221 | -0.705372 | 1.775882 |
| H | -6.388990 | -0.603390 | 0.991981 |
| H | 0.997804 | -0.001042 | -3.634599 |
| H | 2.047809 | -1.481439 | -3.572653 |
| H | 2.392697 | -0.079545 | -2.457026 |
| H | -1.399882 | 3.888179 | -0.535351 |
| H | 0.247745 | 4.646514 | -0.475441 |
| H | -0.342840 | 3.647875 | 0.936377 |
| H | 0.380540 | -0.920326 | 3.518480 |
| H | 0.468098 | 0.881838 | 3.426305 |
| H | 1.967199 | -0.081079 | 3.614107 |
| H | 1.756666 | -4.043548 | -2.085697 |
| H | 3.266245 | -5.407317 | -0.596279 |
| H | 3.867492 | -4.558760 | 1.709099 |
| H | 2.985535 | -2.362507 | 2.518344 |
| H | 4.148333 | 0.494726 | 1.854028 |
| H | 5.764000 | 2.238774 | 1.080677 |
| H | 5.055203 | 3.973613 | -0.620033 |
| H | 2.707890 | 3.953255 | -1.533619 |

**6.xyz**

57

| | | | |
|---|---|---|---|
| C | -2.577173 | 2.746197 | 1.174084 |
| C | -1.665916 | 1.890105 | 0.525040 |
| C | -1.145360 | 2.327980 | -0.704806 |
| C | -1.496287 | 3.555783 | -1.280937 |
| C | -2.413459 | 4.376817 | -0.615370 |
| C | -2.950440 | 3.972372 | 0.611661 |
| Si | -1.116371 | 0.193983 | 1.215002 |
| C | -1.246414 | 0.239706 | 3.102765 |
| S | 0.072800 | 1.309326 | -1.593572 |

| | | | |
|---|---|---|---|
| Ir | 0.942455 | -0.317507 | 0.103698 |
| C | 2.759426 | -0.448601 | -1.344789 |
| C | 3.028759 | -1.262409 | -0.234962 |
| C | 4.000476 | -0.883389 | 0.876208 |
| C | 3.329231 | -0.189340 | 2.081910 |
| C | 2.115139 | 0.640193 | 1.713923 |
| C | 2.060033 | 1.534072 | 0.615707 |
| C | 3.249654 | 1.840212 | -0.296010 |
| C | 3.341266 | 0.936146 | -1.546360 |
| C | -2.372861 | -1.092910 | 0.560021 |
| C | -1.967876 | -2.054588 | -0.376741 |
| C | -2.852959 | -2.973665 | -0.958864 |
| C | -4.193489 | -2.957574 | -0.564890 |
| C | -4.632634 | -2.022812 | 0.381425 |
| C | -3.734698 | -1.101399 | 0.927697 |
| S | -0.230085 | -2.107141 | -0.927735 |
| C | 0.290468 | -3.689002 | -0.154501 |
| C | -1.015269 | 0.487025 | -2.822843 |
| H | -1.051613 | 3.876853 | -2.225918 |
| H | -2.692577 | 5.338917 | -1.049351 |
| H | -3.654936 | 4.620377 | 1.137580 |
| H | -2.998412 | 2.455326 | 2.140476 |
| H | -4.102135 | -0.369024 | 1.652253 |
| H | -4.894920 | -3.669304 | -1.004685 |
| H | -5.681467 | -2.008191 | 0.685221 |
| H | -2.510254 | -3.688630 | -1.711223 |
| H | -0.396976 | -0.222708 | -3.387453 |
| H | -1.392883 | 1.264626 | -3.498542 |
| H | -1.848865 | -0.028133 | -2.330178 |
| H | 1.337813 | -3.865043 | -0.427840 |
| H | -0.334297 | -4.485857 | -0.576747 |
| H | 0.173256 | -3.632129 | 0.933329 |
| H | 2.856860 | -2.334301 | -0.358437 |
| H | 3.012261 | -0.948330 | 2.813267 |
| H | 4.054041 | 0.458778 | 2.609152 |
| H | 4.173170 | 1.773713 | 0.299674 |
| H | 3.177186 | 2.889209 | -0.618438 |
| H | 2.410298 | -0.949276 | -2.255061 |
| H | 2.812406 | 1.418386 | -2.381359 |
| H | 4.393894 | 0.843542 | -1.871704 |
| H | 4.791153 | -0.244312 | 0.454705 |
| H | 4.506370 | -1.795253 | 1.226165 |
| H | 1.319842 | 2.335936 | 0.706702 |
| H | 1.447795 | 0.851356 | 2.553833 |
| H | 1.056261 | -1.349428 | 1.311236 |
| H | -2.293322 | 0.364041 | 3.424010 |
| H | -0.879913 | -0.700659 | 3.541454 |
| H | -0.671048 | 1.071344 | 3.537816 |

**5_l1.xyz**

57

| | | | |
|---|---|---|---|
| C | 2.831787 | -2.646063 | 1.463799 |
| C | 1.950553 | -1.857725 | 0.653153 |
| C | 1.604413 | -2.389679 | -0.628832 |
| C | 2.095107 | -3.637642 | -1.101106 |
| C | 2.981958 | -4.383614 | -0.277568 |
| C | 3.346783 | -3.888674 | 1.003297 |
| S | 0.379810 | -1.457510 | -1.703477 |
| C | 1.539607 | -0.655408 | -2.993491 |
| Si | 1.230071 | -0.126440 | 1.190166 |
| Ir | -0.767786 | 0.142152 | -0.108900 |
| C | 1.081638 | -0.028190 | 3.118346 |
| C | 2.458695 | 1.270675 | 0.582049 |
| C | 2.042774 | 2.255828 | -0.362338 |
| C | 2.921130 | 3.254322 | -0.871693 |
| C | 4.260020 | 3.296886 | -0.400360 |
| C | 4.708764 | 2.338177 | 0.549067 |
| C | 3.822059 | 1.336166 | 1.024845 |
| S | 0.284027 | 2.206486 | -1.019333 |
| C | -0.449246 | 3.756892 | -0.185331 |
| C | -2.424575 | 0.986515 | 1.159995 |
| C | -3.620203 | 1.538537 | 0.307527 |
| C | -5.051595 | 0.959130 | 0.714034 |
| C | -5.586962 | -0.245443 | -0.150795 |
| C | -4.836714 | -1.629287 | -0.081959 |
| C | -3.338645 | -1.643285 | -0.634365 |
| C | -2.249797 | -1.474492 | 0.475488 |
| C | -2.182523 | -0.419731 | 1.471710 |
| H | -1.721106 | -0.660386 | 2.444688 |
| H | -2.137781 | 1.668806 | 1.981617 |
| H | -1.833588 | -2.438788 | 0.821376 |
| H | -3.472171 | 1.381655 | -0.786347 |
| H | -3.628814 | 2.641737 | 0.450314 |
| H | -3.138921 | -2.617779 | -1.130868 |
| H | -3.251816 | -0.878291 | -1.441550 |
| H | -5.049133 | 0.688091 | 1.795581 |
| H | -5.786947 | 1.789211 | 0.606146 |
| H | -4.850651 | -2.024868 | 0.960391 |
| H | -5.423101 | -2.351740 | -0.694763 |
| H | -6.642945 | -0.428181 | 0.158298 |
| H | -5.635882 | 0.079476 | -1.219070 |
| H | 0.899619 | -0.012977 | -3.631077 |
| H | 1.976682 | -1.474755 | -3.597362 |
| H | 2.330623 | -0.063887 | -2.495983 |
| H | -1.495308 | 3.836755 | -0.539223 |
| H | 0.135925 | 4.631562 | -0.530664 |
| H | -0.403574 | 3.652584 | 0.914944 |

| | | | |
|---|---|---|---|
| H | 0.520198 | -0.888625 | 3.544130 |
| H | 0.580098 | 0.913945 | 3.431979 |
| H | 2.097542 | -0.027162 | 3.577024 |
| H | 1.785641 | -4.033473 | -2.082943 |
| H | 3.370233 | -5.353114 | -0.632024 |
| H | 4.024521 | -4.474139 | 1.647413 |
| H | 3.120555 | -2.291492 | 2.468565 |
| H | 4.200660 | 0.593485 | 1.749218 |
| H | 5.750139 | 2.367401 | 0.911739 |
| H | 4.949049 | 4.068738 | -0.782174 |
| H | 2.577174 | 3.983680 | -1.624273 |

**5_I2.xyz**

57

| | | | |
|---|---|---|---|
| C | -2.655402 | 2.706732 | 1.197051 |
| C | -1.753571 | 1.868681 | 0.511630 |
| C | -1.252141 | 2.332967 | -0.719623 |
| C | -1.618552 | 3.573886 | -1.256322 |
| C | -2.529721 | 4.374803 | -0.559063 |
| C | -3.045413 | 3.941868 | 0.667312 |
| Si | -1.205322 | 0.167959 | 1.181118 |
| C | -1.201408 | 0.195684 | 3.068552 |
| S | -0.037028 | 1.344992 | -1.644505 |
| Ir | 0.786706 | -0.287627 | 0.062577 |
| C | 2.146752 | 0.517732 | 1.601576 |
| C | 3.396792 | -0.258593 | 2.024341 |
| C | 4.669213 | -0.306656 | 1.162462 |
| C | 4.602239 | -1.060495 | -0.172911 |
| C | 3.580895 | -0.479494 | -1.173078 |
| C | 3.657290 | 1.016187 | -1.268364 |
| C | 2.974053 | 1.863275 | -0.478017 |
| C | 1.989012 | 1.499093 | 0.574259 |
| C | -2.448018 | -1.151665 | 0.577726 |
| C | -2.049985 | -2.109297 | -0.367417 |
| C | -2.925806 | -3.070932 | -0.889586 |
| C | -4.244369 | -3.100203 | -0.427003 |
| C | -4.674270 | -2.166049 | 0.523867 |
| C | -3.788069 | -1.201339 | 1.012582 |
| S | -0.347731 | -2.058517 | -1.007439 |
| C | 0.321659 | -3.638895 | -0.357900 |
| C | -1.140519 | 0.550499 | -2.878796 |
| H | -0.628681 | 1.045512 | 3.469277 |
| H | -0.776822 | -0.736216 | 3.470278 |
| H | -2.231683 | 0.278871 | 3.451973 |
| H | -1.189709 | 3.918782 | -2.200175 |
| H | -2.821847 | 5.343840 | -0.968473 |
| H | -3.745533 | 4.573693 | 1.217998 |

| | | | |
|---|---|---|---|
| H | -3.058115 | 2.394779 | 2.164895 |
| H | -4.147699 | -0.473772 | 1.745854 |
| H | -4.937715 | -3.847364 | -0.818106 |
| H | -5.706452 | -2.187539 | 0.879515 |
| H | -2.593764 | -3.784885 | -1.647336 |
| H | -0.524996 | -0.137954 | -3.471741 |
| H | -1.534280 | 1.342245 | -3.528212 |
| H | -1.963768 | 0.014042 | -2.391166 |
| H | 1.386675 | -3.662949 | -0.620395 |
| H | -0.202112 | -4.463424 | -0.858006 |
| H | 0.187562 | -3.684323 | 0.728364 |
| H | 1.500651 | 0.680854 | 2.469988 |
| H | 4.375524 | -2.127703 | -0.006725 |
| H | 3.091040 | -1.281379 | 2.302887 |
| H | 3.688379 | 0.216753 | 2.979972 |
| H | 3.112410 | 2.939880 | -0.620381 |
| H | 2.547253 | -0.810946 | -0.842587 |
| H | 4.379028 | 1.428650 | -1.980291 |
| H | 5.024186 | 0.720188 | 0.984389 |
| H | 5.446342 | -0.787446 | 1.779267 |
| H | 1.295368 | 2.311841 | 0.819929 |
| H | 1.119030 | -1.417840 | 1.127236 |
| H | 3.698155 | -0.951312 | -2.161861 |
| H | 5.601895 | -1.029367 | -0.639022 |

**5_I2b.xyz**

57

| | | | |
|---|---|---|---|
| C | -3.940936 | -1.204564 | 0.865290 |
| C | -2.554357 | -1.188962 | 0.496642 |
| C | -2.132582 | -2.175970 | -0.441733 |
| C | -3.020273 | -3.128370 | -1.017758 |
| C | -4.383061 | -3.121010 | -0.618614 |
| C | -4.841554 | -2.159542 | 0.323500 |
| Si | -1.292554 | 0.140596 | 1.190104 |
| Ir | 0.799043 | -0.327575 | 0.129520 |
| C | 2.150440 | 1.501535 | 0.648008 |
| C | 3.283253 | 1.948808 | -0.335946 |
| C | 3.822741 | 0.996379 | -1.482946 |
| C | 4.859894 | -0.119252 | -1.102058 |
| C | 4.323039 | -1.240656 | -0.116085 |
| C | 4.411229 | -0.892309 | 1.377488 |
| S | -0.341584 | -2.168448 | -1.016621 |
| C | 0.296721 | -3.809997 | -0.283629 |
| C | -1.838361 | 1.903075 | 0.545161 |
| C | -2.751320 | 2.733788 | 1.276914 |
| C | -3.165652 | 4.000231 | 0.782651 |

| | | | |
|---|---|---|---|
| C | -2.663293 | 4.481060 | -0.455605 |
| C | -1.740432 | 3.695743 | -1.197777 |
| C | -1.350069 | 2.420905 | -0.698836 |
| S | -0.078310 | 1.464414 | -1.690413 |
| C | -1.149342 | 0.704654 | -3.069281 |
| C | -1.324660 | 0.090601 | 3.124242 |
| C | 2.291110 | 0.584255 | 1.744690 |
| C | 3.527164 | -0.178583 | 2.134837 |
| H | -0.740576 | 0.924316 | 3.572777 |
| H | -0.907974 | -0.871155 | 3.496157 |
| H | -2.370515 | 0.168367 | 3.501391 |
| H | -1.323972 | 4.079894 | -2.143925 |
| H | -2.971609 | 5.468535 | -0.837954 |
| H | -3.871173 | 4.613667 | 1.368278 |
| H | -3.146936 | 2.391881 | 2.249022 |
| H | -4.326069 | -0.460322 | 1.584413 |
| H | -5.081971 | -3.856823 | -1.050296 |
| H | -5.901222 | -2.150807 | 0.629801 |
| H | -2.667960 | -3.859870 | -1.764397 |
| H | -0.478136 | 0.056945 | -3.668290 |
| H | -1.527391 | 1.537482 | -3.693745 |
| H | -1.987276 | 0.121254 | -2.643709 |
| H | 1.382669 | -3.844292 | -0.498606 |
| H | -0.225017 | -4.633770 | -0.809135 |
| H | 0.103182 | -3.834570 | 0.804696 |
| H | 1.621420 | 0.764387 | 2.602769 |
| H | 1.151929 | -1.446388 | 1.221419 |
| H | 3.264426 | -1.483547 | -0.396414 |
| H | 5.297634 | -1.294938 | 1.902768 |
| H | 3.735521 | -0.105638 | 3.220093 |
| H | 4.148936 | 2.268940 | 0.294495 |
| H | 2.907799 | 2.869031 | -0.833998 |
| H | 4.311686 | 1.659158 | -2.233501 |
| H | 2.959884 | 0.525827 | -2.013728 |
| H | 4.904898 | -2.173846 | -0.288924 |
| H | 5.177361 | -0.616175 | -2.047789 |
| H | 5.775850 | 0.345509 | -0.668348 |
| H | 1.414155 | 2.305518 | 0.827764 |

**5_I3.xyz**

57

| | | | |
|---|---|---|---|
| C | 3.212212 | -2.189617 | 1.317396 |
| C | 2.190593 | -1.558295 | 0.581053 |
| C | 1.879938 | -2.098374 | -0.681489 |
| C | 2.543533 | -3.213164 | -1.206454 |
| C | 3.564304 | -3.808167 | -0.456709 |
| C | 3.894885 | -3.298549 | 0.804008 |

| | | | |
|---|---|---|---|
| Si | 1.223460 | -0.024966 | 1.173897 |
| C | 1.150504 | -0.009946 | 3.061730 |
| S | 0.523704 | -1.369656 | -1.649509 |
| C | 1.486573 | -0.339422 | -2.832504 |
| C | 2.114103 | 1.541093 | 0.543899 |
| C | 1.463172 | 2.373429 | -0.378404 |
| C | 2.067053 | 3.508476 | -0.935374 |
| C | 3.362755 | 3.844948 | -0.532290 |
| C | 4.038925 | 3.042565 | 0.395767 |
| C | 3.423849 | 1.901490 | 0.920203 |
| S | -0.220425 | 1.944636 | -0.931435 |
| C | -1.174292 | 3.274994 | -0.098701 |
| Ir | -0.772944 | -0.107273 | -0.031345 |
| C | -2.182326 | -1.237218 | 1.428749 |
| C | -3.464028 | -1.984894 | 0.978731 |
| C | -3.722328 | -2.091336 | -0.539353 |
| C | -3.466849 | - 0.753105 | -1.264555 |
| C | -4.406635 | 0.357228 | -0.919621 |
| C | -4.378167 | 1.104376 | 0.198026 |
| C | -3.452214 | 1.085527 | 1.390798 |
| C | -2.159645 | 0.268620 | 1.500901 |
| H | 2.260087 | -3.623420 | -2.178697 |
| H | 4.088633 | -4.680187 | -0.852576 |
| H | 4.682095 | -3.773379 | 1.393518 |
| H | 3.478328 | -1.816267 | 2.310322 |
| H | 3.975317 | 1.279685 | 1.631381 |
| H | 3.847267 | 4.728656 | -0.952113 |
| H | 5.053284 | 3.304605 | 0.703815 |
| H | 1.543637 | 4.118966 | -1.675480 |
| H | 0.761509 | 0.195102 | -3.459901 |
| H | 2.086973 | -1.013255 | -3.456491 |
| H | 2.131057 | 0.366688 | -2.294974 |
| H | -2.227605 | 3.111764 | -0.359552 |
| H | -0.833709 | 4.235726 | -0.506495 |
| H | -1.019030 | 3.232167 | 0.985277 |
| H | -3.186257 | 2.134683 | 1.612399 |
| H | -4.081012 | 0.805618 | 2.264176 |
| H | -1.636415 | 0.608300 | 2.405014 |
| H | -1.280993 | -1.672134 | 0.650323 |
| H | 0.670555 | -0.916766 | 3.460132 |
| H | 2.170406 | 0.035412 | 3.478566 |
| H | 0.608255 | 0.870533 | 3.436773 |
| H | -4.753600 | -2.440006 | -0.708385 |
| H | -3.051138 | -2.853549 | -0.970640 |
| H | -3.436826 | -3.001139 | 1.399713 |
| H | -4.309349 | -1.468275 | 1.463381 |
| H | -1.745224 | -1.692171 | 2.329163 |
| H | -3.329818 | -0.882765 | -2.345495 |
| H | -2.467389 | -0.513248 | -0.806881 |
| H | -5.170993 | 1.854447 | 0.303824 |

H -5.207785 0.550092 -1.640833

**5_l4.xyz**

57

C 4.062074 -0.924810 0.934099
C 2.701449 -0.996285 0.482526
C 2.396429 -2.018387 -0.465999
C 3.366471 -2.951516 -0.931035
C 4.704323 -2.841586 -0.469947
C 5.052157 -1.824924 0.460555
Si 1.323173 0.212454 1.166769
C 1.408079 0.214518 3.101068
S 0.623624 -2.239306 -1.053050
C 0.781054 -1.926022 -2.926730
C 1.639046 2.020628 0.491389
C 1.028817 2.489580 -0.717237
C 1.291617 3.782717 -1.249503
C 2.160955 4.659648 -0.545483
C 2.773075 4.236070 0.662784
C 2.517655 2.932353 1.166056
S -0.044069 1.280864 -1.664752
Ir -0.739836 -0.516113 0.159975
C -2.185967 -0.224161 1.930689
C -2.128758 1.006067 1.191317
C -3.349241 1.708239 0.513670
C -4.402251 1.038016 -0.397076
C -4.553483 -0.228371 -0.871938
C -3.668651 -1.461156 -0.623721
C -3.779221 -2.108123 0.809918
C -3.446064 -1.148877 2.019853
C -1.370956 2.363188 -2.486368
H 1.181010 -0.797484 3.503318
H 0.695064 0.942511 3.548076
H 2.428624 0.488193 3.454345
H 3.091766 -3.758872 -1.629998
H 5.464891 -3.555578 -0.827669
H 6.090468 -1.740425 0.823207
H 4.357152 -0.150845 1.664089
H 3.004431 2.626466 2.108145
H 2.358972 5.666724 -0.949327
H 3.446350 4.916037 1.211345
H 0.839732 4.117683 -2.196542
H -0.250993 -1.947399 -3.331070
H 1.364895 -2.768039 -3.346797
H 1.270083 -0.956441 -3.129033
H -2.221201 1.692208 -2.717749
H -0.947111 2.775406 -3.422763

| | | | |
|---|---|---|---|
| H | -1.686829 | 3.174399 | -1.804636 |
| H | -1.435292 | 1.767930 | 1.592389 |
| H | -0.755487 | -1.796643 | 1.129345 |
| H | -3.922825 | 2.143483 | 1.376086 |
| H | -2.973899 | 2.611599 | -0.019846 |
| H | -5.182858 | 1.766106 | -0.694707 |
| H | -5.443038 | -0.415409 | -1.502810 |
| H | -3.900605 | -2.242885 | -1.381807 |
| H | -2.580027 | -1.202251 | -0.839941 |
| H | -3.106736 | -2.994493 | 0.844565 |
| H | -4.817105 | -2.487473 | 0.950904 |
| H | -3.337916 | -1.780603 | 2.928563 |
| H | -4.321261 | -0.482178 | 2.204173 |
| H | -1.531841 | -0.291121 | 2.814810 |

**5_I4b.xyz**

57

| | | | |
|---|---|---|---|
| C | 3.650784 | -1.498299 | 1.204998 |
| C | 2.444699 | -1.159404 | 0.561726 |
| C | 2.213502 | -1.743829 | -0.695253 |
| C | 3.113558 | -2.627805 | -1.302265 |
| C | 4.305930 | -2.934965 | -0.637925 |
| C | 4.571245 | -2.372526 | 0.615471 |
| Si | 1.147132 | 0.062804 | 1.263120 |
| C | 1.207557 | 0.025623 | 3.152390 |
| S | 0.649888 | -1.412059 | -1.573561 |
| C | 1.232879 | -0.230052 | -2.855162 |
| C | 1.719225 | 1.768033 | 0.621267 |
| C | 1.004354 | 2.417928 | -0.394693 |
| C | 1.473639 | 3.586853 | -1.015259 |
| C | 2.672414 | 4.154335 | -0.576312 |
| C | 3.395408 | 3.548080 | 0.458739 |
| C | 2.928043 | 2.365405 | 1.037116 |
| S | -0.589062 | 1.750484 | -0.986294 |
| C | -1.653622 | 3.132924 | -0.420646 |
| Ir | -0.831811 | -0.484412 | 0.066699 |
| C | -2.155924 | -1.165985 | 1.706948 |
| C | -2.974838 | -2.190614 | 0.929156 |
| C | -2.503689 | -1.978917 | -0.512244 |
| C | -2.776889 | -0.881144 | -1.326666 |
| C | -3.897582 | 0.131667 | -1.235245 |
| C | -4.548197 | 0.381119 | 0.128217 |
| C | -3.621123 | 0.946092 | 1.214807 |
| C | -2.332538 | 0.233742 | 1.595455 |
| H | 2.885192 | -3.087481 | -2.267069 |
| H | 5.016075 | -3.627409 | -1.094074 |
| H | 5.495561 | -2.624574 | 1.139736 |

| | | | |
|---|---|---|---|
| H | 3.873532 | -1.079009 | 2.190149 |
| H | 3.519630 | 1.891695 | 1.825894 |
| H | 3.043719 | 5.065698 | -1.049174 |
| H | 4.331440 | 3.992602 | 0.803341 |
| H | 0.917936 | 4.050636 | -1.834267 |
| H | 0.350418 | 0.128751 | -3.399694 |
| H | 1.883486 | -0.795362 | -3.534433 |
| H | 1.782236 | 0.605065 | -2.405104 |
| H | -2.672596 | 2.954297 | -0.780997 |
| H | -1.262750 | 4.044118 | -0.889755 |
| H | -1.624230 | 3.228002 | 0.670855 |
| H | -3.556410 | 1.084426 | -1.677554 |
| H | -3.384528 | 1.991513 | 0.976631 |
| H | -4.200021 | 1.004413 | 2.156933 |
| H | -4.059403 | -2.099237 | 1.077289 |
| H | -2.687736 | -3.201307 | 1.249682 |
| H | -2.381633 | -0.972012 | -2.345923 |
| H | -1.984586 | -2.823421 | -0.972390 |
| H | -5.047776 | -0.533287 | 0.476781 |
| H | -5.362935 | 1.109984 | -0.015015 |
| H | -1.556595 | -1.536059 | 2.541678 |
| H | -1.766738 | 0.806933 | 2.339147 |
| H | -0.342613 | -1.862891 | 0.700614 |
| H | 0.473827 | 0.718759 | 3.591622 |
| H | 1.004686 | -0.984425 | 3.540230 |
| H | 2.199163 | 0.330119 | 3.524553 |
| H | -4.682994 | -0.224427 | -1.929254 |

**5_I5.xyz**

57

| | | | |
|---|---|---|---|
| C | 1.401167 | -2.366684 | -0.675968 |
| C | 1.895259 | -1.845716 | 0.557398 |
| C | 2.876786 | -2.638135 | 1.238203 |
| C | 3.334517 | -3.873365 | 0.703009 |
| C | 2.816552 | -4.355780 | -0.529074 |
| C | 1.833112 | -3.603460 | -1.227567 |
| Si | 1.204027 | -0.128036 | 1.188169 |
| C | 1.205125 | -0.087243 | 3.128072 |
| S | 0.048299 | -1.426566 | -1.594426 |
| C | 1.069945 | -0.616559 | -2.994269 |
| C | 2.409831 | 1.275291 | 0.534702 |
| C | 3.791098 | 1.332017 | 0.921994 |
| C | 4.669495 | 2.322972 | 0.409836 |
| C | 4.193120 | 3.284797 | -0.522375 |
| C | 2.835332 | 3.255565 | -0.935936 |
| C | 1.964972 | 2.266453 | -0.392793 |
| S | 0.180149 | 2.262403 | -0.980860 |

| | | | |
|---|---|---|---|
| C | -0.490486 | 3.779601 | -0.040418 |
| Ir | -0.884511 | 0.132802 | 0.020025 |
| C | -3.421702 | 0.994201 | -0.951676 |
| C | -4.109896 | 1.506035 | 0.340211 |
| C | -3.877117 | 0.672927 | 1.669756 |
| C | -2.436599 | 0.046585 | 1.829043 |
| C | -2.044889 | -1.275591 | 1.164970 |
| C | -3.052631 | -2.203836 | 0.412916 |
| C | -3.986970 | -1.528010 | -0.685637 |
| C | -3.367160 | -0.309476 | -1.400921 |
| H | 1.407655 | -3.986922 | -2.170463 |
| H | 3.160793 | -5.319296 | -0.940742 |
| H | 4.088452 | -4.463302 | 1.251355 |
| H | 3.288602 | -2.293154 | 2.202633 |
| H | 4.191620 | 0.587330 | 1.632399 |
| H | 4.873918 | 4.048628 | -0.934214 |
| H | 5.725160 | 2.340525 | 0.729892 |
| H | 2.466762 | 3.988948 | -1.672894 |
| H | 0.372923 | 0.029702 | -3.563621 |
| H | 1.443052 | -1.438517 | -3.636713 |
| H | 1.907915 | -0.030754 | -2.572881 |
| H | -1.556206 | 3.885392 | -0.324717 |
| H | 0.076106 | 4.670229 | -0.375592 |
| H | -0.382237 | 3.630626 | 1.051437 |
| H | 0.792597 | 0.876097 | 3.504356 |
| H | 0.608290 | -0.919494 | 3.563718 |
| H | 2.241865 | -0.173895 | 3.527174 |
| H | -3.074732 | 1.783857 | -1.642639 |
| H | -4.061396 | 1.350293 | 2.532711 |
| H | -4.616480 | -0.150970 | 1.761823 |
| H | -3.696644 | -2.738671 | 1.154427 |
| H | -2.441596 | -2.994980 | -0.076997 |
| H | -2.946075 | -0.484508 | -2.407414 |
| H | -4.238983 | -2.297587 | -1.447439 |
| H | -4.951840 | -1.227391 | -0.222439 |
| H | -5.209132 | 1.582751 | 0.156828 |
| H | -3.766977 | 2.549713 | 0.518078 |
| H | -1.418503 | -1.899966 | 1.833703 |
| H | -2.074103 | 0.102636 | 2.876743 |
| H | -1.668146 | 0.990494 | 1.398884 |

**5_TS1.xyz**

57

| | | | |
|---|---|---|---|
| C | -2.978962 | 2.558103 | 1.288867 |
| C | -2.000415 | 1.796436 | 0.567370 |
| C | -1.536303 | 2.353272 | -0.666547 |
| C | -2.002499 | 3.596274 | -1.174572 |

| | | | |
|---|---|---|---|
| C | -2.985477 | 4.313107 | -0.441330 |
| C | -3.469236 | 3.795654 | 0.789358 |
| S | -0.192021 | 1.469529 | -1.634244 |
| C | -1.211219 | 0.648030 | -3.022840 |
| Si | -1.287210 | 0.081512 | 1.174059 |
| Ir | 0.790135 | -0.116386 | 0.011387 |
| C | -1.245475 | 0.019332 | 3.109453 |
| C | -2.444479 | -1.351253 | 0.510133 |
| C | -1.965063 | -2.315316 | -0.427709 |
| C | -2.797032 | -3.335363 | -0.972170 |
| C | -4.149400 | -3.422383 | -0.548147 |
| C | -4.659269 | -2.486048 | 0.392414 |
| C | -3.819466 | -1.462655 | 0.905919 |
| S | -0.191218 | -2.208504 | -1.031458 |
| C | 0.570807 | -3.727612 | -0.167595 |
| C | 2.350105 | 0.170709 | 1.756240 |
| C | 2.037877 | 1.420094 | 1.021082 |
| C | 3.057572 | 2.181887 | 0.200518 |
| C | 3.898958 | 1.714993 | -0.767702 |
| C | 3.977332 | 0.284972 | -1.332529 |
| C | 4.976120 | -0.669337 | -0.553033 |
| C | 4.382723 | -1.379396 | 0.716603 |
| C | 3.777622 | -0.488078 | 1.875065 |
| H | 3.114688 | 3.256805 | 0.451582 |
| H | 1.377281 | 2.103101 | 1.587529 |
| H | 4.623173 | 2.430300 | -1.199270 |
| H | 1.510556 | -1.082525 | 1.143803 |
| H | 1.801708 | 0.086983 | 2.713902 |
| H | 4.294522 | 0.344165 | -2.398382 |
| H | 2.957838 | -0.191265 | -1.356456 |
| H | 4.474183 | 0.355836 | 2.093393 |
| H | 3.746236 | -1.121788 | 2.790038 |
| H | 5.881002 | -0.085501 | -0.269369 |
| H | 5.321850 | -1.468552 | -1.248750 |
| H | 5.202507 | -1.978391 | 1.177440 |
| H | 3.608480 | -2.119508 | 0.399019 |
| H | -0.503747 | 0.023411 | -3.604158 |
| H | -1.613208 | 1.462279 | -3.658866 |
| H | -2.029786 | 0.036810 | -2.598080 |
| H | 1.643181 | -3.739158 | -0.446216 |
| H | 0.066281 | -4.630519 | -0.564021 |
| H | 0.444206 | -3.644172 | 0.928981 |
| H | -0.678229 | 0.874252 | 3.542767 |
| H | -0.785787 | -0.929181 | 3.467086 |
| H | -2.278762 | 0.058202 | 3.522457 |
| H | -1.600585 | 4.009200 | -2.115097 |
| H | -3.354442 | 5.278900 | -0.823158 |
| H | -4.222716 | 4.359638 | 1.364811 |
| H | -3.362069 | 2.186783 | 2.254501 |
| H | -4.245007 | -0.739426 | 1.623960 |

| | | | |
|---|---|---|---|
| H | -5.711076 | -2.549170 | 0.718971 |
| H | -4.801160 | -4.211366 | -0.959360 |
| H | -2.405309 | -4.047778 | -1.717535 |

**5_TS2.xyz**

57

| | | | |
|---|---|---|---|
| C | -2.052170 | -2.275480 | -0.475981 |
| C | -2.510792 | -1.300868 | 0.462714 |
| C | -3.889733 | -1.377109 | 0.852828 |
| C | -4.753396 | -2.378120 | 0.334401 |
| C | -4.263941 | -3.326632 | -0.604745 |
| C | -2.908302 | -3.273322 | -1.023773 |
| Si | -1.316188 | 0.089706 | 1.150526 |
| C | -1.272925 | -0.012634 | 3.084287 |
| S | -0.274832 | -2.210509 | -1.072474 |
| C | 0.460970 | -3.737830 | -0.197748 |
| C | -1.969316 | 1.839096 | 0.584115 |
| C | -1.447911 | 2.417299 | -0.613798 |
| C | -1.855866 | 3.688418 | -1.101559 |
| C | -2.842168 | 4.413493 | -0.378749 |
| C | -3.385640 | 3.872979 | 0.817729 |
| C | -2.949526 | 2.606713 | 1.294566 |
| S | -0.101648 | 1.505503 | -1.562455 |
| C | -1.116187 | 0.780380 | -3.015409 |
| Ir | 0.762609 | -0.128838 | -0.003939 |
| C | 2.098350 | 1.156072 | 1.107873 |
| C | 3.264778 | 1.947617 | 0.404329 |
| C | 3.838319 | 1.500169 | -1.005063 |
| C | 4.882378 | 0.326234 | -1.077838 |
| C | 4.372613 | -1.080303 | -0.542723 |
| C | 4.545370 | -1.240661 | 0.975213 |
| C | 3.684243 | -0.870785 | 1.960935 |
| C | 2.317093 | -0.185880 | 1.831609 |
| H | -0.845976 | -0.981752 | 3.426276 |
| H | -2.308399 | 0.048542 | 3.492479 |
| H | -0.683801 | 0.816703 | 3.534727 |
| H | -1.410421 | 4.117437 | -2.014859 |
| H | -3.169769 | 5.401225 | -0.743745 |
| H | -4.142275 | 4.441476 | 1.384509 |
| H | -3.378421 | 2.218006 | 2.234604 |
| H | -4.299590 | -0.644415 | 1.570424 |
| H | -4.933910 | -4.098833 | -1.018612 |
| H | -5.807764 | -2.414672 | 0.656733 |
| H | -2.531015 | -3.995109 | -1.767640 |
| H | -0.423040 | 0.137280 | -3.593106 |
| H | -1.446787 | 1.638663 | -3.633318 |
| H | -1.983385 | 0.204477 | -2.641044 |

| | | | |
|---|---|---|---|
| H | 1.539320 | -3.753608 | -0.453741 |
| H | -0.037021 | -4.641591 | -0.600274 |
| H | 0.313590 | -3.655911 | 0.896391 |
| H | 1.799138 | -0.197014 | 2.810438 |
| H | 3.304676 | -1.220787 | -0.851047 |
| H | 5.511345 | -1.675236 | 1.295524 |
| H | 3.973208 | -1.056734 | 3.011940 |
| H | 4.111156 | 2.043470 | 1.128798 |
| H | 2.869492 | 2.979863 | 0.267279 |
| H | 4.335439 | 2.398392 | -1.440181 |
| H | 2.989101 | 1.271018 | -1.691989 |
| H | 4.946434 | -1.888055 | -1.050091 |
| H | 5.176787 | 0.206082 | -2.146040 |
| H | 5.809942 | 0.609138 | -0.527769 |
| H | 1.538340 | 1.859357 | 1.756819 |
| H | 1.435551 | -1.155723 | 1.022051 |

**5_TS3.xyz**

57

| | | | |
|---|---|---|---|
| C | 3.358626 | -2.142046 | 1.348300 |
| C | 2.293192 | -1.553107 | 0.590428 |
| C | 2.004021 | -2.144709 | -0.680407 |
| C | 2.722336 | -3.263169 | -1.186765 |
| C | 3.783510 | -3.809261 | -0.415004 |
| C | 4.098696 | -3.249538 | 0.852057 |
| Si | 1.258481 | -0.008962 | 1.196911 |
| C | 1.202440 | 0.024449 | 3.133349 |
| S | 0.567917 | -1.492155 | -1.695566 |
| C | 1.481764 | -0.502030 | -3.051140 |
| C | 2.140434 | 1.613354 | 0.546243 |
| C | 1.508446 | 2.461646 | -0.411029 |
| C | 2.147687 | 3.605498 | -0.969041 |
| C | 3.455206 | 3.944473 | -0.531364 |
| C | 4.111993 | 3.133174 | 0.434120 |
| C | 3.465964 | 1.981307 | 0.955561 |
| S | -0.216593 | 2.039182 | -1.031412 |
| C | -1.224185 | 3.465141 | -0.268429 |
| Ir | -0.810218 | -0.139529 | -0.003412 |
| C | -2.247815 | -1.160956 | 1.541962 |
| C | -3.468668 | -2.037789 | 1.076553 |
| C | -3.724688 | -2.187408 | -0.472765 |
| C | -3.672155 | -0.855070 | -1.318448 |
| C | -4.653472 | 0.251138 | -0.895549 |
| C | -4.597784 | 1.056529 | 0.199647 |
| C | -3.604558 | 1.162068 | 1.378764 |
| C | -2.280529 | 0.334780 | 1.551996 |
| H | 2.455002 | -3.714505 | -2.157005 |

| | | | |
|---|---|---|---|
| H | 4.346973 | -4.676603 | -0.797840 |
| H | 4.914046 | -3.680286 | 1.457657 |
| H | 3.617230 | -1.735492 | 2.341417 |
| H | 4.005701 | 1.358217 | 1.690375 |
| H | 3.958626 | 4.831541 | -0.950832 |
| H | 5.129198 | 3.393359 | 0.772470 |
| H | 1.644882 | 4.221696 | -1.733422 |
| H | 0.698582 | -0.007563 | -3.659900 |
| H | 2.040348 | -1.230982 | -3.670450 |
| H | 2.166411 | 0.241834 | -2.601945 |
| H | -2.276445 | 3.296399 | -0.568103 |
| H | -0.848363 | 4.407897 | -0.711821 |
| H | -1.108507 | 3.467474 | 0.831610 |
| H | -3.329715 | 2.238440 | 1.480863 |
| H | -4.205690 | 0.963062 | 2.306458 |
| H | -1.740446 | 0.755186 | 2.422629 |
| H | -1.189320 | -1.672066 | 0.611246 |
| H | 0.744335 | -0.899566 | 3.551594 |
| H | 2.232419 | 0.106102 | 3.551242 |
| H | 0.629026 | 0.902420 | 3.504344 |
| H | -4.724996 | -2.658318 | -0.607295 |
| H | -2.979569 | -2.898825 | -0.898539 |
| H | -3.339995 | -3.058202 | 1.500527 |
| H | -4.370433 | -1.602614 | 1.565364 |
| H | -1.721031 | -1.602899 | 2.409468 |
| H | -3.845201 | -1.116087 | -2.386696 |
| H | -2.610276 | -0.452483 | -1.316642 |
| H | -5.428182 | 1.781247 | 0.315617 |
| H | -5.520518 | 0.387498 | -1.568971 |

**5_TS4.xyz**

57

| | | | |
|---|---|---|---|
| C | 1.303204 | 2.510435 | -0.401811 |
| C | 2.002602 | 1.719192 | 0.555744 |
| C | 3.310109 | 2.174530 | 0.933493 |
| C | 3.875131 | 3.353583 | 0.379565 |
| C | 3.153234 | 4.104867 | -0.588143 |
| C | 1.859790 | 3.680455 | -0.992822 |
| Si | 1.232460 | 0.048486 | 1.224930 |
| Ir | -0.809217 | -0.251927 | 0.013510 |
| S | -0.424921 | 1.998469 | -0.956284 |
| C | -1.437631 | 3.347605 | -0.064321 |
| C | 2.389671 | -1.407842 | 0.616257 |
| C | 2.174768 | -1.987912 | -0.675081 |
| C | 2.988495 | -3.035065 | -1.189777 |
| C | 4.070988 | -3.518197 | -0.405602 |
| C | 4.313537 | -2.968713 | 0.881712 |

| | | | |
|---|---|---|---|
| C | 3.479678 | -1.933360 | 1.385308 |
| S | 0.711619 | -1.423629 | -1.707174 |
| C | 1.571682 | -0.338387 | -3.024948 |
| C | 1.186549 | 0.087774 | 3.162043 |
| C | -2.304214 | -0.060051 | 1.616122 |
| C | -3.660554 | 0.741064 | 1.578848 |
| C | -4.852216 | 0.396364 | 0.601641 |
| C | -4.554953 | 0.387126 | -0.939508 |
| C | -3.655565 | -0.717137 | -1.523337 |
| C | -3.137954 | -1.857032 | -0.964736 |
| C | -3.178641 | -2.350573 | 0.511079 |
| C | -2.173071 | -1.538494 | 1.400387 |
| H | 2.778545 | -3.481130 | -2.176485 |
| H | 4.707773 | -4.330168 | -0.795029 |
| H | 5.145579 | -3.351660 | 1.496755 |
| H | 3.683316 | -1.532453 | 2.393349 |
| H | 3.899897 | 1.597504 | 1.667521 |
| H | 3.594667 | 5.011991 | -1.033797 |
| H | 4.880589 | 3.681414 | 0.693550 |
| H | 1.304467 | 4.251451 | -1.756025 |
| H | 0.763878 | 0.099570 | -3.645061 |
| H | 2.203353 | -1.006716 | -3.642421 |
| H | 2.180544 | 0.451938 | -2.547590 |
| H | -2.493540 | 3.211395 | -0.365815 |
| H | -1.065586 | 4.325676 | -0.427035 |
| H | -1.312716 | 3.254975 | 1.030897 |
| H | -4.139141 | 1.376391 | -1.253527 |
| H | -3.402349 | 1.816671 | 1.455104 |
| H | -4.076704 | 0.669276 | 2.614721 |
| H | -4.191597 | -2.300595 | 0.961763 |
| H | -2.878827 | -3.420766 | 0.529325 |
| H | -3.460494 | -0.587098 | -2.606913 |
| H | -2.589368 | -2.532435 | -1.646002 |
| H | -5.336043 | -0.559087 | 0.896255 |
| H | -5.627958 | 1.176837 | 0.780380 |
| H | -1.769326 | -2.109165 | 2.263048 |
| H | -1.766270 | 0.255449 | 2.531657 |
| H | -0.936213 | -1.811133 | 0.681381 |
| H | 0.553168 | 0.925669 | 3.528889 |
| H | 0.793118 | -0.862330 | 3.588121 |
| H | 2.208918 | 0.242951 | 3.577480 |
| H | -5.531401 | 0.316349 | -1.481113 |

**5_TS5.xyz**

57

| | | | |
|---|---|---|---|
| C | -2.773439 | 2.610237 | 1.257803 |
| C | -1.810860 | 1.820764 | 0.584563 |
| C | -1.321660 | 2.319287 | -0.640665 |

| | | | |
|---|---|---|---|
| C | -1.744250 | 3.540048 | -1.197211 |
| C | -2.707579 | 4.296146 | -0.505110 |
| C | -3.218742 | 3.832055 | 0.720305 |
| Si | -1.130431 | 0.135149 | 1.178876 |
| C | -1.122525 | 0.110084 | 3.084912 |
| S | -0.050915 | 1.364120 | -1.549114 |
| Ir | 0.929442 | -0.170410 | -0.028522 |
| C | 2.841060 | 0.232004 | -1.438098 |
| C | 3.077156 | -0.966081 | -0.748336 |
| C | 4.073965 | -1.183634 | 0.420232 |
| C | 3.639836 | -0.607852 | 1.810948 |
| C | 2.221515 | -0.034500 | 1.860915 |
| C | 1.994360 | 1.252523 | 1.117535 |
| C | 3.232937 | 1.904106 | 0.452666 |
| C | 3.351093 | 1.612748 | -1.059055 |
| C | -2.330412 | -1.225561 | 0.553054 |
| C | -1.882034 | -2.185762 | -0.380967 |
| C | -2.731929 | -3.171349 | -0.923526 |
| C | -4.070370 | -3.224014 | -0.500496 |
| C | -4.548261 | -2.289824 | 0.437586 |
| C | -3.689384 | -1.302980 | 0.949677 |
| S | -0.147808 | -2.149620 | -0.960758 |
| C | 0.512828 | -3.624828 | -0.060416 |
| C | -1.123141 | 0.524391 | -2.801741 |
| H | -1.322907 | 3.906765 | -2.140609 |
| H | -3.043485 | 5.253841 | -0.917275 |
| H | -3.959135 | 4.429769 | 1.263496 |
| H | -3.177706 | 2.273813 | 2.220548 |
| H | -4.086759 | -0.574610 | 1.667919 |
| H | -4.740225 | -3.986929 | -0.911907 |
| H | -5.594364 | -2.326388 | 0.761352 |
| H | -2.359339 | -3.884382 | -1.668314 |
| H | -0.477916 | -0.148841 | -3.387556 |
| H | -1.540797 | 1.305325 | -3.456324 |
| H | -1.929930 | -0.038038 | -2.308675 |
| H | 1.581284 | -3.710341 | -0.312015 |
| H | -0.019510 | -4.521740 | -0.413102 |
| H | 0.379849 | -3.498870 | 1.025135 |
| H | 2.896123 | -1.870356 | -1.345232 |
| H | 3.743473 | -1.387110 | 2.586973 |
| H | 4.318127 | 0.202456 | 2.134089 |
| H | 4.154874 | 1.568240 | 0.961723 |
| H | 3.196145 | 2.995927 | 0.610883 |
| H | 2.501348 | 0.128828 | -2.479266 |
| H | 2.764229 | 2.354734 | -1.629369 |
| H | 4.400612 | 1.726504 | -1.402142 |
| H | 5.044746 | -0.743303 | 0.110954 |
| H | 4.239526 | -2.267606 | 0.514027 |
| H | 1.350452 | 1.973815 | 1.640462 |
| H | 1.774490 | -0.067936 | 2.868529 |

| | | | |
|---|---|---|---|
| H | 1.528860 | -1.031987 | 1.427891 |
| H | -2.153537 | 0.189648 | 3.476460 |
| H | -0.704413 | -0.834313 | 3.476252 |
| H | -0.546497 | 0.952540 | 3.507508 |

**5_l1b.xyz**

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| | | | |
|---|---|---|---|
| C | -3.054754 | 2.324433 | 1.227068 |
| C | -2.029047 | 1.638079 | 0.549295 |
| C | -1.601995 | 2.170449 | -0.679067 |
| C | -2.151361 | 3.331561 | -1.232967 |
| C | -3.178623 | 3.983946 | -0.541021 |
| C | -3.626343 | 3.482764 | 0.686560 |
| Si | -1.198925 | 0.033654 | 1.149034 |
| C | -1.326987 | -0.074103 | 3.033089 |
| S | -0.243148 | 1.348593 | -1.568108 |
| C | -1.205396 | 0.382326 | -2.804928 |
| C | -2.170115 | -1.435904 | 0.406541 |
| C | -1.519337 | -2.355488 | -0.428732 |
| C | -2.180093 | -3.434312 | -1.031754 |
| C | -3.541633 | -3.617480 | -0.772483 |
| C | -4.222462 | -2.720878 | 0.061142 |
| C | -3.545564 | -1.641198 | 0.637332 |
| S | 0.245541 | -2.118856 | -0.782123 |
| C | 0.963845 | -3.449864 | 0.260725 |
| Ir | 0.891082 | 0.003748 | 0.072245 |
| C | 1.785618 | 0.737446 | 1.845850 |
| C | 1.931293 | 1.770578 | 0.857595 |
| C | 3.267027 | 2.138394 | 0.178826 |
| C | 3.602397 | 1.512610 | -1.183848 |
| C | 3.385569 | 0.005357 | -1.324254 |
| C | 4.082556 | -0.964112 | -0.364889 |
| C | 3.777457 | -0.831877 | 1.139985 |
| C | 2.323007 | -0.580095 | 1.598455 |
| H | -1.778365 | 3.732683 | -2.178337 |
| H | -3.616448 | 4.893936 | -0.956062 |
| H | -4.418114 | 4.003049 | 1.229744 |
| H | -3.409871 | 1.956560 | 2.193884 |
| H | -4.100275 | -0.944330 | 1.272536 |
| H | -4.072393 | -4.454096 | -1.231114 |
| H | -5.287878 | -2.861369 | 0.255337 |
| H | -1.646835 | -4.117274 | -1.697539 |
| H | -0.487780 | -0.238573 | -3.357082 |
| H | -1.680084 | 1.095057 | -3.491172 |
| H | -1.960611 | -0.240945 | -2.311270 |
| H | 2.053829 | -3.389422 | 0.152597 |
| H | 0.605849 | -4.414402 | -0.121594 |

| | | | |
|---|---|---|---|
| H | 0.669805 | -3.312443 | 1.307459 |
| H | -0.743080 | -0.917249 | 3.432105 |
| H | -1.000654 | 0.848737 | 3.535596 |
| H | -2.378345 | -0.250681 | 3.314776 |
| H | 5.173926 | -0.870784 | -0.505240 |
| H | 4.657011 | 1.739829 | -1.419895 |
| H | 3.004323 | 2.009325 | -1.965974 |
| H | 1.100892 | 0.887061 | 2.684561 |
| H | 4.407640 | -0.040684 | 1.574075 |
| H | 1.965462 | -1.328989 | 2.313316 |
| H | 2.262546 | -0.216772 | -1.334091 |
| H | 3.642826 | -0.288064 | -2.357826 |
| H | 1.284080 | 2.636991 | 1.033067 |
| H | 3.269692 | 3.231687 | 0.050475 |
| H | 4.078821 | 1.927641 | 0.891676 |
| H | 3.832808 | -1.986903 | -0.696794 |
| H | 4.114197 | -1.760939 | 1.626022 |

**5_TS1b.xyz**

57

| | | | |
|---|---|---|---|
| C | -2.674985 | 2.774489 | 1.254624 |
| C | -1.759951 | 1.927231 | 0.546316 |
| C | -1.267405 | 2.422002 | -0.697349 |
| C | -1.643812 | 3.683205 | -1.236162 |
| C | -2.562116 | 4.490661 | -0.511097 |
| C | -3.073430 | 4.036231 | 0.733747 |
| Si | -1.183897 | 0.163503 | 1.167928 |
| C | -1.326285 | 0.119155 | 3.107855 |
| S | -0.003823 | 1.418251 | -1.656012 |
| C | -1.109400 | 0.596515 | -2.980006 |
| C | -2.472891 | -1.145525 | 0.488058 |
| C | -2.073712 | -2.207668 | -0.372669 |
| C | -2.995810 | -3.146576 | -0.921958 |
| C | -4.368466 | -3.045055 | -0.575610 |
| C | -4.804083 | -2.006427 | 0.292413 |
| C | -3.870960 | -1.069790 | 0.809376 |
| S | -0.279474 | -2.372296 | -0.881218 |
| C | 0.253638 | -3.857816 | 0.182016 |
| Ir | 1.040264 | -0.234144 | -0.063818 |
| C | 1.969427 | -0.268357 | 1.964609 |
| C | 1.992305 | 1.129118 | 1.517482 |
| C | 3.262496 | 1.908066 | 1.027717 |
| C | 3.431300 | 1.841565 | -0.526593 |
| C | 3.158773 | 0.430136 | -1.133499 |
| C | 4.199311 | -0.695707 | -0.820213 |
| C | 4.093498 | -1.262383 | 0.641706 |
| C | 2.633095 | -1.324430 | 1.223966 |

| | | | |
|---|---|---|---|
| H | -1.220849 | 4.042702 | -2.189275 |
| H | -2.858818 | 5.474384 | -0.911699 |
| H | -3.775308 | 4.667860 | 1.304329 |
| H | -3.080949 | 2.452824 | 2.228953 |
| H | -4.240303 | -0.263468 | 1.466688 |
| H | -5.091727 | -3.767051 | -0.990271 |
| H | -5.871469 | -1.921497 | 0.557960 |
| H | -2.655733 | -3.938304 | -1.610415 |
| H | -0.451727 | -0.075803 | -3.565971 |
| H | -1.498536 | 1.408464 | -3.625548 |
| H | -1.936478 | 0.036602 | -2.505638 |
| H | 1.310638 | -4.068817 | -0.073043 |
| H | -0.384494 | -4.716070 | -0.106068 |
| H | 0.137520 | -3.623731 | 1.257522 |
| H | -1.059298 | -0.884597 | 3.508622 |
| H | -0.686039 | 0.878525 | 3.609506 |
| H | -2.377673 | 0.317821 | 3.418411 |
| H | 5.231228 | -0.304586 | -1.002739 |
| H | 4.471127 | 2.144015 | -0.815857 |
| H | 2.750210 | 2.579753 | -1.003165 |
| H | 1.298724 | -0.554483 | 2.790020 |
| H | 4.722676 | -0.665242 | 1.338149 |
| H | 2.342425 | -2.336564 | 1.558041 |
| H | 1.797647 | -0.824617 | -1.397085 |
| H | 3.033074 | 0.536112 | -2.230629 |
| H | 1.273906 | 1.778621 | 2.048658 |
| H | 3.164207 | 2.969042 | 1.345906 |
| H | 4.165549 | 1.513002 | 1.542430 |
| H | 4.043734 | -1.528733 | -1.541764 |
| H | 4.510504 | -2.293194 | 0.664262 |