Electronic Supplementary Information

Does the Metal Protect the Ancillary Ligands? C-H Strengthening and Deactivation in Amines and Phosphines upon Metal-Binding

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Computational Details

All calculations were carried out with Gaussian09[1] at the DFT(M06) level.[2–4] Geometries were fully optimized without any geometry or symmetry constraints by using the double-ζ 6-31G** basis set[5,6] (C, N, O and H) with LANL08(f,d) quasi-relativistic pseudo-potentials on the heaviest atoms (metal, Cl and P).[7] Frequencies were computed analytically in order to classify all stationary points as either minima (reactants and products) or saddle points (transition states) in the potential energy surface. These calculations were also used to estimate the thermochemistry, including the zero-point, thermal and entropy energies, T. The nature of the transition states was further confirmed by means of IRC calculations.[8,9] Potential energies were refined by means of single point calculations with the triple-ζ 6-311++G** basis set with LANL08(f) pseudo-potentials on the metal atoms (E).[5–7] The single point coupled-cluster calculations were performed at the CCSD(T) level[10–14] with the cc-pVTZ basis set for all elements except the metal, which was described with the cc-pVTZ-PP (E).[15–17] Spin densities and NLMOs were obtained from NBO analysis (version 5.9).[18] Deletion calculations with NBO showed that the total energy of the system changes by 20.2 and 8.2 kcal mol^{-1} in the free tacn and $[Ir(tacn)(Cl)_3]$ systems (**7**), respectively, when the N(LP) → σ*(C-H) interaction is supressed. All relative energies discussed in the text were obtained from G, which was calculated by adding the thermochemistry energies (T) to the triple-ζ potential energies (E). The influence of the nature of the DFT functional on $\Delta\Delta G^{\ddagger}$ was explored for complexes **2**, **7** and **8** by means of single point calculations with the PBE0,[19] TPSSh[20] and B3LYP[21]+GD3[22] functionals (Table S1).

Theoretical References

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Additional Figures (S1, S2 and S3)

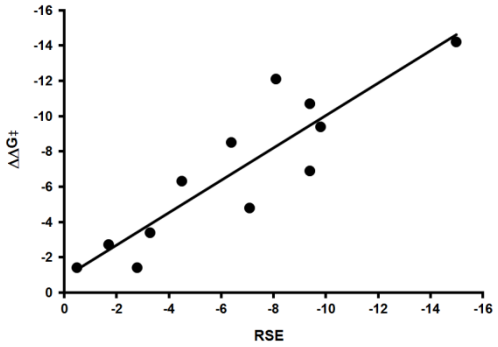

Fig. S1 Plot and linear regression of $\Delta\Delta G^{\ddagger}$ vs. RSE (kcal mol^{-1}).

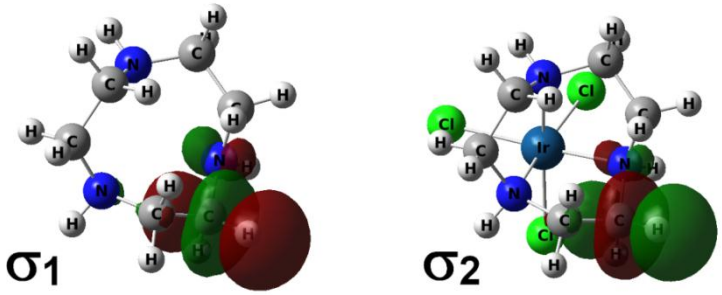

Fig. S2 NLMOs (natural localized molecular orbitals) of the σ*(C-H) orbitals in free tacn (σ_1) and [Ir(tacn)Cl_3] (σ_2) from NBO analysis.

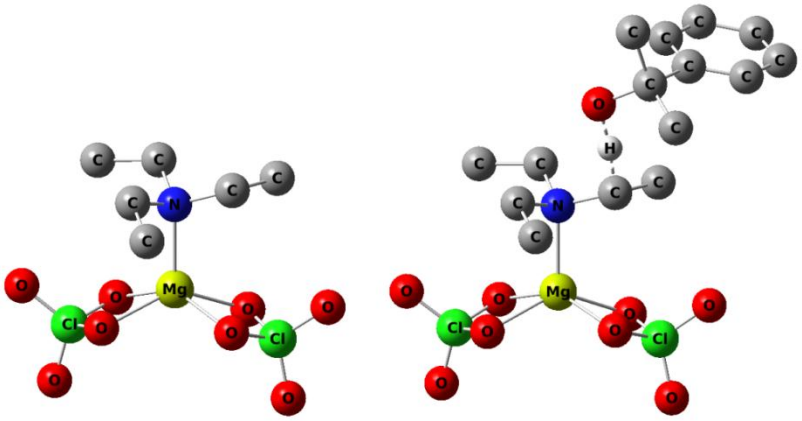

Fig. S3 Optimized geometries of the Mg-TEA complex, **9** (left), and the TS for H abstraction by the cumyloxyl radical (right).

Influence of the DFT Functional on $\Delta\Delta G^{\ddagger}$

Table S1 $\Delta\Delta G^{\ddagger}$ values, in kcal mol^{-1}, for complexes **2**, **7** and **8** with different DFT functionals.

Complex	M/L	Position	M06	PBE0	TPSSh	B3LYP+GD3
2	Pt/dmpe	$CH_2(PMe_2)$	-6.3	-6.4	-5.7	-7.2
7	Ir/tacn	CH_2(NHR)	-14.2	-15.5	-13.4	-15.9
8	Pt/bpym	β-CH(NR)	-12.1	-11.3	-11.5	-12.5

Optimized Energies and Geometries (RSE)

Optimized energies (G, in hartrees) and geometries (Å) of all species used in the calculation of the RSE.

Complex **1**

ML(C•) G = -1236,907709

Pd	0.17281900	-0.00003600	0.01958100
Cl	1.75911000	-1.66602200	0.00783500
Cl	1.62928500	1.77944600	-0.06229600
C	-2.70644500	0.55341000	0.21173200
C	-2.50255700	-0.79364800	-0.38291900
H	-2.85358400	0.48037700	1.29882100
N	-1.36972000	-1.47823700	0.11567800
N	-1.45963700	1.35433500	0.00734300
H	-1.32736200	2.08573300	0.70500600
H	-1.43656300	1.80395900	-0.90694500
H	-3.58865700	1.04781300	-0.20907200
H	-2.79288500	-1.02073500	-1.40393700
H	-1.40697400	-1.70683600	1.10984700
H	-1.08687300	-2.30813500	-0.40265900

L(C-H) G = -190,318548

C	-0.71100100	0.61060500	-0.25827600
C	0.71863700	0.61013300	0.25206200
H	0.70273300	0.74356100	1.34749700
H	-0.69708300	0.71290100	-1.35597800
N	1.39744800	-0.63776500	-0.05678700
N	-1.38995500	-0.63098200	0.07397800
H	-2.39362500	-0.53417200	-0.02720700
H	-1.19780500	-0.88900100	1.03697800
H	-1.19989700	1.52441900	0.12884700
H	1.21179400	1.51148900	-0.15564900
H	1.07541400	-1.00548500	-0.94579400
H	2.40019800	-0.50690900	-0.11174900

ML(C-H) G = -1237,557836

Pd	0.20135600	0.00003800	-0.00007200
Cl	1.72773900	1.72238900	-0.03996200
Cl	1.72800500	-1.72226500	0.04010500
C	-2.61410200	-0.68698000	-0.32339000
C	-2.61416000	0.68662400	0.32363800
H	-2.61349000	0.58336000	1.41545900
H	-2.61381100	-0.58373500	-1.41521300
N	-1.37551800	1.39795200	-0.05192200
N	-1.37516700	-1.39803300	0.05179500
H	-1.14736400	-2.17134600	-0.57113400
H	-1.41437800	-1.77997100	0.99591000
H	-3.51674500	-1.24569900	-0.04267700
H	-3.51703200	1.24511900	0.04321200
H	-1.41502100	1.77967200	-0.99611100
H	-1.14781300	2.17143100	0.57083200

L(C•) G = -189,683337

C	0.69762800	0.66360800	0.18128000
C	-0.73285100	0.61385700	-0.20951200
H	0.82078300	0.85723300	1.26767100
N	-1.45271200	-0.55239700	0.01300200
N	1.32470800	-0.63774500	-0.06443700
H	2.27961900	-0.64618900	0.27810900
H	1.35405900	-0.81617200	-1.06444100
H	1.18456100	1.51474800	-0.32905800
H	-1.28375700	1.50802800	-0.48010400
H	-0.88251700	-1.28714000	0.41658500
H	-2.36538300	-0.46430400	0.44067200

Complex **2**

ML(C•) G = -1959,662887

Pt	-0.02313400	-0.53662500	0.01101600
Cl	-1.87597600	-2.04955500	-0.00788300
Cl	1.67777600	-2.21724400	-0.02735000
C	0.82530900	2.67395100	0.38408900
C	-0.56749900	2.68355400	-0.12978900
H	0.85055200	2.75960200	1.48567700
H	1.43658100	3.49331500	-0.01563100
H	-0.98932500	3.57769400	-0.58944000
P	-1.52430200	1.14172400	-0.00439800
P	1.61196500	1.00709200	0.00951200
C	2.43135900	1.21897600	-1.61670700
H	3.21543900	1.98314100	-1.56903200
H	2.86279700	0.25250400	-1.89736900
H	1.68071700	1.49569900	-2.36370800
C	2.98364700	0.83225000	1.20812200
H	3.50721700	-0.10072600	0.97730100
H	3.67027000	1.68362800	1.14131400
H	2.57383700	0.75280100	2.21919900
C	-2.56708200	1.25074500	1.50698200
H	-3.27277800	2.08565800	1.44158300
H	-3.10383300	0.29872600	1.58728900
H	-1.92511000	1.36587800	2.38486100
C	-2.73049400	1.17676600	-1.38223800
H	-3.33248600	0.26513000	-1.31077600
H	-3.37087800	2.06327900	-1.31547300
H	-2.19550900	1.16633300	-2.33549800

L(C-H) G = -920,617649

C	0.66049200	-0.38043900	1.05395200
C	-0.66050400	0.38051500	1.05394700
H	-0.47523100	1.45857800	1.16866800
H	0.47522000	-1.45849800	1.16871400
H	1.27579000	-0.07234600	1.91336700
H	-1.27578400	0.07244900	1.91338200
P	-1.67952300	0.18452200	-0.51905800
P	1.67949800	-0.18452200	-0.51906500
C	2.02204900	1.64768000	-0.40775100
H	2.29272900	1.94893300	0.61306000
H	2.84837700	1.89864500	-1.08164500
H	1.14239200	2.21333100	-0.73253600
C	3.30093100	-0.79657500	0.18134200
H	4.09451600	-0.66251400	-0.56137600
H	3.57867700	-0.26299700	1.09977600
H	3.22531900	-1.86726000	0.40138200
C	-2.02194500	-1.64769300	-0.40772400
H	-2.29268500	-1.94896000	0.61306600
H	-2.84817600	-1.89875800	-1.08170100
H	-1.14218100	-2.21322600	-0.73242300
C	-3.30099700	0.79652000	0.18131000
H	-4.09456700	0.66237800	-0.56141000
H	-3.57872800	0.26297400	1.09976700
H	-3.22545300	1.86722100	0.40129700

ML(C-H) G = -1960,312966

Pt	0.00000000	0.55655400	0.00000000
Cl	-1.77878600	2.15678600	-0.02341400
Cl	1.77878700	2.15678500	0.02341400
C	0.68558500	-2.67880800	-0.33425000
C	-0.68558600	-2.67880700	0.33425300
H	-0.58580100	-2.75825700	1.42618700
H	0.58580000	-2.75826000	-1.42618300
H	1.30718500	-3.52034500	-0.00141000
H	-1.30718500	-3.52034500	0.00141600
P	-1.56220700	-1.05987800	0.01300100
P	1.56220700	-1.05987900	-0.01300000
C	2.46170400	-1.27484800	1.57116300
H	3.19308200	-2.08817400	1.50139600
H	2.97002700	-0.33003000	1.79051000
H	1.75076800	-1.47696100	2.37801100
C	2.88260700	-0.96522400	-1.27624400
H	3.46654200	-0.06082500	-1.07961300
H	3.52422100	-1.85260100	-1.23285700
H	2.43049300	-0.87231800	-2.26786100
C	-2.46170100	-1.27485100	-1.57116400
H	-3.19307800	-2.08817800	-1.50139700
H	-2.97002700	-0.33003400	-1.79051200
H	-1.75076400	-1.47696200	-2.37801100
C	-2.88260900	-0.96522100	1.27624200
H	-3.46654300	-0.06082300	1.07960900
H	-3.52422400	-1.85259800	1.23285400
H	-2.43049700	-0.87231600	2.26786000

L(C•) G = -919,974731

C	-0.59118100	0.24333000	1.03274400
C	0.63079100	-0.55831600	0.80657200

H	-0.36222000	1.30560400	1.21308200
H	-1.16129900	-0.12949200	1.89582000
H	0.64353900	-1.58105300	1.19128200
P	1.82959800	-0.20522500	-0.50020600
P	-1.74631600	0.22991700	-0.48786600
C	-2.11622600	-1.59810000	-0.50340900
H	-2.39539100	-1.96318000	0.49367300
H	-2.93593000	-1.80034100	-1.20095000
H	-1.23058200	-2.14147100	-0.85069600
C	-3.30124700	0.81913100	0.36655000
H	-4.14849400	0.75651300	-0.32483100
H	-3.52647000	0.22161300	1.25913300
H	-3.18432600	1.86821900	0.65999500
C	1.94847500	1.65460200	-0.40156400
H	2.11765000	1.99856400	0.62550700
H	2.77992000	1.98570900	-1.03263200
H	1.02916800	2.10304300	-0.79327700
C	3.41554800	-0.67148700	0.37602200
H	4.26670700	-0.46106400	-0.28040200
H	3.53288000	-0.12202000	1.31629900
H	3.40866000	-1.74599100	0.58758800

Complex **3** (α-N)

ML(C•) G = -2891,036533

Ru	-0.00055400	-0.19701300	-0.01301600
Cl	-0.00990500	2.26115900	0.02370600
Cl	0.01503200	-2.66705500	-0.04913200
C	-2.21542100	-0.27250000	2.38613600
H	-2.23605600	-1.35185900	2.59619300
H	-3.08644700	0.18134600	2.87457300
P	-2.30311700	-0.14038800	0.51871400
C	-3.25350100	1.40350800	0.17227700
C	-3.84271400	1.53928900	-1.08817200
C	-3.31381300	2.47269800	1.06579100
C	-4.48426800	2.71896900	-1.44612300
H	-3.81557400	0.70456400	-1.79086300
C	-3.96047200	3.65219500	0.71006300
H	-2.83765900	2.40200700	2.04175000
C	-4.54375000	3.77913600	-0.54562800
H	-4.94239000	2.80979000	-2.42857600
H	-3.99708500	4.47921900	1.41529400
H	-5.04464400	4.70347800	-0.82368200
C	-3.58149500	-1.41086000	0.09708100
C	-3.29701400	-2.44077700	-0.80042700
C	-4.85896500	-1.32919600	0.66502800
C	-4.27651600	-3.37814200	-1.12266000
H	-2.29239300	-2.53502400	-1.20880100
C	-5.83031900	-2.27056000	0.34943300
H	-5.09966000	-0.51375000	1.34760800
C	-5.53912700	-3.29597600	-0.54830300
H	-4.04369600	-4.18126800	-1.81803000
H	-6.81898000	-2.20004600	0.79766400
H	-6.30059000	-4.03181600	-0.79725600
C	-0.91896200	0.33977500	2.88219900
H	-0.90091900	1.42164400	2.70501800
H	-0.79657400	0.16733200	3.96147600
N	0.22530600	-0.22154900	2.12886800
H	1.06790500	0.29993900	2.36582200
H	0.37547100	-1.20006700	2.38318400
C	2.23698500	-0.26586300	-2.42854600
H	2.26445600	-1.35026700	-2.62038200
H	3.10073900	0.19946400	-2.91509300
P	2.33133100	-0.13997100	-0.53127200
C	3.24970200	1.42514100	-0.20351700
C	3.87622100	1.57311400	1.03798800
C	3.23085800	2.50609500	-1.08490200
C	4.47980400	2.77582700	1.38641800
H	3.90680900	0.73254000	1.73296200
C	3.84143700	3.70731200	-0.73936400
H	2.71816400	2.42631700	-2.04114500
C	4.46413800	3.84574200	0.49626600
H	4.96713300	2.87626300	2.35379000
H	3.81726200	4.54246500	-1.43538100
H	4.93576400	4.78754100	0.76691400
C	3.61915100	-1.39284300	-0.09395000
C	3.32002700	-2.45186900	0.76501000
C	4.90860800	-1.28603000	-0.63015000
C	4.30012400	-3.38885600	1.08584300
H	2.30570500	-2.56574200	1.14368200
C	5.88037900	-2.22729000	-0.31570600
H	5.15577300	-0.45140700	-1.28666100
C	5.57610600	-3.27930900	0.54627800
H	4.05739100	-4.21387600	1.75159000
H	6.87860600	-2.13753400	-0.73855200
H	6.33769100	-4.01555500	0.79368900
C	0.95506900	0.33904600	-2.83526600
H	0.88190100	1.39770500	-3.07077200
N	-0.19930200	-0.21031700	-2.20928400
H	-1.04242100	0.29442600	-2.47104700
H	-0.31733200	-1.20723200	-2.40733200

L(C-H) G = -938,612702

C	-0.37274900	2.07365900	0.64488500
H	0.19069400	2.99886700	0.44964000
H	0.01515200	1.64129100	1.57716700
P	-0.04427600	0.90942900	-0.80482600
C	-1.10017100	-0.51819700	-0.24510200
C	-2.27079300	-0.77662000	-0.96310200
C	-0.80577000	-1.30222200	0.87526500
C	-3.13039700	-1.79964600	-0.57237400
H	-2.50929200	-0.15909000	-1.82808600
C	-1.66217100	-2.32607800	1.26434300
H	0.10915600	-1.11446100	1.43769400
C	-2.82550600	-2.57677000	0.53995300
H	-4.03785400	-1.99265800	-1.14072500
H	-1.42076700	-2.93268900	2.13486700
H	-3.49263900	-3.38076600	0.84350200
C	1.63842900	0.26918200	-0.33383500
C	2.50995000	0.92082500	0.54294100
C	2.09247100	-0.88736400	-0.98247800
C	3.79262400	0.42610800	0.77195300
H	2.19575800	1.82653100	1.05881700
C	3.36542700	-1.38811800	-0.74608000
H	1.43003500	-1.40582400	-1.67657600
C	4.22283400	-0.73006600	0.13341500
H	4.45564400	0.94889500	1.45838300
H	3.69257700	-2.29349700	-1.25306700
H	5.22281200	-1.11724500	0.31533500
C	-1.85104700	2.38695300	0.80356900
H	-2.37023800	1.48105100	1.14648900
H	-1.96663200	3.13731300	1.60867600
N	-2.43770900	2.78175300	-0.46843100
H	-3.42201400	3.00002800	-0.35829900
H	-1.98306100	3.61868200	-0.82253500

ML(C-H) G = -2891,683876

Ru	0.00007300	0.19932200	0.00008800
Cl	-0.00001800	-2.26121200	0.00040800
Cl	-0.00001500	2.66926200	-0.00011400
C	-2.22843600	0.25153600	-2.39742200
H	-2.25310900	1.32906300	-2.61625000
H	-3.09985800	-0.20882100	-2.87916400
P	-2.31009500	0.13434400	-0.52891100
C	-3.25334700	-1.41173300	-0.17018900
C	-3.84778700	-1.54026900	1.08875100
C	-3.29862100	-2.49173900	-1.05177700
C	-4.47797900	-2.72308600	1.45682900
H	-3.83370700	-0.69766400	1.78218900
C	-3.93398300	-3.67425300	-0.68610300
H	-2.81919500	-2.42706200	-2.02643500
C	-4.52136800	-3.79403700	0.56835800
H	-4.93995000	-2.80782900	2.43805200
H	-3.95802200	-4.50934100	-1.38231000
H	-5.01292400	-4.72089600	0.85463100
C	-3.59141700	1.40317100	-0.11186600
C	-3.30354200	2.44077000	0.77576000
C	-4.87184300	1.31434300	-0.67180700
C	-4.28327900	3.37846400	1.09638000
H	-2.29610400	2.53989600	1.17625600
C	-5.84352800	2.25591700	-0.35763000
H	-5.11434700	0.49317000	-1.34685500
C	-5.54917700	3.28890800	0.53034000
H	-4.04804700	4.18794200	1.78356900
H	-6.83465500	2.17993800	-0.79951900
H	-6.31077700	4.02505800	0.77806900
C	-0.93144500	-0.36000800	-2.89389200

H	-0.90825500	-1.44044200	-2.70816300
H	-0.81680700	-0.19701100	-3.97559700
N	0.21396000	0.21135900	-2.15105100
H	1.05777600	-0.30430800	-2.39449900
H	0.35504600	1.19022300	-2.40928500
C	2.22871200	0.25170000	2.39749000
H	2.25357800	1.32925000	2.61619100
H	3.10009400	-0.20874000	2.87923000
P	2.31027200	0.13432600	0.52898100
C	3.25328200	-1.41188500	0.17022600
C	3.84795200	-1.54041600	-1.08861000
C	3.29785000	-2.49212100	1.05157200
C	4.47766000	-2.72345500	-1.45681900
H	3.83444900	-0.69764700	-1.78185900
C	3.93273100	-3.67485100	0.68577000
H	2.81824100	-2.42744400	2.02613600
C	4.52032400	-3.79463500	-0.56859600
H	4.93981300	-2.80818600	-2.43795800
H	3.95619800	-4.51011700	1.38178100
H	5.01147500	-4.72167300	-0.85498200
C	3.59167300	1.40301400	0.11174700
C	3.30365600	2.44086000	-0.77554600
C	4.87227100	1.31388300	0.67125500
C	4.28343000	3.37847600	-1.09628400
H	2.29611000	2.54021000	-1.17571400
C	5.84399500	2.25537700	0.35695700
H	5.11487500	0.49253800	1.34605900
C	5.54950600	3.28860300	-0.53069500
H	4.04809100	4.18813200	-1.78322700
H	6.83525600	2.17915400	0.79850100
H	6.31113700	4.02468500	-0.77852900
C	0.93164600	-0.35955100	2.89412600
H	0.90826500	-1.44001400	2.70860600
H	0.81708800	-0.19632600	3.97580400
N	-0.21372700	0.21181900	2.15123400
H	-1.05758400	-0.30370800	2.39483300
H	-0.35469300	1.19075200	2.40927800

L(C•) G = -937,975573

C	-0.02165000	2.04413900	0.77617400
H	0.76720000	2.78532100	0.56740800
H	0.29372700	1.48198400	1.66253500
P	0.04883000	0.88074700	-0.77610600
C	-1.25080200	-0.35843000	-0.32128300
C	-1.95643300	-0.95486800	-1.36999000
C	-1.57202200	-0.71898500	0.99225400
C	-2.94696400	-1.89986700	-1.11846200
H	-1.72421900	-0.66725800	-2.39527100
C	-2.56575200	-1.65761000	1.24749100
H	-1.03048100	-0.27049100	1.82473300
C	-3.25336500	-2.25095900	0.19177600
H	-3.48295100	-2.35783000	-1.94688700
H	-2.80400200	-1.92924000	2.27379700
H	-4.03023400	-2.98563100	0.39194200
C	1.61946900	-0.00129700	-0.32413700
C	2.81290500	0.67732600	-0.60536500
C	1.69462200	-1.25965300	0.28132900
C	4.04455600	0.12480000	-0.27493000
H	2.77281000	1.65014600	-1.09846300
C	2.92898700	-1.81966700	0.59723400
H	0.78079900	-1.80863700	0.50290200
C	4.10603300	-1.12941800	0.32639400
H	4.95962100	0.66983300	-0.49760500
H	2.97006000	-2.80346900	1.06065200
H	5.06863500	-1.56955300	0.57688300
C	-1.33890200	2.65904500	0.96544000
H	-2.07389900	2.17459900	1.60474000
N	-1.87228000	3.40111700	-0.08474100
H	-2.69893200	3.93915500	0.13422000
H	-1.19872200	3.94470800	-0.61037500

Complex **3** (α-P)

ML(C•) G = -2891,034071

Ru	0.00974700	-0.14981300	0.00017400
Cl	-0.10411100	2.27369200	-0.43881800
Cl	0.04680100	-2.55829800	0.53881400
C	-2.19279100	-0.02329200	2.39593500
H	-2.07449200	-1.06604400	2.72350800
H	-3.10895400	0.37126300	2.85243300
P	-2.29643400	-0.10661400	0.53185500
C	-3.30219000	1.36170000	0.03490900
C	-3.73893500	1.41743600	-1.29212400
C	-3.58740500	2.43068700	0.88244500
C	-4.44565900	2.51658000	-1.76115100
H	-3.52968500	0.58462800	-1.96559200
C	-4.29415900	3.53527500	0.41325100
H	-3.25069000	2.42251400	1.91743000
C	-4.72296600	3.58138800	-0.90758200
H	-4.77990900	2.54401800	-2.79583000
H	-4.50450700	4.36442400	1.08495700
H	-5.27219500	4.44561400	-1.27359900
C	-3.52861300	-1.45363300	0.23458900
C	-3.19181300	-2.55704400	-0.54930900
C	-4.82057600	-1.35472900	0.76352100
C	-4.13425400	-3.55194000	-0.79899900
H	-2.17529900	-2.65258000	-0.92549900
C	-5.75606800	-2.35310200	0.52140500
H	-5.09996300	-0.48308400	1.35626200
C	-5.41284000	-3.45212600	-0.26332700
H	-3.86128700	-4.41247600	-1.40547200
H	-6.75726800	-2.27009900	0.93854200
H	-6.14684900	-4.23169300	-0.45517600
C	-0.97563400	0.79901800	2.78061300
H	-1.08365600	1.83727200	2.44359600
H	-0.83923800	0.80771300	3.87161400
N	0.22870000	0.26454400	2.10472700
H	0.99710000	0.92478900	2.21658600
H	0.50631300	-0.62495400	2.52529800
C	2.19586700	0.15665000	-2.35088500
H	3.04407500	0.44240900	-2.97450000
P	2.31796000	-0.03285400	-0.54468800
C	3.33175500	1.42153400	-0.00753200
C	4.13925200	1.31867000	1.12995700
C	3.22533900	2.65227400	-0.66108700
C	4.83421500	2.42788100	1.60221200
H	4.24067400	0.36048800	1.64075500
C	3.93114600	3.75579900	-0.19284300
H	2.56673900	2.75141300	-1.52179100
C	4.73350000	3.64702400	0.93889000
H	5.46325500	2.33544900	2.48490300
H	3.84201000	4.70862200	-0.70956700
H	5.28117500	4.51298700	1.30384700
C	3.55459300	-1.39305200	-0.31218700
C	3.39497100	-2.29422000	0.74147600
C	4.68711800	-1.48385900	-1.12827900
C	4.35575500	-3.27570800	0.97392100
H	2.49657000	-2.24919900	1.35405700
C	5.63973500	-2.46935600	-0.89970200
H	4.83193800	-0.77225400	-1.94065000
C	5.47413300	-3.36622200	0.15382600
H	4.21925200	-3.97871800	1.79233300
H	6.51662200	-2.53401800	-1.54015300
H	6.22037100	-4.13738900	0.33206400
C	0.84327000	0.15599600	-2.95788600
H	0.46220800	1.19134800	-3.00044300
H	0.86791400	-0.23054100	-3.98870600
N	-0.12180400	-0.59567000	-2.12016800
H	-1.06308300	-0.41801700	-2.46232600
H	0.04463800	-1.60169000	-2.19023300

L(C•) G = -937,965589

C	-0.24167800	2.10653000	0.62771900
H	0.59312200	2.29821700	1.30258700
P	-0.01769300	0.94315900	-0.73937300
C	-1.18137600	-0.45096700	-0.31507500
C	-1.47325500	-1.37677500	-1.31962500
C	-1.76199400	-0.61276900	0.94505000
C	-2.31391600	-2.45511500	-1.06440000
H	-1.03772500	-1.24651800	-2.31057700
C	-2.61034900	-1.68554200	1.19880100
H	-1.54193100	0.10918800	1.73173500
C	-2.88515100	-2.60987000	0.19520500
H	-2.52958200	-3.17280100	-1.85318400
H	-3.05773600	-1.80187300	2.18399100

H	-3.54826700	-3.44903100	0.39368000
C	1.60844800	0.19408900	-0.22550000
C	2.68965200	0.29994400	-1.10248200
C	1.78965600	-0.46309200	0.99595800
C	3.93209600	-0.23273700	-0.76560100
H	2.55241100	0.80465000	-2.05866500
C	3.02794600	-0.99425000	1.33465800
H	0.94748600	-0.56534400	1.68001300
C	4.10116700	-0.87916400	0.45326900
H	4.76653800	-0.14378500	-1.45789800
H	3.15802900	-1.50362500	2.28730900
H	5.06953700	-1.29837100	0.71792800
C	-1.47016500	2.93796400	0.76309400
H	-2.07749800	2.56282300	1.60784800
H	-1.18555400	3.96911700	1.05563200
N	-2.29578500	2.85627800	-0.43203200
H	-3.19697300	3.29605400	-0.28498200
H	-1.84244500	3.33049100	-1.20702100

Complex **4**

ML(C•) G = -2423,723896

Pt	0.04825600	-1.20787000	0.04468700
Cl	1.88132500	-2.76431200	0.09557700
Cl	-1.67765600	-2.87307600	0.19795100
C	4.13381100	0.29300900	-0.69864400
C	4.08698900	0.94356100	0.68080800
C	2.77964400	0.50859700	1.34823100
C	2.81295800	0.59563000	-1.41719400
H	4.98436100	0.64150700	-1.29827200
H	4.23103700	-0.79662300	-0.58773200
H	4.11297000	2.04222900	0.58681900
H	4.94813800	0.66048500	1.29962700
H	2.85497500	-0.56179200	1.59495800
H	2.80145800	1.65691800	-1.71400300
P	1.53539100	0.47257800	-0.05082100
C	0.59403600	2.06539600	-0.03761800
C	-0.80234800	1.99753800	0.05267700
C	1.22026400	3.31505500	-0.05326800
C	-1.55399700	3.16973100	0.16245500
C	0.46558300	4.47893200	0.03708000
H	2.30531900	3.38389300	-0.12656900
C	-0.92078600	4.40732900	0.15432100
H	-2.63827100	3.10886900	0.25839900
H	0.96112300	5.44669100	0.02799200
H	-1.50833600	5.31829100	0.23774300
C	-2.93502500	0.26552200	1.16805500
C	-2.73212900	0.23447200	-1.50000100
C	-4.24516800	0.11055300	0.46300800
C	-4.09315600	0.67213100	-0.95350100
H	-2.75659700	-0.85042400	-1.68849200
H	-4.49717300	-0.96516000	0.41850300
H	-5.05899900	0.59596300	1.02117200
H	-4.89987500	0.33692700	-1.61766100
H	-4.13934600	1.77227700	-0.92663300
P	-1.58914200	0.32152300	-0.02567200
C	2.52415000	-0.28948000	-2.61567500
H	1.57954400	-0.01820500	-3.10184800
H	3.32554300	-0.19405200	-3.35871400
H	2.45453500	-1.34024300	-2.30816100
C	2.35859600	1.29041900	2.57584900
H	1.39287900	0.93878200	2.96163100
H	3.09914300	1.16863100	3.37512300
H	2.26868100	2.36382800	2.36594200
C	-2.25230000	0.96600400	-2.73716400
H	-2.93660800	0.78941800	-3.57539100
H	-2.20131600	2.04995700	-2.57238200
H	-1.25678200	0.62192600	-3.04533000
C	-2.73940200	0.00907500	2.61274900
H	-3.56714200	0.41105200	3.21078800
H	-2.69239400	-1.07709900	2.79762600
H	-1.79729400	0.43303000	2.98371700

L(C-H) G = -1384,651937

C	-4.23748900	-0.31916600	-0.15232100
C	-3.36204200	-0.99369400	-1.20078800
C	-2.22540400	-1.69639300	-0.46933400
C	-3.36124000	0.29848000	0.96095100
H	-4.90816600	0.42896000	-0.59564500
H	-4.88717600	-1.08103300	0.30585000
H	-2.93552200	-0.25268200	-1.89396600
H	-3.93646400	-1.70208200	-1.81625300
H	-2.65353800	-2.49457200	0.16140800
H	-3.29008200	1.38733800	0.84903000
P	-1.60649200	-0.42686400	0.81221700
C	-0.74476600	0.79395600	-0.32921000
C	0.65567300	0.68160800	-0.50087200
C	-1.41681300	1.83894500	-0.97350300
C	1.31598200	1.62470100	-1.29559500
C	-0.74327100	2.76418700	-1.76381800
H	-2.49429200	1.94510700	-0.86400000
C	0.63147000	2.65954500	-1.92334900
H	2.39483600	1.56321400	-1.42810900
H	-1.29595600	3.56338700	-2.25306400
H	1.17412800	3.38001800	-2.53143500
C	3.12468000	-0.95920400	-0.66934200
C	2.48610300	0.21328100	1.73515000
C	4.27949500	-0.57289600	0.26200900
H	3.09568200	-0.26286600	-1.51708600
C	3.82903200	0.59893900	1.12000900
H	2.66770900	-0.56350000	2.49517700
H	4.50841600	-1.43025700	0.91685100
H	5.19465100	-0.35959100	-0.30726500
H	4.56466500	0.85589300	1.89607900
H	3.70117200	1.49936800	0.49762100
P	1.54161300	-0.72960300	0.36712800
C	-3.91523600	-0.00254600	2.34902700
H	-3.32890100	0.48076000	3.13852100
H	-4.95524900	0.33902200	2.43877900
H	-3.90597300	-1.08396400	2.54725300
C	-1.17832000	-2.29111900	-1.39089700
H	-0.38068500	-2.79725500	-0.83545700
H	-1.63792000	-3.01882400	-2.07301000
H	-0.71393800	-1.50928200	-2.00760700
C	1.72946100	1.36096200	2.37549300
H	2.31635100	1.80285700	3.19156000
H	1.52407200	2.15256700	1.64385900
H	0.76918400	1.03180800	2.79020700
C	3.23280100	-2.37857000	-1.20395300
H	4.17581800	-2.52699000	-1.74712600
H	3.20072800	-3.10785400	-0.38320300
H	2.40895000	-2.61863000	-1.88706600

ML(C-H) G = -2424,362664

Pt	0.00006100	-1.19027900	-0.00009200
Cl	1.76598400	-2.81801000	0.00648900
Cl	-1.76591000	-2.81793600	-0.00663300
C	4.15594000	0.09568000	-0.62361000
C	4.12604100	0.74052600	0.75881800
C	2.78341800	0.38556000	1.40309100
C	2.87064300	0.49123500	-1.36113100
H	5.03757500	0.39263200	-1.20592400
H	4.17982600	-0.99876700	-0.51899000
H	4.22073700	1.83606300	0.67074700
H	4.95710500	0.40250800	1.39095100
H	2.78990100	-0.68624500	1.65413100
H	2.93054800	1.55753700	-1.63357900
P	1.56388500	0.42202500	-0.01789200
C	0.70037000	2.05837500	-0.02498200
C	-0.70044500	2.05831600	0.02511500
C	1.39077700	3.27348600	-0.05294500
C	-1.39100100	3.27333800	0.05314800
C	0.69558800	4.47661100	-0.02732400
H	2.47961300	3.28180500	-0.09287000
C	-0.69594400	4.47654000	0.02761000
H	-2.47984200	3.28151500	0.09307700
H	1.24023700	5.41734300	-0.04718100
H	-1.24069000	5.41721400	0.04752800
C	-2.87056200	0.49080200	1.36132100
C	-2.78361200	0.38556300	-1.40305500
C	-4.15597500	0.09557300	0.62382200
H	-2.93034800	1.55699300	1.63420500
C	-4.12604900	0.74057700	-0.75852500
H	-2.79006500	-0.68621200	-1.65421600
H	-4.18008300	-0.99885600	0.51915600
H	-5.03751200	0.39268300	1.20620500
H	-4.95729300	0.40290400	-1.39061200

H	-4.22046400	1.83612400	-0.67023300
P	-1.56381700	0.42192300	0.01789800
C	2.55477600	-0.34326900	-2.58851300
H	1.63482700	-0.00649300	-3.08119600
H	3.37323500	-0.26921600	-3.31520300
H	2.42393400	-1.39715100	-2.31439000
C	2.39103400	1.19770700	2.62035600
H	1.40643600	0.89831400	3.00139700
H	3.11820400	1.04710300	3.42700400
H	2.35582300	2.27219800	2.39983700
C	-2.39135300	1.19795000	-2.62020600
H	-3.11853200	1.04740900	-3.42685700
H	-2.35624100	2.27240600	-2.39950100
H	-1.40673300	0.89871500	-3.00131800
C	-2.55460000	-0.34430200	2.58828700
H	-3.37327000	-0.27099800	3.31482200
H	-2.42331900	-1.39798000	2.31352500
H	-1.63489900	-0.00748600	3.08138600

L(C•) G = -1384,018366

C	4.29369600	0.33369700	-0.23976900
C	3.78739000	-0.97193000	-0.83317800
C	2.49995400	-0.64998100	-1.58637900
C	3.13808400	1.00923400	0.50899400
H	5.16468700	0.19557800	0.41532000
H	4.61893800	0.99695200	-1.05873300
H	3.57240600	-1.69783100	-0.03274800
H	4.52825500	-1.44488200	-1.49426500
H	2.76502300	-0.06956900	-2.48494400
H	3.02901500	0.55117500	1.50082100
P	1.57205400	0.62270300	-0.50686300
C	0.59656900	-0.51272200	0.62322900
C	-0.79810100	-0.60039000	0.42127600
C	1.17633500	-1.28569700	1.63513600
C	-1.55205300	-1.45905100	1.22817400
C	0.41375600	-2.13300900	2.43252200
H	2.24961100	-1.23854600	1.81044600
C	-0.95720000	-2.22031300	2.22813400
H	-2.62853500	-1.52992600	1.06987500
H	0.89452700	-2.72502800	3.20836200
H	-1.56546400	-2.87719700	2.84646800
C	-3.31133300	-0.28059700	-0.92609700
C	-2.17862200	1.94523600	-0.10133800
C	-4.25964400	0.60374100	-0.17742400
C	-3.42370100	1.54294500	0.68750500
H	-2.48406100	2.59745000	-0.93625700
H	-4.88758800	1.18218500	-0.88179000
H	-4.96782800	0.00694900	0.42217000
H	-3.98804100	2.42873300	1.01286400
H	-3.10340400	1.01631100	1.59993300
P	-1.60641600	0.35752600	-0.99184400
C	3.33041800	2.50786500	0.67923000
H	2.50264500	2.96260900	1.23680100
H	4.26220500	2.72971000	1.21677400
H	3.38110300	3.00689800	-0.29800800
C	1.68710900	-1.86031300	-2.00576700
H	0.77542500	-1.57007700	-2.54185100
H	2.27575300	-2.50910800	-2.66784900
H	1.38589100	-2.45634600	-1.13480700
C	-1.14027600	2.66083900	0.74135500
H	-1.57963100	3.54658500	1.21971600
H	-0.76549800	2.00455800	1.53905700
H	-0.28053300	2.98600000	0.14472900
C	-3.78127300	-1.50712400	-1.61892600
H	-4.25660600	-2.20844500	-0.91284300
H	-4.54559000	-1.28210100	-2.38062200
H	-2.96390200	-2.04064800	-2.11806800

Complex **5** (tertiary)

ML(C•) G = -2040,346793

Fe	0.12601600	-0.85666900	-0.02803500
Cl	-0.00644700	-2.57365500	1.52336700
Cl	0.64754500	-2.33721400	-1.74976000
C	-0.15821600	4.43705400	-0.24127200
C	0.21677800	3.30222000	-1.18114300
C	0.33409100	1.98941700	-0.40624600
C	-0.80761000	1.71968300	0.49025800
C	-1.45629100	2.87152100	1.21490300
C	-1.51782400	4.13901300	0.37087100
H	-0.57232000	3.22781400	-1.94042000
H	1.15490500	3.51703000	-1.71254700
H	0.59499600	4.53195400	0.55904600
H	-0.16572800	5.39162000	-0.78264900
H	-2.47903100	2.62931400	1.54670000
H	-0.90607500	3.14139200	2.14792300
H	-2.25260000	4.01219400	-0.43894500
H	-1.86373700	4.97823000	0.98812700
H	1.32823700	2.03417300	0.11094000
N	-0.50910600	0.55335300	1.34193900
N	0.48197900	0.76561300	-1.30878100
C	-0.45071600	0.78418200	-2.44307400
H	-0.15379900	1.53295700	-3.19072700
H	-0.45159600	-0.20507500	-2.90864100
H	-1.44533100	1.02672300	-2.05522200
C	1.86427700	0.62976200	-1.78608900
H	1.87121700	-0.13203200	-2.57697100
H	2.24260300	1.57201300	-2.21266700
C	2.73082700	0.14417000	-0.67477100
C	4.09659600	0.39547700	-0.62416500
C	4.85335200	-0.18617600	0.38173500
H	4.54875800	1.03544100	-1.37779000
C	2.85245200	-1.20469700	1.20382700
C	4.22030800	-1.00823800	1.30733400
H	5.92393000	-0.00635000	0.43979500
H	2.30094000	-1.84920000	1.88479800
H	4.77199100	-1.49882400	2.10308200
N	2.11626700	-0.62846200	0.24236700
C	0.43624000	0.77483900	2.45335300
H	-0.01364100	1.43478500	3.20851000
H	0.68922500	-0.18370800	2.91779900
H	1.34685800	1.24819400	2.07425400
C	-1.77317200	0.01184100	1.87234100
H	-1.53768000	-0.80764300	2.56549600
H	-2.32998100	0.77997000	2.42667900
C	-2.57137100	-0.54614000	0.74548300
C	-3.95663300	-0.61541600	0.75803900
C	-4.60845700	-1.25886200	-0.28729600
H	-4.50671500	-0.16907100	1.58260700
C	-2.47092400	-1.71559100	-1.25494500
C	-3.85449500	-1.82363400	-1.30655600
H	-5.69362000	-1.32448900	-0.30016000
H	-1.81982400	-2.15528000	-2.00734400
H	-4.32084900	-2.34884600	-2.13419700
N	-1.84792100	-1.07588700	-0.26058300

L(C-H) G = -996,995128

C	-0.61970500	2.93160200	0.44311400
C	-0.69116200	1.66274700	1.28478100
C	-0.65962300	0.41114000	0.39323600
C	0.65962300	0.41114300	-0.39323600
C	0.69116100	1.66275400	-1.28477600
C	0.61970300	2.93160500	-0.44310300
H	0.15493100	1.63466000	1.99002700
H	-1.60478600	1.66901400	1.89506700
H	-1.51979600	2.98378000	-0.19188600
H	-0.63877000	3.82365600	1.08287900
H	1.47365400	0.53142600	0.34406000
H	1.60478500	1.66902400	-1.89506200
H	-0.15493200	1.63466900	-1.99002200
H	1.51979400	2.98377900	0.19189700
H	0.63876700	3.82366200	-1.08286400
H	-1.47365300	0.53142500	-0.34406000
N	0.91870400	-0.85124700	-1.07322100
N	-0.91870200	-0.85125300	1.07321400
C	0.10919000	-1.28590000	1.99508500
H	0.22280100	-0.62458400	2.87844400
H	-0.15154900	-2.28377800	2.36896900
H	1.07116800	-1.37614300	1.47955000
C	-2.23529300	-0.94576000	1.66983700
H	-2.35913400	-1.98295700	2.01659700
H	-2.35335500	-0.30392300	2.57017000
C	-3.35458100	-0.64183100	0.70831300
C	-4.25326600	0.39502800	0.96218500
C	-5.27705300	0.64222900	0.05580700
H	-4.14421900	0.99652700	1.86266500
C	-4.42471400	-1.16134100	-1.24654600

C	-5.36820700	-0.15137100	-1.07920200
H	-5.98985000	1.44472200	0.23260400
H	-4.46638900	-1.80637600	-2.12582600
H	-6.14813500	0.00273900	-1.82002500
N	-3.44305400	-1.41277100	-0.38333300
C	-0.10918800	-1.28589000	-1.99509300
H	-0.22279800	-0.62457100	-2.87845000
H	0.15155100	-2.28376700	-2.36898100
H	-1.07116600	-1.37613400	-1.47956000
C	2.23529500	-0.94574900	-1.66984300
H	2.35913700	-1.98294400	-2.01661000
H	2.35335800	-0.30390700	-2.57017300
C	3.35458200	-0.64182600	-0.70831600
C	4.25327000	0.39503300	-0.96218100
C	5.27705400	0.64222700	-0.05579900
H	4.14422700	0.99653600	-1.86265900
C	4.42471000	-1.16134700	1.24654300
C	5.36820500	-0.15137700	1.07920600
H	5.98985400	1.44472000	-0.23259100
H	4.46638100	-1.80638700	2.12582000
H	6.14813100	0.00272700	1.82003200
N	3.44305100	-1.41277100	0.38332700

ML(C-H) G = -2040,997815

Fe	0.00000000	-0.87371000	0.00000100
Cl	0.36260600	-2.49511000	-1.68272200
Cl	-0.36260400	-2.49510800	1.68272600
C	-0.57195400	4.46076800	0.50257600
C	-0.50077700	3.21221000	1.37156800
C	-0.54645700	1.93618700	0.52997400
C	0.54645700	1.93618500	-0.52997500
C	0.50077900	3.21220900	-1.37157000
C	0.57196000	4.46076600	-0.50257800
H	0.44136300	3.24561100	1.93795500
H	-1.31170800	3.20502200	2.11208300
H	-1.53207100	4.48971800	-0.03666900
H	-0.54055800	5.35746700	1.13307900
H	1.51573700	1.91467800	-0.00340700
H	1.31170900	3.20501900	-2.11208500
H	-0.44136100	3.24561200	-1.93795600
H	1.53207700	4.48971400	0.03666700
H	0.54056600	5.35746500	-1.13308100
H	-1.51573800	1.91468000	0.00340600
N	0.48988400	0.66895900	-1.32011300
N	-0.48988600	0.66896100	1.32011400
C	0.42668400	0.73181200	2.46966400
H	0.06091800	1.41577500	3.24959100
H	0.50257600	-0.27892700	2.88104100
H	1.42012200	1.05620700	2.14531000
C	-1.84260100	0.33053700	1.80592800
H	-1.72229600	-0.46393500	2.55417300
H	-2.33268900	1.19444600	2.28620300
C	-2.66945300	-0.22759600	0.69532600
C	-4.05566100	-0.15619900	0.68835600
C	-4.75769300	-0.81011100	-0.31645700
H	-4.56963900	0.39087400	1.47552300
C	-2.65702600	-1.52572600	-1.21495100
C	-4.04350800	-1.51583500	-1.27601000
H	-5.84397800	-0.77679300	-0.34266100
H	-2.03904200	-2.07625200	-1.92250100
H	-4.54713300	-2.06058400	-2.06900200
N	-1.97546400	-0.87673900	-0.25902300
C	-0.42668700	0.73181000	-2.46966200
H	-0.06092100	1.41577100	-3.24959100
H	-0.50258000	-0.27892900	-2.88103900
H	-1.42012400	1.05620600	-2.14530800
C	1.84259800	0.33053300	-1.80592900
H	1.72229000	-0.46394000	-2.55417200
H	2.33268600	1.19444100	-2.28620700
C	2.66945200	-0.22759700	-0.69532800
C	4.05565900	-0.15620300	-0.68836000
C	4.75769300	-0.81011300	0.31645200
H	4.56963600	0.39086800	-1.47553000
C	2.65702700	-1.52572300	1.21495200
C	4.04350900	-1.51583400	1.27600900
H	5.84397700	-0.77679600	0.34265400
H	2.03904400	-2.07624700	1.92250500
H	4.54713500	-2.06058100	2.06900100
N	1.97546400	-0.87673800	0.25902300

L(C$^{\bullet}$) G = -996,355490

C	0.16461100	2.73986000	-0.84194600
C	-0.25072300	2.00132100	0.42284400
C	-0.62596900	0.53415800	0.13316900
C	0.50555600	-0.13279500	-0.59777700
C	1.00126800	0.59279300	-1.81348400
C	1.34607400	2.05000900	-1.50934500
H	0.58575500	2.01113000	1.13967200
H	-1.09972400	2.51107000	0.90403300
H	-0.68479300	2.75876500	-1.54574700
H	0.40289400	3.78733600	-0.61430900
H	1.86182200	0.08111600	-2.26372400
H	0.21075700	0.58786100	-2.59407700
H	2.21700500	2.08123800	-0.83462200
H	1.63405100	2.57639900	-2.42928100
H	-1.49962700	0.57213300	-0.55369900
N	0.80939400	-1.47424000	-0.35554100
N	-1.07080700	-0.21176200	1.30683200
C	-0.11937300	-0.26367700	2.39987600
H	-0.07632100	0.67771500	2.98451800
H	-0.41183400	-1.06422800	3.09213400
H	0.88223300	-0.48754100	2.01795900
C	-2.38909400	0.14657600	1.78325900
H	-2.62608100	-0.53574400	2.61400900
H	-2.43450500	1.17390400	2.20728000
C	-3.46527100	-0.00233800	0.74121300
C	-4.24537000	1.08894500	0.35817000
C	-5.23872400	0.90925100	-0.59655700
H	-4.06384300	2.06469800	0.80557900
C	-4.58631400	-1.38043300	-0.69978700
C	-5.41727700	-0.35467000	-1.14263000
H	-5.85937800	1.74520500	-0.91184700
H	-4.69910100	-2.38660700	-1.10729700
H	-6.17860200	-0.54663100	-1.89386800
N	-3.63533600	-1.22333500	0.21772700
C	-0.21559300	-2.48278900	-0.57803000
H	-0.31125500	-2.74933000	-1.64787900
H	0.04053500	-3.39602700	-0.02444800
H	-1.17813800	-2.12003700	-0.20456800
C	2.13882500	-1.91772400	-0.69586400
H	2.28303900	-2.90522600	-0.22835400
H	2.27613800	-2.07984700	-1.78652900
C	3.22295500	-0.99149600	-0.20233800
C	4.29537300	-0.65791000	-1.03058000
C	5.28438800	0.19089800	-0.55014800
H	4.33954200	-1.05353400	-2.04384800
C	4.06776900	0.29028700	1.49512000
C	5.16930700	0.68602100	0.74198500
H	6.12757800	0.46764400	-1.17918600
H	3.94509100	0.65406500	2.51666700
H	5.91068400	1.36135000	1.16030500
N	3.11840100	-0.52846500	1.04787200

Complex **5** (benzyl)

ML(C$^{\bullet}$) G = -2040,383304

Fe	0.20231400	-0.95741100	0.04646900
Cl	0.96537000	-2.23797000	-1.81962500
Cl	0.08572100	-2.50925400	1.91133800
C	-1.61799600	4.31175700	0.45569500
C	-1.37191800	3.08761800	1.32718500
C	-1.01852200	1.84981100	0.49695200
C	0.15310600	2.13359400	-0.43778600
C	-0.04980100	3.41035200	-1.25399300
C	-0.37847700	4.60865200	-0.37601900
H	-0.53991500	3.31902600	2.00793600
H	-2.24356200	2.87480300	1.96066400
H	-2.47432500	4.13295100	-0.21394300
H	-1.88594800	5.17027100	1.08335600
H	1.04763900	2.27637000	0.18885500
H	0.84903900	3.59049000	-1.86044600
H	-0.88250900	3.26554400	-1.95768700
H	0.46678700	4.82840700	0.29528800
H	-0.52473800	5.50030600	-0.99744800
H	-1.89343100	1.60131300	-0.12824100
N	0.45532300	0.95061400	-1.30107200
N	-0.74325400	0.63958200	1.31260300

C	0.08626400	0.88707700	2.49981400
H	-0.45671600	1.44072500	3.28087900
H	0.39496700	-0.08565400	2.89663600
H	0.98442200	1.44948400	2.22584300
C	-1.99696100	-0.01820500	1.70792300
H	-1.74362700	-0.75319000	2.48366100
H	-2.72533800	0.69444800	2.13215600
C	-2.59135800	-0.77490200	0.56363500
C	-3.96185600	-0.94978100	0.43213000
C	-4.44960100	-1.75410100	-0.59018300
H	-4.63067400	-0.46693700	1.14090700
C	-2.18545500	-2.11951100	-1.27556800
C	-3.54131600	-2.35370000	-1.45220000
H	-5.51885900	-1.91129000	-0.70753000
H	-1.42443600	-2.55968500	-1.91783500
H	-3.86830400	-3.00063700	-2.26061100
N	-1.71174900	-1.33492100	-0.29368400
C	-0.36364000	0.82611000	-2.51101100
H	-0.09896800	1.57530800	-3.27295100
H	-0.19529000	-0.17708600	-2.91532500
H	-1.42470900	0.93102100	-2.26105400
C	1.83072100	0.86048200	-1.58852900
H	2.20181900	1.21384900	-2.55340600
C	2.69973900	0.26879600	-0.64588200
C	4.09624900	0.41970300	-0.72496900
C	4.90154900	-0.19620000	0.21305400
H	4.51416600	1.02123700	-1.52862400
C	2.91885100	-1.09392300	1.22530200
C	4.30464400	-0.95989200	1.21419400
H	5.98242700	-0.09027600	0.16484200
H	2.40426300	-1.72875600	1.94602100
H	4.89568800	-1.47379300	1.96570700
N	2.12483700	-0.49887400	0.33309500

L(C$^{\bullet}$) G = -996,381378

C	-0.92382500	3.10190600	-0.55275600
C	-0.92068900	2.18052200	0.66072500
C	-0.75767300	0.71458600	0.23823700
C	0.56266100	0.57226600	-0.52651600
C	0.58380200	1.48939700	-1.75192700
C	0.36373600	2.94328700	-1.35268700
H	-0.09463000	2.46097300	1.33309700
H	-1.84893600	2.30539700	1.23572700
H	-1.78605900	2.84695600	-1.19161900
H	-1.06282200	4.14610500	-0.24436200
H	1.38596600	0.89656300	0.11883300
H	1.55337400	1.36515500	-2.25301100
H	-0.19420400	1.17864800	-2.46886400
H	1.21472300	3.27269600	-0.73561500
H	0.35363700	3.58730400	-2.24130700
H	-1.57757400	0.48942900	-0.46646400
N	0.85531800	-0.81033500	-0.90057500
N	-0.86926300	-0.26511900	1.31672300
C	0.14416700	-0.16316800	2.34755000
H	0.02960000	0.73044300	2.99290100
H	0.08618100	-1.04586400	2.99616900
H	1.14804700	-0.13944900	1.91024900
C	-2.19206100	-0.35013100	1.91161400
H	-2.18018600	-1.20466000	2.60413200
H	-2.44628500	0.54346000	2.52135200
C	-3.28434000	-0.58341800	0.90204300
C	-4.27319400	0.37445400	0.67554500
C	-5.25289300	0.12409400	-0.27769600
H	-4.26520800	1.30386700	1.24190100
C	-4.19262300	-1.97256700	-0.67432300
C	-5.21441800	-1.07607100	-0.97436200
H	-6.03199600	0.85737400	-0.47371900
H	-4.13551100	-2.92925900	-1.19626600
H	-5.95630700	-1.31779200	-1.73051500
N	-3.24979400	-1.74601500	0.23787400
C	-0.22568500	-1.60012800	-1.45913600
H	-0.76982700	-1.03304400	-2.22745200
H	0.18452600	-2.49316300	-1.93883700
H	-0.93724200	-1.90385000	-0.67987600
C	2.10049000	-1.35684200	-0.84024900
H	2.15094600	-2.36021500	-1.26035200
C	3.31489200	-0.85589600	-0.32207800
C	4.46763500	-1.68955400	-0.43448700
C	5.67486400	-1.26173200	0.05960500
H	4.37398100	-2.66407500	-0.91117900
C	4.59000800	0.75130200	0.74445000
C	5.75807400	-0.00144800	0.67235700
H	6.55509700	-1.89625100	-0.02230900
H	4.61499200	1.73698100	1.21580200
H	6.69113900	0.37903500	1.07726900
N	3.40759600	0.37033500	0.27724400

Complex **6** (α-NH)

ML(C$^{\bullet}$) G = -1849,363922

Co	0.32395400	-0.00766800	0.04148900
Cl	-0.30598300	0.88479300	2.05636400
Cl	2.47186800	-0.02455800	0.63672100
Cl	0.79201200	-0.88522900	-2.01878700
N	-1.58031400	-0.02391600	-0.55095400
C	-2.28142100	-1.01411500	0.28288900
H	-3.25345000	-1.28535000	-0.14789700
H	-2.43475200	-0.56099100	1.26810800
C	-1.94571800	1.33673400	-0.58051000
H	-2.56088900	1.70669500	0.23313700
C	-0.90329600	2.16126200	-1.25757000
C	-1.36374800	-2.22603000	0.37038000
N	-0.00640700	-1.78287700	0.76374900
N	0.42979800	1.80496000	-0.67522200
H	-1.76706900	-2.97316400	1.06340900
H	-1.27292600	-2.69296900	-0.61750000
H	0.72510200	-2.40049600	0.41283700
H	0.10393600	-1.67837600	1.77308700
H	-0.84977700	1.91201400	-2.32666300
H	-1.11152400	3.23175500	-1.17106200
H	-1.40331800	-0.39281900	-1.49551900
H	1.18618400	1.84583300	-1.35820300
H	0.67102900	2.38551600	0.12885600

L(C-H) G = -324,151981

N	0.00003400	-0.30572700	-0.24669700
C	1.21659600	-0.90234700	0.28091100
H	1.28233500	-1.99094400	0.07772100
H	1.19368300	-0.79297500	1.37745700
C	-1.21655900	-0.90244800	0.28071500
H	-1.28228900	-1.99100400	0.07727700
H	-1.19367000	-0.79335400	1.37729100
C	-2.44194500	-0.18692900	-0.27056900
C	2.44196300	-0.18694200	-0.27053300
N	2.52769700	1.22787700	0.05116500
N	-2.52777500	1.22785000	0.05130400
H	3.35057500	-0.69030700	0.08418500
H	2.45048600	-0.29475900	-1.36736900
H	2.66518000	1.33552400	1.05256600
H	1.62334700	1.64807200	-0.15039300
H	-2.45057500	-0.29465700	-1.36741700
H	-3.35051600	-0.69034800	0.08416600
H	0.00013000	-0.40691600	-1.26135800
H	-2.66514700	1.33542300	1.05272700
H	-1.62355500	1.64823900	-0.15039100

ML(C-H) G = -1850,015699

Co	-0.33699600	0.00002500	0.02814400
Cl	0.21385800	-0.00268900	2.25458500
Cl	-2.51039800	-0.00048600	0.52401200
Cl	-0.77278900	0.00260300	-2.21643000
N	1.55522900	0.00047000	-0.46970100
C	2.13192300	1.27725500	-0.01792400
H	3.11146300	1.46737800	-0.47786700
H	2.25060800	1.22260500	1.06916200
C	2.13181900	-1.27742000	-0.02095400
H	3.11115600	-1.46673500	-0.48171400
H	2.25136500	-1.22536100	1.06616400
C	1.12647500	-2.35315900	-0.41233700
C	1.12683900	2.35403600	-0.40704800
N	-0.22423600	1.94153000	0.04184000
N	-0.22451700	-1.94157700	0.03774000
H	1.41241900	3.32861300	0.00483300
H	1.08749800	2.44814100	-1.49857200
H	-0.96507300	2.29805800	-0.56107700
H	-0.42395300	2.20838500	1.00639700
H	1.08702500	-2.44463800	-1.50411100

H	1.41209000	-3.32874300	-0.00287500
H	1.48487900	0.00161300	-1.49261300
H	-0.96558500	-2.29670900	-0.56573300
H	-0.42405300	-2.21079100	1.00170000

L(C•) G = -323,515851

N	0.01979300	-0.38997600	0.21704300
C	-1.20407000	-0.92038500	-0.32636000
H	-1.25947300	-1.99681300	-0.10407800
H	-1.24649500	-0.83030700	-1.43193400
C	1.22875800	-0.94101600	-0.17044800
H	1.24228000	-2.02201400	-0.30647100
C	2.45967300	-0.22882200	0.25576300
C	-2.39973000	-0.21101100	0.27697500
N	-2.32900000	1.21026100	-0.03812200
N	2.37555500	1.18231300	-0.13250600
H	-3.32483500	-0.71084900	-0.06353900
H	-2.35411200	-0.31985200	1.36859700
H	-3.03238700	1.73249700	0.47175900
H	-2.50706000	1.35700600	-1.02757500
H	2.57150800	-0.23915500	1.35807600
H	3.33942200	-0.76437400	-0.14504300
H	0.03021500	0.62760200	0.25536200
H	3.16779800	1.70246900	0.23018000
H	2.40092000	1.25300200	-1.14581300

Complex **6** (α-NH_2)

ML(C•) G = -1849,362175

Co	0.32980000	-0.01677900	0.02222100
Cl	-0.22886400	-0.31591800	2.22741600
Cl	2.49180200	-0.28665400	0.48526700
Cl	0.76399800	0.31395700	-2.19283700
N	-1.55883000	0.22913900	-0.44433400
C	-2.25448100	-1.04171500	-0.18277300
H	-3.24777700	-1.06987700	-0.65078200
H	-2.36343600	-1.14616900	0.90175900
C	-2.00900500	1.49620400	0.18884500
H	-2.94157500	1.86653400	-0.25388200
H	-2.17779400	1.27973800	1.25244600
C	-0.88077900	2.45012300	-0.01349500
C	-1.35147900	-2.12901400	-0.75283600
N	0.03398900	-1.91360000	-0.27137100
N	0.39045600	1.92601600	0.36405300
H	-1.71988200	-3.12771500	-0.49209200
H	-1.32570200	-2.05303000	-1.84611900
H	0.73578700	-2.23353100	-0.93828700
H	0.21545100	-2.34741400	0.63463100
H	-0.89419900	3.19490200	-0.80322100
H	-1.48052100	0.37828600	-1.45582600
H	1.17955000	2.33468300	-0.13547700
H	0.57275400	1.93859300	1.37261100

L(C•) G = -323,513443

N	-0.08055300	0.08261800	-0.10908900
C	1.11655700	0.84722800	-0.37782100
H	1.34560500	1.57866100	0.42999600
H	0.97189500	1.44173200	-1.29295800
C	-1.21597800	0.90521400	0.28691500
H	-1.02114100	1.50913000	1.19683200
H	-1.35289200	1.64821700	-0.53077700
C	-2.42506100	0.06999300	0.48420500
C	2.30463600	-0.07793200	-0.54980100
N	2.53142500	-0.81527000	0.68869600
N	-2.65004900	-1.00382900	-0.36825900
H	2.06461000	-0.80399500	-1.33771900
H	3.17553800	0.50639400	-0.89772100
H	2.91896900	-0.19632700	1.39508700
H	3.20211100	-1.56260800	0.54989700
H	-3.23643000	0.38165200	1.13272800
H	0.13341100	-0.59323600	0.62338400
H	-3.57842500	-1.10405600	-0.75811600
H	-1.90993100	-1.11722500	-1.05105400

Complex **7**

ML(C•) G = -1886,247778

Ir	0.34845300	0.00596800	0.00610500
Cl	1.70465600	-0.48392900	-1.88048200
Cl	1.56463600	-1.44236800	1.44021000
Cl	1.58484400	1.93769800	0.62411100
N	-0.94048600	1.14250700	-1.18278100
N	-1.07667100	0.41456500	1.47859800
N	-0.95425900	-1.55260300	-0.46908000
C	-1.58699500	2.12493400	-0.26536000
C	-2.09305100	1.38591100	0.96382900
C	-1.64674100	-0.90710600	1.84902100
C	-2.00847300	-1.68023200	0.58819000
C	-1.51597400	-1.20549400	-1.80773000
C	-1.87325500	0.23539600	-1.80423400
H	-0.35716700	1.63190000	-1.87354000
H	-0.57189800	0.81401700	2.27337100
H	-0.39029300	-2.40413700	-0.52821700
H	-2.41715700	2.64536000	-0.76424700
H	-0.80660400	2.84376400	0.00479900
H	-2.36757900	2.09989400	1.74751800
H	-2.99841300	0.81971300	0.71029700
H	-2.53327500	-0.79680500	2.49037800
H	-0.85862100	-1.43038400	2.39949900
H	-2.16909700	-2.73495500	0.83547600
H	-2.94574100	-1.30527300	0.15664200
H	-2.38356000	-1.83082900	-2.06186200
H	-0.70762100	-1.40579900	-2.53089500
H	-2.69734300	0.64845200	-2.38403000

L(C-H) G = -401,462375

N	-0.13626000	1.69026300	-0.49699400
N	1.53244800	-0.72838300	-0.49930700
N	-1.39693500	-0.96263300	-0.49881900
C	1.23393200	1.70300200	-0.03788900
C	1.73948200	0.34331000	0.44916000
C	0.85754000	-1.91978000	-0.03683000
C	-0.57173300	-1.67441900	0.45208900
C	-2.09299100	0.21770400	-0.03966500
C	-1.16617800	1.33094800	0.45260700
H	-0.36048700	2.53477700	-1.00396600
H	2.37474000	-0.95881400	-1.00706700
H	-2.01664600	-1.57916600	-1.00511200
H	1.43042000	2.43033800	0.78138600
H	1.85708500	2.01670300	-0.88768300
H	2.80299200	0.47043000	0.71592400
H	1.24790000	0.08959500	1.40037500
H	1.39019800	-2.45175500	0.78295500
H	0.81503300	-2.61827500	-0.88481800
H	-0.99423700	-2.65704100	0.72477300
H	-0.54177600	-1.11652100	1.40002900
H	-2.82484900	0.02389700	0.77626300
H	-2.67156100	0.60472100	-0.89077300
H	-1.80550600	2.18808600	0.72662000
H	-0.69839700	1.02371000	1.40010300

ML(C-H) G = -1886,895527

Ir	0.35543500	-0.00036100	-0.00030600
Cl	1.63077700	1.98879700	-0.26610000
Cl	1.63175700	-1.22418800	-1.58988000
Cl	1.63431000	-0.76384300	1.85290000
N	-0.97810700	1.00837500	1.24293300
N	-0.97988100	-1.58104900	0.25239700
N	-0.98086400	0.57172900	-1.49382900
C	-1.55924600	-0.03255200	2.13012600
C	-1.99012000	-1.23816000	1.30315000
C	-1.56389900	-1.82753700	-1.09197700
C	-1.99373200	-0.50749100	-1.72044900
C	-1.56063500	1.86122100	-1.03563100
C	-1.98934100	1.74750400	0.42226600
H	-0.41953900	1.66321200	1.79549600
H	-0.42288800	-2.38829700	0.54266200
H	-0.42393800	0.72100500	-2.33879900
H	-2.41307500	0.35829100	2.70262500
H	-0.75877400	-0.31981000	2.81956400
H	-2.15314000	-2.09650100	1.96360800
H	-2.94620300	-1.04607100	0.79960000
H	-2.41873700	-2.51726600	-1.03773800
H	-0.76502600	-2.28238000	-1.68646700
H	-2.16011900	-0.64917800	-2.79366100
H	-2.94805500	-0.16594200	-1.29926400
H	-2.41517400	2.16161400	-1.65930500
H	-0.75953800	2.60105300	-1.13355500

H	-2.15133900	2.74840000	0.83649300
H	-2.94548300	1.21536700	0.50926200

L(C•) G = -400,838456

N	-0.42745000	-1.55692800	-0.54340400
N	-1.19257400	1.13055600	-0.47777700
N	1.68614900	0.34836300	-0.48337000
C	-1.74795800	-1.21352600	-0.03638800
C	-1.78462900	0.22337000	0.49679500
C	-0.13362000	2.01644800	-0.02902300
C	1.12153900	1.29783300	0.46620000
C	1.90072400	-0.99997800	0.05225100
C	0.59656000	-1.62088800	0.39419000
H	-0.17783700	-0.85522200	-1.24306100
H	-1.90044000	1.65258400	-0.97695400
H	2.53642800	0.70306600	-0.90346800
H	-2.03309800	-1.92383400	0.75251200
H	-2.47271700	-1.32902500	-0.85414700
H	-2.81601200	0.50612900	0.76121200
H	-1.20564600	0.25766400	1.43043200
H	-0.44940100	2.70489500	0.78322600
H	0.14053100	2.64783300	-0.88619300
H	1.84823800	2.07633300	0.75017100
H	0.88560300	0.76008800	1.39716900
H	2.55002800	-1.02353400	0.94981200
H	2.44304100	-1.55922800	-0.73472200
H	0.47271800	-2.29124000	1.24171500

Complex **8** (β-Pt)

ML(C•) G = -1566,030315

Pt	0.86556700	0.02365500	-0.00000300
Cl	2.44486400	1.71409400	-0.00001000
Cl	2.43864400	-1.66764100	-0.00001100
C	-1.95822000	0.66903800	0.00000800
N	-0.74602600	1.28259400	0.00000400
C	-0.72049700	2.62457300	0.00000400
C	-1.90325000	3.34343600	0.00000900
C	-3.09269300	2.62216700	0.00001300
N	-3.12213600	1.29019600	0.00001300
H	0.27363500	3.07216600	0.00000100
H	-1.89228300	4.42798000	0.00001000
H	-4.05710600	3.12809500	0.00001700
C	-1.90364400	-0.80651300	0.00000700
N	-0.63559600	-1.31974700	0.00000200
C	-0.51935100	-2.62724800	0.00000200
C	-1.58845100	-3.49082900	0.00000600
C	-2.83959800	-2.86798600	0.00001000
N	-2.99298300	-1.54311100	0.00001100
H	-1.47412000	-4.56934200	0.00000500
H	-3.75259900	-3.46304200	0.00001300

L(C-H) G = -527,064118

C	0.00000000	0.74712600	-0.00001600
N	-0.28748600	1.34802500	1.15749600
C	-0.28946600	2.67787200	1.14188100
C	0.00000000	3.41405400	0.00001600
C	0.28946100	2.67789800	-1.14186700
N	0.28747800	1.34805000	-1.15751600
H	-0.53280300	3.17497300	2.08231500
H	0.00000000	4.49953200	0.00003000
H	0.53279200	3.17502100	-2.08229200
C	0.00000000	-0.74712600	-0.00001600
N	0.28748600	-1.34802500	1.15749600
C	0.28946600	-2.67787200	1.14188100
C	0.00000000	-3.41405400	0.00001600
C	-0.28946100	-2.67789800	-1.14186700
N	-0.28747800	-1.34805000	-1.15751600
H	0.53280300	-3.17497300	2.08231500
H	0.00000000	-4.49953200	0.00003000
H	-0.53279200	-3.17502100	-2.08229200

ML(C-H) G = -1566,705802

Pt	0.86547200	-0.00002400	-0.00000800
Cl	2.47763100	1.65798500	0.00000500
Cl	2.47755900	-1.65811500	0.00002800
C	-1.93302900	0.73808800	0.00001500
N	-0.70232000	1.30816600	-0.00002500
C	-0.63095500	2.64920000	-0.00003600
C	-1.78774500	3.40849100	-0.00000900
C	-3.00122600	2.72851800	0.00005000
N	-3.07521600	1.39907200	0.00005800
H	0.37725600	3.06298900	-0.00006600
H	-1.73839300	4.49198800	-0.00002300
H	-3.94784700	3.26730600	0.00009500
C	-1.93308500	-0.73797900	-0.00001600
N	-0.70241900	-1.30814600	0.00000300
C	-0.63114200	-2.64918400	0.00002100
C	-1.78797900	-3.40839800	0.00001300
C	-3.00141300	-2.72834300	-0.00002900
N	-3.07531800	-1.39888900	-0.00004200
H	0.37704400	-3.06303900	0.00003900
H	-1.73870000	-4.49189700	0.00003300
H	-3.94807100	-3.26706400	-0.00003800

L(C•) G = -526,401496

C	0.71681100	-0.00246200	-0.00000100
N	1.33167600	-1.18732100	-0.00001500
C	2.66097800	-1.15887700	-0.00001400
C	3.38377400	0.02735700	0.00000100
C	2.63393400	1.19691600	0.00001500
N	1.30446300	1.19678900	0.00001200
H	3.16807700	-2.12483600	-0.00002700
H	4.46909300	0.04014800	0.00000200
H	3.11940000	2.17402600	0.00002700
C	-0.77456800	-0.02382900	0.00000000
N	-1.38400600	-1.22771600	0.00001600
C	-2.66885400	-1.23789900	0.00001900
C	-3.47758800	-0.11259700	0.00000100
C	-2.75736800	1.07997400	-0.00001500
N	-1.42602700	1.13243900	-0.00001600
H	-4.56213300	-0.13894900	0.00000400
H	-3.27988600	2.03877100	-0.00002600

Complex **8** (δ-Pt)

ML(C•) G = -1566,038663

Pt	-0.83636800	-0.11488400	-0.00000400
Cl	-2.17028800	-2.00133500	-0.00001800
Cl	-2.67844500	1.28103800	-0.00000900
C	2.04259100	-0.41622600	0.00000900
N	0.91307800	-1.16690400	0.00000100
C	1.05041100	-2.50261500	-0.00000200
C	2.31170000	-3.07300200	0.00000300
C	3.40683400	-2.21489800	0.00001100
N	3.27402000	-0.88975200	0.00001400
H	0.11796100	-3.06644300	-0.00000800
H	2.43054300	-4.15116900	0.00000100
H	4.42514500	-2.60072900	0.00001600
C	1.81156900	1.03764800	0.00001100
N	0.51724800	1.42253400	0.00000700
C	0.23298700	2.73973800	0.00000900
C	1.24639000	3.68508100	0.00001600
C	2.52637000	3.15267500	0.00001900
N	2.82671900	1.89767600	0.00001800
H	-0.83101900	2.98135500	0.00000600
H	1.03198800	4.74775400	0.00001700

Complex **9**

ML(C•) G = -2012,958714

Mg	-0.03627100	-0.32674400	-0.01416200
Cl	-2.60131100	-1.11895600	-0.00909200
O	-1.74772600	-0.59910900	1.14592500
O	-1.55090300	-1.13807800	-1.12762400
O	-3.64757200	-0.16256800	-0.32591200
O	-3.08734200	-2.45322800	0.25879300
Cl	2.40922600	-1.40263500	-0.02264500
O	1.36310500	-1.30532600	1.09358800
O	1.63186900	-0.76158500	-1.17414100
O	2.71772300	-2.78443100	-0.31615000
O	3.57174200	-0.60057900	0.31185300
N	0.14499000	1.80782000	0.02531400
C	-0.81792200	2.41556200	1.00428400
H	-1.82078800	2.08339800	0.71275000
H	-0.77255100	3.50967100	0.87735600
C	-0.08299700	2.38623200	-1.33174700
H	0.64529300	1.92021200	-2.00604300
H	0.15799200	3.46055700	-1.28910000

C	1.51435400	1.96054300	0.44720100
H	1.71140400	1.65798100	1.47043000
C	-1.48236100	2.18939700	-1.87672500
H	-2.24238200	2.73418100	-1.30861600
H	-1.51278900	2.56692600	-2.90335800
H	-1.77546200	1.13407600	-1.91286000
C	-0.57282700	2.04669700	2.45215200
H	0.32561100	2.51825800	2.86043500
H	-1.42411500	2.38914000	3.04786700
H	-0.50187000	0.96234100	2.60362400
C	2.62128000	2.36971200	-0.44746800
H	2.48216500	3.37283500	-0.87639800
H	3.55085600	2.37841200	0.12688100
H	2.77810300	1.67561500	-1.28753100

L(C-H) G = -292,041483

N	0.00093900	-0.00062600	-0.02636900
C	-0.15480100	1.37976500	0.42127300
H	0.82098200	1.87601500	0.34383600
H	-0.42643400	1.41446400	1.49878200
C	1.27438000	-0.55443200	0.42255400
H	1.21498600	-1.64795500	0.35087200
H	1.44129000	-0.33138000	1.49884700
C	-1.11383200	-0.82611600	0.42745400
H	-2.03105100	-0.22661600	0.36670300
H	-0.99555800	-1.08820100	1.50124500
C	2.45206800	-0.08300900	-0.40911600
H	2.60085100	1.00100000	-0.34545300
H	3.37977100	-0.55859200	-0.07214300
H	2.29269500	-0.33560500	-1.46271700
C	-1.15674300	2.16107800	-0.40739100
H	-2.16864100	1.74526400	-0.33992100
H	-1.21006600	3.20246200	-0.07124100
H	-0.86230500	2.14949900	-1.46211600
C	-1.30162100	-2.07678400	-0.41019600
H	-0.43229100	-2.74292200	-0.36559100
H	-2.16893400	-2.64994800	-0.06430300
H	-1.45857700	-1.80611500	-1.45968600

ML(C-H) G = -2013,606552

Mg	0.00924000	-0.27930100	-0.10452300
Cl	-2.46361900	-1.32549000	-0.04835800
O	-1.50887600	-1.00164300	1.10036700
O	-1.57971400	-0.94917600	-1.24230800
O	-3.62500300	-0.45444300	0.00832000
O	-2.78909700	-2.73356100	-0.07415900
Cl	2.50738100	-1.27357100	-0.03997500
O	1.59932200	-0.85445800	1.11467100
O	1.57952900	-0.97780800	-1.22646600
O	2.81568300	-2.68458600	0.02563400
O	3.67890500	-0.41829300	-0.09381200
N	-0.03023200	1.84252300	0.05587200
C	-0.82510300	2.17824800	1.27668100
H	-1.82522500	1.74879400	1.14684800
H	-0.94284500	3.27572700	1.31204900
C	-0.63515200	2.53683400	-1.12319900
H	-0.10375600	2.18222900	-2.01491600
H	-0.41158300	3.61413300	-1.02507800
C	1.36669700	2.35451100	0.23647400
H	1.84750500	1.73610100	1.00371600
H	1.29733700	3.38017400	0.63930200
C	-2.12435500	2.34517800	-1.32289900
H	-2.72437100	2.81498900	-0.53804300
H	-2.40411900	2.81921100	-2.26901200
H	-2.40910700	1.29152500	-1.39281900
C	-0.23778000	1.67755600	2.58121600
H	0.69418100	2.18266600	2.85101800
H	-0.95852900	1.86871800	3.38186900
H	-0.05216400	0.59668900	2.57816500
C	2.22068400	2.35178200	-1.01719500
H	1.92734200	3.12924500	-1.72882600
H	3.25985900	2.54033300	-0.73185700
H	2.20633600	1.38454500	-1.53200800

L(C$^{\bullet}$) G = -291,401824

N	-0.06969400	-0.11468700	-0.25451800
C	1.21009000	-0.69256400	-0.62496700
H	1.82409200	0.08809000	-1.09458500
H	1.05499000	-1.46332400	-1.39899300
C	-0.24093300	1.30550900	-0.49499300
H	-1.29830400	1.55279900	-0.35188700
H	-0.00763500	1.55321700	-1.54787600
C	-1.16380000	-0.97454400	-0.23227100
H	-0.90147500	-2.02968300	-0.26724800
C	0.60677200	2.15131500	0.43899600
H	1.67652200	1.94468300	0.31014000
H	0.45231100	3.22005000	0.25233100
H	0.34969900	1.93643700	1.48271000
C	1.94346300	-1.28780300	0.56528000
H	1.32819100	-2.05560300	1.04865300
H	2.88977200	-1.75065500	0.26224000
H	2.15671300	-0.51556600	1.31372300
C	-2.45344000	-0.55649900	0.37207700
H	-3.01627800	0.17141800	-0.23534800
H	-3.10706100	-1.42578900	0.49408000
H	-2.32658500	-0.09575100	1.36895200

Optimized Energies and Geometries ($\Delta\Delta G^{\ddagger}$)

Optimized energies (G, in hartrees) and geometries (Å) of all species used in the calculation of $\Delta\Delta G^{\ddagger}$.

Complex **1**

Reactant (L) G = -305,345731

C	0.75869800	-0.67648600	-0.43274000
C	0.66158100	0.73310400	0.13433100
H	0.35761100	0.66278400	1.19359200
H	1.05569700	-0.61497200	-1.49011900
N	1.88502500	1.51362700	0.06372900
N	1.78474500	-1.42333400	0.28367000
H	1.96437500	-2.31719700	-0.16018600
H	1.47159900	-1.62201500	1.22996000
H	-0.24679600	-1.14401300	-0.42309400
H	-0.15036700	1.26694100	-0.37867700
H	2.64409900	0.91719500	0.38774900
H	2.09207400	1.71530500	-0.91105600
O	-2.25317600	-0.08603800	-0.72935300
C	-2.75198500	0.08411800	0.52283100
H	-3.85574700	0.03572700	0.41859800
H	-2.49223500	-0.74541800	1.20556800
H	-2.51306800	1.05749700	0.98415000

TS (L) G = -305,339146

C	0.93344900	-0.78387600	-0.25523400
C	0.35554700	0.49460200	0.30955000
H	0.12923500	0.41844900	1.38731100
H	0.81903700	-0.75696000	-1.34981700
N	1.14520400	1.63485500	0.04302100
N	2.34912400	-0.91993800	0.05447300
H	2.68420900	-1.83767300	-0.21889800
H	2.49811600	-0.83094500	1.05530300
H	0.29035100	-1.61369900	0.09159900
H	-0.74295600	0.52806000	-0.19106200
H	1.60203400	1.61968800	-0.86035700
H	0.69991400	2.52321900	0.22894600
O	-1.96473700	0.11491900	-0.69016000
C	-2.64075000	-0.41435700	0.38594600
H	-3.61761700	-0.77542000	0.02107600
H	-2.14108000	-1.29156200	0.84255700
H	-2.85311500	0.31485400	1.19059500

Reactant (ML) G = -1352,596786

Pd	0.97523500	0.00041900	0.00620100
Cl	2.41741900	1.79486300	-0.08957000
Cl	2.57867500	-1.65264200	-0.05192100
C	-1.82758400	-0.80865400	-0.11538700
C	-1.82591800	0.55183200	0.55580100
H	-1.71445300	0.43671600	1.64120800
H	-1.94185200	-0.68528200	-1.19871300
N	-0.66107200	1.32144200	0.07394300
N	-0.52852300	-1.46973100	0.13061600
H	-0.32091900	-2.21305400	-0.53412400
H	-0.46620000	-1.88000500	1.06134100
H	-2.67947800	-1.40919600	0.22986900
H	-2.77598100	1.06828400	0.36070500
H	-0.80496200	1.69058500	-0.86528400
H	-0.42048000	2.11141700	0.67063300
O	-4.61663300	0.21077900	-0.70255000
C	-5.61012500	-0.04370400	0.18611900
H	-6.50395300	-0.28324500	-0.42850200
H	-5.43192400	-0.94116100	0.80506200
H	-5.89218600	0.82287300	0.80718900

TS (ML) G = -1352,579203

Pd	0.90650600	0.00409600	-0.02490100
Cl	2.02974600	2.00811300	0.04105000
Cl	2.75620000	-1.34659100	0.15552100
C	-1.71016600	-1.25438400	-0.37934200
C	-1.93972900	0.10537600	0.23398500
H	-1.99362300	0.09303500	1.32919900
H	-1.79382900	-1.18083500	-1.47083700
N	-0.93495400	1.04787300	-0.20735500
N	-0.33528500	-1.70730600	-0.06101800
H	0.03259000	-2.38516200	-0.72688800
H	-0.26646000	-2.13131700	0.86310800
H	-2.47599800	-1.96362300	-0.04109500
H	-3.10206700	0.42389700	-0.16101600
H	-1.02372400	1.30282300	-1.19092400
H	-0.88686900	1.90768600	0.33770400
O	-4.28182800	0.38896900	-0.54101200
C	-5.07943900	0.12493300	0.56338100
H	-6.11938400	0.13179900	0.20333500
H	-4.90469700	-0.87176200	1.00489300
H	-5.00397900	0.88787800	1.35483500

Complex **2**

Reactant (L) G = -1035,658256

C	-0.33425700	-0.17605300	-0.83138500
C	0.74042700	0.75202000	-0.28446100
H	0.33024000	1.38372000	0.51857900
H	0.00892500	-0.64486500	-1.76574600
H	-1.24459300	0.39780900	-1.08679500
H	1.09138700	1.43412000	-1.07527700
P	2.23422500	-0.12380700	0.46220400
P	-0.84864900	-1.57616400	0.31579800
C	-1.60096100	-0.55881600	1.68737900
H	-2.27487000	0.20490700	1.27521400
H	-2.17056100	-1.21886200	2.35066300
H	-0.81307100	-0.08563500	2.28397900
C	-2.42779800	-2.02489300	-0.57233300
H	-2.98081700	-2.76512300	0.01574600
H	-3.05851000	-1.14079400	-0.72885600
H	-2.18996700	-2.47543400	-1.54231100
C	2.89377600	-0.93015000	-1.08662400
H	2.88146300	-0.24019000	-1.94076900
H	3.92421500	-1.25663700	-0.90891800
H	2.29962300	-1.81770100	-1.32851200
C	3.37353200	1.35868700	0.49185000
H	4.37565000	1.04519600	0.80320400
H	3.44208000	1.84412300	-0.49048800
H	3.00794400	2.08737500	1.22396100
O	-2.90021900	1.57991800	-0.56345300
C	-2.27431200	2.72124200	-0.17013600
H	-3.06542100	3.49832100	-0.12195400
H	-1.84020300	2.66533000	0.84467700
H	-1.52783900	3.09233800	-0.89456000

TS (L) G = -1035,653894

C	-0.41109800	0.00306100	-0.68864500
C	0.73915600	0.76166900	-0.08079300
H	0.42727600	1.27753800	0.83974300
H	-0.21806800	-0.27158000	-1.73565300
H	-1.39356800	0.73899500	-0.73385200
H	1.10770000	1.53057200	-0.77718300
P	2.20634100	-0.33216200	0.41850400
P	-1.02956300	-1.47552700	0.23656000
C	-1.66391600	-0.63620700	1.77247600
H	-2.23854400	0.25465500	1.48948500
H	-2.30899300	-1.32954200	2.32185400
H	-0.82941700	-0.36034300	2.42542900
C	-2.64226700	-1.72430000	-0.66377700
H	-3.21151100	-2.51801600	-0.16925600
H	-3.22824000	-0.79875300	-0.67547600
H	-2.44117100	-2.04108200	-1.69268900
C	2.68474800	-0.94790900	-1.27639500
H	2.69187400	-0.13802000	-2.01757200
H	3.68567500	-1.38987400	-1.22500300
H	1.98949800	-1.72969900	-1.59974400
C	3.47091100	1.03537400	0.56935900
H	4.46112900	0.59946500	0.74043000
H	3.50877600	1.65961700	-0.33253700
H	3.22872600	1.66723100	1.43091300
O	-2.40628900	1.60991700	-0.64552200
C	-1.89536300	2.78186900	-0.13011700
H	-2.68386700	3.55024800	-0.20577500
H	-1.61195200	2.72009400	0.93833600
H	-1.02970600	3.17314500	-0.69588500

Reactant (ML) G = -2075,368798

Pt	-0.88647900	-0.28030500	-0.09221300
Cl	-1.44015900	-2.58305300	-0.44994100
Cl	-2.97343000	0.60006000	-0.87415800
C	1.60583900	1.79164800	0.67024800
C	1.96532900	0.52246000	1.43561100
H	1.60347700	0.57076100	2.47272600
H	2.13765100	1.80848600	-0.29035400
H	1.89414500	2.69719900	1.22033400
H	3.05189100	0.36789400	1.45457000
O	4.35625700	0.63894800	-0.62042400
C	5.24994300	0.19136200	-1.54049100
H	6.00211200	1.00279300	-1.63805400
H	5.80791200	-0.70485500	-1.22223700
H	4.81819600	0.06039700	-2.54707600
P	-0.21589200	1.83384200	0.27791300
P	1.11791600	-0.95667500	0.67487900
C	2.23204000	-1.59902900	-0.63383700
H	3.20072800	-1.89410000	-0.21264600
H	1.73528400	-2.46096100	-1.09166100
H	2.37195700	-0.82781700	-1.39794600
C	1.14955400	-2.25091700	1.96857000
H	0.70898600	-3.15860900	1.54453200
H	2.17726800	-2.44106800	2.29856800
H	0.53425700	-1.93347300	2.81546700
C	-0.39257200	3.03637200	-1.09045800
H	-1.45819800	3.12017700	-1.32455300
H	0.01639200	4.01165700	-0.80279600
H	0.12574100	2.65568400	-1.97523200
C	-1.02971200	2.64755900	1.70736700
H	-0.66118400	3.67180200	1.83631900
H	-2.10761500	2.65614100	1.51522000
H	-0.84558600	2.06676700	2.61659800

TS (ML) G = -2075,354319

Pt	-0.95881100	-0.22840500	-0.00022800
Cl	-3.09642500	0.84309000	-0.07378600
Cl	-1.79049300	-2.46594200	-0.04881500
C	2.22791000	0.31952400	0.51647500
C	1.82663300	1.60119100	-0.16941800
H	2.02053700	1.54354500	-1.25099900
H	2.30701100	0.40631800	1.60856100
H	3.35740100	-0.06298700	0.13522300
H	2.35605100	2.47906100	0.22295000
P	-0.03121000	1.82417600	0.01638300
P	1.12016900	-1.09430900	0.06948700
C	1.72326900	-1.73298600	-1.53894700
H	2.76396600	-2.06339800	-1.45914900
H	1.07071100	-2.56591200	-1.82139800
H	1.63613900	-0.95331500	-2.30162500
C	1.51274100	-2.41129900	1.27367600
H	0.91800500	-3.29239200	1.01504200
H	2.58346900	-2.64236900	1.23438000
H	1.22818600	-2.08528900	2.27805100
C	-0.25621200	2.75652000	1.57934500
H	0.23383400	3.73548300	1.52754200
H	-1.33288600	2.88171900	1.73473300
H	0.14747300	2.17688400	2.41513200
C	-0.51889300	2.99983800	-1.29921300
H	-1.59208200	3.18692100	-1.19195600
H	0.04348300	3.93635200	-1.21326500
H	-0.34667400	2.54261400	-2.27777400
O	4.50638100	-0.37890500	-0.25899400
C	5.35192100	0.69109400	-0.01205200
H	6.35809000	0.37075800	-0.32419700
H	5.10467300	1.59130500	-0.60001100
H	5.41782400	0.95870900	1.05547700

Complex **3** (α-N)

Reactant (L) G = -1053,664119

C	0.25114300	-2.05033300	0.44815700
H	-0.37755300	-2.95229300	0.50529800
H	0.13420900	-1.48211600	1.37854500
P	-0.38340500	-1.04104600	-1.01065800
C	0.69615500	0.46465500	-0.78717200
C	1.90963800	0.49662000	-1.48414000
C	0.35807600	1.54949600	0.02962900
C	2.76747100	1.58655500	-1.36139600
H	2.18061800	-0.35164100	-2.11361700
C	1.20297600	2.65134200	0.13036200
H	-0.57552500	1.53178300	0.58985900
C	2.40950700	2.67236300	-0.56214000
H	3.70882800	1.59852000	-1.90726600
H	0.92139300	3.49059400	0.76268000
H	3.06997100	3.53350900	-0.48487500
C	-1.98236000	-0.39290100	-0.31672700
C	-2.48238500	-0.65433900	0.96180400
C	-2.74262700	0.41213300	-1.17557300
C	-3.70158300	-0.11935400	1.37177600
H	-1.92136100	-1.27488300	1.65712400
C	-3.95001700	0.96038800	-0.76279400
H	-2.37153500	0.61427400	-2.18135200
C	-4.43488400	0.69327800	0.51529800
H	-4.07457800	-0.33528600	2.37087900
H	-4.51948700	1.59128200	-1.44198400
H	-5.38405500	1.11385500	0.83984700
C	1.71480900	-2.42673000	0.30453800
H	2.31738100	-1.51339100	0.40556800
H	1.98956100	-3.07447700	1.15884200
N	1.99406300	-3.00703900	-1.00189500
H	2.94763300	-3.35023200	-1.04763200
H	1.38299600	-3.80079300	-1.17272700
O	1.59649400	0.23020500	2.36610900
C	2.92678500	0.46059300	2.25770700
H	3.30801300	1.20054600	2.98398700
H	3.54215900	-0.45809100	2.27127900
H	3.08577400	0.91957100	1.25383200

TS (L) G = -1053,658911

C	0.69869300	-1.47210600	-0.59202000
H	0.44163000	-2.42041600	-1.08644100
H	0.45430900	-1.58024000	0.47317300
P	-0.35725400	-0.10242300	-1.36503200
C	0.32208500	1.31027500	-0.36378500
C	1.09394100	2.26855300	-1.02482800
C	0.17019200	1.40009200	1.02437900
C	1.70475300	3.29916300	-0.31417600
H	1.22011700	2.19572600	-2.10485300
C	0.77817900	2.42848400	1.73379400
H	-0.43503600	0.66054300	1.54910000
C	1.54696100	3.37935200	1.06487500
H	2.30244700	4.04067500	-0.83984800
H	0.65307100	2.49127100	2.81270100
H	2.02183900	4.18445600	1.62129200
C	-1.96408500	-0.38288700	-0.47297200
C	-2.33291800	-1.60404900	0.09755600
C	-2.88731400	0.67120800	-0.44724800
C	-3.58460800	-1.76303400	0.68846500
H	-1.64451000	-2.44716400	0.08995600
C	-4.13080300	0.51593600	0.14994700
H	-2.61858100	1.63057600	-0.89044500
C	-4.48442900	-0.70483300	0.72064800
H	-3.85236000	-2.72063300	1.13009900
H	-4.82850800	1.35040100	0.16921000
H	-5.45967200	-0.82930400	1.18577300
C	2.17376100	-1.20081300	-0.74097400
H	2.47884500	-0.29418800	-0.19506900
H	2.70328000	-2.08026900	-0.10109900
N	2.60335800	-1.12392200	-2.09141000
H	3.59651000	-0.96154300	-2.19871000
H	2.31554900	-1.91683400	-2.65405800
O	3.04604700	-2.89070400	0.96193400
C	3.18513600	-2.03630800	2.03201800
H	3.37328000	-2.65134400	2.92851300
H	4.03371800	-1.33197100	1.94394700
H	2.27373400	-1.44449800	2.25258700

Reactant (ML) G = -3006,786698

Ru	0.06785600	-0.41615900	-0.07358200
Cl	-0.04236700	1.97157500	-0.65889900
Cl	0.16996300	-2.82917500	0.42402000
C	2.38141900	-0.89912400	-2.34753200
H	2.43237600	-1.99703400	-2.31136600
H	3.26067700	-0.54120900	-2.89711700
P	2.39452800	-0.35746200	-0.55639500
C	3.24782500	1.28020900	-0.54063200

C	3.71293300	1.75045900	0.69141800
C	3.36544100	2.09739100	-1.66428400
C	4.28769900	3.01063000	0.79764700
H	3.64155100	1.11339600	1.57473800
C	3.94423100	3.35917700	-1.55966000
H	2.98929800	1.76455400	-2.63005400
C	4.40306100	3.81890300	-0.33062700
H	4.65040000	3.36191100	1.76110400
H	4.02635700	3.98811400	-2.44306400
H	4.85115500	4.80651200	-0.24998100
C	3.72712900	-1.42099700	0.16324500
C	3.45962300	-2.27539500	1.23310000
C	5.02621300	-1.35619400	-0.35551100
C	4.47813300	-3.05559900	1.77713400
H	2.44184100	-2.36034000	1.60857500
C	6.03745100	-2.14178700	0.18277600
H	5.24999100	-0.67558400	-1.17730500
C	5.76358000	-2.99096900	1.25323200
H	4.25884200	-3.72245600	2.60774800
H	7.04325900	-2.08596000	-0.22769300
H	6.55648800	-3.60315700	1.67720200
C	1.08905800	-0.45066800	-3.00381700
H	1.03359900	0.64335000	-3.05845900
H	1.01530300	-0.84768700	-4.02676900
N	-0.06595800	-0.88701600	-2.18707800
H	-0.91471800	-0.46931100	-2.56394300
H	-0.16752700	-1.90286800	-2.23382800
C	-2.20942100	-0.30581500	2.27294100
H	-2.12808600	-1.35231400	2.60025000
H	-3.13634400	0.10598800	2.69058800
P	-2.25432200	-0.39187600	0.40662400
C	-3.23923100	1.06826600	-0.13953500
C	-3.66645900	1.10148100	-1.47101800
C	-3.47725700	2.17220000	0.67583300
C	-4.31146700	2.22159000	-1.97803700
H	-3.49755800	0.23779600	-2.11662200
C	-4.11539600	3.30011900	0.16504700
H	-3.14105300	2.19854600	1.71045000
C	-4.53252500	3.32794400	-1.16009900
H	-4.63938100	2.23451500	-3.01510800
H	-4.27095400	4.15820800	0.81584000
H	-5.02847000	4.20969800	-1.55950000
C	-3.46956800	-1.75072200	0.09183500
C	-3.10447100	-2.87771900	-0.64439900
C	-4.78023500	-1.63854700	0.57055200
C	-4.03704400	-3.88070000	-0.89953400
H	-2.07494500	-2.98587000	-0.97865300
C	-5.70576600	-2.64491800	0.32401600
H	-5.08032600	-0.75103900	1.12834400
C	-5.33464300	-3.76612000	-0.41547100
H	-3.74187200	-4.75817700	-1.47035000
H	-6.72116500	-2.55131100	0.70273500
H	-6.06137500	-4.55140900	-0.61153200
C	-0.99914700	0.49131600	2.72173200
H	-1.10349300	1.55323800	2.46844500
H	-0.88458600	0.43254900	3.81327900
N	0.22310000	-0.01006200	2.04619700
H	0.98002900	0.65385300	2.19879500
H	0.50337700	-0.90316900	2.45619300
O	-1.76327800	3.76398900	2.65096900
C	-0.99659200	4.36440900	1.72322500
H	-0.77872000	3.58628500	0.93480000
H	-1.48803400	5.19703400	1.18721100
H	0.00495100	4.65831600	2.08910100

TS (ML) G = -3006,768006

Ru	0.08335000	-0.26559500	-0.23100500
Cl	0.09762200	2.16908800	-0.50731400
Cl	0.07053600	-2.72606900	-0.06922500
C	2.41759900	-0.66229800	-2.46976800
H	2.37077200	-1.75930700	-2.52591700
H	3.34107000	-0.34281400	-2.96841700
P	2.41921800	-0.25604400	-0.64426900
C	3.34133700	1.33646500	-0.50351700
C	3.71419800	1.75206400	0.77834300
C	3.61769200	2.16684300	-1.58854900
C	4.34971300	2.97125600	0.97110700
H	3.51447900	1.10814900	1.63634400
C	4.25476700	3.39003100	-1.39669500
H	3.32560400	1.87739800	-2.59642900
C	4.62037200	3.79495900	-0.11872000
H	4.63454000	3.28033500	1.97417900
H	4.45986500	4.02965800	-2.25203100
H	5.11365400	4.75255800	0.03027700
C	3.67034000	-1.42939200	0.04781000
C	3.30399700	-2.38311800	0.99876900
C	5.00483300	-1.34954500	-0.36814300
C	4.26246600	-3.24408400	1.52882900
H	2.25863500	-2.47859200	1.28711700
C	5.95572800	-2.21676400	0.15454500
H	5.30175600	-0.59256100	-1.09443100
C	5.58459700	-3.16265200	1.10828000
H	3.96812900	-3.98653100	2.26689300
H	6.99000700	-2.14972200	-0.17545800
H	6.33018000	-3.83825100	1.52166400
C	1.19046100	-0.04048100	-3.11190700
H	1.23077000	1.05426300	-3.05574800
H	1.11633100	-0.32633900	-4.17090100
N	-0.02731900	-0.44965900	-2.37421700
H	-0.81695400	0.10870600	-2.69629200
H	-0.23671900	-1.43386200	-2.55227500
C	-2.26932000	-0.09404100	2.03485700
H	-2.33783100	-1.13579100	2.38155800
H	-3.13251200	0.45202000	2.43346300
P	-2.27269300	-0.17445500	0.15914200
C	-3.17810800	1.33519900	-0.38962700
C	-3.72295300	1.33469200	-1.67759000
C	-3.23052700	2.50365900	0.37003600
C	-4.31296700	2.48168400	-2.19504500
H	-3.69943000	0.42078300	-2.27382200
C	-3.82757200	3.64967300	-0.14581000
H	-2.78473200	2.53597200	1.36283400
C	-4.36594600	3.64184300	-1.42809900
H	-4.73696000	2.46778000	-3.19662400
H	-3.85924000	4.55596700	0.45424200
H	-4.82611000	4.54110300	-1.83086700
C	-3.52909900	-1.47881300	-0.20755800
C	-3.20645800	-2.56898400	-1.01604800
C	-4.82365400	-1.36871900	0.31457400
C	-4.16642700	-3.53843600	-1.29843900
H	-2.18873200	-2.67990700	-1.38452400
C	-5.77569600	-2.34198200	0.03960700
H	-5.09112300	-0.50976100	0.93052600
C	-5.44675900	-3.42766700	-0.76998800
H	-3.90433300	-4.38914000	-1.92316800
H	-6.77777900	-2.25153300	0.45281300
H	-6.19297000	-4.18933500	-0.98492900
C	-0.96684900	0.52046300	2.47153800
H	-0.85618400	1.57917900	2.20260600
H	-0.97565100	0.50500800	3.72001000
N	0.17044400	-0.21604700	1.94558600
H	1.04134400	0.20780700	2.25779800
H	0.16231100	-1.19252300	2.25065200
O	-1.23218500	0.62393100	4.96806700
C	-1.86892200	1.84188400	5.10993400
H	-2.81617200	1.91601800	4.54131900
H	-2.13684700	1.95122400	6.17295300
H	-1.23859500	2.71043600	4.84640400

Complex **3** (α-P)

TS (L) G = -1053,650967

C	-0.25819200	1.72127600	-0.76514800
H	0.50334300	2.32369000	-1.28403600
H	-0.00333800	1.87279400	0.42971200
P	-0.08343100	-0.04180900	-1.25184300
C	-1.28850800	-0.86750500	-0.11063200
C	-2.24956400	-1.69943800	-0.68981800
C	-1.29464700	-0.67568300	1.27623000
C	-3.19646300	-2.34420800	0.10110700
H	-2.25600400	-1.83283500	-1.77095400
C	-2.24395200	-1.31811000	2.06286200
H	-0.57204500	-0.00769000	1.74330400
C	-3.19165200	-2.15524700	1.47830000
H	-3.93892000	-2.99162500	-0.36022100
H	-2.24587800	-1.16161500	3.13934500
H	-3.93087300	-2.65639600	2.09945500

C	1.58466800	-0.50206000	-0.57890300
C	2.13427200	-0.02262200	0.61695200
C	2.32514500	-1.40603900	-1.34848100
C	3.39178500	-0.45164600	1.02870700
H	1.57890700	0.68491100	1.23154000
C	3.58067100	-1.83678800	-0.93185400
H	1.90954100	-1.77190000	-2.28732200
C	4.11516600	-1.35885200	0.25956100
H	3.80883000	-0.07436900	1.96025500
H	4.14264300	-2.54140400	-1.54088200
H	5.09770300	-1.69037200	0.58853300
C	-1.65772200	2.28594800	-0.89071400
H	-2.28585200	1.82212200	-0.11704700
H	-1.61497600	3.36480000	-0.64700300
N	-2.24429600	1.97748200	-2.18911800
H	-3.17698200	2.37168900	-2.25836400
H	-1.68874600	2.39020800	-2.93316300
O	0.13886400	2.35478800	1.64683800
C	1.02792600	3.41000000	1.54212900
H	0.65421000	4.23412800	0.90793100
H	1.16967500	3.82679400	2.55233900
H	2.02579400	3.10936100	1.17156100

TS (ML) G = -3006,769218

Ru	0.22276000	-0.15517600	-0.15573400
Cl	0.26184800	2.26041400	-0.08447400
Cl	0.20645900	-2.59499000	-0.32668800
C	2.66825900	-0.22278100	-2.33509700
H	2.66011900	-1.29512700	-2.57735300
H	3.59906600	0.20258700	-2.72938600
P	2.59483300	-0.14319200	-0.46842300
C	3.54653000	1.36497600	0.00361500
C	3.98108600	1.46483600	1.32924700
C	3.77600000	2.43102700	-0.86568700
C	4.63746700	2.60552400	1.77419800
H	3.82221400	0.63137000	2.01563400
C	4.43652800	3.57264700	-0.42076100
H	3.42742000	2.38959500	-1.89600300
C	4.86692700	3.66282500	0.89808500
H	4.97489700	2.66743800	2.80626200
H	4.60727300	4.39716000	-1.10884800
H	5.38013800	4.55666300	1.24442400
C	3.78207900	-1.46183000	0.04528700
C	3.38851000	-2.47418100	0.92059300
C	5.10265600	-1.42877500	-0.41844900
C	4.30327100	-3.44323200	1.32653200
H	2.35283300	-2.52489600	1.24883100
C	6.01004900	-2.40196200	-0.01990600
H	5.42794200	-0.62805500	-1.08300900
C	5.61035000	-3.40955900	0.85585100
H	3.98587100	-4.23207600	2.00433100
H	7.03359900	-2.37086100	-0.38641000
H	6.32242600	-4.16909700	1.17053500
C	1.45070000	0.46368600	-2.92685400
H	1.45863300	1.53811700	-2.70791000
H	1.42737100	0.33895200	-4.01863000
N	0.21440300	-0.07786800	-2.31532500
H	-0.58163800	0.48716400	-2.60744100
H	0.05484300	-1.03845700	-2.62599900
C	-2.20421200	-0.31528300	1.94576800
H	-2.24191400	-1.39358200	2.16363500
H	-3.29605400	0.13064500	2.38663100
P	-2.14447200	-0.13235700	0.12570000
C	-2.99957700	1.43411400	-0.32550300
C	-3.23117100	1.66963900	-1.68408600
C	-3.33197100	2.41529500	0.60728300
C	-3.77105400	2.87660200	-2.10882200
H	-3.00618000	0.89125300	-2.41692300
C	-3.87117300	3.62476600	0.17884700
H	-3.19244500	2.23475900	1.67092800
C	-4.08337600	3.86121100	-1.17473900
H	-3.95140000	3.04904800	-3.16764800
H	-4.12783000	4.38572700	0.91200900
H	-4.50080300	4.81004900	-1.50389500
C	-3.35160500	-1.39144800	-0.46490300
C	-3.04026400	-2.29072900	-1.48378800
C	-4.63062400	-1.39770400	0.10774000
C	-4.00189600	-3.19117700	-1.93593200
H	-2.03165600	-2.31639800	-1.89132000
C	-5.58093600	-2.30722700	-0.34142700
H	-4.87202800	-0.69168800	0.90642900
C	-5.26973700	-3.19938700	-1.36546600
H	-3.75282400	-3.89547100	-2.72635700
H	-6.57186300	-2.31574400	0.10724900
H	-6.01840700	-3.90653300	-1.71611800
C	-1.03167000	0.35648600	2.60668500
H	-1.04957700	1.44078400	2.44141900
H	-1.03606000	0.17732800	3.69114600
N	0.24327600	-0.13558100	2.00365400
H	1.02522200	0.43548400	2.32664900
H	0.41017300	-1.09736800	2.30058100
O	-4.42270300	0.46270500	2.92141600
C	-4.74370900	-0.53336300	3.81730200
H	-3.98040000	-0.68287400	4.60684400
H	-5.67523000	-0.25779500	4.34073100
H	-4.92858200	-1.51680700	3.33858400

Complex **4**

Reactant (L) G = -1499,712727

C	-3.45634800	-1.52450300	1.08681000
C	-2.92090500	-2.21002400	-0.16381500
C	-1.39951700	-1.97772200	-0.28389300
C	-2.82985000	-0.13437700	1.10936000
H	-4.55581900	-1.46490500	1.09036300
H	-3.16912500	-2.07621600	1.99757100
H	-3.40546400	-1.74658500	-1.03693900
H	-3.16075000	-3.28058600	-0.19118300
H	-0.84966500	-2.84485100	0.10713400
H	-3.13956700	0.37465500	0.17472500
P	-1.00486300	-0.56282700	0.95153300
C	-0.28089100	0.81135600	-0.08388600
C	1.09875200	0.76964000	-0.38789400
C	-1.03075500	1.92630400	-0.47047500
C	1.67204500	1.84636900	-1.06890500
C	-0.44005300	2.98861000	-1.14756500
H	-2.09655400	1.97306700	-0.25864000
C	0.91501800	2.95143000	-1.44638700
H	2.73387400	1.83776100	-1.30949800
H	-1.04502400	3.84291100	-1.44355800
H	1.38763400	3.77926400	-1.97065100
C	3.54859200	-0.78237900	-1.01041000
C	3.10283100	-0.01504500	1.59216100
C	4.77314800	-0.49100700	-0.13561900
H	3.42320400	0.02532800	-1.74331500
C	4.37563700	0.51280100	0.93493600
H	3.36833200	-0.90185800	2.19002300
H	5.08865200	-1.42862000	0.35187400
H	5.62320500	-0.15377400	-0.74454000
H	5.17149700	0.66971900	1.67748200
H	4.17118600	1.49578100	0.48074100
P	2.05384900	-0.74235500	0.17292600
C	-3.18504900	0.70327200	2.31956900
H	-2.70650600	1.68985500	2.28910400
H	-4.27078300	0.85914200	2.38936600
H	-2.85972800	0.20585000	3.24338900
C	-0.99119400	-1.73532900	-1.72625000
H	0.09441100	-1.63033400	-1.84085800
H	-1.31217500	-2.57725200	-2.35531500
H	-1.46417200	-0.82476800	-2.11872600
C	2.38968800	0.98467600	2.48254500
H	3.04439200	1.30319600	3.30456500
H	2.10213500	1.88056400	1.91788400
H	1.47861000	0.56164100	2.92192800
C	3.65497900	-2.10674200	-1.74992500
H	4.56141700	-2.13765100	-2.36960600
H	3.70555100	-2.94543800	-1.04264600
H	2.79520700	-2.28190400	-2.40686800
O	-4.22462800	0.74618900	-1.37021300
C	-5.49422300	0.49475000	-0.94868800
H	-5.79207400	1.08762800	-0.06475300
H	-6.16316900	0.82131000	-1.77094900
H	-5.70792700	-0.57719900	-0.78329500

TS (L) G = -1499,709174

C	-3.47016100	-1.56912500	1.04607900
C	-2.91198900	-2.29344100	-0.17606400

C	-1.40322300	-1.99945400	-0.33918400
C	-2.85356400	-0.17933900	1.03819400
H	-4.56845000	-1.50826000	1.02173900
H	-3.20848200	-2.09057200	1.98262400
H	-3.42942700	-1.90267200	-1.06389800
H	-3.10049600	-3.37335900	-0.13968500
H	-0.80494200	-2.83326700	0.05264000
H	-3.22015000	0.29457700	-0.02703600
P	-1.04662400	-0.55022900	0.84859700
C	-0.29852000	0.82780600	-0.15075800
C	1.09204800	0.78692800	-0.39287200
C	-1.03992000	1.94055800	-0.56077400
C	1.69344900	1.86887600	-1.04038100
C	-0.41733900	3.00807900	-1.20005100
H	-2.11766200	1.96885700	-0.41843100
C	0.95046000	2.97642200	-1.43724400
H	2.76390000	1.86144800	-1.23856000
H	-1.01031800	3.86196000	-1.52007000
H	1.44309000	3.80964100	-1.93384700
C	3.53498400	-0.79278600	-0.95227600
C	3.03550200	-0.02698600	1.64189800
C	4.74081900	-0.53074800	-0.04331600
H	3.44133200	0.02617100	-1.67777700
C	4.33413900	0.47890600	1.01864900
H	3.26951100	-0.91877800	2.24542700
H	5.02375400	-1.47604800	0.44916300
H	5.61345800	-0.20889400	-0.62795700
H	5.11332600	0.62133900	1.78131900
H	4.15785200	1.46513200	0.56006000
P	2.01356500	-0.73301500	0.19357800
C	-3.28531200	0.74930800	2.14267800
H	-2.79586000	1.72792200	2.07475600
H	-4.37188200	0.91194600	2.11307100
H	-3.04490500	0.32165100	3.12683000
C	-1.03376400	-1.75197300	-1.79131000
H	0.04243800	-1.58492600	-1.92283400
H	-1.31411900	-2.61923400	-2.40463800
H	-1.56795500	-0.87573600	-2.18145400
C	2.31113900	0.98218800	2.51240300
H	2.94562800	1.29209000	3.35315300
H	2.04943000	1.88154700	1.94062300
H	1.38283100	0.56988000	2.92568800
C	3.63451200	-2.11032100	-1.70415600
H	4.55296100	-2.14970900	-2.30513800
H	3.65585800	-2.95776900	-1.00595300
H	2.78570100	-2.26234900	-2.38081900
O	-3.91366700	0.75387400	-1.08239400
C	-5.25977300	0.58510800	-0.83892900
H	-5.60720900	1.07181500	0.09228200
H	-5.81387600	1.06701000	-1.66249300
H	-5.58103500	-0.47376400	-0.81777800

Reactant (ML) G = -2539,436742

Pt	-0.75020900	-1.17585300	-0.03697900
Cl	-2.95471800	-2.08238400	-0.34879600
Cl	0.31672400	-3.32755100	0.00021300
C	-4.26045700	1.41965900	0.30163600
C	-3.86078200	2.08667600	-1.01094900
C	-2.64605200	1.33310800	-1.55973100
C	-3.00945700	1.33386000	1.18318000
H	-5.05902300	1.96370900	0.82223200
H	-4.62566600	0.40114300	0.10334500
H	-3.59741300	3.14334700	-0.83463300
H	-4.67827700	2.08292600	-1.74317400
H	-2.97951900	0.34307600	-1.90639500
H	-2.74583000	2.34976900	1.51967400
P	-1.65685800	0.87856800	-0.03405600
C	-0.29502400	2.10893400	0.18529800
C	1.02055900	1.62724100	0.24671800
C	-0.53247200	3.48473100	0.24979500
C	2.08374400	2.52836500	0.35842100
C	0.52876900	4.37389700	0.36971500
H	-1.55142400	3.86775600	0.19850400
C	1.83504200	3.89501500	0.41948800
H	3.11132900	2.16949400	0.38722000
H	0.33696700	5.44306800	0.41760900
H	2.66670300	4.58981100	0.50639200
C	2.65230800	-0.57815400	-0.98237400
C	2.22144900	-0.72273000	1.74618000
C	3.57607900	-1.48441700	-0.16205500
H	3.15413500	0.39331000	-1.13236600
C	3.65846600	-0.90915000	1.24818500
H	1.79338100	-1.71588200	1.94969200
H	3.14272700	-2.49468000	-0.12879700
H	4.56103600	-1.56847600	-0.64258600
H	4.21794700	-1.56227400	1.93037700
H	4.18060800	0.06280800	1.22634900
P	1.26299600	-0.20560200	0.21870500
C	-3.12374400	0.40601100	2.37790500
H	-2.20139800	0.39257400	2.97100800
H	-3.94086700	0.73383800	3.03246500
H	-3.32938000	-0.61994900	2.05157100
C	-1.86469300	2.02831300	-2.65564500
H	-0.99966300	1.43076900	-2.97081200
H	-2.49990200	2.18332600	-3.53577600
H	-1.49484100	3.00973000	-2.33276300
C	2.04104900	0.17059700	2.95662100
H	2.55456600	-0.25857500	3.82520700
H	2.45191700	1.17394900	2.78698700
H	0.98057600	0.27967900	3.21826500
C	2.20601900	-1.15125200	-2.31306800
H	3.07864300	-1.35079700	-2.94897600
H	1.66220900	-2.09157600	-2.16312200
H	1.54713000	-0.46094100	-2.85327400
O	5.08058100	1.50989000	-0.61505800
C	6.06167900	0.71675100	-1.11644500
H	5.76019900	0.18938500	-2.03975800
H	6.87349400	1.40703500	-1.42868600
H	6.50023700	0.01974900	-0.38204200

TS (ML) G = -2539,427740

Pt	-0.63824000	-1.19557500	-0.04642400
Cl	-2.78344900	-2.19945800	-0.43870100
Cl	0.52113300	-3.29890000	-0.03261800
C	-4.28465500	1.23265900	0.21443100
C	-3.87118600	1.92861900	-1.07923500
C	-2.60987000	1.22932400	-1.59412300
C	-3.06064600	1.18157700	1.13688000
H	-5.11994300	1.73880000	0.71504300
H	-4.60223700	0.20310300	-0.00577300
H	-3.65773100	2.99367600	-0.88753500
H	-4.66410400	1.89674300	-1.83723700
H	-2.89182500	0.22799100	-1.95417200
H	-2.85255900	2.19896000	1.50564600
P	-1.64995800	0.81187600	-0.04236200
C	-0.36111400	2.10677500	0.23313900
C	0.97592800	1.69505300	0.33797700
C	-0.67231500	3.46695300	0.31087200
C	1.98474600	2.64690100	0.51355400
C	0.33524400	4.40753300	0.48811700
H	-1.70718500	3.79764100	0.22657900
C	1.66167600	3.99690900	0.58483300
H	3.02734200	2.34039600	0.55760300
H	0.08486100	5.46412500	0.54367200
H	2.45136300	4.73259400	0.71460500
C	2.74245500	-0.51725500	-0.79366100
C	2.19902400	-0.62062300	1.89391700
C	3.64867900	-1.38996200	0.05519300
H	3.34637000	0.55926000	-0.91343900
C	3.65798000	-0.80736300	1.46556200
H	1.76617200	-1.61311100	2.08925900
H	3.23230600	-2.41079100	0.06641900
H	4.65296300	-1.45569300	-0.38696900
H	4.18616800	-1.45394700	2.17724200
H	4.17526500	0.16586300	1.46354800
P	1.30498600	-0.12262800	0.32104800
C	-3.17664900	0.22135100	2.30619200
H	-2.27484000	0.23009500	2.93033500
H	-4.02785200	0.50097800	2.93919000
H	-3.32969000	-0.80400100	1.94997200
C	-1.82261400	1.95956100	-2.66269000
H	-0.92632500	1.39602700	-2.95211200
H	-2.43548600	2.09347300	-3.56181300
H	-1.50005100	2.95271500	-2.32551300
C	1.96352000	0.28503100	3.08544000
H	2.43800400	-0.13475100	3.98029800

H	2.38073500	1.28691000	2.92367500
H	0.89239900	0.39634000	3.29804400
C	2.43183900	-0.98067900	-2.18930800
H	3.35726100	-1.11318800	-2.76598000
H	1.91163400	-1.94909000	-2.15378400
H	1.79189400	-0.26918200	-2.72403700
O	4.21241200	1.50842400	-1.14638400
C	5.38924400	0.94170000	-1.59937200
H	5.24164400	0.26410600	-2.45835400
H	6.02323200	1.76774400	-1.96073400
H	5.95987600	0.41265600	-0.81568000

Complex **5** (tertiary)
Reactant (L) G = -1112,054192

C	-1.32630800	3.21914000	-0.23269100
C	-1.20661100	2.13388000	0.82432400
C	-0.98853300	0.73594500	0.22266100
C	0.28154100	0.72654800	-0.64441900
C	0.16279400	1.85497700	-1.68789800
C	-0.06672400	3.23142100	-1.08301800
H	-0.36029100	2.37035100	1.48555600
H	-2.10574600	2.11154000	1.45677000
H	-2.20308000	3.01583000	-0.87077100
H	-1.49711400	4.19738000	0.23571200
H	1.13554800	0.98575000	0.03574500
H	1.05605900	1.87152600	-2.32620900
H	-0.67639700	1.59223800	-2.35216400
H	0.78991300	3.49818500	-0.44500600
H	-0.13091200	3.98629600	-1.87774000
H	-1.82798200	0.53267000	-0.46676800
N	0.57566800	-0.51790700	-1.34116800
N	-1.02055800	-0.32000700	1.23448700
C	-0.03923500	-0.20158400	2.29567300
H	-0.33716600	0.51997100	3.08251700
H	0.09127300	-1.18208200	2.77588300
H	0.93114800	0.10442100	1.89599500
C	-2.33121200	-0.57708400	1.80499700
H	-2.24038500	-1.48407400	2.42110900
H	-2.65890100	0.23330200	2.49268000
C	-3.41709500	-0.81681500	0.79065800
C	-4.44016500	0.11423100	0.60272300
C	-5.42717300	-0.14398400	-0.34017800
H	-4.45099500	1.02972000	1.19147200
C	-4.30579000	-2.19338700	-0.80821700
C	-5.36327900	-1.32600200	-1.06571500
H	-6.23235800	0.56849800	-0.50541100
H	-4.22479200	-3.13293700	-1.35724400
H	-6.11145100	-1.57458300	-1.81347400
N	-3.35409100	-1.95833300	0.09301600
C	-0.03796800	-1.79373200	-1.02262500
H	0.15849400	-2.47041300	-1.86720900
H	0.35341500	-2.25798300	-0.10529100
H	-1.11937000	-1.70723800	-0.90689900
C	1.92817000	-0.64323000	-1.80909800
H	1.95563900	-1.37281400	-2.63526500
H	2.26166000	0.30772500	-2.25431700
C	2.98097900	-1.04542100	-0.79043700
C	4.28953300	-1.29141400	-1.22148000
C	5.25922400	-1.60024300	-0.28055900
H	4.53113000	-1.23438000	-2.28221400
C	3.57103800	-1.40773200	1.38985100
C	4.89768600	-1.65479400	1.06333900
H	6.28476800	-1.79563900	-0.58693600
H	3.24138100	-1.44358100	2.43015800
H	5.62441100	-1.88757300	1.83674700
N	2.62958000	-1.11314200	0.49153600
O	2.28646000	2.12052100	1.06129600
C	3.34644800	2.31317700	0.22937800
H	4.06556600	2.95843900	0.77467400
H	3.89667700	1.38778800	-0.02726600
H	3.09006500	2.86982900	-0.69390900

TS (L) G = -1112,051800

C	-1.50185500	3.19141200	-0.10519000
C	-1.31023100	2.08696300	0.92128900
C	-1.02000100	0.72927700	0.26283300
C	0.24770800	0.82943300	-0.59713700
C	0.09239500	1.98571400	-1.60413900
C	-0.24696400	3.31921200	-0.95511600
H	-0.47121200	2.34615500	1.58188100
H	-2.20484300	1.99151600	1.55273400
H	-2.36486900	2.94733300	-0.74841500
H	-1.73718200	4.14289800	0.38901300
H	1.11142500	1.23009800	0.15655800
H	1.00211400	2.08681300	-2.20980600
H	-0.70913700	1.69368100	-2.30406400
H	0.58856100	3.62573800	-0.31015400
H	-0.36824400	4.08853900	-1.72891900
H	-1.84684900	0.52347000	-0.44401400
N	0.68000200	-0.36383000	-1.24816000
N	-1.00658300	-0.38261700	1.20965000
C	-0.01867800	-0.29721900	2.26985800
H	-0.31170900	0.40122600	3.07858600
H	0.10689200	-1.29262100	2.71891100
H	0.95022200	0.02159100	1.87636300
C	-2.30655200	-0.71176000	1.76645000
H	-2.18347300	-1.64482200	2.33614600
H	-2.66285300	0.05025700	2.49329700
C	-3.38096700	-0.93726900	0.73660900
C	-4.45947400	-0.05885500	0.62092000
C	-5.43432200	-0.30509900	-0.33790100
H	-4.52104500	0.80771700	1.27678000
C	-4.19036300	-2.23806800	-0.96503700
C	-5.30221600	-1.42189400	-1.15214100
H	-6.28281000	0.36663000	-0.44750900
H	-4.05361200	-3.12447600	-1.58648000
H	-6.03839700	-1.65850000	-1.91548900
N	-3.24974200	-2.01416400	-0.04960800
C	0.09595100	-1.68083100	-1.07413900
H	0.32798800	-2.26345800	-1.97777400
H	0.50053500	-2.21255500	-0.20239900
H	-0.98696900	-1.63423900	-0.95737700
C	2.02769000	-0.38830100	-1.75132800
H	2.06318500	-0.99611700	-2.67076500
H	2.33237400	0.62457900	-2.05170400
C	3.08353100	-0.90810900	-0.79147800
C	4.39695400	-1.05934300	-1.24715600
C	5.37346800	-1.46083700	-0.34955700
H	4.63927100	-0.84952600	-2.28824000
C	3.67587600	-1.54865100	1.32029000
C	5.01063900	-1.70537700	0.97200000
H	6.40554900	-1.57901900	-0.67244500
H	3.34515000	-1.73885500	2.34291900
H	5.74251900	-2.01646300	1.71222900
N	2.72767800	-1.16364300	0.46452700
O	1.95633600	1.97232700	1.02636200
C	3.09546400	2.31580600	0.34034400
H	3.69971500	2.98077500	0.98420800
H	3.74708400	1.45892300	0.07487100
H	2.90214400	2.89665300	-0.58633300

Reactant (ML) G = -2156,085885

Fe	-0.90168700	-0.91304200	-0.07873700
Cl	-1.11722600	-2.24390000	-2.06621200
Cl	-2.29939900	-2.09175900	1.50844000
C	1.48398600	3.99835100	1.10882200
C	0.74654400	2.85971500	1.80099800
C	0.15708000	1.86436200	0.79732500
C	1.23729000	1.34114100	-0.14620100
C	1.98527300	2.49524000	-0.81502200
C	2.58320400	3.44297200	0.21320400
H	1.46309300	2.33735100	2.45209200
H	-0.04621800	3.24717600	2.45578300
H	0.77943600	4.58445000	0.49753100
H	1.89527700	4.68663600	1.85740600
H	1.97274200	0.78560900	0.45913900
H	2.76730200	2.09252200	-1.47110900
H	1.29030300	3.06482300	-1.45089900
H	3.32454500	2.90007300	0.82103100
H	3.12174100	4.25585900	-0.29069200
H	-0.58545300	2.40378900	0.18384300
N	0.67285600	0.36297900	-1.11043400
N	-0.57961600	0.74030300	1.42720800
C	0.06073300	0.19701100	2.63108100
H	0.00609800	0.89197200	3.48321300
H	-0.45499000	-0.73347800	2.89078300

H	1.11224700	-0.03219600	2.42851400
C	-1.96426000	1.13185300	1.72308400
H	-2.38302600	0.36722900	2.39170700
H	-2.01854900	2.10676800	2.23877000
C	-2.80010500	1.13820200	0.48138100
C	-3.88611100	1.98954000	0.33179300
C	-4.69258400	1.87292100	-0.79343600
H	-4.09642900	2.72459600	1.10527000
C	-3.26708500	0.10053200	-1.53569800
C	-4.37996800	0.90382600	-1.73760700
H	-5.55224200	2.52487700	-0.92635200
H	-2.96898500	-0.68030300	-2.23383800
H	-4.98554800	0.76178000	-2.62748500
N	-2.47969400	0.22068300	-0.45497000
C	0.10187000	0.96721800	-2.31887000
H	0.87496400	1.38442900	-2.98214100
H	-0.44941100	0.18755600	-2.85433300
H	-0.59836600	1.76474000	-2.04842500
C	1.68065700	-0.64101700	-1.46399100
H	1.31654500	-1.17449900	-2.35312500
H	2.65861000	-0.17919300	-1.70036400
C	1.84222100	-1.65232400	-0.37291500
C	3.05694700	-2.28365300	-0.13913200
C	3.12083700	-3.30137300	0.80317700
H	3.93421100	-1.94970500	-0.68595500
C	0.79101700	-2.95842700	1.22418800
C	1.96306200	-3.65262100	1.48473000
H	4.06039200	-3.81197700	1.00013900
H	-0.14755900	-3.17774200	1.73093700
H	1.95618300	-4.45232000	2.21923500
N	0.72975400	-1.96349600	0.32454600
O	4.47089400	0.53259200	-0.61635600
C	5.46632400	1.25194000	-1.19298100
H	6.26569500	1.35074700	-0.42695500
H	5.94232300	0.74999100	-2.05354900
H	5.17972600	2.28727200	-1.45807600

TS (ML) G = -2156,075821

Fe	0.55660900	-0.91289600	0.00992600
Cl	0.86057900	-2.54662000	1.58634700
Cl	1.39341500	-2.26639000	-1.64492000
C	-0.72252900	4.28246300	-0.36855000
C	-0.44367000	3.08515900	-1.26853000
C	0.08844900	1.91505400	-0.44005100
C	-0.90749200	1.53146100	0.61537300
C	-1.18085600	2.72425100	1.52515700
C	-1.72183200	3.89891100	0.71426000
H	-1.39038600	2.77898700	-1.73210900
H	0.26096200	3.35870700	-2.06781500
H	0.21434500	4.62621600	0.10119700
H	-1.09651900	5.11999700	-0.97054900
H	-2.07286700	1.22674500	-0.05470000
H	-1.89655000	2.45984500	2.31814600
H	-0.26566500	3.08253000	2.03981000
H	-2.67476500	3.61584800	0.24555000
H	-1.92120600	4.75231100	1.37512800
H	1.05988100	2.23413700	0.00071100
N	-0.36245200	0.32977300	1.36829500
N	0.43973800	0.69748100	-1.27490000
C	-0.50623900	0.46170900	-2.39421900
H	-0.36818300	1.23013800	-3.16635200
H	-0.27558200	-0.51434100	-2.82880000
H	-1.53847900	0.49411300	-2.03243100
C	1.79554500	0.87377400	-1.82840300
H	1.93711400	0.12958300	-2.62238000
H	1.90949300	1.87464500	-2.27219300
C	2.81898300	0.62204000	-0.77497000
C	4.09916000	1.15730900	-0.82489100
C	5.02240100	0.78742900	0.14310500
H	4.35907200	1.84678200	-1.62400100
C	3.33970300	-0.59641500	1.12660700
C	4.63813600	-0.11115100	1.13055300
H	6.03165100	1.19069300	0.12279900
H	2.98351600	-1.31839100	1.85792500
H	5.33050200	-0.44230600	1.89802100
N	2.44319600	-0.22315600	0.20246500
C	0.53806400	0.66919500	2.48986300
H	-0.01670000	1.17655000	3.28922100
H	0.97569600	-0.24853000	2.89234200
H	1.33352200	1.33364300	2.14118800
C	-1.50846300	-0.43950000	1.89515700
H	-1.14363600	-1.13194700	2.66630300
H	-2.24095600	0.23909200	2.35616000
C	-2.12979500	-1.23859800	0.80254400
C	-3.43906300	-1.69492000	0.85992200
C	-3.92109200	-2.48370300	-0.17061200
H	-4.07024800	-1.39777400	1.69340800
C	-1.76684100	-2.35199500	-1.19561900
C	-3.07162500	-2.81161500	-1.22087600
H	-4.94916700	-2.83642800	-0.15858900
H	-1.04714300	-2.60958300	-1.96758800
H	-3.40336800	-3.42909400	-2.04943600
N	-1.30477000	-1.58059700	-0.20160600
O	-3.05327500	1.03151700	-0.75995100
C	-4.21280400	1.32544200	-0.09466500
H	-4.80873300	2.13044400	-0.57259100
H	-4.90306400	0.45751400	-0.00165900
H	-4.03486400	1.67191000	0.95385600

Complex **5** (benzyl)
Reactant (L) G = -1112,061368

C	-0.80540800	0.15917800	2.96917000
C	-1.02141600	-0.99344200	1.99436300
C	-0.92910100	-0.51111000	0.53809600
C	0.46661100	0.08813400	0.32008700
C	0.63593800	1.29846000	1.25417200
C	0.52154700	0.86144600	2.70966000
H	-0.26561100	-1.77628400	2.16789500
H	-1.99981800	-1.45927100	2.17616700
H	-1.62727100	0.88398100	2.84569500
H	-0.86017400	-0.19773200	4.00594000
H	1.20114600	-0.66595900	0.65155100
H	1.60286400	1.78806600	1.07483200
H	-0.14651200	2.04235500	1.02703900
H	1.35131000	0.17104900	2.93499800
H	0.64260600	1.72061500	3.38178800
H	-1.65558300	0.31383700	0.42940400
N	0.77051800	0.35481200	-1.07792100
N	-1.28716200	-1.49782000	-0.47479700
C	-0.37563800	-2.61536100	-0.60412700
H	-0.34863000	-3.27219200	0.28895200
H	-0.69305500	-3.23349800	-1.45291600
H	0.63651500	-2.26104100	-0.82630200
C	-2.66246500	-1.94866600	-0.40571400
H	-2.84628900	-2.56245300	-1.30062100
H	-2.85954000	-2.60857600	0.46673800
C	-3.66885400	-0.82716900	-0.40169500
C	-4.57808400	-0.68889000	0.64744900
C	-5.50736200	0.34341000	0.60786900
H	-4.55297600	-1.38856100	1.48064200
C	-4.54698700	0.99455400	-1.47294200
C	-5.49535100	1.20952100	-0.47670200
H	-6.22783800	0.46960300	1.41297300
H	-4.50965100	1.65428500	-2.34143000
H	-6.20042100	2.03261200	-0.55498100
N	-3.65576900	0.00603100	-1.45052800
C	-0.18563800	1.14672900	-1.81955400
H	-0.23353100	2.20046700	-1.48288900
H	0.10658400	1.15453200	-2.87611700
H	-1.18276700	0.69789600	-1.75762500
C	2.13802100	0.67956700	-1.36928900
H	2.25429600	0.68485500	-2.46343700
H	2.42161100	1.71649700	-1.02638600
C	3.13711700	-0.28775200	-0.78458400
C	4.07523500	0.13614500	0.15775200
C	4.97921500	-0.79061000	0.66332600
H	4.08411000	1.17753400	0.47148100
C	3.94546200	-2.42701300	-0.72686100
C	4.91703900	-2.10350400	0.21577300
H	5.72178000	-0.48890300	1.39891600
H	3.86912800	-3.44795200	-1.10493700
H	5.60299200	-2.86233300	0.58294800
N	3.07340500	-1.55191000	-1.22348300
O	3.13037200	3.18310200	-0.15195700
C	2.20605200	4.17228300	-0.31406000
H	2.62736900	5.08647800	0.15171400

H	2.01705300	4.43357400	-1.37114000
H	1.24478700	3.97843300	0.19873100

TS (L) G = -1112,058510

C	-0.94189200	-0.22048300	3.03338500
C	-1.10011000	-1.26649200	1.93643600
C	-0.95819700	-0.63094400	0.54606000
C	0.43981100	-0.00722200	0.44099400
C	0.58713800	1.08102800	1.51788200
C	0.39834500	0.49404200	2.91154200
H	-0.33974600	-2.05428100	2.05964700
H	-2.07767300	-1.76067000	2.02339300
H	-1.75763100	0.51592600	2.94048900
H	-1.04948700	-0.68020300	4.02448300
H	1.17646700	-0.79317400	0.67053500
H	1.56617800	1.57229800	1.42540600
H	-0.17249900	1.86125800	1.34237500
H	1.20888600	-0.22571100	3.10931200
H	0.49161000	1.28052800	3.67116900
H	-1.68226900	0.20164800	0.50515200
N	0.75847000	0.46935000	-0.90086500
N	-1.28432100	-1.50223900	-0.57814800
C	-0.40021900	-2.63622400	-0.76079300
H	-0.47039300	-3.38518700	0.05388100
H	-0.66916100	-3.14638500	-1.69401800
H	0.63973900	-2.30616200	-0.85902400
C	-2.67401000	-1.92028100	-0.61804900
H	-2.82469700	-2.44275100	-1.57443600
H	-2.92606700	-2.65226800	0.17921200
C	-3.65066300	-0.77526400	-0.55611100
C	-4.55778500	-0.66318800	0.49812100
C	-5.44402000	0.40692800	0.51825600
H	-4.56076900	-1.40959100	1.29016000
C	-4.45375900	1.13757700	-1.52215000
C	-5.39361600	1.33351300	-0.51415300
H	-6.16045600	0.51612300	1.32937300
H	-4.38803900	1.84410300	-2.35120900
H	-6.06274300	2.18912500	-0.54319900
N	-3.60274000	0.11430500	-1.55625200
C	-0.24613800	1.27165500	-1.56950600
H	-0.52061800	2.17359900	-0.99413000
H	0.14975900	1.60393100	-2.53491300
H	-1.14707800	0.67478700	-1.75284700
C	2.10354500	0.84105600	-1.14268000
H	2.21890100	1.07488700	-2.21268400
H	2.38935500	1.83653700	-0.60802600
C	3.16704000	-0.14675000	-0.73103100
C	4.35698500	0.33049800	-0.17635500
C	5.36204400	-0.57774800	0.12905300
H	4.46890300	1.39686700	0.00638000
C	3.92143600	-2.30620200	-0.65259700
C	5.14617700	-1.92843100	-0.11352100
H	6.30064700	-0.23346300	0.55790100
H	3.71101500	-3.35880200	-0.84969200
H	5.90248600	-2.67549100	0.11198600
N	2.95037000	-1.44790700	-0.96275800
O	2.91678700	3.06925200	0.17059900
C	2.02909100	4.05818400	-0.16515300
H	2.41167500	5.01713200	0.23254700
H	1.92409200	4.20680100	-1.25788800
H	1.01564600	3.91849700	0.26225900

Reactant (ML) G = -2156,087612

Fe	0.78349400	-0.97891700	0.09668000
Cl	0.59441000	-2.24042300	2.13921800
Cl	2.21975000	-2.35246200	-1.27394600
C	-0.90605000	4.11055200	-1.50748400
C	-0.18479700	2.89051900	-2.06280900
C	0.13859100	1.87038000	-0.96947300
C	-1.11035900	1.47794900	-0.18395100
C	-1.87382200	2.70682800	0.31887400
C	-2.18777200	3.67894200	-0.81008500
H	-0.83526600	2.42273000	-2.81683200
H	0.73665300	3.18286400	-2.58524200
H	-0.25681400	4.63755400	-0.79003200
H	-1.11788100	4.82041300	-2.31639300
H	-1.78198400	0.93744900	-0.87251000
H	-2.80017300	2.38286400	0.81272600
H	-1.26590500	3.23672500	1.06736000
H	-2.85845700	3.19884100	-1.53985600
H	-2.73006700	4.54602000	-0.41378100
H	0.83408500	2.35133100	-0.25972800
N	-0.76325200	0.50706500	0.88565700
N	0.83952700	0.65909800	-1.47072100
C	0.32496500	0.15130800	-2.74857300
H	0.57461900	0.81169700	-3.59316100
H	0.77395000	-0.83262300	-2.91843700
H	-0.76289800	0.03189300	-2.70355800
C	2.28430700	0.89992300	-1.57327600
H	2.70932700	0.07364500	-2.15882900
H	2.51186900	1.84519900	-2.09645000
C	2.93503800	0.86559300	-0.22682600
C	4.05708600	1.62928700	0.06488800
C	4.68273000	1.47587000	1.29559700
H	4.43626900	2.32552700	-0.67964600
C	3.02310300	-0.15723300	1.84838800
C	4.15966200	0.55828000	2.19656300
H	5.56568900	2.05983700	1.54324600
H	2.56444800	-0.89131600	2.50964000
H	4.61910700	0.38979200	3.16590000
N	2.40786400	0.00116600	0.66545000
C	-0.29411300	1.11763900	2.13299000
H	-1.10307400	1.63504400	2.67268000
H	0.10683500	0.31816700	2.76430200
H	0.50784800	1.83537300	1.92977200
C	-1.88521100	-0.39144600	1.14916800
H	-1.66273300	-0.93648700	2.07717500
H	-2.83642700	0.16184700	1.28337500
C	-2.03832200	-1.39611200	0.05428800
C	-3.28677900	-1.86632500	-0.32959800
C	-3.36190200	-2.87657200	-1.28028200
H	-4.17261100	-1.42159600	0.11966300
C	-0.97038200	-2.84050500	-1.40398500
C	-2.18196100	-3.38074300	-1.81170800
H	-4.32624100	-3.26461900	-1.59903400
H	-0.01251700	-3.18667700	-1.79011000
H	-2.18689200	-4.18247800	-2.54406800
N	-0.89424300	-1.84965400	-0.50127500
O	-4.67972400	0.82740500	1.15666900
C	-4.96364800	1.08583900	2.46388000
H	-5.98865200	1.51053800	2.48518100
H	-5.00256200	0.18157100	3.09574500
H	-4.30479700	1.84694500	2.92095700

TS (ML) G = -2156,082542

Fe	0.68952800	-0.99110700	0.07351700
Cl	0.37515600	-2.20914600	2.07882600
Cl	2.06264900	-2.47629200	-1.26504700
C	-0.60242700	4.18173100	-1.52583300
C	0.01356400	2.90124500	-2.07328300
C	0.23138200	1.86092000	-0.97233100
C	-1.06650200	1.57611800	-0.22311400
C	-1.73610100	2.86424200	0.26837500
C	-1.93346600	3.86692700	-0.85969600
H	-0.67006300	2.49408800	-2.83268400
H	0.96267300	3.11002300	-2.58539800
H	0.07748900	4.64132100	-0.79072500
H	-0.72795900	4.91142200	-2.33491600
H	-1.76538100	1.08872100	-0.92321300
H	-2.69627100	2.60580300	0.73412400
H	-1.10235900	3.33389400	1.03541100
H	-2.63074400	3.45723000	-1.60710200
H	-2.40130500	4.77736800	-0.46628000
H	0.94657500	2.28666700	-0.24744100
N	-0.84058800	0.59479400	0.87324600
N	0.85210900	0.59530900	-1.45393100
C	0.31320300	0.11723300	-2.73692900
H	0.61094900	0.76165000	-3.57701700
H	0.70379100	-0.89174800	-2.90234900
H	-0.77939600	0.06607300	-2.69628700
C	2.31335900	0.75185500	-1.56357500
H	2.68516300	-0.10445600	-2.14269000
H	2.58974300	1.67739100	-2.09599000
C	2.95968400	0.68707700	-0.21721800
C	4.13441300	1.36625000	0.07435000
C	4.73964400	1.17357400	1.30993100

H	4.56899300	2.02665300	-0.67235300
C	2.95818900	-0.32500100	1.86529000
C	4.14367600	0.30504400	2.21447700
H	5.66324400	1.69020200	1.55857300
H	2.44385300	-1.01734700	2.52967100
H	4.58452900	0.10996000	3.18734600
N	2.36481700	-0.12980400	0.67702500
C	-0.32436200	1.16305500	2.12316400
H	-1.09770200	1.72917300	2.66255800
H	0.02313800	0.33263200	2.74574000
H	0.52256900	1.82631100	1.91993600
C	-1.97930400	-0.24392400	1.09401400
H	-1.90127900	-0.73359600	2.07508600
H	-3.02578000	0.40264800	1.15304900
C	-2.16493900	-1.26783100	0.03021000
C	-3.43026600	-1.73648500	-0.30297500
C	-3.54366400	-2.76783400	-1.22544700
H	-4.29345000	-1.27018200	0.16665100
C	-1.15646900	-2.76635900	-1.41766900
C	-2.38595400	-3.29752800	-1.78079800
H	-4.52128500	-3.15438100	-1.50261300
H	-0.21431000	-3.14486200	-1.81221100
H	-2.42149800	-4.11713800	-2.49215100
N	-1.04069100	-1.75630800	-0.54103700
O	-4.23816100	0.94605800	1.26644400
C	-4.40166900	1.23431000	2.60946600
H	-5.46244300	1.47925700	2.78304300
H	-4.17088800	0.37935700	3.27035900
H	-3.80721400	2.10299100	2.95306600

Complex **6** (α-NH)

Reactant (L) G = -439,181637

N	-0.32550300	-1.20102900	-0.44176100
C	-0.86737300	-0.32986900	0.55170700
H	-0.15128700	0.48548500	0.86845300
H	-1.05395800	-0.91740200	1.46819500
C	0.83262600	-1.98142900	-0.06448200
H	0.53502500	-2.68987900	0.72507300
H	1.12871700	-2.57628100	-0.93826300
C	2.03217800	-1.16448600	0.41952500
C	-2.14151700	0.36005700	0.10466800
N	-3.16454300	-0.59123400	-0.29587500
N	2.39571800	-0.13477000	-0.55000300
H	-2.43518000	1.04812100	0.92051000
H	-1.90905700	1.00162600	-0.76122500
H	-4.06684900	-0.13408000	-0.36882500
H	-3.25336800	-1.32267500	0.40296600
H	1.79053800	-0.71547400	1.39618000
H	2.86533700	-1.85791000	0.60190800
H	-0.17647900	-0.72303600	-1.32597500
H	2.20898500	0.77629100	-0.13800400
H	3.38167800	-0.17635400	-0.77484400
O	0.78250700	2.06970800	0.76105900
C	0.39946100	2.55173300	-0.45629400
H	1.14079800	3.31475700	-0.76853100
H	0.45909500	1.77269600	-1.24485400
H	-0.59601300	3.02965400	-0.46850700

TS (L) G = -439,180781

N	-0.15871200	-1.13729500	-0.44760100
C	-0.80975600	-0.32917600	0.50285700
H	-0.18119000	0.64600100	0.75784300
H	-0.87156200	-0.86576300	1.46494500
C	1.03132700	-1.86710900	-0.06765700
H	0.75985700	-2.58832200	0.71868900
H	1.35534300	-2.44028700	-0.94464800
C	2.18875500	-0.99331800	0.41576300
C	-2.16523200	0.18050100	0.05784400
N	-3.08303300	-0.90941100	-0.23469900
N	2.47917200	0.05471100	-0.55374100
H	-2.51134400	0.89126900	0.83251100
H	-2.03409800	0.77658600	-0.85946900
H	-4.01393000	-0.54578600	-0.41058800
H	-3.15439000	-1.52637400	0.56928100
H	1.94654400	-0.59276700	1.41663000
H	3.06286700	-1.64521700	0.54691900
H	-0.10109500	-0.72419700	-1.37250900
H	1.99115700	0.89678100	-0.24564300
H	3.46844500	0.27416100	-0.54411700
O	0.50860600	1.95995400	0.73907500
C	0.04473900	2.57316900	-0.40072600
H	0.69183400	3.44274300	-0.61707800
H	0.11198700	1.92636300	-1.30139000
H	-0.99025400	2.95473100	-0.32018000

Reactant (ML) G = -1965,059076

Co	0.91268600	0.00388400	0.04465300
Cl	0.25544700	0.08073500	2.24395000
Cl	3.06233700	0.04475900	0.64461200
Cl	1.46003900	-0.07169400	-2.17240800
N	-0.95193800	-0.03504200	-0.54284300
C	-1.53872900	-1.30250300	-0.07470900
H	-2.49761400	-1.50721400	-0.57126900
H	-1.70303800	-1.21138600	1.00498300
C	-1.56115400	1.25527400	-0.17892900
H	-2.51624900	1.40825900	-0.70068800
H	-1.73940300	1.24629200	0.90253700
C	-0.54284800	2.32059200	-0.56162000
C	-0.50531200	-2.37876600	-0.37857000
N	0.81775200	-1.93662500	0.12319900
N	0.78298900	1.94337600	-0.01705600
H	-0.80050100	-3.34375200	0.04905800
H	-0.41043700	-2.50618000	-1.46327500
H	1.59226700	-2.30633500	-0.42705400
H	0.97003000	-2.16553500	1.10587100
H	-0.44109200	2.35761200	-1.65266700
H	-0.85752500	3.31261900	-0.21778400
H	-0.83970200	-0.07398900	-1.56114600
H	1.55622700	2.28802600	-0.58513600
H	0.91957500	2.24575500	0.94802200
O	-4.30100500	-0.05612000	-0.71318000
C	-4.85330900	0.05023600	0.52353700
H	-5.94926300	-0.03786200	0.36644800
H	-4.58359200	-0.77780100	1.20176700
H	-4.69064600	1.03001700	1.00415300

TS (ML) G = -1965,043277

Co	0.89480000	-0.05418400	0.01817300
Cl	0.51459700	0.06359200	2.27867600
Cl	3.05154000	-0.48846900	0.35215800
Cl	1.15074300	-0.14865200	-2.24794300
N	-1.00063600	0.32746900	-0.34538300
C	-1.74593300	-0.78218600	0.19644200
H	-2.91206200	-0.71090900	-0.30041200
H	-1.87594800	-0.66892400	1.27845400
C	-1.27433600	1.70614700	0.08832900
H	-2.22431100	2.06679200	-0.32737400
H	-1.33321900	1.70430000	1.18218500
C	-0.09628800	2.53790700	-0.40084800
C	-1.05586200	-2.06037800	-0.23517400
N	0.39457600	-1.93856900	0.07195400
N	1.16590000	1.87289900	0.00291900
H	-1.50232800	-2.93755700	0.24416900
H	-1.14710100	-2.18354600	-1.32111200
H	0.98289300	-2.44047600	-0.59298300
H	0.62582900	-2.24169200	1.01857700
H	-0.09987900	2.57362000	-1.49640500
H	-0.15352000	3.56615600	-0.02646500
H	-0.99955200	0.28004500	-1.37128900
H	1.93655300	2.07327300	-0.63384100
H	1.45341600	2.10568000	0.95430500
O	-3.98872800	-0.26935700	-0.72528600
C	-4.80930300	-0.03479200	0.37034800
H	-5.74787400	0.37862200	-0.02893000
H	-5.06616400	-0.94623800	0.93306600
H	-4.40203100	0.71588400	1.06951500

Complex **6** (α-NH_2)

Reactant (L) G = -439,184420

N	-0.45109100	0.28434100	-0.04614200
C	-1.37327000	-0.54684000	-0.80255100
H	-0.88458600	-1.45720900	-1.20905200
H	-1.71310900	0.03505400	-1.67401300
C	0.74535600	0.64479200	-0.78313500
H	1.31546300	-0.25160900	-1.12096400
H	0.43930000	1.19356000	-1.68610900

C	1.65117500	1.52249400	0.05198200
C	-2.56724200	-0.93246800	0.05767400
N	-3.35571900	0.17969000	0.56103800
N	1.00186000	2.79488900	0.30883700
H	-3.22201100	-1.60882400	-0.50629300
H	-2.20273800	-1.51986200	0.91793700
H	-3.82038100	0.63888700	-0.21764700
H	-2.71571800	0.87118300	0.94453400
H	1.93792100	0.95350000	0.96220900
H	2.58471900	1.69134100	-0.50066500
H	-0.18456000	-0.20304100	0.81026900
H	0.08899000	2.61779000	0.71754500
H	1.53409800	3.35159600	0.96787900
O	2.52875200	-1.63814100	-0.30841400
C	1.78520400	-2.16903600	0.69503400
H	2.30658100	-3.09764500	1.00609400
H	1.71562500	-1.53570400	1.59967000
H	0.77770400	-2.49998400	0.37576200

TS (L) G = -439,176311

N	-0.99555700	-0.05865200	0.28649500
C	-1.94296900	-1.05595700	-0.19072900
H	-1.67213100	-2.08429000	0.12271700
H	-1.90655700	-1.04840500	-1.29187300
C	0.36378500	-0.29518500	-0.18244200
H	0.75968700	-1.28937300	0.09718900
H	0.34859000	-0.26910400	-1.28237100
C	1.31339900	0.77258100	0.30553300
C	-3.35227200	-0.71566500	0.27330000
N	-3.86590000	0.56198600	-0.19110800
N	0.87757800	2.06405200	-0.04322400
H	-4.04095000	-1.51176100	-0.03733600
H	-3.37162700	-0.71822500	1.37522200
H	-3.99238700	0.52692900	-1.19900700
H	-3.15077500	1.26583300	-0.02534800
H	1.59574600	0.64391800	1.36852000
H	2.35188700	0.47526600	-0.25897500
H	-0.99957600	-0.06567800	1.30622500
H	-0.11606000	2.11313600	-0.23705700
H	1.20964100	2.82401500	0.53042300
O	3.35124700	-0.28961300	-0.75637900
C	3.91273900	-0.90351000	0.34089800
H	4.68315100	-1.60277700	-0.02534000
H	4.41479600	-0.21036600	1.04176700
H	3.19565700	-1.51750000	0.92178200

Reactant (ML) G = -1965,066060

Co	-0.68460900	-0.22341100	-0.02154700
Cl	-2.19848600	1.43816200	-0.46560700
Cl	-2.28774400	-1.76672800	-0.24203500
Cl	0.86013700	-1.85083400	0.44680900
N	0.74360900	1.09270600	0.17593000
C	0.94397800	1.74207600	-1.13087200
H	1.90223800	2.27772400	-1.16014400
H	0.12041200	2.44358200	-1.29637900
C	0.43502400	1.90991700	1.36048500
H	1.30884900	2.49124900	1.68592200
H	-0.37623800	2.59695100	1.09847400
C	-0.00300100	0.92816500	2.43951300
C	0.93302800	0.61715400	-2.15682200
N	-0.23902900	-0.25851000	-1.91323400
N	-1.03225100	0.02402400	1.87566400
H	0.93966600	1.00960800	-3.18000500
H	1.83216400	0.00357500	-2.02595100
H	-0.07024400	-1.22854600	-2.17667200
H	-1.08473900	0.06745400	-2.38254300
H	0.84683100	0.30035200	2.73280400
H	-0.36433000	1.44974000	3.33324200
H	1.59470200	0.54976600	0.36892900
H	-1.03277200	-0.89640600	2.31415000
H	-1.97465400	0.41321600	1.92140800
O	3.56638700	0.35869900	-0.19302000
C	4.16484500	-0.81558100	0.10909500
H	4.33397600	-0.93115800	1.19564500
H	3.39643600	-1.60130000	-0.09534000
H	5.07507000	-1.03144000	-0.47036200

TS (ML) G = -1965,040896

Co	-0.77864200	-0.25039300	-0.01248800
Cl	-0.58689900	0.18599500	-2.25339000
Cl	-1.98622300	-2.07614500	-0.42060800
Cl	-0.90010500	-0.58893400	2.24409300
N	0.27455100	1.34528200	0.42251700
C	1.64666400	1.10821300	-0.06513000
H	2.37143600	1.81011000	0.36947600
H	1.64562700	1.22514200	-1.15455100
C	-0.49647400	2.52028100	-0.01536900
H	-0.10377500	3.45072000	0.41688400
H	-0.43142300	2.57528900	-1.10686400
C	-1.92873200	2.26806800	0.44065400
C	1.97082500	-0.31791600	0.32595600
N	0.92911500	-1.22689500	-0.11768600
N	-2.33732400	0.90360800	0.03030100
H	3.09559700	-0.55604900	-0.22151700
H	2.14493500	-0.44457000	1.40113000
H	0.85954900	-2.07758600	0.43964300
H	0.98573900	-1.46803300	-1.11002300
H	-1.98180100	2.30297900	1.53497600
H	-2.61062700	3.02953500	0.04551600
H	0.26953000	1.29552600	1.44667300
H	-3.01366000	0.48537800	0.66867500
H	-2.71102100	0.86730400	-0.91906700
O	4.23966400	-0.43094600	-0.65187200
C	5.06727900	-0.11741900	0.41690200
H	6.07788000	0.00345400	-0.00105200
H	4.81049900	0.83988000	0.90389500
H	5.12062600	-0.90780000	1.18273700

Complex **7**

Reactant (L) G = -516,510011

N	2.19578300	0.82835100	-0.66828500
N	0.62540300	-1.66871400	-0.46523000
N	-0.57252300	0.83485300	-0.14850600
C	2.81303200	-0.45651500	-0.39522300
C	1.87503200	-1.47777600	0.25163300
C	-0.59622700	-1.57388400	0.31973300
C	-0.79203300	-0.16884900	0.88065200
C	0.23358000	1.97445000	0.25777500
C	1.71128500	1.60851400	0.46235400
H	2.78212400	1.38084000	-1.27919800
H	0.63436400	-2.51053800	-1.02519500
H	-0.05736300	0.38102300	-0.90884100
H	3.71060700	-0.38707400	0.25427400
H	3.15416900	-0.85958800	-1.35921300
H	2.44120400	-2.41732600	0.35950400
H	1.65211400	-1.16620500	1.28219300
H	-0.64957000	-2.29128600	1.16050100
H	-1.44236200	-1.79912700	-0.34310600
H	-1.82519200	-0.10928800	1.26824900
H	-0.13048200	-0.00718200	1.74960700
H	-0.18359400	2.41922100	1.17202900
H	0.16307600	2.73937800	-0.52843500
H	2.29983100	2.52631300	0.61646900
H	1.82729800	1.02708600	1.38866500
O	-3.68875000	-0.42849600	0.25242200
C	-3.59770900	0.47301300	-0.73855500
H	-4.24803300	1.36089400	-0.61912900
H	-2.53158000	0.86176900	-0.70982200
H	-3.70901000	0.04389800	-1.75399700

TS (L) G = -516,505280

N	2.25507500	0.83412800	-0.58356700
N	0.68049100	-1.68573700	-0.50087400
N	-0.51977900	0.80241600	-0.32063300
C	2.83704800	-0.44586800	-0.21840800
C	1.83548000	-1.44937000	0.35225800
C	-0.61780100	-1.58843500	0.15267100
C	-0.90336600	-0.17058100	0.62570300
C	0.20436300	1.97024900	0.13813800
C	1.66108200	1.63105300	0.48186900
H	2.91215600	1.37532000	-1.12947000
H	0.76299600	-2.55506100	-1.01214100
H	-0.00262300	0.36805400	-1.08811900
H	3.66038500	-0.35811200	0.52084600
H	3.27750200	-0.87175200	-1.13081100

H	2.39003000	-2.37679600	0.56940600
H	1.48420200	-1.09694700	1.33307900
H	-0.74798700	-2.27257400	1.01118800
H	-1.38425000	-1.86421700	-0.58586500
H	-2.12995500	-0.16870400	0.76038700
H	-0.54027800	0.05310400	1.64182900
H	-0.31076400	2.40667800	1.00419900
H	0.18533000	2.72395100	-0.66053900
H	2.22242500	2.55935700	0.66866600
H	1.69194900	1.06973400	1.42743000
O	-3.42777300	-0.27974800	0.53502200
C	-3.65697900	0.36647200	-0.65491700
H	-4.36880800	1.20560500	-0.54737500
H	-2.71595300	0.81474800	-1.04703200
H	-4.03365300	-0.31117600	-1.44422700

Reactant (ML) G = -2001,957256

Ir	-0.17315500	-0.36342300	-0.00217600
Cl	1.23318300	-1.18298800	1.74953200
Cl	1.19624800	-1.18663800	-1.77392600
Cl	-1.50925400	-2.33882300	0.01521600
N	-1.38885700	0.55413400	1.41580600
N	-1.47956200	0.52530400	-1.35119600
N	0.74351900	1.50764400	-0.05845000
C	-2.74313200	0.59955800	0.80434200
C	-2.64805100	1.11818200	-0.62420200
C	-0.67510200	1.52133200	-2.10769500
C	0.14924800	2.35389600	-1.13592600
C	0.59246600	2.07283100	1.30278400
C	-0.83922700	1.89805300	1.79158500
H	-1.40062700	-0.06481100	2.22976800
H	-1.79368100	-0.21832900	-1.97954400
H	1.75748400	1.37814500	-0.22781200
H	-3.42634700	1.22868600	1.39308800
H	-3.10573700	-0.43321500	0.80197300
H	-3.57661900	0.89412200	-1.16009600
H	-2.53181000	2.20890800	-0.63904000
H	-1.31791600	2.16741400	-2.72286400
H	-0.01481500	0.94000600	-2.75892200
H	0.94639200	2.87236900	-1.68051200
H	-0.46427900	3.13457900	-0.66693500
H	0.87640900	3.13507100	1.32736900
H	1.28253800	1.50988000	1.94003900
H	-0.88299100	2.02751900	2.87805400
H	-1.49797900	2.66156500	1.35833600
O	3.57408700	1.28402500	-0.00506700
C	3.99757000	0.00466300	-0.00173200
H	3.41291900	-0.54227400	0.78662100
H	3.62737000	-0.54579000	-0.89340000
H	5.07857400	-0.11953300	0.15993100

TS (ML) G = -2001,929949

Ir	-0.46872400	-0.30515000	0.02038800
Cl	-1.07577700	-1.31752900	2.07974500
Cl	0.79892900	-2.16983100	-0.71828500
Cl	-2.42819500	-1.05242800	-1.09263400
N	-1.40230800	1.47061800	0.59390300
N	0.08111800	0.81509100	-1.65141800
N	1.19920200	0.60612500	0.88235000
C	-1.80735400	2.13209700	-0.67414800
C	-0.63759600	2.12956000	-1.65026300
C	1.56689600	0.94582000	-1.56648200
C	1.97255600	1.31398000	-0.15704700
C	0.67825400	1.47943500	1.96695400
C	-0.48965900	2.29988800	1.44308500
H	-2.23313700	1.19888900	1.12544900
H	-0.17557100	0.26684900	-2.47640200
H	1.78397200	-0.12799200	1.29599800
H	-2.15073800	3.16138400	-0.49597000
H	-2.63213200	1.53449700	-1.07512400
H	-0.99806000	2.36297700	-2.65769400
H	0.09239700	2.90655400	-1.38912000
H	1.94551900	1.69079300	-2.28023200
H	1.96146300	-0.04120100	-1.83726600
H	3.19489800	0.93796400	0.04180200
H	2.00742600	2.39203800	0.04293000
H	1.46754900	2.13684700	2.35747900
H	0.34035200	0.80322900	2.75920700
H	-1.04590000	2.73399300	2.28051700
H	-0.13331800	3.13943600	0.83383400
O	4.15424100	0.30943100	0.43244500
C	4.26962700	-0.87522800	-0.28517900
H	4.94679600	-1.52697700	0.28825100
H	3.31435600	-1.43089300	-0.35664900
H	4.69527100	-0.73702100	-1.29184000

Complex **8** (β-Pt)

Reactant (L) G = -642,104995

C	-1.23400200	0.23018100	-0.00423100
N	-2.29754500	1.03124800	-0.09421400
C	-3.48592600	0.43534800	-0.08593900
C	-3.63280000	-0.94265400	0.01391200
C	-2.45560000	-1.67448500	0.10077600
N	-1.25454100	-1.10351800	0.09090900
H	-4.35715800	1.08777300	-0.16149200
H	-4.60830700	-1.41862300	0.02260000
H	-2.47708400	-2.76215800	0.18227300
C	0.11285000	0.88169400	-0.00818000
N	0.15546300	2.21069600	0.09484700
C	1.36854200	2.75824400	0.09624600
C	2.53465300	2.00922100	-0.00401500
C	2.37022700	0.63321000	-0.10785500
N	1.16628200	0.06955200	-0.11028100
H	1.40916500	3.84499400	0.18358300
H	3.51672800	2.47131600	0.00015300
H	3.21807400	-0.05278200	-0.18816400
O	3.35810800	-2.25400000	0.09524300
C	2.19177200	-2.91041200	-0.05959900
H	1.40325700	-2.11086100	-0.02884100
H	2.07197100	-3.39317100	-1.04728700
H	1.95258500	-3.61242300	0.75971300

TS (L) G = -642,084491

C	1.38138000	0.13519000	0.00197500
N	2.43131300	0.95665100	-0.05382800
C	3.62778100	0.37649200	-0.05484900
C	3.79189800	-1.00239400	-0.00017300
C	2.62484000	-1.75402800	0.05473200
N	1.41657600	-1.19862400	0.05585600
H	4.49085400	1.04211800	-0.10050100
H	4.77391000	-1.46487100	-0.00080000
H	2.66027900	-2.84327300	0.09988400
C	0.02769800	0.76256900	0.00519600
N	-0.06792700	2.08677300	0.01864300
C	-1.29651400	2.60115800	0.02323700
C	-2.45198700	1.82534000	0.01383500
C	-2.22552200	0.45256800	-0.00091000
N	-1.03243300	-0.06034000	-0.00460100
H	-1.36499300	3.69023900	0.03557000
H	-3.44402000	2.26406900	0.01801800
H	-3.18446000	-0.44033300	-0.01111600
O	-3.80926400	-1.44755600	-0.01494800
C	-2.93069300	-2.51540400	-0.03138200
H	-1.87797000	-2.16498800	-0.00892300
H	-3.06434700	-3.16205500	0.85090200
H	-3.04113500	-3.12061300	-0.94589800

Reactant (ML) G = -1681,762300

Pt	-0.83577500	0.19981300	-0.27139700
Cl	-2.33623000	1.93838800	0.02410100
Cl	-2.56454200	-1.34817800	-0.42051200
C	1.99852300	0.72572000	-0.09057100
N	0.81059300	1.37955900	-0.07067800
C	0.82338100	2.70855800	0.11464600
C	2.02437000	3.37717600	0.27410000
C	3.18863000	2.61827100	0.23684300
N	3.17798700	1.29882000	0.05477000
H	-0.15532300	3.18745600	0.13394200
H	2.04496900	4.45133600	0.42318400
H	4.16669200	3.08258900	0.35726100
C	1.89932400	-0.73224900	-0.30533400
N	0.63836700	-1.19337400	-0.48352400
C	0.47205300	-2.50935100	-0.67639300
C	1.56665600	-3.35541500	-0.69218500
C	2.81857400	-2.78488200	-0.49493500
N	2.98706900	-1.47707000	-0.30830500

H	-0.55847200	-2.83986800	-0.80043400
H	1.44077300	-4.42198900	-0.84393100
H	3.72027100	-3.39587300	-0.48773600
O	0.45903000	-1.40329800	2.29642100
C	-0.74752700	-1.62144600	2.87648000
H	-1.08618000	-0.80266400	3.53242000
H	-1.48832000	-1.66527900	2.04114000
H	-0.81509200	-2.60215000	3.37900700

TS (ML) G = -1681,722517

Pt	-0.00962700	-0.83877200	-0.11085200
Cl	-0.93679700	-2.95624800	0.01544400
Cl	2.06851700	-1.71936000	-0.59203000
C	-1.74863200	1.46327400	0.04333500
N	-1.78967200	0.11454300	0.17213700
C	-2.98073200	-0.45958200	0.40686800
C	-4.11994800	0.31859500	0.51175300
C	-3.97372100	1.69340500	0.35739700
N	-2.79377300	2.26494500	0.12493300
H	-2.96710900	-1.54571700	0.49188300
H	-5.08609900	-0.13675300	0.70128300
H	-4.83184000	2.36114900	0.42065600
C	-0.40091800	2.02602500	-0.17845200
N	0.61401000	1.10769300	-0.19469700
C	1.85418200	1.57813900	-0.28158100
C	2.10890000	2.93300200	-0.40657400
C	1.00524900	3.77628300	-0.45235000
N	-0.24142300	3.32390400	-0.31382100
H	2.97176200	0.81982800	-0.13008500
H	3.13012700	3.29680100	-0.45433100
H	1.12215600	4.85211600	-0.57903200
O	3.98469100	0.78353000	0.41969900
C	3.81226200	0.20495200	1.67647500
H	3.46287700	0.92617100	2.43206300
H	3.15694300	-0.67716200	1.64200300
H	4.81148200	-0.13727400	1.98530600

Complex **8** (δ-Pt)
Reactant (ML) G = -1681,755630

Pt	-1.35591800	-0.17468700	-0.00302200
Cl	-3.28760900	1.09672500	-0.03341800
Cl	-2.56104300	-2.14642600	-0.00216900
C	1.21098600	1.15961300	0.02055100
N	-0.11374900	1.44529800	0.00157700
C	-0.47866500	2.73751700	-0.01083800
C	0.48311700	3.73253500	-0.00420900
C	1.81639600	3.33687100	0.01600600
N	2.18164800	2.05572100	0.02865700
H	-1.55354400	2.91748200	-0.02577300
H	0.19774700	4.77891900	-0.01426300
H	2.62039800	4.07137600	0.02243600
C	1.53286700	-0.28072700	0.03206000
N	0.46024500	-1.10821700	0.02237100
C	0.69138600	-2.43165900	0.02988800
C	1.98817000	-2.91447600	0.04778900
C	3.02470900	-1.98593200	0.05804700
N	2.79134600	-0.67267700	0.04994200
H	-0.19915900	-3.05990200	0.02156000
H	2.17948300	-3.98216400	0.05345300
H	4.07610200	-2.27657100	0.07123500
O	5.82084800	-0.92249800	-0.33650700
C	5.84891300	0.34738900	0.12817900
H	4.79114000	0.69677400	0.05779700
H	6.10326100	0.42115800	1.20076000
H	6.46276000	1.03578200	-0.47710100

TS (ML) G = -1681,732871

Pt	-1.30893000	-0.32142500	0.00191200
Cl	-3.45184100	0.54292200	0.00980100
Cl	-2.10527300	-2.48936900	0.01169600
C	0.95054600	1.49068500	-0.01189300
N	-0.40534200	1.50955000	-0.00676600
C	-1.01557400	2.70583300	-0.00720300
C	-0.26591800	3.86896700	-0.01277400
C	1.11959700	3.74214200	-0.01795900
N	1.72818400	2.55707000	-0.01745800
H	-2.10476400	2.67373900	-0.00275900
H	-0.75053600	4.83942900	-0.01302500
H	1.76462800	4.61953300	-0.02242600
C	1.54193400	0.14126700	-0.01022500
N	0.65818700	-0.88067500	-0.00521000
C	1.13505800	-2.13945200	-0.00562300
C	2.49805900	-2.38087600	-0.00917600
C	3.31651800	-1.25342400	-0.01030500
N	2.85578000	-0.03254800	-0.01315000
H	0.37513400	-2.92213900	-0.00221300
H	2.88970400	-3.39189100	-0.00951500
H	4.65015300	-1.33712800	-0.02009600
O	5.76998400	-1.09876600	-0.13938600
C	5.98399200	0.24293900	0.14587300
H	5.10613400	0.85817900	-0.12409400
H	6.21794900	0.42805600	1.20579700
H	6.81624900	0.60082000	-0.47739400

Complex **9**
Reactant (L) G = -716,463740

N	-2.54060500	-0.40067600	0.27950500
C	-3.40007100	0.70277900	-0.14355200
H	-3.98226500	0.37178000	-1.01213700
H	-2.77776800	1.55114700	-0.49657600
C	-2.05296900	-1.16774500	-0.86389300
H	-1.21013500	-1.78432900	-0.52800600
H	-1.63656200	-0.48104500	-1.62995100
C	-1.45796100	0.08867200	1.10932500
H	-1.87683000	0.80703600	1.82725900
H	-0.75196100	0.67952300	0.46828200
C	-3.10969800	-2.08004400	-1.45753200
H	-3.96313000	-1.52774000	-1.86706100
H	-2.68708800	-2.67447400	-2.27496800
H	-3.49156000	-2.76446700	-0.69239000
C	-4.36313800	1.15256500	0.93953800
H	-3.84546100	1.54341000	1.82277300
H	-5.01733800	1.94878100	0.56776800
H	-4.98718500	0.31279400	1.26340600
C	-0.70373200	-0.98365500	1.87175100
H	-0.10660300	-1.63077000	1.21861300
H	-0.00393700	-0.52038400	2.57700400
H	-1.40235300	-1.60960800	2.43844800
O	0.15627400	1.53874200	-1.04533700
C	1.39863900	1.63117800	-0.45885900
C	1.34997700	2.55543600	0.75848600
H	2.34853000	2.84532500	1.10514300
H	0.80451700	3.46300000	0.48099400
H	0.81952900	2.07355200	1.58902600
C	2.25940100	2.29654900	-1.56481400
H	3.28725600	2.39374100	-1.19637000
H	2.26112900	1.67651500	-2.46612200
H	1.86006300	3.28701800	-1.80576800
C	1.97986800	0.25076000	-0.15766600
C	2.86359900	0.02814200	0.89851600
C	1.63030800	-0.82553500	-0.97526600
C	3.37265100	-1.24523300	1.14193600
H	3.15588700	0.84954500	1.55033300
C	2.13874900	-2.09657300	-0.73614100
H	0.93454800	-0.65155200	-1.79380200
C	3.00995000	-2.31247000	0.32897100
H	4.05481600	-1.40145700	1.97485700
H	1.84942200	-2.92419700	-1.38082100
H	3.40509000	-3.30730800	0.52141700

TS (L) G = -716,464522

N	-2.45366900	-0.30134300	0.23404900
C	-3.35637200	0.73963500	-0.25592100
H	-3.80522100	0.39418700	-1.19525600
H	-2.76994300	1.63957900	-0.51004800
C	-2.10711800	-1.30701900	-0.76353400
H	-1.21221600	-1.84188400	-0.42540100
H	-1.82648000	-0.80768800	-1.70916700
C	-1.38989600	0.20932000	1.02298300
H	-1.77468700	1.02043900	1.65839900
H	-0.66000000	0.77637900	0.25481500
C	-3.23851700	-2.29454100	-0.97980700
H	-4.15775900	-1.79581700	-1.31066800
H	-2.97143400	-3.03333900	-1.74292400
H	-3.46509500	-2.82271400	-0.04729900
C	-4.45323100	1.05583400	0.74335800

H	-4.03993900	1.40225900	1.69789500
H	-5.11748800	1.84010000	0.36439300
H	-5.05068700	0.15946300	0.94574100
C	-0.60944700	-0.79651400	1.83992300
H	0.00971900	-1.45918700	1.22454100
H	0.07173200	-0.27539700	2.52114800
H	-1.29094900	-1.41232700	2.44028900
O	-0.00242400	1.41553800	-0.85457300
C	1.31119300	1.60546300	-0.43849500
C	1.34869300	2.53901100	0.77225200
H	2.36192600	2.87760800	1.02008700
H	0.74033100	3.42003000	0.54195400
H	0.92363900	2.05025700	1.65892100
C	2.01112800	2.29205500	-1.62374600
H	3.06860600	2.46693300	-1.38945100
H	1.94931900	1.66088700	-2.51635000
H	1.52476400	3.25081200	-1.83638800
C	1.99919100	0.26513000	-0.17625000
C	2.96300000	0.08718500	0.81689100
C	1.65420200	-0.83407400	-0.96802700
C	3.54804300	-1.15910200	1.02987700
H	3.25723800	0.92409700	1.44794100
C	2.24024100	-2.07717700	-0.76352000
H	0.89613800	-0.69948700	-1.73760600
C	3.18700200	-2.24702500	0.24440200
H	4.28907900	-1.27820100	1.81781400
H	1.95401900	-2.92018200	-1.38991600
H	3.64179000	-3.22079700	0.41245900

Reactant (ML) G = -2438,057767

Mg	2.14748900	0.17481800	-0.11375300
Cl	3.94134700	-1.81609600	0.06531100
O	3.23483600	-1.03387900	1.17023400
O	3.39441600	-1.08975300	-1.16821600
O	3.49647000	-3.19927500	0.06856400
O	5.37661400	-1.66437800	0.15553000
Cl	2.27065400	2.86297400	-0.04642600
O	2.10861800	1.86747100	1.10040800
O	2.36393300	1.89281100	-1.22968500
O	3.49565600	3.61977200	0.09118700
O	1.08411800	3.69117800	-0.16743000
N	0.15720800	-0.54298000	-0.12510900
C	-0.01217100	-1.43513700	1.06601600
H	0.73556000	-2.23303800	0.98627300
H	-1.01133500	-1.89849600	1.00228500
C	-0.21088400	-1.30530800	-1.35847700
H	0.02918800	-0.66462100	-2.21671300
H	-1.30704100	-1.43831800	-1.35608500
C	-0.78880500	0.61272600	0.01384000
H	-0.39910600	1.26840300	0.80321100
H	-1.75026800	0.20469600	0.36472700
C	0.46649700	-2.64912300	-1.53248100
H	0.14133500	-3.38754000	-0.79353800
H	0.19974600	-3.04099300	-2.51922900
H	1.55787800	-2.58138800	-1.49597100
C	0.13652700	-0.74344800	2.40638500
H	-0.70426400	-0.07852100	2.62839400
H	0.15436400	-1.50824000	3.18852900
H	1.07046800	-0.17437200	2.49604400
C	-1.02586300	1.42533400	-1.24406100
H	-1.62562500	0.88438000	-1.98375200
H	-1.58763500	2.32476100	-0.96862500
H	-0.09378900	1.76185400	-1.71300800
O	-3.15095200	-1.04872200	1.97280800
C	-4.11609400	-0.16794700	1.55880300
C	-3.87584100	1.21460000	2.16738400
H	-4.74809700	1.86731400	2.05402700
H	-3.66873200	1.09635600	3.23544800
H	-3.01407900	1.70511500	1.69781800
C	-5.40437400	-0.77810700	2.19242600
H	-6.25014200	-0.14956200	1.89217100
H	-5.56525500	-1.79488000	1.82406300
H	-5.31729100	-0.79004400	3.28263800
C	-4.27290900	-0.16947800	0.04001500
C	-4.63330200	0.97570000	-0.66968400
C	-4.06628400	-1.35975200	-0.66176700
C	-4.77874500	0.93372000	-2.05462600
H	-4.79533700	1.91674400	-0.14776800
C	-4.21410000	-1.40389800	-2.04276100
H	-3.77172600	-2.25062800	-0.10888100
C	-4.56947900	-0.25420300	-2.74530400
H	-5.05461500	1.83698700	-2.59390100
H	-4.04952200	-2.33919700	-2.57375900
H	-4.68375100	-0.28656000	-3.82608200

TS (ML) G = -2438,048288

Mg	2.11686100	0.31513600	-0.10924000
Cl	4.33672700	-1.17013500	-0.33880000
O	3.63572700	-0.62727000	0.90799100
O	3.43508100	-0.57952700	-1.42700500
O	4.26495300	-2.62050200	-0.36039200
O	5.68095700	-0.64930500	-0.44651700
Cl	1.57295500	2.92038400	0.26230400
O	1.74472200	1.80670900	1.29381700
O	1.83364900	2.12670000	-1.02553500
O	2.57092200	3.95164000	0.43610700
O	0.20784500	3.41380200	0.28009800
N	0.34716100	-0.89624600	-0.03255900
C	0.54352000	-1.84455900	1.11776000
H	1.47355400	-2.39159800	0.92337900
H	-0.28573100	-2.56600000	1.10409400
C	0.06910000	-1.67054900	-1.28811800
H	0.12468700	-0.96097900	-2.12317100
H	-0.97334700	-2.02279600	-1.22637400
C	-0.77689300	0.01368500	0.22928900
H	-0.56321500	0.61773700	1.11892000
H	-1.71132800	-0.74985400	0.60194800
C	0.98900200	-2.84133500	-1.56286600
H	0.86686800	-3.65324300	-0.84038200
H	0.73607400	-3.24564200	-2.54806500
H	2.04369200	-2.55486300	-1.59217500
C	0.61855300	-1.18375200	2.47827800
H	-0.35288100	-0.79673100	2.80127500
H	0.92927200	-1.93633100	3.20904900
H	1.35338800	-0.37060900	2.52900600
C	-1.27455700	0.84224500	-0.92556700
H	-1.79961700	0.24681700	-1.67953500
H	-1.98199700	1.58711100	-0.54776200
H	-0.46136800	1.39577700	-1.41681000
O	-2.56320100	-1.62497800	0.99088100
C	-3.75468500	-0.93747800	1.28952900
C	-3.52357200	0.04218700	2.43541500
H	-4.46296700	0.45616600	2.81947800
H	-3.02852300	-0.48904500	3.25583900
H	-2.88581000	0.88130800	2.12824700
C	-4.70869300	-2.04648800	1.75882000
H	-5.68693600	-1.61157000	1.99502400
H	-4.84135800	-2.79860600	0.97512500
H	-4.30554000	-2.53428300	2.65294900
C	-4.31895300	-0.28420900	0.03233900
C	-4.89975200	0.98372500	0.03081800
C	-4.25003400	-0.98836600	-1.17391400
C	-5.37567800	1.54598600	-1.15215100
H	-4.97286000	1.55501400	0.95368500
C	-4.72886800	-0.43316500	-2.35314100
H	-3.79111700	-1.97605500	-1.17712400
C	-5.28732000	0.84323200	-2.34720200
H	-5.81357400	2.54148800	-1.13549700
H	-4.66330800	-0.99479100	-3.28264700
H	-5.65536200	1.28431600	-3.27052300