

Zirconocene-catalyzed dimerization of α -olefins: DFT modeling of the Zr-Al binuclear reaction mechanism

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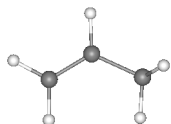
SUPPORTING INFORMATION

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S1. DFT calculations data: molecular structures, energies and cartesian coordinates

S1.1. Olefins and organoaluminium compounds

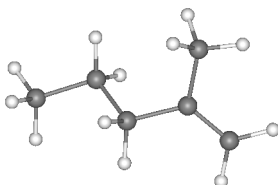
C3 Propylene



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 211398.7 (Joules/Mol) |
| | 50.52549 (Kcal/Mol) |
| Zero-point correction | 0.080517 (Hartree/Particle) |
| Thermal correction to Energy | 0.084591 |
| Thermal correction to Enthalpy | 0.085535 |
| Thermal correction to Gibbs Free Energy | 0.055526 |
| Sum of electronic and zero-point Energies | -117.762918 |
| Sum of electronic and Thermal Energies | -117.758845 |
| Sum of electronic and Thermal Enthalpies | -117.757900 |
| Sum of electronic and Thermal Free Energies | -117.787910 |

| | | | | cartesian | | | |
|---|-------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 1 | -0.27033332 | 1.58850002 | 0.00021111 | 1 | 1.70376670 | 0.18960002 | -0.88008893 |
| 6 | -0.23303331 | 0.49990001 | 0.00011111 | 1 | 1.70386672 | 0.18940002 | 0.88001108 |
| 6 | -1.37853336 | -0.18249999 | 0.00001111 | 1 | -1.38873339 | -1.27020001 | -0.00008889 |
| 6 | 1.13336670 | -0.12299998 | -0.00008889 | 1 | -2.34013319 | 0.32170001 | 0.00011111 |
| 1 | 1.06976664 | -1.21340001 | -0.00018889 | | | | |

C6 2-methylpent-1-ene

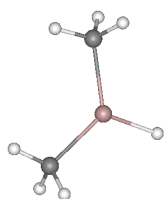


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 437755.2 (Joules/Mol) |
| | 104.62601 (Kcal/Mol) |
| Zero-point correction | 0.166732 (Hartree/Particle) |
| Thermal correction to Energy | 0.174743 |
| Thermal correction to Enthalpy | 0.175687 |
| Thermal correction to Gibbs Free Energy | 0.133949 |

| | |
|---|-------------|
| Sum of electronic and zero-point Energies | -235.567243 |
| Sum of electronic and Thermal Energies | -235.559233 |
| Sum of electronic and Thermal Enthalpies | -235.558288 |
| Sum of electronic and Thermal Free Energies | -235.600026 |

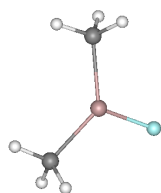
| cartesian | | | | | | | |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | 2.11586118 | -1.19247782 | 0.22433333 | 6 | -1.17973888 | 0.21752222 | 0.40563333 |
| 6 | 1.28416109 | -0.19617778 | -0.09466667 | 1 | -0.29373884 | -0.08927779 | -1.53176665 |
| 6 | 1.72116113 | 1.24642217 | -0.05856667 | 1 | -0.32783884 | -1.53517783 | -0.52496666 |
| 6 | -0.14513884 | -0.45527780 | -0.50626665 | 6 | -2.61013889 | -0.14387779 | 0.00683333 |
| 1 | 1.79176116 | -2.22987771 | 0.20183334 | 1 | -1.05713880 | 1.30512214 | 0.36623335 |
| 1 | 3.14576125 | -1.00127780 | 0.51553333 | 1 | -0.99213886 | -0.08297779 | 1.44253337 |
| 1 | 1.46976113 | 1.75102222 | -0.99796665 | 1 | -3.34213877 | 0.34442219 | 0.65543336 |
| 1 | 1.21206117 | 1.79022217 | 0.74383336 | 1 | -2.77293897 | -1.22397780 | 0.07083333 |
| 1 | 2.79746103 | 1.33322215 | 0.10443333 | 1 | -2.81703877 | 0.16242221 | -1.02326667 |

Me₂AlH



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 206187.7 (Joules/Mol) |
| | 49.28004 (Kcal/Mol) |
| Zero-point correction | 0.078533 (Hartree/Particle) |
| Thermal correction to Energy | 0.084839 |
| Thermal correction to Enthalpy | 0.085783 |
| Thermal correction to Gibbs Free Energy | 0.049544 |
| Sum of electronic and zero-point Energies | -322.675915 |
| Sum of electronic and Thermal Energies | -322.669609 |
| Sum of electronic and Thermal Enthalpies | -322.668665 |
| Sum of electronic and Thermal Free Energies | -322.704904 |

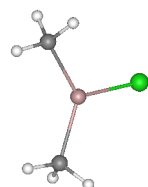
| cartesian | | | | | | | |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 13 | 0.00000995 | 0.69409001 | 0.00005000 | 1 | -2.31759000 | 0.04249001 | -0.87424999 |
| 6 | -1.71979010 | -0.24191001 | 0.00005000 | 1 | 2.31751013 | 0.04159001 | -0.87465000 |
| 6 | 1.71980989 | -0.24191001 | 0.00005000 | 1 | 2.31810999 | 0.04289000 | 0.87395000 |
| 1 | -1.62759006 | -1.33160996 | -0.00025000 | 1 | 1.62750995 | -1.33160996 | 0.00085000 |
| 1 | -2.31788993 | 0.04209000 | 0.87424999 | 1 | -0.00009005 | 2.28389001 | -0.00005000 |

Me₂AlF

| | |
|---|-----------------------------|
| Zero-point vibrational energy | 195987.5 (Joules/Mol) |
| | 46.84214 (Kcal/Mol) |
| Zero-point correction | 0.074648 (Hartree/Particle) |
| Thermal correction to Energy | 0.081673 |
| Thermal correction to Enthalpy | 0.082617 |
| Thermal correction to Gibbs Free Energy | 0.043727 |
| Sum of electronic and zero-point Energies | -422.008060 |
| Sum of electronic and Thermal Energies | -422.001034 |
| Sum of electronic and Thermal Enthalpies | -422.000090 |
| Sum of electronic and Thermal Free Energies | -422.038981 |

cartesian

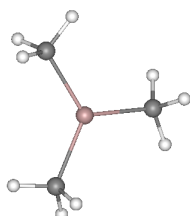
| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 9 | -0.00026001 | 2.27294993 | -0.00003000 | 1 | -2.33186007 | 0.07445005 | -0.87582999 |
| 13 | -0.00006001 | 0.58705002 | -0.00003000 | 1 | -1.71665990 | -1.33574986 | -0.00043000 |
| 6 | -1.75565994 | -0.24314994 | -0.00003000 | 1 | 2.33153987 | 0.07435006 | 0.87617004 |
| 6 | 1.75574005 | -0.24284995 | -0.00003000 | 1 | 1.71684003 | -1.33544993 | -0.00013000 |
| 1 | -2.33156013 | 0.07385004 | 0.87617004 | 1 | 2.33193994 | 0.07455003 | -0.87582999 |

Me₂AlCl

| | |
|---|-----------------------------|
| Zero-point vibrational energy | 193594.6 (Joules/Mol) |
| | 46.27022 (Kcal/Mol) |
| Zero-point correction | 0.073736 (Hartree/Particle) |
| Thermal correction to Energy | 0.081041 |
| Thermal correction to Enthalpy | 0.081985 |
| Thermal correction to Gibbs Free Energy | 0.041705 |
| Sum of electronic and zero-point Energies | -782.313017 |
| Sum of electronic and Thermal Energies | -782.305712 |
| Sum of electronic and Thermal Enthalpies | -782.304768 |
| Sum of electronic and Thermal Free Energies | -782.345048 |

| cartesian | | | | | | | |
|-----------|-------------|-------------|------------|---|-------------|-------------|-------------|
| 17 | -2.68446016 | -0.00012997 | 0.00012000 | 1 | -0.02626008 | -2.33113003 | 0.87361997 |
| 13 | -0.55946004 | -0.00002997 | 0.00052000 | 1 | -0.01906008 | -2.32693005 | -0.87867999 |
| 6 | 0.28773999 | -1.74942994 | 0.00012000 | 1 | -0.01836008 | 2.32646990 | -0.87927997 |
| 6 | 0.28753996 | 1.74947011 | 0.00022000 | 1 | -0.02736008 | 2.33156991 | 0.87301999 |
| 1 | 1.37994003 | -1.69572997 | 0.00462000 | 1 | 1.37974000 | 1.69587004 | 0.00572000 |

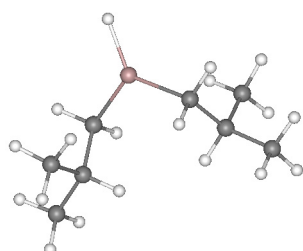
Me₃Al



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 281420.0 (Joules/Mol) |
| | 67.26100 (Kcal/Mol) |
| Zero-point correction | 0.107187 (Hartree/Particle) |
| Thermal correction to Energy | 0.114008 |
| Thermal correction to Enthalpy | 0.114952 |
| Thermal correction to Gibbs Free Energy | 0.076672 |
| Sum of electronic and zero-point Energies | -361.960633 |
| Sum of electronic and Thermal Energies | -361.953812 |
| Sum of electronic and Thermal Enthalpies | -361.952868 |
| Sum of electronic and Thermal Free Energies | -361.991148 |

| cartesian | | | | | | | |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 13 | 0.00673848 | -0.00203843 | 0.01049999 | 1 | -1.73296154 | 1.79556155 | 0.64690000 |
| 6 | 1.96193850 | -0.15483843 | 0.00679999 | 1 | -0.17346153 | 2.57096148 | 0.32240000 |
| 6 | -0.84406149 | 1.76556158 | 0.00699999 | 6 | -1.11116147 | -1.61333847 | -0.00300001 |
| 1 | 2.43583846 | 0.58226156 | 0.66439998 | 1 | -1.29386151 | -1.95633841 | 1.02420008 |
| 1 | 2.31593847 | -1.14763844 | 0.30170000 | 1 | -0.63736153 | -2.45083833 | -0.52580005 |
| 1 | 2.35833836 | 0.03676157 | -0.99900001 | 1 | -2.09526157 | -1.44513845 | -0.45260000 |
| 1 | -1.19066155 | 2.01906157 | -1.00349998 | | | | |

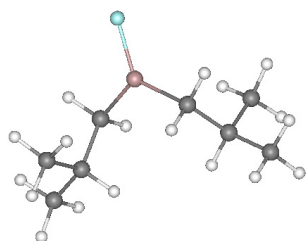
ⁱBu₂AlH



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 660384.6 (Joules/Mol) |
| | 157.83571 (Kcal/Mol) |
| Zero-point correction | 0.251527 (Hartree/Particle) |
| Thermal correction to Energy | 0.265239 |
| Thermal correction to Enthalpy | 0.266183 |
| Thermal correction to Gibbs Free Energy | 0.210572 |
| Sum of electronic and zero-point Energies | -558.270078 |
| Sum of electronic and Thermal Energies | -558.256366 |
| Sum of electronic and Thermal Enthalpies | -558.255422 |
| Sum of electronic and Thermal Free Energies | -558.311033 |

| cartesian | | | | | | | | | | | |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|--|--|--|--|
| 13 | -0.00905002 | 1.78803933 | 0.04104284 | 1 | 3.35724998 | 0.96273929 | 1.08924282 | | | | |
| 6 | 1.42435002 | 0.79663926 | -0.87575716 | 1 | 3.43794990 | -1.97056055 | -0.11415716 | | | | |
| 6 | -1.40014994 | 0.71213931 | 0.92934281 | 1 | 3.90965009 | -0.50746071 | -0.99635720 | | | | |
| 1 | 1.03775001 | 0.36833930 | -1.81295717 | 1 | 2.66144991 | -1.57246065 | -1.65705717 | | | | |
| 6 | 1.99284995 | -0.33396071 | 0.00484284 | 6 | -3.05664992 | -1.20196068 | 0.65544283 | | | | |
| 1 | 2.24175000 | 1.46893930 | -1.17325723 | 1 | -1.18355000 | -1.00696063 | -0.36185715 | | | | |
| 6 | -1.99205005 | -0.34066069 | -0.03015716 | 6 | -2.57975006 | 0.33543932 | -1.27325714 | | | | |
| 1 | -2.21134996 | 1.35123932 | 1.30594277 | 1 | -3.02935004 | -0.38956070 | -1.95875716 | | | | |
| 1 | -0.98374999 | 0.20463930 | 1.81224287 | 1 | -1.81464994 | 0.88173926 | -1.84415722 | | | | |
| 6 | 2.56664991 | 0.23533930 | 1.30634284 | 1 | -3.35505009 | 1.05503929 | -0.98575717 | | | | |
| 6 | 3.06084991 | -1.14796066 | -0.73135716 | 1 | -3.45315003 | -1.96756077 | -0.02015716 | | | | |
| 1 | 1.17375004 | -1.01656067 | 0.27134284 | 1 | -3.89385009 | -0.57706070 | 0.98654282 | | | | |
| 1 | 2.99394989 | -0.54726070 | 1.94084287 | 1 | -2.64615011 | -1.70436060 | 1.53634286 | | | | |
| 1 | 1.79834998 | 0.74753928 | 1.90314281 | 1 | -0.04805002 | 3.37653923 | 0.05234284 | | | | |

ⁱBu₂AlF

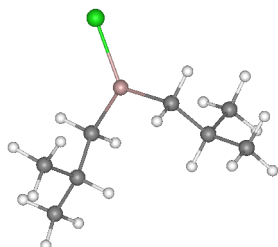


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 650028.3 (Joules/Mol) |
| | 155.36048 (Kcal/Mol) |
| Zero-point correction | 0.247583 (Hartree/Particle) |
| Thermal correction to Energy | 0.262147 |
| Thermal correction to Enthalpy | 0.263092 |
| Thermal correction to Gibbs Free Energy | 0.204262 |
| Sum of electronic and zero-point Energies | -657.602812 |

| | |
|---|-------------|
| Sum of electronic and thermal Energies | -657.588247 |
| Sum of electronic and thermal Enthalpies | -657.587303 |
| Sum of electronic and thermal Free Energies | -657.646132 |

| cartesian | | | | | | | | | | | |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|--|--|--|--|
| 13 | -0.00083931 | 1.62581789 | 0.00134998 | 1 | -3.27653933 | 1.03181791 | -1.18494999 | | | | |
| 6 | -1.48273921 | 0.71481788 | 0.88824999 | 1 | -3.69283938 | -1.86618221 | 0.04264998 | | | | |
| 6 | 1.48306072 | 0.71841788 | -0.88605005 | 1 | -4.07253933 | -0.35048211 | 0.87914997 | | | | |
| 1 | -1.15173924 | 0.26341787 | 1.83404994 | 1 | -2.96673918 | -1.51538217 | 1.62144995 | | | | |
| 6 | -2.09923935 | -0.37168211 | -0.01665002 | 6 | 3.27536082 | -1.06898212 | -0.67275000 | | | | |
| 1 | -2.25613928 | 1.44801784 | 1.15674996 | 1 | 1.33286071 | -1.12918210 | 0.22544998 | | | | |
| 6 | 2.09946084 | -0.37058210 | 0.01594998 | 6 | 2.54836082 | 0.22761787 | 1.35294998 | | | | |
| 1 | 2.25616074 | 1.45291781 | -1.15155005 | 1 | 3.01356077 | -0.52248210 | 1.99934995 | | | | |
| 1 | 1.15326071 | 0.26981789 | -1.83354998 | 1 | 1.70636070 | 0.65481788 | 1.91715002 | | | | |
| 6 | -2.54833937 | 0.23021787 | -1.35195005 | 1 | 3.27666068 | 1.02961779 | 1.18814993 | | | | |
| 6 | -3.27503920 | -1.07208216 | 0.67025000 | 1 | 3.69326067 | -1.86468208 | -0.04735002 | | | | |
| 1 | -1.33253932 | -1.12968218 | -0.22835001 | 1 | 4.07286072 | -0.34658211 | -0.87975001 | | | | |
| 1 | -3.01363921 | -0.51818210 | -2.00035024 | 1 | 2.96716070 | -1.50978208 | -1.62514997 | | | | |
| 1 | -1.70643926 | 0.65871787 | -1.91534996 | 9 | -0.00303931 | 3.30991793 | 0.00084998 | | | | |

ⁱBu₂AlCl

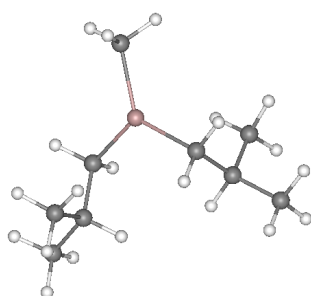


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 647950.8 (Joules/Mol) |
| | 154.86396 (Kcal/Mol) |
| Zero-point correction | 0.246791 (Hartree/Particle) |
| Thermal correction to Energy | 0.261656 |
| Thermal correction to Enthalpy | 0.262600 |
| Thermal correction to Gibbs Free Energy | 0.202152 |
| Sum of electronic and zero-point Energies | -1017.907594 |
| Sum of electronic and thermal Energies | -1017.892730 |
| Sum of electronic and thermal Enthalpies | -1017.891785 |
| Sum of electronic and thermal Free Energies | -1017.952233 |

| cartesian | | | | | | | | | | | |
|-----------|-------------|------------|------------|---|-------------|------------|-------------|--|--|--|--|
| 13 | -0.06489286 | 1.68887162 | 0.03645718 | 1 | -3.32349300 | 0.89927155 | -1.14404285 | | | | |

| | | | | | | | |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | -1.48939288 | 0.67107153 | 0.90525717 | 1 | -3.49249291 | -2.05762839 | 0.00965718 |
| 6 | 1.46210718 | 0.84097153 | -0.84174281 | 1 | -3.98659301 | -0.60142845 | 0.89065719 |
| 1 | -1.12339282 | 0.22377151 | 1.84025717 | 1 | -2.78029299 | -1.68992829 | 1.59075713 |
| 6 | -2.02699280 | -0.43702847 | -0.02354282 | 6 | 3.21220708 | -0.99402851 | -0.72484285 |
| 1 | -2.31259298 | 1.34007156 | 1.19085717 | 1 | 1.27090716 | -1.05602837 | 0.17645717 |
| 6 | 2.05410695 | -0.30512851 | 0.00285718 | 6 | 2.51980710 | 0.21337152 | 1.36685717 |
| 1 | 2.24210715 | 1.58667159 | -1.04854286 | 1 | 2.96510696 | -0.58172852 | 1.97245717 |
| 1 | 1.15020716 | 0.45337152 | -1.82264280 | 1 | 1.69090712 | 0.63567156 | 1.95235717 |
| 6 | -2.53739285 | 0.16107154 | -1.33854282 | 1 | 3.27080703 | 1.00127149 | 1.24025714 |
| 6 | -3.13449287 | -1.24852848 | 0.65475720 | 1 | 3.61580706 | -1.82712841 | -0.13994282 |
| 1 | -1.20429277 | -1.12512851 | -0.26314282 | 1 | 4.02360725 | -0.27942842 | -0.90194285 |
| 1 | -2.95069289 | -0.60562843 | -2.00064278 | 1 | 2.89050698 | -1.38312840 | -1.69504285 |
| 1 | -1.73899281 | 0.66847152 | -1.89944279 | 17 | -0.20219284 | 3.80797148 | 0.01415718 |

ⁱBu₂AlMe



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 737304.7 (Joules/Mol) |
| | 176.22006 (Kcal/Mol) |
| Zero-point correction | 0.280825 (Hartree/Particle) |
| Thermal correction to Energy | 0.296627 |
| Thermal correction to Enthalpy | 0.297571 |
| Thermal correction to Gibbs Free Energy | 0.235473 |
| Sum of electronic and zero-point Energies | -597.554227 |
| Sum of electronic and thermal Energies | -597.538424 |
| Sum of electronic and thermal Enthalpies | -597.537480 |
| Sum of electronic and thermal Free Energies | -597.599578 |

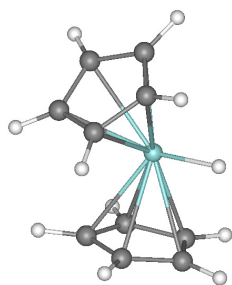
cartesian

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 13 | 0.05293867 | 1.37268722 | -0.06253873 | 1 | 3.82563877 | -1.15381277 | -0.97243875 |
| 6 | 1.35613859 | 0.18758714 | -0.95083874 | 1 | 2.54563880 | -2.27741289 | -1.45113873 |
| 6 | -1.45526135 | 0.47948712 | 0.84056127 | 6 | -3.17076135 | -1.39791286 | 0.77626127 |
| 1 | 0.89103872 | -0.36101288 | -1.78273869 | 1 | -1.25826132 | -1.40891278 | -0.18803872 |
| 6 | 1.94393861 | -0.82491285 | 0.05426127 | 6 | -2.57526135 | -0.16751285 | -1.32983863 |
| 1 | 2.17963886 | 0.76628715 | -1.39473867 | 1 | -3.02166128 | -0.97101289 | -1.92413867 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | -2.05246115 | -0.67751288 | 0.01676127 | 1 | -1.77416134 | 0.27608714 | -1.93713868 |
| 1 | -2.25116134 | 1.20058715 | 1.07966125 | 1 | -3.34116125 | 0.60148716 | -1.17553866 |
| 1 | -1.11336136 | 0.09148714 | 1.81306136 | 1 | -3.57396126 | -2.23901272 | 0.20206128 |
| 6 | 2.56573868 | -0.09781286 | 1.25176132 | 1 | -3.99346113 | -0.70381290 | 0.98286122 |
| 6 | 2.97973871 | -1.74331284 | -0.60073876 | 1 | -2.80936122 | -1.78201282 | 1.73476136 |
| 1 | 1.12683868 | -1.45481277 | 0.43276128 | 6 | 0.29583865 | 3.31778717 | -0.04273873 |
| 1 | 3.02243876 | -0.79481286 | 1.96136129 | 1 | -0.39176133 | 3.83878708 | 0.63046128 |
| 1 | 1.81953859 | 0.48318714 | 1.81386125 | 1 | 0.14733867 | 3.73778725 | -1.04583871 |
| 1 | 3.34213877 | 0.59928715 | 0.91536123 | 1 | 1.31843865 | 3.58768725 | 0.24706128 |
| 1 | 3.36903882 | -2.48461270 | 0.10556127 | | | | |

S1.2. Reaction profile without Zr–Al coordination

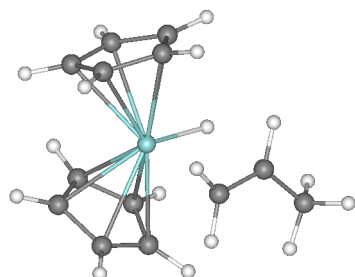
I-0



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 463865.2 (Joules/Mol) |
| | 110.86645 (Kcal/Mol) |
| Zero-point correction | 0.176677 (Hartree/Particle) |
| Thermal correction to Energy | 0.186380 |
| Thermal correction to Enthalpy | 0.187324 |
| Thermal correction to Gibbs Free Energy | 0.139040 |
| Sum of electronic and zero-point Energies | -3927.913963 |
| Sum of electronic and thermal Energies | -3927.904260 |
| Sum of electronic and thermal Enthalpies | -3927.903316 |
| Sum of electronic and thermal Free Energies | -3927.951600 |

| | | | | cartesian | | | |
|---|-------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 6 | 1.65699995 | 1.40859997 | -0.11290000 | 6 | -1.66550004 | 0.75360000 | 1.15439999 |
| 6 | 1.66520000 | 0.75440001 | 1.15390003 | 6 | -2.18300009 | -0.55739999 | 0.97310001 |
| 6 | 2.18269992 | -0.55669999 | 0.97380000 | 6 | -2.45650005 | -0.72270000 | -0.41110000 |
| 6 | 2.45659995 | -0.72320002 | -0.41020000 | 1 | -2.87129998 | -1.61310005 | -0.87099999 |
| 6 | 2.14969993 | 0.49720001 | -1.07449996 | 1 | -2.27640009 | 0.69980001 | -2.13269997 |
| 1 | 2.27710009 | 0.69800001 | -2.13290000 | 1 | -1.35899997 | 2.43260002 | -0.29990000 |
| 1 | 1.35930002 | 2.43239999 | -0.30180001 | 1 | -2.35560012 | -1.28989995 | 1.74940002 |
| 1 | 2.35509992 | -1.28859997 | 1.75059998 | 40 | 0.00000000 | -0.44040000 | -0.21110000 |
| 1 | 2.87140012 | -1.61389995 | -0.86930001 | 1 | 0.00000000 | -1.79999995 | 0.99080002 |
| 6 | -2.14930010 | 0.49810001 | -1.07439995 | 1 | -1.38110006 | 1.19669998 | 2.10080004 |
| 6 | -1.65690005 | 1.40869999 | -0.11190000 | 1 | 1.38059998 | 1.19830000 | 2.09990001 |

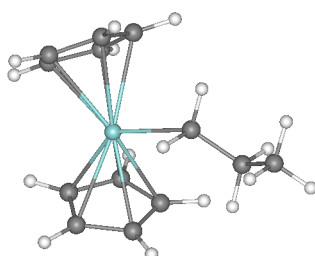
I-1



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 679571.4 (Joules/Mol) |
| | 162.42147 (Kcal/Mol) |
| Zero-point correction | 0.258835 (Hartree/Particle) |
| Thermal correction to Energy | 0.272972 |
| Thermal correction to Enthalpy | 0.273916 |
| Thermal correction to Gibbs Free Energy | 0.217132 |
| Sum of electronic and zero-point Energies | -4045.725664 |
| Sum of electronic and thermal Energies | -4045.711527 |
| Sum of electronic and thermal Enthalpies | -4045.710583 |
| Sum of electronic and thermal Free Energies | -4045.767368 |

| cartesian | | | | | | | |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | -1.47160006 | 1.97000003 | 0.09150000 | 1 | 1.12310004 | -2.31660008 | 1.93949997 |
| 6 | -0.56910002 | 2.12630010 | 1.17659998 | 1 | 2.63319993 | -0.09750000 | 1.92200005 |
| 6 | 0.72579998 | 2.33270001 | 0.63309997 | 40 | 0.11790000 | 0.02150000 | 0.00490000 |
| 6 | 0.61890000 | 2.32189989 | -0.78759998 | 6 | -1.86329997 | -1.14859998 | -1.27929997 |
| 6 | -0.74040002 | 2.10500002 | -1.11650002 | 6 | -2.20580006 | -1.71319997 | -0.09920000 |
| 1 | -1.14909995 | 2.05559993 | -2.11969995 | 6 | -3.37770009 | -1.29939997 | 0.72960001 |
| 1 | -2.53900003 | 1.80550003 | 0.17850000 | 1 | -2.47569990 | -0.36019999 | -1.71150005 |
| 1 | -0.82840002 | 2.11129999 | 2.22639990 | 1 | -1.11179996 | -1.61179996 | -1.92429996 |
| 1 | 1.63170004 | 2.50999999 | 1.19939995 | 1 | -0.59230000 | -0.41630000 | 1.62849998 |
| 6 | 1.25500000 | -2.18289995 | -0.28979999 | 1 | -3.08450007 | -1.14110005 | 1.76950002 |
| 6 | 1.47889996 | -1.80180001 | 1.05739999 | 1 | -4.11250019 | -2.11190009 | 0.72030002 |
| 6 | 2.28320003 | -0.63069999 | 1.04639995 | 1 | -3.85570002 | -0.40059999 | 0.33710000 |
| 6 | 2.58380008 | -0.31169999 | -0.30500001 | 1 | 3.20120001 | 0.51190001 | -0.64170003 |
| 6 | 1.94140005 | -1.26110005 | -1.13259995 | 1 | 1.42410004 | 2.48889995 | -1.49220002 |
| 1 | 1.99220002 | -1.29729998 | -2.21510005 | 1 | -1.63660002 | -2.57159996 | 0.26040000 |
| 1 | 0.70889997 | -3.05839992 | -0.62210000 | | | | |

I-2_a

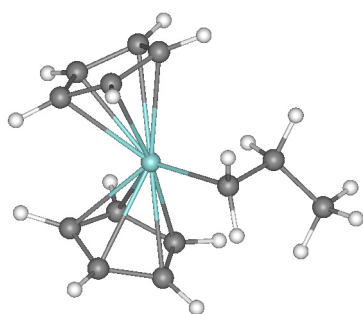


| | |
|--------------------------------|-----------------------------|
| Zero-point vibrational energy | 692418.1 (Joules/Mol) |
| | 165.49189 (Kcal/Mol) |
| Zero-point correction | 0.263728 (Hartree/Particle) |
| Thermal correction to Energy | 0.278005 |
| Thermal correction to Enthalpy | 0.278949 |

| | |
|---|--------------|
| Thermal correction to Gibbs Free Energy | 0.221886 |
| Sum of electronic and zero-point Energies | -4045.724543 |
| Sum of electronic and thermal Energies | -4045.710267 |
| Sum of electronic and thermal Enthalpies | -4045.709323 |
| Sum of electronic and thermal Free Energies | -4045.766386 |

| | | | | cartesian | | | |
|----|-------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 6 | 1.25453222 | -0.82727426 | 0.13028066 | 1 | 1.19003224 | -1.90927410 | -0.02301934 |
| 6 | -1.45456779 | -1.94137430 | -0.85861933 | 6 | 2.61503220 | -0.33497423 | -0.34651935 |
| 6 | -2.37816763 | -0.90597433 | -1.16931939 | 1 | 1.19263220 | -0.69377428 | 1.26388061 |
| 6 | -3.09626770 | -0.58437425 | 0.01858066 | 6 | 3.77413225 | -1.14177418 | 0.24828066 |
| 6 | -2.59786797 | -1.40057421 | 1.05988061 | 1 | 2.75553226 | 0.72402573 | -0.11071934 |
| 6 | -1.57646775 | -2.23247433 | 0.52178067 | 1 | 4.73403215 | -0.77677429 | -0.12361935 |
| 1 | -3.89386797 | 0.14262575 | 0.10568066 | 1 | 3.78363228 | -1.06487417 | 1.33928061 |
| 1 | -2.94536781 | -1.40387416 | 2.08758068 | 1 | 3.69023228 | -2.19967413 | -0.01401935 |
| 6 | -0.95916778 | 2.09132576 | -1.12651932 | 1 | -0.77886778 | -2.42087412 | -1.55491936 |
| 6 | -1.65726781 | 2.42062569 | 0.07118066 | 1 | -1.01036787 | -2.97737432 | 1.06878066 |
| 6 | -0.70566779 | 2.52432585 | 1.11248064 | 1 | -2.55206776 | -0.48367426 | -2.15131927 |
| 6 | 0.58053219 | 2.26062584 | 0.56568062 | 1 | -0.91856778 | 2.77552581 | 2.14618063 |
| 6 | 0.42583221 | 2.00902581 | -0.82101929 | 1 | -2.72306776 | 2.58802581 | 0.16358066 |
| 1 | 1.22183216 | 1.79592574 | -1.52311933 | 1 | -1.40016770 | 1.98142576 | -2.10931921 |
| 1 | 1.51633227 | 2.27682590 | 1.11218059 | 1 | 2.63953209 | -0.41937426 | -1.43901932 |
| 40 | -0.72606778 | 0.12802576 | 0.35578066 | | | | |

I-2_b

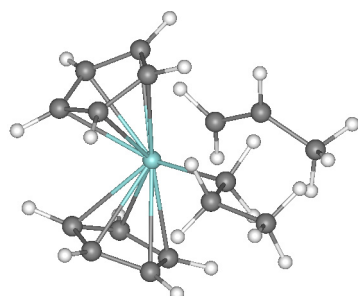


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 691916.6 (Joules/Mol) |
| | 165.37203 (Kcal/Mol) |
| Zero-point correction | 0.263537 (Hartree/Particle) |
| Thermal correction to Energy | 0.277639 |
| Thermal correction to Enthalpy | 0.278583 |
| Thermal correction to Gibbs Free Energy | 0.221509 |
| Sum of electronic and zero-point Energies | -4045.741248 |
| Sum of electronic and thermal Energies | -4045.727146 |

| | |
|---|--------------|
| Sum of electronic and thermal Enthalpies | -4045.726202 |
| Sum of electronic and thermal Free Energies | -4045.783276 |

| cartesian | | | | | | | | | | | |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|--|--|--|--|
| 6 | -2.11848068 | -1.58108389 | -0.14251934 | 1 | 2.20761919 | 1.20691609 | -1.50481939 | | | | |
| 6 | -2.27318048 | -0.70938390 | -1.25841939 | 1 | -0.07478060 | 2.50741625 | -2.10351944 | | | | |
| 6 | -2.69238043 | 0.55231607 | -0.77201939 | 40 | -0.37938058 | 0.23621611 | 0.09298065 | | | | |
| 6 | -2.78158045 | 0.46861610 | 0.64678061 | 6 | 2.74611950 | -1.76658392 | -0.46151933 | | | | |
| 6 | -2.44428062 | -0.86048388 | 1.02758062 | 6 | 0.79401934 | -1.34388387 | 1.16368067 | | | | |
| 1 | -2.42968082 | -1.24948394 | 2.03858066 | 6 | 1.23741937 | -1.80138385 | -0.21391934 | | | | |
| 1 | -1.81658065 | -2.62068367 | -0.18491934 | 1 | 0.19241941 | -2.08668375 | 1.68658066 | | | | |
| 1 | -2.12528062 | -0.97538388 | -2.29921937 | 1 | 1.62921941 | -1.02328384 | 1.78578067 | | | | |
| 1 | -2.91318083 | 1.42621613 | -1.37261939 | 1 | 0.79541945 | -1.15248394 | -1.06351936 | | | | |
| 6 | 1.65331936 | 1.61761606 | 0.62318063 | 1 | 2.99111938 | -1.98818386 | -1.50201941 | | | | |
| 6 | 1.50821936 | 1.62441611 | -0.78911936 | 1 | 3.16401958 | -0.78938389 | -0.20491935 | | | | |
| 6 | 0.30511940 | 2.31311607 | -1.10721934 | 1 | -1.20548058 | 3.30591631 | 0.20648065 | | | | |
| 6 | -0.28788060 | 2.73841619 | 0.10958065 | 1 | -3.10838079 | 1.25901616 | 1.31188059 | | | | |
| 6 | 0.53871942 | 2.30051613 | 1.17718065 | 1 | 3.22941923 | -2.51198387 | 0.17298065 | | | | |
| 1 | 0.36231941 | 2.47731590 | 2.23238063 | 1 | 0.81471944 | -2.77388382 | -0.47601935 | | | | |
| 1 | 2.48131943 | 1.20021605 | 1.18068063 | | | | | | | | |

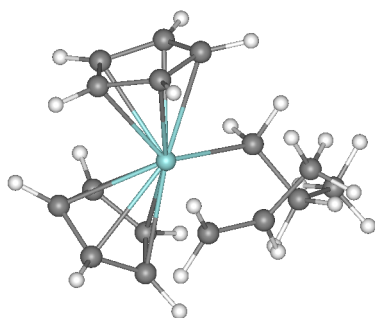
I-3



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 911019.4 (Joules/Mol) |
| | 217.73885 (Kcal/Mol) |
| Zero-point correction | 0.346989 (Hartree/Particle) |
| Thermal correction to Energy | 0.366459 |
| Thermal correction to Enthalpy | 0.367403 |
| Thermal correction to Gibbs Free Energy | 0.299219 |
| Sum of electronic and zero-point Energies | -4163.530477 |
| Sum of electronic and thermal Energies | -4163.511007 |
| Sum of electronic and thermal Enthalpies | -4163.510063 |
| Sum of electronic and thermal Free Energies | -4163.578247 |

| cartesian | | | | | | | | | |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|--|--|
| 6 | 0.02170000 | -1.44910002 | -2.03469992 | 1 | 2.11450005 | -1.92340004 | 1.23619998 | | |
| 6 | -0.50770003 | -2.28489995 | -1.01929998 | 40 | -0.40869999 | 0.01480000 | -0.00610000 | | |
| 6 | -1.85259998 | -1.89600003 | -0.78579998 | 1 | 2.29940009 | -2.24810004 | -0.47409999 | | |
| 6 | -2.14610004 | -0.79799998 | -1.62689996 | 6 | 1.85060000 | -0.17240000 | -0.04180000 | | |
| 6 | -0.98369998 | -0.52380002 | -2.40420008 | 6 | 2.52390003 | -1.51100004 | 0.30500001 | | |
| 1 | -0.90619999 | 0.22570001 | -3.18350005 | 6 | 4.04409981 | -1.38339996 | 0.44180000 | | |
| 1 | 1.01689994 | -1.51479995 | -2.45490003 | 1 | 2.23550010 | 0.60850000 | 0.63150001 | | |
| 1 | 0.01410000 | -3.09649992 | -0.52600002 | 1 | 2.16520000 | 0.11550000 | -1.05820000 | | |
| 1 | -2.53550005 | -2.36389995 | -0.08840000 | 1 | 4.50610018 | -2.35039997 | 0.65560001 | | |
| 1 | -3.09920001 | -0.28529999 | -1.69250000 | 1 | 4.30600023 | -0.69700003 | 1.25209999 | | |
| 6 | -0.28110000 | 1.26209998 | 2.19239998 | 1 | 4.48369980 | -0.99510002 | -0.48130000 | | |
| 6 | 0.23480000 | -0.03180000 | 2.43390012 | 6 | -0.70580000 | 2.53150010 | -0.91079998 | | |
| 6 | -0.81660002 | -0.96499997 | 2.24020004 | 6 | 0.53799999 | 2.43989992 | -1.42700005 | | |
| 6 | -1.99839997 | -0.23480000 | 1.92270005 | 6 | 1.73640001 | 3.14240003 | -0.87599999 | | |
| 6 | -1.66680002 | 1.13540006 | 1.88919997 | 1 | -1.57149994 | 2.14129996 | -1.45150006 | | |
| 1 | -2.35599995 | 1.94620001 | 1.68359995 | 1 | -0.90120000 | 3.17050004 | -0.05350000 | | |
| 1 | 0.27710000 | 2.18889999 | 2.25850010 | 1 | 0.68480003 | 1.87320006 | -2.34759998 | | |
| 1 | 1.25409997 | -0.27020001 | 2.70810008 | 1 | 2.60139990 | 2.47830009 | -0.82260001 | | |
| 1 | -0.74519998 | -2.03940010 | 2.36260009 | 1 | 1.54020000 | 3.57410002 | 0.10710000 | | |
| 1 | -2.98200011 | -0.65249997 | 1.75020003 | 1 | 2.00020003 | 3.95569992 | -1.56140006 | | |

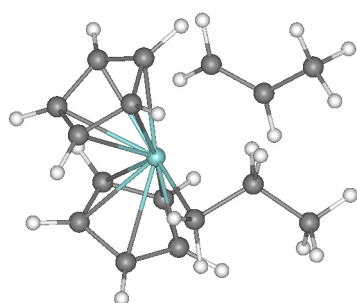
I-3_a



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 911998.7 (Joules/Mol) |
| | 217.97293 (Kcal/Mol) |
| Zero-point correction | 0.347362 (Hartree/Particle) |
| Thermal correction to Energy | 0.366687 |
| Thermal correction to Enthalpy | 0.367631 |
| Thermal correction to Gibbs Free Energy | 0.300474 |
| Sum of electronic and zero-point Energies | -4163.527795 |
| Sum of electronic and thermal Energies | -4163.508470 |
| Sum of electronic and thermal Enthalpies | -4163.507526 |
| Sum of electronic and thermal Free Energies | -4163.574683 |

| cartesian | | | | | | | |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | 0.26818997 | -2.53561258 | -0.11927500 | 40 | -0.77161002 | -0.23171255 | -0.02197501 |
| 6 | -1.00251007 | -2.65811253 | 0.50132501 | 1 | 2.86349010 | 0.68998742 | -0.10307501 |
| 6 | -1.99821007 | -2.38921261 | -0.47967499 | 6 | 1.19678998 | 0.00528744 | 1.09912503 |
| 6 | -1.34471011 | -2.05821252 | -1.68327498 | 6 | 2.55209017 | -0.23171255 | 0.40342501 |
| 6 | 0.06208995 | -2.13901258 | -1.45927501 | 6 | 3.65189028 | -0.63451254 | 1.39072502 |
| 1 | 0.83698988 | -1.97401249 | -2.19977498 | 1 | 1.08908999 | -0.72651255 | 1.91982496 |
| 1 | 1.22448993 | -2.70611262 | 0.35742500 | 1 | 1.22958994 | 0.97618747 | 1.60962498 |
| 1 | -1.18241000 | -2.96021247 | 1.52632499 | 1 | 4.61659002 | -0.74931252 | 0.89022499 |
| 1 | -3.06971025 | -2.42731261 | -0.32807499 | 1 | 3.40828991 | -1.58471251 | 1.87612498 |
| 1 | -1.83481002 | -1.81591249 | -2.61897492 | 1 | 3.76209021 | 0.11948743 | 2.17472506 |
| 6 | -1.36191010 | 1.85478747 | 1.32422495 | 6 | -0.47171006 | 1.08268750 | -2.47327495 |
| 6 | -1.58151007 | 0.73658741 | 2.16422510 | 6 | 0.67548990 | 1.40638745 | -1.84117496 |
| 6 | -2.64070988 | -0.02681255 | 1.60972500 | 6 | 0.94368994 | 2.70998740 | -1.15517497 |
| 6 | -3.07711029 | 0.62138748 | 0.42212498 | 1 | -0.53421009 | 0.18768746 | -3.08547497 |
| 6 | -2.29030991 | 1.78908741 | 0.25522500 | 1 | -1.30440998 | 1.78028750 | -2.52627492 |
| 1 | -2.40701008 | 2.52398753 | -0.53167498 | 1 | 1.50808990 | 0.70228744 | -1.89867496 |
| 1 | -0.62631005 | 2.63288736 | 1.48542500 | 1 | 1.37388992 | 2.56218743 | -0.16077501 |
| 1 | -1.03331006 | 0.50548744 | 3.06932497 | 1 | 0.04578993 | 3.32738757 | -1.08437502 |
| 1 | -3.06341028 | -0.92901254 | 2.03362489 | 1 | 1.68989003 | 3.25808740 | -1.74137497 |
| 1 | -3.89000988 | 0.30148745 | -0.21857500 | 1 | 2.48739004 | -0.99561250 | -0.38257501 |

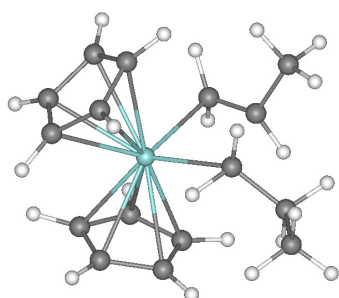
I-3_b



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 913477.1 (Joules/Mol) |
| | 218.32626 (Kcal/Mol) |
| Zero-point correction | 0.347925 (Hartree/Particle) |
| Thermal correction to Energy | 0.366985 |
| Thermal correction to Enthalpy | 0.367929 |
| Thermal correction to Gibbs Free Energy | 0.300920 |
| Sum of electronic and zero-point Energies | -4163.529300 |
| Sum of electronic and thermal Energies | -4163.510240 |
| Sum of electronic and thermal Enthalpies | -4163.509296 |
| Sum of electronic and thermal Free Energies | -4163.576305 |

| cartesian | | | | | | | |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | 0.64131999 | -2.50299239 | -0.15420251 | 1 | -2.28688002 | 2.10580754 | -1.19280255 |
| 6 | 1.71011996 | -2.15159249 | 0.72099745 | 1 | -2.65637994 | 1.50290751 | -2.81060243 |
| 6 | 2.70562005 | -1.51049244 | -0.05050251 | 6 | -0.05888000 | 0.63030750 | -2.08400249 |
| 6 | 2.24832010 | -1.43409240 | -1.39190257 | 6 | -1.43247998 | 0.15750751 | -1.65060258 |
| 6 | 0.98342001 | -2.07109237 | -1.45490253 | 1 | 0.33052000 | 0.10360751 | -2.95280242 |
| 1 | 0.37911999 | -2.19419241 | -2.34430242 | 1 | -0.05478001 | 1.70230758 | -2.27790260 |
| 1 | -0.26097998 | -3.03849244 | 0.11759749 | 1 | -1.44728005 | -0.16219249 | -0.55910254 |
| 1 | 1.77751994 | -2.37509251 | 1.77839744 | 1 | -3.50377989 | 0.83470750 | -1.41160250 |
| 1 | 2.78062010 | -0.99189252 | -2.22500253 | 6 | -0.65157998 | -0.88539249 | 2.34319758 |
| 6 | 0.78711998 | 1.92920756 | 1.66569746 | 6 | -1.74088013 | -0.28729248 | 1.82159746 |
| 6 | 2.06172013 | 1.31680763 | 1.62759745 | 6 | -2.93847990 | -1.03849244 | 1.31619751 |
| 6 | 2.62551999 | 1.58000755 | 0.34439752 | 1 | 0.11412001 | -0.33339250 | 2.88099742 |
| 6 | 1.68911994 | 2.32440758 | -0.40500250 | 1 | -0.59958005 | -1.97009242 | 2.39229751 |
| 6 | 0.53711998 | 2.52140760 | 0.40469751 | 1 | -1.82828009 | 0.79960752 | 1.86989748 |
| 1 | -0.35007998 | 3.07740760 | 0.12509750 | 1 | -3.35807991 | -0.59629250 | 0.41059750 |
| 1 | 0.11802000 | 1.94850755 | 2.51789737 | 1 | -2.70867991 | -2.09019232 | 1.13269746 |
| 1 | 2.54952002 | 0.79620749 | 2.44289756 | 1 | -3.71998000 | -0.99119252 | 2.08199739 |
| 1 | 1.83491993 | 2.69230747 | -1.41110253 | 1 | 3.61482000 | 1.29470754 | 0.01129749 |
| 40 | 0.71032000 | 0.01990751 | -0.03390251 | 1 | 3.65622020 | -1.14999247 | 0.32019749 |
| 6 | -2.54038000 | 1.20920753 | -1.76530254 | 1 | -1.71768010 | -0.77239251 | -2.15070248 |

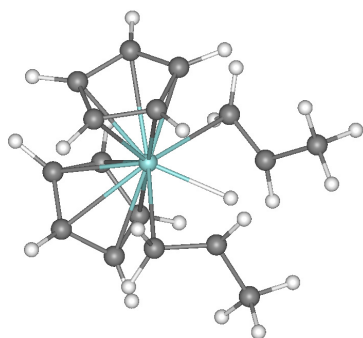
TS-2



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 916072.3 (Joules/Mol) |
| | 218.94652 (Kcal/Mol) |
| Zero-point correction | 0.348913 (Hartree/Particle) |
| Thermal correction to Energy | 0.366397 |
| Thermal correction to Enthalpy | 0.367341 |
| Thermal correction to Gibbs Free Energy | 0.304683 |
| Sum of electronic and zero-point Energies | -4163.517412 |
| Sum of electronic and thermal Energies | -4163.499929 |
| Sum of electronic and thermal Enthalpies | -4163.498984 |
| Sum of electronic and thermal Free Energies | -4163.561642 |

| cartesian | | | | | | |
|-----------|-------------|-------------|-------------|----|-------------|-------------------------|
| 6 | -0.23428001 | 2.28946257 | -1.20005500 | 40 | -0.90178001 | 0.12046253 -0.05215501 |
| 6 | -0.19028001 | 2.55216265 | 0.18854499 | 1 | 3.32031989 | -0.04233747 -0.10835501 |
| 6 | -1.50668001 | 2.43206263 | 0.70444500 | 6 | 1.29981995 | -0.24453747 0.58984500 |
| 6 | -2.37177992 | 2.13006258 | -0.38245502 | 6 | 2.60112000 | 0.53916252 0.47784498 |
| 6 | -1.58738005 | 2.03696251 | -1.55615497 | 6 | 3.20971990 | 0.84326249 1.85044503 |
| 1 | -1.96138000 | 1.83326256 | -2.55185509 | 1 | 0.68751991 | 0.28586254 1.38804495 |
| 1 | 0.61052001 | 2.30816269 | -1.87875497 | 1 | 1.47231996 | -1.24063754 1.00634503 |
| 1 | 0.69271994 | 2.80306268 | 0.76474500 | 1 | 4.15952015 | 1.37146246 1.74454498 |
| 1 | -1.80568004 | 2.59806252 | 1.73214495 | 1 | 2.54202008 | 1.46966255 2.45024490 |
| 1 | -3.44657993 | 2.01376247 | -0.32515502 | 1 | 3.39511991 | -0.07853747 2.40804482 |
| 6 | -1.29478002 | -2.25733733 | 0.73824501 | 6 | -0.18988001 | -0.79013747 -2.12965512 |
| 6 | -1.47328007 | -1.42693746 | 1.87254500 | 6 | 1.10061991 | -0.83013749 -1.55525506 |
| 6 | -2.60088015 | -0.60203749 | 1.64324498 | 6 | 1.79931998 | -2.15523744 -1.37545502 |
| 6 | -3.13698006 | -0.94113743 | 0.36914498 | 1 | -0.38398001 | -0.00813747 -2.85755515 |
| 6 | -2.33687997 | -1.96943748 | -0.18305501 | 1 | -0.66158003 | -1.74553752 -2.33925509 |
| 1 | -2.51187992 | -2.46573734 | -1.12815499 | 1 | 1.75022006 | 0.01586253 -1.76735497 |
| 1 | -0.52968001 | -3.01463747 | 0.62204498 | 1 | 2.65192008 | -2.11193728 -0.69705498 |
| 1 | -0.85337996 | -1.42023754 | 2.76144481 | 1 | 1.10601997 | -2.92963743 -1.04135501 |
| 1 | -3.00678015 | 0.12846252 | 2.33194494 | 1 | 2.17371988 | -2.45393729 -2.36025524 |
| 1 | -4.02417994 | -0.51633751 | -0.08345501 | 1 | 2.43741989 | 1.47336257 -0.07105501 |

TS-3



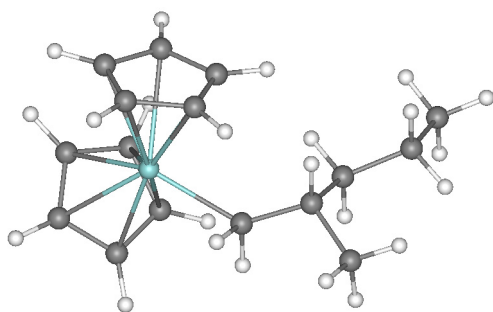
| | |
|---|-----------------------------|
| Zero-point vibrational energy | 904319.0 (Joules/Mol) |
| | 216.13742 (Kcal/Mol) |
| Zero-point correction | 0.344437 (Hartree/Particle) |
| Thermal correction to Energy | 0.362458 |
| Thermal correction to Enthalpy | 0.363403 |
| Thermal correction to Gibbs Free Energy | 0.299638 |
| Sum of electronic and zero-point Energies | -4163.506150 |
| Sum of electronic and thermal Energies | -4163.488129 |
| Sum of electronic and thermal Enthalpies | -4163.487185 |

Sum of electronic and thermal Free Energies

-4163.550949

| | | | | cartesian | | | |
|----|-------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 6 | 0.69806993 | -2.56201506 | 0.10210251 | 1 | -2.12783003 | 2.32648492 | -0.96729749 |
| 6 | 1.92306995 | -2.09351492 | 0.64990252 | 1 | -3.18313003 | 1.52488494 | -2.13369727 |
| 6 | 2.65977001 | -1.49601507 | -0.40149748 | 6 | -0.39673007 | 0.55068499 | -2.18329740 |
| 6 | 1.87786984 | -1.54741502 | -1.58069754 | 6 | -1.58293009 | 0.28858498 | -1.48019755 |
| 6 | 0.66736996 | -2.22441506 | -1.26609755 | 1 | -2.00393009 | -0.71101505 | -1.60389745 |
| 1 | -0.13163006 | -2.45931506 | -1.95959747 | 1 | -0.01453006 | -0.19981501 | -2.86399746 |
| 1 | -0.06673005 | -3.10931492 | 0.63760251 | 1 | -0.16813004 | 1.57868493 | -2.44529748 |
| 1 | 2.25856996 | -2.21831512 | 1.67180252 | 1 | -1.33582997 | 0.00008499 | 0.00000251 |
| 1 | 2.17837000 | -1.18441498 | -2.55539727 | 1 | -3.30573010 | 1.11568499 | -0.42079750 |
| 6 | 0.66766995 | 2.22438502 | 1.26620245 | 6 | -0.39673007 | -0.55061501 | 2.18330264 |
| 6 | 1.87817001 | 1.54718494 | 1.58060253 | 6 | -1.58293009 | -0.28841501 | 1.48020256 |
| 6 | 2.65997005 | 1.49578500 | 0.40130252 | 6 | -2.60512996 | -1.37731504 | 1.21680248 |
| 6 | 1.92316985 | 2.09338498 | -0.64989752 | 1 | -0.01443005 | 0.19978499 | 2.86400270 |
| 6 | 0.69816995 | 2.56198502 | -0.10209749 | 1 | -0.16813004 | -1.57861507 | 2.44530272 |
| 1 | -0.06653005 | 3.10938501 | -0.63749748 | 1 | -2.00382996 | 0.71118498 | 1.60400248 |
| 1 | -0.13133007 | 2.45928502 | 1.95980251 | 1 | -3.30573010 | -1.11551499 | 0.42090249 |
| 1 | 2.17866993 | 1.18418503 | 2.55530262 | 1 | -2.12792993 | -2.32631493 | 0.96730250 |
| 1 | 2.25856996 | 2.21818495 | -1.67189753 | 1 | -3.18313003 | -1.52471507 | 2.13370252 |
| 40 | 0.66036993 | -0.00001501 | 0.00000251 | 1 | 3.66017008 | 1.09268498 | 0.32430249 |
| 6 | -2.60512996 | 1.37748504 | -1.21679747 | 1 | 3.66006994 | -1.09291506 | -0.32449749 |

I-4_a



Zero-point vibrational energy

917695.1 (Joules/Mol)

219.33440 (Kcal/Mol)

Zero-point correction

0.349532 (Hartree/Particle)

Thermal correction to Energy

0.367821

Thermal correction to Enthalpy

0.368765

Thermal correction to Gibbs Free Energy

0.301980

Sum of electronic and zero-point Energies

-4163.528347

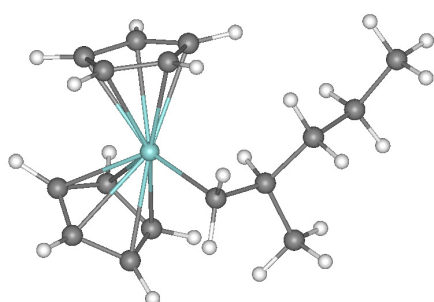
Sum of electronic and thermal Energies

-4163.510058

| | |
|---|--------------|
| Sum of electronic and thermal Enthalpies | -4163.509114 |
| Sum of electronic and thermal Free Energies | -4163.575899 |

| cartesian | | | | | |
|-----------|-------------|-------------|-------------|---|-------------------------------------|
| 6 | 0.27660000 | 2.43810010 | 0.44749999 | 6 | -0.83260000 -0.37979999 1.23679996 |
| 6 | 1.69649994 | 2.50600004 | 0.45739999 | 6 | -2.23799992 0.17299999 1.02219999 |
| 6 | 2.17000008 | 2.02230000 | -0.78689998 | 6 | -2.84349990 -0.51200002 -0.21349999 |
| 6 | 1.03900003 | 1.64830005 | -1.56680000 | 1 | -0.90579998 -1.43929994 1.51090002 |
| 6 | -0.13020000 | 1.91760004 | -0.80430001 | 1 | -0.34740001 0.13150001 2.12879992 |
| 1 | -1.15190005 | 1.75940001 | -1.12779999 | 1 | -2.18210006 1.25150001 0.82620001 |
| 1 | -0.37909999 | 2.74340010 | 1.25460005 | 6 | -4.20989990 0.02870000 -0.63830000 |
| 1 | 2.30970001 | 2.88290000 | 1.26909995 | 1 | -2.92630005 -1.59010005 -0.01370000 |
| 1 | 3.20630002 | 1.97060001 | -1.09749997 | 1 | -2.14439988 -0.41389999 -1.05820000 |
| 6 | 1.68499994 | -2.34910011 | 0.72759998 | 1 | -2.63380003 0.40799999 3.15499997 |
| 6 | 2.91499996 | -1.70669997 | 0.40720001 | 1 | -3.25799990 -1.09819996 2.46329999 |
| 6 | 2.84089994 | -1.25430000 | -0.92909998 | 1 | 1.20560002 -1.44149995 -2.44989991 |
| 6 | 1.55970001 | -1.61230004 | -1.44060004 | 1 | 1.06400001 1.27800000 -2.58389997 |
| 6 | 0.85740000 | -2.31110001 | -0.42120001 | 1 | -4.08629990 0.43630001 2.15490007 |
| 1 | -0.13480000 | -2.73410010 | -0.51029998 | 6 | -4.69540024 -0.60920000 -1.93949997 |
| 1 | 1.43949997 | -2.81500006 | 1.67509997 | 1 | -4.94479990 -0.15640000 0.15060000 |
| 1 | 3.76679993 | -1.59689999 | 1.07009995 | 1 | -4.14870024 1.11759996 -0.75849998 |
| 1 | 3.62339997 | -0.73930001 | -1.47210002 | 1 | -5.67460012 -0.22280000 -2.22979999 |
| 40 | 1.12940001 | 0.06400000 | 0.33149999 | 1 | -4.00019979 -0.40889999 -2.76049995 |
| 6 | -3.10570002 | -0.03080000 | 2.27110004 | 1 | -4.78329992 -1.69430006 -1.83299994 |

I-4_b

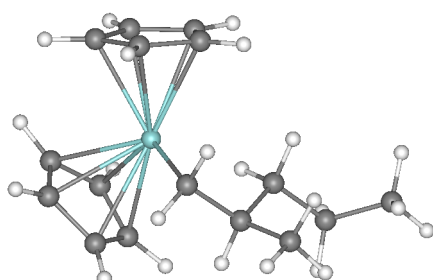


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 918784.4 (Joules/Mol) |
| | 219.59475 (Kcal/Mol) |
| Zero-point correction | 0.349947 (Hartree/Particle) |
| Thermal correction to Energy | 0.367846 |
| Thermal correction to Enthalpy | 0.368790 |
| Thermal correction to Gibbs Free Energy | 0.303902 |
| Sum of electronic and zero-point Energies | -4163.545046 |
| Sum of electronic and thermal Energies | -4163.527147 |

| | |
|---|--------------|
| Sum of electronic and thermal Enthalpies | -4163.526203 |
| Sum of electronic and thermal Free Energies | -4163.591091 |

| cartesian | | | | | | | |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | 0.25549507 | 2.35509753 | 0.96692002 | 6 | -0.05660492 | -0.68800247 | 1.67331994 |
| 6 | -0.01800489 | 2.24369740 | -0.42147997 | 6 | -0.96850491 | -0.96370250 | 0.49622002 |
| 6 | 1.21089506 | 2.36619735 | -1.12608004 | 6 | -2.29060483 | -0.18170251 | 0.54332000 |
| 6 | 2.24189520 | 2.56249738 | -0.17197998 | 1 | -0.49130487 | -0.00070250 | 2.39931989 |
| 6 | 1.65459514 | 2.54329753 | 1.11961997 | 1 | 0.29239509 | -1.59430254 | 2.16872001 |
| 1 | 2.17869520 | 2.67769742 | 2.05942011 | 1 | -0.48820496 | -0.57560247 | -0.49787995 |
| 1 | -0.47070491 | 2.33469748 | 1.76852000 | 6 | -3.08430481 | -0.17680250 | -0.76337999 |
| 1 | -0.99590492 | 2.11339760 | -0.87228000 | 1 | -2.89600492 | -0.62450248 | 1.34361994 |
| 1 | 1.33409500 | 2.34949756 | -2.20248008 | 1 | -2.09200501 | 0.85129750 | 0.85332000 |
| 6 | 2.42749500 | -2.03290248 | 0.31212002 | 1 | -1.61760497 | -2.62700248 | -0.77377999 |
| 6 | 2.03749514 | -1.84130251 | -1.03978002 | 1 | -0.23800492 | -3.01190257 | 0.26982000 |
| 6 | 2.81529498 | -0.78010249 | -1.57798004 | 1 | 4.43609524 | 0.45619750 | -0.66387999 |
| 6 | 3.69199514 | -0.32300252 | -0.56028003 | 1 | 3.28989506 | 2.72279739 | -0.39037997 |
| 6 | 3.44489503 | -1.08860254 | 0.60872000 | 1 | -1.85250497 | -2.86500263 | 0.96661997 |
| 1 | 3.95959496 | -0.98590249 | 1.55762005 | 6 | -4.30530500 | 0.73919749 | -0.68217999 |
| 1 | 2.04859495 | -2.78540254 | 0.99052000 | 1 | -3.40990496 | -1.19260252 | -1.00777996 |
| 1 | 1.29459500 | -2.41800261 | -1.57897997 | 1 | -2.43400502 | 0.14569750 | -1.58917999 |
| 1 | 2.77199507 | -0.40880251 | -2.59507990 | 1 | -4.87470484 | 0.72309750 | -1.61318004 |
| 40 | 1.35839510 | 0.23709750 | 0.18092002 | 1 | -4.01070499 | 1.77469742 | -0.48577997 |
| 6 | -1.17630494 | -2.45560265 | 0.21062002 | 1 | -4.97320509 | 0.42529750 | 0.12452002 |

I-4_g

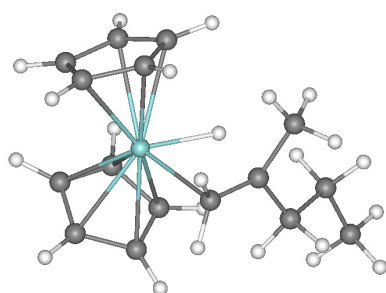


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 920011.5 (Joules/Mol) |
| | 219.88803 (Kcal/Mol) |
| Zero-point correction | 0.350414 (Hartree/Particle) |
| Thermal correction to Energy | 0.368487 |
| Thermal correction to Enthalpy | 0.369431 |
| Thermal correction to Gibbs Free Energy | 0.304050 |
| Sum of electronic and zero-point Energies | -4163.536704 |
| Sum of electronic and thermal Energies | -4163.518631 |

| | |
|---|--------------|
| Sum of electronic and thermal Enthalpies | -4163.517687 |
| Sum of electronic and thermal Free Energies | -4163.583068 |

| cartesian | | | | | | | | | | | |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|--|--|--|--|
| 6 | -1.00805748 | -2.36746240 | 0.76401752 | 40 | -1.23915744 | 0.02073751 | 0.03131752 | | | | |
| 6 | -2.08315754 | -1.80846250 | 1.51451755 | 1 | 3.02844262 | -1.33566248 | 0.90371752 | | | | |
| 6 | -3.13335752 | -1.51686251 | 0.61431748 | 6 | 1.49374247 | 0.13323750 | 0.48291752 | | | | |
| 6 | -2.70685744 | -1.87586248 | -0.69378251 | 6 | 2.71984243 | -0.35926250 | 1.29121745 | | | | |
| 6 | -1.40235758 | -2.42136240 | -0.59598249 | 6 | 3.88924265 | 0.62683749 | 1.26041746 | | | | |
| 1 | -0.81575751 | -2.81106257 | -1.41728246 | 1 | 2.43214250 | -0.52226251 | 2.33291769 | | | | |
| 1 | -0.06915754 | -2.72596240 | 1.17121744 | 1 | 4.74504232 | 0.21973750 | 1.80281746 | | | | |
| 1 | -2.10415745 | -1.65706253 | 2.58761764 | 1 | 3.61074257 | 1.57013750 | 1.73831749 | | | | |
| 1 | -4.09535742 | -1.09396255 | 0.87611753 | 1 | 4.21314240 | 0.84933752 | 0.24151751 | | | | |
| 1 | -3.28945756 | -1.78286254 | -1.60298252 | 6 | 0.10204250 | -0.07616249 | -1.74098253 | | | | |
| 6 | -1.02385747 | 2.52543759 | -0.27388248 | 6 | 1.34744239 | -0.52896249 | -0.91978252 | | | | |
| 6 | -1.41905749 | 2.30973744 | 1.07301748 | 6 | 2.61734247 | -0.25336251 | -1.74338245 | | | | |
| 6 | -2.71535754 | 1.73983753 | 1.06471753 | 1 | -0.07735750 | -0.78436249 | -2.55208230 | | | | |
| 6 | -3.12085748 | 1.60253751 | -0.29278249 | 1 | 0.29794246 | 0.90333748 | -2.18818235 | | | | |
| 6 | -2.07665753 | 2.10013747 | -1.11708248 | 1 | 1.29374242 | -1.61166251 | -0.75438249 | | | | |
| 1 | -2.08295751 | 2.14093757 | -2.19888234 | 1 | 3.50724268 | -0.68986249 | -1.28308249 | | | | |
| 1 | -0.08305752 | 2.94993758 | -0.60248250 | 1 | 2.77534246 | 0.82333750 | -1.86068249 | | | | |
| 1 | -0.83695751 | 2.55243754 | 1.95521748 | 1 | 2.50534248 | -0.68796247 | -2.73888230 | | | | |
| 1 | -3.29965734 | 1.47063756 | 1.93611753 | 1 | 0.64384252 | -0.07906249 | 1.19101751 | | | | |
| 1 | -4.07615757 | 1.22623754 | -0.63748252 | 1 | 1.53614259 | 1.22493756 | 0.38101754 | | | | |

TS-4

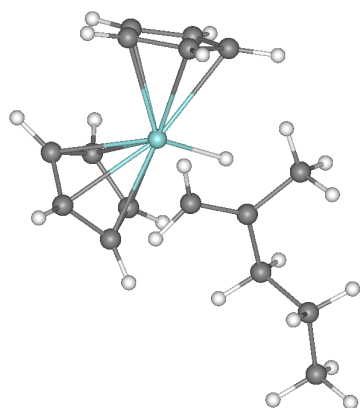


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 906276.5 (Joules/Mol) |
| | 216.60528 (Kcal/Mol) |
| Zero-point correction | 0.345182 (Hartree/Particle) |
| Thermal correction to Energy | 0.363060 |
| Thermal correction to Enthalpy | 0.364004 |
| Thermal correction to Gibbs Free Energy | 0.299366 |
| Sum of electronic and zero-point Energies | -4163.531410 |
| Sum of electronic and thermal Energies | -4163.513533 |

| | |
|---|--------------|
| Sum of electronic and thermal Enthalpies | -4163.512588 |
| Sum of electronic and thermal Free Energies | -4163.577226 |

| cartesian | | | | | | |
|-----------|-------------|-------------|-------------|---|-------------|-------------------------|
| 6 | -2.36525011 | -2.05958486 | 0.22251251 | 6 | 0.22614992 | -0.83908498 1.87041259 |
| 6 | -1.93115008 | -1.79458487 | -1.10248744 | 6 | 1.10144997 | -1.09188485 0.81771255 |
| 6 | -2.69115019 | -0.70088494 | -1.59728742 | 6 | 1.18324995 | -2.47228479 0.21381250 |
| 6 | -3.61105013 | -0.31058496 | -0.58828747 | 1 | -0.35195008 | -1.66618490 2.27991247 |
| 6 | -3.40264988 | -1.13918495 | 0.53921252 | 1 | 0.46024990 | -0.02528495 2.55551243 |
| 1 | -3.95905018 | -1.09958494 | 1.46901250 | 1 | 0.19284993 | -0.36558497 -0.65458745 |
| 1 | -2.01605010 | -2.85828495 | 0.86451250 | 1 | 1.37114990 | -2.44318485 -0.86008745 |
| 1 | -1.17815006 | -2.34258485 | -1.65348744 | 1 | 0.28884989 | -3.06368494 0.41351250 |
| 1 | -2.60914993 | -0.26948494 | -2.58738756 | 6 | 2.94374990 | -0.19498493 -0.77328748 |
| 6 | -0.17995009 | 2.32681513 | 1.01381254 | 1 | 2.09065008 | 0.80981505 0.95191252 |
| 6 | 0.05994993 | 2.21611500 | -0.38048750 | 1 | -3.24755001 | 2.70441508 -0.25398749 |
| 6 | -1.18965006 | 2.33481503 | -1.04638743 | 1 | -4.35335016 | 0.47271508 -0.67088747 |
| 6 | -2.19425011 | 2.54321504 | -0.06448749 | 1 | 3.05805016 | -0.59408498 1.33681250 |
| 6 | -1.57455003 | 2.52621508 | 1.20711255 | 6 | 4.06754971 | 0.83681506 -0.86698747 |
| 1 | -2.07185006 | 2.67181516 | 2.15961242 | 1 | 2.17254972 | 0.01981506 -1.52308750 |
| 1 | 0.56864989 | 2.31981516 | 1.79621255 | 1 | 3.34284973 | -1.18598485 -1.01048744 |
| 1 | 1.02324986 | 2.09281516 | -0.85978746 | 1 | 4.85154963 | 0.63361502 -0.13248751 |
| 1 | -1.34105015 | 2.31101513 | -2.11848760 | 1 | 3.69324970 | 1.84851515 -0.68098748 |
| 40 | -1.30395007 | 0.21201506 | 0.26451251 | 1 | 4.52654982 | 0.82711506 -1.85718751 |
| 6 | 2.31624985 | -0.20918493 | 0.62171251 | 1 | 2.03294992 | -2.98128486 0.68481255 |

I-5

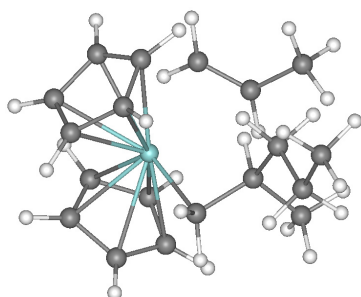


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 907054.2 (Joules/Mol) |
| | 216.79116 (Kcal/Mol) |
| Zero-point correction | 0.345479 (Hartree/Particle) |
| Thermal correction to Energy | 0.364444 |
| Thermal correction to Enthalpy | 0.365388 |
| Thermal correction to Gibbs Free Energy | 0.296641 |
| Sum of electronic and zero-point Energies | -4163.535388 |
| Sum of electronic and thermal Energies | -4163.516423 |
| Sum of electronic and thermal Enthalpies | -4163.515479 |
| Sum of electronic and thermal Free Energies | -4163.584225 |

| cartesian | | | | | |
|-----------|-------------|-------------|-------------|---|-------------------------------------|
| 6 | -2.15187001 | -2.20005250 | 0.61726499 | 6 | 0.63773000 -0.43695250 1.57796502 |
| 6 | -1.95137000 | -2.18965244 | -0.78273499 | 6 | 1.39903009 -0.78105253 0.50266498 |
| 6 | -2.91267014 | -1.31425250 | -1.35593498 | 6 | 1.43203008 -2.18635249 -0.02413500 |
| 6 | -3.71497011 | -0.79975253 | -0.30983499 | 1 | 0.11682999 -1.20715249 2.14896512 |
| 6 | -3.23497009 | -1.32505250 | 0.91786498 | 1 | 0.77803004 0.53164750 2.05506492 |
| 1 | -3.65877008 | -1.14295256 | 1.89846504 | 1 | -0.47057000 -0.03665251 -1.50003505 |
| 1 | -1.60687006 | -2.79745245 | 1.33836496 | 1 | 1.35413003 -2.19615245 -1.11523497 |
| 1 | -1.20687008 | -2.74975252 | -1.33373499 | 1 | 2.40063000 -2.62845230 0.23406500 |
| 1 | -3.01606989 | -1.09665251 | -2.41163492 | 1 | 0.65513003 -2.81655240 0.41156501 |
| 6 | -0.53276998 | 2.48724747 | 0.24736500 | 1 | 2.09852982 0.28024748 -1.21043503 |
| 6 | -1.14636993 | 2.38504767 | -1.02803504 | 1 | 2.20602989 1.19084752 0.30546501 |
| 6 | -2.53337002 | 2.16574764 | -0.82003498 | 1 | -3.74057007 2.03954744 1.06326497 |
| 6 | -2.77747011 | 2.15674758 | 0.58216500 | 1 | -4.54946995 -0.11965252 -0.42493498 |
| 6 | -1.54136992 | 2.35554767 | 1.23866498 | 6 | 3.81162977 -0.22355250 0.01256500 |
| 1 | -1.39446998 | 2.40794754 | 2.31166506 | 6 | 4.75342989 0.85994744 -0.50893497 |
| 1 | 0.51682997 | 2.67984748 | 0.42956501 | 1 | 3.98732996 -1.15365255 -0.53543502 |
| 1 | -0.65206999 | 2.48264766 | -1.98463511 | 1 | 4.02022982 -0.42635250 1.06836498 |
| 1 | -3.28046989 | 2.05904746 | -1.59703505 | 1 | 5.79442978 0.54634750 -0.41203499 |

| | | | | | | | |
|----|-------------|------------|-------------|---|------------|------------|-------------|
| 40 | -1.41936994 | 0.13664749 | 0.05176500 | 1 | 4.63103008 | 1.79194748 | 0.04936500 |
| 6 | 2.33723021 | 0.20134750 | -0.14283499 | 1 | 4.56253004 | 1.06974745 | -1.56483495 |

I-6



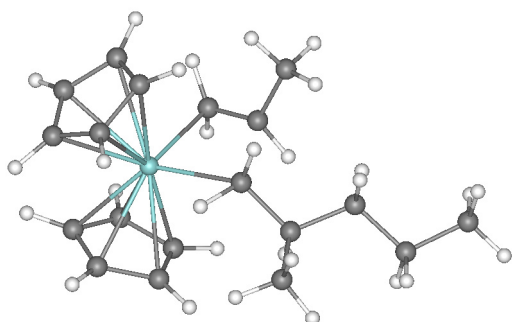
| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1137201.0 (Joules/Mol) |
| | 271.79755 (Kcal/Mol) |
| Zero-point correction | 0.433137 (Hartree/Particle) |
| Thermal correction to Energy | 0.456374 |
| Thermal correction to Enthalpy | 0.457318 |
| Thermal correction to Gibbs Free Energy | 0.380895 |
| Sum of electronic and zero-point Energies | -4281.331907 |
| Sum of electronic and thermal Energies | -4281.308670 |
| Sum of electronic and thermal Enthalpies | -4281.307725 |
| Sum of electronic and thermal Free Energies | 4281.384149 |

cartesian

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | 0.64018160 | -0.72293872 | -2.39606524 | 6 | -1.77121830 | -1.76503873 | 1.06543469 |
| 6 | 0.74558163 | -1.95013881 | -1.69546533 | 1 | -0.60611838 | 0.81356132 | 1.17053473 |
| 6 | 2.12268162 | -2.22893882 | -1.50486529 | 1 | -0.57471842 | 1.04966140 | -0.58036530 |
| 6 | 2.87168169 | -1.16253877 | -2.06256533 | 1 | -3.09471846 | 0.68496132 | 1.14333475 |
| 6 | 1.94948149 | -0.23413870 | -2.62066531 | 1 | -2.98331833 | 1.04776120 | -0.57316530 |
| 1 | 2.20928168 | 0.66736132 | -3.16396523 | 6 | 2.82458162 | 2.22926116 | -0.47336531 |
| 1 | -0.28211838 | -0.24603869 | -2.70456529 | 6 | 1.59028161 | 2.68606114 | -0.76936531 |
| 1 | -0.07981843 | -2.57683873 | -1.37976527 | 6 | 0.77818161 | 3.56086135 | 0.13303469 |
| 1 | 2.53058171 | -3.11223865 | -1.03006530 | 1 | 3.44348168 | 1.73076129 | -1.22106528 |
| 1 | 3.95278168 | -1.09173870 | -2.09446526 | 1 | 3.30388165 | 2.51516128 | 0.45903468 |
| 6 | 2.20478153 | 0.35146132 | 2.29093480 | 1 | 1.17118168 | 2.47206116 | -1.75426531 |
| 6 | 1.33968163 | -0.76603872 | 2.33343458 | 1 | -0.24421841 | 3.19166136 | 0.24093468 |
| 6 | 2.00528169 | -1.85613871 | 1.71523476 | 1 | 1.23748159 | 3.66266131 | 1.11773467 |
| 6 | 3.30908155 | -1.42113876 | 1.34023476 | 1 | 0.71128160 | 4.55596113 | -0.32006532 |
| 6 | 3.43018174 | -0.06283869 | 1.69093466 | 1 | -1.88081837 | -1.37403870 | 2.08433461 |
| 1 | 4.31238174 | 0.54866129 | 1.54293466 | 1 | -2.59981823 | -2.45513868 | 0.89023471 |
| 1 | 1.98848152 | 1.33786130 | 2.68533468 | 1 | -0.84371835 | -2.34813881 | 1.02523470 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 0.34248161 | -0.78903872 | 2.75053477 | 6 | -4.34901857 | -0.54603869 | -0.11156531 |
| 1 | 1.61108160 | -2.85903883 | 1.60283470 | 1 | -4.50321865 | -1.29843879 | 0.66803467 |
| 1 | 4.07468176 | -2.02573872 | 0.87043470 | 1 | -4.26681852 | -1.08933878 | -1.06096530 |
| 40 | 1.64498162 | -0.20613870 | -0.10806531 | 6 | -5.56041861 | 0.38546133 | -0.15436532 |
| 1 | -1.74681830 | -1.05983877 | -0.95936531 | 1 | -5.67401838 | 0.91996127 | 0.79333472 |
| 6 | -0.52931839 | 0.27396131 | 0.21353470 | 1 | -6.48321867 | -0.16943869 | -0.33706534 |
| 6 | -1.76701832 | -0.62093866 | 0.04793468 | 1 | -5.45461845 | 1.13116121 | -0.94766527 |
| 6 | -3.05061841 | 0.22176132 | 0.14763469 | | | | |

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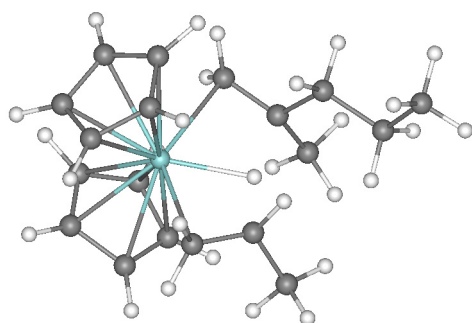


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1142195.1 (Joules/Mol) |
| | 272.99118 (Kcal/Mol) |
| Zero-point correction | 0.435039 (Hartree/Particle) |
| Thermal correction to Energy | 0.456539 |
| Thermal correction to Enthalpy | 0.457483 |
| Thermal correction to Gibbs Free Energy | 0.385706 |
| Sum of electronic and zero-point Energies | -4281.316222 |
| Sum of electronic and thermal Energies | -4281.294723 |
| Sum of electronic and thermal Enthalpies | -4281.293778 |
| Sum of electronic and thermal Free Energies | -4281.365555 |

| cartesian | | | | | | | |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | -1.12747550 | -2.19465518 | 1.37963676 | 6 | 2.86632442 | 0.22094485 | -0.23706324 |
| 6 | -1.11807537 | -2.56295514 | 0.01573674 | 1 | -0.33147544 | -0.31345513 | -1.40266323 |
| 6 | -2.44707537 | -2.47755527 | -0.47616327 | 1 | 0.55252457 | 1.17614484 | -1.16566324 |
| 6 | -3.28457546 | -2.09325528 | 0.60683674 | 6 | 4.17112446 | -0.57855511 | -0.16076325 |
| 6 | -2.47107553 | -1.91155517 | 1.74913681 | 1 | 2.97302437 | 1.01294482 | -0.99206322 |
| 1 | -2.81827545 | -1.62645519 | 2.73443675 | 1 | 2.73262453 | 0.72894490 | 0.72443676 |
| 1 | -0.26467544 | -2.16045523 | 2.03463674 | 6 | -1.07837546 | 0.91314489 | 2.07633662 |
| 1 | -0.24807543 | -2.86075521 | -0.55646324 | 6 | 0.15002453 | 1.09234476 | 1.39653683 |
| 1 | -2.77117538 | -2.71545529 | -1.48216319 | 6 | 0.59272456 | 2.49244475 | 1.04453683 |
| 1 | -4.35977554 | -1.97065520 | 0.56863672 | 1 | -1.10897541 | 0.14814484 | 2.84503675 |
| 6 | -2.21507549 | 2.01844478 | -1.22686327 | 1 | -1.65577543 | 1.80604482 | 2.29633665 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | -2.76357555 | 0.95504493 | -1.99706328 | 1 | 0.93782461 | 0.38484484 | 1.63933682 |
| 6 | -3.86907530 | 0.42854485 | -1.28976321 | 1 | -0.24767545 | 3.09404492 | 0.68923676 |
| 6 | -4.00077534 | 1.15324485 | -0.07426326 | 1 | 0.96042454 | 2.95454478 | 1.96723676 |
| 6 | -2.99217558 | 2.15004492 | -0.05186326 | 6 | 1.83742464 | -1.35315514 | -1.91656315 |
| 1 | -2.86097527 | 2.89784479 | 0.71873671 | 6 | 5.31352472 | 0.25964484 | 0.41223672 |
| 1 | -1.37997544 | 2.64464474 | -1.51506317 | 1 | 4.45212460 | -0.93475515 | -1.15566325 |
| 1 | -2.41227531 | 0.62124485 | -2.96646333 | 1 | 4.01682472 | -1.46895516 | 0.46113673 |
| 1 | -4.50637531 | -0.38195515 | -1.62056315 | 1 | 0.94652462 | -1.90975523 | -2.22536325 |
| 1 | -4.76437521 | 1.00214481 | 0.67933673 | 1 | 2.66242456 | -2.06555510 | -1.85246325 |
| 40 | -1.83397543 | -0.11885515 | 0.08243674 | 1 | 5.09392452 | 0.57894486 | 1.43523681 |
| 1 | 1.50122464 | -1.38195515 | 0.20833674 | 1 | 5.48052454 | 1.15724480 | -0.19046324 |
| 6 | 0.34952462 | 0.22594485 | -0.66586328 | 1 | 6.24682474 | -0.30655515 | 0.43203673 |
| 6 | 1.62582457 | -0.62415510 | -0.57836324 | 1 | 2.06992435 | -0.63405514 | -2.70936322 |
| | | | | 1 | 1.39792454 | 2.52794480 | 0.31143674 |

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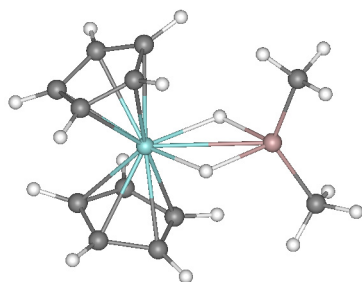
| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1127819.9 (Joules/Mol) |
| | 269.55543 (Kcal/Mol) |
| Zero-point correction | 0.429564 (Hartree/Particle) |
| Thermal correction to Energy | 0.451801 |
| Thermal correction to Enthalpy | 0.452745 |
| Thermal correction to Gibbs Free Energy | 0.379531 |
| Sum of electronic and zero-point Energies | -4281.305669 |
| Sum of electronic and thermal Energies | -4281.283432 |
| Sum of electronic and thermal Enthalpies | -4281.282488 |
| Sum of electronic and thermal Free Energies | -4281.355702 |

| cartesian | | | | | | | |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | -1.58554292 | -2.32785296 | 0.35126126 | 6 | 1.50915718 | -1.61075306 | 1.63716125 |
| 6 | -2.44114280 | -1.98185301 | -0.72603869 | 1 | -0.40554282 | -0.24655306 | 2.84546113 |
| 6 | -3.44764280 | -1.12305307 | -0.23593874 | 1 | 0.10305721 | 1.42594695 | 2.31916118 |
| 6 | -3.24044275 | -0.96305311 | 1.16486132 | 1 | 0.57195717 | -0.42385307 | -0.20563874 |
| 6 | -2.10634279 | -1.72205305 | 1.52476132 | 1 | 1.99595714 | -2.12135315 | 0.80676126 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | -1.72804284 | -1.85035300 | 2.52926111 | 1 | 2.22965717 | -1.56965303 | 2.46296120 |
| 1 | -0.74154282 | -3.00475311 | 0.30076125 | 1 | 0.65655714 | -2.20245314 | 1.97416127 |
| 1 | -2.36164284 | -2.34525299 | -1.74103868 | 1 | 1.81465721 | 1.58964694 | 0.29606125 |
| 1 | -3.86184287 | -0.39085308 | 1.84246123 | 6 | -0.68984282 | -0.10875309 | -2.38213873 |
| 6 | -1.13614273 | 2.57264686 | -0.95963871 | 6 | 0.53785723 | -0.49445310 | -1.84033871 |
| 6 | -2.46724272 | 2.10384703 | -1.16813874 | 6 | 1.00645709 | -1.92705297 | -1.98303878 |
| 6 | -3.08874273 | 2.00814700 | 0.09886126 | 1 | -0.78724283 | 0.88284695 | -2.80263877 |
| 6 | -2.13734293 | 2.34734702 | 1.09026122 | 1 | -1.32654285 | -0.86455309 | -2.82593894 |
| 6 | -0.93804282 | 2.72634697 | 0.42106125 | 1 | 1.32045722 | 0.26574692 | -1.82763875 |
| 1 | -0.03304282 | 3.09274697 | 0.88876128 | 1 | 1.77745724 | -2.20915294 | -1.26693869 |
| 1 | -0.40554282 | 2.79574704 | -1.72793877 | 1 | 0.17175716 | -2.62615299 | -1.90153873 |
| 1 | -2.94044280 | 1.91814697 | -2.12423873 | 1 | 1.42975712 | -2.03415298 | -2.98693895 |
| 1 | -2.31134272 | 2.37604690 | 2.15876126 | 1 | -4.11474276 | 1.71444690 | 0.28016126 |
| 40 | -1.32024288 | 0.19504693 | 0.02556126 | 1 | -4.25384283 | -0.69335306 | -0.81753874 |
| 6 | 2.23335719 | 0.76174688 | 0.88146126 | 1 | 3.04755735 | -0.45135310 | -0.73483872 |
| 1 | 2.62815714 | 1.21694696 | 1.79916131 | 1 | 3.91605735 | -0.58525312 | 0.77956128 |
| 6 | 3.40225720 | 0.12594692 | 0.12526126 | 6 | 4.39515686 | 1.18694699 | -0.34983876 |
| 6 | 0.06315720 | 0.36854693 | 2.08646107 | 1 | 5.24865723 | 0.72944689 | -0.85323870 |
| 6 | 1.11035728 | -0.17925307 | 1.32936132 | 1 | 4.77655697 | 1.77044690 | 0.49266124 |
| | | | | 1 | 3.92405725 | 1.88244700 | -1.05123878 |

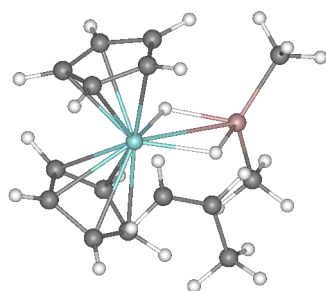
S1.3. Me₂AlH reaction profile

I-OH



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 679540.8 (Joules/Mol) |
| | 162.41414 (Kcal/Mol) |
| Zero-point correction | 0.258823 (Hartree/Particle) |
| Thermal correction to Energy | 0.274570 |
| Thermal correction to Enthalpy | 0.275514 |
| Thermal correction to Gibbs Free Energy | 0.214702 |
| Sum of electronic and zero-point Energies | -4250.669473 |
| Sum of electronic and thermal Energies | -4250.653726 |
| Sum of electronic and thermal Enthalpies | -4250.652782 |
| Sum of electronic and thermal Free Energies | -4250.713595 |

| cartesian | | | | | | | |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | 1.82288432 | -1.90424991 | 1.15558445 | 1 | 3.58228421 | 1.38665009 | 0.31368440 |
| 6 | 2.63388443 | -1.61284995 | 0.02818439 | 1 | 2.37378430 | 1.76175010 | -2.06411576 |
| 6 | 1.87768435 | -1.89014995 | -1.14011562 | 1 | -0.14301562 | 2.61045003 | -1.59161556 |
| 6 | 0.60298437 | -2.37514997 | -0.73471558 | 1 | -0.49281561 | 2.73134995 | 1.07608438 |
| 6 | 0.56868434 | -2.38364983 | 0.68458438 | 40 | 0.72808439 | 0.00415001 | -0.00681561 |
| 1 | -0.25921559 | -2.71374989 | 1.29998446 | 1 | -0.88371557 | -0.02334999 | 1.09408438 |
| 1 | 2.11988449 | -1.80964994 | 2.19408417 | 1 | -0.87391561 | -0.03134999 | -1.12851560 |
| 1 | 3.65698433 | -1.25914991 | 0.05418439 | 13 | -2.28861570 | -0.03524999 | -0.02131561 |
| 1 | 2.22418427 | -1.78444993 | -2.16191578 | 6 | -3.11041570 | 1.72725010 | 0.00058439 |
| 1 | -0.19281563 | -2.69914985 | -1.39391565 | 6 | -3.09901571 | -1.80065000 | 0.00608439 |
| 6 | 2.55578423 | 1.69675004 | 0.16368438 | 1 | -4.12461567 | 1.69525003 | -0.41031560 |
| 6 | 1.91688442 | 1.89345002 | -1.08991563 | 1 | -3.20421576 | 2.10275006 | 1.02638435 |
| 6 | 0.59158438 | 2.34695005 | -0.84061557 | 1 | -2.55761576 | 2.48045015 | -0.57031560 |
| 6 | 0.40728438 | 2.41094995 | 0.56558442 | 1 | -3.87501574 | -1.88974988 | -0.76151562 |
| 6 | 1.62208438 | 2.00475001 | 1.18498445 | 1 | -2.39351559 | -2.62214994 | -0.15121561 |
| 1 | 1.80838442 | 1.96175003 | 2.25228429 | 1 | -3.59481573 | -1.97994995 | 0.96688437 |

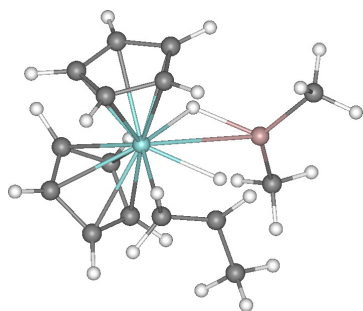
I-1H

| | |
|---|-----------------------------|
| Zero-point vibrational energy | 901973.9 (Joules/Mol) |
| | 215.57695 (Kcal/Mol) |
| Zero-point correction | 0.343544 (Hartree/Particle) |
| Thermal correction to Energy | 0.364822 |
| Thermal correction to Enthalpy | 0.365766 |
| Thermal correction to Gibbs Free Energy | 0.293380 |
| Sum of electronic and zero-point Energies | -4368.459600 |
| Sum of electronic and thermal Energies | -4368.438321 |
| Sum of electronic and thermal Enthalpies | -4368.437377 |
| Sum of electronic and thermal Free Energies | -4368.509764 |

cartesian

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | -1.34009516 | -2.25256109 | 0.69904149 | 1 | 0.72410482 | 0.94093907 | 1.27554142 |
| 6 | -2.24829531 | -1.43406093 | 1.40644145 | 1 | 1.06780481 | 0.04693904 | -0.64055860 |
| 6 | -1.51449513 | -0.74176097 | 2.41314149 | 13 | 2.25710487 | 0.75943905 | 0.42284143 |
| 6 | -0.15979518 | -1.14236093 | 2.32164145 | 6 | 2.86430478 | 2.47483897 | -0.27495858 |
| 6 | -0.04059519 | -2.05366111 | 1.23734140 | 6 | 3.35040474 | -0.62576097 | 1.24874151 |
| 1 | 0.86580479 | -2.55826116 | 0.92534137 | 1 | 3.95330477 | 2.49063897 | -0.38585857 |
| 1 | -1.59869516 | -2.93856096 | -0.09625857 | 1 | 2.44090486 | 2.71153903 | -1.25745857 |
| 1 | -3.31699514 | -1.37576091 | 1.23944151 | 1 | 2.61120486 | 3.30493903 | 0.39504144 |
| 1 | -1.92439520 | -0.05916096 | 3.14704156 | 1 | 4.08660460 | -0.18786095 | 1.93164146 |
| 1 | 0.64330482 | -0.81586093 | 2.96924138 | 1 | 2.79580474 | -1.38046098 | 1.81474149 |
| 6 | -1.45969522 | 2.06483889 | -1.24815857 | 1 | 3.92920494 | -1.16066098 | 0.48554143 |
| 6 | -2.63249516 | 1.46653903 | -0.69585860 | 6 | -1.34509516 | -1.00266099 | -2.29835844 |
| 6 | -2.63099527 | 1.72253907 | 0.69644141 | 6 | -0.00389519 | -1.13206100 | -2.40525866 |
| 6 | -1.44629514 | 2.42663884 | 1.01614141 | 6 | 0.77520478 | -2.38176107 | -2.12525845 |
| 6 | -0.73329520 | 2.65663886 | -0.19715858 | 1 | -1.97279513 | -1.83566093 | -1.99405861 |
| 1 | 0.20570481 | 3.18853903 | -0.29015857 | 1 | -1.84909523 | -0.14706096 | -2.73315859 |
| 1 | -1.17539525 | 2.07813907 | -2.29375863 | 1 | 1.11290479 | -2.79196095 | -3.08295846 |
| 1 | -3.42239523 | 0.96793908 | -1.24415851 | 1 | 1.66930485 | -2.17716098 | -1.53135860 |
| 1 | -3.39969516 | 1.41923904 | 1.39594150 | 1 | 0.17200482 | -3.14456105 | -1.62995851 |
| 1 | -1.14799523 | 2.76893902 | 1.99904144 | 1 | 0.55240482 | -0.30896097 | -2.85175848 |
| 40 | -0.71489519 | 0.15933904 | 0.23614143 | | | | |

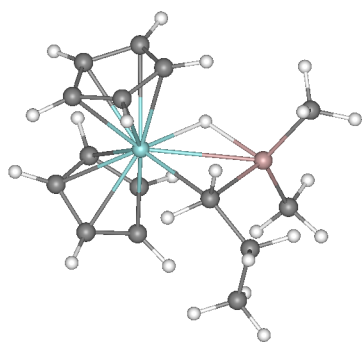
TS-1H



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 898825.0 (Joules/Mol) |
| | 214.82433 (Kcal/Mol) |
| Zero-point correction | 0.342344 (Hartree/Particle) |
| Thermal correction to Energy | 0.362787 |
| Thermal correction to Enthalpy | 0.363732 |
| Thermal correction to Gibbs Free Energy | 0.294205 |
| Sum of electronic and zero-point Energies | -4368.451149 |
| Sum of electronic and thermal Energies | -4368.430706 |
| Sum of electronic and thermal Enthalpies | -4368.429762 |
| Sum of electronic and thermal Free Energies | -4368.499289 |

| cartesian | | | | | |
|-----------|-------------|-------------|-------------|----|-------------------------------------|
| 6 | -0.01282695 | -2.32699752 | -0.68525368 | 1 | -1.18342686 0.97610247 2.24504638 |
| 6 | 0.60637307 | -1.82679772 | -1.86725354 | 6 | -0.81252682 -0.03589760 2.07914639 |
| 6 | 1.98907316 | -1.69919765 | -1.61625361 | 6 | 0.54927307 -0.26239762 2.33864641 |
| 6 | 2.23827291 | -2.12579751 | -0.27905366 | 6 | -1.83982694 -1.13259768 2.25014639 |
| 6 | 1.00487304 | -2.54159737 | 0.27774635 | 1 | -1.46282685 -2.09289742 1.89234650 |
| 1 | 0.87027311 | -2.97439742 | 1.25984645 | 1 | -2.78182697 -0.90679753 1.74674642 |
| 1 | -1.06352687 | -2.56959748 | -0.57625365 | 1 | -2.04222703 -1.22899771 3.32114625 |
| 1 | 0.10497306 | -1.59549761 | -2.79825377 | 1 | -1.00742686 0.15550239 0.55124635 |
| 1 | 2.73257303 | -1.35269761 | -2.32305360 | 1 | 0.85097313 -1.25769770 2.64714622 |
| 1 | 3.20577312 | -2.17969751 | 0.20534635 | 1 | 1.11847305 0.55200243 2.77084637 |
| 6 | 2.20667291 | 1.64550233 | -1.40995359 | 13 | -1.98312676 0.70570242 -0.98735368 |
| 6 | 3.11117291 | 1.08690238 | -0.46805364 | 1 | -0.37092692 0.53270245 -1.52625358 |
| 6 | 2.68677306 | 1.46050239 | 0.82624632 | 6 | -2.44362688 2.54780269 -0.56675369 |
| 6 | 1.52917314 | 2.28320265 | 0.68634635 | 6 | -3.10442710 -0.77159756 -1.57225358 |
| 6 | 1.25117314 | 2.41340256 | -0.69055367 | 1 | -3.41822696 -1.40669763 -0.73495370 |
| 1 | 0.44477305 | 2.99010253 | -1.12675357 | 1 | -2.60292697 -1.42229772 -2.29655361 |
| 1 | 2.26307297 | 1.55000234 | -2.48715377 | 1 | -4.02272701 -0.40789762 -2.04455352 |
| 1 | 3.97527289 | 0.47700238 | -0.70035368 | 1 | -3.46752691 2.63430262 -0.18885365 |
| 1 | 3.18277311 | 1.20160234 | 1.75314641 | 1 | -2.39362693 3.17780256 -1.46325350 |
| 1 | 0.98457313 | 2.76110268 | 1.49274647 | 1 | -1.78012693 3.00200248 0.17744637 |
| 40 | 0.88737309 | -0.03519760 | -0.11235365 | | |

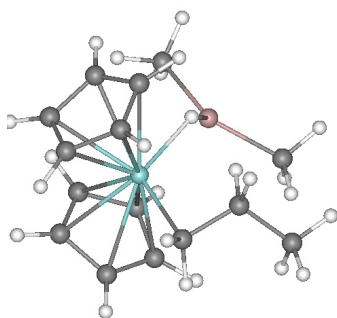
I-2H_a



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 909914.3 (Joules/Mol) |
| | 217.47475 (Kcal/Mol) |
| Zero-point correction | 0.346568 (Hartree/Particle) |
| Thermal correction to Energy | 0.367351 |
| Thermal correction to Enthalpy | 0.368295 |
| Thermal correction to Gibbs Free Energy | 0.296995 |
| Sum of electronic and zero-point Energies | -4368.473827 |
| Sum of electronic and thermal Energies | -4368.453044 |
| Sum of electronic and thermal Enthalpies | -4368.452100 |
| Sum of electronic and thermal Free Energies | -4368.523400 |

| cartesian | | | | | | | | | | | |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|--|--|--|--|
| 6 | 1.72529995 | -1.90310001 | -1.28160000 | 1 | 1.31099999 | 2.03509998 | 2.37949991 | | | | |
| 6 | 0.32040000 | -2.05739999 | -1.42200005 | 1 | 3.35050011 | 0.39340001 | 1.75979996 | | | | |
| 6 | -0.21160001 | -2.38599992 | -0.15050000 | 13 | -1.96010005 | 0.78479999 | -0.87309998 | | | | |
| 6 | 0.86900002 | -2.45919991 | 0.77329999 | 6 | -3.03040004 | -0.60869998 | -1.71840000 | | | | |
| 6 | 2.06450009 | -2.16669989 | 0.07450000 | 6 | -2.35290003 | 2.69519997 | -0.94010001 | | | | |
| 40 | 0.71950001 | -0.06530000 | 0.05400000 | 1 | -3.10319996 | -0.39060000 | -2.79150009 | | | | |
| 6 | -1.32449996 | 0.47830001 | 1.20360005 | 1 | -4.06150007 | -0.61229998 | -1.34549999 | | | | |
| 1 | -0.28830001 | 0.51840001 | -1.46599996 | 1 | -2.65310001 | -1.63259995 | -1.63189995 | | | | |
| 6 | 1.19640005 | 2.40479994 | 0.18160000 | 1 | -1.70850003 | 3.21180010 | -1.66190004 | | | | |
| 6 | 1.97529995 | 1.89250004 | -0.89469999 | 1 | -2.22569990 | 3.20449996 | 0.02230000 | | | | |
| 6 | 2.93700004 | 1.00590003 | -0.35479999 | 1 | -3.38240004 | 2.88269997 | -1.26259995 | | | | |
| 6 | 2.75119996 | 0.95719999 | 1.05509996 | 1 | -0.66960001 | -0.19149999 | 1.82490003 | | | | |
| 6 | 1.68630004 | 1.83959997 | 1.38150001 | 1 | -1.11090004 | 1.49710000 | 1.54400003 | | | | |
| 1 | -1.25000000 | -2.59030008 | 0.07240000 | 6 | -2.75860000 | 0.13290000 | 1.69120002 | | | | |
| 1 | 0.79329997 | -2.71860003 | 1.82369995 | 6 | -3.09960008 | -1.35350001 | 1.68700004 | | | | |
| 1 | -0.24360000 | -1.94589996 | -2.33949995 | 1 | -3.50760007 | 0.68650001 | 1.10510004 | | | | |
| 1 | 2.42000008 | -1.67019999 | -2.07949996 | 1 | -4.07049990 | -1.51880002 | 2.15869999 | | | | |
| 1 | 3.06279993 | -2.15799999 | 0.49439999 | 1 | -2.35770011 | -1.92690003 | 2.25340009 | | | | |
| 1 | 3.69260001 | 0.46810001 | -0.91360003 | 1 | -3.15809989 | -1.75790000 | 0.67430001 | | | | |
| 1 | 1.85769999 | 2.15100002 | -1.93970001 | 1 | -2.86409998 | 0.52730000 | 2.70650005 | | | | |
| 1 | 0.38270000 | 3.11509991 | 0.08990000 | | | | | | | | |

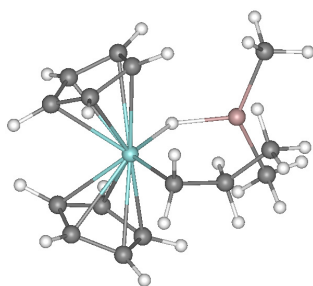
I-2H_bi



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 906854.6 (Joules/Mol) |
| | 216.74345 (Kcal/Mol) |
| Zero-point correction | 0.345403 (Hartree/Particle) |
| Thermal correction to Energy | 0.366043 |
| Thermal correction to Enthalpy | 0.366987 |
| Thermal correction to Gibbs Free Energy | 0.295655 |
| Sum of electronic and zero-point Energies | -4368.459386 |
| Sum of electronic and thermal Energies | -4368.438745 |
| Sum of electronic and thermal Enthalpies | -4368.437801 |
| Sum of electronic and thermal Free Energies | -4368.509134 |

| cartesian | | | | | | |
|-----------|-------------|-------------|-------------|----|-------------|-------------------------|
| 6 | 2.64969993 | -0.19610000 | -1.34940004 | 1 | -0.94970000 | -0.18770000 -1.23099995 |
| 6 | 2.84920001 | -1.00440001 | -0.20200001 | 1 | -0.07820000 | 1.69959998 -1.18579996 |
| 6 | 1.93610001 | -2.09220004 | -0.27320001 | 13 | -2.54719996 | -0.40930000 -0.82999998 |
| 6 | 1.14950001 | -1.93320000 | -1.43529999 | 6 | -3.50690007 | 1.27269995 -0.75940001 |
| 6 | 1.59080005 | -0.75349998 | -2.10260010 | 6 | -3.10229993 | -2.25460005 -1.03009999 |
| 1 | 1.19970000 | -0.36989999 | -3.03719997 | 1 | -3.91020012 | 1.53139997 -1.74510002 |
| 1 | 3.20810008 | 0.69520003 | -1.60259998 | 1 | -2.87290001 | 2.11019993 -0.44830000 |
| 1 | 3.58999991 | -0.83929998 | 0.57090002 | 1 | -4.36439991 | 1.23380005 -0.07920000 |
| 1 | 1.85749996 | -2.90310001 | 0.44010001 | 1 | -2.31830001 | -2.96580005 -0.75070000 |
| 1 | 0.36289999 | -2.59780002 | -1.77119994 | 1 | -3.36610007 | -2.46880007 -2.07200003 |
| 6 | -0.93269998 | 0.73689997 | 2.04329991 | 1 | -3.99070001 | -2.48830009 -0.43430001 |
| 6 | 0.33199999 | 0.40419999 | 2.57329988 | 6 | 1.53610003 | 2.00580001 0.31240001 |
| 6 | 0.53619999 | -0.99030000 | 2.39129996 | 6 | 0.68260002 | 2.47779989 -0.85100001 |
| 6 | -0.61299998 | -1.53219998 | 1.76650000 | 6 | -0.16190000 | 3.72510004 -0.56980002 |
| 6 | -1.52830005 | -0.46529999 | 1.55780005 | 1 | 2.60570002 | 2.09949994 0.13890000 |
| 1 | -2.59759998 | -0.59469998 | 1.38429999 | 1 | 1.27349997 | 2.53020000 1.23160005 |
| 1 | -1.39800000 | 1.71589994 | 2.05399990 | 1 | -0.81349999 | 3.97119999 -1.41120005 |
| 1 | 1.02639997 | 1.08749998 | 3.04279995 | 1 | 0.49349999 | 4.57700014 -0.37799999 |
| 1 | 1.40840006 | -1.54849994 | 2.70860004 | 1 | -0.78490001 | 3.57859993 0.31760001 |
| 1 | -0.78829998 | -2.57529998 | 1.53240001 | 1 | 1.27880001 | 2.60310006 -1.75899994 |
| 40 | 0.56339997 | -0.02450000 | 0.07110000 | | | |

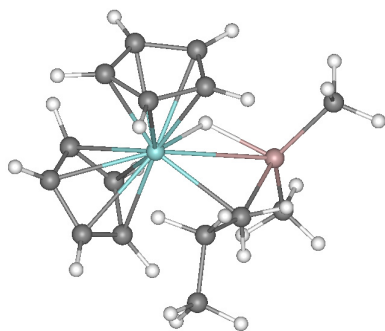
I-2H_b'



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 905923.6 (Joules/Mol) |
| | 216.52093 (Kcal/Mol) |
| Zero-point correction | 0.345048 (Hartree/Particle) |
| Thermal correction to Energy | 0.366394 |
| Thermal correction to Enthalpy | 0.367338 |
| Thermal correction to Gibbs Free Energy | 0.293828 |
| Sum of electronic and zero-point Energies | -4368.457077 |
| Sum of electronic and thermal Energies | -4368.435731 |
| Sum of electronic and thermal Enthalpies | -4368.434787 |
| Sum of electronic and thermal Free Energies | -4368.508297 |

| cartesian | | | | | | |
|-----------|-------------|-------------|-------------|---|-------------|-------------|
| 6 | 1.61150002 | 2.22346354 | -0.96474630 | 1 | -0.56909990 | 0.26316339 |
| 6 | 0.73910010 | 2.52486348 | 0.10855365 | 6 | -3.01130009 | -1.44233668 |
| 6 | 1.40260005 | 2.18386340 | 1.32305360 | 6 | -2.90100002 | 2.12356353 |
| 6 | 2.66899991 | 1.65826333 | 0.99275368 | 1 | -3.94039989 | 2.18856359 |
| 6 | 2.79369998 | 1.65926337 | -0.42564636 | 1 | -2.88540006 | 2.46436357 |
| 1 | 3.65649986 | 1.32926333 | -0.99184638 | 1 | -2.31590009 | 2.84106350 |
| 1 | 1.41420007 | 2.39876342 | -2.01374650 | 1 | -4.01639986 | -1.44163668 |
| 6 | 1.97640014 | -1.45163667 | 1.87145364 | 1 | -3.10739994 | -1.82073665 |
| 6 | 2.83360004 | -1.53673661 | 0.73545367 | 1 | -2.40919995 | -2.17403650 |
| 6 | 2.12980008 | -2.19403648 | -0.29904634 | 1 | 1.00670004 | 2.31126356 |
| 6 | 0.83320010 | -2.51463652 | 0.19035365 | 1 | -0.23899993 | 2.98516345 |
| 6 | 0.75530005 | -2.08463645 | 1.53735363 | 1 | 2.51539993 | -2.41993642 |
| 1 | -0.09449995 | -2.20953655 | 2.19725370 | 1 | 0.06090006 | -3.04223657 |
| 1 | 2.22889996 | -1.02233660 | 2.83315349 | 1 | 3.41669989 | 1.31476331 |
| 40 | 0.98760009 | 0.01606340 | 0.11495364 | 1 | 3.85529995 | -1.18223667 |
| 6 | -0.85069990 | 0.09866340 | -1.88674641 | 6 | -1.93679988 | -0.88433659 |
| 6 | 0.57500005 | -0.33483660 | -2.11134648 | 1 | -1.04089987 | 1.10876334 |
| 1 | -1.05419993 | 0.25426340 | -0.75354636 | 1 | -2.93810010 | -0.54663658 |
| 1 | 1.10590005 | 0.27906340 | -2.83504629 | 1 | -1.76719987 | -1.87233663 |
| 1 | 0.62890005 | -1.38323665 | -2.40484643 | 1 | -1.90659988 | -0.98933655 |
| 13 | -2.21210003 | 0.32096338 | 1.20055366 | | | |

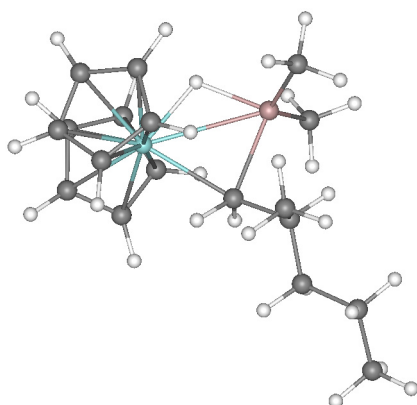
I-2H_bo



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 911044.0 (Joules/Mol) |
| | 217.74473 (Kcal/Mol) |
| Zero-point correction | 0.346998 (Hartree/Particle) |
| Thermal correction to Energy | 0.367848 |
| Thermal correction to Enthalpy | 0.368792 |
| Thermal correction to Gibbs Free Energy | 0.297628 |
| Sum of electronic and zero-point Energies | -4368.483495 |
| Sum of electronic and thermal Energies | -4368.462645 |
| Sum of electronic and thermal Enthalpies | -4368.461701 |
| Sum of electronic and thermal Free Energies | -4368.532865 |

| cartesian | | | | | |
|-----------|-------------|-------------|-------------|---|-------------------------------------|
| 6 | -0.55215120 | 2.41029024 | -0.87821954 | 6 | 3.00974870 -1.20140982 1.56788039 |
| 6 | -1.86345124 | 1.94829011 | -1.19521952 | 6 | 2.94754887 2.07719016 0.41238046 |
| 6 | -2.61555123 | 1.90769017 | 0.00138044 | 1 | 2.33484888 -2.04440975 1.75418043 |
| 6 | -1.77455127 | 2.33789039 | 1.06358051 | 1 | 3.46884871 -0.94110984 2.52788043 |
| 6 | -0.51125121 | 2.67649031 | 0.51238048 | 1 | 3.82334900 -1.57660985 0.93598044 |
| 1 | 0.33714879 | 3.06689024 | 1.06008053 | 1 | 2.99124885 2.68329024 1.32518053 |
| 1 | 0.25014877 | 2.58599019 | -1.58461952 | 1 | 2.43634868 2.67869020 -0.34721953 |
| 1 | -2.23085117 | 1.69899011 | -2.18381953 | 1 | 3.98574877 1.96349013 0.08018044 |
| 1 | -2.05945110 | 2.44009018 | 2.10348034 | 6 | 0.13364878 -1.95320976 -2.86871958 |
| 6 | -0.70195121 | -2.23020983 | 0.92288047 | 6 | 1.15544879 -0.46440980 -1.04951954 |
| 6 | -1.89645123 | -2.08630967 | 0.16598044 | 6 | 0.08064878 -0.60950977 -2.13641953 |
| 6 | -2.76955128 | -1.22810984 | 0.87718046 | 1 | 0.13444880 0.22169019 -2.84261942 |
| 6 | -2.12215137 | -0.85060978 | 2.08648038 | 1 | 1.95484877 0.14599019 -1.49601960 |
| 6 | -0.85375124 | -1.48360980 | 2.12148046 | 1 | 1.57234883 -1.45730984 -0.84991950 |
| 1 | -0.12975122 | -1.41590989 | 2.92338061 | 1 | -0.99045122 -0.54990977 -1.77411962 |
| 1 | 0.14974877 | -2.84630966 | 0.66208047 | 1 | 0.04404879 -2.78300977 -2.16191959 |
| 1 | -2.11285114 | -2.56470966 | -0.78261954 | 1 | 1.09194875 -2.05330968 -3.38241959 |
| 1 | -2.54085112 | -0.22310981 | 2.86348057 | 1 | -3.76955128 -0.94680983 0.57228041 |
| 40 | -0.80635118 | 0.18589020 | 0.24208045 | 1 | -3.65475130 1.61749017 0.08918045 |
| 1 | 0.58164877 | 0.56099021 | 1.51158047 | 1 | -0.66545117 -2.03630972 -3.60831952 |
| 13 | 2.13734889 | 0.33889019 | 0.75908047 | | |

I-4H_a

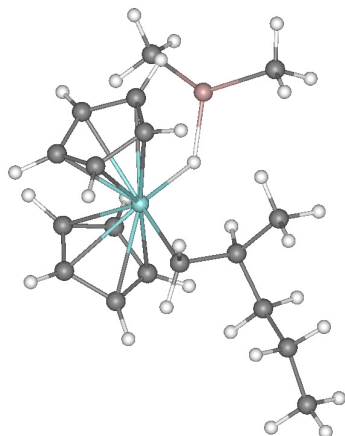


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1135934.0 (Joules/Mol) |
| | 271.49475 (Kcal/Mol) |
| Zero-point correction | 0.432654 (Hartree/Particle) |
| Thermal correction to Energy | 0.457474 |
| Thermal correction to Enthalpy | 0.458418 |
| Thermal correction to Gibbs Free Energy | 0.378226 |
| Sum of electronic and zero-point Energies | -4486.277142 |
| Sum of electronic and thermal Energies | -4486.252323 |
| Sum of electronic and thermal Enthalpies | -4486.251378 |
| Sum of electronic and thermal Free Energies | -4486.331571 |

| | | | | cartesian | | | |
|----|-------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 6 | 3.79535007 | 1.53163600 | 0.42124194 | 6 | -0.57705003 | -1.00206399 | -3.04495811 |
| 6 | 2.67135000 | 2.24483609 | -0.07365809 | 1 | 0.19114992 | 2.59593606 | -3.24925804 |
| 6 | 1.67124987 | 2.23413610 | 0.92924196 | 1 | -1.31675005 | 2.61943603 | -2.36105824 |
| 6 | 2.18674994 | 1.53393602 | 2.05694175 | 1 | 0.18524992 | 3.06133604 | -1.55365813 |
| 6 | 3.50014997 | 1.10823596 | 1.74604189 | 1 | 0.26644990 | -1.48646402 | -3.55165815 |
| 40 | 1.97904992 | -0.15386397 | 0.21994191 | 1 | -1.11525011 | -1.78786397 | -2.50085807 |
| 6 | -0.41965014 | -0.26406395 | 0.11154191 | 1 | -1.24855018 | -0.65226400 | -3.83615804 |
| 1 | 1.77924991 | 0.30593604 | -1.62315810 | 1 | -0.07805008 | -0.11676396 | 1.17224193 |
| 6 | 1.86034989 | -2.49946380 | -0.69595808 | 1 | -0.53025013 | -1.34636402 | -0.02005809 |
| 6 | 3.10894990 | -1.96166396 | -1.11535811 | 6 | -1.86115003 | 0.32623604 | 0.11694191 |
| 6 | 3.89864993 | -1.73966396 | 0.03894191 | 6 | -2.80145001 | -0.65096396 | 0.84584194 |
| 6 | 3.13984990 | -2.13526392 | 1.17604184 | 6 | -1.90895009 | 1.73133600 | 0.71544194 |
| 6 | 1.88714981 | -2.61906385 | 0.71334195 | 1 | -2.23605013 | 0.38573605 | -0.92045808 |
| 1 | 0.70154989 | 2.70923615 | 0.86754191 | 1 | -2.92435002 | 2.13113618 | 0.68804193 |
| 1 | 1.67444992 | 1.37713599 | 2.99984193 | 1 | -1.58575010 | 1.71223605 | 1.76384187 |
| 1 | 2.59314990 | 2.71393609 | -1.04625809 | 1 | -1.27775002 | 2.43033624 | 0.16264191 |
| 1 | 4.73084974 | 1.37973607 | -0.10335809 | 6 | -4.26865005 | -0.21776398 | 0.88534194 |
| 1 | 4.16694975 | 0.56573600 | 2.40484190 | 1 | -2.73655009 | -1.62856400 | 0.35134190 |
| 1 | 4.91074991 | -1.35506403 | 0.05434191 | 1 | -2.43355012 | -0.79456401 | 1.87194192 |
| 1 | 3.40415001 | -1.77056396 | -2.13935804 | 6 | -5.16975021 | -1.32906401 | 1.42374182 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 1.04294991 | -2.77996397 | -1.35005808 | 1 | -4.59215021 | 0.06523603 | -0.12345809 |
| 1 | 1.08874989 | -3.00496387 | 1.33714187 | 1 | -4.38105011 | 0.67083603 | 1.51354182 |
| 1 | 3.47654986 | -2.12466383 | 2.20544195 | 1 | -6.21054983 | -1.00286400 | 1.47234190 |
| 13 | 0.00724989 | 0.46763602 | -1.90015817 | 1 | -4.86495018 | -1.62556398 | 2.43154192 |
| 6 | -0.25425011 | 2.36333609 | -2.27365804 | 1 | -5.12585020 | -2.21586394 | 0.78534192 |

I-4H_bi



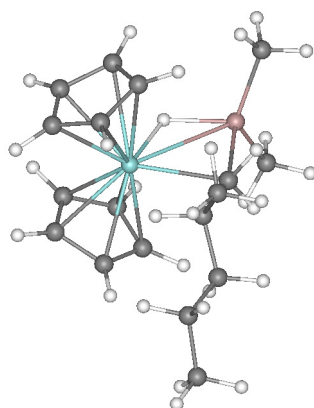
| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1132658.0 (Joules/Mol) |
| | 270.71177 (Kcal/Mol) |
| Zero-point correction | 0.431407 (Hartree/Particle) |
| Thermal correction to Energy | 0.456920 |
| Thermal correction to Enthalpy | 0.457864 |
| Thermal correction to Gibbs Free Energy | 0.374211 |
| Sum of electronic and zero-point Energies | -4486.262023 |
| Sum of electronic and thermal Energies | -4486.236510 |
| Sum of electronic and thermal Enthalpies | -4486.235565 |
| Sum of electronic and thermal Free Energies | -4486.319218 |

cartesian

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | 0.74059618 | -2.64763188 | 0.74807203 | 6 | -4.13320398 | 0.81736803 | 1.82127202 |
| 6 | -0.39710388 | -3.26193190 | 0.16937199 | 1 | -1.54820383 | 3.85746813 | 1.60007203 |
| 6 | -1.53660393 | -2.88573194 | 0.93757200 | 1 | -1.19450390 | 3.45346808 | -0.07312801 |
| 6 | -1.10700393 | -2.01593208 | 1.95987189 | 1 | -2.80740404 | 4.01726818 | 0.38817197 |
| 6 | 0.30379611 | -1.85083199 | 1.83387196 | 1 | -4.08170366 | -0.26583201 | 1.97057211 |
| 1 | 0.93189609 | -1.25483203 | 2.48547196 | 1 | -4.35890388 | 1.26656806 | 2.79477191 |
| 1 | 1.76199615 | -2.77703190 | 0.41977197 | 1 | -5.00230360 | 1.02306807 | 1.18537199 |
| 1 | -0.38940388 | -3.94103193 | -0.67452800 | 6 | 1.27469611 | -0.51973200 | -1.28932798 |
| 1 | -2.55440378 | -3.21563196 | 0.76947200 | 6 | 1.56589615 | 0.59946799 | -0.30442804 |
| 1 | -1.73480392 | -1.55963194 | 2.71507192 | 6 | 1.54889607 | 1.99656796 | -0.94052798 |
| 6 | -1.61170387 | 0.46216801 | -2.29222822 | 6 | 2.82599592 | 0.35586801 | 0.54927200 |
| 6 | -1.44690382 | -0.88843203 | -2.66732812 | 1 | 2.01279593 | -1.31973195 | -1.26752794 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|------------|-------------|-------------|
| 6 | -2.37600374 | -1.66823196 | -1.92862797 | 1 | 1.17049611 | -0.15413201 | -2.31162810 |
| 6 | -3.12540388 | -0.80273199 | -1.09722805 | 1 | 1.73029602 | 2.77396798 | -0.19212802 |
| 6 | -2.65820408 | 0.52266800 | -1.32942796 | 1 | 2.32029629 | 2.07026792 | -1.71082795 |
| 1 | -3.18700409 | 1.44276798 | -1.07652795 | 1 | 0.58679610 | 2.20476794 | -1.41732800 |
| 1 | -1.07950389 | 1.30936801 | -2.70662808 | 6 | 4.13439608 | 0.53656793 | -0.22412801 |
| 1 | -0.74140388 | -1.26483202 | -3.39642811 | 1 | 2.82159615 | 1.03626800 | 1.41007197 |
| 1 | -2.50800371 | -2.74013209 | -2.00652814 | 1 | 2.79269600 | -0.66303205 | 0.95487201 |
| 1 | -3.94110394 | -1.08463204 | -0.44212800 | 6 | 5.34229612 | 0.12006798 | 0.61517203 |
| 40 | -0.70920384 | -0.82533205 | -0.22892801 | 1 | 4.24569607 | 1.58406806 | -0.52092803 |
| 1 | -1.21230388 | 0.53636801 | 1.15707195 | 1 | 4.10329628 | -0.05113202 | -1.14902794 |
| 1 | 0.74629617 | 0.67096794 | 0.49017203 | 1 | 6.27499628 | 0.28006801 | 0.07057199 |
| 13 | -2.50930405 | 1.56966805 | 1.07397199 | 1 | 5.28899622 | -0.93873203 | 0.88497198 |
| 6 | -1.96620393 | 3.39036798 | 0.70097202 | 1 | 5.39309645 | 0.69936800 | 1.54157197 |

I-4H_bo



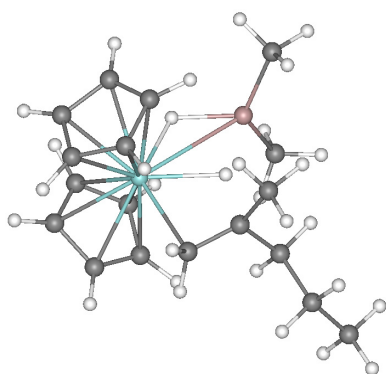
| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1139139.7 (Joules/Mol) |
| | 272.26093 (Kcal/Mol) |
| Zero-point correction | 0.433875 (Hartree/Particle) |
| Thermal correction to Energy | 0.458266 |
| Thermal correction to Enthalpy | 0.459210 |
| Thermal correction to Gibbs Free Energy | 0.381441 |
| Sum of electronic and zero-point Energies | -4486.286925 |
| Sum of electronic and thermal Energies | -4486.262534 |
| Sum of electronic and thermal Enthalpies | -4486.261590 |
| Sum of electronic and thermal Free Energies | -4486.339359 |

cartesian

| | | | | | | | |
|---|------------|-------------|------------|---|------------|------------|-------------|
| 6 | 1.92533588 | -0.78495610 | 2.07330608 | 1 | 2.53123593 | 2.94004393 | -2.80459404 |
| 6 | 0.97023594 | -1.83825612 | 2.12290597 | 1 | 1.17353594 | 3.77494383 | -2.08329391 |
| 6 | 1.39263606 | -2.85825610 | 1.23830605 | 1 | 4.20723581 | 2.58024383 | 0.46180600 |
| 6 | 2.61973596 | -2.44485617 | 0.64750600 | 1 | 3.20363593 | 1.91594386 | 1.74660599 |
| 6 | 2.95713592 | -1.17555606 | 1.18000603 | 1 | 2.92183614 | 3.54744387 | 1.14750600 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 3.84803605 | -0.60475612 | 0.95150602 | 6 | -2.46706390 | 0.79034388 | 0.20740598 |
| 1 | 1.91113591 | 0.12424389 | 2.66100597 | 6 | -3.61456394 | -0.13305610 | 0.62010598 |
| 1 | 0.07963598 | -1.86415613 | 2.74020600 | 6 | -4.82616425 | 0.02754390 | -0.29829401 |
| 1 | 3.21733594 | -3.01955605 | -0.04879401 | 1 | -3.27536392 | -1.17865610 | 0.60660601 |
| 6 | -0.35676402 | -0.48655611 | -2.35649395 | 1 | -5.65096426 | -0.61325610 | 0.01840599 |
| 6 | -1.00306392 | -1.58495617 | -1.72439396 | 1 | -4.57616425 | -0.23135610 | -1.33189404 |
| 6 | -0.08806404 | -2.66345620 | -1.67149401 | 1 | -5.18366432 | 1.06084383 | -0.29239401 |
| 6 | 1.12523603 | -2.23845601 | -2.28109407 | 6 | 0.01843596 | 1.35424387 | 0.34610599 |
| 6 | 0.94993597 | -0.90215611 | -2.72119403 | 6 | -1.13476396 | 0.51914394 | 0.92810595 |
| 1 | 1.68233585 | -0.30425611 | -3.24839401 | 6 | -1.27256393 | 0.68734396 | 2.44660592 |
| 1 | -0.79636401 | 0.47864392 | -2.57619405 | 1 | 0.39013597 | 1.99734378 | 1.15630603 |
| 1 | -2.02426386 | -1.60285616 | -1.35999405 | 1 | -0.40446401 | 2.00254393 | -0.43179402 |
| 1 | 2.01193595 | -2.84245610 | -2.42679405 | 1 | -1.00086403 | -0.60725611 | 0.79530597 |
| 40 | 0.87153596 | -0.87595606 | -0.20179401 | 1 | -1.95856404 | -0.04895610 | 2.87180591 |
| 1 | 2.30023599 | 0.21184391 | -0.86399400 | 1 | -1.67046404 | 1.68464386 | 2.65790606 |
| 1 | -3.91156411 | 0.07824391 | 1.65180600 | 1 | -0.31166404 | 0.59764385 | 2.95730591 |
| 13 | 1.97093606 | 1.88674378 | -0.54809403 | 1 | -2.31616402 | 0.72164392 | -0.87629402 |
| 6 | 1.60593605 | 2.77984381 | -2.23949409 | 1 | -2.74236393 | 1.83294392 | 0.40880597 |
| 6 | 3.17913604 | 2.52764392 | 0.83870602 | 1 | -0.28996402 | -3.64865613 | -1.27059400 |
| 1 | 0.92063594 | 2.23354387 | -2.89689398 | 1 | 0.89073598 | -3.80295610 | 1.07230604 |

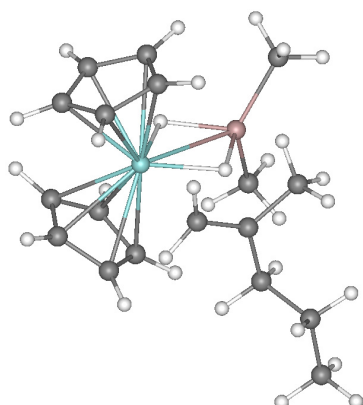
TS-4H



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1126129.9 (Joules/Mol) |
| | 269.15151 (Kcal/Mol) |
| Zero-point correction | 0.428920 (Hartree/Particle) |
| Thermal correction to Energy | 0.453290 |
| Thermal correction to Enthalpy | 0.454234 |
| Thermal correction to Gibbs Free Energy | 0.376326 |
| Sum of electronic and zero-point Energies | -4486.258626 |
| Sum of electronic and thermal Energies | -4486.234257 |
| Sum of electronic and thermal Enthalpies | -4486.233313 |
| Sum of electronic and thermal Free Energies | -4486.311221 |

| cartesian | | | | | | | | | |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|--|--|
| 6 | 2.16737223 | 1.84116399 | 1.12143600 | 1 | -0.35892797 | 1.73096406 | 2.26183581 | | |
| 6 | 3.17787218 | 1.54126406 | 0.16233599 | 1 | -1.76322806 | 2.10246396 | 1.23463607 | | |
| 6 | 3.83667183 | 0.36466402 | 0.57593602 | 1 | -1.95472801 | 1.12216401 | 2.69613600 | | |
| 6 | 3.24047184 | -0.07343599 | 1.79353607 | 1 | -0.31092793 | 0.63176399 | -0.08656400 | | |
| 6 | 2.23467207 | 0.86016405 | 2.14063597 | 1 | -2.64212799 | 0.39746398 | -0.37336400 | | |
| 1 | 1.63857210 | 0.83426404 | 3.04283595 | 1 | -2.00602818 | -1.24683595 | -0.37686399 | | |
| 1 | 1.51587200 | 2.70706391 | 1.10213602 | 1 | 0.15937206 | -0.77963597 | 2.64273596 | | |
| 1 | 3.40537214 | 2.12066388 | -0.72296399 | 1 | -0.50862789 | -1.98393595 | 1.44043601 | | |
| 1 | 4.66047239 | -0.11483599 | 0.06273600 | 13 | -0.14272797 | 1.63626397 | -1.69666398 | | |
| 1 | 3.54097223 | -0.93323600 | 2.37993598 | 1 | 1.36157203 | 0.84706402 | -1.55146396 | | |
| 6 | 2.69257212 | -1.69493604 | -1.70136404 | 6 | -1.29182792 | 0.74136400 | -2.98686409 | | |
| 6 | 2.78457212 | -2.43263602 | -0.48916399 | 6 | -0.04772794 | 3.51176381 | -1.18546402 | | |
| 6 | 1.48697209 | -2.86173606 | -0.13546400 | 1 | 0.98367202 | 3.88206387 | -1.17616403 | | |
| 6 | 0.58687204 | -2.40823603 | -1.14336395 | 1 | -0.61152792 | 4.14436436 | -1.87826395 | | |
| 6 | 1.33587205 | -1.71243596 | -2.11746407 | 1 | -0.46042794 | 3.69506383 | -0.18646401 | | |
| 1 | 0.94497204 | -1.26303601 | -3.02196407 | 1 | -2.28612804 | 1.19766402 | -3.03766418 | | |
| 1 | 3.51497221 | -1.23923600 | -2.23886418 | 1 | -0.86772799 | 0.81596404 | -3.99606419 | | |
| 1 | 3.69197226 | -2.63703609 | 0.06513600 | 1 | -1.43062794 | -0.32473600 | -2.77626419 | | |
| 1 | 1.23227203 | -3.46133614 | 0.72883600 | 6 | -3.44142771 | -0.86223596 | 1.18863606 | | |
| 1 | -0.47502792 | -2.61553621 | -1.18776405 | 6 | -4.60552788 | -1.42143595 | 0.37173602 | | |
| 40 | 1.49457204 | -0.33933598 | 0.02403600 | 1 | -3.78922796 | -0.01433600 | 1.78643596 | | |
| 6 | -2.28962803 | -0.41423601 | 0.27443600 | 1 | -3.07642794 | -1.61923599 | 1.89063597 | | |
| 6 | -1.08642793 | 0.03966400 | 1.09043598 | 1 | -5.42672777 | -1.72563601 | 1.02323604 | | |
| 6 | -0.23692793 | -0.95233595 | 1.64683604 | 1 | -4.29632759 | -2.29563618 | -0.20806399 | | |
| 6 | -1.28962791 | 1.33596396 | 1.85343599 | 1 | -4.99192762 | -0.67403597 | -0.32656398 | | |

I-5H



Zero-point vibrational energy

1127761.5 (Joules/Mol)

269.54147 (Kcal/Mol)

Zero-point correction

0.429542 (Hartree/Particle)

Thermal correction to Energy

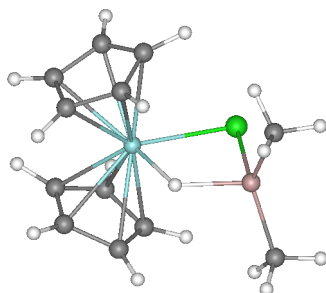
0.454940

| | |
|---|--------------|
| Thermal correction to Enthalpy | 0.455885 |
| Thermal correction to Gibbs Free Energy | 0.374290 |
| Sum of electronic and zero-point Energies | -4486.269371 |
| Sum of electronic and thermal Energies | -4486.243972 |
| Sum of electronic and thermal Enthalpies | -4486.243028 |
| Sum of electronic and thermal Free Energies | -4486.324622 |

| cartesian | | | | | | | |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | 0.27738017 | -2.27340412 | -1.45063996 | 6 | -0.42251986 | 2.48339605 | -2.56674004 |
| 6 | 1.64218020 | -2.61960411 | -1.33133996 | 1 | 0.24998015 | 4.57549572 | 0.32236004 |
| 6 | 2.39988017 | -1.64460397 | -2.04323983 | 1 | 0.90948015 | 3.39349604 | 1.45046008 |
| 6 | 1.49738014 | -0.70370400 | -2.59204006 | 1 | 1.94748020 | 4.14899588 | 0.23986004 |
| 6 | 0.18058017 | -1.07170391 | -2.19933987 | 1 | -0.32661986 | 3.49049616 | -2.98513985 |
| 1 | -0.73241985 | -0.55820400 | -2.47663999 | 1 | -0.08011985 | 1.78359604 | -3.33624005 |
| 1 | -0.55191982 | -2.84430408 | -1.05514002 | 1 | -1.49731982 | 2.30649614 | -2.43463993 |
| 1 | 2.03578019 | -3.49620390 | -0.83133996 | 6 | -0.54321980 | -1.46150398 | 1.61926007 |
| 1 | 3.47478008 | -1.64200401 | -2.17353988 | 6 | -1.42461979 | -0.47810400 | 1.29255998 |
| 1 | 1.76428020 | 0.14299601 | -3.21034002 | 6 | -1.56641996 | 0.74979603 | 2.15186000 |
| 6 | 2.28388023 | 0.05889602 | 2.23415995 | 6 | -2.43151999 | -0.63250399 | 0.18516006 |
| 6 | 2.63878012 | -1.29430401 | 1.94176006 | 1 | -0.60081983 | -2.44010401 | 1.14936006 |
| 6 | 3.59267998 | -1.27340400 | 0.89966005 | 1 | 0.00218016 | -1.39960396 | 2.55636001 |
| 6 | 3.79038000 | 0.07279602 | 0.50676006 | 1 | -1.83351982 | 1.62889600 | 1.55956006 |
| 6 | 2.99978018 | 0.89759600 | 1.35876000 | 1 | -2.37712002 | 0.57859600 | 2.86886001 |
| 1 | 2.95148039 | 1.97919595 | 1.32705998 | 1 | -0.66011989 | 0.96429598 | 2.72076011 |
| 1 | 1.60938013 | 0.38869601 | 3.01476002 | 6 | -3.86391973 | -0.76000398 | 0.74016005 |
| 1 | 2.29317999 | -2.17730379 | 2.46496010 | 1 | -2.38741970 | 0.24229601 | -0.47633997 |
| 1 | 4.07378006 | -2.14000416 | 0.46396005 | 1 | -2.20711994 | -1.51810396 | -0.41623998 |
| 1 | 4.46018028 | 0.42359602 | -0.26853997 | 6 | -4.87201977 | -0.99090397 | -0.38413996 |
| 40 | 1.41578019 | -0.46090397 | -0.08653995 | 1 | -4.12951994 | 0.14789602 | 1.28965998 |
| 1 | 1.86578012 | 1.19379604 | -1.00243998 | 1 | -3.89971972 | -1.58930397 | 1.45436001 |
| 1 | -0.02061987 | 0.90959597 | -0.01983995 | 1 | -5.88431978 | -1.07980394 | 0.01426005 |
| 13 | 0.52008015 | 2.32309580 | -0.86703998 | 1 | -4.64691973 | -1.90910399 | -0.93363994 |
| 6 | 0.94638014 | 3.73479605 | 0.40966004 | 1 | -4.86301994 | -0.16010398 | -1.09524000 |

S1.4. Me₂AlCl reaction profile

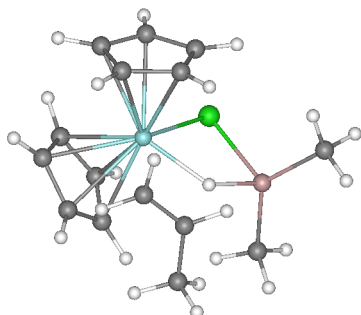
I-OCI



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 663989.4 (Joules/Mol) |
| | 158.69729 (Kcal/Mol) |
| Zero-point correction | 0.252900 (Hartree/Particle) |
| Thermal correction to Energy | 0.270165 |
| Thermal correction to Enthalpy | 0.271110 |
| Thermal correction to Gibbs Free Energy | 0.207188 |
| Sum of electronic and zero-point Energies | -4710.301965 |
| Sum of electronic and thermal Energies | -4710.284700 |
| Sum of electronic and thermal Enthalpies | -4710.283755 |
| Sum of electronic and thermal Free Energies | -4710.347677 |

| cartesian | | | | | | | | | |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|--|--|
| 6 | 1.81931889 | 2.07045937 | -1.25137496 | 1 | 3.65041876 | -1.26364052 | -0.39337498 | | |
| 6 | 2.61931896 | 1.61115944 | -0.17537498 | 1 | 2.33161879 | -1.39874053 | 1.95592511 | | |
| 6 | 1.85041881 | 1.70965946 | 1.01562500 | 1 | -0.10728115 | -2.44374061 | 1.47752500 | | |
| 6 | 0.58321881 | 2.25915956 | 0.67512500 | 1 | -0.30758116 | -2.90054059 | -1.17137504 | | |
| 6 | 0.56011885 | 2.46955943 | -0.72627497 | 40 | 0.73171884 | -0.00224057 | -0.38787499 | | |
| 1 | -0.26728114 | 2.86725950 | -1.30117500 | 17 | -1.28428113 | -0.02334057 | -1.98977494 | | |
| 1 | 2.11941886 | 2.12165952 | -2.29237509 | 1 | -0.80218112 | -0.00834057 | 0.79312503 | | |
| 1 | 3.64481878 | 1.27195942 | -0.24567498 | 13 | -2.44878125 | -0.00714057 | 0.07582501 | | |
| 1 | 2.18751884 | 1.46015954 | 2.01432490 | 6 | -3.16248107 | -1.78194046 | 0.38492504 | | |
| 1 | -0.22078115 | 2.48135948 | 1.36562502 | 6 | -3.14838123 | 1.77915943 | 0.35252503 | | |
| 6 | 2.63251877 | -1.60334051 | -0.25187498 | 1 | -3.35298109 | -1.95224047 | 1.45012510 | | |
| 6 | 1.93651879 | -1.67584050 | 0.98622501 | 1 | -4.12128162 | -1.91184056 | -0.12797499 | | |
| 6 | 0.65461886 | -2.23784041 | 0.73602509 | 1 | -2.50388122 | -2.58344054 | 0.03572503 | | |
| 6 | 0.54961884 | -2.48424053 | -0.65667498 | 1 | -3.30028105 | 1.98655951 | 1.41742504 | | |
| 6 | 1.77301884 | -2.09704041 | -1.26507497 | 1 | -2.50088120 | 2.56515956 | -0.04907499 | | |
| 1 | 2.00891876 | -2.17274046 | -2.32107496 | 1 | -4.12478161 | 1.89495945 | -0.12967499 | | |

I-1Cl

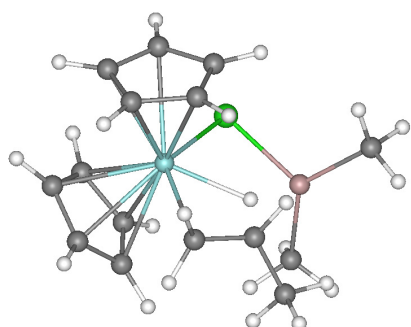


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 886300.5 (Joules/Mol) |
| | 211.83090 (Kcal/Mol) |
| Zero-point correction | 0.337574 (Hartree/Particle) |
| Thermal correction to Energy | 0.360321 |
| Thermal correction to Enthalpy | 0.361265 |
| Thermal correction to Gibbs Free Energy | 0.286333 |
| Sum of electronic and zero-point Energies | -4828.077044 |
| Sum of electronic and thermal Energies | -4828.054296 |
| Sum of electronic and thermal Enthalpies | -4828.053352 |
| Sum of electronic and thermal Free Energies | -4828.128284 |

cartesian

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | 1.52011204 | 1.95962679 | 1.03774643 | 17 | -1.05428791 | -1.84017313 | 1.72124624 |
| 6 | 2.51931214 | 1.04612684 | 1.43884635 | 1 | -1.04538774 | 0.01212683 | -0.27745366 |
| 6 | 1.95701218 | 0.20122683 | 2.44234633 | 13 | -2.49988770 | -0.75367320 | 0.32654634 |
| 6 | 0.62111211 | 0.61262685 | 2.65604639 | 6 | -3.08978772 | -1.92587316 | -1.11035371 |
| 6 | 0.33071214 | 1.67402685 | 1.76224637 | 6 | -3.48288774 | 0.60022682 | 1.31964636 |
| 1 | -0.60638785 | 2.21302700 | 1.69674635 | 1 | -3.64418769 | -1.37327313 | -1.87695360 |
| 1 | 1.65171218 | 2.76282692 | 0.32644635 | 1 | -2.26448774 | -2.44017315 | -1.61465359 |
| 1 | 3.54111218 | 1.02512681 | 1.08104634 | 1 | -3.76758790 | -2.70067310 | -0.73585361 |
| 1 | 2.47231221 | -0.58597314 | 2.97894645 | 1 | -4.33438778 | 0.14432684 | 1.83764625 |
| 1 | -0.07178786 | 0.17102683 | 3.35934639 | 1 | -2.87848783 | 1.09422684 | 2.08794641 |
| 6 | 1.32961226 | -1.85487318 | -1.64675355 | 1 | -3.90038776 | 1.37732685 | 0.66984636 |
| 6 | 2.55641222 | -1.27277327 | -1.19535375 | 6 | 1.03871214 | 1.31382680 | -2.06195354 |
| 6 | 2.84091210 | -1.80537319 | 0.08394635 | 6 | -0.29548785 | 1.48292685 | -1.92375350 |
| 6 | 1.77311206 | -2.65357304 | 0.45644635 | 6 | -0.97128791 | 2.65372705 | -1.27965355 |
| 6 | 0.85351211 | -2.70347309 | -0.63385367 | 1 | 1.74791217 | 2.05722666 | -1.70945358 |
| 1 | -0.06358786 | -3.27837324 | -0.65725362 | 1 | 1.42141223 | 0.56222683 | -2.74205351 |
| 1 | 0.84841216 | -1.68577313 | -2.60285354 | 1 | -1.45858788 | 3.23732662 | -2.06815362 |
| 1 | 3.19911218 | -0.60637319 | -1.75735354 | 1 | -1.75638795 | 2.33652687 | -0.58735365 |
| 1 | 3.71551228 | -1.58367312 | 0.68224633 | 1 | -0.26928785 | 3.31142664 | -0.76455361 |
| 1 | 1.67991209 | -3.20027304 | 1.38684630 | 1 | -0.95038790 | 0.77152681 | -2.42635369 |
| 40 | 0.78701216 | -0.35627317 | 0.31984636 | | | | |

TS-1Cl

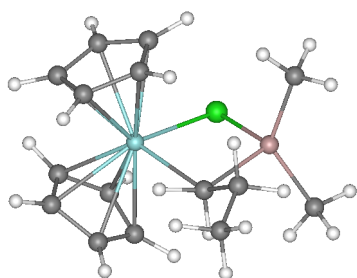


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 882100.4 (Joules/Mol) |
| | 210.82706 (Kcal/Mol) |
| Zero-point correction | 0.335974 (Hartree/Particle) |
| Thermal correction to Energy | 0.357878 |
| Thermal correction to Enthalpy | 0.358822 |
| Thermal correction to Gibbs Free Energy | 0.285805 |
| Sum of electronic and zero-point Energies | -4828.071225 |
| Sum of electronic and thermal Energies | -4828.049321 |
| Sum of electronic and thermal Enthalpies | -4828.048377 |
| Sum of electronic and thermal Free Energies | -4828.121395 |

cartesian

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | 0.73094153 | 2.45389509 | 0.27595359 | 17 | -0.72865850 | -0.76130480 | 2.40195370 |
| 6 | 2.07494140 | 2.16149521 | -0.10484639 | 1 | -0.93825847 | -0.20400481 | -0.33934641 |
| 6 | 2.72334146 | 1.58519518 | 1.00895357 | 13 | -2.36355853 | -0.42780480 | 0.92095363 |
| 6 | 1.77984142 | 1.47719514 | 2.06645346 | 6 | -3.10505867 | -2.07290483 | 0.20625360 |
| 6 | 0.56024146 | 2.05169511 | 1.61545360 | 6 | -3.12155867 | 1.35149515 | 1.12085366 |
| 1 | -0.35055852 | 2.13279510 | 2.19585371 | 1 | -2.35075855 | -2.85010481 | 0.04835361 |
| 1 | -0.01745850 | 2.93179512 | -0.34514642 | 1 | -3.84585857 | -2.49020481 | 0.89775360 |
| 1 | 2.53484154 | 2.38199520 | -1.05954635 | 1 | -3.62505865 | -1.91480482 | -0.74494636 |
| 1 | 3.76334143 | 1.28979516 | 1.04625368 | 1 | -3.36505866 | 1.54659522 | 2.17155361 |
| 1 | 1.96494150 | 1.07569516 | 3.05545378 | 1 | -2.44265866 | 2.15059519 | 0.80225360 |
| 6 | 1.58744144 | -2.22710490 | -0.90364635 | 1 | -4.04915857 | 1.46999514 | 0.55125362 |
| 6 | 2.79384136 | -1.51150477 | -0.67234635 | 6 | 0.58274150 | 0.41609520 | -2.12044621 |
| 6 | 3.01904154 | -1.49240482 | 0.72985363 | 6 | -0.72935849 | -0.03110481 | -1.91874635 |
| 6 | 1.93324161 | -2.13600469 | 1.36065364 | 6 | -1.91295862 | 0.88219517 | -2.13104630 |
| 6 | 1.04564142 | -2.59620476 | 0.34495360 | 1 | 0.71664149 | 1.47299516 | -2.32914639 |
| 1 | 0.12654150 | -3.14460492 | 0.51145363 | 1 | 1.29444146 | -0.24960482 | -2.59554625 |
| 1 | 1.15514147 | -2.44860482 | -1.87204635 | 1 | -2.04785848 | 0.98729515 | -3.21234655 |
| 1 | 3.45714140 | -1.10810483 | -1.42814636 | 1 | -2.83965850 | 0.47739518 | -1.71874630 |
| 1 | 3.87794137 | -1.06660485 | 1.23105359 | 1 | -1.73935866 | 1.87619519 | -1.71474636 |
| 1 | 1.80424142 | -2.27530479 | 2.42645359 | 1 | -0.93165857 | -1.09170485 | -2.07224655 |
| 40 | 0.97804147 | -0.07240481 | 0.29305360 | | | | |

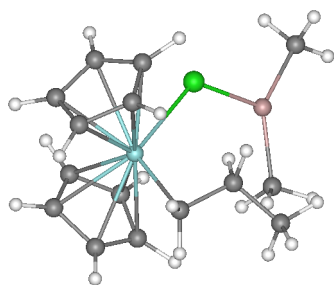
I-2Cl_a



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 893577.6 (Joules/Mol) |
| | 213.57016 (Kcal/Mol) |
| Zero-point correction | 0.340346 (Hartree/Particle) |
| Thermal correction to Energy | 0.361888 |
| Thermal correction to Enthalpy | 0.362832 |
| Thermal correction to Gibbs Free Energy | 0.290111 |
| Sum of electronic and zero-point Energies | -4828.098749 |
| Sum of electronic and thermal Energies | -4828.077207 |
| Sum of electronic and thermal Enthalpies | -4828.076263 |
| Sum of electronic and thermal Free Energies | -4828.148984 |

| cartesian | | | | | | | | | | | |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|--|--|--|--|
| 6 | -2.28972912 | 1.75091469 | 1.66371226 | 1 | -1.32642913 | -1.78958523 | -2.33068776 | | | | |
| 6 | -0.91312921 | 2.10431480 | 1.58761215 | 1 | -3.54362917 | -0.38498530 | -1.75498772 | | | | |
| 6 | -0.60262918 | 2.36191463 | 0.23611219 | 13 | 1.84377098 | -0.46448532 | 1.17191219 | | | | |
| 6 | -1.78762913 | 2.17091465 | -0.53528780 | 6 | 2.55637097 | 1.21871471 | 1.84741211 | | | | |
| 6 | -2.83262920 | 1.82361472 | 0.35631219 | 6 | 2.72697091 | -2.18988514 | 1.01851225 | | | | |
| 40 | -1.21112919 | -0.07758530 | 0.36131218 | 1 | 2.54077077 | 1.22591472 | 2.94361234 | | | | |
| 6 | 0.92787081 | -0.26558530 | -0.80238777 | 1 | 3.60577106 | 1.34241474 | 1.55591226 | | | | |
| 17 | -0.06372917 | -0.88248533 | 2.51171231 | 1 | 2.03507090 | 2.12391472 | 1.51751208 | | | | |
| 6 | -1.47002912 | -2.51238537 | -0.22158778 | 1 | 3.24137092 | -2.44648528 | 1.95081210 | | | | |
| 6 | -2.42632914 | -2.24078536 | 0.79221219 | 1 | 2.02317095 | -3.00428534 | 0.81411219 | | | | |
| 6 | -3.36802912 | -1.32008529 | 0.27611220 | 1 | 3.48587084 | -2.21058536 | 0.22831219 | | | | |
| 6 | -3.00462914 | -1.02998531 | -1.07198787 | 1 | 0.08757085 | 0.17641470 | -1.40438771 | | | | |
| 6 | -1.84462929 | -1.78398526 | -1.37888789 | 1 | 1.00807071 | -1.28998530 | -1.18778777 | | | | |
| 1 | 0.36317080 | 2.66301465 | -0.15008783 | 6 | 2.14607096 | 0.52951467 | -1.34428787 | | | | |
| 1 | -1.88542914 | 2.31911469 | -1.60468769 | 6 | 2.22877097 | 0.47621471 | -2.87108779 | | | | |
| 1 | -0.22312918 | 2.14261484 | 2.42181230 | 1 | 3.07937098 | 0.11761469 | -0.93818778 | | | | |
| 1 | -2.83232903 | 1.50221479 | 2.56871223 | 1 | 3.10207081 | 1.02381480 | -3.23178768 | | | | |
| 1 | -3.86472917 | 1.64021480 | 0.08561221 | 1 | 2.30737090 | -0.55618531 | -3.22148776 | | | | |
| 1 | -4.22822905 | -0.92748529 | 0.80431223 | 1 | 1.33937073 | 0.92341465 | -3.32598782 | | | | |
| 1 | -2.41742921 | -2.64948535 | 1.79501224 | 1 | 2.10687089 | 1.56811476 | -1.00328779 | | | | |
| 1 | -0.62012917 | -3.17858529 | -0.12978780 | | | | | | | | |

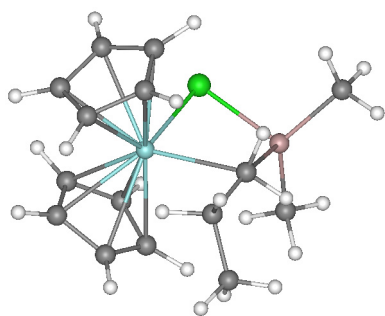
I-2Cl_bi



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 892664.4 (Joules/Mol) |
| | 213.35190 (Kcal/Mol) |
| Zero-point correction | 0.339998 (Hartree/Particle) |
| Thermal correction to Energy | 0.362896 |
| Thermal correction to Enthalpy | 0.363840 |
| Thermal correction to Gibbs Free Energy | 0.286421 |
| Sum of electronic and zero-point Energies | -4828.085847 |
| Sum of electronic and thermal Energies | -4828.062949 |
| Sum of electronic and thermal Enthalpies | -4828.062005 |
| Sum of electronic and thermal Free Energies | -4828.139424 |

| cartesian | | | | | | | | | | | |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|--|--|--|--|
| 6 | -2.22079992 | -1.09200001 | 1.86969995 | 17 | 1.58840001 | -1.34500003 | -0.05870000 | | | | |
| 6 | -3.11680007 | -0.95260000 | 0.77929997 | 1 | 0.67930001 | 0.79259998 | 1.36880004 | | | | |
| 6 | -2.66709995 | -1.80739999 | -0.26280001 | 13 | 3.55819988 | -0.33820000 | -0.14420000 | | | | |
| 6 | -1.47469997 | -2.43409991 | 0.16329999 | 6 | 3.35859990 | 1.56710005 | -0.41909999 | | | | |
| 6 | -1.19970000 | -1.99030006 | 1.48959994 | 6 | 4.99060011 | -1.60630000 | 0.05920000 | | | | |
| 1 | -0.36269999 | -2.30340004 | 2.10220003 | 1 | 4.26639986 | 2.11520004 | -0.14990000 | | | | |
| 1 | -2.30119991 | -0.58759999 | 2.82360005 | 1 | 2.53130007 | 1.98029995 | 0.16830000 | | | | |
| 1 | -4.00229979 | -0.32920000 | 0.75950003 | 1 | 3.15260005 | 1.79209995 | -1.47259998 | | | | |
| 1 | -3.15149999 | -1.95510006 | -1.21940005 | 1 | 4.90070009 | -2.41149998 | -0.67699999 | | | | |
| 1 | -0.88429999 | -3.13949990 | -0.40880001 | 1 | 4.94840002 | -2.07920003 | 1.04610002 | | | | |
| 6 | -0.28150001 | 1.90369999 | -1.58369994 | 1 | 5.97629976 | -1.14859998 | -0.05400000 | | | | |
| 6 | -1.70229995 | 1.87020004 | -1.54620004 | 6 | -1.33589995 | 1.70340002 | 1.40380001 | | | | |
| 6 | -2.12430000 | 0.65009999 | -2.12030005 | 6 | 0.02070000 | 1.42449999 | 2.03760004 | | | | |
| 6 | -0.96509999 | -0.07700000 | -2.52449989 | 6 | 0.85619998 | 2.67750001 | 2.32599998 | | | | |
| 6 | 0.16310000 | 0.71730000 | -2.21650004 | 1 | -0.07500000 | 0.81150001 | 2.93849993 | | | | |
| 1 | 1.19190001 | 0.44990000 | -2.41989994 | 1 | -2.15869999 | 1.61740005 | 2.11100006 | | | | |
| 1 | 0.34599999 | 2.71499991 | -1.23230004 | 1 | -1.35529995 | 2.69740009 | 0.95630002 | | | | |
| 1 | -2.35069990 | 2.64269996 | -1.15649998 | 1 | 1.84909999 | 2.42820001 | 2.70989990 | | | | |
| 1 | -3.15229988 | 0.34040001 | -2.25799990 | 1 | 0.34540001 | 3.29119992 | 3.07089996 | | | | |
| 1 | -0.95160002 | -1.04190004 | -3.01629996 | 1 | 0.97229999 | 3.28230000 | 1.42200005 | | | | |
| 40 | -0.93699998 | -0.00050000 | -0.03180000 | | | | | | | | |

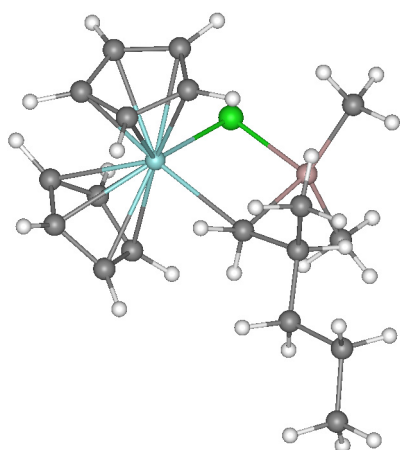
I-2Cl_bo



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 897505.9 (Joules/Mol) |
| | 214.50906 (Kcal/Mol) |
| Zero-point correction | 0.341842 (Hartree/Particle) |
| Thermal correction to Energy | 0.363494 |
| Thermal correction to Enthalpy | 0.364438 |
| Thermal correction to Gibbs Free Energy | 0.293390 |
| Sum of electronic and zero-point Energies | -4828.096474 |
| Sum of electronic and thermal Energies | -4828.074822 |
| Sum of electronic and thermal Enthalpies | -4828.073878 |
| Sum of electronic and thermal Free Energies | -4828.144926 |

| cartesian | | | | | | | | | |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|--|--|
| 6 | 1.74558544 | -1.90562677 | -1.35178053 | 6 | -3.06921458 | 1.04487324 | 1.31771946 | | |
| 6 | 2.84668541 | -1.15162683 | -0.84918046 | 6 | -3.40121460 | -2.04962683 | -0.28008050 | | |
| 6 | 3.03618550 | -1.52202678 | 0.50891954 | 1 | -3.14421463 | 1.86887324 | 0.59751952 | | |
| 6 | 2.02738523 | -2.44582677 | 0.85731953 | 1 | -2.48741460 | 1.40507317 | 2.17241955 | | |
| 6 | 1.23208547 | -2.68862677 | -0.30148047 | 1 | -4.08621454 | 0.87787318 | 1.69101954 | | |
| 1 | 0.37538540 | -3.34992671 | -0.35048050 | 1 | -4.13761473 | -2.45152664 | 0.42431951 | | |
| 1 | 1.36478543 | -1.87192678 | -2.36528063 | 1 | -2.76891470 | -2.89012671 | -0.58608049 | | |
| 1 | 3.47138548 | -0.47602680 | -1.42158043 | 1 | -3.96181440 | -1.72312677 | -1.16348052 | | |
| 1 | 1.88728535 | -2.90572667 | 1.82791948 | 6 | -0.49411458 | 2.10327339 | -2.25248051 | | |
| 6 | 0.20588541 | 2.02077341 | 1.19911957 | 6 | -0.99941456 | -0.19112681 | -1.19978046 | | |
| 6 | 1.43208539 | 2.18257332 | 0.49171954 | 6 | -0.00321458 | 0.67877316 | -1.99518049 | | |
| 6 | 2.44088531 | 1.48217320 | 1.18961954 | 1 | 0.23938541 | 0.18797319 | -2.94118071 | | |
| 6 | 1.84608543 | 0.88967323 | 2.34131956 | 1 | -1.09171462 | -1.17292678 | -1.67398059 | | |
| 6 | 0.47778541 | 1.25197315 | 2.35611963 | 1 | -1.96441460 | 0.31007320 | -1.37218046 | | |
| 1 | -0.24201459 | 0.96027315 | 3.10971975 | 1 | 1.02288532 | 0.78127313 | -1.54158044 | | |
| 1 | -0.75041461 | 2.45917320 | 0.94401950 | 1 | -0.80111456 | 2.59817338 | -1.32788050 | | |
| 1 | 1.57398546 | 2.76047325 | -0.41408050 | 1 | -1.36101460 | 2.07457328 | -2.91668034 | | |
| 1 | 2.35688543 | 0.30507320 | 3.09711933 | 1 | 3.48558545 | 1.43157315 | 0.90921950 | | |
| 40 | 0.85878539 | -0.27692682 | 0.36881953 | 1 | 3.81178546 | -1.15302682 | 1.16771960 | | |
| 17 | -0.85721457 | -1.55542684 | 1.93821955 | 1 | 0.27568540 | 2.71067333 | -2.73378038 | | |
| 13 | -2.39321470 | -0.60402679 | 0.52831954 | | | | | | |

I-4Cl_a

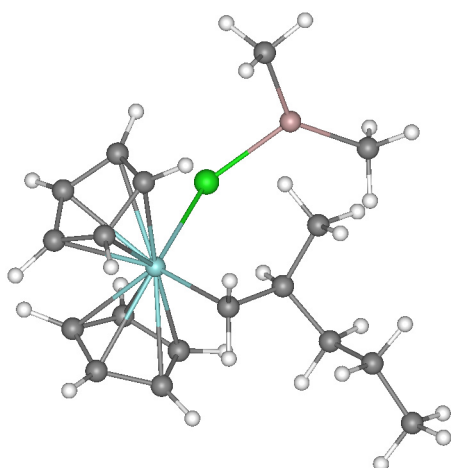


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1121463.1 (Joules/Mol) |
| | 268.03612 (Kcal/Mol) |
| Zero-point correction | 0.427143 (Hartree/Particle) |
| Thermal correction to Energy | 0.453303 |
| Thermal correction to Enthalpy | 0.454248 |
| Thermal correction to Gibbs Free Energy | 0.371644 |
| Sum of electronic and zero-point Energies | -4945.898348 |
| Sum of electronic and thermal Energies | -4945.872188 |
| Sum of electronic and thermal Enthalpies | -4945.871243 |
| Sum of electronic and thermal Free Energies | -4945.953847 |

| cartesian | | | | | | | | | | | |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|--|--|--|--|
| 6 | -3.85750389 | 0.51789600 | -1.51404810 | 6 | 0.90799600 | 2.01249599 | 2.65585208 | | | | |
| 6 | -2.77520394 | 1.40999603 | -1.75204802 | 1 | -0.09090394 | 4.32889605 | -0.11764802 | | | | |
| 6 | -1.69720387 | 0.66319597 | -2.26854801 | 1 | 1.29529619 | 3.52269602 | -0.82704800 | | | | |
| 6 | -2.11020398 | -0.70000398 | -2.36664796 | 1 | -0.32900396 | 3.17499614 | -1.41724801 | | | | |
| 6 | -3.45330381 | -0.77830398 | -1.92854786 | 1 | 0.78809601 | 2.98659611 | 3.14245200 | | | | |
| 40 | -2.08080387 | -0.18720397 | 0.07555199 | 1 | 0.45999604 | 1.27139604 | 3.32735205 | | | | |
| 6 | 0.36529607 | -0.03070398 | 0.27485198 | 1 | 1.98449612 | 1.80979598 | 2.62435198 | | | | |
| 17 | -2.24750400 | 2.03099608 | 1.35465193 | 1 | 0.00319606 | -0.83250403 | -0.42584801 | | | | |
| 6 | -1.94300389 | -1.25110400 | 2.35325193 | 1 | 0.51289600 | -0.54180402 | 1.23315191 | | | | |
| 6 | -3.30500388 | -0.89850402 | 2.15845203 | 6 | 1.79939604 | 0.23929602 | -0.29474801 | | | | |
| 6 | -3.81170392 | -1.66960406 | 1.08775198 | 6 | 2.71369600 | -0.93880403 | 0.08285198 | | | | |
| 6 | -2.76250386 | -2.51480389 | 0.62045199 | 6 | 1.78699613 | 0.50829601 | -1.79784799 | | | | |
| 6 | -1.61920404 | -2.26680398 | 1.42045188 | 1 | 2.23349619 | 1.12679601 | 0.19335198 | | | | |
| 1 | -0.73390394 | 1.05479598 | -2.56234789 | 1 | 2.79939604 | 0.67829597 | -2.16964793 | | | | |
| 1 | -1.51760387 | -1.52050400 | -2.75594807 | 1 | 1.37279606 | -0.34950399 | -2.34324789 | | | | |
| 1 | -2.77510405 | 2.47219610 | -1.54144812 | 1 | 1.20849609 | 1.40129602 | -2.04234791 | | | | |
| 1 | -4.83260393 | 0.79069597 | -1.12704802 | 6 | 4.17359591 | -0.78160399 | -0.34864801 | | | | |

| | | | | | | | |
|----|-------------|-------------|-------------|---|------------|-------------|-------------|
| 1 | -4.06500387 | -1.67130399 | -1.91064787 | 1 | 2.68369603 | -1.06190395 | 1.17325187 |
| 1 | -4.82420397 | -1.63800406 | 0.70495200 | 1 | 2.30049610 | -1.86280406 | -0.34774801 |
| 1 | -3.84970379 | -0.14910397 | 2.71925211 | 6 | 5.06279612 | -1.86440396 | 0.26265198 |
| 1 | -1.27980399 | -0.82420403 | 3.09635210 | 1 | 4.53609610 | 0.20819601 | -0.04644802 |
| 1 | -0.65780395 | -2.75650382 | 1.31805205 | 1 | 4.25189590 | -0.82690400 | -1.43884802 |
| 1 | -2.83740401 | -3.25110388 | -0.17004803 | 1 | 6.09769630 | -1.75690401 | -0.06814802 |
| 13 | 0.08729607 | 2.02329612 | 0.88985199 | 1 | 4.72119617 | -2.86170387 | -0.02944802 |
| 6 | 0.25749606 | 3.36639619 | -0.51174802 | 1 | 5.05239630 | -1.81190395 | 1.35485196 |

I-4Cl_bi



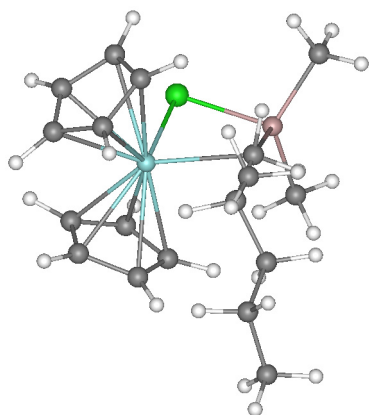
| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1119945.6 (Joules/Mol) |
| | 267.67343 (Kcal/Mol) |
| Zero-point correction | 0.426565 (Hartree/Particle) |
| Thermal correction to Energy | 0.453157 |
| Thermal correction to Enthalpy | 0.454101 |
| Thermal correction to Gibbs Free Energy | 0.369415 |
| Sum of electronic and zero-point Energies | -4945.889515 |
| Sum of electronic and thermal Energies | -4945.862922 |
| Sum of electronic and thermal Enthalpies | -4945.861978 |
| Sum of electronic and thermal Free Energies | -4945.946664 |

cartesian

| | | | | | | | |
|---|------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | 1.25066984 | -2.47885180 | -1.32474601 | 6 | -2.48753023 | 3.07384801 | -1.69074607 |
| 6 | 2.62376976 | -2.39255190 | -0.98774600 | 1 | -0.91933024 | 4.97424793 | 1.14855397 |
| 6 | 3.20726991 | -1.36635208 | -1.78484607 | 1 | 0.18696982 | 3.67574811 | 1.59285402 |
| 6 | 2.19056988 | -0.79925203 | -2.57924581 | 1 | 0.69576979 | 4.90564775 | 0.44005403 |
| 6 | 0.97276986 | -1.47845209 | -2.28784585 | 1 | -2.47463012 | 3.72124815 | -2.57494593 |
| 1 | 0.01356983 | -1.28725207 | -2.75514579 | 1 | -2.64323020 | 2.05224800 | -2.05194592 |
| 1 | 0.54846984 | -3.19655180 | -0.92474604 | 1 | -3.35433006 | 3.36514807 | -1.09054601 |
| 1 | 3.14476991 | -3.03065181 | -0.28454599 | 6 | 0.04706985 | -1.23505199 | 1.10515404 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 4.24916983 | -1.07185209 | -1.78184605 | 6 | -1.03293014 | -0.49245203 | 0.31695399 |
| 1 | 2.31216979 | 0.01234798 | -3.28614593 | 6 | -1.63173008 | 0.69124794 | 1.08975399 |
| 6 | 2.05426979 | 0.99994797 | 2.00615406 | 6 | -2.11823010 | -1.41845202 | -0.26614600 |
| 6 | 2.75146985 | -0.23855202 | 2.08165407 | 1 | -0.07433015 | -2.31695199 | 1.06375396 |
| 6 | 3.77436972 | -0.21825202 | 1.10655403 | 1 | 0.07356983 | -0.92735207 | 2.15155411 |
| 6 | 3.69876981 | 1.01994801 | 0.40715399 | 1 | -2.40673018 | 1.20224798 | 0.50265396 |
| 6 | 2.65566993 | 1.77964795 | 0.99515402 | 1 | -2.10303020 | 0.35154799 | 2.01625419 |
| 1 | 2.36596966 | 2.78024817 | 0.69955397 | 1 | -0.85853016 | 1.41354799 | 1.38875401 |
| 1 | 1.23036981 | 1.29814792 | 2.64345407 | 6 | -3.04083014 | -2.03555202 | 0.78695405 |
| 1 | 2.54626989 | -1.04375207 | 2.77505422 | 1 | -2.72383022 | -0.85795200 | -0.99064600 |
| 1 | 4.49796963 | -1.00405204 | 0.93105400 | 1 | -1.62613010 | -2.22185183 | -0.82904601 |
| 1 | 4.35446978 | 1.34934795 | -0.38924599 | 6 | -3.98953009 | -3.06285191 | 0.16885400 |
| 40 | 1.63516986 | -0.24965201 | -0.18164599 | 1 | -3.63003016 | -1.24895203 | 1.26975393 |
| 17 | 0.76306981 | 1.99504793 | -1.64904606 | 1 | -2.44153023 | -2.50775194 | 1.57355392 |
| 1 | -0.59763014 | -0.03565201 | -0.61784601 | 1 | -4.66583014 | -3.47685194 | 0.91935396 |
| 13 | -0.83333015 | 3.23924804 | -0.71484601 | 1 | -3.43443012 | -3.89305186 | -0.27694601 |
| 6 | -0.15673018 | 4.29484797 | 0.75675404 | 1 | -4.60002995 | -2.60875201 | -0.61684597 |

I-4Cl_bo

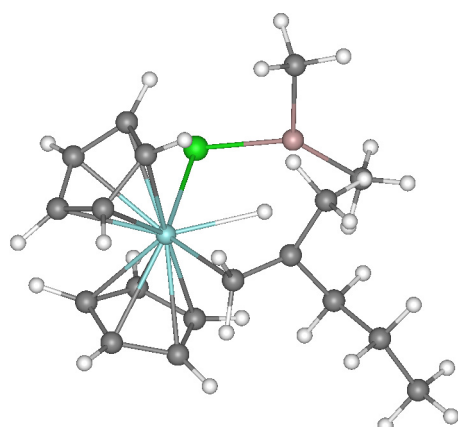


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1124103.1 (Joules/Mol) |
| | 268.66709 (Kcal/Mol) |
| Zero-point correction | 0.428148 (Hartree/Particle) |
| Thermal correction to Energy | 0.453960 |
| Thermal correction to Enthalpy | 0.454904 |
| Thermal correction to Gibbs Free Energy | 0.374265 |
| Sum of electronic and zero-point Energies | -4945.898112 |
| Sum of electronic and thermal Energies | -4945.872300 |
| Sum of electronic and thermal Enthalpies | -4945.871356 |
| Sum of electronic and thermal Free Energies | -4945.951995 |

cartesian

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | 1.88147402 | -1.40067208 | 2.08391380 | 1 | 0.93317401 | 2.69902802 | -2.69308615 |
| 6 | 1.13177407 | -2.49937201 | 1.56531405 | 1 | 0.89007401 | 4.24642801 | -1.87358594 |
| 6 | 1.88127398 | -3.07407212 | 0.51121402 | 1 | 2.95017409 | 4.17752838 | 1.03381395 |
| 6 | 3.06767416 | -2.31247211 | 0.34661400 | 1 | 2.69927406 | 2.78552794 | 2.07831383 |
| 6 | 3.07547402 | -1.30127203 | 1.34481406 | 1 | 1.42597413 | 3.99492812 | 1.88791406 |
| 1 | 3.85147405 | -0.56127203 | 1.48901403 | 6 | -2.26642585 | 0.56752801 | 0.28871399 |
| 1 | 1.61407399 | -0.77787203 | 2.92681384 | 6 | -3.45242572 | -0.40177202 | 0.27301401 |
| 1 | 0.18237406 | -2.86147213 | 1.94371402 | 6 | -4.48212624 | -0.01817201 | -0.78948599 |
| 1 | 3.85487413 | -2.49787211 | -0.37418601 | 1 | -3.10382581 | -1.42947209 | 0.09991400 |
| 6 | -0.06992596 | -0.11327201 | -2.37778616 | 1 | -5.34562635 | -0.68527198 | -0.76498598 |
| 6 | -0.71052593 | -1.28997207 | -1.90208602 | 1 | -4.04972601 | -0.06367201 | -1.79438603 |
| 6 | 0.20647407 | -2.36067200 | -1.98598599 | 1 | -4.84262609 | 1.00182796 | -0.63048601 |
| 6 | 1.42017412 | -1.85397208 | -2.53708601 | 6 | 0.14627406 | 1.05822790 | 0.94181395 |
| 6 | 1.23227406 | -0.47817200 | -2.80208611 | 6 | -1.03602600 | 0.07152799 | 1.06551397 |
| 1 | 1.96957397 | 0.19022797 | -3.22628617 | 6 | -1.38872600 | -0.22967201 | 2.52811384 |
| 1 | -0.51422590 | 0.86922795 | -2.47368622 | 1 | 0.63817406 | 1.16302788 | 1.91371405 |
| 1 | -1.73262596 | -1.36397207 | -1.55178595 | 1 | -0.35752594 | 2.02322793 | 0.76781398 |
| 1 | 2.31087399 | -2.42897201 | -2.75878620 | 1 | -0.82082599 | -0.95357198 | 0.62931401 |
| 40 | 1.17717409 | -0.79677200 | -0.28058600 | 1 | -2.15072584 | -1.00907207 | 2.60301399 |
| 17 | 3.10797405 | 0.95862800 | -0.79718602 | 1 | -1.78112578 | 0.67912799 | 2.99471378 |
| 1 | -3.93242574 | -0.41227204 | 1.25611401 | 1 | -0.51922590 | -0.54887199 | 3.10511398 |
| 13 | 1.49947405 | 2.46732783 | -0.17078601 | 1 | -1.97552586 | 0.82152802 | -0.73708600 |
| 6 | 0.62877405 | 3.18792796 | -1.76128602 | 1 | -2.58562589 | 1.51142788 | 0.74871403 |
| 6 | 2.20487404 | 3.44042802 | 1.35211396 | 1 | -0.00322592 | -3.39037204 | -1.72788596 |
| 1 | -0.46622592 | 3.14992785 | -1.70858598 | 1 | 1.60607409 | -3.95027208 | -0.05998601 |

TS-4Cl



Zero-point vibrational energy

1109215.9 (Joules/Mol)

265.10896 (Kcal/Mol)

Zero-point correction

0.422478 (Hartree/Particle)

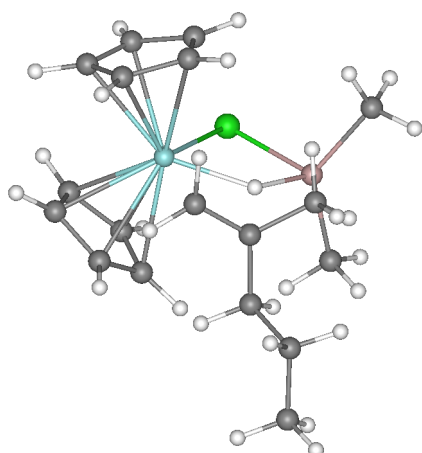
Thermal correction to Energy

0.448209

| | |
|---|--------------|
| Thermal correction to Enthalpy | 0.449153 |
| Thermal correction to Gibbs Free Energy | 0.367905 |
| Sum of electronic and zero-point Energies | -4945.877504 |
| Sum of electronic and thermal Energies | -4945.851774 |
| Sum of electronic and thermal Enthalpies | -4945.850829 |
| Sum of electronic and thermal Free Energies | -4945.932077 |

| cartesian | | | | | | |
|-----------|-------------|-------------|-------------|---|-------------|-------------------------|
| 6 | -0.65492600 | -2.45834994 | 1.22455001 | 6 | 1.75667405 | 2.34835005 2.13194990 |
| 6 | -2.00132608 | -2.69575000 | 0.86074996 | 1 | 0.88317400 | 4.09644985 -0.99984998 |
| 6 | -2.82352614 | -1.88354993 | 1.69704986 | 1 | -0.61442602 | 3.26364994 -1.41534996 |
| 6 | -1.98232603 | -1.12915003 | 2.53604984 | 1 | -0.62872601 | 4.56134987 -0.22985002 |
| 6 | -0.63152599 | -1.45795000 | 2.22665000 | 1 | 1.68027401 | 3.16904998 2.85564995 |
| 1 | 0.24637401 | -1.05875003 | 2.72144985 | 1 | 1.76037383 | 1.42035007 2.71224999 |
| 1 | 0.20387399 | -2.97224998 | 0.81604999 | 1 | 2.73317385 | 2.45274997 1.64754987 |
| 1 | -2.34652591 | -3.41284990 | 0.12584996 | 6 | 0.16907400 | -1.12564993 -1.39645004 |
| 1 | -3.90572596 | -1.85895002 | 1.70114994 | 6 | 1.09647393 | -0.17874998 -0.89035004 |
| 1 | -2.30502605 | -0.41514999 | 3.28164983 | 6 | 1.51957393 | 0.96364999 -1.79135013 |
| 6 | -2.29072595 | 0.72075003 | -2.04365015 | 6 | 2.15647388 | -0.63604999 0.09484997 |
| 6 | -2.78782606 | -0.61675000 | -2.02955008 | 1 | 0.34837401 | -2.16864991 -1.15534997 |
| 6 | -3.75852609 | -0.70515001 | -1.00865006 | 1 | -0.17562598 | -0.95535004 -2.41235018 |
| 6 | -3.83352613 | 0.55445004 | -0.35625005 | 1 | 2.08567405 | 1.72784996 -1.25014997 |
| 6 | -2.94892597 | 1.44115007 | -1.02835011 | 1 | 2.17507386 | 0.54405004 -2.56165004 |
| 1 | -2.79392600 | 2.48315001 | -0.77845001 | 1 | 0.67357403 | 1.43445003 -2.29325008 |
| 1 | -1.56482601 | 1.12185001 | -2.74065018 | 6 | 3.35767388 | -1.24994993 -0.64925003 |
| 1 | -2.50552607 | -1.41355002 | -2.70565009 | 1 | 2.50517392 | 0.20535001 0.70144999 |
| 1 | -4.33952570 | -1.58544993 | -0.76575005 | 1 | 1.74527383 | -1.38265002 0.77924997 |
| 1 | -4.48142576 | 0.81375003 | 0.47224995 | 6 | 4.35527372 | -1.85874999 0.33544996 |
| 40 | -1.56362605 | -0.33604997 | 0.15934998 | 1 | 3.85627413 | -0.47904998 -1.24425006 |
| 17 | -1.66102600 | 1.88625002 | 1.84504986 | 1 | 3.00587392 | -2.01615000 -1.34864998 |
| 1 | 0.23197401 | 0.71495003 | 0.10064997 | 1 | 5.21427393 | -2.27784991 -0.19185004 |
| 13 | 0.26827401 | 2.47285008 | 0.89244998 | 1 | 3.89377403 | -2.66225004 0.91634995 |
| 6 | -0.04942602 | 3.70024991 | -0.58475006 | 1 | 4.72647381 | -1.10595000 1.03594995 |

I-5Cl



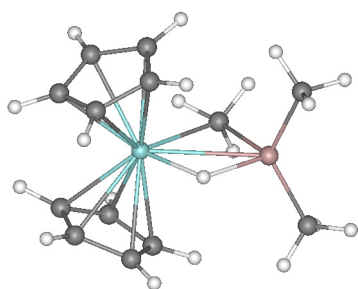
| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1111432.5 (Joules/Mol) |
| | 265.63873 (Kcal/Mol) |
| Zero-point correction | 0.423322 (Hartree/Particle) |
| Thermal correction to Energy | 0.450254 |
| Thermal correction to Enthalpy | 0.451199 |
| Thermal correction to Gibbs Free Energy | 0.365918 |
| Sum of electronic and zero-point Energies | -4945.888445 |
| Sum of electronic and thermal Energies | -4945.861513 |
| Sum of electronic and thermal Enthalpies | -4945.860569 |
| Sum of electronic and thermal Free Energies | -4945.945849 |

| cartesian | | | | | | | | | | | |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|--|--|--|--|
| 6 | -0.52789795 | -2.31204200 | 1.42805803 | 6 | 1.09200203 | 2.66735792 | 2.04695797 | | | | |
| 6 | -1.91659796 | -2.55604196 | 1.37955797 | 1 | 0.58060205 | 4.04815817 | -1.36214197 | | | | |
| 6 | -2.56339788 | -1.54694211 | 2.15365791 | 1 | -0.90289795 | 3.20575809 | -1.80704200 | | | | |
| 6 | -1.56049800 | -0.70564210 | 2.69035792 | 1 | -0.96549797 | 4.60625792 | -0.74264205 | | | | |
| 6 | -0.30269796 | -1.14644206 | 2.21265793 | 1 | 1.01990199 | 3.62675810 | 2.57135797 | | | | |
| 1 | 0.65870202 | -0.71334207 | 2.45875788 | 1 | 0.94660199 | 1.88505793 | 2.79995775 | | | | |
| 1 | 0.23340201 | -2.93374205 | 0.97785795 | 1 | 2.12420225 | 2.59225798 | 1.68505800 | | | | |
| 1 | -2.39639807 | -3.38744187 | 0.87905800 | 6 | 0.42090201 | -1.43794203 | -1.52874196 | | | | |
| 1 | -3.62729788 | -1.46674204 | 2.34115791 | 6 | 1.33890212 | -0.51464206 | -1.13394201 | | | | |
| 1 | -1.72999799 | 0.15235795 | 3.32645798 | 6 | 1.57480204 | 0.73045790 | -1.94504201 | | | | |
| 6 | -2.35969782 | -0.03494206 | -2.22314215 | 6 | 2.27900219 | -0.73934209 | 0.01675797 | | | | |
| 6 | -2.69549799 | -1.37484205 | -1.85184205 | 1 | 0.40920198 | -2.43504190 | -1.09844196 | | | | |
| 6 | -3.70929813 | -1.30594206 | -0.86754203 | 1 | -0.06849796 | -1.31904209 | -2.49014211 | | | | |
| 6 | -3.95029783 | 0.05685795 | -0.57584202 | 1 | 1.90080202 | 1.56545794 | -1.31724203 | | | | |
| 6 | -3.13279819 | 0.84055793 | -1.44244206 | 1 | 2.38160181 | 0.53085792 | -2.65954208 | | | | |
| 1 | -3.10099792 | 1.92255795 | -1.47094202 | 1 | 0.69100201 | 1.03335798 | -2.51044202 | | | | |
| 1 | -1.64979792 | 0.26255795 | -2.98514223 | 6 | 3.74280214 | -0.83174211 | -0.45764205 | | | | |

| | | | | | | | |
|----|-------------|-------------|-------------|---|------------|-------------|-------------|
| 1 | -2.29869795 | -2.28274202 | -2.28974223 | 1 | 2.19360209 | 0.10035795 | 0.72045791 |
| 1 | -4.20229816 | -2.14974189 | -0.40224203 | 1 | 2.02340221 | -1.65804207 | 0.55435795 |
| 1 | -4.65759802 | 0.44565794 | 0.14635795 | 6 | 4.68240213 | -1.12684202 | 0.71005797 |
| 40 | -1.60219789 | -0.38744205 | 0.17165796 | 1 | 4.03550196 | 0.10845795 | -0.93424201 |
| 17 | -2.27229786 | 2.00445795 | 1.36645794 | 1 | 3.82700205 | -1.61614203 | -1.21694195 |
| 1 | -0.14999795 | 0.92485791 | 0.03655796 | 1 | 5.71870232 | -1.17784202 | 0.37095797 |
| 13 | -0.19959795 | 2.57145810 | 0.59305799 | 1 | 4.43800211 | -2.08214188 | 1.18265796 |
| 6 | -0.38709795 | 3.70615792 | -0.97954202 | 1 | 4.61680222 | -0.34524205 | 1.47235799 |

S1.5. Me₃Al reaction profile

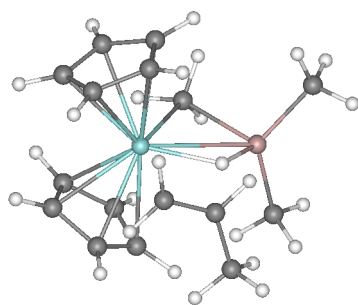
I-OMe



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 756308.5 (Joules/Mol) |
| | 180.76206 (Kcal/Mol) |
| Zero-point correction | 0.288063 (Hartree/Particle) |
| Thermal correction to Energy | 0.306404 |
| Thermal correction to Enthalpy | 0.307348 |
| Thermal correction to Gibbs Free Energy | 0.241768 |
| Sum of electronic and zero-point Energies | -4289.944549 |
| Sum of electronic and thermal Energies | -4289.926207 |
| Sum of electronic and thermal Enthalpies | -4289.925263 |
| Sum of electronic and thermal Free Energies | -4289.990843 |

| cartesian | | | | | | |
|-----------|-------------|-------------|-------------|----|-------------|-------------|
| 6 | 1.87194288 | 2.07636285 | -0.97703713 | 1 | 0.53124285 | -2.24743700 |
| 6 | 2.60044265 | 1.72656274 | 0.18646285 | 1 | -0.33765718 | -2.96673703 |
| 6 | 1.73514283 | 1.86256278 | 1.30386281 | 40 | 0.79464281 | 0.01516281 |
| 6 | 0.47844282 | 2.33396292 | 0.83226287 | 6 | -0.98575711 | -0.15933719 |
| 6 | 0.55694282 | 2.45326281 | -0.57603717 | 1 | -0.67775714 | -0.04123720 |
| 1 | -0.23205718 | 2.80126286 | -1.23163712 | 13 | -2.17385721 | -0.05953719 |
| 1 | 2.25974274 | 2.09016299 | -1.98973703 | 6 | -3.00885725 | -1.80603719 |
| 1 | 3.63704276 | 1.41396272 | 0.21836285 | 6 | -3.00695729 | 1.69266284 |
| 1 | 1.99694288 | 1.68186283 | 2.33976293 | 1 | -4.01125717 | -1.71743727 |
| 1 | -0.38615718 | 2.56306291 | 1.44276285 | 1 | -3.12455726 | -2.33653712 |
| 6 | 2.69874263 | -1.56183720 | -0.30443716 | 1 | -2.43865728 | -2.46363711 |
| 6 | 2.35464263 | -1.53013718 | 1.07676280 | 1 | -3.19015718 | 1.94626284 |
| 6 | 1.06844282 | -2.10943699 | 1.22216284 | 1 | -2.42955732 | 2.51636291 |
| 6 | 0.61064279 | -2.49113703 | -0.06833715 | 1 | -3.98955750 | 1.70446277 |
| 6 | 1.62264287 | -2.16513705 | -1.00583720 | 1 | -1.27295721 | -1.15063727 |
| 1 | 1.58214283 | -2.34603715 | -2.07423711 | 1 | -0.05875719 | 0.08756280 |
| 1 | 3.63274264 | -1.22593725 | -0.73823714 | 1 | -1.68745720 | 0.56886280 |
| 1 | 2.97944283 | -1.15613723 | 1.87866282 | | | |

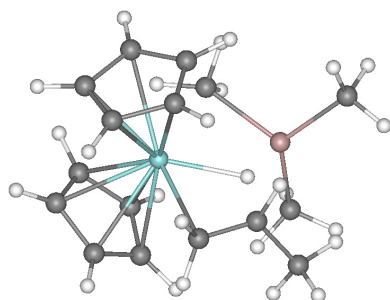
I-1Me



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 976497.1 (Joules/Mol) |
| | 233.38840 (Kcal/Mol) |
| Zero-point correction | 0.371928 (Hartree/Particle) |
| Thermal correction to Energy | 0.395214 |
| Thermal correction to Enthalpy | 0.396158 |
| Thermal correction to Gibbs Free Energy | 0.321046 |
| Sum of electronic and zero-point Energies | -4407.715485 |
| Sum of electronic and thermal Energies | -4407.692199 |
| Sum of electronic and thermal Enthalpies | -4407.691255 |
| Sum of electronic and thermal Free Energies | -4407.766368 |

| cartesian | | | | | | | |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | 1.21529317 | 2.30450678 | 0.81071818 | 1 | -0.93450677 | -0.01689314 | -0.67538184 |
| 6 | 2.21419334 | 1.53380692 | 1.44131815 | 13 | -2.16730666 | -0.83109313 | 0.20821816 |
| 6 | 1.57749319 | 0.70910686 | 2.41421819 | 6 | -2.83330679 | -2.28829312 | -0.90168184 |
| 6 | 0.19079325 | 0.99730688 | 2.38501835 | 6 | -3.28770685 | 0.50490683 | 1.09581816 |
| 6 | -0.04490677 | 1.95500696 | 1.36941814 | 1 | -3.56970668 | -1.93279314 | -1.63078189 |
| 1 | -1.00500679 | 2.38860679 | 1.11671817 | 1 | -2.04750681 | -2.80169320 | -1.46698189 |
| 1 | 1.38589323 | 3.06210685 | 0.05921817 | 1 | -3.34420681 | -3.04949331 | -0.30058181 |
| 1 | 3.27779317 | 1.58660686 | 1.24391818 | 1 | -4.19280720 | 0.03500685 | 1.49871814 |
| 1 | 2.07429314 | 0.02450686 | 3.09171820 | 1 | -2.81100678 | 1.02810693 | 1.93241811 |
| 1 | -0.56430674 | 0.55330688 | 3.02071834 | 1 | -3.64310670 | 1.27370691 | 0.39891815 |
| 6 | 1.75029325 | -1.58899307 | -1.64098179 | 6 | 1.17199326 | 1.48630691 | -2.30208182 |
| 6 | 2.83529329 | -0.86309314 | -1.06218183 | 6 | -0.17760676 | 1.48910689 | -2.31828165 |
| 6 | 3.02439332 | -1.34769309 | 0.25461817 | 6 | -1.05470681 | 2.59780669 | -1.82328188 |
| 6 | 2.03559327 | -2.32319331 | 0.51081818 | 1 | 1.74019325 | 2.32980680 | -1.92098176 |
| 6 | 1.25589323 | -2.48109317 | -0.67168182 | 1 | 1.72429323 | 0.74990684 | -2.87328172 |
| 1 | 0.43099326 | -3.16959310 | -0.80648184 | 1 | -1.51300681 | 3.08470678 | -2.69058180 |
| 1 | 1.36689329 | -1.48649311 | -2.64888167 | 1 | -1.87110686 | 2.21820688 | -1.20268190 |
| 1 | 3.45419335 | -0.12359314 | -1.55478179 | 1 | -0.49610674 | 3.35640669 | -1.27168190 |
| 1 | 3.78859329 | -1.02029312 | 0.94831812 | 1 | -1.58510673 | -1.53429306 | 2.20991826 |
| 1 | 1.92019320 | -2.88619328 | 1.42831814 | 1 | 0.09719324 | -1.64719307 | 2.24221826 |
| 40 | 0.80119324 | -0.13319315 | 0.20031816 | 1 | -0.77830672 | -2.72949314 | 1.19101810 |
| 6 | -0.72900677 | -1.68909311 | 1.52671814 | 1 | -0.68260676 | 0.67490685 | -2.83608174 |

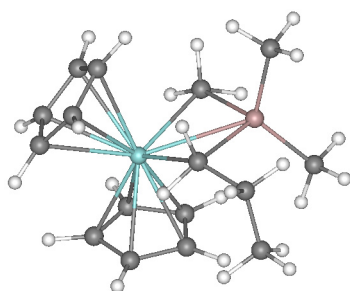
TS-1Me



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 975298.2 (Joules/Mol) |
| | 233.10186 (Kcal/Mol) |
| Zero-point correction | 0.371471 (Hartree/Particle) |
| Thermal correction to Energy | 0.393554 |
| Thermal correction to Enthalpy | 0.394498 |
| Thermal correction to Gibbs Free Energy | 0.322593 |
| Sum of electronic and zero-point Energies | -4407.708612 |
| Sum of electronic and thermal Energies | -4407.686530 |
| Sum of electronic and thermal Enthalpies | -4407.685585 |
| Sum of electronic and thermal Free Energies | -4407.757490 |

| cartesian | | | | | |
|-----------|-------------|-------------|-------------|----|-------------------------------------|
| 6 | -1.17124319 | 2.48448658 | 0.28614089 | 6 | 0.73735678 0.21368636 -2.15925908 |
| 6 | -2.05224323 | 1.90878642 | 1.24614096 | 6 | -0.53704315 -0.29631364 -2.42135906 |
| 6 | -3.08704329 | 1.24798632 | 0.54944092 | 1 | 0.89485681 0.28268635 -0.57145911 |
| 6 | -2.84084320 | 1.38428640 | -0.84205908 | 1 | 2.85695672 -0.19271363 -1.88005912 |
| 6 | -1.67134321 | 2.17648649 | -0.99635911 | 1 | 1.84825683 -1.64531362 -2.08315897 |
| 1 | -1.23754311 | 2.49408650 | -1.93685913 | 1 | -1.29274321 0.35598636 -2.84415913 |
| 1 | -0.29034317 | 3.07658648 | 0.50254089 | 1 | -0.59564316 -1.33971369 -2.71375918 |
| 1 | -1.96544313 | 1.99288642 | 2.32174087 | 13 | 2.02805686 0.34808636 0.87544090 |
| 1 | -3.92684317 | 0.73688638 | 1.00234091 | 6 | 0.49965683 0.58448637 2.22494102 |
| 1 | -3.46574330 | 0.99908638 | -1.63895905 | 6 | 2.92665672 -1.39001369 0.91324091 |
| 6 | -1.83184314 | -1.76481366 | 1.63324094 | 6 | 2.91675687 2.05048656 0.53204089 |
| 6 | -2.64214325 | -1.86801362 | 0.46884087 | 1 | 3.61145687 1.98828638 -0.31335911 |
| 6 | -1.83134317 | -2.32191348 | -0.59095907 | 1 | 2.22685671 2.87568641 0.32404089 |
| 6 | -0.51214314 | -2.51701355 | -0.08405910 | 1 | 3.52115679 2.35828638 1.39364088 |
| 6 | -0.52454317 | -2.19951344 | 1.29124093 | 1 | 3.86785674 -1.36251366 0.35314089 |
| 1 | 0.32635686 | -2.25181341 | 1.95974088 | 1 | 3.19495678 -1.67191362 1.93954086 |
| 1 | -2.17154312 | -1.46571362 | 2.61774087 | 1 | 2.34265685 -2.22381353 0.50824088 |
| 1 | -3.70094323 | -1.65311360 | 0.40564087 | 1 | 1.21485686 0.10158636 2.91954088 |
| 1 | -2.17024302 | -2.52531362 | -1.59775913 | 1 | 0.52415681 1.65468633 2.45334101 |
| 1 | 0.33765683 | -2.89011359 | -0.64345908 | 1 | -0.44134316 0.20198636 2.62354088 |
| 40 | -0.96274316 | -0.03001363 | 0.04884089 | 1 | 2.18425679 -0.59471363 -3.46585917 |
| 6 | 1.98415685 | -0.60631365 | -2.38955903 | 1 | 0.87795687 1.29318631 -2.22185898 |

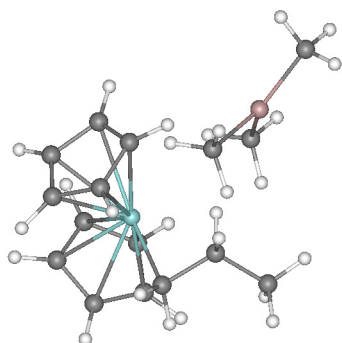
I-2Me_a



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 988223.4 (Joules/Mol) |
| | 236.19106 (Kcal/Mol) |
| Zero-point correction | 0.376394 (Hartree/Particle) |
| Thermal correction to Energy | 0.398577 |
| Thermal correction to Enthalpy | 0.399521 |
| Thermal correction to Gibbs Free Energy | 0.327728 |
| Sum of electronic and zero-point Energies | -4407.738140 |
| Sum of electronic and thermal Energies | -4407.715958 |
| Sum of electronic and thermal Enthalpies | -4407.715014 |
| Sum of electronic and thermal Free Energies | -4407.786807 |

| cartesian | | | | | |
|-----------|-------------|-------------|-------------|---|-------------------------------------|
| 6 | -1.66079998 | 1.92719996 | -1.37240005 | 6 | 3.15790009 0.67970002 -1.43840003 |
| 6 | -2.06949997 | 2.16249990 | -0.03370000 | 1 | 3.54579997 -2.72350001 -0.00020000 |
| 6 | -0.91219997 | 2.41890001 | 0.73920000 | 1 | 2.92630005 -2.98379993 -1.61539996 |
| 6 | 0.21430001 | 2.37820005 | -0.13230000 | 1 | 1.90009999 -3.30150008 -0.22260000 |
| 6 | -0.24730000 | 2.07940006 | -1.43210006 | 1 | 2.71280003 1.67949998 -1.49199998 |
| 1 | 0.36690000 | 1.98959994 | -2.31979990 | 1 | 3.44449997 0.41530001 -2.46499991 |
| 1 | -2.31739998 | 1.71809995 | -2.20930004 | 1 | 4.10330009 0.78240001 -0.89279997 |
| 1 | 1.24039996 | 2.56640005 | 0.14900000 | 6 | 1.26370001 -0.42309999 1.28069997 |
| 6 | -2.25149989 | -1.92060006 | -0.55269998 | 6 | 2.62809992 0.01370000 1.89479995 |
| 6 | -3.06229997 | -0.89109999 | -0.02120000 | 6 | 2.88809991 1.51590002 1.91589999 |
| 6 | -2.69039989 | -0.70039999 | 1.34070003 | 1 | 0.52460003 0.20100001 1.84840000 |
| 6 | -1.65970004 | -1.62489998 | 1.64100003 | 1 | 1.08669996 -1.44830000 1.62399995 |
| 6 | -1.36919999 | -2.36360002 | 0.46799999 | 1 | 3.45849991 -0.49300000 1.38590002 |
| 1 | -0.62540001 | -3.14549994 | 0.37009999 | 1 | 3.78940010 1.73130000 2.49410009 |
| 1 | -2.29710007 | -2.30629992 | -1.56369996 | 1 | 2.06019998 2.05430007 2.39050007 |
| 1 | -3.84629989 | -0.36149999 | -0.54830003 | 1 | 3.04480004 1.91960001 0.91380000 |
| 40 | -0.73559999 | 0.03820000 | -0.02920000 | 1 | -1.17209995 -1.73549998 2.60209990 |
| 1 | -3.08850002 | 2.14730000 | 0.33199999 | 1 | -0.89200002 2.64870000 1.79869998 |
| 1 | -3.14339995 | -0.00460000 | 2.03640008 | 1 | 0.23170000 -2.00000000 -2.10069990 |
| 6 | 0.26240000 | -0.91189998 | -1.99090004 | 1 | 0.97570002 -0.52160001 -2.73210001 |
| 13 | 2.04410005 | -0.75529999 | -0.70889997 | 1 | -0.68980002 -0.55260003 -2.42389989 |
| 6 | 2.65070009 | -2.60929990 | -0.62260002 | 1 | 2.65510011 -0.36849999 2.91969991 |

I-2Me_bi

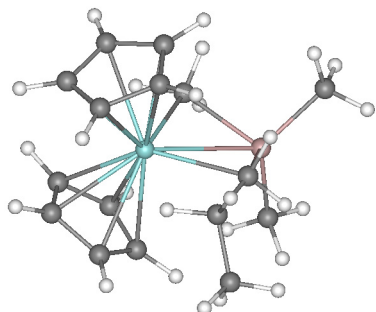


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 983941.6 (Joules/Mol) |
| | 235.16768 (Kcal/Mol) |
| Zero-point correction | 0.374764 (Hartree/Particle) |
| Thermal correction to Energy | 0.398247 |
| Thermal correction to Enthalpy | 0.399191 |
| Thermal correction to Gibbs Free Energy | 0.319781 |
| Sum of electronic and zero-point Energies | -4407.722020 |
| Sum of electronic and thermal Energies | -4407.698537 |
| Sum of electronic and thermal Enthalpies | -4407.697592 |
| Sum of electronic and thermal Free Energies | -4407.777003 |

| | | | | cartesian | | | |
|---|-------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 6 | 2.30430007 | 1.86909997 | -0.94700003 | 1 | 0.02810000 | 1.63789999 | 1.23450005 |
| 6 | 2.74790001 | 0.67570001 | -1.56710005 | 13 | -3.87030005 | 0.08950000 | -0.22380000 |
| 6 | 1.70589995 | 0.21060000 | -2.41759992 | 6 | -4.35699987 | -1.76950002 | 0.08350000 |
| 6 | 0.61269999 | 1.09410000 | -2.29299998 | 6 | -4.99149990 | 1.62890005 | -0.58870000 |
| 6 | 0.97799999 | 2.11820006 | -1.37390006 | 1 | -5.43720007 | -1.93649995 | 0.05000000 |
| 1 | 0.36730000 | 2.96639991 | -1.08780003 | 1 | -4.00869989 | -2.12220001 | 1.06200004 |
| 1 | 2.88150001 | 2.48490000 | -0.27100000 | 1 | -3.90750003 | -2.43600011 | -0.66310000 |
| 1 | 3.72449994 | 0.22310001 | -1.44560003 | 1 | -6.05569983 | 1.38230002 | -0.62730002 |
| 1 | 1.74460006 | -0.66570002 | -3.05229998 | 1 | -4.72690010 | 2.09829998 | -1.54330003 |
| 1 | -0.33019999 | 1.01680005 | -2.82069993 | 1 | -4.86049986 | 2.40240002 | 0.17700000 |
| 6 | 0.64859998 | -2.08949995 | 1.44089997 | 6 | 1.98780000 | 0.74839997 | 1.75899994 |
| 6 | 1.96949995 | -2.10529995 | 0.91119999 | 6 | 0.84780002 | 1.73169994 | 2.00340009 |
| 6 | 1.87399995 | -2.29270005 | -0.48550001 | 6 | 0.15090001 | 1.58070004 | 3.35829997 |
| 6 | 0.49360001 | -2.38829994 | -0.82880002 | 1 | 2.95810008 | 1.22790003 | 1.64510000 |
| 6 | -0.25170001 | -2.29859996 | 0.37250000 | 1 | 2.05089998 | 0.01730000 | 2.56640005 |
| 1 | -1.33120000 | -2.36209989 | 0.45390001 | 1 | -0.68470001 | 2.27659988 | 3.46300006 |
| 1 | 0.38499999 | -1.97880006 | 2.48629999 | 1 | 0.86040002 | 1.77260005 | 4.16569996 |
| 1 | 2.88619995 | -2.00629997 | 1.47720003 | 1 | -0.23170000 | 0.56300002 | 3.48790002 |
| 1 | 2.70670009 | -2.37400007 | -1.17240000 | 1 | -1.65369999 | 1.46519995 | -0.30599999 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 0.09210000 | -2.56719995 | -1.81889999 | 1 | -1.62220001 | 0.07610000 | 0.88270003 |
| 40 | 0.89340001 | -0.03970000 | -0.05350000 | 1 | -1.48500001 | -0.25080001 | -0.91409999 |
| 6 | -1.87919998 | 0.41180000 | -0.13100000 | 1 | 1.17700005 | 2.76209998 | 1.84119999 |

I-2Me_bo



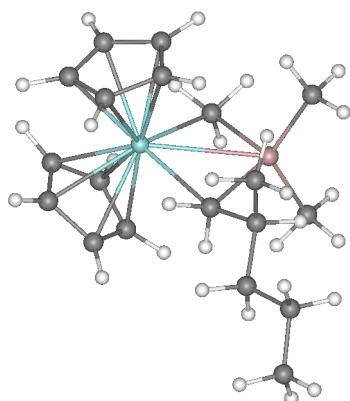
| | |
|---|-----------------------------|
| Zero-point vibrational energy | 990513.4 (Joules/Mol) |
| | 236.73838 (Kcal/Mol) |
| Zero-point correction | 0.377267 (Hartree/Particle) |
| Thermal correction to Energy | 0.399244 |
| Thermal correction to Enthalpy | 0.400188 |
| Thermal correction to Gibbs Free Energy | 0.328627 |
| Sum of electronic and zero-point Energies | -4407.740304 |
| Sum of electronic and thermal Energies | -4407.718327 |
| Sum of electronic and thermal Enthalpies | -4407.717383 |
| Sum of electronic and thermal Free Energies | -4407.788944 |

cartesian

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | 1.81025004 | -1.84350681 | -1.33039093 | 6 | -2.93874979 | -2.28250670 | 0.10210910 |
| 6 | 2.87745023 | -0.96920681 | -0.98009092 | 1 | -3.25204992 | 1.68839324 | 0.22940910 |
| 6 | 3.13735008 | -1.13940680 | 0.40530911 | 1 | -2.56874990 | 1.61699319 | 1.84880900 |
| 6 | 2.21115017 | -2.07810688 | 0.91280907 | 1 | -4.02355003 | 0.72079319 | 1.46250916 |
| 6 | 1.38884997 | -2.51450682 | -0.16459090 | 1 | -3.46894979 | -2.68030667 | 0.97530907 |
| 1 | 0.58725011 | -3.24040675 | -0.10249090 | 1 | -2.24534988 | -3.06560683 | -0.22799090 |
| 1 | 1.39125013 | -1.96950674 | -2.32099080 | 1 | -3.69334984 | -2.17490673 | -0.68569088 |
| 1 | 3.43315005 | -0.33320680 | -1.65939093 | 6 | -0.62824988 | 1.90789318 | -2.70649076 |
| 1 | 2.15575004 | -2.42750669 | 1.93640900 | 6 | -0.96934992 | -0.26360682 | -1.36899090 |
| 6 | 0.05075008 | 2.28669333 | 0.72270912 | 6 | -0.04044992 | 0.56379318 | -2.27699089 |
| 6 | 1.27375007 | 2.44809318 | 0.01310910 | 1 | 0.23055008 | -0.02480681 | -3.15729094 |
| 6 | 2.31675005 | 1.91159320 | 0.79920912 | 1 | -1.02144980 | -1.29450679 | -1.73029089 |
| 6 | 1.74664998 | 1.42759323 | 2.01150918 | 1 | -1.97174978 | 0.16179320 | -1.53119087 |
| 6 | 0.35485008 | 1.68639326 | 1.96880913 | 1 | 0.97465008 | 0.78549320 | -1.84809089 |
| 1 | -0.35774994 | 1.45909321 | 2.75130916 | 1 | -0.96114987 | 2.49669313 | -1.84829092 |
| 1 | -0.92854995 | 2.62649322 | 0.41110909 | 1 | -1.49615002 | 1.73639321 | -3.34749079 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 1.38985014 | 2.91549325 | -0.95769089 | 1 | 3.36695004 | 1.89919317 | 0.53590906 |
| 1 | 2.28995013 | 0.98279315 | 2.83730912 | 1 | 3.91155005 | -0.64010686 | 0.97410911 |
| 40 | 0.86915010 | -0.05340681 | 0.20040910 | 1 | 0.32335010 | -0.96310681 | 2.53970909 |
| 6 | -0.54454988 | -1.17110682 | 1.90180922 | 1 | -0.60974991 | -2.25980687 | 1.82470918 |
| 13 | -2.06344986 | -0.59000683 | 0.51100910 | 1 | -1.36084986 | -0.85210681 | 2.57420921 |
| 6 | -3.04274988 | 1.01209319 | 1.06810904 | 1 | 0.09575009 | 2.49749327 | -3.27329087 |

I-4Me_a

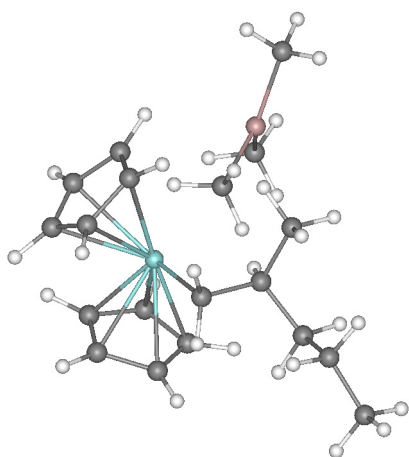


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1214479.1 (Joules/Mol) |
| | 290.26747 (Kcal/Mol) |
| Zero-point correction | 0.462571 (Hartree/Particle) |
| Thermal correction to Energy | 0.488850 |
| Thermal correction to Enthalpy | 0.489795 |
| Thermal correction to Gibbs Free Energy | 0.408318 |
| Sum of electronic and zero-point Energies | -4525.541047 |
| Sum of electronic and thermal Energies | -4525.514768 |
| Sum of electronic and thermal Enthalpies | -4525.513823 |
| Sum of electronic and thermal Free Energies | -4525.595301 |

| cartesian | | | | | | | |
|-----------|------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | 3.68165469 | 1.04619050 | 1.27288687 | 1 | -0.07034528 | 3.89369059 | -1.44131315 |
| 6 | 3.30075479 | 0.02129056 | 2.17718673 | 1 | -1.43244529 | 3.37219048 | -0.48331314 |
| 6 | 1.96095467 | 0.25649056 | 2.56698680 | 6 | -2.88064528 | -1.00580943 | 0.45018685 |
| 6 | 1.52265477 | 1.45279050 | 1.92898679 | 6 | -0.52264529 | -0.27410945 | -0.04671317 |
| 6 | 2.58315468 | 1.94009042 | 1.13518679 | 6 | -1.95584512 | 0.21909055 | 0.33348686 |
| 1 | 2.56505466 | 2.83849049 | 0.53068686 | 6 | -1.96624517 | 1.07329059 | 1.59948683 |
| 1 | 4.65525436 | 1.15379047 | 0.80818683 | 1 | -0.17024529 | -0.75060946 | 0.90638685 |
| 1 | 0.55525476 | 1.91749048 | 2.05418682 | 1 | -0.66624528 | -1.10710943 | -0.74451315 |
| 6 | 3.13125491 | -1.70420945 | -1.57491314 | 1 | -2.36204529 | 0.83139056 | -0.48751318 |
| 6 | 3.67055488 | -1.99910951 | -0.30091316 | 1 | -2.98474526 | 1.37039053 | 1.85768688 |
| 6 | 2.65125489 | -2.62810946 | 0.47038680 | 1 | -1.55784512 | 0.51259053 | 2.45008683 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | 1.49275470 | -2.72320938 | -0.33891320 | 1 | -1.39434528 | 1.99439049 | 1.47138679 |
| 6 | 1.77815485 | -2.13200951 | -1.59441316 | 1 | -2.83414531 | -1.56380951 | -0.49391317 |
| 1 | 1.09455466 | -2.04220939 | -2.43031335 | 1 | -2.48724532 | -1.67580950 | 1.22888684 |
| 1 | 3.65915489 | -1.23150945 | -2.39371324 | 1 | 0.54705477 | -3.15880942 | -0.03841317 |
| 1 | 4.68705463 | -1.80790949 | 0.02048683 | 1 | 1.38455474 | -0.34510943 | 3.26078677 |
| 40 | 1.90465474 | -0.26570946 | 0.11468682 | 6 | -4.34614563 | -0.68260950 | 0.75018686 |
| 1 | 3.92595482 | -0.79810947 | 2.50868678 | 1 | 1.98875475 | 0.69179052 | -2.78671336 |
| 1 | 2.75435472 | -3.00700951 | 1.47978687 | 1 | 1.95465469 | 2.24529052 | -1.93591321 |
| 6 | 2.06885481 | 1.15929055 | -1.80091321 | 1 | 3.14225483 | 1.10259056 | -1.54141319 |
| 13 | -0.09464526 | 1.36059058 | -1.37651312 | 6 | -5.23174524 | -1.92240942 | 0.62518686 |
| 6 | -0.87114531 | 0.75739056 | -3.06461334 | 1 | -4.69654560 | 0.09299055 | 0.05868683 |
| 6 | -0.37304527 | 3.16649055 | -0.67611319 | 1 | -4.44424534 | -0.27290946 | 1.75968683 |
| 1 | -1.96664524 | 0.79429054 | -3.05541325 | 1 | -6.27254534 | -1.68920946 | 0.85858685 |
| 1 | -0.55614525 | 1.39359057 | -3.90001321 | 1 | -4.90284538 | -2.70780945 | 1.31198680 |
| 1 | -0.59354526 | -0.26970944 | -3.33071327 | 1 | -5.19804525 | -2.32850957 | -0.38971317 |
| 1 | 0.17175475 | 3.43549061 | 0.23588683 | | | | |

I-4Me_bi



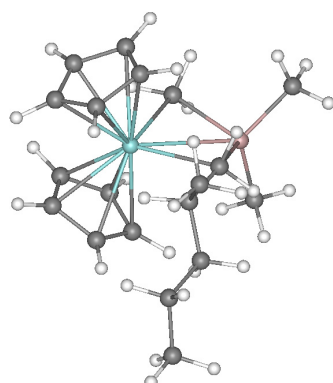
| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1209446.8 (Joules/Mol) |
| | 289.06473 (Kcal/Mol) |
| Zero-point correction | 0.460654 (Hartree/Particle) |
| Thermal correction to Energy | 0.487280 |
| Thermal correction to Enthalpy | 0.488224 |
| Thermal correction to Gibbs Free Energy | 0.403106 |
| Sum of electronic and zero-point Energies | -4525.525096 |
| Sum of electronic and thermal Energies | -4525.498470 |
| Sum of electronic and thermal Enthalpies | -4525.497526 |
| Sum of electronic and thermal Free Energies | -4525.582644 |

cartesian

| | | | | | | | |
|---|-------------|-------------|-------------|---|------------|------------|------------|
| 6 | -1.59097171 | -1.47669435 | -2.02832079 | 1 | 3.79692841 | 2.87390566 | 1.91007924 |
|---|-------------|-------------|-------------|---|------------|------------|------------|

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | -1.06317163 | -2.77479434 | -1.82632077 | 1 | 4.59122801 | 1.33650565 | 2.18707919 |
| 6 | 0.32752836 | -2.73589420 | -2.13322091 | 1 | 5.49582815 | 2.29030561 | -2.03972077 |
| 6 | 0.65822840 | -1.41229439 | -2.48772073 | 1 | 4.89062834 | 0.67850566 | -2.40752077 |
| 6 | -0.52587163 | -0.62429434 | -2.40782094 | 1 | 3.89062834 | 2.07950568 | -2.74352074 |
| 1 | -0.60977161 | 0.42930564 | -2.64932084 | 6 | -1.97667158 | -0.63629436 | 0.79827923 |
| 1 | -2.62897158 | -1.19469428 | -1.92402077 | 6 | -1.49557161 | 0.79480565 | 0.58047920 |
| 1 | -1.63087165 | -3.65119433 | -1.53892076 | 6 | -1.10677171 | 1.50770569 | 1.88297927 |
| 1 | 1.01022840 | -3.57579422 | -2.10592079 | 6 | -2.44247150 | 1.63610578 | -0.29682076 |
| 1 | 1.63952827 | -1.05979431 | -2.78252077 | 1 | -2.90017152 | -0.86239433 | 0.26717925 |
| 6 | 0.31092834 | -1.98219430 | 2.42617917 | 1 | -2.11577153 | -0.86359429 | 1.85567927 |
| 6 | -0.43157163 | -3.03509426 | 1.82177925 | 1 | -0.74937165 | 2.52380562 | 1.68857932 |
| 6 | 0.40792835 | -3.67109442 | 0.88027924 | 1 | -1.96827161 | 1.56940579 | 2.55227923 |
| 6 | 1.66222835 | -2.99949431 | 0.87597924 | 1 | -0.31707165 | 0.96810567 | 2.41727924 |
| 6 | 1.60212839 | -1.97759426 | 1.86097932 | 6 | -3.75697160 | 2.00450563 | 0.39467925 |
| 1 | 2.40882850 | -1.30529428 | 2.12827921 | 1 | -1.93037164 | 2.55660582 | -0.60572076 |
| 1 | -0.04947165 | -1.31879437 | 3.20257926 | 1 | -2.66507149 | 1.07830572 | -1.21582067 |
| 1 | -1.45177162 | -3.31059432 | 2.05567908 | 1 | 1.47172832 | 0.86810565 | -0.99352080 |
| 1 | 0.14562836 | -4.52999449 | 0.27597925 | 1 | 1.65512836 | 0.65030575 | 0.81677920 |
| 1 | 2.52822852 | -3.27059436 | 0.28427926 | 1 | 2.41192842 | -0.55119431 | -0.34962076 |
| 40 | -0.00957164 | -1.38149428 | -0.04322076 | 6 | -4.72307158 | 2.69830561 | -0.56522077 |
| 6 | 2.08762836 | 0.48440567 | -0.17522076 | 1 | -3.55397153 | 2.66660571 | 1.24237931 |
| 1 | -0.54257166 | 0.80130565 | -0.03252076 | 1 | -4.22387171 | 1.10190570 | 0.80537921 |
| 13 | 3.82432842 | 1.51160574 | -0.24552077 | 1 | -5.64877176 | 2.97760582 | -0.05812076 |
| 6 | 4.49052811 | 2.15260577 | 1.46157932 | 1 | -4.98387194 | 2.04530573 | -1.40322077 |
| 6 | 4.60052824 | 1.66300559 | -2.01992083 | 1 | -4.28027201 | 3.60980582 | -0.97702080 |
| 1 | 5.46452808 | 2.64290571 | 1.38367927 | | | | |

I-4Me_bo

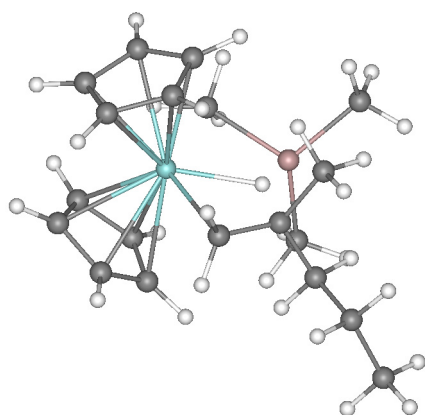


| | |
|--------------------------------|-----------------------------|
| Zero-point vibrational energy | 1215723.6 (Joules/Mol) |
| | 290.56491 (Kcal/Mol) |
| Zero-point correction | 0.463045 (Hartree/Particle) |
| Thermal correction to Energy | 0.489087 |
| Thermal correction to Enthalpy | 0.490031 |

| | |
|---|--------------|
| Thermal correction to Gibbs Free Energy | 0.409666 |
| Sum of electronic and zero-point Energies | -4525.542152 |
| Sum of electronic and thermal Energies | -4525.516110 |
| Sum of electronic and thermal Enthalpies | -4525.515166 |
| Sum of electronic and thermal Free Energies | -4525.595531 |

| cartesian | | | | | | | | |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|--|
| 6 | 1.77506614 | -1.37285662 | 2.06002069 | 1 | 2.92746615 | 3.83044338 | 1.07942069 | |
| 6 | 1.02806616 | -2.47475672 | 1.55212069 | 1 | 2.52306604 | 2.50444341 | 2.16422081 | |
| 6 | 1.74676621 | -3.02325654 | 0.46402076 | 1 | 1.40196621 | 3.84474325 | 1.93952060 | |
| 6 | 2.92506599 | -2.25335670 | 0.28152072 | 6 | -2.54303384 | 0.38414335 | 0.41672072 | |
| 6 | 2.94876599 | -1.25155663 | 1.28652072 | 6 | -3.66523409 | -0.65765667 | 0.38882074 | |
| 1 | 3.73386598 | -0.52405667 | 1.44092071 | 6 | -4.76123381 | -0.28335667 | -0.60867923 | |
| 1 | 1.52526617 | -0.76355666 | 2.91852069 | 1 | -3.25863385 | -1.64815664 | 0.14062074 | |
| 1 | 0.09166616 | -2.85065651 | 1.94842076 | 1 | -5.57543373 | -1.01025665 | -0.59447926 | |
| 1 | 3.69736600 | -2.43525672 | -0.45647928 | 1 | -4.36833382 | -0.23665665 | -1.62947929 | |
| 6 | -0.34913382 | 0.00744335 | -2.29927921 | 1 | -5.18343401 | 0.69704336 | -0.37157926 | |
| 6 | -0.89033377 | -1.24535656 | -1.90287924 | 6 | -0.14463383 | 0.98794335 | 1.03562069 | |
| 6 | 0.10056616 | -2.23515654 | -2.08347917 | 6 | -1.26303387 | -0.06825665 | 1.13772070 | |
| 6 | 1.26086617 | -1.60105658 | -2.61277938 | 6 | -1.55663383 | -0.45435664 | 2.59362078 | |
| 6 | 0.96886611 | -0.22485664 | -2.76567936 | 1 | 0.33546615 | 1.10814345 | 2.01122069 | |
| 1 | 1.63766623 | 0.52434331 | -3.16857934 | 1 | -0.67073381 | 1.93784332 | 0.84562075 | |
| 1 | -0.86583376 | 0.95834333 | -2.31727934 | 1 | -0.99373376 | -1.05235660 | 0.64742076 | |
| 1 | -1.89533389 | -1.41935658 | -1.53807926 | 1 | -2.25593400 | -1.29185665 | 2.65182066 | |
| 1 | 2.18346620 | -2.09525657 | -2.89357924 | 1 | -2.00443387 | 0.40184331 | 3.10722065 | |
| 40 | 0.99916613 | -0.72885668 | -0.27467927 | 1 | -0.65173388 | -0.73065668 | 3.13782072 | |
| 6 | 2.79956603 | 0.92204338 | -0.74897921 | 1 | -2.29943395 | 0.69704336 | -0.60477924 | |
| 1 | -4.10203409 | -0.75635666 | 1.38692069 | 1 | -2.90543389 | 1.28614342 | 0.92592078 | |
| 13 | 1.26466620 | 2.25484347 | -0.07657926 | 1 | -0.02493384 | -3.29405665 | -1.89967930 | |
| 6 | 0.41946617 | 3.18414330 | -1.58067930 | 1 | 1.46196616 | -3.89415669 | -0.11067926 | |
| 6 | 2.10506606 | 3.18754339 | 1.41422069 | 1 | 3.23006606 | 0.05444334 | -1.26507926 | |
| 1 | -0.67233384 | 3.24864340 | -1.48887932 | 1 | 3.52276611 | 1.17984343 | 0.02932074 | |
| 1 | 0.62906617 | 2.75924349 | -2.56927919 | 1 | 2.88266611 | 1.69594336 | -1.52997935 | |
| 1 | 0.77526617 | 4.22074318 | -1.61427927 | | | | | |

TS-4Me

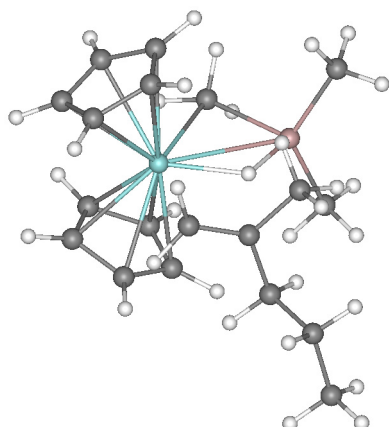


| | |
|--|-----------------------------|
| Zero-point vibrational energy | 1201249.4 (Joules/Mol) |
| | 287.10549 (Kcal/Mol) |
| Zero-point correction= | 0.457532 (Hartree/Particle) |
| Thermal correction to Energy= | 0.483782 |
| Thermal correction to Enthalpy= | 0.484726 |
| Thermal correction to Gibbs Free Energy= | 0.403324 |
| Sum of electronic and zero-point Energies= | -4525.515384 |
| Sum of electronic and thermal Energies= | -4525.489134 |
| Sum of electronic and thermal Enthalpies= | -4525.488190 |
| Sum of electronic and thermal Free Energies= | -4525.569592 |

| cartesian | | | | | | |
|-----------|------------|-------------|-------------|----|-------------|-------------------------|
| 6 | 2.24909449 | 1.15650380 | 1.92583585 | 1 | -1.93640554 | -0.16109625 3.01843596 |
| 6 | 3.33119440 | 1.14360380 | 0.99923581 | 1 | -0.33690554 | 0.51560372 0.18973584 |
| 6 | 3.84129429 | -0.16699624 | 0.93233585 | 1 | -2.70150566 | 0.34430376 -0.10066415 |
| 6 | 3.07809448 | -0.98299628 | 1.81463587 | 1 | -2.05660534 | -1.16969621 -0.74026418 |
| 6 | 2.12889433 | -0.14939624 | 2.45473599 | 1 | 0.19129446 | -1.86269617 2.15253592 |
| 1 | 1.43989444 | -0.46299624 | 3.22663593 | 1 | -0.48270553 | -2.48259640 0.57113582 |
| 1 | 1.67099452 | 2.02680373 | 2.21433592 | 13 | -0.45960552 | 1.96280372 -0.93646419 |
| 1 | 3.71229458 | 1.99740374 | 0.45573583 | 6 | 1.56749451 | 2.11490369 -1.21106410 |
| 1 | 4.67819452 | -0.48929623 | 0.32603583 | 6 | -1.46570551 | 1.35080385 -2.50176406 |
| 1 | 3.23599434 | -2.03679633 | 2.01023579 | 6 | -1.04970551 | 3.37360358 0.27703583 |
| 6 | 2.73649454 | -0.88939625 | -2.11686420 | 1 | -2.11950541 | 3.31690359 0.50683582 |
| 6 | 2.77659464 | -2.05529618 | -1.30436409 | 1 | -0.50790548 | 3.38330364 1.22973585 |
| 6 | 1.46289444 | -2.55089641 | -1.18276405 | 1 | -0.89280558 | 4.35820389 -0.18066417 |
| 6 | 0.60209447 | -1.70329618 | -1.93976414 | 1 | -2.53070545 | 1.59120381 -2.40796399 |
| 6 | 1.39329445 | -0.69599628 | -2.53206420 | 1 | -1.12150550 | 1.85730386 -3.41296411 |
| 1 | 1.03209448 | 0.09690376 | -3.17606401 | 1 | -1.40330553 | 0.27570376 -2.70306420 |
| 1 | 3.59099436 | -0.29299623 | -2.41366410 | 1 | 1.26069450 | 2.57320356 -2.17156410 |
| 1 | 3.66089439 | -2.49469638 | -0.86086416 | 1 | 1.83859444 | 2.94340372 -0.54926413 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 1.17479444 | -3.44059634 | -0.63886416 | 1 | 2.49999452 | 1.63650382 | -1.51556408 |
| 1 | -0.46280551 | -1.83849621 | -2.08126402 | 6 | -3.46680546 | -1.41899621 | 0.87783581 |
| 40 | 1.49989450 | -0.29679623 | -0.01916416 | 6 | -4.64610529 | -1.62739623 | -0.07156416 |
| 6 | -2.33080530 | -0.64809626 | 0.18193583 | 1 | -3.80130529 | -0.86369628 | 1.75903594 |
| 6 | -1.12540555 | -0.52999622 | 1.09763587 | 1 | -3.09070539 | -2.38489628 | 1.23103595 |
| 6 | -0.23230553 | -1.62129617 | 1.18323588 | 1 | -5.45990562 | -2.15399623 | 0.43033585 |
| 6 | -1.32830548 | 0.38430378 | 2.28883600 | 1 | -4.35100555 | -2.21739626 | -0.94356418 |
| 1 | -0.39450550 | 0.66130376 | 2.77623582 | 1 | -5.03610563 | -0.67049628 | -0.42886415 |
| 1 | -1.86310542 | 1.29470384 | 2.00963593 | | | | |

I-5Me



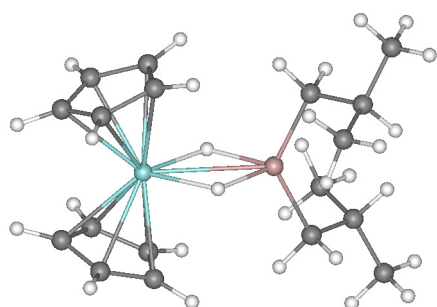
| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1201249.4 (Joules/Mol) |
| | 287.10549 (Kcal/Mol) |
| Zero-point correction | 0.457532 (Hartree/Particle) |
| Thermal correction to Energy | 0.483782 |
| Thermal correction to Enthalpy | 0.484726 |
| Thermal correction to Gibbs Free Energy | 0.403324 |
| Sum of electronic and zero-point Energies | -4525.515384 |
| Sum of electronic and thermal Energies | -4525.489134 |
| Sum of electronic and thermal Enthalpies | -4525.488190 |
| Sum of electronic and thermal Free Energies | -4525.569592 |

| cartesian | | | | | | | |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | 0.30487162 | -2.28994155 | -1.48408866 | 1 | 0.85947156 | 3.17795849 | 1.83051133 |
| 6 | 1.69587159 | -2.51814151 | -1.53198874 | 1 | 0.95997161 | 4.47655869 | 0.64471132 |
| 6 | 2.29237151 | -1.43084145 | -2.23328876 | 1 | -0.80872840 | 3.47915840 | -2.54448867 |
| 6 | 1.25467157 | -0.55114150 | -2.63038874 | 1 | -0.74502844 | 1.75395846 | -2.87728858 |
| 6 | 0.02807161 | -1.05854154 | -2.13998866 | 1 | -1.97892833 | 2.41205835 | -1.80658865 |
| 1 | -0.94792837 | -0.61384153 | -2.29038858 | 6 | -0.63732845 | -1.68244147 | 1.56531131 |
| 1 | -0.42592841 | -2.96174169 | -1.05588865 | 6 | -1.52532840 | -0.69794154 | 1.27081132 |
| 1 | 2.20957160 | -3.38444161 | -1.13458872 | 6 | -1.69662833 | 0.48975846 | 2.17971134 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 3.34557176 | -1.32624149 | -2.46698880 | 6 | -2.50172830 | -0.80874157 | 0.13281132 |
| 1 | 1.37557161 | 0.36315849 | -3.19708872 | 1 | -0.66652840 | -2.63564157 | 1.04611135 |
| 6 | 2.15797162 | -0.37384152 | 2.32601142 | 1 | -0.11172837 | -1.66414154 | 2.51421142 |
| 6 | 2.49117160 | -1.66884148 | 1.82541132 | 1 | -1.96742845 | 1.39005852 | 1.62031126 |
| 6 | 3.52667165 | -1.50834155 | 0.87421131 | 1 | -2.51522827 | 0.28115848 | 2.87751126 |
| 6 | 3.79007173 | -0.12674153 | 0.73841131 | 1 | -0.79952842 | 0.69545853 | 2.76711130 |
| 6 | 2.95227170 | 0.57245851 | 1.65541136 | 6 | -3.94942856 | -0.94394147 | 0.64341134 |
| 1 | 2.93167162 | 1.64295852 | 1.81531131 | 1 | -2.43412828 | 0.09035848 | -0.49508870 |
| 1 | 1.43597162 | -0.15004152 | 3.10101128 | 1 | -2.26522827 | -1.67624152 | -0.49258870 |
| 1 | 2.08087158 | -2.61364150 | 2.16051126 | 1 | 1.95887160 | 2.37875843 | -1.94058871 |
| 1 | 4.02497149 | -2.30414152 | 0.33541131 | 1 | 2.99087167 | 1.12015855 | -1.49088871 |
| 1 | 4.53597164 | 0.31785849 | 0.09161133 | 1 | 2.77777171 | 2.44255829 | -0.37728870 |
| 40 | 1.42487168 | -0.46704152 | -0.10498868 | 6 | -4.92972851 | -1.13254154 | -0.51248866 |
| 6 | 2.23337150 | 1.77715850 | -1.05478871 | 1 | -4.22352839 | -0.05194152 | 1.21451128 |
| 1 | -0.05562842 | 0.76265848 | 0.15231133 | 1 | -4.00862837 | -1.79464149 | 1.33041131 |
| 13 | 0.24547160 | 2.30535841 | -0.52528870 | 1 | -5.95242834 | -1.22724152 | -0.14268868 |
| 6 | 0.37977159 | 3.59305835 | 0.93611133 | 1 | -4.69602823 | -2.03454161 | -1.08478868 |
| 6 | -0.92052835 | 2.49005842 | -2.08458877 | 1 | -4.89842844 | -0.27994153 | -1.19678867 |
| 1 | -0.60292834 | 3.96475816 | 1.24671125 | | | | |

S3.6. ⁱBu₂AlH reaction profile

I-OH

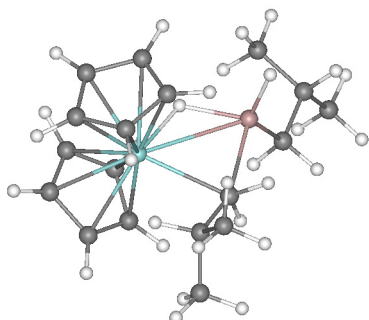


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1134721.8 (Joules/Mol) |
| | 271.20502 (Kcal/Mol) |
| Zero-point correction | 0.432193 (Hartree/Particle) |
| Thermal correction to Energy | 0.456539 |
| Thermal correction to Enthalpy | 0.457484 |
| Thermal correction to Gibbs Free Energy | 0.373872 |
| Sum of electronic and zero-point Energies | -4486.266924 |
| Sum of electronic and thermal Energies | -4486.242577 |
| Sum of electronic and thermal Enthalpies | -4486.241633 |
| Sum of electronic and thermal Free Energies | -4486.325245 |

| | | | | cartesian | | | |
|---|-------------|-------------|-------------|-----------|------------|-------------|-------------|
| 6 | -3.42163610 | 1.52515006 | 1.65658605 | 6 | 1.56366396 | -1.64485002 | -0.57961398 |
| 6 | -4.19173622 | 1.57825005 | 0.46678603 | 1 | 2.01516390 | 1.50534999 | 1.59268606 |
| 6 | -3.38523602 | 2.14665008 | -0.55361396 | 6 | 2.63566399 | 2.12145019 | -0.39971399 |
| 6 | -2.12053609 | 2.46795011 | 0.01268600 | 1 | 0.82786393 | 2.46835017 | 0.73948604 |
| 6 | -2.14083600 | 2.08075023 | 1.37868607 | 6 | 2.65516400 | -2.11554980 | 0.40668601 |
| 1 | -1.33253598 | 2.20485020 | 2.08898592 | 1 | 0.83746397 | -2.46024990 | -0.71701401 |
| 1 | -3.76123595 | 1.15495002 | 2.61738586 | 1 | 2.00936389 | -1.47885001 | -1.57081401 |
| 1 | -5.22033596 | 1.25744998 | 0.36018598 | 6 | 3.32476401 | 3.40105009 | 0.08018599 |
| 1 | -3.69143605 | 2.33525014 | -1.57631397 | 6 | 2.02676392 | 2.33135009 | -1.78921402 |
| 1 | -1.29273605 | 2.93685007 | -0.50481397 | 1 | 3.39986396 | 1.33685005 | -0.48091400 |
| 6 | -4.17973614 | -1.59614992 | -0.48251402 | 6 | 3.33596396 | -3.39364982 | -0.08861400 |
| 6 | -3.39493608 | -1.47025001 | -1.65911400 | 6 | 2.06616402 | -2.33034992 | 1.80408597 |
| 6 | -2.11723614 | -2.03914976 | -1.39881396 | 1 | 3.42106414 | -1.33194995 | 0.47988600 |
| 6 | -2.10863590 | -2.49894977 | -0.05541400 | 1 | 4.13176441 | -3.71154976 | 0.59128600 |
| 6 | -3.38363600 | -2.21944976 | 0.51158601 | 1 | 3.77446389 | -3.24894977 | -1.07951403 |
| 1 | -3.70063615 | -2.46644974 | 1.51858604 | 1 | 2.60736394 | -4.20924997 | -0.15901400 |
| 1 | -5.21123600 | -1.28684998 | -0.36951399 | 1 | 4.11016369 | 3.71585011 | -0.61321402 |
| 1 | -3.72553611 | -1.04855001 | -2.60151410 | 1 | 3.77836394 | 3.25945020 | 1.06478596 |
| 1 | -1.29963613 | -2.12004995 | -2.10451412 | 1 | 2.59776402 | 4.21725035 | 0.15898600 |
| 1 | -1.28463602 | -2.99284983 | 0.44478601 | 1 | 2.76966405 | 2.69105005 | -2.50621414 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|------------|-------------|-------------|
| 40 | -2.31443596 | -0.01794996 | 0.04678600 | 1 | 1.22226393 | 3.07625008 | -1.74611402 |
| 1 | -0.70073605 | -0.34654996 | 1.09818602 | 1 | 1.60496402 | 1.40455008 | -2.20351410 |
| 1 | -0.72603607 | 0.32815003 | -1.01891398 | 1 | 2.81736398 | -2.69884992 | 2.50778580 |
| 13 | 0.70166397 | -0.00144996 | 0.02798600 | 1 | 1.25566399 | -3.06924987 | 1.76898599 |
| 6 | 1.55806398 | 1.65614998 | 0.60418600 | 1 | 1.65686393 | -1.40324998 | 2.23028588 |

I-OH_bo



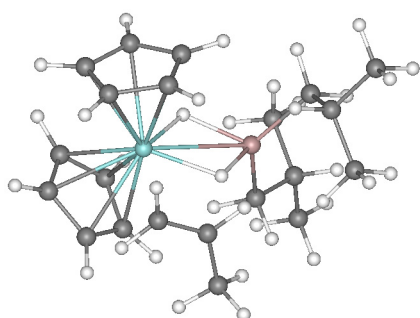
| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1138711.1 (Joules/Mol) |
| | 272.15848 (Kcal/Mol) |
| Zero-point correction | 0.433712 (Hartree/Particle) |
| Thermal correction to Energy | 0.457216 |
| Thermal correction to Enthalpy | 0.458160 |
| Thermal correction to Gibbs Free Energy | 0.381281 |
| Sum of electronic and zero-point Energies | -4486.265712 |
| Sum of electronic and thermal Energies | -4486.242208 |
| Sum of electronic and thermal Enthalpies | -4486.241264 |
| Sum of electronic and thermal Free Energies | -4486.318143 |

cartesian

| | | | | | | | |
|---|-------------|-------------|-------------|----|------------|-------------|-------------|
| 6 | -1.97790194 | -0.45687792 | -2.45889997 | 1 | 0.41819799 | 1.82142198 | -0.71950006 |
| 6 | -2.36900187 | -1.74417794 | -2.01889992 | 13 | 1.30609798 | 0.27172208 | 1.02049994 |
| 6 | -1.19210196 | -2.47617793 | -1.70300007 | 1 | 1.19829798 | 0.27852207 | 2.59529996 |
| 6 | -0.07340199 | -1.64467788 | -1.96970010 | 6 | 2.90639782 | 0.55772209 | -0.05730003 |
| 6 | -0.55660200 | -0.38967791 | -2.41799998 | 6 | 4.13219786 | -0.19927791 | 0.49449998 |
| 1 | 0.05639800 | 0.44882208 | -2.72449994 | 1 | 2.72229815 | 0.23362209 | -1.09460008 |
| 1 | -2.64690208 | 0.32812208 | -2.79250002 | 1 | 3.13419819 | 1.63102210 | -0.12110004 |
| 1 | -3.38490200 | -2.11357784 | -1.95940006 | 6 | 5.36079788 | 0.00892209 | -0.39370003 |
| 1 | -1.15020204 | -3.50357795 | -1.36380005 | 6 | 3.82539797 | -1.69227791 | 0.64399993 |
| 1 | 0.96659803 | -1.92247796 | -1.85520005 | 1 | 4.36229801 | 0.19882210 | 1.49099994 |
| 6 | -3.34920216 | -1.56407785 | 1.09549999 | 1 | 6.24329805 | -0.48397791 | 0.02439997 |
| 6 | -2.26350212 | -2.43537807 | 1.39629996 | 1 | 5.58929777 | 1.07212210 | -0.50770009 |
| 6 | -1.35010195 | -1.73037791 | 2.21670008 | 1 | 5.18429804 | -0.40657791 | -1.39220011 |
| 6 | -1.85020196 | -0.41297793 | 2.40400004 | 1 | 4.69749784 | -2.25147796 | 0.99409997 |
| 6 | -3.09980202 | -0.32517791 | 1.73219991 | 1 | 3.52249813 | -2.12077785 | -0.31960005 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | -3.75660181 | 0.53662211 | 1.71409988 | 1 | 3.01759815 | -1.87797785 | 1.36669993 |
| 1 | -4.23260212 | -1.81667793 | 0.52269995 | 6 | -2.23670197 | 2.84602189 | 1.03469992 |
| 1 | -2.17250204 | -3.46857810 | 1.08589995 | 1 | -2.39850187 | 1.21772206 | -0.31280002 |
| 1 | -0.43360201 | -2.12287807 | 2.63779998 | 6 | -1.74220204 | 2.87582207 | -1.43660009 |
| 1 | -1.38120198 | 0.35292208 | 3.00920010 | 1 | -3.29870176 | 3.05372190 | 0.87940001 |
| 40 | -1.32710195 | -0.62057793 | -0.03880003 | 1 | -1.71610200 | 3.80462217 | 1.11459994 |
| 6 | -0.21890199 | 1.56532204 | 0.13299996 | 1 | -2.11630201 | 2.32242203 | 1.98529994 |
| 1 | 0.44219798 | -1.14207792 | 0.48499995 | 1 | -2.77960205 | 3.14052200 | -1.65860009 |
| 1 | 0.13989800 | 2.15762186 | 0.99210000 | 1 | -1.32950199 | 2.33782196 | -2.29340005 |
| 6 | -1.64920199 | 2.05882192 | -0.14190003 | 1 | -1.17260194 | 3.80152178 | -1.31730008 |

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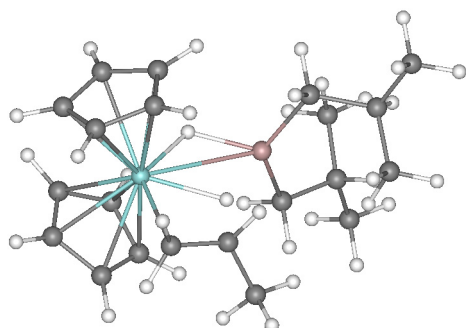
| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1356959.8 (Joules/Mol) |
| | 324.32118 (Kcal/Mol) |
| Zero-point correction | 0.516839 (Hartree/Particle) |
| Thermal correction to Energy | 0.545555 |
| Thermal correction to Enthalpy | 0.546499 |
| Thermal correction to Gibbs Free Energy | 0.457341 |
| Sum of electronic and zero-point Energies | -4604.058621 |
| Sum of electronic and thermal Energies | -4604.029905 |
| Sum of electronic and thermal Enthalpies | -4604.028960 |
| Sum of electronic and thermal Free Energies | -4604.118119 |

cartesian

| | | | | | | | |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | -2.65861034 | -2.27949309 | -1.15430343 | 1 | -1.47221017 | -0.96759319 | -3.49750352 |
| 6 | -3.45611024 | -2.30199313 | 0.01249658 | 1 | -1.08941019 | 1.79580677 | -2.11910343 |
| 6 | -2.60261035 | -2.60389328 | 1.11369658 | 13 | 1.09728980 | -0.07769318 | 0.39239657 |
| 6 | -1.28681016 | -2.76279330 | 0.61819655 | 6 | 2.11408973 | -1.61049318 | -0.27930343 |
| 6 | -1.31081021 | -2.52939320 | -0.78490341 | 6 | 1.79778981 | 1.65520680 | 0.98199660 |
| 1 | -0.46201020 | -2.59639311 | -1.45540345 | 1 | 2.23378968 | -1.52379322 | -1.37040341 |
| 1 | -3.02061033 | -2.12679315 | -2.16210341 | 6 | 3.50418997 | -1.71139324 | 0.38369656 |
| 1 | -4.52941036 | -2.16099310 | 0.05559658 | 1 | 1.58298969 | -2.56079316 | -0.11810343 |
| 1 | -2.90961027 | -2.72909307 | 2.14439654 | 6 | 1.35778975 | 2.80770683 | 0.05409658 |
| 1 | -0.41591018 | -3.02469325 | 1.20469654 | 1 | 1.52228975 | 1.87780678 | 2.02229667 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|------------|-------------|-------------|
| 6 | -2.66781020 | 1.99760675 | 0.90239662 | 1 | 2.89738965 | 1.61190677 | 0.98369658 |
| 6 | -3.81021023 | 1.14790678 | 1.00709653 | 6 | 4.29988956 | -2.89659309 | -0.16820343 |
| 6 | -3.59481025 | 0.27150682 | 2.09809661 | 6 | 3.36448979 | -1.82219315 | 1.90479648 |
| 6 | -2.31231022 | 0.53610682 | 2.63329649 | 1 | 4.06448984 | -0.79389322 | 0.15979658 |
| 6 | -1.74871016 | 1.62240684 | 1.90039659 | 6 | 1.83868980 | 2.55570674 | -1.37890351 |
| 1 | -0.77971017 | 2.07340670 | 2.07719660 | 6 | 1.86488986 | 4.16250706 | 0.55519658 |
| 1 | -2.52541018 | 2.79990673 | 0.18779658 | 1 | 0.25608981 | 2.84800673 | 0.03499658 |
| 1 | -4.71191025 | 1.20160675 | 0.40939659 | 1 | 1.52698970 | 3.35470676 | -2.05880356 |
| 1 | -4.29000998 | -0.47889319 | 2.45279646 | 1 | 1.45518970 | 1.60770679 | -1.78560352 |
| 1 | -1.85101008 | 0.03260682 | 3.47349644 | 1 | 2.93238974 | 2.50040674 | -1.41030347 |
| 40 | -1.92521024 | -0.34659317 | 0.31619656 | 1 | 5.29738998 | -2.95139313 | 0.27779657 |
| 1 | -0.30151021 | -0.59039319 | 1.35029650 | 1 | 4.41798973 | -2.82249308 | -1.25290346 |
| 1 | -0.29471019 | 0.26200682 | -0.60650343 | 1 | 3.78148985 | -3.83679318 | 0.05069657 |
| 6 | -2.94131017 | 0.80590683 | -2.08550358 | 1 | 4.33668995 | -1.92679322 | 2.39409661 |
| 6 | -1.63331008 | 0.89820683 | -2.41560340 | 1 | 2.76338983 | -2.70019317 | 2.17099643 |
| 6 | -0.90421021 | -0.05309319 | -3.31700349 | 1 | 2.88148975 | -0.93629318 | 2.34149647 |
| 1 | -3.56571031 | 0.00370681 | -2.46910357 | 1 | 1.53698969 | 4.98090696 | -0.09310342 |
| 1 | -3.45351028 | 1.64150679 | -1.62220347 | 1 | 2.95958972 | 4.16960716 | 0.57969660 |
| 1 | -0.75211018 | 0.44230682 | -4.28200340 | 1 | 1.50778985 | 4.36690712 | 1.56869650 |
| 1 | 0.08408982 | -0.30869317 | -2.92710352 | | | | |

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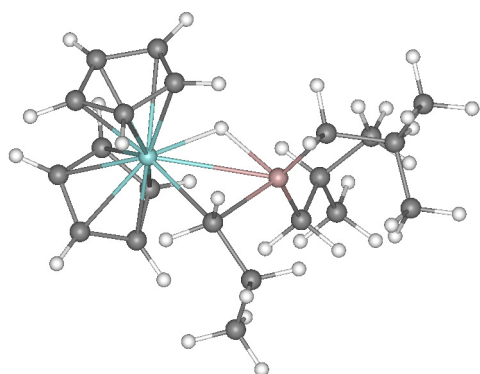


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1353632.3 (Joules/Mol) |
| | 323.52589 (Kcal/Mol) |
| Zero-point correction | 0.515571 (Hartree/Particle) |
| Thermal correction to Energy | 0.543544 |
| Thermal correction to Enthalpy | 0.544488 |
| Thermal correction to Gibbs Free Energy | 0.457231 |
| Sum of electronic and zero-point Energies | -4604.050627 |
| Sum of electronic and thermal Energies | -4604.022655 |
| Sum of electronic and thermal Enthalpies | -4604.021711 |
| Sum of electronic and thermal Free Energies | -4604.108967 |

cartesian

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | 1.85980844 | 2.42909479 | -0.42229149 | 1 | 2.99940825 | -1.74520516 | -2.08349156 |
| 6 | 2.10580850 | 2.40209484 | 0.98080844 | 1 | 0.74140847 | 0.26479489 | 1.31520855 |
| 6 | 3.44800854 | 2.01589489 | 1.18260849 | 13 | -0.74729156 | 0.05779488 | 0.49130848 |
| 6 | 4.04690838 | 1.80889487 | -0.09469152 | 6 | -1.62359154 | 1.76719487 | 0.11920848 |
| 6 | 3.07110834 | 2.09699488 | -1.07889152 | 6 | -1.48909152 | -1.73240519 | 0.76380849 |
| 1 | 3.23280859 | 2.09039474 | -2.14829159 | 1 | -1.54469144 | 2.01629496 | -0.94999152 |
| 1 | 0.93100846 | 2.72409487 | -0.89739150 | 6 | -3.10429144 | 1.80619490 | 0.55370849 |
| 1 | 1.39010847 | 2.64289474 | 1.75620854 | 1 | -1.08359158 | 2.57119489 | 0.64480847 |
| 1 | 3.93960857 | 1.91029489 | 2.14170861 | 6 | -2.86919165 | -1.94430518 | 0.11010848 |
| 1 | 5.07890844 | 1.53749490 | -0.28179151 | 1 | -0.78939152 | -2.48340511 | 0.35960847 |
| 6 | 2.93800831 | -1.12210512 | 2.32390857 | 1 | -1.55219162 | -1.94800520 | 1.84110856 |
| 6 | 4.12310839 | -1.10220516 | 1.54270852 | 6 | -3.72559166 | 3.17609477 | 0.26890847 |
| 6 | 3.91900826 | -1.92130518 | 0.40960848 | 6 | -3.24279165 | 1.45539486 | 2.03810835 |
| 6 | 2.60990858 | -2.48030519 | 0.50550848 | 1 | -3.65879154 | 1.05789483 | -0.02849152 |
| 6 | 2.01740837 | -2.00310516 | 1.69340849 | 6 | -3.36779165 | -3.37710524 | 0.31500849 |
| 1 | 1.02880847 | -2.25440526 | 2.05740857 | 6 | -2.81709146 | -1.60360515 | -1.38239145 |
| 1 | 2.77740860 | -0.60060507 | 3.25920844 | 1 | -3.58879137 | -1.26640511 | 0.58780849 |
| 1 | 5.02700853 | -0.55150509 | 1.77110851 | 1 | -4.36159134 | -3.51980519 | -0.11909152 |
| 1 | 4.64650822 | -2.11800504 | -0.36779150 | 1 | -3.42369127 | -3.62620521 | 1.37810850 |
| 1 | 2.16030836 | -3.17720509 | -0.19249150 | 1 | -2.68569136 | -4.08970499 | -0.16229150 |
| 40 | 2.32710838 | 0.01739488 | 0.18270847 | 1 | -4.78189135 | 3.19979477 | 0.55210847 |
| 1 | 0.59670842 | -1.64520514 | -2.07489157 | 1 | -3.65389156 | 3.43089485 | -0.79199153 |
| 6 | 1.13770843 | -0.70910507 | -2.21849155 | 1 | -3.20669174 | 3.95469475 | 0.83890843 |
| 6 | 2.53780842 | -0.76890510 | -2.17279148 | 1 | -4.28509140 | 1.49629486 | 2.36570859 |
| 6 | 0.42150843 | 0.32749486 | -3.05359149 | 1 | -2.67379141 | 2.16229486 | 2.65350842 |
| 1 | 0.92580843 | 1.29519486 | -3.00759149 | 1 | -2.87799168 | 0.44269487 | 2.26160860 |
| 1 | -0.62299156 | 0.45169488 | -2.76139140 | 1 | -3.77979136 | -1.77270520 | -1.87269151 |
| 1 | 0.44500846 | -0.01480512 | -4.09269190 | 1 | -2.07349157 | -2.22980523 | -1.89279151 |
| 1 | 0.60140848 | -0.21940511 | -0.82599151 | 1 | -2.55449152 | -0.54920512 | -1.55319142 |
| 1 | 3.09980822 | -0.03340512 | -2.73809147 | | | | |

I-2H_a



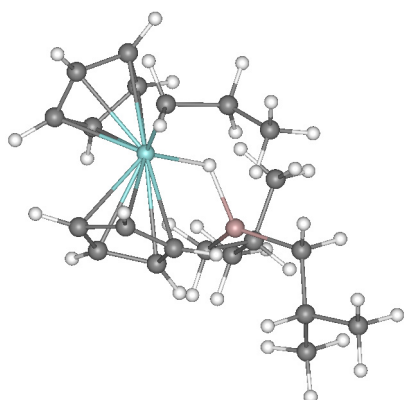
| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1365071.3 (Joules/Mol) |
| | 326.25987 (Kcal/Mol) |
| Zero-point correction | 0.519928 (Hartree/Particle) |
| Thermal correction to Energy | 0.548206 |
| Thermal correction to Enthalpy | 0.549150 |
| Thermal correction to Gibbs Free Energy | 0.461586 |
| Sum of electronic and zero-point Energies | -4604.069359 |
| Sum of electronic and thermal Energies | -4604.041082 |
| Sum of electronic and thermal Enthalpies | -4604.040138 |
| Sum of electronic and thermal Free Energies | -4604.127702 |

cartesian

| | | | | | | | |
|----|------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | 3.41094589 | 1.67184234 | 1.17716777 | 1 | -0.20835423 | 1.85004234 | -2.57713223 |
| 6 | 2.24434566 | 2.17704248 | 0.54206777 | 13 | -0.61325419 | -0.09695762 | 0.00306778 |
| 6 | 2.41054583 | 2.03294230 | -0.85603219 | 6 | -1.21695423 | 1.77244234 | -0.03773221 |
| 6 | 3.69244576 | 1.45604241 | -1.08963227 | 6 | -1.59135425 | -1.75725758 | 0.40286779 |
| 6 | 4.31324577 | 1.24714243 | 0.16516778 | 1 | -2.12775421 | 1.86504233 | -0.64923221 |
| 40 | 2.34764576 | -0.29625762 | 0.08646779 | 6 | -1.52395427 | 2.34054232 | 1.36746776 |
| 6 | 0.73014575 | -0.75995761 | -1.62403226 | 1 | -0.47755420 | 2.42444229 | -0.52353221 |
| 1 | 0.78224576 | 0.01374238 | 1.14416778 | 6 | -3.13385439 | -1.74215758 | 0.36676779 |
| 6 | 1.91674578 | -2.67765760 | 0.78896779 | 1 | -1.24845421 | -2.54205751 | -0.29313222 |
| 6 | 2.38544583 | -1.98945761 | 1.94286776 | 1 | -1.26645422 | -2.10035753 | 1.39866769 |
| 6 | 3.72594595 | -1.60065758 | 1.70546770 | 6 | -2.57315445 | 1.49714243 | 2.09586763 |
| 6 | 4.08984566 | -2.04225779 | 0.40256780 | 6 | -1.97745430 | 3.80014229 | 1.27926779 |
| 6 | 2.97264576 | -2.72195768 | -0.15123221 | 1 | -0.60535419 | 2.31014228 | 1.97226775 |
| 1 | 1.70654583 | 2.34254241 | -1.61703229 | 6 | -3.69625425 | -3.12715769 | 0.70086777 |
| 1 | 4.13124561 | 1.24644244 | -2.05903220 | 6 | -3.65695429 | -1.27325761 | -0.99233216 |
| 1 | 1.38144577 | 2.60064244 | 1.04076779 | 1 | -3.49595404 | -1.04125762 | 1.12766778 |
| 1 | 3.59584570 | 1.65744233 | 2.24446774 | 1 | -4.78995419 | -3.11945772 | 0.72006780 |
| 1 | 5.30304575 | 0.83734238 | 0.32426780 | 1 | -3.34425402 | -3.47395754 | 1.67666769 |
| 1 | 4.36794567 | -1.07225764 | 2.39906764 | 1 | -3.37875414 | -3.85875750 | -0.05103222 |
| 1 | 1.81754577 | -1.80705762 | 2.84646773 | 1 | -2.83565426 | 1.93724227 | 3.06206775 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 0.92694581 | -3.10145760 | 0.66506779 | 1 | -2.21995401 | 0.47594237 | 2.28936768 |
| 1 | 2.93634558 | -3.18665767 | -1.13003230 | 1 | -3.49015427 | 1.42794240 | 1.49886775 |
| 1 | 5.06094599 | -1.92825758 | -0.06343221 | 1 | -2.15195417 | 4.22554255 | 2.27196765 |
| 1 | 1.73824573 | -0.53795761 | -2.07093215 | 1 | -2.91195440 | 3.87134242 | 0.71246779 |
| 1 | 0.67284578 | -1.85175765 | -1.56103230 | 1 | -1.23125422 | 4.41874218 | 0.77096778 |
| 6 | -0.26475424 | -0.32695761 | -2.73543239 | 1 | -4.74895430 | -1.31585765 | -1.03493226 |
| 6 | -0.02775425 | 1.06444240 | -3.31363225 | 1 | -3.27145433 | -1.91375756 | -1.79573226 |
| 1 | -1.30195427 | -0.40175763 | -2.37523222 | 1 | -3.36565399 | -0.23755762 | -1.20843232 |
| 1 | -0.70515418 | 1.24334240 | -4.15133190 | 1 | -0.20395422 | -1.06785762 | -3.53873229 |
| 1 | 0.99544579 | 1.16234243 | -3.69223237 | | | | |

I-2H_bi



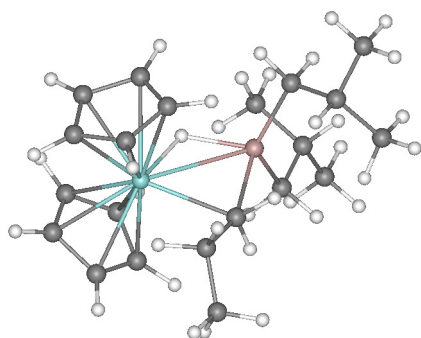
| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1362944.2 (Joules/Mol) |
| | 325.75147 (Kcal/Mol) |
| Zero-point correction | 0.519118 (Hartree/Particle) |
| Thermal correction to Energy | 0.548034 |
| Thermal correction to Enthalpy | 0.548978 |
| Thermal correction to Gibbs Free Energy | 0.456332 |
| Sum of electronic and zero-point Energies | -4604.057475 |
| Sum of electronic and thermal Energies | -4604.028559 |
| Sum of electronic and thermal Enthalpies | -4604.027615 |
| Sum of electronic and thermal Free Energies | -4604.120260 |

cartesian

| | | | | | | | |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | -4.18676949 | -1.67005587 | 0.10166949 | 1 | -1.81656957 | 3.39204407 | 1.10836947 |
| 6 | -3.45776939 | -2.18865609 | -0.99433053 | 1 | -2.64466953 | 0.97214413 | 2.83156967 |
| 6 | -2.21226954 | -2.67595601 | -0.50843048 | 13 | 1.08293045 | -0.29475588 | 0.02226950 |
| 6 | -2.19206953 | -2.48385596 | 0.89676952 | 6 | 1.78163040 | 1.41334414 | 0.65376949 |
| 6 | -3.39606953 | -1.84215581 | 1.27026951 | 6 | 1.90723050 | -1.88895583 | -0.73743051 |
| 1 | -3.67626953 | -1.55015588 | 2.27516937 | 1 | 2.47323036 | 1.21364415 | 1.48766947 |
| 1 | -5.17426920 | -1.22975588 | 0.05746950 | 6 | 2.53573036 | 2.26214409 | -0.39493051 |
| 1 | -3.79796934 | -2.22945595 | -2.02143049 | 1 | 0.96493053 | 2.00244403 | 1.09726954 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|------------|-------------|-------------|
| 1 | -1.43806958 | -3.15285587 | -1.09693050 | 6 | 2.99843025 | -2.40985608 | 0.22536948 |
| 1 | -1.38786960 | -2.76715589 | 1.56416953 | 1 | 1.15583050 | -2.67985606 | -0.88113052 |
| 6 | -1.06056952 | 1.79844415 | -1.42873049 | 1 | 2.34293032 | -1.70035589 | -1.72773051 |
| 6 | -2.40056944 | 1.73654413 | -1.86003053 | 6 | 3.73373079 | 1.49604416 | -0.96373051 |
| 6 | -2.58266973 | 0.51894414 | -2.57323027 | 6 | 2.99203062 | 3.59234405 | 0.20996949 |
| 6 | -1.34016955 | -0.15915588 | -2.61763048 | 1 | 1.85573041 | 2.49464393 | -1.22793055 |
| 6 | -0.39546952 | 0.62694412 | -1.91023052 | 6 | 3.63043070 | -3.70265603 | -0.29423052 |
| 1 | 0.68463051 | 0.50944412 | -2.01743054 | 6 | 2.41543055 | -2.62265587 | 1.62636948 |
| 1 | -0.59136951 | 2.61224413 | -0.88673049 | 1 | 3.78943062 | -1.65105581 | 0.29776949 |
| 1 | -3.15776968 | 2.49004412 | -1.69703054 | 1 | 4.42273045 | -4.05455589 | 0.37266952 |
| 1 | -3.50156975 | 0.19634412 | -3.04723072 | 1 | 4.06333065 | -3.55775595 | -1.28753054 |
| 1 | -1.13386953 | -1.09265590 | -3.12713051 | 1 | 2.87483025 | -4.49255610 | -0.36743051 |
| 40 | -2.17176962 | -0.20305587 | -0.20443051 | 1 | 4.28863049 | 2.10384393 | -1.68323052 |
| 1 | -0.42496952 | -0.59725589 | 0.66176951 | 1 | 3.43713045 | 0.57224417 | -1.47713053 |
| 1 | -1.46666956 | 0.93684411 | 1.56916952 | 1 | 4.42413044 | 1.21864414 | -0.15893051 |
| 6 | -3.56516933 | 1.22354412 | 0.87956953 | 1 | 3.50033045 | 4.21304417 | -0.53353047 |
| 6 | -2.43686962 | 1.45004416 | 1.87086952 | 1 | 3.68983078 | 3.41334391 | 1.03496945 |
| 6 | -2.03776956 | 2.91644406 | 2.06826973 | 1 | 2.14473057 | 4.16084385 | 0.60506952 |
| 1 | -4.44576931 | 0.77734417 | 1.33676946 | 1 | 3.16053057 | -3.01485586 | 2.32336950 |
| 1 | -3.85056973 | 2.14524412 | 0.37536949 | 1 | 1.58323038 | -3.33605599 | 1.59156954 |
| 1 | -1.16196954 | 3.01454401 | 2.71396971 | 1 | 2.03863049 | -1.68705583 | 2.07116938 |
| 1 | -2.86616945 | 3.46144414 | 2.52536964 | | | | |

I-2H_bo

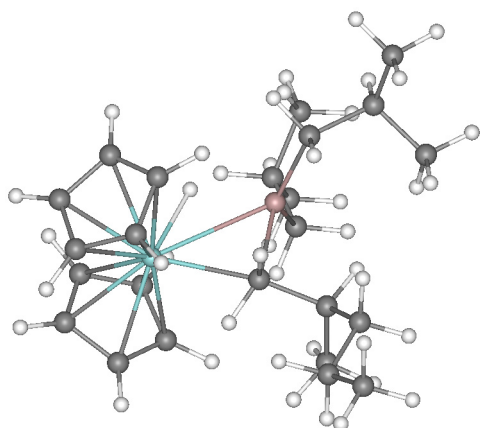


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1367094.0 (Joules/Mol) |
| | 326.74332 (Kcal/Mol) |
| Zero-point correction | 0.520699 (Hartree/Particle) |
| Thermal correction to Energy | 0.548879 |
| Thermal correction to Enthalpy | 0.549823 |
| Thermal correction to Gibbs Free Energy | 0.461991 |
| Sum of electronic and zero-point Energies | -4604.080319 |
| Sum of electronic and thermal Energies | -4604.052139 |
| Sum of electronic and thermal Enthalpies | -4604.051195 |
| Sum of electronic and thermal Free Energies | -4604.139027 |

cartesian

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | 1.61622548 | -2.28887296 | 1.10839832 | 1 | 4.81002569 | -1.30877292 | 1.28319836 |
| 6 | 2.94332528 | -2.31967306 | 0.60099828 | 1 | 2.79842544 | -0.96687287 | -3.98620200 |
| 6 | 3.74712539 | -1.47647297 | 1.40399837 | 13 | -0.91267461 | 0.13922711 | 0.21269830 |
| 6 | 2.92162538 | -0.93847287 | 2.43189812 | 6 | -1.82037473 | -1.42397296 | 0.98109829 |
| 6 | 1.61412549 | -1.45427299 | 2.25999832 | 6 | -1.78547478 | 1.77192700 | -0.41950169 |
| 1 | 0.76402539 | -1.25097299 | 2.89809823 | 1 | -2.71377468 | -1.05357289 | 1.50879836 |
| 1 | 0.76802540 | -2.84287286 | 0.72189832 | 6 | -2.28897476 | -2.47207284 | -0.05280171 |
| 1 | 3.28632522 | -2.89457297 | -0.25090170 | 1 | -1.22227454 | -1.92127299 | 1.75719833 |
| 1 | 3.24562526 | -0.28527290 | 3.23229814 | 6 | -2.88587475 | 2.24932694 | 0.55049831 |
| 6 | 2.13332534 | 2.25042701 | -0.88960171 | 1 | -1.05387473 | 2.58582711 | -0.55200171 |
| 6 | 3.42402530 | 1.67882705 | -1.06530166 | 1 | -2.22387457 | 1.60812700 | -1.41480172 |
| 6 | 4.04372549 | 1.58942699 | 0.20489830 | 6 | -3.19637465 | -1.83307290 | -1.10960174 |
| 6 | 3.14082527 | 2.11592698 | 1.16959834 | 6 | -3.00937462 | -3.63967299 | 0.62689829 |
| 6 | 1.96952534 | 2.53822708 | 0.49009830 | 1 | -1.40707469 | -2.88757300 | -0.56720173 |
| 1 | 1.10372543 | 3.00322700 | 0.94419825 | 6 | -3.56807446 | 3.52252698 | 0.04469829 |
| 1 | 1.41882539 | 2.47412705 | -1.67250168 | 6 | -2.31087470 | 2.47292709 | 1.95249832 |
| 1 | 3.86832523 | 1.38222706 | -2.00880170 | 1 | -3.64957452 | 1.46272707 | 0.62059832 |
| 1 | 3.33002543 | 2.22012711 | 2.23059821 | 1 | -4.36967468 | 3.84202695 | 0.71739829 |
| 40 | 2.08302546 | 0.03272711 | 0.29049829 | 1 | -3.99977469 | 3.37042713 | -0.94830167 |
| 1 | 0.47622538 | 0.56562710 | 1.18199837 | 1 | -2.84187460 | 4.34012747 | -0.02620171 |
| 6 | 1.89132547 | -0.54267287 | -3.55040169 | 1 | -3.55757451 | -2.57207298 | -1.83010173 |
| 6 | 0.43942538 | -0.43237290 | -1.44040167 | 1 | -2.69157457 | -1.04167295 | -1.68050170 |
| 6 | 1.67982531 | -1.03167295 | -2.11510181 | 1 | -4.07087421 | -1.37807298 | -0.63100171 |
| 1 | 1.64412546 | -2.12227297 | -2.07500172 | 1 | -3.31587458 | -4.39817286 | -0.09960170 |
| 1 | -0.34177464 | -1.20387292 | -1.51610172 | 1 | -3.90777469 | -3.28057289 | 1.13989830 |
| 1 | 0.10992539 | 0.42882711 | -2.03080177 | 1 | -2.36847472 | -4.12017250 | 1.37199831 |
| 1 | 2.66712523 | -0.80097288 | -1.61020172 | 1 | -3.07137465 | 2.83382702 | 2.65029812 |
| 1 | 1.96702528 | 0.54792714 | -3.58100176 | 1 | -1.50917459 | 3.22162700 | 1.92169833 |
| 1 | 1.04012537 | -0.83687288 | -4.16750145 | 1 | -1.89387465 | 1.55092704 | 2.38289809 |
| 1 | 5.04282570 | 1.22052705 | 0.39959830 | | | | |

I-4H_a

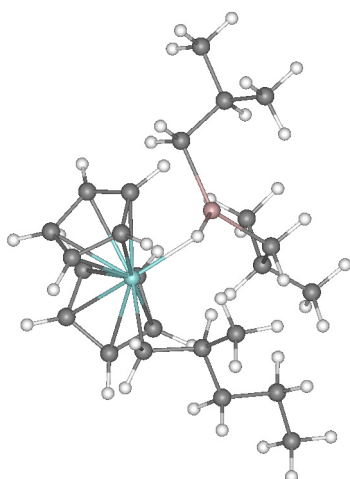


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1592853.6 (Joules/Mol) |
| | 380.70114 (Kcal/Mol) |
| Zero-point correction | 0.606686 (Hartree/Particle) |
| Thermal correction to Energy | 0.638819 |
| Thermal correction to Enthalpy | 0.639763 |
| Thermal correction to Gibbs Free Energy | 0.543141 |
| Sum of electronic and zero-point Energies | -4721.872707 |
| Sum of electronic and thermal Energies | -4721.840574 |
| Sum of electronic and thermal Enthalpies | -4721.839629 |
| Sum of electronic and thermal Free Energies | -4721.936252 |

| | | | | cartesian | | | |
|----|------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 6 | 3.61376929 | -2.25745869 | 0.43127060 | 6 | 0.20796928 | 4.01534128 | 1.35607064 |
| 6 | 2.44126940 | -2.17995882 | 1.23077059 | 6 | -0.20163071 | 5.46624088 | 1.09997058 |
| 6 | 2.50286913 | -0.98265880 | 1.98187065 | 1 | 1.08776927 | 3.77654123 | 0.74397063 |
| 6 | 3.72586918 | -0.32425880 | 1.66177058 | 1 | 0.51346928 | 3.90564132 | 2.40227056 |
| 6 | 4.41646957 | -1.12145889 | 0.71777064 | 1 | 0.61056930 | 6.15614128 | 1.33807063 |
| 40 | 2.35176945 | -0.28675881 | -0.42382944 | 1 | -1.06443071 | 5.74044085 | 1.71287060 |
| 6 | 0.53156924 | 1.10364115 | 0.26827061 | 1 | -0.47643077 | 5.61724091 | 0.05217059 |
| 1 | 0.93486929 | -1.48775887 | -0.88472939 | 13 | -0.58153069 | -0.71945882 | -0.24742940 |
| 6 | 1.84626925 | 0.64174116 | -2.71442938 | 6 | -1.04073071 | -1.95775878 | 1.20877063 |
| 6 | 2.46776915 | -0.62215883 | -2.91432929 | 6 | -1.62733078 | -0.09505881 | -1.79262936 |
| 6 | 3.79926920 | -0.53415883 | -2.44132948 | 1 | -2.01413083 | -1.68555880 | 1.64507055 |
| 6 | 4.00466919 | 0.78284115 | -1.94242942 | 6 | -1.12083077 | -3.42985868 | 0.74427062 |
| 6 | 2.79836917 | 1.50904119 | -2.12932944 | 1 | -0.32563072 | -1.88725889 | 2.04117060 |
| 1 | 1.76666927 | -0.63805884 | 2.69587064 | 6 | -3.15953064 | -0.27505881 | -1.78382945 |
| 1 | 4.08236933 | 0.60564119 | 2.09077072 | 1 | -1.41953063 | 0.98034120 | -1.93282938 |
| 1 | 1.64296925 | -2.91085863 | 1.25827062 | 1 | -1.22163069 | -0.58075881 | -2.69482946 |
| 1 | 3.86796927 | -3.06525874 | -0.24452940 | 6 | -2.14173079 | -3.60265875 | -0.38342941 |
| 1 | 5.38656950 | -0.90295881 | 0.28857058 | 6 | -1.45313072 | -4.35805893 | 1.91567063 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 4.53746939 | -1.32625878 | -2.46742940 | 1 | -0.14173073 | -3.73275876 | 0.34327060 |
| 1 | 2.00386930 | -1.49165881 | -3.36242938 | 6 | -3.78083086 | 0.30634120 | -3.05732942 |
| 1 | 0.82436925 | 0.89034116 | -2.97632933 | 6 | -3.79273081 | 0.36664119 | -0.54702944 |
| 1 | 2.63596916 | 2.54654121 | -1.85892940 | 1 | -3.38643074 | -1.34735882 | -1.76082945 |
| 1 | 4.92976904 | 1.17834115 | -1.54122937 | 1 | -4.86193085 | 0.14094120 | -3.08462930 |
| 1 | 1.47966933 | 1.43064117 | 0.77487063 | 1 | -3.34713078 | -0.14745881 | -3.95312929 |
| 1 | 0.44276929 | 1.73084116 | -0.62632936 | 1 | -3.60513067 | 1.38694119 | -3.10832930 |
| 6 | -0.59413075 | 1.55434120 | 1.24697065 | 1 | -2.24803066 | -4.65385914 | -0.66592938 |
| 6 | -0.92933071 | 3.04324126 | 1.04047060 | 1 | -1.85503078 | -3.05035877 | -1.28762937 |
| 6 | -0.26783073 | 1.22814119 | 2.70607066 | 1 | -3.12653065 | -3.23905873 | -0.06702940 |
| 1 | -1.53223062 | 1.02454114 | 1.00517058 | 1 | -1.46903062 | -5.40655899 | 1.60347056 |
| 1 | -1.01723075 | 1.67004120 | 3.36827064 | 1 | -2.43903065 | -4.11285877 | 2.32487059 |
| 1 | 0.70856929 | 1.63164115 | 2.99567056 | 1 | -0.72213078 | -4.25535917 | 2.72387052 |
| 1 | -0.26933074 | 0.15104121 | 2.88877058 | 1 | -4.88403082 | 0.30084121 | -0.57892942 |
| 1 | -1.79353070 | 3.28744125 | 1.67017066 | 1 | -3.52923059 | 1.43074119 | -0.48632944 |
| 1 | -1.25543070 | 3.18964124 | 0.00207059 | 1 | -3.46733093 | -0.12125881 | 0.38017058 |

I-4H_bi

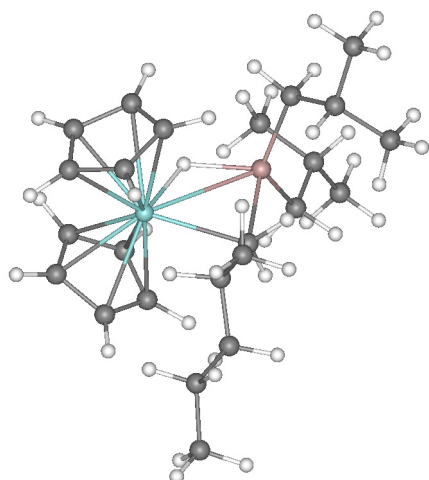


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1589067.4 (Joules/Mol) |
| | 379.79623 (Kcal/Mol) |
| Zero-point correction | 0.605244 (Hartree/Particle) |
| Thermal correction to Energy | 0.638056 |
| Thermal correction to Enthalpy | 0.639001 |
| Thermal correction to Gibbs Free Energy | 0.539447 |
| Sum of electronic and zero-point Energies | -4721.861016 |
| Sum of electronic and thermal Energies | -4721.828203 |
| Sum of electronic and thermal Enthalpies | -4721.827259 |
| Sum of electronic and thermal Free Energies | -4721.926813 |

cartesian

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | -2.80794263 | -3.53673816 | 0.00375737 | 6 | 2.69075727 | -1.76053822 | -0.11804263 |
| 6 | -1.80404258 | -3.80743814 | -0.95384264 | 1 | 2.48825741 | 1.76246190 | 1.13385737 |
| 6 | -0.53574264 | -3.65253830 | -0.32464263 | 6 | 2.17145729 | 2.38806176 | -0.90374261 |
| 6 | -0.76614261 | -3.31633830 | 1.03285742 | 1 | 0.81195736 | 2.09076190 | 0.77575737 |
| 6 | -2.16324258 | -3.21833825 | 1.23055732 | 6 | 4.00375748 | -1.49593818 | 0.65215737 |
| 1 | -2.65974259 | -2.98253822 | 2.16345739 | 1 | 2.27005744 | -2.71513820 | 0.23015738 |
| 1 | -3.87604260 | -3.57423830 | -0.16514263 | 1 | 2.90615749 | -1.89953816 | -1.18794262 |
| 1 | -1.97014260 | -4.10433817 | -1.98194265 | 6 | 3.46085739 | 1.79146171 | -1.47524261 |
| 1 | 0.43045738 | -3.81853819 | -0.78544265 | 6 | 2.36295748 | 3.87666202 | -0.60024261 |
| 1 | -0.00464264 | -3.15323830 | 1.78575742 | 1 | 1.39015734 | 2.31106186 | -1.67314267 |
| 6 | -1.04664266 | 0.69616175 | -1.87054265 | 6 | 5.03145742 | -2.59953809 | 0.39135736 |
| 6 | -2.20554256 | 0.09736177 | -2.39994264 | 6 | 3.72175741 | -1.37113822 | 2.15225744 |
| 6 | -1.85394263 | -1.19023824 | -2.89634252 | 1 | 4.42985725 | -0.54593825 | 0.30235738 |
| 6 | -0.46454263 | -1.37323821 | -2.70744252 | 1 | 5.97015762 | -2.40013838 | 0.91625738 |
| 6 | 0.04115736 | -0.21543823 | -2.06294250 | 1 | 5.25305748 | -2.68933821 | -0.67554265 |
| 1 | 1.09935737 | 0.05136177 | -2.03994274 | 1 | 4.64875746 | -3.56483817 | 0.74025738 |
| 1 | -0.97194266 | 1.68706179 | -1.43314266 | 1 | 3.79255724 | 2.33676171 | -2.36274266 |
| 1 | -3.19084263 | 0.53946173 | -2.44284272 | 1 | 3.35005736 | 0.73646176 | -1.76464260 |
| 1 | -2.52904272 | -1.88643825 | -3.37884259 | 1 | 4.26425743 | 1.84216189 | -0.73154265 |
| 1 | 0.11805737 | -2.23303819 | -3.01464272 | 1 | 2.65385747 | 4.43086147 | -1.49724269 |
| 40 | -1.57074261 | -1.38133824 | -0.40934262 | 1 | 3.14725733 | 4.01376152 | 0.15145737 |
| 1 | -0.05804265 | -0.77073824 | 0.75035739 | 1 | 1.44245744 | 4.32086134 | -0.20954263 |
| 1 | -1.79684258 | 0.42306176 | 0.87195742 | 1 | 4.63525724 | -1.18073821 | 2.72165728 |
| 6 | -3.62334251 | -0.60703826 | 0.17205736 | 1 | 3.27625728 | -2.29633832 | 2.53615737 |
| 6 | -2.93394256 | 0.46946177 | 0.99505734 | 1 | 3.03025746 | -0.54613823 | 2.38135743 |
| 6 | -3.27644253 | 1.89036179 | 0.51545739 | 1 | -4.17824268 | 0.48536178 | 2.76135731 |
| 1 | -4.18314266 | -1.30573821 | 0.79465735 | 1 | -2.50564265 | 0.98496175 | 3.08005738 |
| 1 | -4.28234291 | -0.20553824 | -0.59714264 | 1 | -2.88654256 | -0.72003824 | 2.82745743 |
| 6 | -2.38144255 | 2.99746180 | 1.07095742 | 6 | -2.68644261 | 4.35326147 | 0.43435735 |
| 1 | -4.32164240 | 2.08446169 | 0.78725737 | 1 | -1.32854259 | 2.73716187 | 0.89235735 |
| 1 | -3.24144268 | 1.92006183 | -0.58034265 | 1 | -2.50004268 | 3.07066178 | 2.15645742 |
| 6 | -3.13104272 | 0.29636177 | 2.50715733 | 1 | -2.04494262 | 5.13686132 | 0.84285736 |
| 13 | 1.43095744 | -0.29513824 | 0.15645736 | 1 | -3.72514272 | 4.64356136 | 0.61465734 |
| 6 | 1.71565747 | 1.62466168 | 0.36075735 | 1 | -2.53314257 | 4.32306147 | -0.64904261 |

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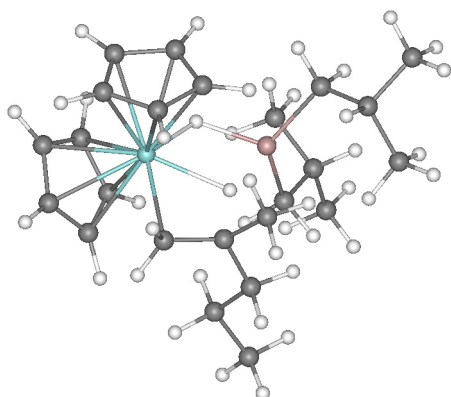


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1591929.3 (Joules/Mol) |
| | 380.48023 (Kcal/Mol) |
| Zero-point correction | 0.606334 (Hartree/Particle) |
| Thermal correction to Energy | 0.638491 |
| Thermal correction to Enthalpy | 0.639436 |
| Thermal correction to Gibbs Free Energy | 0.542098 |
| Sum of electronic and zero-point Energies | -4721.885706 |
| Sum of electronic and thermal Energies | -4721.853548 |
| Sum of electronic and thermal Enthalpies | -4721.852604 |
| Sum of electronic and thermal Free Energies | -4721.949942 |

| cartesian | | | | | | | |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | -0.62101316 | 1.18547797 | 2.63040280 | 1 | -2.78311324 | 2.97777796 | -0.20739710 |
| 6 | -2.04071307 | 1.19587803 | 2.58180285 | 1 | -1.37281322 | 3.16987777 | -1.25949717 |
| 6 | -2.51521325 | 0.00997794 | 3.19090295 | 1 | -1.14741325 | 2.83397794 | 0.45960289 |
| 6 | -1.38591325 | -0.72762209 | 3.64660287 | 1 | -2.41051316 | -0.24542207 | -2.30199718 |
| 6 | -0.22101320 | 0.00397794 | 3.31410289 | 1 | -1.95311320 | 1.34797800 | -2.87159705 |
| 1 | 0.79608679 | -0.28152207 | 3.54920292 | 1 | -3.90641332 | -2.39892220 | 1.79190290 |
| 1 | 0.04408678 | 1.96137798 | 2.26840305 | 1 | -3.55461335 | -0.26152205 | 3.32670283 |
| 1 | -2.65911317 | 1.97687805 | 2.15540290 | 13 | 1.51678681 | -0.28472206 | 0.12930287 |
| 1 | -1.41411328 | -1.66462207 | 4.18800259 | 6 | 2.53508687 | 1.04847801 | 1.15160286 |
| 6 | -1.65671325 | -2.41412210 | -0.68199718 | 6 | 2.23518682 | -1.42202199 | -1.29199708 |
| 6 | -2.94141316 | -2.05152202 | -0.18899715 | 1 | 3.58818674 | 0.72517794 | 1.14800286 |
| 6 | -3.04081321 | -2.50112224 | 1.14970291 | 6 | 2.48448682 | 2.48647785 | 0.59350288 |
| 6 | -1.81891322 | -3.14412212 | 1.48820293 | 1 | 2.24978685 | 1.05807793 | 2.21260285 |
| 6 | -0.97281325 | -3.10542226 | 0.35020289 | 6 | 3.62088680 | -1.99492204 | -0.92949712 |
| 1 | 0.01958680 | -3.53232217 | 0.28020287 | 1 | 1.55178678 | -2.26022220 | -1.50679708 |
| 1 | -1.27831316 | -2.24102211 | -1.68199706 | 1 | 2.30838680 | -0.85692209 | -2.23279715 |
| 1 | -3.71961331 | -1.53962207 | -0.74439716 | 6 | 3.02858686 | 2.53707790 | -0.83809710 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|------------|-------------|-------------|
| 1 | -1.58881319 | -3.62112212 | 2.43250299 | 6 | 3.25688672 | 3.46047783 | 1.48760283 |
| 40 | -1.26751316 | -0.73322207 | 1.14770293 | 1 | 1.43588674 | 2.82697797 | 0.56900287 |
| 1 | 0.57128680 | -1.25842202 | 1.22630286 | 6 | 4.15998697 | -2.90212226 | -2.03809714 |
| 1 | -4.05241299 | 2.32197785 | -2.01899719 | 6 | 3.56058669 | -2.75522208 | 0.39900288 |
| 6 | -2.49341321 | 0.82417792 | -2.07339716 | 1 | 4.32048702 | -1.15692210 | -0.80839717 |
| 6 | -3.96661329 | 1.23327804 | -2.08949709 | 1 | 5.15928698 | -3.27762222 | -1.79819703 |
| 6 | -4.67581320 | 0.74977791 | -3.35419703 | 1 | 4.21778679 | -2.36842203 | -2.99069715 |
| 1 | -4.47281313 | 0.82537788 | -1.20289707 | 1 | 3.49948668 | -3.76562214 | -2.17589712 |
| 1 | -5.72201300 | 1.06107795 | -3.36409712 | 1 | 2.99808669 | 3.55217791 | -1.24379706 |
| 1 | -4.64871311 | -0.34162205 | -3.42969704 | 1 | 2.46828675 | 1.89127791 | -1.52779710 |
| 1 | -4.19681311 | 1.15717793 | -4.24849701 | 1 | 4.07088709 | 2.20027781 | -0.85689712 |
| 6 | -0.34651321 | 0.52757794 | -0.73249710 | 1 | 3.19848680 | 4.48507786 | 1.10820293 |
| 6 | -1.76511323 | 1.11597800 | -0.74999714 | 1 | 4.31348705 | 3.17577791 | 1.53040290 |
| 6 | -1.77371323 | 2.61097789 | -0.40789711 | 1 | 2.86788678 | 3.45317793 | 2.51040292 |
| 1 | 0.33538678 | 1.39267802 | -0.77279711 | 1 | 4.52658701 | -3.19792223 | 0.65770292 |
| 1 | -0.18891320 | -0.04982206 | -1.64929712 | 1 | 2.82868671 | -3.57052207 | 0.33890289 |
| 1 | -2.46761322 | 0.64797789 | 0.01860288 | 1 | 3.27208686 | -2.10542202 | 1.23790288 |

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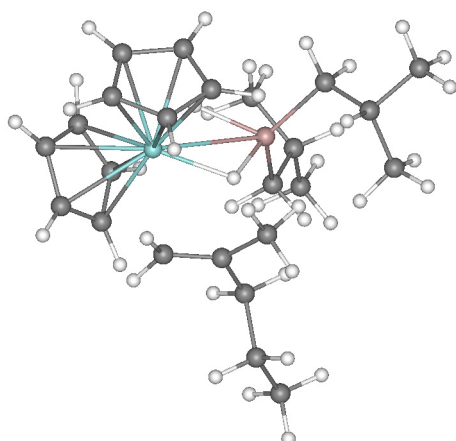


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1580072.3 (Joules/Mol) |
| | 377.64633 (Kcal/Mol) |
| Zero-point correction | 0.601818 (Hartree/Particle) |
| Thermal correction to Energy | 0.633588 |
| Thermal correction to Enthalpy | 0.634532 |
| Thermal correction to Gibbs Free Energy | 0.539886 |
| Sum of electronic and zero-point Energies | -4721.854443 |
| Sum of electronic and thermal Energies | -4721.822673 |
| Sum of electronic and thermal Enthalpies | -4721.821729 |
| Sum of electronic and thermal Free Energies | -4721.916374 |

cartesian

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | -2.07542920 | -2.21796179 | 1.30722070 | 6 | 1.60037065 | 2.05113816 | 0.99902058 |
| 6 | -2.81762934 | -1.42776167 | 2.23362064 | 1 | 2.36197066 | -1.46936166 | -0.37327939 |
| 6 | -4.05502939 | -1.10296166 | 1.62892067 | 6 | 2.91507077 | -1.43786168 | 1.72832060 |
| 6 | -4.06182957 | -1.63376176 | 0.31602061 | 1 | 1.22217059 | -2.28486180 | 0.68162060 |
| 6 | -2.84552932 | -2.34816194 | 0.13482061 | 6 | 2.17897081 | 2.78053808 | -0.23147939 |
| 1 | -2.57122922 | -2.91306186 | -0.74457937 | 1 | 0.91337067 | 2.72013807 | 1.53372061 |
| 1 | -1.09842932 | -2.65116191 | 1.48612070 | 1 | 2.43277073 | 1.88093829 | 1.70352066 |
| 1 | -2.50442934 | -1.16226172 | 3.23572063 | 6 | 3.71427059 | -2.74226189 | 1.68232071 |
| 1 | -4.85772943 | -0.53766179 | 2.08432055 | 6 | 2.24907064 | -1.26556170 | 3.09742069 |
| 1 | -4.87172937 | -1.56036174 | -0.39937943 | 1 | 3.61747074 | -0.60586178 | 1.58302069 |
| 6 | -3.33482933 | 1.89063823 | 1.79352069 | 6 | 3.09397078 | 1.85803831 | -1.04127932 |
| 6 | -3.97352934 | 1.93993831 | 0.52072060 | 6 | 2.93387079 | 4.04633808 | 0.18392061 |
| 6 | -3.03122926 | 2.42493820 | -0.41687942 | 1 | 1.34807062 | 3.09323812 | -0.87997943 |
| 6 | -1.80062938 | 2.63013816 | 0.25772062 | 1 | 3.54117060 | 2.37693810 | -1.89407945 |
| 6 | -2.00162935 | 2.31753826 | 1.63182068 | 1 | 2.55887079 | 0.98223823 | -1.43547940 |
| 1 | -1.26372933 | 2.40103817 | 2.41892076 | 1 | 3.91077089 | 1.48283827 | -0.41317940 |
| 1 | -3.79272914 | 1.59523833 | 2.72862077 | 1 | 4.49437094 | -2.76016188 | 2.44912076 |
| 1 | -5.01022911 | 1.70173824 | 0.31512061 | 1 | 4.19227076 | -2.87656188 | 0.70812058 |
| 1 | -3.23392916 | 2.62693810 | -1.45987940 | 1 | 3.05277085 | -3.59866190 | 1.85462070 |
| 1 | -0.88292933 | 3.01663828 | -0.17127939 | 1 | 2.97247076 | -1.34496176 | 3.91342068 |
| 40 | -2.25522923 | 0.13513824 | 0.36082059 | 1 | 1.48547077 | -2.03746176 | 3.25222063 |
| 6 | -0.52242929 | 1.47813833 | -2.67097926 | 1 | 1.76057076 | -0.28516176 | 3.20502067 |
| 6 | -0.96062928 | 0.11593823 | -2.16267943 | 1 | 3.29677081 | 4.59793806 | -0.68847942 |
| 6 | -2.35592937 | -0.14036176 | -2.06837940 | 1 | 3.79957056 | 3.78613806 | 0.80232060 |
| 6 | 0.01557070 | -0.98186177 | -2.57307935 | 1 | 2.29407072 | 4.71433830 | 0.76712060 |
| 6 | -0.23582929 | -2.39846182 | -2.07377934 | 1 | 0.51067072 | 1.70453823 | -2.39617944 |
| 1 | 1.03347063 | -0.67226177 | -2.30567932 | 1 | -1.17172933 | 2.28733826 | -2.33837938 |
| 1 | -0.01782930 | -0.98016173 | -3.67177939 | 1 | -0.57582927 | 1.43863833 | -3.76447940 |
| 1 | -0.47362930 | 0.23853824 | -0.71687943 | 6 | 0.87167066 | -3.35416174 | -2.51987934 |
| 1 | -2.68712926 | -1.15826166 | -2.24797940 | 1 | -1.19542933 | -2.76346183 | -2.45577931 |
| 1 | -3.02542925 | 0.62403822 | -2.45237923 | 1 | -0.29772928 | -2.39566183 | -0.97887939 |
| 1 | -0.66822928 | 0.08883823 | 1.52492070 | 1 | 0.68007070 | -4.36876202 | -2.16517925 |
| 13 | 0.83107072 | 0.26843822 | 0.72542059 | 1 | 1.84277081 | -3.03936195 | -2.12787938 |
| 6 | 1.85857081 | -1.39136171 | 0.60072058 | 1 | 0.94297069 | -3.38716173 | -3.61047935 |

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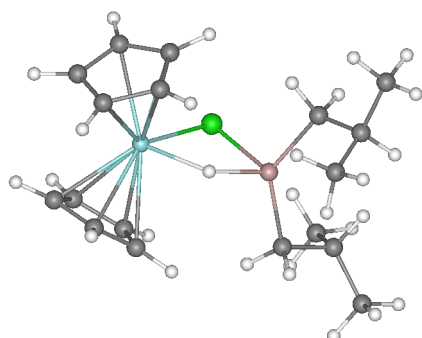
| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1579373.0 (Joules/Mol) |
| | 377.47920 (Kcal/Mol) |
| Zero-point correction | 0.601551 (Hartree/Particle) |
| Thermal correction to Energy | 0.633967 |
| Thermal correction to Enthalpy | 0.634911 |
| Thermal correction to Gibbs Free Energy | 0.536965 |
| Sum of electronic and zero-point Energies | -4721.867363 |
| Sum of electronic and thermal Energies | -4721.834948 |
| Sum of electronic and thermal Enthalpies | -4721.834003 |
| Sum of electronic and thermal Free Energies | -4721.931949 |

| cartesian | | | | | | | |
|-----------|------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | 3.63226628 | -0.11810585 | 1.98063087 | 1 | 0.33316630 | 2.15319419 | 1.63293087 |
| 6 | 3.91916633 | -1.44790590 | 1.60383093 | 6 | -1.07463360 | 4.49129438 | 1.99563098 |
| 6 | 2.75856638 | -2.23060584 | 1.82583094 | 1 | -0.17423373 | 4.73259401 | 0.05063094 |
| 6 | 1.76996636 | -1.38910592 | 2.41013098 | 1 | 0.99206626 | 4.55089426 | 1.35273087 |
| 6 | 2.29656625 | -0.08580586 | 2.49143100 | 1 | -1.14113379 | 5.56279421 | 2.19323111 |
| 1 | 1.79216623 | 0.77639419 | 2.91053104 | 1 | -0.88233370 | 3.98599434 | 2.94623113 |
| 1 | 4.32716608 | 0.71169418 | 1.94383097 | 1 | -2.04813361 | 4.15629435 | 1.62723088 |
| 1 | 4.85746622 | -1.80330586 | 1.19693089 | 13 | -0.86703366 | -1.03900588 | -0.12396906 |
| 1 | 2.65196633 | -3.29180574 | 1.63753092 | 6 | -1.88453364 | -0.78800583 | 1.53073096 |
| 1 | 0.78156626 | -1.70230591 | 2.72083116 | 6 | -1.63583374 | -1.52480590 | -1.86386907 |
| 6 | 3.08996630 | -0.07580586 | -2.25926900 | 1 | -2.45203376 | 0.15179415 | 1.44833088 |
| 6 | 3.99066639 | -0.94670582 | -1.60356903 | 6 | -2.86353374 | -1.94930589 | 1.80293095 |
| 6 | 3.34176636 | -2.20540595 | -1.44956911 | 1 | -1.23473382 | -0.65150583 | 2.40853095 |
| 6 | 2.04396629 | -2.10010576 | -2.00216913 | 6 | -2.06423354 | -0.32230586 | -2.73276901 |
| 6 | 1.87476635 | -0.77160585 | -2.48356891 | 1 | -0.98093373 | -2.18330574 | -2.45046902 |
| 1 | 0.99256629 | -0.38410586 | -2.97926903 | 1 | -2.53443360 | -2.12780595 | -1.65696907 |
| 1 | 3.30746627 | 0.94119412 | -2.55606890 | 6 | -3.66723347 | -1.71810591 | 3.08483100 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 5.00836658 | -0.71100587 | -1.31736910 | 6 | -2.11623359 | -3.28410578 | 1.87523091 |
| 1 | 3.77496624 | -3.09720588 | -1.01466906 | 1 | -3.57313347 | -2.00490594 | 0.96633095 |
| 1 | 1.31156635 | -2.89410567 | -2.05926895 | 6 | -2.90583372 | 0.67259419 | -1.92826903 |
| 40 | 2.12746620 | -0.60810584 | 0.02253094 | 6 | -2.82573366 | -0.78040582 | -3.97956896 |
| 1 | 0.67006630 | -1.88570595 | 0.10753094 | 1 | -1.16093373 | 0.20559414 | -3.07386899 |
| 1 | 0.33396631 | 0.20039414 | -0.25916907 | 1 | -3.26063371 | 1.49929416 | -2.55086899 |
| 6 | 2.48286629 | 2.15429425 | 0.07193094 | 1 | -2.33813357 | 1.11439407 | -1.09606910 |
| 6 | 1.20196629 | 2.38839412 | -0.32066908 | 1 | -3.78353357 | 0.17669414 | -1.49726903 |
| 6 | 0.81046629 | 2.55869412 | -1.76016903 | 1 | -4.39183378 | -2.52020574 | 3.25373101 |
| 6 | 0.12666631 | 2.68089414 | 0.69563091 | 1 | -4.21333361 | -0.77170587 | 3.04213095 |
| 1 | 2.73716640 | 2.25789428 | 1.12293088 | 1 | -2.99783373 | -1.68110585 | 3.95173097 |
| 1 | 3.30656624 | 2.18709421 | -0.63726908 | 1 | -2.79203367 | -4.11680603 | 2.08913112 |
| 1 | -0.03973371 | 1.91579401 | -2.01016903 | 1 | -1.36283374 | -3.25860572 | 2.67283106 |
| 1 | 0.47936630 | 3.59209418 | -1.91156912 | 1 | -1.60073376 | -3.52270579 | 0.93373090 |
| 1 | 1.63116622 | 2.36699414 | -2.45256901 | 1 | -3.08813357 | 0.06469415 | -4.62306929 |
| 6 | 0.02726626 | 4.19179440 | 0.98063093 | 1 | -3.75373363 | -1.28500593 | -3.69016886 |
| 1 | -0.84223372 | 2.32219434 | 0.32973093 | 1 | -2.23153377 | -1.48540592 | -4.56766939 |

S3.7. ⁱBu₂AlCl reaction profile

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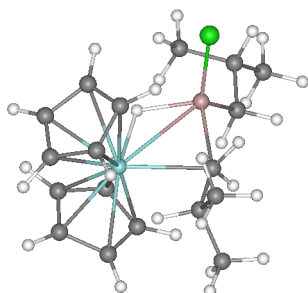


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1119848.7 (Joules/Mol) |
| | 267.65027 (Kcal/Mol) |
| Zero-point correction | 0.426528 (Hartree/Particle) |
| Thermal correction to Energy | 0.452154 |
| Thermal correction to Enthalpy | 0.453098 |
| Thermal correction to Gibbs Free Energy | 0.369347 |
| Sum of electronic and zero-point Energies | -4945.900440 |
| Sum of electronic and thermal Energies | -4945.874813 |
| Sum of electronic and thermal Enthalpies | -4945.873869 |
| Sum of electronic and thermal Free Energies | -4945.957621 |

| cartesian | | | | | | |
|-----------|-------------|-------------|-------------|---|------------|-------------|
| 6 | -3.43925595 | 1.94134998 | 1.52393806 | 6 | 1.38784409 | 1.80414999 |
| 6 | -4.44755602 | 1.54955006 | 0.60443801 | 1 | 1.36404395 | -1.83284998 |
| 6 | -3.95105600 | 1.78174996 | -0.71056199 | 6 | 2.78894401 | -1.91114998 |
| 6 | -2.63965583 | 2.30804992 | -0.59676194 | 1 | 0.71694404 | -2.51594996 |
| 6 | -2.31985593 | 2.39575005 | 0.78533804 | 6 | 2.84104395 | 1.89915001 |
| 1 | -1.38275599 | 2.74675012 | 1.20203805 | 1 | 0.78184408 | 2.54935002 |
| 1 | -3.50315595 | 1.88454998 | 2.60483813 | 1 | 1.34554410 | 2.09225011 |
| 1 | -5.43445587 | 1.18355000 | 0.86033797 | 6 | 3.31814384 | -3.30905008 |
| 1 | -4.49005604 | 1.60895002 | -1.63406193 | 6 | 2.82764411 | -1.66425002 |
| 1 | -1.99345589 | 2.59555006 | -1.41696191 | 1 | 3.45084381 | -1.17935002 |
| 6 | -4.41365576 | -1.49304998 | -0.63116205 | 6 | 3.41994381 | 3.29434991 |
| 6 | -3.39445591 | -1.45525002 | -1.61736190 | 6 | 2.91644406 | 1.54955006 |
| 6 | -2.25095582 | -2.12325001 | -1.09286201 | 1 | 3.45574379 | 1.17684996 |
| 6 | -2.55595589 | -2.54305005 | 0.22353801 | 1 | 4.45774412 | 3.35945010 |
| 6 | -3.89255595 | -2.14785004 | 0.51343799 | 1 | 3.39474392 | 3.55005002 |
| 1 | -4.42735577 | -2.33964992 | 1.43713808 | 1 | 2.84034395 | 4.04885006 |
| 1 | -5.41505575 | -1.09445000 | -0.73596203 | 1 | 4.34494400 | -3.43785000 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|------------|-------------|-------------|
| 1 | -3.48355603 | -1.03215003 | -2.61086202 | 1 | 3.30624390 | -3.49324989 | -1.20296192 |
| 1 | -1.31255591 | -2.28244996 | -1.60956192 | 1 | 2.69814396 | -4.07375002 | 0.35603800 |
| 1 | -1.88915586 | -3.06734991 | 0.89713800 | 1 | 3.82514381 | -1.84235001 | 2.12573791 |
| 40 | -2.58945584 | -0.04455002 | 0.26353800 | 1 | 2.12844396 | -2.33084989 | 2.23373795 |
| 17 | -0.79275590 | -0.36265004 | 2.05763793 | 1 | 2.55884409 | -0.62994999 | 1.97693801 |
| 1 | -0.93835592 | 0.18874997 | -0.71976197 | 1 | 3.94054413 | 1.61975002 | -2.01246190 |
| 13 | 0.62074405 | 0.02064998 | 0.15833801 | 1 | 2.29934406 | 2.24055004 | -2.22236204 |
| 6 | 1.35984397 | -1.71194994 | -0.34856197 | 1 | 2.56704402 | 0.52875000 | -1.84296203 |

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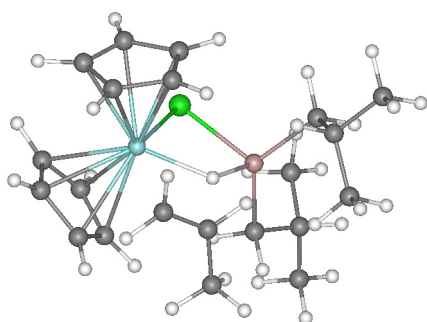


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1123566.6 (Joules/Mol) |
| | 268.53886 (Kcal/Mol) |
| Zero-point correction | 0.427944 (Hartree/Particle) |
| Thermal correction to Energy | 0.452808 |
| Thermal correction to Enthalpy | 0.453752 |
| Thermal correction to Gibbs Free Energy | 0.372702 |
| Sum of electronic and zero-point Energies | -4945.899293 |
| Sum of electronic and thermal Energies | -4945.874429 |
| Sum of electronic and thermal Enthalpies | -4945.873485 |
| Sum of electronic and thermal Free Energies | -4945.954535 |

| cartesian | | | | | | | |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | 2.06536794 | 2.21805620 | -0.67464805 | 1 | -0.41083199 | -0.32044393 | -1.98104811 |
| 6 | 2.46676803 | 2.39315605 | 0.67135197 | 13 | -1.39463198 | -0.89634395 | 0.14105196 |
| 6 | 1.29386806 | 2.49715614 | 1.46885192 | 17 | -1.63243198 | -2.79774380 | 1.04805195 |
| 6 | 0.16946800 | 2.40605617 | 0.60885197 | 6 | -2.89883208 | 0.06755607 | -0.61674798 |
| 6 | 0.64246798 | 2.21025610 | -0.71384811 | 6 | -4.13183212 | 0.09225607 | 0.31075197 |
| 1 | 0.02376799 | 2.13365626 | -1.59974802 | 1 | -2.59863210 | 1.10415602 | -0.84274805 |
| 1 | 2.73046803 | 2.12965608 | -1.52624810 | 1 | -3.17303205 | -0.37704393 | -1.58364809 |
| 1 | 3.48716784 | 2.46775627 | 1.02505195 | 6 | -5.28433228 | 0.86905599 | -0.32984802 |
| 1 | 1.26096809 | 2.66715622 | 2.53755188 | 6 | -3.77643204 | 0.68935609 | 1.67505193 |
| 1 | -0.86823207 | 2.47875619 | 0.91005194 | 1 | -4.46293211 | -0.94124389 | 0.46985197 |
| 6 | 3.28446794 | -0.47154394 | 1.99325192 | 1 | -6.17323208 | 0.85795605 | 0.30715197 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | 2.17026806 | -0.33644393 | 2.87005186 | 1 | -5.55753231 | 0.44225606 | -1.29874802 |
| 6 | 1.24626803 | -1.36644399 | 2.56685185 | 1 | -4.99803209 | 1.91455615 | -0.49064800 |
| 6 | 1.76796806 | -2.12214398 | 1.48245192 | 1 | -4.64993191 | 0.74065602 | 2.33045197 |
| 6 | 3.04006791 | -1.58114398 | 1.14925194 | 1 | -3.39123201 | 1.71045601 | 1.55905199 |
| 1 | 3.71616793 | -1.95704401 | 0.38985199 | 1 | -3.01733208 | 0.09555608 | 2.20335197 |
| 1 | 4.18116808 | 0.13515607 | 2.00025201 | 6 | 2.18596792 | -2.38904381 | -2.01574802 |
| 1 | 2.06656790 | 0.39755610 | 3.65925193 | 1 | 2.39146781 | -0.45594394 | -1.17244804 |
| 1 | 0.30706799 | -1.55824399 | 3.07065201 | 6 | 1.76946807 | -0.18504393 | -3.16684794 |
| 1 | 1.29356802 | -2.99474382 | 1.05025196 | 1 | 3.24896789 | -2.37124395 | -2.26994801 |
| 40 | 1.32876801 | 0.16855606 | 0.57785201 | 1 | 1.65386808 | -2.88494396 | -2.83224797 |
| 6 | 0.19206800 | -0.95134389 | -1.31774807 | 1 | 2.04966807 | -2.99224377 | -1.11594808 |
| 1 | -0.46293199 | 0.01225607 | 1.26645195 | 1 | 2.81416798 | -0.13234393 | -3.48494816 |
| 1 | -0.18183200 | -1.98244393 | -1.42394805 | 1 | 1.37816799 | 0.83165610 | -3.08294797 |
| 6 | 1.63546801 | -0.96724391 | -1.85404801 | 1 | 1.20226800 | -0.69824398 | -3.94814801 |

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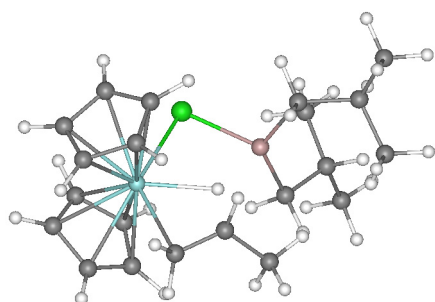
| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1340335.2 (Joules/Mol) |
| | 320.34781 (Kcal/Mol) |
| Zero-point correction | 0.510507 (Hartree/Particle) |
| Thermal correction to Energy | 0.540765 |
| Thermal correction to Enthalpy | 0.541709 |
| Thermal correction to Gibbs Free Energy | 0.448968 |
| Sum of electronic and zero-point Energies | -5063.676833 |
| Sum of electronic and thermal Energies | -5063.646575 |
| Sum of electronic and thermal Enthalpies | -5063.645631 |
| Sum of electronic and thermal Free Energies | -5063.738372 |

cartesian

| | | | | | | | |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | -2.73219657 | -2.01865935 | -1.46533215 | 1 | -1.10809660 | -0.69795930 | -3.51973224 |
| 6 | -3.74439669 | -2.04245949 | -0.48023215 | 1 | -0.66049665 | 1.80604064 | -1.72613215 |
| 6 | -3.18379664 | -2.61755943 | 0.69996786 | 13 | 1.22750330 | -0.17745931 | 0.66956782 |
| 6 | -1.83629656 | -2.94415951 | 0.42536786 | 6 | 1.79800344 | 1.61084068 | 1.23236787 |
| 6 | -1.53609669 | -2.53595924 | -0.89953220 | 6 | 2.22050333 | -1.57875931 | -0.26693216 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|------------|-------------|-------------|
| 1 | -0.58589667 | -2.66125917 | -1.40543222 | 1 | 2.89430332 | 1.61984074 | 1.33066785 |
| 1 | -2.85359669 | -1.68935931 | -2.48713207 | 6 | 1.39010334 | 2.71534061 | 0.23856786 |
| 1 | -4.77229643 | -1.72825933 | -0.61433220 | 1 | 1.41590333 | 1.84304059 | 2.23586798 |
| 1 | -3.70619655 | -2.81585932 | 1.62756777 | 6 | 3.66650343 | -1.68085933 | 0.26856786 |
| 1 | -1.14119673 | -3.39615917 | 1.11946785 | 1 | 1.72550344 | -2.55285931 | -0.12813213 |
| 6 | -2.75599670 | 1.95464075 | 0.93006790 | 1 | 2.24800348 | -1.40145934 | -1.35163212 |
| 6 | -3.94619656 | 1.19024074 | 0.73406786 | 6 | 1.96170330 | 2.42484045 | -1.15343213 |
| 6 | -4.03999662 | 0.26114067 | 1.80006778 | 6 | 1.83020329 | 4.10204077 | 0.71476781 |
| 6 | -2.89049673 | 0.39944071 | 2.60766792 | 1 | 0.28960335 | 2.72354078 | 0.16276786 |
| 6 | -2.10089660 | 1.46164072 | 2.07206798 | 6 | 4.43770361 | -2.80565929 | -0.42583212 |
| 1 | -1.15599668 | 1.81344068 | 2.46956778 | 6 | 3.66990328 | -1.88665926 | 1.78646779 |
| 1 | -2.40369678 | 2.77104092 | 0.31066787 | 1 | 4.18130350 | -0.73465931 | 0.05256785 |
| 1 | -4.68929672 | 1.33984065 | -0.03953215 | 1 | 5.47390318 | -2.85245943 | -0.07783213 |
| 1 | -4.84549665 | -0.44535932 | 1.95516777 | 1 | 4.45020342 | -2.66515923 | -1.51033223 |
| 1 | -2.65279651 | -0.18155931 | 3.48956776 | 1 | 3.96830320 | -3.77325916 | -0.21613213 |
| 40 | -2.06379676 | -0.41785932 | 0.38426787 | 1 | 1.65980339 | 3.17974091 | -1.88713217 |
| 17 | -0.15869668 | -1.09195924 | 2.24346781 | 1 | 1.64800334 | 1.44234073 | -1.53653216 |
| 1 | -0.26839668 | 0.10984069 | -0.21573213 | 1 | 3.05680346 | 2.41554070 | -1.11833215 |
| 6 | -2.58569670 | 1.07814074 | -2.12173223 | 1 | 1.51470327 | 4.88674068 | 0.01986787 |
| 6 | -1.23909664 | 1.01884067 | -2.20903206 | 1 | 2.92130327 | 4.14334059 | 0.79696786 |
| 6 | -0.46689668 | 0.05614069 | -3.05903220 | 1 | 1.41350341 | 4.33004045 | 1.69986784 |
| 1 | -3.22379661 | 0.40524065 | -2.68743229 | 1 | 4.68510342 | -2.00895929 | 2.17356777 |
| 1 | -3.07199669 | 1.93454063 | -1.67033219 | 1 | 3.09860349 | -2.78305912 | 2.05466795 |
| 1 | 0.01640332 | 0.62194067 | -3.86283207 | 1 | 3.22690344 | -1.03615928 | 2.32446790 |
| 1 | 0.32950330 | -0.43755931 | -2.49483228 | | | | |

TS-1Cl

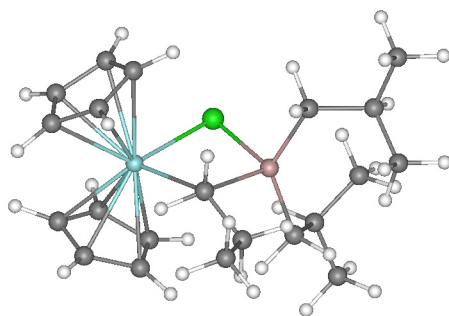


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1336885.7 (Joules/Mol) |
| | 319.52335 (Kcal/Mol) |
| Zero-point correction | 0.509193 (Hartree/Particle) |
| Thermal correction to Energy | 0.538692 |
| Thermal correction to Enthalpy | 0.539636 |
| Thermal correction to Gibbs Free Energy | 0.448350 |
| Sum of electronic and zero-point Energies | -5063.668796 |

| | |
|---|--------------|
| Sum of electronic and thermal Energies | -5063.639296 |
| Sum of electronic and thermal Enthalpies | -5063.638352 |
| Sum of electronic and thermal Free Energies | -5063.729638 |

| cartesian | | | | | | | | | |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|---|--|
| 6 | 2.57411003 | 2.25316954 | -1.02201188 | 1 | 0.16791016 | 0.80236953 | -2.84051180 | 1 | |
| 6 | 3.88921022 | 1.69696951 | -1.06941187 | | 0.79261017 | -1.95683050 | -1.58831191 | | |
| 6 | 4.39601040 | 1.67216945 | 0.24698816 | 13 | -0.93638980 | 0.10036954 | 0.49388814 | | |
| 6 | 3.39141011 | 2.17396951 | 1.11988819 | 6 | -1.64888978 | -1.70873046 | 0.71478814 | | |
| 6 | 2.28551006 | 2.56876969 | 0.32008815 | 6 | -1.70918989 | 1.73626947 | -0.24771182 | | |
| 1 | 1.36301017 | 2.99736953 | 0.68968815 | 1 | -1.47458982 | -2.00373030 | 1.76008809 | | |
| 1 | 1.92411017 | 2.43446970 | -1.86991191 | 6 | -3.14728975 | -1.86543036 | 0.37508816 | | |
| 1 | 4.42621040 | 1.39106965 | -1.95771194 | 1 | -1.08018982 | -2.43363047 | 0.10938817 | | |
| 1 | 5.38200998 | 1.33206964 | 0.53558815 | 6 | -3.08898973 | 2.00916958 | 0.39968818 | | |
| 1 | 3.47081017 | 2.28566957 | 2.19448829 | 1 | -1.04628980 | 2.58576965 | -0.02301185 | | |
| 6 | 3.02271008 | -2.44453049 | 0.25268817 | 1 | -1.81578994 | 1.71276951 | -1.33931184 | | |
| 6 | 4.24400997 | -1.73983049 | 0.41288817 | 6 | -3.64208984 | -3.26833034 | 0.73818815 | | |
| 6 | 4.20261002 | -1.09173036 | 1.67918813 | 6 | -3.41189003 | -1.57713056 | -1.10461187 | | |
| 6 | 2.94921017 | -1.35473037 | 2.26708817 | 1 | -3.72248983 | -1.14303041 | 0.97038817 | | |
| 6 | 2.20851016 | -2.18573046 | 1.37748814 | 6 | -3.63598967 | 3.37316966 | -0.02811183 | | |
| 1 | 1.21051025 | -2.57213044 | 1.55138814 | 6 | -3.01208973 | 1.91936946 | 1.92738807 | | |
| 1 | 2.75791025 | -3.07263041 | -0.58881181 | 1 | -3.79158974 | 1.24056959 | 0.05138816 | | |
| 1 | 5.08201027 | -1.74353051 | -0.27411181 | 1 | -4.63348961 | 3.54736948 | 0.38568819 | | |
| 1 | 4.99711037 | -0.50543046 | 2.12248826 | 1 | -3.70208979 | 3.44866967 | -1.11701190 | | |
| 1 | 2.60711002 | -0.99203044 | 3.22728801 | 1 | -2.97898984 | 4.17446947 | 0.32748818 | | |
| 40 | 2.49221015 | 0.04026954 | 0.21528816 | 1 | -4.71038961 | -3.37973046 | 0.53148818 | | |
| 17 | 0.53211015 | 0.61926955 | 2.10658813 | 1 | -3.47789001 | -3.48363042 | 1.79758811 | | |
| 1 | 0.64241016 | -0.30903047 | -0.54491180 | 1 | -3.10508990 | -4.02353048 | 0.15328816 | | |
| 6 | 2.41111016 | -0.68773049 | -2.16611195 | 1 | -4.46598959 | -1.72333050 | -1.35631192 | | |
| 6 | 1.05501020 | -0.96263045 | -1.95191193 | 1 | -2.82508993 | -2.25553036 | -1.73701191 | | |
| 6 | -0.02158982 | -0.26923046 | -2.75101185 | 1 | -3.15468979 | -0.54593045 | -1.37891185 | | |
| 1 | 2.64311028 | 0.13076954 | -2.84041190 | 1 | -3.97238970 | 2.16026950 | 2.39148808 | | |
| 1 | 3.12441015 | -1.50443053 | -2.15891194 | 1 | -2.26428986 | 2.61706948 | 2.32218814 | | |
| 1 | -0.00718981 | -0.70313048 | -3.75611186 | 1 | -2.74378991 | 0.91036952 | 2.27718806 | | |
| 1 | -1.01828980 | -0.42703047 | -2.33361197 | | | | | | |

I-2Cl_a

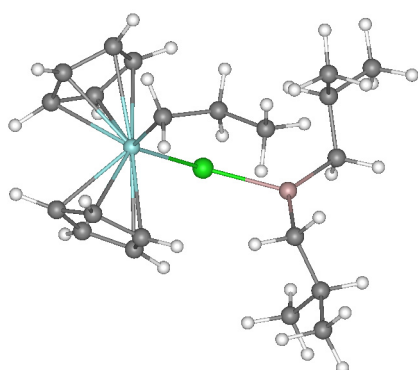


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1349531.2 (Joules/Mol) |
| | 322.54569 (Kcal/Mol) |
| Zero-point correction | 0.514009 (Hartree/Particle) |
| Thermal correction to Energy | 0.543849 |
| Thermal correction to Enthalpy | 0.544793 |
| Thermal correction to Gibbs Free Energy | 0.453673 |
| Sum of electronic and zero-point Energies | -5063.695489 |
| Sum of electronic and thermal Energies | -5063.665649 |
| Sum of electronic and thermal Enthalpies | -5063.664705 |
| Sum of electronic and thermal Free Energies | -5063.755825 |

| cartesian | | | | | | | | | | | | |
|-----------|------------|-------------|-------------|----|-------------|-------------|-------------|--|--|--|--|--|
| 6 | 3.35046101 | 2.24961877 | 0.77360332 | 1 | 1.20366096 | -1.27238142 | -3.86959672 | | | | | |
| 6 | 2.14476109 | 2.43821883 | 0.04100335 | 1 | -0.11673898 | 0.46501866 | -2.58759665 | | | | | |
| 6 | 2.31876111 | 1.87341869 | -1.23949671 | 13 | -0.75833899 | -0.04178134 | 0.25740334 | | | | | |
| 6 | 3.63526106 | 1.32781863 | -1.30799663 | 6 | -1.31753898 | 1.74061859 | -0.35539666 | | | | | |
| 6 | 4.27726126 | 1.59071863 | -0.07189667 | 6 | -1.71873903 | -1.68058133 | 0.76020336 | | | | | |
| 40 | 2.43686104 | -0.04068134 | 0.39200336 | 1 | -2.16883898 | 1.61121869 | -1.04199672 | | | | | |
| 6 | 0.73846102 | -0.90958136 | -1.11199665 | 6 | -1.75713897 | 2.70281887 | 0.76700330 | | | | | |
| 17 | 0.62086105 | 0.47061867 | 2.12980342 | 1 | -0.54403895 | 2.22621870 | -0.96949673 | | | | | |
| 6 | 2.43616104 | -2.36538124 | 1.35400331 | 6 | -3.25883889 | -1.62028134 | 0.82500339 | | | | | |
| 6 | 3.11436105 | -1.54468131 | 2.29340339 | 1 | -1.44633889 | -2.48168135 | 0.05320334 | | | | | |
| 6 | 4.30016088 | -1.06698132 | 1.68890333 | 1 | -1.32873893 | -2.01058125 | 1.73470330 | | | | | |
| 6 | 4.36846113 | -1.60618138 | 0.37060332 | 6 | -2.81183910 | 2.04851866 | 1.66400325 | | | | | |
| 6 | 3.22596097 | -2.42228127 | 0.17820334 | 6 | -2.28513908 | 4.01951885 | 0.19070333 | | | | | |
| 1 | 1.58426106 | 1.85691857 | -2.03539658 | 1 | -0.88723892 | 2.93561864 | 1.39750326 | | | | | |
| 1 | 4.08456087 | 0.84801865 | -2.16989660 | 6 | -3.83393908 | -2.95688128 | 1.30240333 | | | | | |
| 1 | 1.24266100 | 2.90651870 | 0.41730332 | 6 | -3.85213900 | -1.24828136 | -0.53599668 | | | | | |
| 1 | 3.53386092 | 2.58051872 | 1.78960335 | 1 | -3.55453920 | -0.85098135 | 1.54890335 | | | | | |
| 1 | 5.29676104 | 1.32891858 | 0.18170333 | 1 | -4.92453909 | -2.91578126 | 1.37800336 | | | | | |
| 1 | 5.03776121 | -0.42618135 | 2.15600348 | 1 | -3.43713903 | -3.23178124 | 2.28380322 | | | | | |
| 1 | 2.76616096 | -1.30508137 | 3.29030323 | 1 | -3.57573891 | -3.75578117 | 0.59790337 | | | | | |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 1.48696113 | -2.86318135 | 1.51670337 | 1 | -3.18133903 | 2.74371886 | 2.42300320 |
| 1 | 2.99026108 | -2.97778130 | -0.72169662 | 1 | -2.41393900 | 1.17341864 | 2.19570327 |
| 1 | 5.16886091 | -1.45348132 | -0.34289667 | 1 | -3.67083883 | 1.71771860 | 1.06730330 |
| 1 | 1.76166105 | -0.81248134 | -1.56789672 | 1 | -2.54973912 | 4.72451830 | 0.98440337 |
| 1 | 0.64756107 | -1.98278129 | -0.90809667 | 1 | -3.18213892 | 3.83811879 | -0.41119668 |
| 6 | -0.17413896 | -0.59608138 | -2.32789660 | 1 | -1.54143906 | 4.49771833 | -0.45439664 |
| 6 | 0.17576104 | -1.45838141 | -3.54249668 | 1 | -4.94533920 | -1.23598135 | -0.50519669 |
| 1 | -1.22643900 | -0.78588134 | -2.07019663 | 1 | -3.55253887 | -1.98078144 | -1.29639673 |
| 1 | -0.48873895 | -1.23678136 | -4.38029623 | 1 | -3.52543879 | -0.25708133 | -0.87239671 |
| 1 | 0.08106107 | -2.52158117 | -3.30649662 | | | | |

I-2Cl_bi



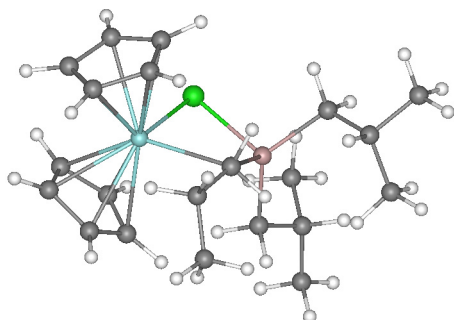
| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1346417.7 (Joules/Mol) |
| | 321.80156 (Kcal/Mol) |
| Zero-point correction | 0.512823 (Hartree/Particle) |
| Thermal correction to Energy | 0.543408 |
| Thermal correction to Enthalpy | 0.544352 |
| Thermal correction to Gibbs Free Energy | 0.447967 |
| Sum of electronic and zero-point Energies | -5063.686234 |
| Sum of electronic and thermal Energies | -5063.655649 |
| Sum of electronic and thermal Enthalpies | -5063.654705 |
| Sum of electronic and thermal Free Energies | -5063.751090 |

cartesian

| | | | | | | | |
|---|------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | 3.30522704 | -2.38622546 | -0.42100850 | 1 | 0.51762718 | 0.02107456 | -4.06690836 |
| 6 | 4.38762712 | -1.64132535 | 0.11169152 | 1 | 0.10972717 | 1.27077460 | -2.88340855 |
| 6 | 4.13512707 | -1.43922544 | 1.49589145 | 13 | -1.95447278 | -0.04112544 | 0.65519154 |
| 6 | 2.88222718 | -2.01192546 | 1.80409145 | 6 | -3.31437278 | -1.37552536 | 1.00149155 |
| 6 | 2.36642718 | -2.60022545 | 0.61239153 | 6 | -1.83767295 | 1.62387455 | -0.34270850 |
| 1 | 1.42582726 | -3.13142538 | 0.52459157 | 1 | -4.22407293 | -1.10472536 | 0.44689155 |
| 1 | 3.21162724 | -2.72172546 | -1.44530845 | 6 | -2.81967282 | -2.76172543 | 0.52909154 |
| 1 | 5.26572704 | -1.31682539 | -0.43350849 | 1 | -3.59757280 | -1.41172540 | 2.06019163 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 4.78782701 | -0.93272543 | 2.19539165 | 6 | -2.83727288 | 2.64107466 | 0.25809154 |
| 1 | 2.40372729 | -2.01532555 | 2.77579141 | 1 | -0.82017285 | 2.03837466 | -0.28220847 |
| 6 | 2.09542727 | 2.39847469 | -0.02970847 | 1 | -2.04987288 | 1.47427464 | -1.40880847 |
| 6 | 3.48022723 | 2.12857461 | -0.20720848 | 6 | -2.25087285 | -2.67572546 | -0.89210856 |
| 6 | 3.98942709 | 1.64867461 | 1.02009153 | 6 | -3.94197273 | -3.80012536 | 0.59449148 |
| 6 | 2.92142701 | 1.62017465 | 1.96529150 | 1 | -2.01377296 | -3.08642530 | 1.19929147 |
| 6 | 1.76432729 | 2.11197472 | 1.31639147 | 6 | -2.70617294 | 4.00647449 | -0.41940847 |
| 1 | 0.78702718 | 2.21857452 | 1.77059150 | 6 | -2.63407278 | 2.76907468 | 1.77109146 |
| 1 | 1.42412710 | 2.78857470 | -0.78630853 | 1 | -3.85487270 | 2.26987457 | 0.08179152 |
| 1 | 4.04752731 | 2.27387452 | -1.11660850 | 1 | -3.43557310 | 4.71857452 | -0.02350849 |
| 1 | 5.01972723 | 1.37807465 | 1.21229148 | 1 | -2.86107278 | 3.92707467 | -1.49860847 |
| 1 | 2.98972702 | 1.31557465 | 3.00249147 | 1 | -1.70557284 | 4.42027473 | -0.24960849 |
| 40 | 2.40142727 | -0.10842544 | 0.25269154 | 1 | -1.93617296 | -3.65332532 | -1.26840854 |
| 17 | -0.03487283 | -0.61232543 | 1.62549150 | 1 | -1.35787272 | -2.02622557 | -0.94250846 |
| 1 | 0.51012719 | -0.32752544 | -1.04740846 | 1 | -2.99597287 | -2.27372551 | -1.58870852 |
| 6 | 2.47012711 | -0.02462544 | -2.01100850 | 1 | -3.58407307 | -4.79112530 | 0.30039153 |
| 6 | 1.02682722 | -0.51002544 | -2.03690839 | 1 | -4.75937271 | -3.52152538 | -0.07890847 |
| 6 | 0.12772718 | 0.19177458 | -3.06110859 | 1 | -4.34967279 | -3.87252545 | 1.60579145 |
| 1 | 0.97252715 | -1.59622538 | -2.15890861 | 1 | -3.32417297 | 3.49077463 | 2.21559167 |
| 1 | 3.14532709 | -0.68692547 | -2.55030847 | 1 | -1.61447287 | 3.10187459 | 1.99869144 |
| 1 | 2.54652715 | 0.97867459 | -2.43190861 | 1 | -2.80367279 | 1.81717455 | 2.30149150 |
| 1 | -0.89887279 | -0.18502544 | -3.02170849 | | | | |

I-2Cl_bo

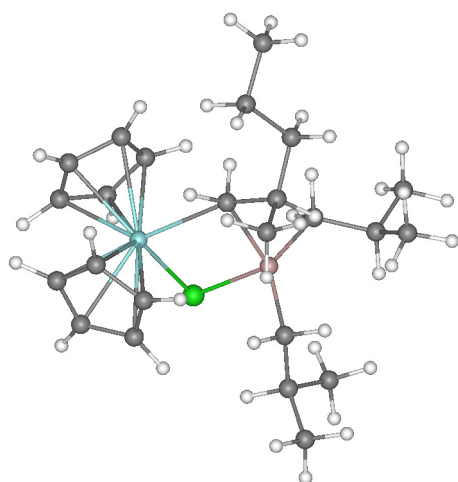


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1352452.8 (Joules/Mol) |
| | 323.24398 (Kcal/Mol) |
| Zero-point correction | 0.515122 (Hartree/Particle) |
| Thermal correction to Energy | 0.544525 |
| Thermal correction to Enthalpy | 0.545469 |
| Thermal correction to Gibbs Free Energy | 0.456382 |
| Sum of electronic and zero-point Energies | -5063.694252 |
| Sum of electronic and thermal Energies | -5063.664850 |
| Sum of electronic and thermal Enthalpies | -5063.663906 |

cartesian

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | -3.17361522 | 2.33361530 | 0.42350847 | 1 | -5.26801491 | -0.01598477 | 1.55290842 |
| 6 | -4.29541540 | 1.48011518 | 0.20600849 | 1 | -1.81921506 | 0.27441522 | -3.98609138 |
| 6 | -4.48141527 | 0.70811522 | 1.38380849 | 13 | 0.93698484 | -0.00478477 | 0.60560846 |
| 6 | -3.45001507 | 1.03361523 | 2.29050851 | 6 | 1.95848489 | 1.58131528 | 1.11830842 |
| 6 | -2.64431524 | 2.04931521 | 1.69560850 | 6 | 1.59038496 | -1.70478475 | -0.11519152 |
| 1 | -1.76971507 | 2.50421524 | 2.14450860 | 1 | 2.75758481 | 1.25531518 | 1.80290842 |
| 1 | -2.78781509 | 3.06431532 | -0.27669153 | 6 | 2.60808492 | 2.38681531 | -0.02639151 |
| 1 | -4.93441534 | 1.47551525 | -0.66909146 | 1 | 1.32208490 | 2.24421525 | 1.72340846 |
| 1 | -3.30031514 | 0.60161525 | 3.27240849 | 6 | 2.96218491 | -2.08068466 | 0.48990849 |
| 6 | -1.74521518 | -2.20498466 | -0.87349153 | 1 | 0.89878482 | -2.53488469 | 0.09340848 |
| 6 | -2.98171520 | -1.76318479 | -1.42659152 | 1 | 1.67818499 | -1.65298474 | -1.21199155 |
| 6 | -3.96151519 | -1.80648482 | -0.41019151 | 6 | 3.52668476 | 1.50441527 | -0.87629151 |
| 6 | -3.33811522 | -2.28408480 | 0.77890849 | 6 | 3.38748503 | 3.58691525 | 0.51960850 |
| 6 | -1.98181510 | -2.55548477 | 0.47730848 | 1 | 1.81718493 | 2.78011513 | -0.68149149 |
| 1 | -1.24481511 | -2.93318486 | 1.17410851 | 6 | 3.50548506 | -3.36868477 | -0.13299152 |
| 1 | -0.80741519 | -2.32188487 | -1.40129149 | 6 | 2.85758495 | -2.22428489 | 2.01100850 |
| 1 | -3.14931512 | -1.46648479 | -2.45549154 | 1 | 3.67498493 | -1.27428472 | 0.27260849 |
| 1 | -3.82221508 | -2.45148468 | 1.73360848 | 1 | 4.49028492 | -3.62178469 | 0.27050850 |
| 40 | -2.33271527 | -0.05058476 | 0.31790850 | 1 | 3.59878492 | -3.27418470 | -1.21869159 |
| 17 | -0.58261514 | -0.40178478 | 2.28170848 | 1 | 2.83098483 | -4.20658493 | 0.07660848 |
| 6 | -1.03671515 | 0.31511524 | -3.22489142 | 1 | 4.00218487 | 2.07671523 | -1.67799151 |
| 6 | -0.48901516 | 1.03431523 | -0.81779158 | 1 | 2.99058485 | 0.66721523 | -1.34489155 |
| 6 | -1.49971509 | 1.07491529 | -1.98259151 | 1 | 4.32258511 | 1.07671523 | -0.25609151 |
| 1 | -1.72741508 | 2.11321521 | -2.23799133 | 1 | 3.81898499 | 4.18501520 | -0.28879151 |
| 1 | -0.37501517 | 2.03651524 | -0.39369151 | 1 | 4.20698500 | 3.24571514 | 1.16100848 |
| 1 | 0.46718484 | 0.81821525 | -1.32159150 | 1 | 2.74398494 | 4.23771524 | 1.11860847 |
| 1 | -2.52991509 | 0.68631524 | -1.74419153 | 1 | 3.81318474 | -2.52228475 | 2.45100856 |
| 1 | -0.73261517 | -0.70578480 | -2.98159146 | 1 | 2.11608481 | -2.98838472 | 2.27390862 |
| 1 | -0.17241517 | 0.82281524 | -3.65989137 | 1 | 2.55658484 | -1.28808475 | 2.49980855 |
| 1 | -5.00601530 | -1.54638481 | -0.52709150 | | | | |

I-4Cl_a

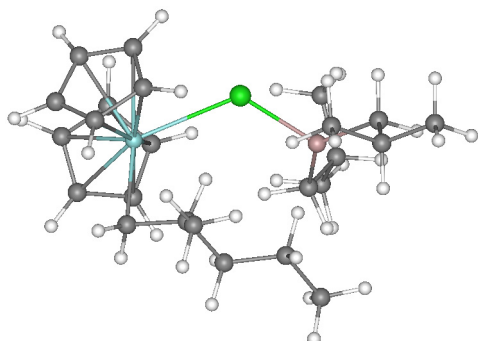


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1575613.1 (Joules/Mol) |
| | 376.58058 (Kcal/Mol) |
| Zero-point correction | 0.600119 (Hartree/Particle) |
| Thermal correction to Energy | 0.633129 |
| Thermal correction to Enthalpy | 0.634073 |
| Thermal correction to Gibbs Free Energy | 0.535962 |
| Sum of electronic and zero-point Energies | -5181.495563 |
| Sum of electronic and thermal Energies | -5181.462553 |
| Sum of electronic and thermal Enthalpies | -5181.461609 |
| Sum of electronic and thermal Free Energies | -5181.559720 |

| | | | | cartesian | | | | |
|----|------------|-------------|-------------|-----------|-------------|-------------|-------------|--|
| 6 | 3.32843232 | -2.84297204 | 0.51105881 | 6 | 0.96963227 | 3.73372769 | 1.25485873 | |
| 6 | 2.10603237 | -2.62567210 | 1.20745873 | 6 | 0.91613233 | 5.23652840 | 0.97635877 | |
| 6 | 2.22683239 | -1.42707205 | 1.93865883 | 1 | 1.78653240 | 3.28922796 | 0.66965878 | |
| 6 | 3.52733231 | -0.89037204 | 1.69945884 | 1 | 1.21513224 | 3.56842804 | 2.30955887 | |
| 6 | 4.21413231 | -1.78757203 | 0.84425879 | 1 | 1.86133218 | 5.72282839 | 1.22675884 | |
| 40 | 2.36283231 | -0.77877206 | -0.49574119 | 1 | 0.12863231 | 5.71252823 | 1.56675875 | |
| 6 | 0.62873226 | 0.82742798 | 0.12955879 | 1 | 0.70393229 | 5.43182802 | -0.07864121 | |
| 17 | 0.56383228 | -2.22937202 | -1.59724116 | 13 | -0.83526772 | -0.69117200 | -0.39614120 | |
| 6 | 2.40373230 | 0.56382799 | -2.62994099 | 6 | -1.41436768 | -1.80257213 | 1.11955881 | |
| 6 | 3.02293229 | -0.67597204 | -2.93104100 | 6 | -1.78886771 | 0.26942798 | -1.82454121 | |
| 6 | 4.21143246 | -0.77387202 | -2.16984105 | 1 | -2.24476767 | -1.29207206 | 1.63335884 | |
| 6 | 4.34313250 | 0.42372796 | -1.40724123 | 6 | -1.89196777 | -3.21907210 | 0.73405880 | |
| 6 | 3.23273230 | 1.25072789 | -1.70634127 | 1 | -0.62896770 | -1.89277208 | 1.88335884 | |
| 1 | 1.46993232 | -0.99077201 | 2.57615900 | 6 | -3.33126783 | 0.25802794 | -1.81534123 | |
| 1 | 3.93643212 | 0.01352796 | 2.13665891 | 1 | -1.46566772 | 1.32412791 | -1.80684125 | |
| 1 | 1.22903228 | -3.26017213 | 1.15945876 | 1 | -1.43306780 | -0.12397204 | -2.78824115 | |
| 1 | 3.55153227 | -3.68607211 | -0.13264120 | 6 | -2.95606780 | -3.16267204 | -0.36424118 | |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 5.23453236 | -1.68197203 | 0.49875879 | 6 | -2.42096782 | -3.97227216 | 1.95745885 |
| 1 | 4.90993214 | -1.60157204 | -2.18574119 | 1 | -1.03596783 | -3.78207207 | 0.33615881 |
| 1 | 2.63393211 | -1.42827213 | -3.60524106 | 6 | -3.88536787 | 1.03432798 | -3.01344109 |
| 1 | 1.46923232 | 0.92192793 | -3.04624104 | 6 | -3.88226795 | 0.83872795 | -0.51074117 |
| 1 | 3.04603219 | 2.23302794 | -1.28764117 | 1 | -3.67806768 | -0.77847207 | -1.89924121 |
| 1 | 5.16383219 | 0.67612791 | -0.74724120 | 1 | -4.97866774 | 1.00072789 | -3.03864121 |
| 1 | 1.61313224 | 0.99322796 | 0.64585876 | 1 | -3.51276779 | 0.62532794 | -3.95684099 |
| 1 | 0.66453230 | 1.47052789 | -0.75614125 | 1 | -3.58256769 | 2.08632803 | -2.95924115 |
| 6 | -0.37126774 | 1.52012789 | 1.11965883 | 1 | -3.35166788 | -4.15687180 | -0.59054118 |
| 6 | -0.35336769 | 3.04662800 | 0.91395879 | 1 | -2.55606771 | -2.75367212 | -1.30154121 |
| 6 | -0.12716770 | 1.13942790 | 2.58115888 | 1 | -3.79686785 | -2.53107214 | -0.05174120 |
| 1 | -1.40356779 | 1.21792793 | 0.88025880 | 1 | -2.71086788 | -4.99547195 | 1.70085883 |
| 1 | -0.75596768 | 1.75032783 | 3.23485899 | 1 | -3.30196786 | -3.46547198 | 2.36615896 |
| 1 | 0.91463232 | 1.31372797 | 2.87325883 | 1 | -1.66766787 | -4.02257204 | 2.75005889 |
| 1 | -0.37796772 | 0.09472796 | 2.77725887 | 1 | -4.97526789 | 0.87732792 | -0.52084118 |
| 1 | -1.14796782 | 3.48202801 | 1.53225875 | 1 | -3.51786757 | 1.86392784 | -0.36424118 |
| 1 | -0.62096769 | 3.26682782 | -0.12784120 | 1 | -3.58676767 | 0.24352798 | 0.36215878 |

I-4Cl_bi



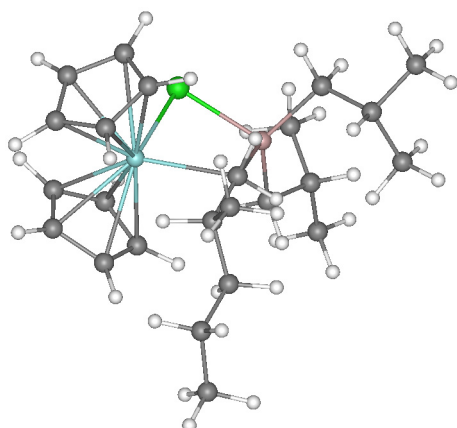
| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1571825.7 (Joules/Mol) |
| | 375.67536 (Kcal/Mol) |
| Zero-point correction | 0.598677 (Hartree/Particle) |
| Thermal correction to Energy | 0.633010 |
| Thermal correction to Enthalpy | 0.633954 |
| Thermal correction to Gibbs Free Energy | 0.530101 |
| Sum of electronic and zero-point Energies | -5181.490555 |
| Sum of electronic and thermal Energies | -5181.456222 |
| Sum of electronic and thermal Enthalpies | -5181.455278 |
| Sum of electronic and thermal Free Energies | -5181.559131 |

cartesian

| | | | | | | | |
|---|-------------|------------|------------|---|------------|-------------|-------------|
| 6 | -3.87484121 | 1.96721029 | 0.72251761 | 6 | 1.99545884 | -2.08998966 | -0.41958237 |
|---|-------------|------------|------------|---|------------|-------------|-------------|

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | -4.74384117 | 0.88931030 | 1.01711762 | 1 | 4.14845896 | 0.31941026 | 1.32691765 |
| 6 | -4.22964144 | 0.21281029 | 2.15951777 | 6 | 3.10615897 | 2.19811034 | 0.99951762 |
| 6 | -3.02954102 | 0.84621024 | 2.53921771 | 1 | 2.99005890 | 0.72491026 | 2.57971764 |
| 6 | -2.79644108 | 1.92691040 | 1.63951766 | 6 | 2.71475887 | -3.22388959 | 0.35441762 |
| 1 | -1.95894122 | 2.61481023 | 1.68011761 | 1 | 0.99335879 | -2.43038964 | -0.71858239 |
| 1 | -4.02764130 | 2.69491029 | -0.06118236 | 1 | 2.53715897 | -1.88198972 | -1.34948242 |
| 1 | -5.66034126 | 0.65291029 | 0.49081761 | 6 | 4.23205900 | 3.00521040 | 1.65301764 |
| 1 | -4.68064117 | -0.63998973 | 2.65081763 | 6 | 1.75425887 | 2.85901022 | 1.28571761 |
| 1 | -2.39054108 | 0.55781025 | 3.36471772 | 1 | 3.27395892 | 2.21251035 | -0.08608235 |
| 6 | -2.20364118 | -2.24978971 | -1.16318238 | 6 | 2.59215879 | -4.55538988 | -0.38878238 |
| 6 | -3.59874105 | -1.97068965 | -1.20618236 | 6 | 2.17955899 | -3.35318971 | 1.78471756 |
| 6 | -4.11924124 | -2.16398978 | 0.09321763 | 1 | 3.77905893 | -2.96628976 | 0.41771764 |
| 6 | -3.04744101 | -2.55168962 | 0.94911760 | 1 | 3.14835882 | -5.34818983 | 0.11951763 |
| 6 | -1.87724113 | -2.63348961 | 0.15701763 | 1 | 2.97415900 | -4.47299004 | -1.40968239 |
| 1 | -0.89634115 | -2.91538978 | 0.51761764 | 1 | 1.54175901 | -4.86379004 | -0.44478238 |
| 1 | -1.52394116 | -2.21398973 | -2.00598216 | 1 | 4.24365902 | 4.03591013 | 1.28681767 |
| 1 | -4.16454124 | -1.67508972 | -2.07968235 | 1 | 5.20925903 | 2.56071043 | 1.44651759 |
| 1 | -5.15634108 | -2.05308962 | 0.38301763 | 1 | 4.09745884 | 3.03381038 | 2.73941779 |
| 1 | -3.11984110 | -2.79178977 | 2.00251770 | 1 | 1.75685883 | 3.90721011 | 0.97141761 |
| 40 | -2.60894108 | -0.18618971 | 0.28241763 | 1 | 1.53305888 | 2.83091044 | 2.35901785 |
| 17 | -0.15214115 | -0.28928971 | 1.64891768 | 1 | 0.92405885 | 2.36011028 | 0.76751763 |
| 1 | -0.92584115 | 1.21361029 | -0.41558236 | 1 | 2.65525889 | -4.17809010 | 2.32181764 |
| 6 | -2.64974117 | 0.84571028 | -1.74148238 | 1 | 1.09825873 | -3.53508973 | 1.78811765 |
| 6 | -1.27824116 | 1.46231031 | -1.46278238 | 1 | 2.36775899 | -2.44948959 | 2.38761783 |
| 6 | -0.18804115 | 0.87901026 | -2.37768221 | 1 | -1.48144114 | 3.33961034 | -2.50728226 |
| 6 | -1.29834116 | 2.99641037 | -1.48438239 | 1 | -0.35654116 | 3.42861032 | -1.13648236 |
| 1 | -3.41494107 | 1.59441030 | -1.94478238 | 1 | -2.09474111 | 3.39381027 | -0.85128236 |
| 1 | -2.60854101 | 0.15131028 | -2.58218217 | 6 | 2.28395891 | 0.65681028 | -2.93998218 |
| 6 | 1.24015880 | 1.27321029 | -2.01258230 | 1 | 1.43325901 | 0.97031027 | -0.96458232 |
| 1 | -0.40024114 | 1.19721031 | -3.40638232 | 1 | 1.35745883 | 2.36161041 | -1.99698246 |
| 1 | -0.26114115 | -0.21728972 | -2.37518215 | 1 | 3.30035901 | 0.85301030 | -2.58838224 |
| 13 | 1.87245893 | -0.51458973 | 0.71301764 | 1 | 2.19115901 | 1.08071029 | -3.94338226 |
| 6 | 3.14295888 | 0.73171026 | 1.48971760 | 1 | 2.15045881 | -0.42498970 | -3.02588224 |

I-4Cl_bo

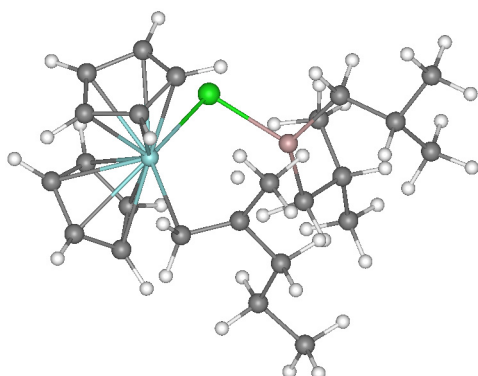


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1577004.0 (Joules/Mol) |
| | 376.91300 (Kcal/Mol) |
| Zero-point correction | 0.600649 (Hartree/Particle) |
| Thermal correction to Energy | 0.634267 |
| Thermal correction to Enthalpy | 0.635211 |
| Thermal correction to Gibbs Free Energy | 0.535875 |
| Sum of electronic and zero-point Energies | -5181.496412 |
| Sum of electronic and thermal Energies | -5181.462794 |
| Sum of electronic and thermal Enthalpies | -5181.461850 |
| Sum of electronic and thermal Free Energies | -5181.561186 |

| | | | | cartesian | | | |
|---|------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 6 | 2.40123534 | -1.30292070 | -2.57488370 | 1 | 2.73113537 | 2.70547938 | -1.91708374 |
| 6 | 3.59213543 | -0.84212065 | -1.93868375 | 1 | 1.00143540 | 2.75747943 | -2.30178380 |
| 6 | 4.10023546 | -1.90062070 | -1.14988375 | 1 | 1.97873545 | 1.38247931 | -2.81768370 |
| 6 | 3.21613550 | -3.00622058 | -1.27278376 | 1 | 0.89123535 | 1.92807937 | 1.33911622 |
| 6 | 2.18913531 | -2.63952065 | -2.18038368 | 1 | 0.32313538 | 3.03647923 | 0.11121619 |
| 1 | 1.36463547 | -3.26732063 | -2.48978376 | 1 | 4.64543533 | -1.01242065 | 1.59521627 |
| 1 | 1.79133534 | -0.75262070 | -3.27878380 | 1 | 5.01643562 | -1.88062072 | -0.57548380 |
| 1 | 4.05103540 | 0.13167930 | -2.06678367 | 13 | -1.36046457 | -0.95142066 | -0.15488382 |
| 1 | 3.33423543 | -3.97652078 | -0.80588382 | 6 | -2.39816451 | -0.91972065 | -1.81258380 |
| 6 | 1.41543531 | -0.52532071 | 2.30001616 | 6 | -1.96446466 | -0.58292067 | 1.67241621 |
| 6 | 2.70593548 | -0.00492066 | 2.00591636 | 1 | -3.31146455 | -1.51272070 | -1.64598370 |
| 6 | 3.58593535 | -1.09032071 | 1.79891622 | 6 | -2.82036448 | 0.46797931 | -2.33798385 |
| 6 | 2.84483552 | -2.29422069 | 1.97851634 | 1 | -1.84816456 | -1.46112061 | -2.59678364 |
| 6 | 1.51763535 | -1.93862069 | 2.31441617 | 6 | -3.43736458 | -1.00602067 | 1.87411630 |
| 1 | 0.71123540 | -2.63142061 | 2.51591635 | 1 | -1.36056471 | -1.12922072 | 2.41301632 |
| 1 | 0.52923536 | 0.04837930 | 2.54001617 | 1 | -1.85686445 | 0.48497933 | 1.92001629 |
| 1 | 2.97763538 | 1.04317927 | 1.96761620 | 6 | -3.60446453 | 1.24897933 | -1.27928376 |
| 1 | 3.23753548 | -3.30162072 | 1.91591620 | 6 | -3.64866447 | 0.34357929 | -3.62038374 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 40 | 1.92933536 | -1.20922065 | -0.08418381 | 1 | -1.91856456 | 1.04667926 | -2.58528376 |
| 17 | -0.13566458 | -2.89152074 | -0.14308381 | 6 | -3.92786455 | -0.64552069 | 3.27841616 |
| 1 | 2.47853541 | 4.10077953 | -0.10858381 | 6 | -3.60916471 | -2.50622082 | 1.61801624 |
| 6 | 1.19403541 | 2.44487929 | 0.42121619 | 1 | -4.06086445 | -0.46382070 | 1.15081620 |
| 6 | 2.36123538 | 3.39117932 | 0.71581620 | 1 | -4.98046446 | -0.91102070 | 3.41371632 |
| 6 | 2.15233541 | 4.16107941 | 2.01981616 | 1 | -3.82176447 | 0.42597932 | 3.47111630 |
| 1 | 3.30443549 | 2.82877922 | 0.76351619 | 1 | -3.34576464 | -1.18392062 | 4.03481627 |
| 1 | 2.96783543 | 4.86357975 | 2.20071626 | 1 | -3.91396475 | 2.22967935 | -1.65208375 |
| 1 | 2.09643531 | 3.48147941 | 2.87641621 | 1 | -3.02256465 | 1.41517937 | -0.36148381 |
| 1 | 1.22003531 | 4.73157978 | 1.98861623 | 1 | -4.50976467 | 0.70017934 | -0.99648380 |
| 6 | 0.29473537 | 0.42367929 | -0.84828383 | 1 | -3.92096472 | 1.32637930 | -4.01738405 |
| 6 | 1.46743536 | 1.41307926 | -0.68518382 | 1 | -4.57396460 | -0.20722067 | -3.42088366 |
| 6 | 1.82613540 | 2.09997940 | -2.00918388 | 1 | -3.09916449 | -0.19652069 | -4.39658356 |
| 1 | 0.10163540 | 0.26557934 | -1.91368377 | 1 | -4.64016438 | -2.82512069 | 1.79511631 |
| 1 | -0.57116467 | 0.99887931 | -0.47698382 | 1 | -2.96106458 | -3.08692074 | 2.28511620 |
| 1 | 2.43613529 | 0.91697931 | -0.36478382 | 1 | -3.35946465 | -2.78682065 | 0.58631617 |

TS-4Cl

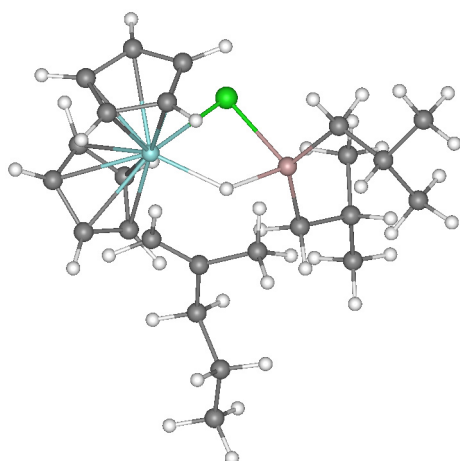


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1565700.3 (Joules/Mol) |
| | 374.21135 (Kcal/Mol) |
| Zero-point correction | 0.596344 (Hartree/Particle) |
| Thermal correction to Energy | 0.629335 |
| Thermal correction to Enthalpy | 0.630279 |
| Thermal correction to Gibbs Free Energy | 0.533415 |
| Sum of electronic and zero-point Energies | -5181.470810 |
| Sum of electronic and thermal Energies | -5181.437819 |
| Sum of electronic and thermal Enthalpies | -5181.436874 |
| Sum of electronic and thermal Free Energies | -5181.533738 |

| cartesian | | | | | | | |
|-----------|-------------|-------------|-------------|---|------------|-------------|------------|
| 6 | -2.60541773 | -2.37368989 | -0.70739561 | 6 | 1.80268228 | -1.57938969 | 0.44980437 |
| 6 | -3.93871784 | -1.87228978 | -0.68539560 | 1 | 2.05448198 | 1.89421022 | 2.15620446 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | -4.34391785 | -1.79048967 | 0.66650438 | 6 | 2.66368198 | 2.45941019 | 0.16990438 |
| 6 | -3.24841785 | -2.16718984 | 1.48200440 | 1 | 0.77038217 | 2.63131022 | 1.24750447 |
| 6 | -2.18081784 | -2.55418992 | 0.62110436 | 6 | 2.98738241 | -1.88628972 | 1.39850450 |
| 1 | -1.21131778 | -2.91308975 | 0.94320440 | 1 | 1.08358216 | -2.40968990 | 0.52000439 |
| 1 | -2.02871776 | -2.59518981 | -1.59419560 | 1 | 2.16698217 | -1.58378971 | -0.58489561 |
| 1 | -4.55011797 | -1.64398968 | -1.54979563 | 6 | 3.84888220 | 1.49991024 | 0.04010439 |
| 1 | -5.31981802 | -1.47888970 | 1.01490438 | 6 | 3.14448214 | 3.84551024 | 0.60890436 |
| 1 | -3.23331785 | -2.19878983 | 2.56450438 | 1 | 2.21928215 | 2.56541014 | -0.82909566 |
| 6 | -3.62571764 | 2.23471022 | 0.05710438 | 6 | 3.56948185 | -3.26908994 | 1.09330440 |
| 6 | -4.61051798 | 1.35161030 | 0.55240440 | 6 | 2.57728243 | -1.78968978 | 2.87080431 |
| 6 | -4.25321770 | 1.01221025 | 1.89250445 | 1 | 3.77428198 | -1.14398968 | 1.21920443 |
| 6 | -3.04761791 | 1.66941023 | 2.20030427 | 1 | 4.44438219 | -3.47858977 | 1.71570444 |
| 6 | -2.63001776 | 2.39921021 | 1.05470443 | 1 | 3.87278223 | -3.34698987 | 0.04520439 |
| 1 | -1.75021780 | 3.02841020 | 0.99450439 | 1 | 2.82368231 | -4.04788971 | 1.28780437 |
| 1 | -3.65501785 | 2.71971011 | -0.90839559 | 1 | 4.62688208 | 1.91911030 | -0.60419559 |
| 1 | -5.50541782 | 1.03981030 | 0.02790439 | 1 | 3.55218220 | 0.53511024 | -0.38969558 |
| 1 | -4.81981802 | 0.38391024 | 2.56760430 | 1 | 4.29798222 | 1.30851030 | 1.02190447 |
| 1 | -2.51691771 | 1.61141026 | 3.14060426 | 1 | 3.86868191 | 4.25801039 | -0.09939560 |
| 40 | -2.54501772 | -0.05028976 | 0.37360439 | 1 | 3.62828207 | 3.78561020 | 1.58980441 |
| 17 | -0.69881779 | -0.33408976 | 2.41840434 | 1 | 2.31008244 | 4.54861021 | 0.69010437 |
| 1 | -0.61541778 | 0.39741024 | -0.31179559 | 1 | 3.40048218 | -2.07788992 | 3.53010440 |
| 6 | -2.26191783 | 0.42491025 | -2.02789569 | 1 | 1.72838223 | -2.44958973 | 3.08510423 |
| 6 | -0.93141782 | 0.86101019 | -1.80829573 | 1 | 2.28548241 | -0.76958978 | 3.15740442 |
| 6 | 0.25138217 | 0.13351025 | -2.43409562 | 1 | 0.15498221 | 2.57581019 | -1.01329565 |
| 1 | -2.39941788 | -0.49928975 | -2.57869577 | 1 | -1.55671787 | 2.90541005 | -1.35639572 |
| 1 | -2.99931765 | 1.19011033 | -2.24869561 | 1 | -0.41001779 | 2.71431017 | -2.67929578 |
| 1 | 0.33468223 | 0.58051026 | -3.43519568 | 6 | 1.42718232 | -1.91928971 | -3.29779577 |
| 1 | 1.17538226 | 0.42291024 | -1.91249561 | 1 | -0.69881779 | -1.65928972 | -3.16699576 |
| 6 | 0.18568218 | -1.38098967 | -2.58389568 | 1 | 0.08898222 | -1.84698975 | -1.59659553 |
| 6 | -0.67811781 | 2.35171008 | -1.68079567 | 1 | 1.40388215 | -3.00898981 | -3.35809565 |
| 13 | 0.91158223 | 0.10061024 | 0.91600436 | 1 | 2.34398222 | -1.63088977 | -2.77559566 |
| 6 | 1.60118210 | 1.91751027 | 1.14950442 | 1 | 1.48898208 | -1.52648973 | -4.31639576 |

I-5Cl



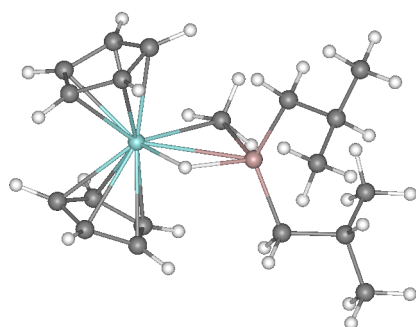
| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1567247.8 (Joules/Mol) |
| | 374.58121 (Kcal/Mol) |
| Zero-point correction | 0.596933 (Hartree/Particle) |
| Thermal correction to Energy | 0.631370 |
| Thermal correction to Enthalpy | 0.632314 |
| Thermal correction to Gibbs Free Energy | 0.529704 |
| Sum of electronic and zero-point Energies | -5181.483996 |
| Sum of electronic and thermal Energies | -5181.449559 |
| Sum of electronic and thermal Enthalpies | -5181.448615 |
| Sum of electronic and thermal Free Energies | -5181.551225 |

| cartesian | | | | | | | | | |
|-----------|------------|-------------|-------------|---|-------------|------------|-------------|--|--|
| 6 | 3.29454541 | 1.48925149 | 1.28334713 | 6 | -0.08085442 | 1.01095152 | -2.36625290 | | |
| 6 | 4.23164558 | 0.46655157 | 1.53904712 | 6 | 0.63854557 | 2.72735167 | -0.62605286 | | |
| 6 | 3.62964559 | -0.46114841 | 2.44024706 | 1 | 3.14754558 | 1.87585163 | -1.40565288 | | |
| 6 | 2.33524561 | 0.01895159 | 2.75204706 | 1 | 2.56084561 | 0.63265157 | -2.64045286 | | |
| 6 | 2.10484552 | 1.20105159 | 2.00994730 | 1 | -1.00215435 | 0.93675160 | -1.77815282 | | |
| 1 | 1.20884562 | 1.80765152 | 2.04474711 | 1 | -0.29955447 | 1.66335154 | -3.21965265 | | |
| 1 | 3.47234559 | 2.36345148 | 0.67224717 | 1 | 0.17994556 | 0.02275157 | -2.75195265 | | |
| 1 | 5.24054527 | 0.42195156 | 1.14954710 | 6 | -0.05635446 | 3.88885164 | -1.36325288 | | |
| 1 | 4.09594584 | -1.34674847 | 2.85474730 | 1 | -0.05905443 | 2.32395148 | 0.12084714 | | |
| 1 | 1.62644553 | -0.45904842 | 3.41444731 | 1 | 1.51334548 | 3.11765146 | -0.09675285 | | |
| 6 | 2.70564556 | -1.91074848 | -1.87565291 | 6 | -0.37835449 | 5.03265142 | -0.40325284 | | |
| 6 | 3.96854544 | -1.35824847 | -1.49355292 | 1 | -0.97895449 | 3.52995157 | -1.82865298 | | |
| 6 | 4.39624548 | -2.03004837 | -0.32515287 | 1 | 0.59344554 | 4.24465132 | -2.16965294 | | |
| 6 | 3.38294554 | -2.94004846 | 0.05754714 | 1 | -0.88425440 | 5.84745169 | -0.92435288 | | |
| 6 | 2.35394549 | -2.88574839 | -0.92685282 | 1 | 0.53194559 | 5.43785143 | 0.04694714 | | |
| 1 | 1.44654560 | -3.47554851 | -0.91925287 | 1 | -1.03335452 | 4.69295168 | 0.40424713 | | |
| 1 | 2.12444568 | -1.64434850 | -2.74995279 | 6 | -3.54525471 | 0.75595152 | 3.35344696 | | |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 1 | 4.53384542 | -0.61024845 | -2.03585291 | 6 | -2.79175448 | -1.61914849 | 3.00824690 |
| 1 | 5.32954550 | -1.86474848 | 0.19724713 | 1 | -3.82525444 | -0.40644842 | 1.57904708 |
| 1 | 3.39664555 | -3.59354854 | 0.92114711 | 6 | -3.13085461 | -2.84264851 | -2.89455271 |
| 40 | 2.36754560 | -0.66074842 | 0.30214715 | 1 | -2.07945442 | -0.99764836 | -2.66225290 |
| 17 | 0.61774558 | -2.29924846 | 1.62374711 | 6 | -3.76125431 | -0.97514844 | -1.33755291 |
| 1 | 0.50594556 | -0.23564842 | -0.14955285 | 1 | -4.47835445 | 0.42705157 | 3.82044697 |
| 13 | -0.91445440 | -1.06314838 | 0.43304715 | 1 | -3.72585440 | 1.72715163 | 2.88364697 |
| 6 | -1.59785461 | -2.25294828 | -0.96995282 | 1 | -2.80375457 | 0.89795160 | 4.14784718 |
| 6 | -1.76955462 | 0.24215159 | 1.62044716 | 1 | -3.66895437 | -1.95314848 | 3.56944704 |
| 6 | -2.59925461 | -1.71114850 | -2.00955296 | 1 | -1.95075440 | -1.55384851 | 3.70924711 |
| 1 | -0.75245446 | -2.72634840 | -1.49175286 | 1 | -2.55825448 | -2.40854836 | 2.28074694 |
| 1 | -2.08615446 | -3.08124852 | -0.42905289 | 1 | -4.50485468 | -0.64954841 | -2.07075310 |
| 6 | -3.04095459 | -0.26784843 | 2.33294725 | 1 | -3.42595434 | -0.08444841 | -0.79115289 |
| 1 | -1.03325438 | 0.52805161 | 2.39114714 | 1 | -4.26735449 | -1.63414848 | -0.62155288 |
| 1 | -2.00745440 | 1.17025161 | 1.07874715 | 1 | -3.81035471 | -2.46234846 | -3.66325283 |
| 6 | 2.32914567 | 1.28115153 | -1.80135286 | 1 | -3.68175459 | -3.57034850 | -2.28885269 |
| 6 | 1.03504562 | 1.62495160 | -1.56665289 | 1 | -2.31515455 | -3.37314844 | -3.39455271 |

S3.8. ⁱBu₂AlMe reaction profile

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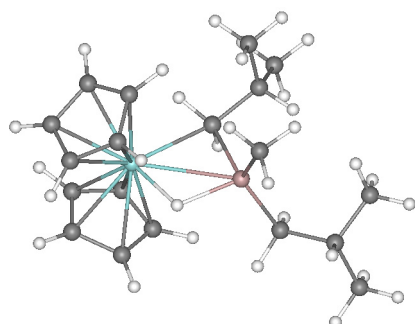


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1209895.9 (Joules/Mol) |
| | 289.17207 (Kcal/Mol) |
| Zero-point correction | 0.460825 (Hartree/Particle) |
| Thermal correction to Energy | 0.486866 |
| Thermal correction to Enthalpy | 0.487810 |
| Thermal correction to Gibbs Free Energy | 0.403556 |
| Sum of electronic and zero-point Energies | -4525.543269 |
| Sum of electronic and thermal Energies | -4525.517228 |
| Sum of electronic and thermal Enthalpies | -4525.516284 |
| Sum of electronic and thermal Free Energies | -4525.600538 |

| cartesian | | | | | |
|-----------|-------------|-------------|-------------|---|------------------------------------|
| 6 | -3.38580179 | 1.90520573 | 1.37410378 | 6 | 1.36719811 -1.69039428 -0.40929621 |
| 6 | -4.36060190 | 1.51810563 | 0.41930377 | 6 | 1.37989795 1.78040564 0.29200378 |
| 6 | -3.83450174 | 1.78890562 | -0.87529624 | 1 | 1.34979808 -1.84479427 -1.49849617 |
| 6 | -2.53860188 | 2.34410572 | -0.71509624 | 6 | 2.81989813 -1.81909430 0.09710379 |
| 6 | -2.25630188 | 2.40360570 | 0.67600381 | 1 | 0.77939808 -2.52229428 0.01380379 |
| 1 | -1.34530199 | 2.78450561 | 1.12200379 | 6 | 2.78319788 1.90980566 -0.33489621 |
| 1 | -3.48820210 | 1.83650565 | 2.45140386 | 1 | 0.73569798 2.55670571 -0.15349621 |
| 1 | -5.34420204 | 1.12150562 | 0.63930380 | 1 | 1.43349802 2.02680564 1.36330378 |
| 1 | -4.34590197 | 1.62600565 | -1.81639624 | 6 | 3.40479803 -3.19439435 -0.23449621 |
| 1 | -1.88060200 | 2.67150569 | -1.51019621 | 6 | 2.89839792 -1.55549431 1.60380375 |
| 6 | -4.24540186 | -1.57829428 | -0.71859622 | 1 | 3.43069792 -1.06309438 -0.41349620 |
| 6 | -3.24500179 | -1.55619431 | -1.72419620 | 6 | 3.35699797 3.31280565 -0.12039621 |
| 6 | -2.07340193 | -2.16479445 | -1.19279623 | 6 | 2.74289799 1.57240570 -1.82809615 |
| 6 | -2.34070206 | -2.53019428 | 0.14740379 | 1 | 3.45269823 1.19410563 0.16020378 |
| 6 | -3.68550205 | -2.16179442 | 0.44520378 | 1 | 4.36529827 3.39980578 -0.53549623 |
| 1 | -4.20330191 | -2.33609438 | 1.38190377 | 1 | 3.40619802 3.56160569 0.94340378 |
| 1 | -5.25910187 | -1.21149433 | -0.82199621 | 1 | 2.72529793 4.06090546 -0.61269623 |
| 1 | -3.36240196 | -1.17899430 | -2.73319602 | 1 | 4.44769812 -3.27159429 0.08680379 |
| 1 | -1.14140201 | -2.32269430 | -1.72089624 | 1 | 3.36639833 -3.39089441 -1.30939627 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|------------|-------------|-------------|
| 1 | -1.65190196 | -3.02349424 | 0.82260376 | 1 | 2.83759785 | -3.98269439 | 0.27310380 |
| 40 | -2.44640207 | -0.03129431 | 0.08350379 | 1 | 3.91719818 | -1.67579436 | 1.98220384 |
| 6 | -0.80440199 | -0.23319432 | 1.79000378 | 1 | 2.26039791 | -2.26139426 | 2.15100384 |
| 1 | -0.88380194 | 0.23170570 | -1.00559616 | 1 | 2.58109808 | -0.53559434 | 1.86580384 |
| 1 | -0.15010196 | -1.05879438 | 2.10480380 | 1 | 3.72789812 | 1.67630565 | -2.29179621 |
| 1 | -1.77720201 | -0.55639434 | 2.23500395 | 1 | 2.05669785 | 2.24770570 | -2.35369611 |
| 1 | -0.52360195 | 0.65090567 | 2.37090397 | 1 | 2.40809822 | 0.54210567 | -2.01079607 |
| 13 | 0.53869808 | 0.02720569 | 0.04480379 | | | | |

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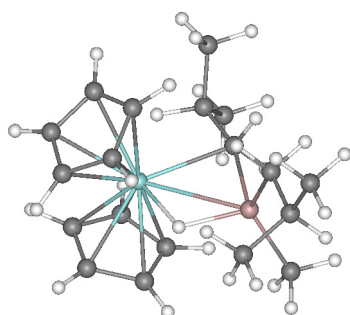


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1212783.3 (Joules/Mol) |
| | 289.86216 (Kcal/Mol) |
| Zero-point correction | 0.461925 (Hartree/Particle) |
| Thermal correction to Energy | 0.487740 |
| Thermal correction to Enthalpy | 0.488684 |
| Thermal correction to Gibbs Free Energy | 0.406455 |
| Sum of electronic and zero-point Energies | -4525.542068 |
| Sum of electronic and thermal Energies | -4525.516252 |
| Sum of electronic and thermal Enthalpies | -4525.515308 |
| Sum of electronic and thermal Free Energies | -4525.597537 |

| | | | | cartesian | | | |
|---|------------|-------------|-------------|-----------|-------------|-------------|-------------|
| 6 | 3.55746412 | 1.63991702 | 0.10151130 | 6 | -2.00773597 | -1.39618301 | 0.35551131 |
| 6 | 4.31506443 | 0.56221700 | 0.61941129 | 6 | -1.05133581 | 1.43671703 | 2.16981125 |
| 6 | 3.71206403 | 0.14921699 | 1.83881128 | 1 | -1.58143592 | -2.35128307 | 0.70151132 |
| 6 | 2.59846425 | 0.99461693 | 2.08751106 | 6 | -3.43903613 | -1.25858295 | 0.91631132 |
| 6 | 2.49266410 | 1.90681696 | 1.00921130 | 1 | -2.07713580 | -1.49178302 | -0.74118870 |
| 1 | 1.75886416 | 2.69551706 | 0.91021127 | 1 | -0.17153585 | 2.04201698 | 2.41371107 |
| 1 | 3.76956415 | 2.18541694 | -0.81138873 | 1 | -1.84583592 | 2.13361692 | 1.87921131 |
| 1 | 5.20396423 | 0.13511698 | 0.17201129 | 6 | -4.27533579 | -2.50038290 | 0.59591132 |
| 1 | 4.06576443 | -0.64028299 | 2.49071121 | 6 | -4.12413549 | -0.00438301 | 0.36811128 |
| 1 | 1.94936419 | 0.95111698 | 2.95281124 | 1 | -3.38163590 | -1.16308296 | 2.00871134 |
| 6 | 3.41796422 | -1.98158300 | -1.29168868 | 1 | -5.28363562 | -2.42048287 | 1.01271129 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | 3.27526402 | -2.55648303 | 0.00201130 | 1 | -3.81363606 | -3.40558290 | 1.00051129 |
| 6 | 1.90906405 | -2.87718296 | 0.19241129 | 1 | -4.36863565 | -2.62568307 | -0.48878872 |
| 6 | 1.20276415 | -2.50598288 | -0.98518872 | 1 | -5.15593576 | 0.07371698 | 0.72171128 |
| 6 | 2.13576412 | -1.96648300 | -1.90238869 | 1 | -4.15063572 | -0.03118301 | -0.72848868 |
| 1 | 1.91316414 | -1.59938300 | -2.89798880 | 1 | -3.60803580 | 0.91331702 | 0.67481130 |
| 1 | 4.34496403 | -1.66068292 | -1.75098872 | 6 | -1.19593573 | 1.81111705 | -2.81128883 |
| 1 | 4.07506418 | -2.73318291 | 0.71021128 | 6 | -0.37943584 | 3.10141706 | -0.80548871 |
| 1 | 1.47606421 | -3.33708286 | 1.07171130 | 1 | -1.80923581 | 1.50601709 | -0.80248868 |
| 1 | 0.13876414 | -2.63228297 | -1.14848876 | 1 | -1.94023585 | 2.58771706 | -3.00488853 |
| 40 | 2.07086420 | -0.37298301 | 0.04341129 | 1 | -1.59623599 | 0.86021692 | -3.17318869 |
| 6 | 0.16666415 | 0.60741699 | -1.05608869 | 1 | -0.29843587 | 2.05081701 | -3.39168882 |
| 1 | 0.76936418 | -0.76498300 | 1.38291132 | 1 | -1.10773587 | 3.87971711 | -1.04658866 |
| 1 | -0.10373586 | -0.21618301 | -1.72648871 | 1 | 0.56706417 | 3.37591696 | -1.28728867 |
| 1 | 1.12566423 | 1.02931702 | -1.46528876 | 1 | -0.24083585 | 3.10911703 | 0.27771130 |
| 6 | -0.86313587 | 1.74531698 | -1.31648874 | 1 | -1.38483596 | 0.97651702 | 3.10871124 |
| 13 | -0.75623578 | 0.03341699 | 0.84401131 | | | | |

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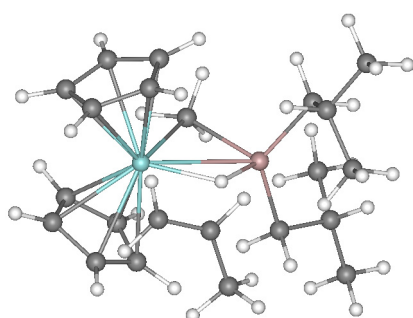


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1212997.1 (Joules/Mol) |
| | 289.91326 (Kcal/Mol) |
| Zero-point correction | 0.462006 (Hartree/Particle) |
| Thermal correction to Energy | 0.487794 |
| Thermal correction to Enthalpy | 0.488738 |
| Thermal correction to Gibbs Free Energy | 0.406857 |
| Sum of electronic and zero-point Energies | -4525.551292 |
| Sum of electronic and thermal Energies | -4525.525504 |
| Sum of electronic and thermal Enthalpies | -4525.524560 |
| Sum of electronic and thermal Free Energies | -4525.606441 |

| cartesian | | | | | | | |
|-----------|------------|-------------|------------|---|-------------|------------|-------------|
| 6 | 1.72263396 | -1.61271322 | 2.13605475 | 6 | -1.41226602 | 1.69148684 | -2.32694530 |
| 6 | 2.24903393 | -2.54761314 | 1.21355462 | 6 | -2.73966599 | 0.25968680 | 0.52695471 |
| 6 | 1.16863394 | -3.04921341 | 0.43475473 | 1 | -2.06626606 | 1.18358684 | -3.04584527 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | -0.02216601 | -2.42771339 | 0.88535476 | 1 | -0.46176600 | 1.87738669 | -2.83894539 |
| 6 | 0.31973398 | -1.51811326 | 1.92135477 | 6 | -4.01106596 | -0.14761320 | -0.24814527 |
| 1 | -0.37906605 | -0.90941322 | 2.48255467 | 1 | -2.49326611 | -0.54021323 | 1.24285483 |
| 1 | 2.29353380 | -1.07591319 | 2.88475466 | 1 | -2.96226597 | 1.14358675 | 1.14285469 |
| 1 | 3.28443408 | -2.85641336 | 1.14415479 | 6 | -5.19256592 | -0.37841320 | 0.69725472 |
| 1 | 1.23793399 | -3.80521297 | -0.33704528 | 6 | -3.75396585 | -1.39931321 | -1.09184527 |
| 1 | -1.01966608 | -2.61321306 | 0.50715470 | 1 | -4.27946615 | 0.67078680 | -0.92944527 |
| 6 | 3.46073389 | -1.15031314 | -1.49574518 | 1 | -6.09996605 | -0.64121318 | 0.14565472 |
| 6 | 2.35023403 | -1.58381319 | -2.27214527 | 1 | -5.40446615 | 0.51548678 | 1.29025483 |
| 6 | 1.61533403 | -0.43661320 | -2.66514540 | 1 | -4.96996593 | -1.19751322 | 1.39015484 |
| 6 | 2.24783397 | 0.70348680 | -2.10624528 | 1 | -4.64606619 | -1.70211315 | -1.64694524 |
| 6 | 3.39993405 | 0.25988680 | -1.39734530 | 1 | -3.46566606 | -2.24031305 | -0.44894528 |
| 1 | 4.11953402 | 0.88948679 | -0.88674527 | 1 | -2.95306611 | -1.24851322 | -1.82964516 |
| 1 | 4.23533392 | -1.78301322 | -1.08144522 | 6 | 2.59473395 | 2.82398701 | 0.72965473 |
| 1 | 2.12813401 | -2.60551310 | -2.55364537 | 1 | 2.45973396 | 0.74778682 | 1.09135485 |
| 1 | 0.73013401 | -0.42981321 | -3.28824544 | 6 | 1.60293400 | 1.71758676 | 2.76265478 |
| 1 | 1.93593395 | 1.73078680 | -2.24904537 | 1 | 3.58723402 | 2.83458662 | 1.18845463 |
| 40 | 1.40003395 | -0.63571322 | -0.16224527 | 1 | 2.08743382 | 3.75478697 | 0.99785477 |
| 6 | 0.41843396 | 1.50058675 | 0.51125473 | 1 | 2.71343398 | 2.80948687 | -0.35574529 |
| 1 | -0.30966604 | -0.75771320 | -1.01324534 | 1 | 2.57413387 | 1.68668675 | 3.26425457 |
| 1 | 0.33023399 | 2.34628677 | -0.18314527 | 1 | 0.98153400 | 0.90938675 | 3.15475464 |
| 6 | 1.76613402 | 1.63878679 | 1.23965478 | 1 | 1.11953402 | 2.66428661 | 3.01935458 |
| 1 | -0.36776602 | 1.60238683 | 1.27095461 | 1 | -1.87186599 | 2.66958666 | -2.14264536 |
| 13 | -1.25266600 | 0.66138679 | -0.67934525 | | | | |

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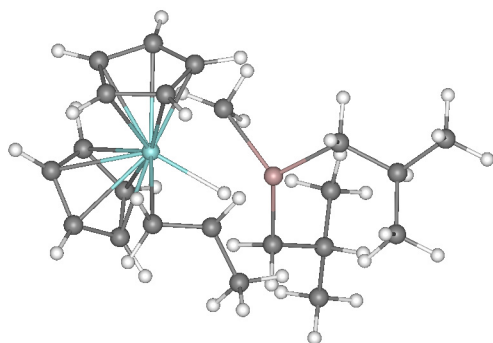


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1431865.4 (Joules/Mol) |
| | 342.22404 (Kcal/Mol) |
| Zero-point correction | 0.545369 (Hartree/Particle) |
| Thermal correction to Energy | 0.575964 |
| Thermal correction to Enthalpy | 0.576908 |
| Thermal correction to Gibbs Free Energy | 0.485519 |
| Sum of electronic and zero-point Energies | -4643.314598 |

| | |
|---|--------------|
| Sum of electronic and thermal Energies | -4643.284003 |
| Sum of electronic and thermal Enthalpies | -4643.283058 |
| Sum of electronic and thermal Free Energies | -4643.374448 |

| cartesian | | | | | | |
|-----------|-------------|-------------|-------------|----|-------------|-------------|
| 6 | -2.69293213 | -2.09581947 | -1.40069187 | 1 | 0.57376766 | -1.44681942 |
| 6 | -3.57553244 | -2.17311931 | -0.30239192 | 1 | -1.07793236 | -1.31291938 |
| 6 | -2.82423210 | -2.60671926 | 0.82900810 | 1 | -0.07723227 | 0.08578062 |
| 6 | -1.48663235 | -2.80881929 | 0.40830809 | 1 | -0.70173228 | 1.79238057 |
| 6 | -1.39063227 | -2.46041942 | -0.95989192 | 13 | 1.04066777 | -0.07851937 |
| 1 | -0.49543229 | -2.52351928 | -1.56739187 | 6 | 1.75536764 | 1.67858064 |
| 1 | -2.96973228 | -1.84051943 | -2.41369200 | 6 | 2.06016779 | -1.55231941 |
| 1 | -4.63983250 | -1.97441947 | -0.32599193 | 1 | 2.84866762 | 1.62138057 |
| 1 | -3.22023249 | -2.79691935 | 1.81990814 | 6 | 1.43336773 | 2.76278067 |
| 1 | -0.66933227 | -3.15551925 | 1.02710807 | 1 | 1.38286769 | 1.99628055 |
| 6 | -2.74803209 | 2.06588078 | 0.61200809 | 6 | 3.51116753 | -1.61001945 |
| 6 | -3.91503239 | 1.25758064 | 0.46900809 | 1 | 1.58186781 | -2.52801919 |
| 6 | -4.00533247 | 0.42538065 | 1.61180806 | 1 | 2.08596754 | -1.44781947 |
| 6 | -2.88183212 | 0.67828065 | 2.42970800 | 6 | 2.01356792 | 2.38138080 |
| 6 | -2.10773230 | 1.70348060 | 1.81180811 | 6 | 1.95006764 | 4.13958025 |
| 1 | -1.18653226 | 2.13088059 | 2.18980813 | 1 | 0.33766770 | 2.83438063 |
| 1 | -2.40203238 | 2.82948065 | -0.07439191 | 6 | 4.29886770 | -2.74891925 |
| 1 | -4.64413261 | 1.31008053 | -0.32989192 | 6 | 3.53376770 | -1.75201941 |
| 1 | -4.79403257 | -0.28741938 | 1.81790817 | 1 | 4.00726748 | -0.66431934 |
| 1 | -2.66773224 | 0.20448063 | 3.37920809 | 1 | 5.33786774 | -2.76401925 |
| 40 | -1.98033226 | -0.32391936 | 0.28390810 | 1 | 4.30246782 | -2.65281940 |
| 6 | -0.26013228 | -0.72991937 | 2.11160803 | 1 | 3.84776783 | -3.71541929 |
| 1 | -0.30183229 | 0.27508062 | -0.48169193 | 1 | 1.78256762 | 3.13008070 |
| 6 | -2.61463213 | 0.97148067 | -2.37939191 | 1 | 1.63806760 | 1.41198063 |
| 6 | -1.27263236 | 0.94338065 | -2.51429200 | 1 | 3.10436773 | 2.29638076 |
| 6 | -0.49753228 | -0.07721937 | -3.28999186 | 1 | 1.70386779 | 4.90898037 |
| 1 | -3.25093222 | 0.22498064 | -2.84569192 | 1 | 3.03916788 | 4.11508036 |
| 1 | -3.10973215 | 1.85348058 | -1.99119186 | 1 | 1.52496779 | 4.44168043 |
| 1 | -0.11033228 | 0.40158063 | -4.19579220 | 1 | 4.55456781 | -1.84151947 |
| 1 | 0.36776769 | -0.43951935 | -2.72779179 | 1 | 2.98706770 | -2.65191936 |
| 1 | -1.11493230 | -0.92381936 | -3.59669185 | 1 | 3.08126783 | -0.88721937 |

TS-1Me

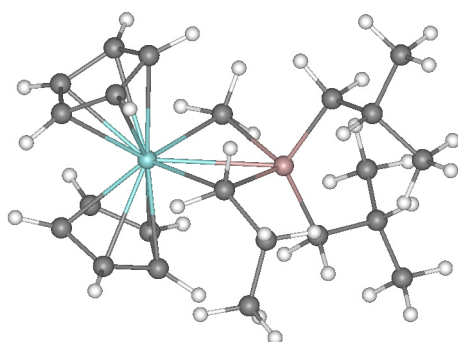


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1430503.6 (Joules/Mol) |
| | 341.89856 (Kcal/Mol) |
| Zero-point correction | 0.544850 (Hartree/Particle) |
| Thermal correction to Energy | 0.574495 |
| Thermal correction to Enthalpy | 0.575439 |
| Thermal correction to Gibbs Free Energy | 0.485963 |
| Sum of electronic and zero-point Energies | -4643.305193 |
| Sum of electronic and thermal Energies | -4643.275548 |
| Sum of electronic and thermal Enthalpies | -4643.274604 |
| Sum of electronic and thermal Free Energies | -4643.364080 |

| cartesian | | | | | | | | | | | |
|-----------|------------|-------------|-------------|----|-------------|-------------|-------------|--|--|--|--|
| 6 | 2.32494211 | -2.28705168 | 1.20394516 | 1 | 0.38244197 | -0.73685163 | 2.58134532 | | | | |
| 6 | 3.06564188 | -1.41925168 | 2.05774522 | 1 | 1.40214193 | 0.68114841 | 2.45234537 | | | | |
| 6 | 4.25264168 | -1.05385160 | 1.38774514 | 1 | 0.01304197 | -0.68405163 | -3.99355483 | | | | |
| 6 | 4.24374199 | -1.66455150 | 0.10684520 | 1 | 0.84414196 | -2.00375175 | -1.90195489 | | | | |
| 6 | 3.06354189 | -2.45085168 | 0.01394520 | 13 | -0.76095808 | -0.03725161 | 0.41474518 | | | | |
| 1 | 2.77794194 | -3.07245159 | -0.82575476 | 6 | -1.53765798 | 1.64064837 | -0.26255479 | | | | |
| 1 | 1.37494195 | -2.75535178 | 1.43444514 | 6 | -1.66175795 | -1.77195168 | 0.62854522 | | | | |
| 1 | 2.78714204 | -1.12145162 | 3.06014538 | 1 | -1.58705807 | 1.65624833 | -1.36045480 | | | | |
| 1 | 5.03374195 | -0.41815162 | 1.78484511 | 6 | -2.94945812 | 1.92134833 | 0.30454519 | | | | |
| 1 | 5.02234173 | -1.58335161 | -0.64195478 | 1 | -0.89015806 | 2.48984838 | 0.00874520 | | | | |
| 6 | 3.21364188 | 2.10254836 | 1.12144518 | 6 | -3.15345812 | -1.83345151 | 0.24174519 | | | | |
| 6 | 4.09384203 | 1.81094837 | 0.03954519 | 1 | -1.12575805 | -2.55005169 | 0.05864520 | | | | |
| 6 | 3.37354207 | 1.96444845 | -1.16195488 | 1 | -1.55295801 | -2.07445168 | 1.68164515 | | | | |
| 6 | 2.03664207 | 2.33954835 | -0.83515477 | 6 | -3.45705795 | 3.29664826 | -0.13605481 | | | | |
| 6 | 1.95894194 | 2.45974827 | 0.57204521 | 6 | -2.96485806 | 1.81274843 | 1.83194518 | | | | |
| 1 | 1.08094192 | 2.74944830 | 1.13524520 | 1 | -3.63965797 | 1.16624832 | -0.09265481 | | | | |
| 1 | 3.47584200 | 2.10304832 | 2.17294526 | 6 | -3.75745821 | -3.19505167 | 0.59734523 | | | | |
| 1 | 5.14074183 | 1.54654837 | 0.11844520 | 6 | -3.35255814 | -1.54015160 | -1.24675488 | | | | |
| 1 | 3.78614187 | 1.85524845 | -2.15475464 | 1 | -3.69565821 | -1.06785154 | 0.81344521 | | | | |
| 1 | 1.23884201 | 2.56214833 | -1.53475487 | 1 | -4.82245827 | -3.23645163 | 0.35034519 | | | | |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 40 | 2.35394192 | -0.00485160 | 0.08614519 | 1 | -3.64925814 | -3.40915155 | 1.66434515 |
| 6 | -0.00735807 | -0.27655160 | -2.97745466 | 1 | -3.25125813 | -3.99225163 | 0.04144520 |
| 6 | 1.07584190 | -0.97965163 | -2.19675469 | 1 | -4.47445822 | 3.47984838 | 0.22184519 |
| 6 | 2.42124200 | -0.63125163 | -2.34985471 | 1 | -3.45985794 | 3.38484836 | -1.22615480 |
| 1 | 0.60684198 | -0.44725162 | -0.76765478 | 1 | -2.81215811 | 4.08724833 | 0.26414520 |
| 1 | -1.00235808 | -0.45035160 | -2.56455469 | 1 | -3.94755793 | 2.05974841 | 2.24344540 |
| 1 | 0.17844194 | 0.79774839 | -3.04075480 | 1 | -2.23935795 | 2.50624824 | 2.27674532 |
| 1 | 3.17444205 | -1.41035151 | -2.35175467 | 1 | -2.72545815 | 0.79674840 | 2.17934537 |
| 1 | 2.63044190 | 0.22484839 | -2.98155475 | 1 | -4.40645790 | -1.61125159 | -1.53085482 |
| 6 | 0.53194195 | 0.18774839 | 2.01594520 | 1 | -2.79705811 | -2.26425171 | -1.85665488 |
| 1 | -0.26735806 | 0.88374841 | 2.33944535 | 1 | -3.01175809 | -0.53255159 | -1.51525486 |

I-2Me_a



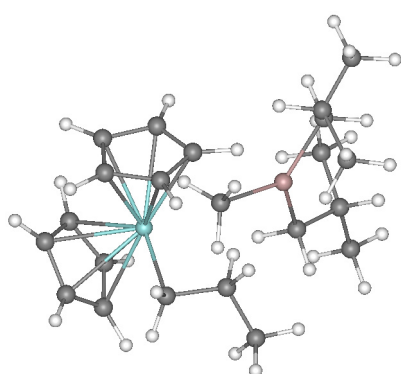
| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1441645.2 (Joules/Mol) |
| | 344.56147 (Kcal/Mol) |
| Zero-point correction | 0.549094 (Hartree/Particle) |
| Thermal correction to Energy | 0.578996 |
| Thermal correction to Enthalpy | 0.579940 |
| Thermal correction to Gibbs Free Energy | 0.490410 |
| Sum of electronic and zero-point Energies | -4643.333929 |
| Sum of electronic and thermal Energies | -4643.304027 |
| Sum of electronic and thermal Enthalpies | -4643.303083 |
| Sum of electronic and thermal Free Energies | -4643.392612 |

cartesian

| | | | | | | | |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | -3.52572870 | -2.09423542 | 0.73813713 | 1 | -0.10582894 | -0.97483546 | 2.20883703 |
| 6 | -2.18292904 | -2.47163534 | 0.46183711 | 1 | -1.72322893 | -0.53913546 | 2.44973707 |
| 6 | -1.93322897 | -2.23363543 | -0.90706289 | 1 | -0.52542889 | 0.72476453 | 2.49733710 |
| 6 | -3.12792873 | -1.72133553 | -1.49006283 | 13 | 0.61807108 | 0.06056455 | 0.26253712 |
| 6 | -4.11352873 | -1.65313542 | -0.47796288 | 6 | 1.55577099 | 1.70786452 | 0.78893709 |
| 40 | -2.36502886 | 0.02956454 | 0.14613712 | 6 | 1.48237097 | -1.68393552 | -0.04616288 |
| 6 | -0.63032889 | 0.79546452 | -1.36576283 | 1 | 2.17357111 | 1.49236453 | 1.67603719 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|------------|-------------|-------------|
| 6 | -0.81002891 | -0.17463546 | 1.94153714 | 6 | 2.45687103 | 2.39496469 | -0.25856286 |
| 6 | -2.50562906 | 2.43566465 | 0.93463707 | 1 | 0.80427110 | 2.43346477 | 1.13993716 |
| 6 | -3.27752876 | 1.67056453 | 1.84993720 | 6 | 2.74467087 | -1.92763543 | 0.81483710 |
| 6 | -4.38412905 | 1.13236451 | 1.15383720 | 1 | 0.78627110 | -2.52003527 | 0.13463712 |
| 6 | -4.30592871 | 1.57196450 | -0.19876289 | 1 | 1.77557099 | -1.77683544 | -1.10206282 |
| 6 | -3.15752888 | 2.39356470 | -0.32056287 | 6 | 3.63217115 | 1.49666452 | -0.65236288 |
| 1 | -1.00562894 | -2.43553543 | -1.42316282 | 6 | 2.97907114 | 3.73826456 | 0.26093712 |
| 1 | -3.27022886 | -1.46383548 | -2.53346300 | 1 | 1.86437118 | 2.60176468 | -1.16266286 |
| 1 | -1.47422886 | -2.87233543 | 1.17613721 | 6 | 3.39537096 | -3.26663542 | 0.45713714 |
| 1 | -4.02862883 | -2.17833543 | 1.69473720 | 6 | 2.43547106 | -1.87673545 | 2.31333709 |
| 1 | -5.13722897 | -1.32503545 | -0.60716289 | 1 | 3.46987104 | -1.13293552 | 0.59923708 |
| 1 | -5.16612911 | 0.51496452 | 1.57843721 | 1 | 4.31627083 | -3.42853546 | 1.02533710 |
| 1 | -3.05732870 | 1.52736449 | 2.90063715 | 1 | 3.64237118 | -3.31353545 | -0.60726291 |
| 1 | -1.59662890 | 2.97756457 | 1.16633713 | 1 | 2.71277094 | -4.09453583 | 0.68073708 |
| 1 | -2.83082914 | 2.89026475 | -1.22606289 | 1 | 4.26547098 | 1.97516453 | -1.40486288 |
| 1 | -5.02332926 | 1.36106455 | -0.98256296 | 1 | 3.30597115 | 0.53066450 | -1.05766284 |
| 1 | -1.62322891 | 0.66356450 | -1.87336290 | 1 | 4.25607109 | 1.28666449 | 0.22413711 |
| 1 | -0.57212889 | 1.87236452 | -1.16556287 | 1 | 3.60477114 | 4.23926449 | -0.48396286 |
| 6 | 0.37147105 | 0.50406456 | -2.52076292 | 1 | 3.58357096 | 3.58566475 | 1.16183710 |
| 6 | 0.11157107 | -0.78063548 | -3.30116296 | 1 | 2.15617085 | 4.41106462 | 0.52003711 |
| 1 | 1.40487111 | 0.49906456 | -2.15216303 | 1 | 3.31847095 | -2.12633538 | 2.90823698 |
| 1 | 0.73427105 | -0.80513549 | -4.19816256 | 1 | 1.65297115 | -2.60243535 | 2.57293701 |
| 1 | -0.93262893 | -0.84443545 | -3.62656307 | 1 | 2.10487127 | -0.88183546 | 2.63693714 |
| 1 | 0.35187113 | -1.67283547 | -2.72106290 | 1 | 0.32457107 | 1.35406458 | -3.20906305 |

I-2Me_bi

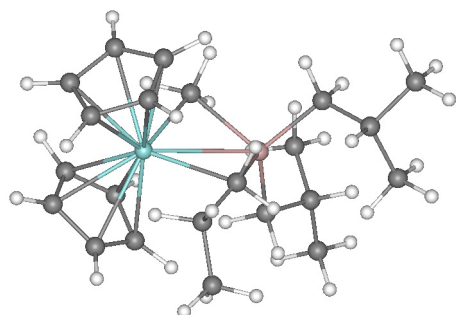


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1438065.7 (Joules/Mol) |
| | 343.70594 (Kcal/Mol) |
| Zero-point correction | 0.547730 (Hartree/Particle) |
| Thermal correction to Energy | 0.578739 |
| Thermal correction to Enthalpy | 0.579683 |
| Thermal correction to Gibbs Free Energy | 0.482591 |

| | |
|---|--------------|
| Sum of electronic and zero-point Energies | -4643.319937 |
| Sum of electronic and thermal Energies | -4643.288928 |
| Sum of electronic and thermal Enthalpies | -4643.287984 |
| Sum of electronic and thermal Free Energies | -4643.385077 |

| cartesian | | | | | | | |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | -3.63423848 | 1.96965325 | 0.01978227 | 1 | -0.20193857 | 0.61075324 | 0.11188227 |
| 6 | -4.33253860 | 1.30425322 | 1.05638230 | 1 | -0.10143858 | -1.17774677 | -0.34761775 |
| 6 | -3.42953849 | 1.11315322 | 2.13968229 | 1 | -0.14953858 | -0.67374676 | 1.40828228 |
| 6 | -2.17173862 | 1.62425327 | 1.75678229 | 1 | -2.36533856 | 1.26135325 | -2.70471764 |
| 6 | -2.29463863 | 2.14985347 | 0.43858224 | 13 | 2.14006138 | -0.18174675 | 0.35148227 |
| 1 | -1.51123857 | 2.64085340 | -0.12951772 | 6 | 2.71456146 | 1.65885329 | 0.68888223 |
| 1 | -4.05253887 | 2.28695345 | -0.92571777 | 6 | 3.19036150 | -1.76474679 | -0.08461772 |
| 1 | -5.37913895 | 1.02505326 | 1.03928232 | 1 | 3.66996169 | 1.84625328 | 0.17628227 |
| 1 | -3.66383862 | 0.65545326 | 3.09248233 | 6 | 1.68816137 | 2.72775340 | 0.26628226 |
| 1 | -1.27553856 | 1.62975323 | 2.36638236 | 1 | 2.94276142 | 1.77355325 | 1.75898230 |
| 6 | -2.83073854 | -2.87484670 | -0.09341772 | 6 | 4.71326113 | -1.60104680 | 0.09088227 |
| 6 | -4.12503862 | -2.39364672 | 0.25138226 | 1 | 2.84636140 | -2.62024665 | 0.51798224 |
| 6 | -4.07003880 | -1.91804671 | 1.57958233 | 1 | 2.96106148 | -2.04684663 | -1.12451768 |
| 6 | -2.73993850 | -2.09444666 | 2.06218219 | 6 | 1.39156151 | 2.64105344 | -1.23491764 |
| 6 | -1.99393868 | -2.71964669 | 1.03338230 | 6 | 2.16116142 | 4.13895321 | 0.62758225 |
| 1 | -0.95373857 | -3.01484656 | 1.09418225 | 1 | 0.75126141 | 2.54565334 | 0.81678224 |
| 1 | -2.54803848 | -3.31664658 | -1.04171765 | 6 | 5.45936108 | -2.85364652 | -0.37611777 |
| 1 | -4.99993896 | -2.40074658 | -0.38491774 | 6 | 5.05956125 | -1.28564680 | 1.54828227 |
| 1 | -4.90103865 | -1.50924671 | 2.14028215 | 1 | 5.04876137 | -0.75814676 | -0.52771777 |
| 1 | -2.38443851 | -1.85484672 | 3.05688238 | 1 | 6.54216146 | -2.73104668 | -0.28001773 |
| 40 | -2.63703847 | -0.35644674 | 0.26268226 | 1 | 5.23606110 | -3.08124661 | -1.42221773 |
| 6 | 0.12766141 | -0.39574674 | 0.38518226 | 1 | 5.16366148 | -3.71884656 | 0.22738227 |
| 1 | -1.44433856 | 0.33275324 | -1.58731771 | 1 | 0.66466147 | 3.39575338 | -1.55291772 |
| 6 | -3.54543853 | -0.33034673 | -1.80811763 | 1 | 0.99716145 | 1.65715325 | -1.53301764 |
| 6 | -2.24203849 | 0.22525325 | -2.37561774 | 1 | 2.30796146 | 2.80775332 | -1.81191766 |
| 6 | -1.60633850 | -0.62964672 | -3.47541761 | 1 | 1.41776156 | 4.89435339 | 0.35408229 |
| 1 | -4.41023874 | 0.29645324 | -2.01931763 | 1 | 3.09046149 | 4.37285328 | 0.09788227 |
| 1 | -3.73813844 | -1.33304679 | -2.19331765 | 1 | 2.35626149 | 4.22535324 | 1.69968235 |
| 1 | -0.65093857 | -0.21604675 | -3.80771780 | 1 | 6.13906145 | -1.18724680 | 1.69138229 |
| 1 | -2.27413869 | -0.68454677 | -4.33761787 | 1 | 4.70926142 | -2.08864665 | 2.20718241 |
| 1 | -1.43403864 | -1.65134680 | -3.12251759 | 1 | 4.60246134 | -0.34634674 | 1.88628232 |

I-2Me_bo

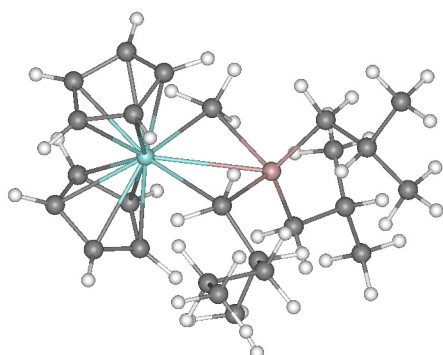


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1445477.8 (Joules/Mol) |
| | 345.47749 (Kcal/Mol) |
| Zero-point correction | 0.550553 (Hartree/Particle) |
| Thermal correction to Energy | 0.579911 |
| Thermal correction to Enthalpy | 0.580855 |
| Thermal correction to Gibbs Free Energy | 0.493244 |
| Sum of electronic and zero-point Energies | -4643.336456 |
| Sum of electronic and thermal Energies | -4643.307099 |
| Sum of electronic and thermal Enthalpies | -4643.306155 |
| Sum of electronic and thermal Free Energies | -4643.393766 |

| cartesian | | | | | | | |
|-----------|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | -3.12375951 | 2.33801627 | 0.08799675 | 1 | -1.42365956 | -0.72818387 | 2.53339672 |
| 6 | -4.23115969 | 1.44631612 | 0.09369675 | 1 | -0.37485963 | 0.66981614 | 2.60379672 |
| 6 | -4.27935982 | 0.82761616 | 1.37209678 | 1 | 0.22524035 | -0.95898384 | 2.27349687 |
| 6 | -3.18795967 | 1.30501616 | 2.13059688 | 1 | -1.92195964 | -0.06658386 | -4.16770315 |
| 6 | -2.46745968 | 2.23731613 | 1.33259678 | 13 | 0.78584039 | 0.02891614 | 0.38569674 |
| 1 | -1.58055961 | 2.78301620 | 1.63219678 | 6 | 1.83474040 | 1.60551620 | 0.91679680 |
| 1 | -2.82925963 | 2.97691607 | -0.73540330 | 6 | 1.58634043 | -1.67228389 | -0.20230326 |
| 1 | -4.94735956 | 1.31121612 | -0.70820320 | 1 | 2.61074042 | 1.28541613 | 1.63069677 |
| 1 | -2.95275950 | 1.02771616 | 3.15039682 | 6 | 2.53324032 | 2.39301610 | -0.21370324 |
| 6 | -1.67495966 | -2.26418376 | -0.86890328 | 1 | 1.19724035 | 2.29921627 | 1.48729682 |
| 6 | -2.95025969 | -1.88348389 | -1.37350321 | 6 | 2.96884036 | -1.94618380 | 0.43169674 |
| 6 | -3.86445951 | -1.86368382 | -0.29750326 | 1 | 0.94924033 | -2.54218388 | 0.02039675 |
| 6 | -3.16145968 | -2.24418378 | 0.88089681 | 1 | 1.69734049 | -1.66948378 | -1.29910326 |
| 6 | -1.81925964 | -2.51388383 | 0.51729679 | 6 | 3.48804045 | 1.50321615 | -1.01400328 |
| 1 | -1.03365970 | -2.84478378 | 1.18479681 | 6 | 3.28994036 | 3.60211611 | 0.34449676 |
| 1 | -0.76935959 | -2.40888381 | -1.44380319 | 1 | 1.77034044 | 2.77591610 | -0.90670323 |
| 1 | -3.18465972 | -1.66348386 | -2.40850329 | 6 | 3.59624052 | -3.22078395 | -0.13890325 |
| 1 | -3.58975959 | -2.35258389 | 1.87049675 | 6 | 2.86334038 | -2.04668379 | 1.95639682 |
| 40 | -2.21565962 | -0.03078386 | 0.20219675 | 1 | 3.63534021 | -1.10738385 | 0.19549675 |
| 6 | -0.57745963 | -0.24048385 | 2.03189683 | 1 | 4.59184027 | -3.39678383 | 0.27939677 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|------------|-------------|-------------|
| 6 | -1.11095965 | 0.04191614 | -3.44400311 | 1 | 3.69204044 | -3.16108394 | -1.22680318 |
| 6 | -0.47505963 | 0.98271620 | -1.13830316 | 1 | 2.97414041 | -4.09158373 | 0.09749675 |
| 6 | -1.53165960 | 0.90581614 | -2.25570321 | 1 | 3.98114061 | 2.06511617 | -1.81250322 |
| 1 | -1.77725959 | 1.91531610 | -2.59640312 | 1 | 2.97854042 | 0.64841616 | -1.47920322 |
| 1 | -0.37375963 | 2.01501608 | -0.79070330 | 1 | 4.26984024 | 1.10161614 | -0.35950324 |
| 1 | 0.47934043 | 0.74771619 | -1.63710320 | 1 | 3.76294041 | 4.18241596 | -0.45360324 |
| 1 | -2.54135966 | 0.53741616 | -1.93000317 | 1 | 4.07584047 | 3.27141619 | 1.03209674 |
| 1 | -0.79055965 | -0.95348382 | -3.12810326 | 1 | 2.62104034 | 4.26761627 | 0.89809680 |
| 1 | -0.26785964 | 0.51361614 | -3.95440340 | 1 | 3.82404041 | -2.31188393 | 2.40679669 |
| 1 | -4.91815948 | -1.62308383 | -0.36370325 | 1 | 2.14194036 | -2.82348394 | 2.24209690 |
| 1 | -5.02525949 | 0.11891615 | 1.70949674 | 1 | 2.54824042 | -1.10078382 | 2.41599679 |

I-4Me_a



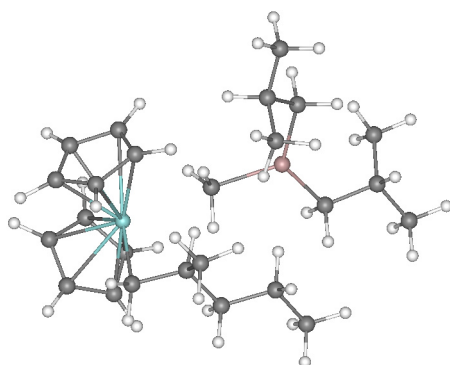
| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1668209.5 (Joules/Mol) |
| | 398.71165 (Kcal/Mol) |
| Zero-point correction | 0.635387 (Hartree/Particle) |
| Thermal correction to Energy | 0.669386 |
| Thermal correction to Enthalpy | 0.670330 |
| Thermal correction to Gibbs Free Energy | 0.571478 |
| Sum of electronic and zero-point Energies | -4761.137088 |
| Sum of electronic and thermal Energies | -4761.103090 |
| Sum of electronic and thermal Enthalpies | -4761.102145 |
| Sum of electronic and thermal Free Energies | -4761.200997 |

cartesian

| | | | | | | | |
|----|------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | 3.43406200 | -2.66643810 | 0.76999581 | 1 | 1.79796195 | 3.32066178 | 0.77989584 |
| 6 | 2.10206199 | -2.72813821 | 1.26329577 | 1 | 1.32886195 | 3.42906189 | 2.47299576 |
| 6 | 1.87066197 | -1.57763815 | 2.04739571 | 1 | 1.97166193 | 5.67136192 | 1.57789576 |
| 6 | 3.06746197 | -0.80463821 | 2.05939579 | 1 | 0.26766199 | 5.66046190 | 2.04229593 |
| 6 | 4.03526211 | -1.48683810 | 1.28619587 | 1 | 0.71696198 | 5.54986191 | 0.33789581 |
| 40 | 2.25566196 | -0.76163816 | -0.32090417 | 1 | -0.01763803 | -2.92883825 | -0.93450421 |
| 6 | 0.55136198 | 0.88356179 | 0.21849582 | 1 | 1.57916200 | -2.80543804 | -1.49140418 |

| | | | | | | | |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | 0.66796196 | -2.18913817 | -1.36750424 | 1 | 0.34266198 | -1.98053813 | -2.39250422 |
| 6 | 2.35296202 | 0.33546180 | -2.60340428 | 13 | -0.73523808 | -0.76303822 | -0.38790417 |
| 6 | 3.11006212 | -0.86223817 | -2.70550418 | 6 | -1.65523803 | 0.00166181 | -1.95020413 |
| 6 | 4.23846197 | -0.74513817 | -1.86170423 | 6 | -1.64433801 | -1.74633813 | 1.05809581 |
| 6 | 4.18856192 | 0.53496182 | -1.23890424 | 1 | -2.29873800 | -0.77233821 | -2.39970422 |
| 6 | 3.03576183 | 1.20416188 | -1.71870422 | 6 | -2.51503801 | 1.26116180 | -1.71920419 |
| 1 | 0.95386195 | -1.34583831 | 2.57009578 | 1 | -0.90373802 | 0.22466180 | -2.72440410 |
| 1 | 3.22286177 | 0.12606180 | 2.59339571 | 6 | -2.89313793 | -2.53843808 | 0.60089582 |
| 1 | 1.38576198 | -3.51673818 | 1.06909585 | 1 | -0.96483803 | -2.44623804 | 1.57369578 |
| 1 | 3.92306185 | -3.41273808 | 0.15469584 | 1 | -1.97333801 | -1.04243827 | 1.83619583 |
| 1 | 5.05656195 | -1.16863823 | 1.11919582 | 6 | -3.69643784 | 0.96776181 | -0.79050416 |
| 1 | 5.01506233 | -1.48823810 | -1.72940421 | 6 | -3.02483797 | 1.83646178 | -3.04430413 |
| 1 | 2.86506176 | -1.71603823 | -3.32500410 | 1 | -1.89173806 | 2.03416181 | -1.24510419 |
| 1 | 1.43386197 | 0.55466181 | -3.13300419 | 6 | -3.57483768 | -3.21063805 | 1.79619586 |
| 1 | 2.72416210 | 2.20336175 | -1.43890417 | 6 | -2.56363821 | -3.58273816 | -0.46870419 |
| 1 | 4.92406225 | 0.94466180 | -0.55750418 | 1 | -3.60633802 | -1.82923818 | 0.16169584 |
| 1 | 1.55966198 | 1.11556172 | 0.65599585 | 1 | -4.48903799 | -3.73093820 | 1.49509585 |
| 1 | 0.50646198 | 1.49606180 | -0.69210416 | 1 | -3.83903790 | -2.47763824 | 2.56379580 |
| 6 | -0.40983802 | 1.55716181 | 1.24589586 | 1 | -2.90313816 | -3.94723821 | 2.25159574 |
| 6 | -0.33153802 | 3.09226179 | 1.12189579 | 1 | -4.28723812 | 1.86876178 | -0.60170418 |
| 6 | -0.16193801 | 1.10606170 | 2.68699574 | 1 | -3.37963820 | 0.56846184 | 0.18109581 |
| 1 | -1.44683802 | 1.29246187 | 0.99299586 | 1 | -4.36013794 | 0.22416180 | -1.24670422 |
| 1 | -0.72693801 | 1.73706174 | 3.37889576 | 1 | -3.62503767 | 2.73756194 | -2.88440418 |
| 1 | 0.89596200 | 1.18796182 | 2.95989585 | 1 | -3.65163803 | 1.10066175 | -3.55950427 |
| 1 | -0.48443806 | 0.07746181 | 2.85619593 | 1 | -2.19633818 | 2.09556198 | -3.71030426 |
| 1 | -1.08933806 | 3.52236176 | 1.78799582 | 1 | -3.44483805 | -4.17893839 | -0.72200418 |
| 1 | -0.61653805 | 3.38666177 | 0.10389582 | 1 | -1.79353797 | -4.27833796 | -0.10920417 |
| 6 | 1.02686203 | 3.71066189 | 1.45809579 | 1 | -2.20943785 | -3.12763810 | -1.40190423 |
| 6 | 0.99706197 | 5.23596191 | 1.34739578 | | | | |

I-4Me_bi



Zero-point vibrational energy

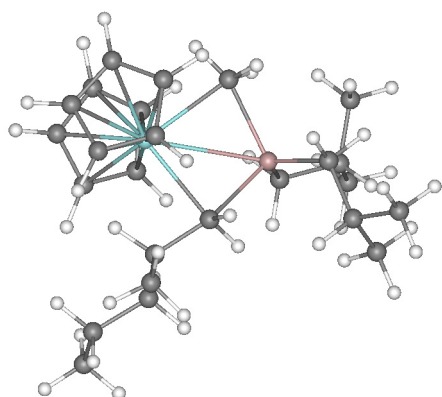
1665611.7 (Joules/Mol)

| | |
|---|-----------------------------|
| | 398.09075 (Kcal/Mol) |
| Zero-point correction | 0.634398 (Hartree/Particle) |
| Thermal correction to Energy | 0.668909 |
| Thermal correction to Enthalpy | 0.669853 |
| Thermal correction to Gibbs Free Energy | 0.567649 |
| Sum of electronic and zero-point Energies | -4761.126077 |
| Sum of electronic and thermal Energies | -4761.091567 |
| Sum of electronic and thermal Enthalpies | -4761.090622 |
| Sum of electronic and thermal Free Energies | -4761.192827 |

| cartesian | | | | | | |
|-----------|-------------|-------------|-------------|---|-------------|-------------|
| 6 | -3.76286173 | 1.82410979 | -0.52804798 | 6 | 2.46563816 | 2.16410995 |
| 6 | -4.52256203 | 1.51990986 | 0.62715209 | 6 | 3.16203833 | -1.29519022 |
| 6 | -3.71416187 | 1.78990984 | 1.76785207 | 1 | 3.42003822 | 2.24830985 |
| 6 | -2.45166183 | 2.22250986 | 1.31485200 | 6 | 1.40043831 | 3.02251005 |
| 6 | -2.47386169 | 2.23410988 | -0.11004797 | 1 | 2.67003822 | 2.58880997 |
| 1 | -1.66126180 | 2.54621005 | -0.75834793 | 6 | 4.67413807 | -0.99769014 |
| 1 | -4.11776161 | 1.76690984 | -1.54704785 | 1 | 2.90713835 | -1.93779016 |
| 1 | -5.55316162 | 1.18690979 | 0.63745201 | 1 | 2.91163826 | -1.90209019 |
| 1 | -4.01486206 | 1.68390989 | 2.80255198 | 6 | 1.12353826 | 2.49430990 |
| 1 | -1.61536181 | 2.50540996 | 1.94365215 | 6 | 1.81463814 | 4.49591017 |
| 6 | -2.91196179 | -2.70409012 | 1.08725202 | 1 | 0.46363819 | 2.96771002 |
| 6 | -4.22316170 | -2.15288997 | 1.10295200 | 6 | 5.48923826 | -2.28928995 |
| 6 | -4.30416203 | -1.26359022 | 2.19795203 | 6 | 5.05853844 | -0.23189013 |
| 6 | -3.03796172 | -1.23879015 | 2.84745193 | 1 | 4.92113829 | -0.36819014 |
| 6 | -2.19486189 | -2.15918994 | 2.17245197 | 1 | 6.56363821 | -2.08349013 |
| 1 | -1.17326176 | -2.39778996 | 2.44065189 | 1 | 5.23983812 | -2.83959007 |
| 1 | -2.54016161 | -3.43409014 | 0.37895203 | 1 | 5.28053808 | -2.94259000 |
| 1 | -5.02176189 | -2.38688993 | 0.41085204 | 1 | 0.40563822 | 3.12180996 |
| 1 | -5.18286180 | -0.70719016 | 2.49785209 | 1 | 0.72453821 | 1.46820986 |
| 1 | -2.78696179 | -0.67309016 | 3.73625207 | 1 | 2.04733825 | 2.47610998 |
| 40 | -2.70476174 | -0.19559012 | 0.60035205 | 1 | 1.04443824 | 5.10991001 |
| 6 | 0.01663822 | -0.05559013 | 1.10085201 | 1 | 2.73853827 | 4.60340977 |
| 1 | -1.25616169 | 0.04790987 | -1.17344785 | 1 | 1.99723816 | 4.89541006 |
| 6 | -3.19966173 | -0.93159014 | -1.48524785 | 1 | 6.13293839 | -0.03259013 |
| 6 | -1.78196180 | -0.58639014 | -1.94574809 | 1 | 4.79753828 | -0.81469017 |
| 6 | -0.89616179 | -1.83479011 | -2.09214807 | 1 | 4.54713821 | 0.73710984 |
| 1 | -3.96906185 | -0.42449012 | -2.06694794 | 1 | -2.14546180 | -0.25019014 |
| 1 | -3.38206172 | -2.00659013 | -1.52804804 | 1 | -0.75666177 | 0.66550982 |
| 6 | 0.58813822 | -1.56079018 | -2.33734798 | 1 | -2.40256166 | 1.18690979 |
| 1 | -1.29566169 | -2.44168997 | -2.91494799 | 6 | 1.41723824 | -2.84439015 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|------------|-------------|-------------|
| 1 | -0.99516177 | -2.45599008 | -1.18964791 | 1 | 0.96553826 | -0.86889017 | -1.56694794 |
| 1 | -0.36076176 | 0.80780983 | 0.54285204 | 1 | 0.72553825 | -1.04939020 | -3.29494810 |
| 1 | -0.14276177 | -1.03219020 | 0.62875205 | 1 | 2.47423816 | -2.64089012 | -2.50564814 |
| 1 | -0.28176177 | -0.04209013 | 2.15425205 | 1 | 1.07053828 | -3.53919005 | -3.08904791 |
| 6 | -1.76316178 | 0.31060988 | -3.18984795 | 1 | 1.33503819 | -3.35229015 | -1.35244799 |
| 13 | 2.00433826 | 0.27340987 | 0.94625205 | | | | |

I-4Me_bo



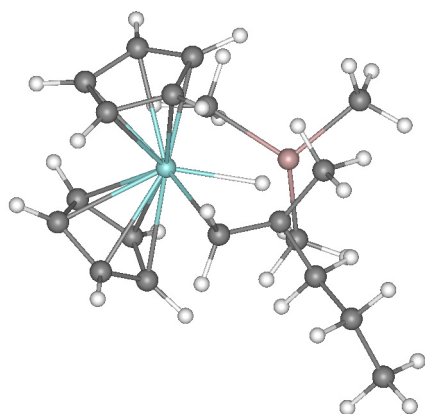
| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1671569.5 (Joules/Mol) |
| | 399.51469 (Kcal/Mol) |
| Zero-point correction | 0.636667 (Hartree/Particle) |
| Thermal correction to Energy | 0.670064 |
| Thermal correction to Enthalpy | 0.671008 |
| Thermal correction to Gibbs Free Energy | 0.574389 |
| Sum of electronic and zero-point Energies | -4761.138220 |
| Sum of electronic and thermal Energies | -4761.104823 |
| Sum of electronic and thermal Enthalpies | -4761.103878 |
| Sum of electronic and thermal Free Energies | -4761.200498 |

cartesian

| | | | | | | | |
|---|------------|-------------|-------------|----|-------------|-------------|-------------|
| 6 | 2.09623671 | -2.15178728 | -1.97207606 | 1 | 2.01823664 | 0.33881265 | -3.15957594 |
| 6 | 3.34543681 | -1.58198738 | -1.59627604 | 1 | 1.14743674 | 2.46521282 | 0.51042396 |
| 6 | 3.83313680 | -2.29548740 | -0.47737604 | 1 | 0.66263676 | 3.11081266 | -1.04047608 |
| 6 | 2.88493681 | -3.30108738 | -0.14917605 | 1 | 4.52553654 | -0.65588737 | 1.89052391 |
| 6 | 1.82763672 | -3.22268724 | -1.09077609 | 1 | 4.78103638 | -2.12828732 | 0.01602396 |
| 1 | 0.96463668 | -3.87298727 | -1.13157606 | 1 | 0.51603675 | -3.05658722 | 1.39822388 |
| 1 | 1.48053670 | -1.86068738 | -2.81347609 | 1 | -0.69676328 | -3.11658716 | 0.15462396 |
| 1 | 3.85243678 | -0.76398736 | -2.09457588 | 1 | -0.98026323 | -2.31418753 | 1.70162392 |
| 1 | 2.98263669 | -4.03488731 | 0.64202398 | 13 | -1.22986329 | -0.68008733 | 0.16382396 |
| 6 | 1.40663671 | 0.47941267 | 2.27842402 | 6 | -2.31626320 | -1.33128738 | -1.34107614 |
| 6 | 2.74693680 | 0.68131262 | 1.85062397 | 6 | -1.93206334 | 0.38131267 | 1.66782391 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | 3.47083664 | -0.50948739 | 2.08192396 | 1 | -3.20376325 | -1.84518731 | -0.93737608 |
| 6 | 2.58213687 | -1.45458734 | 2.66862392 | 6 | -2.80326319 | -0.28778735 | -2.36977601 |
| 6 | 1.31943667 | -0.83078736 | 2.81002402 | 1 | -1.75336313 | -2.11578751 | -1.87277603 |
| 1 | 0.43663672 | -1.27798736 | 3.24812412 | 6 | -3.41526318 | 0.08401266 | 1.98332393 |
| 1 | 0.60713673 | 1.20881259 | 2.26312399 | 1 | -1.36426330 | 0.21171266 | 2.59612393 |
| 1 | 3.15183687 | 1.59611261 | 1.43472385 | 1 | -1.82376313 | 1.45751262 | 1.45612395 |
| 1 | 2.84243679 | -2.45438719 | 2.99502397 | 6 | -3.62666345 | 0.81871259 | -1.70547605 |
| 40 | 1.75883675 | -1.09668732 | 0.32222396 | 6 | -3.62106347 | -0.95078737 | -3.48227596 |
| 6 | -0.24456325 | -2.44688749 | 0.89232397 | 1 | -1.92866325 | 0.18291265 | -2.84147596 |
| 1 | 2.91453671 | 3.77761269 | -1.60687613 | 6 | -3.94036317 | 1.00481260 | 3.08782411 |
| 6 | 1.47453678 | 2.57811260 | -0.52937603 | 6 | -3.60816312 | -1.38218737 | 2.38102412 |
| 6 | 2.74413681 | 3.43261242 | -0.58277601 | 1 | -4.00966358 | 0.26771265 | 1.07972395 |
| 6 | 2.65093684 | 4.64061260 | 0.34922397 | 1 | -4.99936342 | 0.82091260 | 3.29212403 |
| 1 | 3.62203670 | 2.82661247 | -0.31937605 | 1 | -3.82666326 | 2.05701256 | 2.81142402 |
| 1 | 3.54393673 | 5.26481295 | 0.28172398 | 1 | -3.38506317 | 0.83951271 | 4.01822376 |
| 1 | 2.53743672 | 4.32671261 | 1.39182389 | 1 | -3.97296309 | 1.55201268 | -2.43967605 |
| 1 | 1.78773677 | 5.26111269 | 0.09382395 | 1 | -3.05976319 | 1.36301267 | -0.93807608 |
| 6 | 0.32313672 | 0.35341263 | -0.99877602 | 1 | -4.51206350 | 0.39311266 | -1.21967614 |
| 6 | 1.60163677 | 1.19371259 | -1.18477607 | 1 | -3.94206309 | -0.22138736 | -4.23227596 |
| 6 | 1.98793674 | 1.31231260 | -2.66507602 | 1 | -4.51816368 | -1.41948736 | -3.06347609 |
| 1 | 0.07423672 | -0.13758735 | -1.94377601 | 1 | -3.04436326 | -1.72918737 | -3.99047613 |
| 1 | -0.47786328 | 1.09271264 | -0.82707602 | 1 | -4.64506340 | -1.58698738 | 2.66182399 |
| 1 | 2.51293683 | 0.73401260 | -0.69597602 | 1 | -2.97886324 | -1.63308740 | 3.24492407 |
| 1 | 2.96273685 | 1.79031265 | -2.79017591 | 1 | -3.35766315 | -2.07178736 | 1.56442392 |
| 1 | 1.23863673 | 1.92111266 | -3.18067598 | | | | |

TS-4Me



Zero-point vibrational energy

1658046.0 (Joules/Mol)

396.28251 (Kcal/Mol)

Zero-point correction

0.631516 (Hartree/Particle)

Thermal correction to Energy

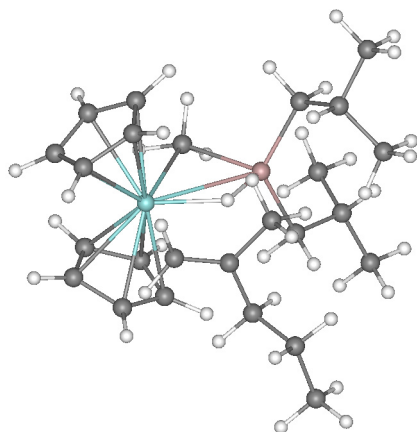
0.664706

| | |
|---|--------------|
| Thermal correction to Enthalpy | 0.665650 |
| Thermal correction to Gibbs Free Energy | 0.569894 |
| Sum of electronic and zero-point Energies | -4761.108600 |
| Sum of electronic and thermal Energies | -4761.075410 |
| Sum of electronic and thermal Enthalpies | -4761.074466 |
| Sum of electronic and thermal Free Energies | -4761.170222 |

| cartesian | | | | | | | |
|-----------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | -1.71688437 | 2.62534785 | -0.09747748 | 6 | 1.92181563 | -1.32375216 | 0.60122252 |
| 6 | -1.98158431 | 2.50264788 | 1.29032254 | 6 | 1.57041574 | 2.10954785 | 0.72782254 |
| 6 | -3.33738446 | 2.14904785 | 1.45462251 | 1 | 2.18921566 | -1.54485214 | -0.44007745 |
| 6 | -3.93028426 | 2.07694793 | 0.15912253 | 6 | 3.23261571 | -1.21845210 | 1.41232252 |
| 6 | -2.93348432 | 2.39204788 | -0.79017746 | 1 | 1.36371565 | -2.20635223 | 0.95412254 |
| 1 | -3.08968425 | 2.47454786 | -1.85677755 | 6 | 2.18521571 | 2.72244787 | -0.54487753 |
| 1 | -0.76568437 | 2.90914798 | -0.53217745 | 1 | 0.88271558 | 2.83584785 | 1.18462253 |
| 1 | -1.26198435 | 2.64864779 | 2.08532262 | 1 | 2.39001560 | 2.01384783 | 1.46442246 |
| 1 | -3.84338427 | 1.99334788 | 2.39952254 | 6 | 4.06621552 | -2.49425220 | 1.26202250 |
| 1 | -4.97008419 | 1.86864781 | -0.05957748 | 6 | 2.96161556 | -0.93605202 | 2.89272261 |
| 6 | -3.39378428 | -1.20645213 | 2.13832259 | 1 | 3.82041550 | -0.38235211 | 1.01002252 |
| 6 | -4.46258450 | -0.75915205 | 1.33052254 | 6 | 3.16971564 | 1.75704789 | -1.21007752 |
| 6 | -4.33378410 | -1.35665214 | 0.05352252 | 6 | 2.87921572 | 4.05334806 | -0.23967749 |
| 6 | -3.21868443 | -2.23925209 | 0.10382252 | 1 | 1.37971568 | 2.93664789 | -1.26137745 |
| 6 | -2.62918425 | -2.13865209 | 1.37512255 | 1 | 3.58851576 | 2.17894793 | -2.12857747 |
| 1 | -1.76608431 | -2.69475222 | 1.71912253 | 1 | 2.70551562 | 0.79484791 | -1.46707749 |
| 1 | -3.22588444 | -0.94245213 | 3.17472267 | 1 | 4.00481558 | 1.54154789 | -0.53377748 |
| 1 | -5.23978424 | -0.06905209 | 1.63282251 | 1 | 5.02121544 | -2.41335225 | 1.78982246 |
| 1 | -5.00258446 | -1.21855211 | -0.78727746 | 1 | 4.27861547 | -2.70615220 | 0.20992252 |
| 1 | -2.88898444 | -2.89095211 | -0.69207752 | 1 | 3.52481556 | -3.35255218 | 1.67582250 |
| 40 | -2.32348442 | 0.16854790 | 0.30192250 | 1 | 3.88451576 | -0.95925206 | 3.47872257 |
| 6 | 0.02121562 | -1.33355212 | -2.41077733 | 1 | 2.28281569 | -1.68855214 | 3.31202269 |
| 6 | -0.89348435 | -0.14265209 | -2.16857743 | 1 | 2.51171565 | 0.05234791 | 3.05232263 |
| 6 | -2.30178452 | -0.30535209 | -2.10777736 | 1 | 3.29241562 | 4.50534821 | -1.14647746 |
| 1 | -0.47798437 | 0.09444790 | -0.67297745 | 1 | 3.70311546 | 3.89834785 | 0.46512252 |
| 1 | 1.05241561 | -1.03905213 | -2.18967748 | 1 | 2.18391562 | 4.76824808 | 0.20962253 |
| 6 | -0.30648437 | -2.64875221 | -1.71537745 | 1 | -0.96028435 | 2.00504804 | -2.58667731 |
| 1 | -2.90428448 | 0.45504791 | -2.59477735 | 1 | -0.33348435 | 0.96824795 | -3.86597729 |
| 1 | -2.67938447 | -1.31415212 | -2.23327732 | 1 | 0.68391562 | 1.32434785 | -2.46787739 |
| 6 | -0.55228436 | 0.00214791 | 2.25122261 | 6 | 0.74921560 | -3.71785212 | -2.00247741 |
| 1 | -0.39678437 | -1.02565217 | 2.58952260 | 1 | -1.27848434 | -3.01675224 | -2.05947733 |
| 1 | 0.22181565 | 0.60694790 | 2.76402259 | 1 | -0.38068438 | -2.48345208 | -0.63197744 |
| 1 | -1.44098437 | 0.37804788 | 2.76142263 | 1 | 0.49631560 | -4.65865183 | -1.50977755 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|------------|-------------|-------------|
| 1 | -0.01828438 | -1.48585212 | -3.49907732 | 1 | 1.73431563 | -3.40675211 | -1.64467752 |
| 6 | -0.34338436 | 1.12854791 | -2.78177738 | 1 | 0.82431567 | -3.91125202 | -3.07617736 |
| 13 | 0.80521560 | 0.29144791 | 0.71902251 | | | | |

I-5Me



| | |
|---|-----------------------------|
| Zero-point vibrational energy | 1658285.3 (Joules/Mol) |
| | 396.33969 (Kcal/Mol) |
| Zero-point correction | 0.631608 (Hartree/Particle) |
| Thermal correction to Energy | 0.666340 |
| Thermal correction to Enthalpy | 0.667284 |
| Thermal correction to Gibbs Free Energy | 0.565558 |
| Sum of electronic and zero-point Energies | -4761.121319 |
| Sum of electronic and thermal Energies | -4761.086587 |
| Sum of electronic and thermal Enthalpies | -4761.085643 |
| Sum of electronic and thermal Free Energies | -4761.187368 |

| cartesian | | | | | | | |
|-----------|------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | 2.92140126 | 1.48615634 | 1.66519439 | 1 | 3.09070134 | 2.35915637 | -0.86220562 |
| 6 | 3.88130140 | 0.47635639 | 1.88119447 | 1 | 2.81860137 | 1.36025643 | -2.38850570 |
| 6 | 3.23360133 | -0.60424364 | 2.54689431 | 1 | -0.83129871 | 1.25335646 | -2.11930561 |
| 6 | 1.88140130 | -0.23524362 | 2.75529432 | 1 | -0.02799869 | 2.36055636 | -3.23070550 |
| 6 | 1.67200136 | 1.03885639 | 2.17809439 | 1 | 0.57400131 | 0.70625639 | -3.06700563 |
| 1 | 0.74170136 | 1.59385645 | 2.18679452 | 6 | -0.23399866 | 4.16235638 | -0.98350567 |
| 1 | 3.11620140 | 2.45315623 | 1.22389436 | 1 | -0.34249866 | 2.32995629 | 0.14689437 |
| 1 | 4.93000126 | 0.53025639 | 1.61679447 | 1 | 1.17430139 | 3.22375631 | 0.35659435 |
| 1 | 3.70650125 | -1.52004361 | 2.88209438 | 1 | -0.02299869 | -2.45954370 | 1.90799439 |
| 1 | 1.12850142 | -0.83034360 | 3.25549436 | 1 | 1.64290130 | -2.64524364 | 1.71269441 |
| 6 | 2.91060138 | -1.26544356 | -2.07600570 | 1 | 0.59880131 | -3.27294374 | 0.46799436 |
| 6 | 4.08740139 | -0.81834358 | -1.40570557 | 6 | -0.80119860 | 5.06615639 | 0.10959436 |
| 6 | 4.37000132 | -1.74214363 | -0.37030566 | 1 | -1.03639865 | 3.86245608 | -1.66390562 |

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | 3.35220122 | -2.72254372 | -0.36500564 | 1 | 0.50490135 | 4.70885658 | -1.57900560 |
| 6 | 2.45510149 | -2.43134379 | -1.43220556 | 1 | -1.27549863 | 5.94955635 | -0.32190564 |
| 1 | 1.57600141 | -3.00084376 | -1.70630562 | 1 | -0.01399869 | 5.40695667 | 0.78799433 |
| 1 | 2.44480133 | -0.80454361 | -2.93750548 | 1 | -1.55349874 | 4.53785658 | 0.70269436 |
| 1 | 4.69510126 | 0.03745639 | -1.67290556 | 6 | -2.85859871 | -2.34434366 | -3.30560565 |
| 1 | 5.21600151 | -1.70344365 | 0.30409437 | 1 | -1.33429861 | -0.93444359 | -2.80170560 |
| 1 | 3.28970122 | -3.57054377 | 0.30479437 | 6 | -3.16039872 | -0.32044363 | -1.85560560 |
| 40 | 2.23300123 | -0.53654361 | 0.25699437 | 6 | -3.80119848 | 0.19635640 | 3.08059430 |
| 6 | 0.75330132 | -2.40904379 | 1.12199438 | 6 | -2.88449860 | -2.10234356 | 2.64829445 |
| 1 | 0.43830132 | -0.10204361 | -0.40320563 | 1 | -3.67939854 | -0.76864362 | 1.17259443 |
| 13 | -0.75629866 | -1.12344360 | 0.30529436 | 1 | -3.83789873 | -2.52404380 | 2.97879434 |
| 6 | -1.64239860 | -2.19944382 | -1.08160555 | 1 | -2.21489859 | -2.08344364 | 3.51759434 |
| 6 | -1.69899869 | -0.08174361 | 1.68429446 | 1 | -2.46579862 | -2.80014372 | 1.91139436 |
| 6 | -2.18249869 | -1.41474354 | -2.29370570 | 1 | -4.78469849 | -0.21334362 | 3.32999444 |
| 1 | -0.97419870 | -2.99664378 | -1.43860555 | 1 | -3.94599867 | 1.20455635 | 2.68179440 |
| 1 | -2.48829865 | -2.72724366 | -0.61180562 | 1 | -3.22659874 | 0.28085637 | 4.00999451 |
| 6 | -3.06119871 | -0.69234359 | 2.07759452 | 1 | -3.51119852 | 0.27045637 | -2.70750570 |
| 1 | -1.09239864 | 0.02165639 | 2.59899449 | 1 | -2.71729875 | 0.37495643 | -1.12830555 |
| 1 | -1.86409855 | 0.94775641 | 1.32979441 | 1 | -4.03979874 | -0.76654363 | -1.37690556 |
| 6 | 2.39690137 | 1.82465637 | -1.50290561 | 1 | -3.22179866 | -1.79204357 | -4.17800570 |
| 6 | 1.05980134 | 2.04235625 | -1.43340564 | 1 | -3.71529865 | -2.84674382 | -2.84380555 |
| 6 | 0.14420134 | 1.54625642 | -2.51760554 | 1 | -2.16799855 | -3.11654377 | -3.65670562 |
| 6 | 0.42820132 | 2.90965629 | -0.38010564 | | | | |

S1.9. Interaction with H₂

H2 Hydrogen

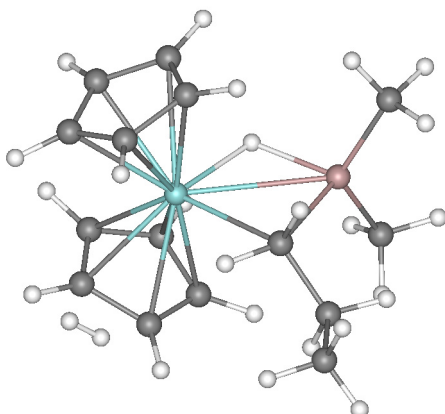


| | |
|---|-----------------------------|
| Zero-point vibrational energy | 27227.7 (Joules/Mol) |
| | 6.50757 (Kcal/Mol) |
| Zero-point correction | 0.010370 (Hartree/Particle) |
| Thermal correction to Energy | 0.012731 |
| Thermal correction to Enthalpy | 0.013675 |
| Thermal correction to Gibbs Free Energy | -0.001099 |
| Sum of electronic and zero-point Energies | -1.153736 |
| Sum of electronic and thermal Energies | -1.151375 |
| Sum of electronic and thermal Enthalpies | -1.150431 |
| Sum of electronic and thermal Free Energies | -1.165205 |

cartesian

| | | | | | | | |
|---|------------|------------|------------|---|------------|------------|-------------|
| 1 | 0.00000000 | 0.00000000 | 0.36780000 | 1 | 0.00000000 | 0.00000000 | -0.36780000 |
|---|------------|------------|------------|---|------------|------------|-------------|

_I-2H_a_H2



| | |
|--|-----------------------------|
| Zero-point vibrational energy | 945988.3 (Joules/Mol) |
| | 226.09663 (Kcal/Mol) |
| Zero-point correction= | 0.360308 (Hartree/Particle) |
| Thermal correction to Energy= | 0.382778 |
| Thermal correction to Enthalpy= | 0.383723 |
| Thermal correction to Gibbs Free Energy= | 0.310018 |
| Sum of electronic and zero-point Energies= | -4369.628294 |
| Sum of electronic and thermal Energies= | -4369.605823 |
| Sum of electronic and thermal Enthalpies= | -4369.604879 |
| Sum of electronic and thermal Free Energies= | -4369.678583 |

cartesian

| | | | | | | | |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| 6 | -0.12040000 | -2.23469996 | -0.91839999 | 6 | -2.94689989 | -0.58560002 | -2.05620003 |
| 6 | 0.52300000 | -2.49469995 | 0.31639999 | 1 | -1.71469998 | 3.30730009 | -0.55430001 |
| 6 | 1.89900005 | -2.17490005 | 0.17600000 | 1 | -2.94129992 | 3.02080011 | -1.78310001 |
| 6 | 2.10780001 | -1.73529994 | -1.16159999 | 1 | -3.32150006 | 2.75399995 | -0.09400000 |
| 6 | 0.86240000 | -1.77230000 | -1.83650005 | 1 | -2.33929992 | -0.97399998 | -2.88229990 |
| 1 | 0.68629998 | -1.50689995 | -2.87159991 | 1 | -3.28870010 | -1.44780004 | -1.47370005 |
| 1 | -1.16910005 | -2.38910007 | -1.14069998 | 1 | -3.84170008 | -0.14760000 | -2.51200008 |
| 1 | 0.04660000 | -2.87540007 | 1.21340001 | 6 | -2.85540009 | -0.97350001 | 2.81669998 |
| 1 | 3.05819988 | -1.44760001 | -1.59340000 | 6 | -1.42780006 | 0.16270000 | 1.03869998 |
| 6 | 0.93199998 | 2.34240007 | 0.77609998 | 6 | -2.61400008 | -0.78369999 | 1.31710005 |
| 6 | 1.73899996 | 1.53269994 | 1.61940002 | 1 | -3.52800012 | -0.37880000 | 0.86309999 |
| 6 | 2.79200006 | 0.99519998 | 0.83829999 | 1 | -1.64129996 | 1.13360000 | 1.50619996 |
| 6 | 2.63949990 | 1.47780001 | -0.49140000 | 1 | -0.60140002 | -0.22849999 | 1.69760001 |
| 6 | 1.49880004 | 2.32170010 | -0.52420002 | 1 | -2.44619989 | -1.75370002 | 0.83710003 |
| 1 | 1.12860000 | 2.85960007 | -1.38759995 | 1 | -1.98210001 | -1.42719996 | 3.29679990 |
| 1 | 0.05810000 | 2.90540004 | 1.08000004 | 1 | -3.04859996 | -0.01550000 | 3.30609989 |
| 1 | 1.58140004 | 1.36259997 | 2.67860007 | 1 | 3.58960009 | 0.35609999 | 1.19700003 |
| 1 | 3.30110002 | 1.27260005 | -1.32379997 | 1 | 2.66090012 | -2.29320002 | 0.93680000 |
| 40 | 0.69550002 | -0.01320000 | -0.05690000 | 1 | -3.71320009 | -1.62530005 | 2.99519992 |
| 1 | -0.29290000 | 0.68250000 | -1.54980004 | 1 | 1.72679996 | -1.33060002 | 3.55399990 |
| 13 | -1.99269998 | 0.77300000 | -1.02760005 | 1 | 1.12179995 | -1.61360002 | 3.24130011 |
| 6 | -2.52979994 | 2.63569999 | -0.84410000 | | | | |

S1.10. Transition states search and proof

As was mentioned in the main article, transition states were found by draft scanning using Priroda program [48] followed by presize scanning with sequential changing of key geometric parameters with a step of 0.01 Å and then by Berny optimization using Gaussian-09 program package [36]. Verification of the geometries of the transition states was performed using the standard IRC procedure as implemented in Gaussian-09 with the command line:

```
# irc=(maxpoints=20,calcf).
```

Note that in some cases the IRC sequences included one artifact point (see Fig. 1a for example), and IRC procedures were repeated in duplicative mode for reverse and forward directions. In view of the visibility of the IRC procedure for the confirmation of the TS identity, we attached animation files named *_IRC.gif to the SI data in addition to animation files that reflect the imaginary frequency vibration for all transition states mentioned in the manuscript.

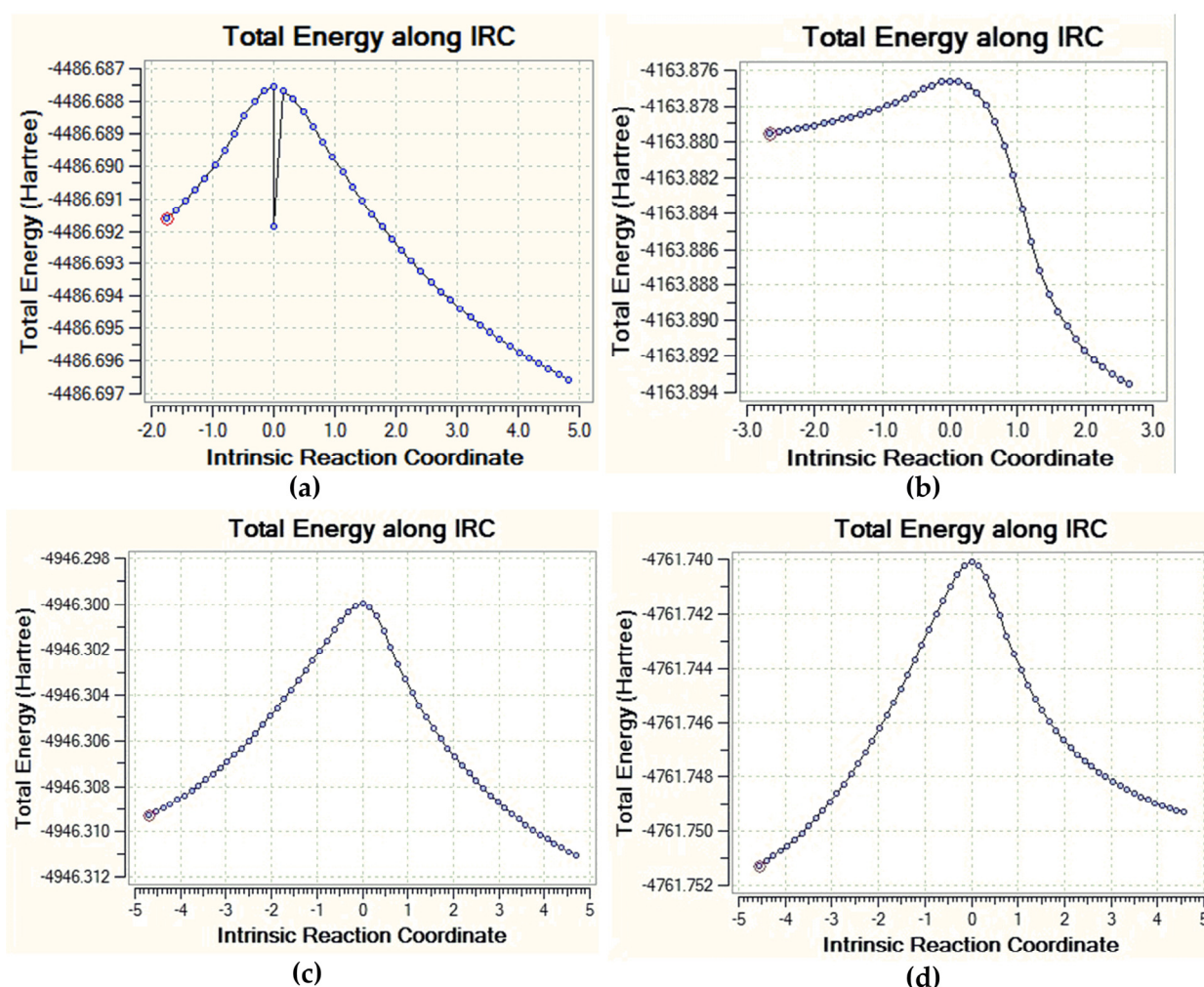


Figure S2. IRC plots (GaussView) for transition states: (a) TS-4H (one artifact point); (b) TS-4-; (c) TS-4Cl; (d) TS-4Me_dibu. Animations for (b–d) can be found in the Supporting Information as *_IRC.gif.

S2. Oligomerization experiments

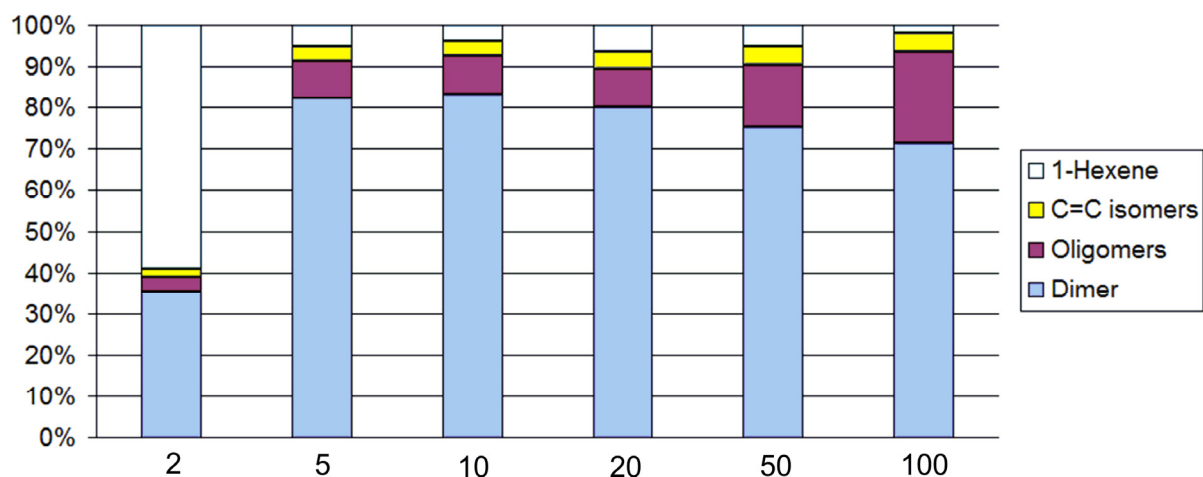


Figure S2. The dependence of the composition of the reaction mixtures (1-hexene oligomerization in bulk, 60 °C, 4 h) from Al_{MMAO-12}/Zr ratio.

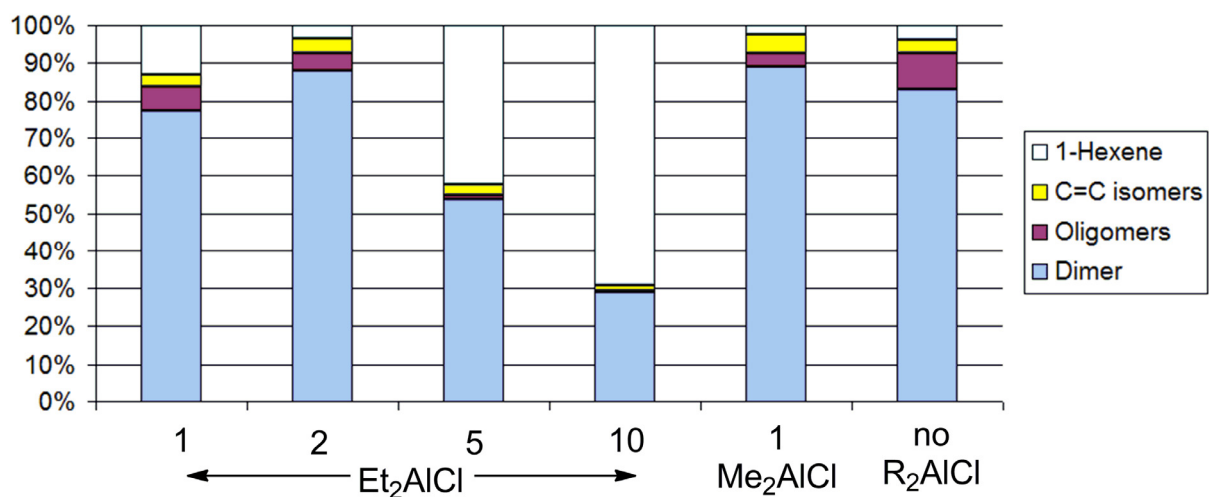


Figure S3. The affect of R₃AlCl on the composition of the reaction mixtures (1-hexene oligomerization in bulk, 60 °C, 4 h, Al_{MMAO-12}/Zr = 10).