Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Back to basics: Identification of reaction intermediates in the mechanism of a classic ligand substitution reaction on Vaska's complex

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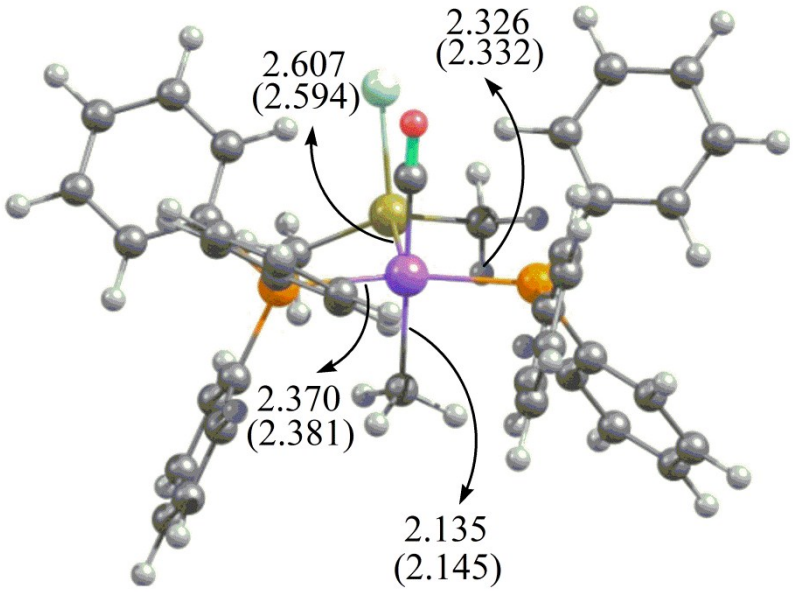
Index



I2

Figure S1. Optimized geometry of the intermediate $[Me_2ClGa)MeIr(CO)(PPh_3)_2]$ (**I2**), calculated at the M05-2X-D3/def2-SVP level. Some representative bond distances, in Å, are shown. In parenthesis, the corresponding computed bond distance values incorporating benzene as solvent are displayed. Atom colour code: C (dark grey), Cl (light blue), Ga (olive green), H (silver white), Ir (purple), O (red), P (orange).

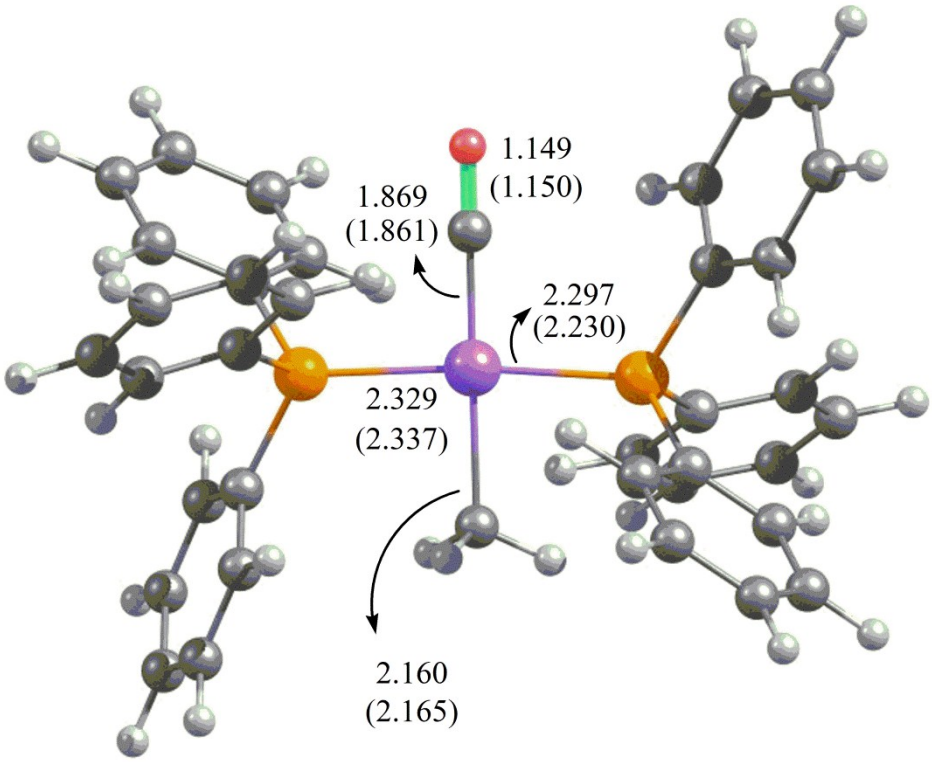


Figure S2. Optimized geometry of *trans*-[MeIr(CO)(PPh_3)$_2$] (**2**), the product of the methylation of Vaska's complex, calculated at the M05-2X-D3/def2-SVP level. Some representative bond distances, in Å, are shown. In parenthesis, the corresponding computed bond distance values incorporating benzene as solvent are displayed. Atom colour code: C (dark grey), H (silver white), Ir (purple), O (red), P (orange).

Scaling Factor

The only C-O stretching vibration assigned unequivocally is that of **1** because the experimental value is available (1951 cm^{-1}). The overestimation of *ab initio* harmonic vibrational frequencies was found to be relatively uniform. In our case, the computed value for such vibration a the M05-2X-D3/def2-SVP is 2135 cm-1. So, we determined a scaling factor of 0.914.

Table S1. Relative energies (in kcal/mol) for the methylation of the Vaska´s complex *trans*-[ClIr(CO)(PPh_3)$_2$] by trimethylgallium computed at different levels.

Level	ΔG			
	RC	TS	PC	Products
B3LYP/def2-SVP	7.6	35.8	18.2	6.4
B3LYP-D3/def2-SVP	-2.9	17.7	-4.5	--
M06-D3/def2-TZVP	-5.1	15.2	-6.7	0.6
M052X-D3/def2-SVP-W06	-5.1	14.0	-5.6	6.3

Cartesian Coordinates of optimized structures computed at M05-2X/def2-SVP including Grimme´s dispersion GD3.

Complex 1

E_{zpe} = -2748.359658

G^{280K} = -2748.4313859

freq= 5.75 cm^{-1}

C	4.207910000	2.168080000	-0.148454000
C	3.055788000	1.651996000	0.450874000
C	2.422004000	2.373869000	1.470204000
C	2.946952000	3.591660000	1.896082000
C	4.097959000	4.103012000	1.296477000
C	4.723368000	3.393542000	0.272751000
P	2.341484000	0.021582000	-0.001077000
C	3.216617000	-1.139196000	1.116218000
C	3.955189000	-0.687983000	2.214025000
C	4.602726000	-1.602921000	3.045096000
C	4.520303000	-2.967590000	2.781185000
C	3.786049000	-3.420556000	1.684376000
C	3.130977000	-2.514232000	0.856395000
C	3.059224000	-0.356784000	-1.646237000
C	2.299839000	-0.078631000	-2.787871000
C	2.833194000	-0.306580000	-4.055558000
C	4.122137000	-0.819582000	-4.189424000
C	4.879880000	-1.106836000	-3.053794000
C	4.352067000	-0.877665000	-1.784832000
Ir	-0.006138000	0.049223000	-0.001575000
P	-2.337813000	-0.043486000	0.041394000
C	-3.192628000	1.398329000	-0.711732000
C	-3.994927000	1.286451000	-1.849849000
C	-4.599042000	2.422493000	-2.392169000
C	-4.410070000	3.668349000	-1.800218000
C	-3.610081000	3.783322000	-0.661824000
C	-3.001262000	2.655273000	-0.122520000
C	0.017687000	1.758951000	-0.596257000
O	0.051674000	2.836708000	-0.994701000
C	-3.097656000	-0.123467000	1.712648000
C	-4.358464000	0.434843000	1.962254000
C	-4.927481000	0.338790000	3.230812000
C	-4.241937000	-0.311123000	4.256492000
C	-2.987607000	-0.867032000	4.010560000
C	-2.411757000	-0.775508000	2.744208000
C	-3.024712000	-1.469600000	-0.875898000
C	-2.312755000	-1.940039000	-1.984330000
C	-2.835889000	-2.971255000	-2.760593000
C	-4.062906000	-3.544186000	-2.425827000

C	-4.766689000	-3.085927000	-1.313017000
C	-4.250621000	-2.048357000	-0.537659000
H	-4.896321000	0.950955000	1.167468000
H	-5.907478000	0.776192000	3.417170000
H	-4.686139000	-0.382264000	5.248728000
H	-2.448244000	-1.376315000	4.807973000
H	-1.438513000	-1.222280000	2.543809000
H	-1.341790000	-1.502419000	-2.218878000
H	-2.276881000	-3.337323000	-3.620520000
H	-4.466823000	-4.356834000	-3.028500000
H	-5.719083000	-3.539995000	-1.042833000
H	-4.799097000	-1.697342000	0.335741000
H	-4.151897000	0.314375000	-2.315074000
H	-5.221230000	2.327763000	-3.281124000
H	-4.882933000	4.552501000	-2.225802000
H	-3.454013000	4.755823000	-0.197310000
H	-2.371634000	2.748412000	0.763738000
H	4.034314000	0.377415000	2.423294000
H	5.176119000	-1.242383000	3.897994000
H	5.027910000	-3.680616000	3.429786000
H	3.713546000	-4.487015000	1.476241000
H	2.543737000	-2.872536000	0.013471000
H	1.285675000	0.304249000	-2.673561000
H	2.235624000	-0.088635000	-4.939531000
H	4.535964000	-1.002661000	-5.180345000
H	5.884860000	-1.514316000	-3.155353000
H	4.942898000	-1.109552000	-0.898678000
H	1.509268000	1.975930000	1.917243000
H	2.449596000	4.146716000	2.690197000
H	4.503021000	5.060186000	1.622549000
H	5.616300000	3.795274000	-0.204245000
H	4.699830000	1.621233000	-0.951433000
Cl	-0.056044000	-2.266660000	0.696260000

Complex 1(benzene)

E_{zpe} = -2748.402537

G^{280K} = -2748.47316294

freq= 8.78 cm^{-1}

C	4.186284000	2.205491000	0.042122000
C	3.023740000	1.640904000	0.574924000
C	2.347401000	2.294943000	1.613004000
C	2.841643000	3.493045000	2.124392000
C	4.003494000	4.052144000	1.591810000
C	4.670713000	3.410972000	0.549084000
P	2.345478000	0.030484000	0.010625000
C	3.229601000	-1.195107000	1.047680000
C	3.956816000	-0.818997000	2.180216000

C	4.610986000	-1.787551000	2.943413000
C	4.544735000	-3.129574000	2.577430000
C	3.817816000	-3.507753000	1.447258000
C	3.156871000	-2.547848000	0.687280000
C	3.070492000	-0.233422000	-1.655184000
C	2.301443000	0.064757000	-2.785586000
C	2.843262000	-0.085183000	-4.061624000
C	4.151657000	-0.539472000	-4.216673000
C	4.919960000	-0.847423000	-3.093370000
C	4.383484000	-0.696251000	-1.816393000
Ir	-0.007146000	0.034825000	0.026032000
P	-2.343444000	-0.055622000	0.038537000
C	-3.176554000	1.388425000	-0.736023000
C	-3.973821000	1.282342000	-1.878265000
C	-4.565524000	2.423688000	-2.424167000
C	-4.370352000	3.668048000	-1.830447000
C	-3.576997000	3.776459000	-0.686494000
C	-2.980443000	2.643287000	-0.143390000
C	0.025913000	1.707900000	-0.653977000
O	0.072310000	2.763332000	-1.110448000
C	-3.167771000	-0.135049000	1.679077000
C	-4.478187000	0.336122000	1.841141000
C	-5.101507000	0.258054000	3.084833000
C	-4.421369000	-0.286439000	4.174384000
C	-3.117811000	-0.753660000	4.016871000
C	-2.488619000	-0.679949000	2.774407000
C	-2.971142000	-1.485703000	-0.915201000
C	-2.272922000	-1.829591000	-2.079274000
C	-2.727820000	-2.869838000	-2.884775000
C	-3.872820000	-3.581359000	-2.523763000
C	-4.560353000	-3.250700000	-1.357161000
C	-4.113970000	-2.202076000	-0.551926000
H	-5.013142000	0.770638000	0.996854000
H	-6.120003000	0.626587000	3.202221000
H	-4.908401000	-0.343468000	5.147476000
H	-2.582012000	-1.179620000	4.864346000
H	-1.476547000	-1.060012000	2.644255000
H	-1.364336000	-1.283744000	-2.338139000
H	-2.179647000	-3.133250000	-3.788508000
H	-4.223700000	-4.401912000	-3.148892000
H	-5.446962000	-3.813529000	-1.067504000
H	-4.651935000	-1.952824000	0.362068000
H	-4.138115000	0.312594000	-2.346276000
H	-5.183417000	2.333641000	-3.316874000
H	-4.833553000	4.556198000	-2.258978000
H	-3.417972000	4.747350000	-0.218887000
H	-2.355727000	2.731807000	0.747430000
H	4.022629000	0.228595000	2.470185000
H	5.177355000	-1.486394000	3.823880000
H	5.058515000	-3.883734000	3.172843000
H	3.757418000	-4.556808000	1.160161000

H	2.580327000	-2.848034000	-0.186065000
H	1.272406000	0.401782000	-2.663051000
H	2.236775000	0.148174000	-4.935826000
H	4.572305000	-0.660719000	-5.214404000
H	5.940865000	-1.209129000	-3.210545000
H	4.986232000	-0.943942000	-0.942645000
H	1.426539000	1.861290000	2.007558000
H	2.312598000	3.995318000	2.933380000
H	4.385170000	4.993934000	1.984875000
H	5.572108000	3.850638000	0.123628000
H	4.711800000	1.713843000	-0.775244000
Cl	-0.062722000	-2.236953000	0.881092000

Intermediate I1

E_{zpe} = -4792.442401

G^{280K} = -4792.52373972

freq= 7.88 cm^{-1}

C	-4.019903000	-2.866458000	-0.643540000
C	-2.892398000	-2.445485000	0.066755000
C	-2.206989000	-3.354492000	0.882422000
C	-2.653893000	-4.668671000	0.995047000
C	-3.779072000	-5.085852000	0.283772000
C	-4.457589000	-4.186203000	-0.536369000
P	-2.297813000	-0.709296000	0.018607000
C	-3.196762000	0.074635000	1.409217000
C	-3.821528000	-0.690921000	2.399250000
C	-4.479208000	-0.062690000	3.456612000
C	-4.521023000	1.327554000	3.527670000
C	-3.902534000	2.093983000	2.539665000
C	-3.237706000	1.473186000	1.485986000
C	-3.068239000	-0.004199000	-1.484440000
C	-2.349572000	-0.065228000	-2.683219000
C	-2.909288000	0.426010000	-3.860079000
C	-4.183752000	0.990050000	-3.843890000
C	-4.902815000	1.055590000	-2.650635000
C	-4.350498000	0.557123000	-1.472127000
Ir	0.054929000	-0.582579000	0.009561000
P	2.395777000	-0.445661000	0.078606000
C	3.254159000	-1.822854000	-0.784139000
C	4.036132000	-1.625672000	-1.924244000
C	4.646762000	-2.716401000	-2.546934000
C	4.483395000	-3.999860000	-2.033310000
C	3.703563000	-4.199066000	-0.892292000
C	3.089588000	-3.116689000	-0.272069000
C	0.117141000	-2.136573000	-0.904937000
O	0.142107000	-3.106040000	-1.518452000
C	3.178162000	-0.496350000	1.738209000

C	4.498980000	-0.945256000	1.880611000
C	5.100572000	-0.963449000	3.136508000
C	4.387085000	-0.541630000	4.258621000
C	3.072474000	-0.101465000	4.121453000
C	2.465004000	-0.077611000	2.866333000
C	3.045030000	1.044960000	-0.753072000
C	2.342242000	1.505304000	-1.871441000
C	2.824661000	2.587584000	-2.603097000
C	4.008911000	3.214329000	-2.217280000
C	4.705042000	2.764332000	-1.095904000
C	4.225902000	1.681412000	-0.360227000
H	5.056348000	-1.288885000	1.009254000
H	6.127163000	-1.312671000	3.238522000
H	4.857019000	-0.559740000	5.241240000
H	2.510303000	0.227096000	4.994279000
H	1.442324000	0.278517000	2.760682000
H	1.409032000	1.016199000	-2.152941000
H	2.262857000	2.951705000	-3.462050000
H	4.380756000	4.068967000	-2.780814000
H	5.619134000	3.266610000	-0.782860000
H	4.764819000	1.342916000	0.523526000
H	4.173382000	-0.623550000	-2.328070000
H	5.254033000	-2.556254000	-3.436736000
H	4.961067000	-4.848184000	-2.521677000
H	3.569188000	-5.201569000	-0.488790000
H	2.475397000	-3.273835000	0.616383000
H	-3.805079000	-1.777920000	2.347840000
H	-4.963344000	-0.666567000	4.222851000
H	-5.036325000	1.816857000	4.353287000
H	-3.922889000	3.181197000	2.588525000
H	-2.753733000	2.080307000	0.722885000
H	-1.341637000	-0.479951000	-2.684214000
H	-2.340624000	0.382859000	-4.787620000
H	-4.615564000	1.387083000	-4.761647000
H	-5.896733000	1.500493000	-2.634473000
H	-4.912985000	0.613880000	-0.540773000
H	-1.317709000	-3.024795000	1.422427000
H	-2.116989000	-5.370205000	1.631904000
H	-4.123315000	-6.116134000	0.364304000
H	-5.331763000	-4.511294000	-1.098716000
H	-4.552649000	-2.167924000	-1.287450000
Cl	-0.007250000	1.600824000	1.162372000
Ga	-0.351752000	3.858247000	-0.079799000
C	1.509372000	4.560985000	0.110472000
H	1.627193000	5.088445000	1.066139000
H	2.241395000	3.745402000	0.075347000
H	1.751633000	5.263960000	-0.699596000
C	-1.026683000	3.184536000	-1.844313000
H	-0.945590000	3.978734000	-2.601597000
H	-0.454098000	2.321338000	-2.205155000
H	-2.082722000	2.885701000	-1.789665000

C	-1.714208000	4.652807000	1.166693000
H	-1.596327000	4.242262000	2.178940000
H	-1.556534000	5.738950000	1.231375000
H	-2.747855000	4.483775000	0.835394000

Intermediate I1 (benzene)

E_{zpe} = -4792.484334

G^{280K} = -4792.56436264

freq= 7.03 cm^{-1}

C	-3.982219000	-2.896202000	-0.579581000
C	-2.854775000	-2.423145000	0.097585000
C	-2.117762000	-3.292515000	0.912502000
C	-2.514529000	-4.619820000	1.057212000
C	-3.639561000	-5.089343000	0.378535000
C	-4.368953000	-4.229128000	-0.440599000
P	-2.319742000	-0.669978000	0.001698000
C	-3.202846000	0.119808000	1.398799000
C	-3.808270000	-0.636230000	2.407649000
C	-4.454501000	0.002722000	3.466232000
C	-4.504533000	1.393625000	3.518894000
C	-3.904315000	2.150630000	2.511831000
C	-3.249760000	1.518918000	1.458095000
C	-3.144146000	-0.014310000	-1.496825000
C	-2.458076000	-0.088971000	-2.714600000
C	-3.057481000	0.368809000	-3.885652000
C	-4.340881000	0.912232000	-3.845864000
C	-5.028982000	0.987865000	-2.635080000
C	-4.436746000	0.522449000	-1.462070000
Ir	0.037593000	-0.504996000	-0.037043000
P	2.381992000	-0.438208000	0.065839000
C	3.208655000	-1.800703000	-0.852694000
C	4.016747000	-1.578021000	-1.969932000
C	4.602723000	-2.658948000	-2.632548000
C	4.388757000	-3.958644000	-2.181833000
C	3.583642000	-4.183670000	-1.063179000
C	2.993637000	-3.110866000	-0.403310000
C	0.076302000	-1.998423000	-1.041551000
O	0.082083000	-2.925403000	-1.719956000
C	3.103032000	-0.630637000	1.743219000
C	4.423516000	-1.079152000	1.893012000
C	4.975043000	-1.219986000	3.163894000
C	4.212013000	-0.922163000	4.293777000
C	2.897323000	-0.484577000	4.149338000
C	2.340526000	-0.338503000	2.878658000
C	3.122569000	1.069405000	-0.654893000
C	2.530716000	1.575832000	-1.818120000

C	3.101254000	2.664253000	-2.474486000
C	4.257467000	3.256424000	-1.966035000
C	4.837616000	2.764913000	-0.797417000
C	4.273436000	1.672465000	-0.139400000
H	5.021329000	-1.325381000	1.015385000
H	6.002079000	-1.567013000	3.271177000
H	4.643397000	-1.035914000	5.287819000
H	2.296074000	-0.254163000	5.027835000
H	1.316339000	0.012514000	2.769941000
H	1.620635000	1.114866000	-2.204775000
H	2.634844000	3.057887000	-3.376704000
H	4.698537000	4.114244000	-2.472517000
H	5.729213000	3.237722000	-0.387466000
H	4.726385000	1.300006000	0.777971000
H	4.197590000	-0.564720000	-2.325724000
H	5.230423000	-2.477588000	-3.504242000
H	4.847843000	-4.799301000	-2.700880000
H	3.410692000	-5.198804000	-0.707994000
H	2.359490000	-3.290249000	0.467159000
H	-3.785609000	-1.723963000	2.371710000
H	-4.923816000	-0.593801000	4.247688000
H	-5.011660000	1.890904000	4.345063000
H	-3.935353000	3.238506000	2.547747000
H	-2.779228000	2.115859000	0.677961000
H	-1.445202000	-0.490544000	-2.741126000
H	-2.513850000	0.313237000	-4.827752000
H	-4.804421000	1.282887000	-4.759488000
H	-6.031096000	1.413557000	-2.600875000
H	-4.979910000	0.584370000	-0.519707000
H	-1.228302000	-2.922896000	1.426247000
H	-1.938606000	-5.290411000	1.693774000
H	-3.943898000	-6.130204000	0.483514000
H	-5.243115000	-4.595140000	-0.977777000
H	-4.556235000	-2.230134000	-1.222748000
Cl	0.012175000	1.628859000	1.244202000
Ga	-0.280963000	3.816708000	-0.083948000
C	1.551798000	4.550174000	0.228366000
H	1.605557000	5.024122000	1.218930000
H	2.316826000	3.765293000	0.185941000
H	1.807929000	5.313507000	-0.521848000
C	-0.824069000	3.061346000	-1.862342000
H	-0.328797000	3.592593000	-2.688739000
H	-0.551017000	1.999908000	-1.933309000
H	-1.909675000	3.137856000	-2.019760000
C	-1.708180000	4.696265000	1.024889000
H	-1.621073000	4.405920000	2.081285000
H	-1.563498000	5.786780000	0.977532000
H	-2.730188000	4.484823000	0.681779000

Transition State TS

E_{zpe} = -4792.416965

G^{280K} = -4792.49360153

freq= -89.90 cm^{-1}

Ir	0.001830000	0.298629000	-0.100342000
P	2.351398000	0.347179000	0.078025000
P	-2.353627000	0.462526000	-0.014476000
C	-0.009372000	2.072558000	-0.341395000
O	-0.074681000	3.212363000	-0.484293000
Cl	-0.455828000	-1.739735000	-1.903913000
Ga	0.078050000	-3.094791000	0.012162000
C	1.936104000	-3.769424000	-0.307729000
H	1.903413000	-4.555828000	-1.074062000
H	2.645437000	-3.006483000	-0.644009000
H	2.327492000	-4.219589000	0.616798000
C	-0.130244000	-1.797123000	1.605940000
H	0.679634000	-2.143000000	2.265544000
H	-0.092635000	-0.691077000	1.746219000
H	-1.089305000	-2.098269000	2.044147000
C	-1.373852000	-4.465469000	0.049718000
H	-2.310504000	-4.043601000	-0.332610000
H	-1.107100000	-5.330996000	-0.571189000
H	-1.555952000	-4.824332000	1.073283000
C	2.859032000	-0.382714000	1.679491000
C	3.679626000	-1.508142000	1.774572000
C	2.310035000	0.172356000	2.844878000
C	3.956627000	-2.065634000	3.024409000
H	4.087640000	-1.968205000	0.877206000
C	2.601655000	-0.375909000	4.089097000
H	1.637243000	1.027870000	2.767969000
C	3.425840000	-1.499484000	4.180158000
H	4.586834000	-2.951532000	3.087393000
H	2.171886000	0.063046000	4.988316000
H	3.644098000	-1.938135000	5.152919000
C	3.440177000	-0.392020000	-1.197847000
C	4.832383000	-0.294842000	-1.054932000
C	2.895616000	-0.972316000	-2.343646000
C	5.669760000	-0.806592000	-2.039681000
H	5.258893000	0.189102000	-0.175442000
C	3.742398000	-1.476487000	-3.333416000
H	1.814804000	-1.051221000	-2.451295000
C	5.123275000	-1.399980000	-3.180899000
H	6.750266000	-0.735707000	-1.922831000
H	3.311755000	-1.936157000	-4.221632000
H	5.780449000	-1.798466000	-3.952983000

C	3.068567000	2.046517000	0.103580000
C	3.763458000	2.586267000	1.187880000
C	2.940559000	2.794997000	-1.073773000
C	4.307976000	3.869260000	1.099205000
H	3.895087000	2.010015000	2.101539000
C	3.484992000	4.071305000	-1.158641000
H	2.410155000	2.373451000	-1.929352000
C	4.168102000	4.613225000	-0.068679000
H	4.848153000	4.282586000	1.949964000
H	3.373701000	4.645342000	-2.077235000
H	4.593280000	5.613889000	-0.133503000
C	-3.383225000	-1.057135000	-0.047706000
C	-3.875378000	-1.564511000	-1.253750000
C	-3.684922000	-1.713749000	1.152302000
C	-4.679034000	-2.703290000	-1.254213000
H	-3.637513000	-1.072108000	-2.194043000
C	-4.488664000	-2.850649000	1.145893000
H	-3.308846000	-1.326004000	2.098159000
C	-4.991737000	-3.343850000	-0.057035000
H	-5.058822000	-3.090733000	-2.198256000
H	-4.718179000	-3.353628000	2.084037000
H	-5.618560000	-4.234428000	-0.061919000
C	-2.957626000	1.458822000	-1.437660000
C	-3.935103000	2.450589000	-1.315344000
C	-2.373907000	1.213344000	-2.688936000
C	-4.338606000	3.175650000	-2.436303000
H	-4.373030000	2.678154000	-0.346032000
C	-2.790951000	1.932525000	-3.806376000
H	-1.591989000	0.458575000	-2.781057000
C	-3.773674000	2.914221000	-3.682400000
H	-5.094474000	3.952483000	-2.329802000
H	-2.336180000	1.730428000	-4.775058000
H	-4.091197000	3.482714000	-4.555636000
C	-2.978347000	1.323594000	1.482074000
C	-4.350091000	1.334909000	1.778954000
C	-2.087501000	1.979648000	2.336071000
C	-4.819255000	2.008342000	2.902554000
H	-5.051021000	0.806056000	1.132916000
C	-2.561529000	2.652836000	3.462944000
H	-1.020941000	1.950064000	2.117302000
C	-3.924397000	2.670573000	3.745431000
H	-5.885570000	2.012211000	3.124232000
H	-1.858753000	3.160660000	4.121754000
H	-4.292761000	3.194674000	4.626460000

Transition State TS(benzene)

E_{zpe} = -4792.458699

G^{280K} = -4792.53483718

freq= -61.44 cm^{-1}

Ir	0.009226000	0.293158000	-0.078290000
P	2.377948000	0.319423000	0.074623000
P	-2.352232000	0.484759000	-0.001989000
C	0.013824000	2.068697000	-0.283609000
O	-0.044868000	3.213372000	-0.393313000
Cl	-0.514994000	-1.757899000	-1.914512000
Ga	-0.007253000	-3.103385000	0.011093000
C	1.843614000	-3.780194000	-0.339969000
H	1.815783000	-4.508135000	-1.163907000
H	2.561290000	-2.998844000	-0.612498000
H	2.228215000	-4.301640000	0.549935000
C	-0.193038000	-1.822399000	1.608387000
H	0.561874000	-2.247618000	2.288666000
H	-0.033928000	-0.727666000	1.745999000
H	-1.182894000	-2.022406000	2.035328000
C	-1.462997000	-4.475106000	0.030571000
H	-2.366488000	-4.089527000	-0.458382000
H	-1.147631000	-5.380665000	-0.507448000
H	-1.731106000	-4.771287000	1.055707000
C	2.925145000	-0.486278000	1.627572000
C	3.797094000	-1.577477000	1.650354000
C	2.381049000	-0.013276000	2.831200000
C	4.125132000	-2.184171000	2.864405000
H	4.212165000	-1.971849000	0.724992000
C	2.723469000	-0.610062000	4.040391000
H	1.677473000	0.820598000	2.815961000
C	3.596046000	-1.700019000	4.057958000
H	4.796817000	-3.041714000	2.869858000
H	2.298018000	-0.232741000	4.969411000
H	3.854954000	-2.176400000	5.002910000
C	3.432676000	-0.363940000	-1.260767000
C	4.825827000	-0.214343000	-1.182828000
C	2.858548000	-0.958928000	-2.384714000
C	5.634210000	-0.681735000	-2.213402000
H	5.277128000	0.275573000	-0.319074000
C	3.675225000	-1.419467000	-3.420181000
H	1.777447000	-1.073950000	-2.445518000
C	5.057732000	-1.285460000	-3.334379000
H	6.715579000	-0.567564000	-2.147770000
H	3.220566000	-1.886083000	-4.293061000
H	5.692428000	-1.646520000	-4.143193000
C	3.086048000	2.020823000	0.163567000
C	3.746054000	2.537031000	1.280800000
C	2.971617000	2.804527000	-0.992668000
C	4.270582000	3.831154000	1.245373000
H	3.868694000	1.936167000	2.179744000
C	3.498788000	4.090969000	-1.025077000
H	2.464110000	2.403689000	-1.872200000

C	4.146642000	4.609163000	0.097732000
H	4.782973000	4.226213000	2.121922000
H	3.399432000	4.691799000	-1.928174000
H	4.557109000	5.618018000	0.074557000
C	-3.418634000	-1.006547000	-0.138656000
C	-3.910777000	-1.423831000	-1.379414000
C	-3.758155000	-1.726690000	1.014050000
C	-4.746609000	-2.536175000	-1.461526000
H	-3.651316000	-0.880705000	-2.285579000
C	-4.595645000	-2.836330000	0.926821000
H	-3.390090000	-1.409919000	1.988893000
C	-5.094041000	-3.241198000	-0.310584000
H	-5.125401000	-2.851020000	-2.432945000
H	-4.854423000	-3.387402000	1.830038000
H	-5.747920000	-4.109900000	-0.378388000
C	-2.917280000	1.570336000	-1.375288000
C	-3.880032000	2.570760000	-1.213311000
C	-2.316833000	1.383989000	-2.628932000
C	-4.250225000	3.364996000	-2.298751000
H	-4.334412000	2.750729000	-0.241309000
C	-2.699679000	2.172302000	-3.711499000
H	-1.547107000	0.620565000	-2.749679000
C	-3.666533000	3.164399000	-3.547706000
H	-4.994992000	4.148089000	-2.161905000
H	-2.230633000	2.016976000	-4.682268000
H	-3.957608000	3.788008000	-4.392356000
C	-2.966483000	1.268394000	1.540126000
C	-4.339129000	1.295066000	1.832701000
C	-2.062772000	1.840843000	2.440350000
C	-4.795310000	1.896799000	3.001702000
H	-5.052429000	0.834362000	1.149147000
C	-2.523936000	2.441984000	3.612405000
H	-0.995715000	1.803604000	2.223421000
C	-3.887222000	2.471908000	3.893155000
H	-5.862291000	1.911873000	3.220721000
H	-1.811053000	2.882875000	4.307902000
H	-4.246024000	2.937649000	4.810480000

Intermediate I2

E_{zpe} = -4792.447661

G^{280K} = -4792.52487113

freq= 14.45 cm^{-1}

C	4.736351000	-0.183927000	-1.292718000
C	3.421607000	-0.618173000	-1.067855000
C	2.953352000	-1.762076000	-1.717055000
C	3.789212000	-2.462351000	-2.588881000
C	5.089401000	-2.023449000	-2.816732000

C	5.563074000	-0.880772000	-2.167018000
P	2.334404000	0.311690000	0.080936000
C	2.292301000	2.016166000	-0.609917000
C	2.476483000	2.250320000	-1.976147000
C	2.303705000	3.534642000	-2.492927000
C	1.947517000	4.587624000	-1.652057000
C	1.747191000	4.354404000	-0.290019000
C	1.911464000	3.072986000	0.230101000
C	3.366925000	0.489418000	1.589863000
C	3.213485000	-0.434128000	2.628398000
C	4.032157000	-0.368224000	3.753417000
C	5.004280000	0.625595000	3.854415000
C	5.153258000	1.557698000	2.828733000
C	4.337854000	1.492722000	1.700212000
Ir	0.040453000	-0.067438000	0.128405000
C	0.003871000	0.605401000	2.154627000
P	-2.298209000	0.311039000	0.061030000
C	-3.487351000	-0.977402000	-0.470364000
C	-4.814909000	-0.980866000	-0.021061000
C	-5.698714000	-1.959459000	-0.471613000
C	-5.264807000	-2.939642000	-1.364824000
C	-3.946071000	-2.935248000	-1.813901000
C	-3.061158000	-1.953039000	-1.374386000
C	0.027423000	-0.434310000	-1.741895000
O	0.016650000	-0.491123000	-2.880450000
C	-2.539942000	1.651716000	-1.176436000
C	-3.695030000	1.733372000	-1.960593000
C	-3.852767000	2.782278000	-2.865545000
C	-2.863262000	3.755924000	-2.990748000
C	-1.708933000	3.678224000	-2.212434000
C	-1.543877000	2.627807000	-1.311869000
C	-3.077640000	0.995882000	1.574170000
C	-3.264031000	0.143415000	2.670367000
C	-3.828571000	0.628707000	3.845747000
C	-4.203405000	1.969839000	3.941390000
C	-4.016756000	2.820486000	2.855072000
C	-3.457233000	2.336892000	1.670995000
H	-0.545879000	1.558376000	2.214645000
H	-0.550277000	-0.107165000	2.782961000
H	0.981105000	0.761531000	2.622432000
H	-4.469295000	0.972567000	-1.873303000
H	-4.752008000	2.833984000	-3.477770000
H	-2.988509000	4.572230000	-3.701031000
H	-0.925032000	4.427513000	-2.307981000
H	-0.631227000	2.568297000	-0.715825000
H	-2.970136000	-0.903209000	2.599553000
H	-3.971776000	-0.042630000	4.691206000
H	-4.641347000	2.349635000	4.863562000
H	-4.310335000	3.867159000	2.922473000
H	-3.321188000	3.008367000	0.824734000
H	-5.159325000	-0.224771000	0.682957000

H	-6.728103000	-1.959545000	-0.115748000
H	-5.954798000	-3.711843000	-1.702864000
H	-3.584180000	-3.705745000	-2.492734000
H	-2.028834000	-1.993415000	-1.712234000
H	2.750920000	1.429414000	-2.638343000
H	2.449993000	3.709666000	-3.557816000
H	1.821481000	5.591031000	-2.057533000
H	1.459094000	5.171689000	0.369821000
H	1.740952000	2.888315000	1.291279000
H	2.443191000	-1.197443000	2.555608000
H	3.902724000	-1.093772000	4.555056000
H	5.641478000	0.678566000	4.736246000
H	5.904901000	2.342083000	2.906076000
H	4.453734000	2.235543000	0.911831000
H	1.945015000	-2.136692000	-1.550834000
H	3.406733000	-3.355870000	-3.079760000
H	5.740227000	-2.571398000	-3.497092000
H	6.581598000	-0.535254000	-2.338341000
H	5.117122000	0.701201000	-0.784844000
Ga	0.072818000	-2.619552000	0.661678000
C	1.838867000	-3.289084000	1.337170000
H	1.864235000	-4.344390000	1.030855000
H	2.725663000	-2.802327000	0.915757000
H	1.897942000	-3.257830000	2.433503000
C	-1.531390000	-3.040527000	1.776369000
H	-2.483029000	-2.766556000	1.308401000
H	-1.531080000	-4.129831000	1.924774000
H	-1.449826000	-2.565490000	2.763379000
Cl	-0.117876000	-3.652245000	-1.386613000

Intermediate I2 (benzene)

E_{zpe} = -4792.490350

G^{280K} = -4792.56590376

freq= 15.19 cm^{-1}

C	4.713706000	-0.156564000	-1.357736000
C	3.410985000	-0.606006000	-1.094819000
C	2.945842000	-1.766214000	-1.716966000
C	3.770954000	-2.469152000	-2.596933000
C	5.059836000	-2.016355000	-2.860039000
C	5.530655000	-0.856505000	-2.239416000
P	2.338311000	0.316638000	0.075538000
C	2.315205000	2.034969000	-0.579400000
C	2.461266000	2.286395000	-1.948064000
C	2.320480000	3.584999000	-2.437571000

C	2.030327000	4.635358000	-1.567970000
C	1.866525000	4.385672000	-0.204109000
C	2.002422000	3.090207000	0.289927000
C	3.369682000	0.439226000	1.591210000
C	3.158566000	-0.468326000	2.633758000
C	3.980540000	-0.450263000	3.758653000
C	5.012857000	0.481309000	3.855682000
C	5.216722000	1.401502000	2.828002000
C	4.399032000	1.383273000	1.699292000
Ir	0.038904000	-0.066004000	0.126285000
C	0.016599000	0.664235000	2.142852000
P	-2.310235000	0.319668000	0.067999000
C	-3.510944000	-0.952822000	-0.476926000
C	-4.846488000	-0.922107000	-0.052747000
C	-5.747052000	-1.877518000	-0.520263000
C	-5.323056000	-2.867147000	-1.407839000
C	-3.996177000	-2.897229000	-1.831992000
C	-3.093300000	-1.940363000	-1.372328000
C	0.008972000	-0.453337000	-1.730678000
O	-0.023940000	-0.508764000	-2.870286000
C	-2.520597000	1.666778000	-1.166863000
C	-3.593929000	1.700319000	-2.062074000
C	-3.711721000	2.751570000	-2.971746000
C	-2.766765000	3.775290000	-2.988580000
C	-1.692830000	3.745335000	-2.098393000
C	-1.565268000	2.692643000	-1.195189000
C	-3.091783000	0.998295000	1.583309000
C	-3.224822000	0.152135000	2.692352000
C	-3.797912000	0.625130000	3.868855000
C	-4.236572000	1.947855000	3.951858000
C	-4.106801000	2.791419000	2.851628000
C	-3.538585000	2.319673000	1.666521000
H	-0.575133000	1.591282000	2.202190000
H	-0.484034000	-0.060836000	2.802684000
H	0.995994000	0.876210000	2.584411000
H	-4.336645000	0.903805000	-2.059349000
H	-4.546660000	2.765183000	-3.671356000
H	-2.861982000	4.593435000	-3.701735000
H	-0.944981000	4.536621000	-2.110059000
H	-0.715612000	2.670784000	-0.509266000
H	-2.881589000	-0.880100000	2.632356000
H	-3.898189000	-0.041283000	4.724609000
H	-4.680315000	2.318669000	4.875197000
H	-4.451617000	3.823211000	2.908403000
H	-3.449706000	2.987232000	0.810963000
H	-5.187072000	-0.156113000	0.642646000
H	-6.782956000	-1.850444000	-0.184226000
H	-6.027210000	-3.619278000	-1.762290000
H	-3.646068000	-3.674351000	-2.509972000
H	-2.055941000	-2.005502000	-1.690721000
H	2.685893000	1.470370000	-2.634681000

H	2.438793000	3.773351000	-3.503843000
H	1.927582000	5.649651000	-1.952732000
H	1.632064000	5.201490000	0.478718000
H	1.866539000	2.898551000	1.354534000
H	2.340299000	-1.181048000	2.566513000
H	3.806649000	-1.164083000	4.562758000
H	5.653564000	0.496449000	4.736738000
H	6.014035000	2.139914000	2.903650000
H	4.560530000	2.116784000	0.910101000
H	1.945276000	-2.147723000	-1.523439000
H	3.389997000	-3.374681000	-3.067376000
H	5.703075000	-2.565789000	-3.546732000
H	6.539787000	-0.498810000	-2.440356000
H	5.093690000	0.744710000	-0.878255000
Ga	0.066423000	-2.606112000	0.652218000
C	1.821620000	-3.308649000	1.325597000
H	1.839898000	-4.362570000	1.010614000
H	2.721379000	-2.829184000	0.922768000
H	1.870559000	-3.293686000	2.423455000
C	-1.529654000	-3.068121000	1.763567000
H	-2.491167000	-2.763684000	1.335444000
H	-1.536270000	-4.165489000	1.848519000
H	-1.430002000	-2.658077000	2.778556000
Cl	-0.143416000	-3.689946000	-1.385260000

Complex 2

E_{zpe} = -2328.071857

G^{280K} = -2044.08273804

freq= 8.12 cm^{-1}

C	-4.303988000	-1.804040000	-0.981701000
C	-3.034237000	-1.639416000	-0.418967000
C	-2.272265000	-2.768326000	-0.094580000
C	-2.782699000	-4.046805000	-0.314729000
C	-4.050041000	-4.205388000	-0.872952000
C	-4.806910000	-3.083553000	-1.210195000
P	-2.316977000	0.008083000	-0.020128000
C	-3.147979000	0.434438000	1.561819000
C	-3.676702000	-0.550051000	2.401024000
C	-4.227032000	-0.198245000	3.634249000
C	-4.253705000	1.135156000	4.035572000
C	-3.725872000	2.121312000	3.201188000
C	-3.171733000	1.773594000	1.972877000
C	-3.115393000	1.168426000	-1.203749000
C	-2.376871000	1.620471000	-2.302440000
C	-2.960112000	2.475192000	-3.237518000
C	-4.279879000	2.891597000	-3.077249000
C	-5.017777000	2.456456000	-1.975864000

C	-4.438996000	1.600967000	-1.041249000
Ir	0.011100000	-0.007302000	-0.073949000
C	0.038915000	1.028888000	1.820557000
P	2.302196000	0.054422000	0.081410000
C	3.273778000	-0.438664000	-1.402118000
C	4.126085000	0.436516000	-2.079969000
C	4.818609000	0.001106000	-3.211831000
C	4.667645000	-1.305719000	-3.667502000
C	3.818099000	-2.183531000	-2.991423000
C	3.122466000	-1.751627000	-1.867236000
C	-0.003318000	-0.898311000	-1.716289000
O	-0.015335000	-1.449859000	-2.723781000
C	3.021347000	-1.049748000	1.364369000
C	4.366919000	-1.438472000	1.317666000
C	4.889272000	-2.275974000	2.300790000
C	4.070200000	-2.739017000	3.331022000
C	2.727667000	-2.367845000	3.372700000
C	2.201059000	-1.527990000	2.391681000
C	2.950253000	1.732813000	0.447979000
C	2.268613000	2.810668000	-0.129751000
C	2.728132000	4.111840000	0.058921000
C	3.861503000	4.345691000	0.838353000
C	4.532106000	3.276224000	1.429073000
C	4.080568000	1.970632000	1.233853000
H	1.022796000	1.161776000	2.292118000
H	-0.362676000	2.043432000	1.662440000
H	-0.616365000	0.541363000	2.558383000
H	5.004219000	-1.095826000	0.501897000
H	5.936080000	-2.573936000	2.257319000
H	4.478479000	-3.397617000	4.096800000
H	2.082385000	-2.736391000	4.168927000
H	1.150411000	-1.240857000	2.407738000
H	1.365606000	2.615241000	-0.711141000
H	2.193290000	4.945717000	-0.393704000
H	4.216282000	5.363923000	0.993467000
H	5.409038000	3.456333000	2.049529000
H	4.604118000	1.141224000	1.706760000
H	4.253630000	1.459119000	-1.727675000
H	5.479557000	0.690378000	-3.735840000
H	5.208941000	-1.642220000	-4.550833000
H	3.691580000	-3.205572000	-3.345593000
H	2.453823000	-2.437030000	-1.344246000
H	-3.663799000	-1.594822000	2.093264000
H	-4.639017000	-0.972614000	4.280020000
H	-4.684877000	1.407777000	4.997996000
H	-3.740144000	3.165462000	3.510592000
H	-2.757684000	2.547101000	1.326054000
H	-1.338561000	1.308457000	-2.409700000
H	-2.376163000	2.820426000	-4.089495000
H	-4.733323000	3.562607000	-3.805858000
H	-6.046518000	2.788007000	-1.840744000

H	-5.014905000	1.277863000	-0.174020000
H	-1.271794000	-2.629226000	0.319002000
H	-2.183111000	-4.919377000	-0.059185000
H	-4.445790000	-5.204080000	-1.053888000
H	-5.792832000	-3.203672000	-1.657300000
H	-4.899311000	-0.934985000	-1.256243000

Complex 2(benzene)

E_{zpe} = -2328.112504

G^{280K} = -2328.18286058

freq= 10.00 cm^{-1}

C	-4.250161000	-1.850244000	-1.022056000
C	-3.003197000	-1.657730000	-0.418383000
C	-2.225896000	-2.770804000	-0.072508000
C	-2.699434000	-4.059971000	-0.311353000
C	-3.944199000	-4.246086000	-0.911439000
C	-4.715436000	-3.140869000	-1.270086000
P	-2.326023000	0.004818000	-0.010099000
C	-3.157881000	0.418653000	1.574487000
C	-3.655352000	-0.574206000	2.423483000
C	-4.197408000	-0.229664000	3.662671000
C	-4.246790000	1.104523000	4.060234000
C	-3.751598000	2.098935000	3.215361000
C	-3.205564000	1.759076000	1.980753000
C	-3.134556000	1.155903000	-1.195156000
C	-2.390533000	1.647389000	-2.273321000
C	-2.982035000	2.500390000	-3.205067000
C	-4.316242000	2.875228000	-3.061791000
C	-5.060475000	2.400411000	-1.980853000
C	-4.473298000	1.546919000	-1.049405000
Ir	0.010105000	0.013817000	-0.057377000
C	0.040613000	0.997270000	1.870977000
P	2.305972000	0.064830000	0.083449000
C	3.251573000	-0.436595000	-1.414134000
C	4.089251000	0.433999000	-2.115631000
C	4.764373000	-0.011472000	-3.254424000
C	4.610627000	-1.324051000	-3.692985000
C	3.774528000	-2.197087000	-2.993699000
C	3.095237000	-1.755111000	-1.863036000
C	-0.016901000	-0.825338000	-1.718738000
O	-0.048182000	-1.343106000	-2.745513000
C	3.035167000	-1.045672000	1.355962000
C	4.389451000	-1.405429000	1.315607000
C	4.918562000	-2.254243000	2.285492000

C	4.098358000	-2.758139000	3.295982000
C	2.747724000	-2.416795000	3.330815000
C	2.214697000	-1.565531000	2.362790000
C	2.952322000	1.746174000	0.440718000
C	2.270042000	2.816321000	-0.152222000
C	2.718465000	4.122133000	0.031785000
C	3.842307000	4.369073000	0.821343000
C	4.512837000	3.308153000	1.427859000
C	4.072363000	1.997703000	1.237644000
H	1.025398000	1.122637000	2.344794000
H	-0.368797000	2.014158000	1.745844000
H	-0.609264000	0.488443000	2.600398000
H	5.030799000	-1.031498000	0.516784000
H	5.972199000	-2.528708000	2.247163000
H	4.512351000	-3.425297000	4.051521000
H	2.101225000	-2.816774000	4.111068000
H	1.157581000	-1.302726000	2.375556000
H	1.375327000	2.612709000	-0.744174000
H	2.183189000	4.949010000	-0.433543000
H	4.188647000	5.391074000	0.972493000
H	5.382259000	3.498534000	2.056213000
H	4.597830000	1.177278000	1.723878000
H	4.221008000	1.461134000	-1.777882000
H	5.414660000	0.674413000	-3.796482000
H	5.139694000	-1.668968000	-4.580773000
H	3.647089000	-3.224147000	-3.333677000
H	2.437165000	-2.437670000	-1.322024000
H	-3.623725000	-1.620501000	2.121668000
H	-4.584096000	-1.010735000	4.316401000
H	-4.670513000	1.371570000	5.027793000
H	-3.784886000	3.143987000	3.521155000
H	-2.816328000	2.540917000	1.327994000
H	-1.341176000	1.370048000	-2.370171000
H	-2.392946000	2.876544000	-4.040586000
H	-4.776330000	3.544671000	-3.788000000
H	-6.101312000	2.698701000	-1.859738000
H	-5.056801000	1.192209000	-0.199586000
H	-1.241414000	-2.613531000	0.372471000
H	-2.088224000	-4.919453000	-0.038433000
H	-4.309969000	-5.253447000	-1.108120000
H	-5.683141000	-3.281705000	-1.750306000
H	-4.858591000	-0.995973000	-1.313879000

Species B

E_{zpe} = -4792.435921

G^{280K} = -4792.51897291

freq= 12.04 cm^{-1}

C	-4.204495000	1.643852000	0.132264000
C	-3.238674000	0.987873000	-0.635887000
C	-2.933848000	1.463068000	-1.918176000
C	-3.593797000	2.576541000	-2.427859000
C	-4.559591000	3.228307000	-1.659361000
C	-4.860788000	2.763495000	-0.381995000
P	-2.388961000	-0.533549000	-0.060598000
C	-3.167516000	-1.828765000	-1.108621000
C	-4.370300000	-1.586668000	-1.784488000
C	-4.958666000	-2.594311000	-2.547564000
C	-4.352745000	-3.845960000	-2.641295000
C	-3.157620000	-4.090387000	-1.966252000
C	-2.563097000	-3.088325000	-1.202179000
C	-3.064638000	-0.801435000	1.615536000
C	-2.397677000	-0.200997000	2.688928000
C	-2.911787000	-0.313710000	3.977630000
C	-4.083880000	-1.037263000	4.200263000
C	-4.741406000	-1.647653000	3.133462000
C	-4.235271000	-1.529973000	1.839171000
Ir	-0.040704000	-0.492519000	-0.086640000
P	2.295436000	-0.714885000	-0.060855000
C	3.248458000	0.743817000	-0.637643000
C	4.191784000	1.391128000	0.163927000
C	4.909240000	2.476420000	-0.343401000
C	4.693340000	2.912138000	-1.647834000
C	3.748024000	2.269607000	-2.449575000
C	3.025424000	1.193527000	-1.946062000
C	0.035473000	1.137922000	-0.812039000
O	0.096367000	2.232013000	-1.202198000
C	2.955447000	-2.054466000	-1.132543000
C	4.205872000	-1.931418000	-1.752639000
C	4.702670000	-2.970692000	-2.537331000
C	3.956081000	-4.135374000	-2.709997000
C	2.712724000	-4.260925000	-2.092578000
C	2.209941000	-3.226353000	-1.305671000
C	2.968059000	-1.048150000	1.605033000
C	2.342799000	-0.436322000	2.696889000
C	2.864800000	-0.599975000	3.977327000
C	4.000626000	-1.385770000	4.173428000
C	4.615584000	-2.007663000	3.087821000
C	4.102887000	-1.839013000	1.802097000
H	4.793351000	-1.022569000	-1.627785000
H	5.674964000	-2.866349000	-3.016968000
H	4.343871000	-4.944867000	-3.327321000
H	2.126008000	-5.169168000	-2.222685000
H	1.247670000	-3.327867000	-0.806803000
H	1.445831000	0.161959000	2.536234000
H	2.376351000	-0.120722000	4.824373000
H	4.402824000	-1.520359000	5.176820000
H	5.496064000	-2.630228000	3.240549000
H	4.581937000	-2.329978000	0.955711000

H	4.370643000	1.050503000	1.182871000
H	5.639603000	2.980111000	0.288198000
H	5.252012000	3.761098000	-2.039439000
H	3.567962000	2.614382000	-3.466668000
H	2.287161000	0.691255000	-2.573553000
H	-4.850450000	-0.611270000	-1.720090000
H	-5.893037000	-2.396582000	-3.071173000
H	-4.812330000	-4.630788000	-3.240952000
H	-2.680902000	-5.067349000	-2.032930000
H	-1.639371000	-3.281250000	-0.658929000
H	-1.468874000	0.341016000	2.506574000
H	-2.389811000	0.154201000	4.810914000
H	-4.480823000	-1.132550000	5.210199000
H	-5.650471000	-2.221684000	3.307404000
H	-4.747913000	-2.010665000	1.006438000
H	-2.182596000	0.951577000	-2.521909000
H	-3.348531000	2.941076000	-3.424243000
H	-5.069374000	4.105778000	-2.054675000
H	-5.606972000	3.274945000	0.224267000
H	-4.448070000	1.283414000	1.130563000
Cl	-0.114279000	-2.554299000	1.193189000
Ga	0.322907000	4.169396000	0.200532000
C	0.855587000	3.068836000	1.781299000
H	0.070466000	2.343802000	2.036859000
H	1.788354000	2.523812000	1.584860000
H	1.021438000	3.708056000	2.660278000
C	1.709845000	5.075509000	-0.905600000
H	2.724580000	4.762307000	-0.634395000
H	1.549260000	4.840690000	-1.966941000
H	1.637660000	6.166532000	-0.795482000
C	-1.583585000	4.715714000	0.025862000
H	-1.810011000	5.096401000	-0.978116000
H	-2.251620000	3.869882000	0.233463000
H	-1.819769000	5.510524000	0.748351000

Species B (benzene)

E_{zpe} = -4792.476310

G^{280K} = -4792.55678701

freq= 10.31 cm^{-1}

C	-4.217000000	1.625080000	0.112476000
C	-3.238056000	0.968601000	-0.638612000
C	-2.919629000	1.435551000	-1.921059000
C	-3.578713000	2.541840000	-2.447676000
C	-4.557792000	3.194461000	-1.696240000
C	-4.872731000	2.737511000	-0.419078000
P	-2.387766000	-0.546158000	-0.045327000
C	-3.122852000	-1.844132000	-1.123234000

C	-4.325526000	-1.618955000	-1.805892000
C	-4.878906000	-2.623490000	-2.598766000
C	-4.238774000	-3.856322000	-2.716049000
C	-3.044747000	-4.085391000	-2.033661000
C	-2.485911000	-3.085509000	-1.239970000
C	-3.098593000	-0.830026000	1.614108000
C	-2.474352000	-0.207930000	2.701344000
C	-3.013211000	-0.333915000	3.978904000
C	-4.168207000	-1.091648000	4.177088000
C	-4.783370000	-1.722807000	3.096890000
C	-4.252098000	-1.592676000	1.813606000
Ir	-0.035165000	-0.481679000	-0.034105000
P	2.308195000	-0.696630000	-0.042842000
C	3.252424000	0.765078000	-0.628758000
C	4.212616000	1.407741000	0.156806000
C	4.930752000	2.486247000	-0.364760000
C	4.698641000	2.919578000	-1.667562000
C	3.734682000	2.283148000	-2.452363000
C	3.011713000	1.213561000	-1.934815000
C	0.025247000	1.148413000	-0.752572000
O	0.070395000	2.242288000	-1.149706000
C	2.939833000	-2.023132000	-1.149046000
C	4.199484000	-1.913258000	-1.753757000
C	4.674492000	-2.936487000	-2.572093000
C	3.897196000	-4.072670000	-2.795284000
C	2.644776000	-4.185756000	-2.193982000
C	2.164528000	-3.166388000	-1.373276000
C	3.011044000	-1.052915000	1.607231000
C	2.440470000	-0.408721000	2.711289000
C	2.974421000	-0.602208000	3.982722000
C	4.068614000	-1.449951000	4.158709000
C	4.630053000	-2.101593000	3.061805000
C	4.104991000	-1.903858000	1.784716000
H	4.812323000	-1.027367000	-1.590744000
H	5.654221000	-2.841842000	-3.038970000
H	4.268389000	-4.869267000	-3.439405000
H	2.033698000	-5.071448000	-2.363619000
H	1.194892000	-3.260903000	-0.888326000
H	1.574929000	0.239366000	2.570147000
H	2.526997000	-0.098456000	4.838543000
H	4.479906000	-1.608491000	5.155171000
H	5.478229000	-2.771388000	3.198336000
H	4.544390000	-2.420131000	0.932065000
H	4.408347000	1.069348000	1.173523000
H	5.676248000	2.984823000	0.253478000
H	5.260484000	3.761086000	-2.071447000
H	3.542477000	2.624696000	-3.468646000
H	2.262032000	0.714829000	-2.551846000
H	-4.834308000	-0.659411000	-1.724285000
H	-5.813208000	-2.437997000	-3.127529000
H	-4.671191000	-4.638394000	-3.339458000

H	-2.541179000	-5.047748000	-2.117580000
H	-1.564554000	-3.269664000	-0.690358000
H	-1.560991000	0.366218000	2.540283000
H	-2.524423000	0.151559000	4.822549000
H	-4.585042000	-1.196397000	5.178304000
H	-5.679704000	-2.322261000	3.251751000
H	-4.734306000	-2.089409000	0.972107000
H	-2.160720000	0.922120000	-2.513964000
H	-3.323669000	2.897880000	-3.445031000
H	-5.068464000	4.065123000	-2.106143000
H	-5.631019000	3.248536000	0.172854000
H	-4.474674000	1.272031000	1.110090000
Cl	-0.092014000	-2.573215000	1.221927000
Ga	0.280487000	4.191034000	0.204401000
C	0.825939000	3.112113000	1.793102000
H	0.071450000	2.344085000	2.016484000
H	1.793990000	2.621417000	1.624358000
H	0.926285000	3.749446000	2.684202000
C	1.646553000	5.097309000	-0.926073000
H	2.658175000	4.716366000	-0.741001000
H	1.414295000	4.963486000	-1.992090000
H	1.644066000	6.179235000	-0.725444000
C	-1.625767000	4.738535000	0.030536000
H	-1.861116000	5.071686000	-0.988823000
H	-2.303790000	3.916398000	0.294944000
H	-1.839560000	5.576110000	0.712093000

Species C

E_{zpe} = -4792.441615

G^{280K} = -4792.51928737

freq= 14.99 cm^{-1}

C	4.061568000	1.530236000	1.947649000
C	3.228842000	0.451156000	1.626561000
C	3.121606000	-0.622754000	2.516854000
C	3.828613000	-0.614369000	3.716646000
C	4.648332000	0.466483000	4.037918000
C	4.764768000	1.535933000	3.151760000
P	2.339792000	0.350718000	0.022490000
C	3.449811000	-0.676971000	-1.009252000
C	4.800457000	-0.831349000	-0.673255000
C	5.627201000	-1.623703000	-1.466992000
C	5.111694000	-2.265070000	-2.592936000
C	3.767890000	-2.109394000	-2.928556000
C	2.934620000	-1.317891000	-2.140471000
C	2.478950000	2.054084000	-0.635367000
C	1.846326000	3.079156000	0.080736000
C	1.866189000	4.383908000	-0.402931000

C	2.505939000	4.668727000	-1.611134000
C	3.129315000	3.648724000	-2.325791000
C	3.118694000	2.340163000	-1.840902000
Ir	0.010878000	-0.031547000	0.086167000
P	-2.333807000	0.276188000	0.034734000
C	-3.099181000	0.495060000	1.690309000
C	-3.632637000	1.720822000	2.100875000
C	-4.176017000	1.852199000	3.379436000
C	-4.196437000	0.764996000	4.249421000
C	-3.668163000	-0.460353000	3.841596000
C	-3.117662000	-0.594894000	2.570803000
C	0.002237000	-0.414599000	1.862961000
O	-0.007517000	-0.658525000	2.981966000
C	-3.394111000	-0.959024000	-0.801441000
C	-4.618876000	-1.379186000	-0.271329000
C	-5.385405000	-2.318965000	-0.959374000
C	-4.936220000	-2.835599000	-2.173748000
C	-3.722825000	-2.403908000	-2.708716000
C	-2.950523000	-1.466427000	-2.027374000
C	-2.734875000	1.853069000	-0.807220000
C	-1.813494000	2.904060000	-0.764102000
C	-2.132833000	4.136379000	-1.327406000
C	-3.370946000	4.323220000	-1.942021000
C	-4.288492000	3.274950000	-1.993193000
C	-3.973568000	2.040217000	-1.426879000
H	-4.974365000	-0.982857000	0.678380000
H	-6.334748000	-2.650025000	-0.540686000
H	-5.533594000	-3.575858000	-2.704537000
H	-3.366663000	-2.802841000	-3.657434000
H	-2.003955000	-1.120623000	-2.441313000
H	-0.835398000	2.749122000	-0.310826000
H	-1.402944000	4.944399000	-1.300718000
H	-3.617399000	5.284789000	-2.390661000
H	-5.252406000	3.414391000	-2.480576000
H	-4.690710000	1.221187000	-1.474055000
H	-3.627605000	2.575107000	1.426209000
H	-4.587196000	2.811136000	3.691822000
H	-4.622336000	0.871221000	5.246305000
H	-3.677163000	-1.315366000	4.515871000
H	-2.704593000	-1.552909000	2.259025000
H	5.206791000	-0.346297000	0.213039000
H	6.675551000	-1.745693000	-1.198414000
H	5.758404000	-2.891114000	-3.206552000
H	3.356432000	-2.611679000	-3.802927000
H	1.886438000	-1.191443000	-2.401776000
H	1.342714000	2.850700000	1.022119000
H	1.379757000	5.178822000	0.161598000
H	2.516576000	5.688044000	-1.994982000
H	3.623717000	3.867890000	-3.271006000
H	3.597307000	1.542477000	-2.407218000
H	2.492589000	-1.473569000	2.267536000

H	3.733591000	-1.455994000	4.400963000
H	5.197637000	0.474960000	4.978497000
H	5.407898000	2.380833000	3.394277000
H	4.167744000	2.366032000	1.258266000
Cl	0.008331000	0.532975000	-2.276039000
Ga	0.083291000	-2.872806000	-0.066171000
C	-0.001273000	-3.158131000	-2.056634000
H	-0.065891000	-2.234038000	-2.640252000
H	0.899817000	-3.704711000	-2.368587000
H	-0.880966000	-3.775083000	-2.286494000
C	1.806619000	-3.440543000	0.805949000
H	1.929864000	-4.493524000	0.505335000
H	2.707990000	-2.910881000	0.474825000
H	1.752827000	-3.428567000	1.903053000
C	-1.499494000	-3.482137000	1.012307000
H	-1.391731000	-3.253765000	2.081211000
H	-2.469495000	-3.123804000	0.647329000
H	-1.505236000	-4.579951000	0.919839000

Species C (benzene)

E_{zpe} = -4792.482370

G^{280K} = -4792.55955286

freq= 12.62 cm^{-1}

C	4.031964000	1.515810000	1.977300000
C	3.224857000	0.427748000	1.622879000
C	3.129002000	-0.667018000	2.489201000
C	3.820863000	-0.671394000	3.697702000
C	4.613898000	0.419314000	4.052799000
C	4.719274000	1.509501000	3.191015000
P	2.347130000	0.342157000	0.010613000
C	3.453927000	-0.692412000	-1.018591000
C	4.812190000	-0.820266000	-0.701077000
C	5.639995000	-1.611637000	-1.495082000
C	5.118461000	-2.278091000	-2.603822000
C	3.767278000	-2.149598000	-2.921348000
C	2.932955000	-1.360126000	-2.131675000
C	2.501430000	2.047991000	-0.636940000
C	1.852212000	3.068876000	0.071088000
C	1.898125000	4.379568000	-0.395295000
C	2.579642000	4.674394000	-1.578169000
C	3.218884000	3.658605000	-2.285231000
C	3.183226000	2.344103000	-1.817300000
Ir	0.011824000	-0.034166000	0.066225000

P	-2.339022000	0.286071000	0.033051000
C	-3.074392000	0.514612000	1.701231000
C	-3.578712000	1.748452000	2.124914000
C	-4.094387000	1.886219000	3.414441000
C	-4.118312000	0.796854000	4.282003000
C	-3.620731000	-0.437052000	3.860926000
C	-3.095859000	-0.577113000	2.579665000
C	0.012949000	-0.392808000	1.843671000
O	0.015277000	-0.606666000	2.969687000
C	-3.413894000	-0.948830000	-0.786754000
C	-4.629288000	-1.374656000	-0.239560000
C	-5.408476000	-2.307200000	-0.924169000
C	-4.983300000	-2.809078000	-2.153467000
C	-3.780305000	-2.370563000	-2.706630000
C	-2.994698000	-1.442603000	-2.027216000
C	-2.746343000	1.859651000	-0.812768000
C	-1.827645000	2.913075000	-0.767707000
C	-2.148007000	4.145039000	-1.331784000
C	-3.384257000	4.328012000	-1.951817000
C	-4.298613000	3.276986000	-2.006141000
C	-3.983783000	2.043425000	-1.436794000
H	-4.971604000	-0.987793000	0.718936000
H	-6.350485000	-2.642900000	-0.492079000
H	-5.591428000	-3.542158000	-2.682499000
H	-3.443736000	-2.755735000	-3.668444000
H	-2.056628000	-1.091995000	-2.456323000
H	-0.852707000	2.760781000	-0.306359000
H	-1.422077000	4.956677000	-1.301872000
H	-3.631715000	5.288799000	-2.402185000
H	-5.261097000	3.413328000	-2.497761000
H	-4.702335000	1.225599000	-1.484838000
H	-3.573265000	2.605686000	1.453905000
H	-4.481415000	2.851996000	3.737156000
H	-4.522886000	0.907678000	5.287482000
H	-3.633198000	-1.293746000	4.533461000
H	-2.704039000	-1.540887000	2.258050000
H	5.226187000	-0.314101000	0.170016000
H	6.694474000	-1.711783000	-1.240741000
H	5.766357000	-2.901958000	-3.218780000
H	3.352421000	-2.669844000	-3.783902000
H	1.879244000	-1.254914000	-2.380329000
H	1.318858000	2.834458000	0.994793000
H	1.399060000	5.171493000	0.162658000
H	2.610199000	5.698555000	-1.948334000
H	3.747110000	3.885452000	-3.210481000
H	3.677353000	1.551987000	-2.378491000
H	2.517866000	-1.523376000	2.214322000
H	3.735183000	-1.529526000	4.362894000
H	5.150925000	0.418804000	5.000691000
H	5.341868000	2.362344000	3.459041000
H	4.133430000	2.368647000	1.308535000

Cl	0.013881000	0.525134000	-2.309224000
Ga	0.048465000	-2.855836000	-0.050758000
C	-0.062278000	-3.163152000	-2.037079000
H	-0.132263000	-2.252834000	-2.641662000
H	0.831382000	-3.721954000	-2.352136000
H	-0.944279000	-3.785986000	-2.245498000
C	1.767484000	-3.483625000	0.790795000
H	1.851091000	-4.535243000	0.468487000
H	2.685232000	-2.981854000	0.459558000
H	1.731788000	-3.494947000	1.889360000
C	-1.513596000	-3.505541000	1.035752000
H	-1.415756000	-3.293387000	2.109364000
H	-2.499403000	-3.180860000	0.679972000
H	-1.482864000	-4.602999000	0.928775000

$(GaMe_3)_2$

E_{zpe} = -4088.117512

G^{280K} = -4088.15862295

freq= 54.18 cm^{-1}

Ga	1.306711000	-0.013277000	-0.000380000
C	2.348040000	1.673428000	0.000467000
H	2.991398000	1.737752000	0.887598000
H	2.993120000	1.737737000	-0.885412000
H	1.677573000	2.542490000	-0.000187000
C	2.041790000	-1.857482000	0.000669000
H	1.244223000	-2.610671000	0.001240000
H	2.668541000	-2.027148000	-0.884857000
H	2.668708000	-2.025918000	0.886311000
C	-0.000249000	0.227612000	1.772198000
H	0.000139000	1.291788000	2.031850000
H	-0.859781000	-0.246780000	2.271164000
H	0.859563000	-0.247233000	2.270231000
Ga	-1.306531000	-0.013251000	0.000190000
C	-2.348549000	1.673038000	-0.000149000
H	-2.992555000	1.737155000	0.886532000
H	-1.678617000	2.542510000	-0.000533000
H	-2.993090000	1.736772000	-0.886463000
C	0.000324000	0.227422000	-1.772426000
H	0.860569000	-0.246074000	-2.271034000
H	-0.858745000	-0.248322000	-2.270872000
H	-0.000856000	1.291591000	-2.032113000
C	-2.041925000	-1.857361000	-0.000227000
H	-2.669292000	-2.026110000	0.885048000
H	-2.668418000	-2.026244000	-0.886087000
H	-1.244652000	-2.610858000	0.000270000

$(GaMe_3)_2$ (benzene)

E_{zpe} = -4088.121189

G^{280K} = -4088.16124613

freq= 54.39 cm^{-1}

Ga	-1.305604000	0.014043000	0.001521000
C	-2.351961000	-1.667905000	0.008072000
H	-3.065178000	-1.689497000	0.843497000
H	-2.928401000	-1.769990000	-0.921906000
H	-1.695382000	-2.543685000	0.097430000
C	-2.038652000	1.859173000	-0.017086000
H	-1.242730000	2.615148000	-0.019215000
H	-2.663295000	2.023937000	-0.906008000
H	-2.669971000	2.036385000	0.864754000
C	-0.000060000	-0.211616000	1.772989000
H	0.000184000	-1.273178000	2.046814000
H	0.858013000	0.266284000	2.273372000
H	-0.858270000	0.265871000	2.273540000
Ga	1.305606000	0.014041000	0.001367000
C	2.351949000	-1.667910000	0.008312000
H	3.064874000	-1.689503000	0.843985000
H	1.695325000	-2.543679000	0.097451000
H	2.928708000	-1.770021000	-0.921465000
C	0.000062000	-0.261309000	-1.762813000
H	-0.858482000	0.199975000	-2.277501000
H	0.858654000	0.199735000	-2.277646000
H	-0.000084000	-1.331461000	-2.001762000
C	2.038657000	1.859170000	-0.016963000
H	2.670021000	2.036230000	0.864875000
H	2.663256000	2.024082000	-0.905888000
H	1.242738000	2.615148000	-0.018928000

$(GaMe_2Cl)_2$

E_{zpe} = -4928.716358

$G_{280.0}$ = -4928.760232

freq= 9.12 cm^{-1}

Ga	1.710348000	0.000000000	0.000059000
C	2.447395000	1.821647000	0.000320000
H	3.065123000	1.989773000	-0.890559000
H	1.628426000	2.550291000	0.001740000
H	3.067333000	1.988779000	0.889848000
C	2.447386000	-1.821651000	-0.000457000
H	3.066059000	-1.989619000	0.889795000
H	1.628411000	-2.550288000	-0.000878000
H	3.066377000	-1.988952000	-0.890614000

Cl	0.000013000	0.000422000	-1.701038000
Ga	-1.710337000	0.000000000	-0.000029000
C	-2.447411000	1.821637000	0.000302000
H	-3.067172000	1.988776000	0.889953000
H	-1.628461000	2.550301000	0.001533000
H	-3.065327000	1.989727000	-0.890455000
C	-2.447409000	-1.821637000	-0.000287000
H	-3.067260000	-1.988780000	-0.889874000
H	-1.628458000	-2.550300000	-0.001604000
H	-3.065233000	-1.989727000	0.890533000
Cl	-0.000009000	-0.000420000	1.701062000

$(GaMe_2Cl)_2$ (benzene)

E_{zpe} = -4928.721348

G^{280K} = -4928.76105274

freq= 56.93 cm^{-1}

Ga	1.717255000	-0.000025000	-0.000023000
C	2.429869000	1.827721000	0.001431000
H	3.048152000	2.000377000	-0.889214000
H	1.608084000	2.554403000	0.002788000
H	3.049647000	1.998641000	0.891363000
C	2.429453000	-1.827932000	-0.001684000
H	3.048421000	-2.000625000	0.888476000
H	1.607499000	-2.554425000	-0.002310000
H	3.048468000	-1.999095000	-0.892102000
Cl	-0.000048000	0.002127000	-1.708902000
Ga	-1.717251000	-0.000025000	0.000036000
C	-2.429875000	1.827717000	0.001589000
H	-3.049473000	1.998630000	0.891648000
H	-1.608097000	2.554407000	0.002786000
H	-3.048342000	2.000370000	-0.888928000
C	-2.429458000	-1.827929000	-0.001383000
H	-3.049176000	-1.999010000	-0.891326000
H	-1.607509000	-2.554427000	-0.002702000
H	-3.047725000	-2.000698000	0.889251000
Cl	0.000049000	-0.001800000	1.708910000

$GaMe_3$

E_{zpe} = -2044.050256

G^{280K} = -2044.08273804

freq= 23.65 cm^{-1}

Ga	-0.001403000	-0.001835000	-0.001034000
C	-1.890538000	-0.618086000	0.002019000

H	-2.075649000	-1.285727000	0.856034000
H	-2.608209000	0.210622000	0.045743000
H	-2.094581000	-1.203052000	-0.907170000
C	0.407474000	1.943144000	-0.001598000
H	1.470340000	2.154745000	-0.173512000
H	-0.182729000	2.465647000	-0.767695000
H	0.126223000	2.378650000	0.969097000
C	1.486443000	-1.320173000	0.001924000
H	2.156319000	-1.133442000	0.853872000
H	1.140929000	-2.360225000	0.051196000
H	2.090565000	-1.199642000	-0.909572000

$GaMe_3$ (benzene)

E_{zpe} = -2044.052522

G^{280K} = -2044.08388837

freq= 30.60 cm^{-1}

Ga	-0.000088000	-0.000079000	-0.000188000
C	0.002890000	1.987562000	0.000397000
H	0.529463000	2.362070000	-0.888902000
H	-1.005737000	2.416357000	0.013270000
H	0.553582000	2.363010000	0.874528000
C	-1.722987000	-0.991289000	0.000023000
H	-1.590811000	-2.079208000	-0.008300000
H	-2.312437000	-0.718757000	0.886999000
H	-2.321932000	-0.705456000	-0.876354000
C	1.720391000	-0.996009000	-0.000021000
H	1.774112000	-1.655691000	-0.877500000
H	2.595728000	-0.336785000	-0.005860000
H	1.778990000	-1.644674000	0.885556000

$GaMe_2Cl$

E_{zpe} = -2464.330596

G^{280K} = -2464.36097452

freq= 47.89 cm^{-1}

Ga	0.000000000	0.000000000	0.333146000
C	0.000000000	1.797113000	1.130855000
H	0.924159000	2.317737000	0.847960000
H	-0.840255000	2.377172000	0.729202000
H	-0.071373000	1.767910000	2.223667000
C	0.000000000	-1.797113000	1.130855000
H	-0.924159000	-2.317737000	0.847960000
H	0.840255000	-2.377172000	0.729202000
H	0.071373000	-1.767910000	2.223667000

Cl	0.000000000	0.000000000	-1.852908000

$GaMe_2Cl$ (benzene)

E_{zpe} = -2464.336940

G^{280K} = -2464.36612697

freq= 119.81 cm^{-1}

Ga	0.000000000	0.000000000	0.346905000
C	0.000000000	1.806167000	1.113939000
H	0.886385000	2.352134000	0.764377000
H	-0.886438000	2.352159000	0.764557000
H	0.000110000	1.788160000	2.210314000
C	0.000000000	-1.806167000	1.113939000
H	-0.886385000	-2.352134000	0.764377000
H	0.886438000	-2.352159000	0.764557000
H	-0.000110000	-1.788160000	2.210314000
Cl	0.000000000	0.000000000	-1.858813000

Infrared spectra