

Electronic Supplementary Information for

Reaction Mechanisms of Iron(III) Catalyzed Carbonyl-Olefin Metatheses in 2,5- and 3,5-Hexadienals: Significant Substituent and Aromaticity Effects

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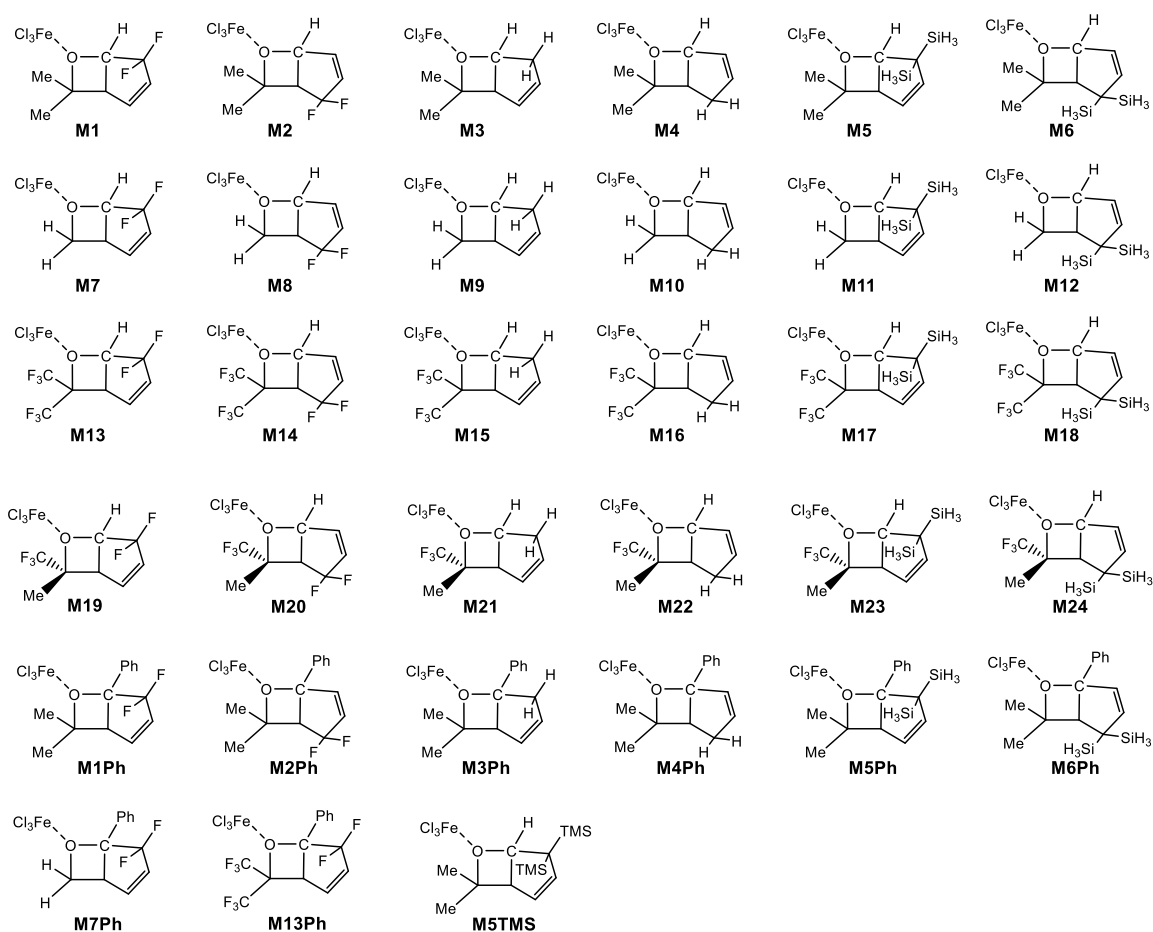
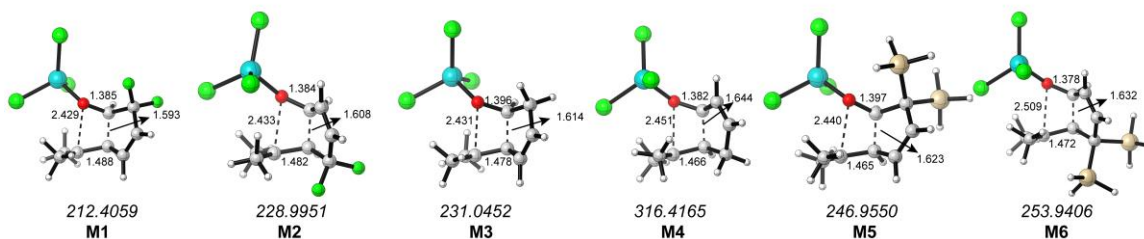


Fig. S1 Oxetane intermediates of the models investigated in this study (33 models in total)

B3LYP-D3BJ/6-31G(d)/LanL2DZ



B3LYP-D3BJ/def2-TZVP

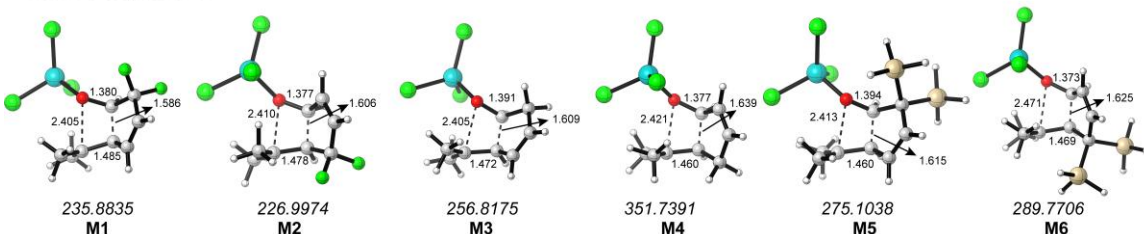


Fig. S2 Comparison between geometries optimized at the B3LYP-D3BJ/6-31G(d)/LanL2DZ and B3LYP-D3BJ/def2TZVP levels. Imaginary frequencies (in *italic*) are given in cm^{-1} .

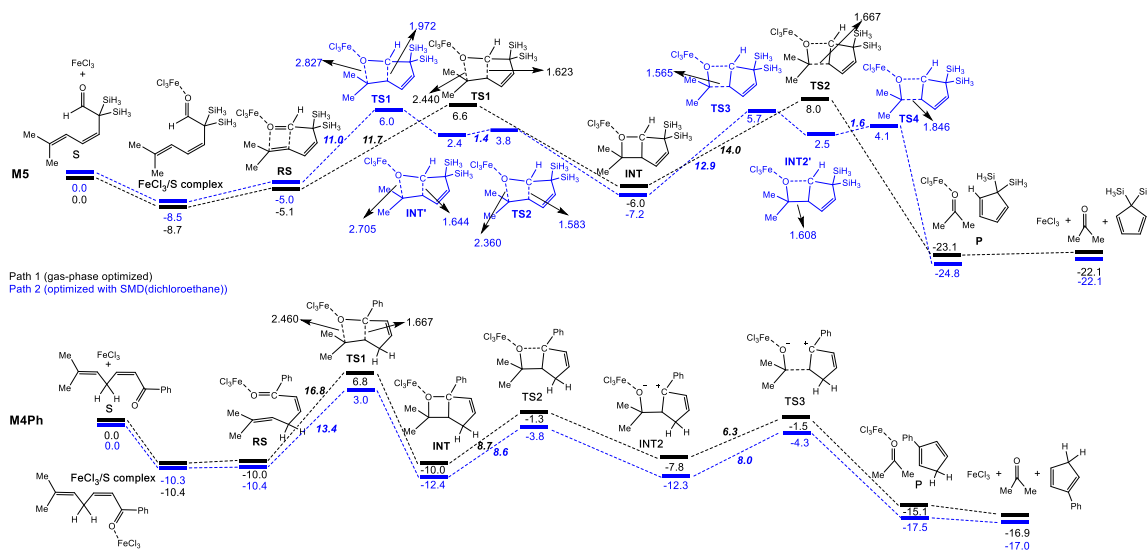


Fig. S3 Reaction profiles of **M5** and **M4Ph** with structures optimized in gas phase (Path 1) and with SMD (solvent: dichloroethane) model (Path 2). Relative Gibbs energies are calculated at 298K and given in kcal mol^{-1} . Bold, italic numbers correspond to intrinsic barriers.

For **M5**, applying the solvent model leads to additional charged-separated intermediates and more transition states in both the cycloaddition and cycloreversion. However, those intermediates (**INT'**,

INT2') of **M5** are not particularly stable, resulting in the potential energy surface (PES) rather similar to that in gas phase. In this context, the cycloaddition and cycloreversion of **M5** could still be considered concerted rather than stepwise, which was also discussed in a similar mechanistic investigation reported by Ludwig et al. (*J. Am. Chem. Soc.* **2017**, *139*, 10832-10842). Moreover, the solvent effect on the PES of **M4Ph** is also not much marked. Neglecting the addition minor barriers caused by the solvation model, the $\Delta G_1^\ddagger$ and $\Delta G_2^\ddagger$ in **M5** (Path 1/Path 2) are 15.3/14.5 and 14.0/12.9 kcal mol⁻¹ respectively while the $\Delta G_1^\ddagger$, $\Delta G_2^\ddagger$, and $\Delta G_3^\ddagger$ in **M4Ph** (Path 1/Path 2) are 17.2/13.4, 8.7/8.6, and 6.3/8.0 kcal mol⁻¹ respectively. Considering that the gas-phase optimization is sufficient for modelling the PES and predicting the reaction barriers and that the SMD optimization is much more costing (especially for sextet species), geometry optimizations for all models investigated in this study were performed in gas phase.

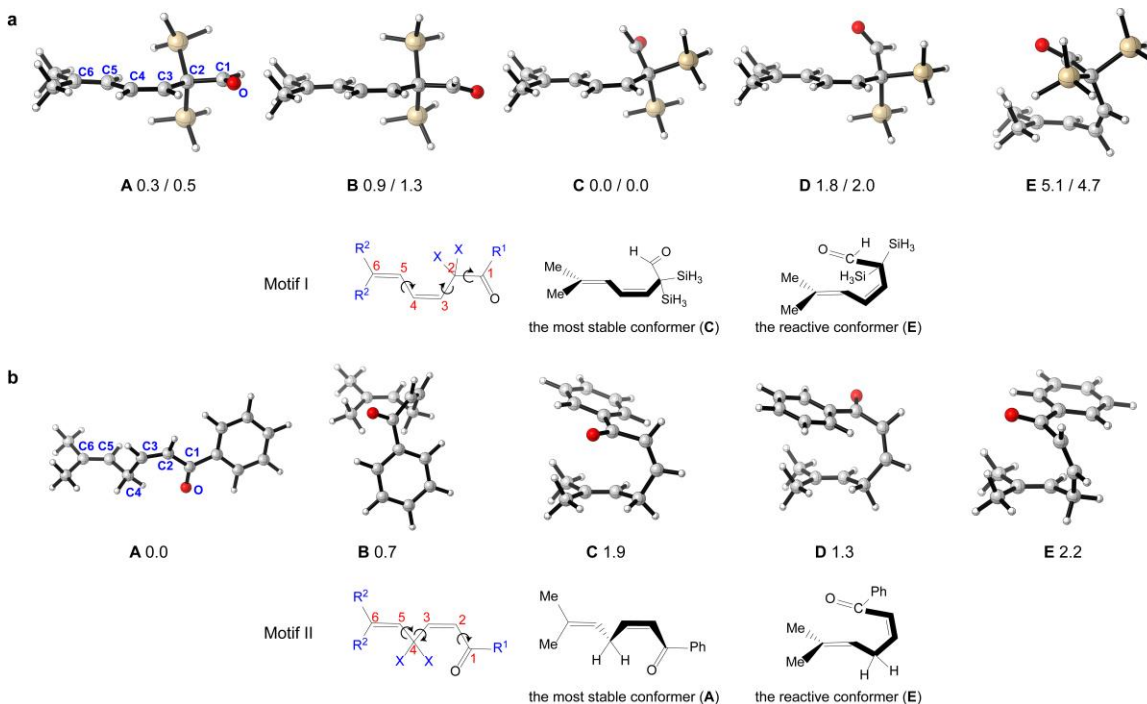


Fig. S4 Illustration of conformational sampling procedures. Motif I (a) and II (b) substrates both have three C-C single bonds that contribute to various conformations via bond rotation. Values before the “/” in a correspond to calculations using gas-phase optimized structures while those behind the “/” correspond to calculations using solvation model in the geometry optimizations.

In the conformational sampling, the rotation interval for each rotating bond was set to 60°, resulting in 216 initial conformer structures. Excluding those with irrational atomic distances, the rest structures were optimized using the PM7 (precise) method implemented in MOPAC2016. The

Molclus was used to submit the calculations and analyze the results, from which the conformers with lower energies were further optimized at the B3LYP-D3(BJ)/6-31G(d)/LanL2DZ level using the Gaussian 09.

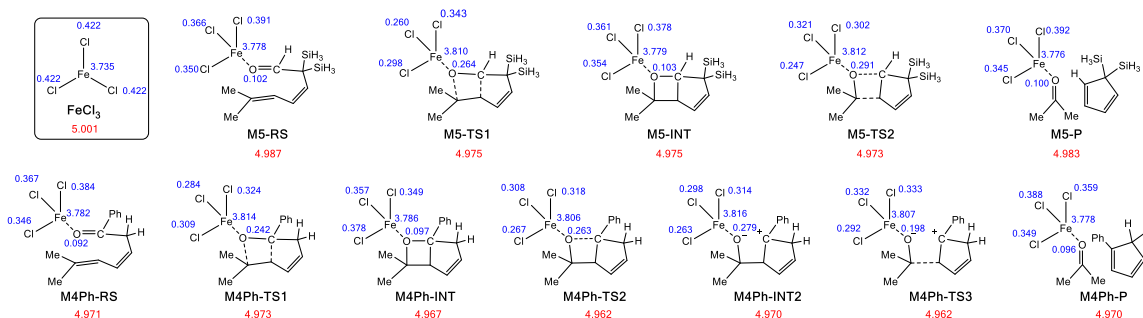


Fig. S5 Spin-density distributions (a.u.) calculated for FeCl_3 and key species of models **M5** and **M4Ph** in the sextet ground state (spin multiplicity = 6). Values in blue are spin densities of Fe, Cl, and O atoms while those in red are sums of spin densities of FeCl_3 -O fragments. After FeCl_3 binds to the reactant, the spin density of the Fe(III) is partially and inevitably delocalized to the ligating atoms including three Cl and one O. Meanwhile, the rest atoms have negligible spin-density distributions along the whole reaction path. Level of theory: UB3LYP-D3(BJ)/6-31G(d)/LanL2DZ.

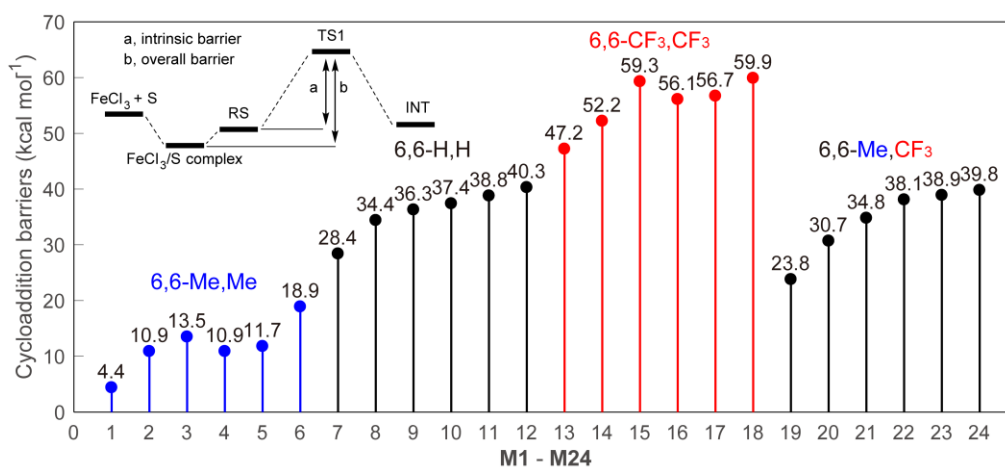


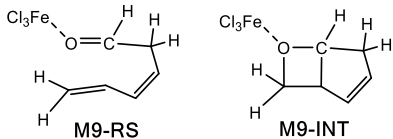
Fig. S6 Intrinsic barriers ($\Delta G_{\text{RS-TS1}}^\ddagger$) of **M1-M24**.

Table S1 Relative energies of **M5-RS** in the lowest quartet and sextet states.

Level of theory	B3LYP-D3(BJ)/6-31G(d)/LanL2DZ	ω B97XD/def2TZVP	ω B97XD/def2TZVP/SMD(dichloroethane)// B3LYP-D3(BJ)/6-31G(d)/LanL2DZ
E_{sextet} (a.u.)	-565.98826	-3613.23023	-3613.2487885
E_{quartet} (a.u.)	-565.94936	-3613.18035	-3613.19674019
ΔE (kcal mol ⁻¹)	24.4	31.3	32.7
G_{sextet} (a.u.)	-565.82617	-3613.06724	0.162083-3613.2487885
G_{quartet} (a.u.)	-565.78962	-3613.01904	0.159733-3613.19674019
ΔG (kcal mol ⁻¹)	22.9	30.2	31.2

E , electronic energy; G , Gibbs energy. $\Delta E = E_{\text{quartet}} - E_{\text{sextet}}$, $\Delta G = G_{\text{quartet}} - G_{\text{sextet}}$.

Table S2 Relative electronic energies between **RS** and **INT** of **M9** calculated at different levels of theory

	
Level of theory	$\Delta E_{\text{INT-RS}}$ /(kcal mol ⁻¹) ^a
CCSD(T)/def2-TZVP	-6.7
U ω B97X-D/def2-TZVP	-5.9
UM06-D3/def2-TZVP	-3.6
UM06-2X-D3/def2-TZVP	-5.2
UM06L-D3/def2-TZVP	-0.3
UBP86-D3(BJ)/def2-TZVP	-2.5
UB97-D3(BJ)/def2-TZVP	3.9
UPBE0-D3(BJ)/def2-TZVP	-8.6
UB3LYP-D3(BJ)/def2-TZVP	0.6
UB2PLYP-D3(BJ)/def2-TZVP	-0.6

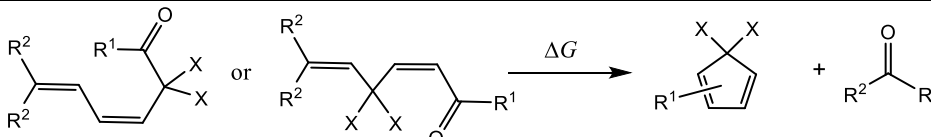
Energies were calculated with the SMD solvation model of dichloroethane. ^a $\Delta E_{\text{INT-RS}} = E_{\text{INT}} - E_{\text{RS}}$ (E_{INT} and E_{RS} are single-point energies of **M9-INT** and **M9-RS**, respectively.)

Table S3 NPA charges of [C1-R¹]^a and [C3-H] moieties in **TS2** of **M1(Ph)**-**M6(Ph)**

Models	M1	M2	M3	M4	M5	M6
[C1-R ¹]	0.41	0.33	0.53	0.34	0.43	0.37
[C3-H]	-0.02	0.20	0.06	0.31	0.03	0.26
Models	M1Ph	M2Ph	M3Ph	M4Ph	M5Ph	M6Ph
[C1-R ¹]	0.62	0.57	0.61	0.50	0.52	0.47
[C3-H]	-0.03	0.12	0.06	0.20	0.03	0.19

^a R¹ = H for **M1-M6**, R¹ = Ph for **M1Ph-M6Ph**.

Table S4 Gibbs energy changes (ΔG) in COM reactions of **M1-M18** (298 K)

							
6,6-Me,Me	M1	M2	M3	M4	M5	M6	Ranges
ΔG (kcal mol ⁻¹)	-12.6	-15.2	-14.8	-18.9	-22.1	-31.7	-31.7 ~ -12.6
6,6-H,H	M7	M8	M9	M10	M11	M12	Ranges
ΔG (kcal mol ⁻¹)	0.2	-0.8	-1.2	-4.3	-8.6	-15.6	-15.6 ~ 0.2
6,6-CF ₃ ,CF ₃	M13	M14	M15	M16	M17	M18	Ranges
ΔG (kcal mol ⁻¹)	3.1	-1.4	4.1	1.3	-3.5	-6.6	-6.6 ~ 4.1

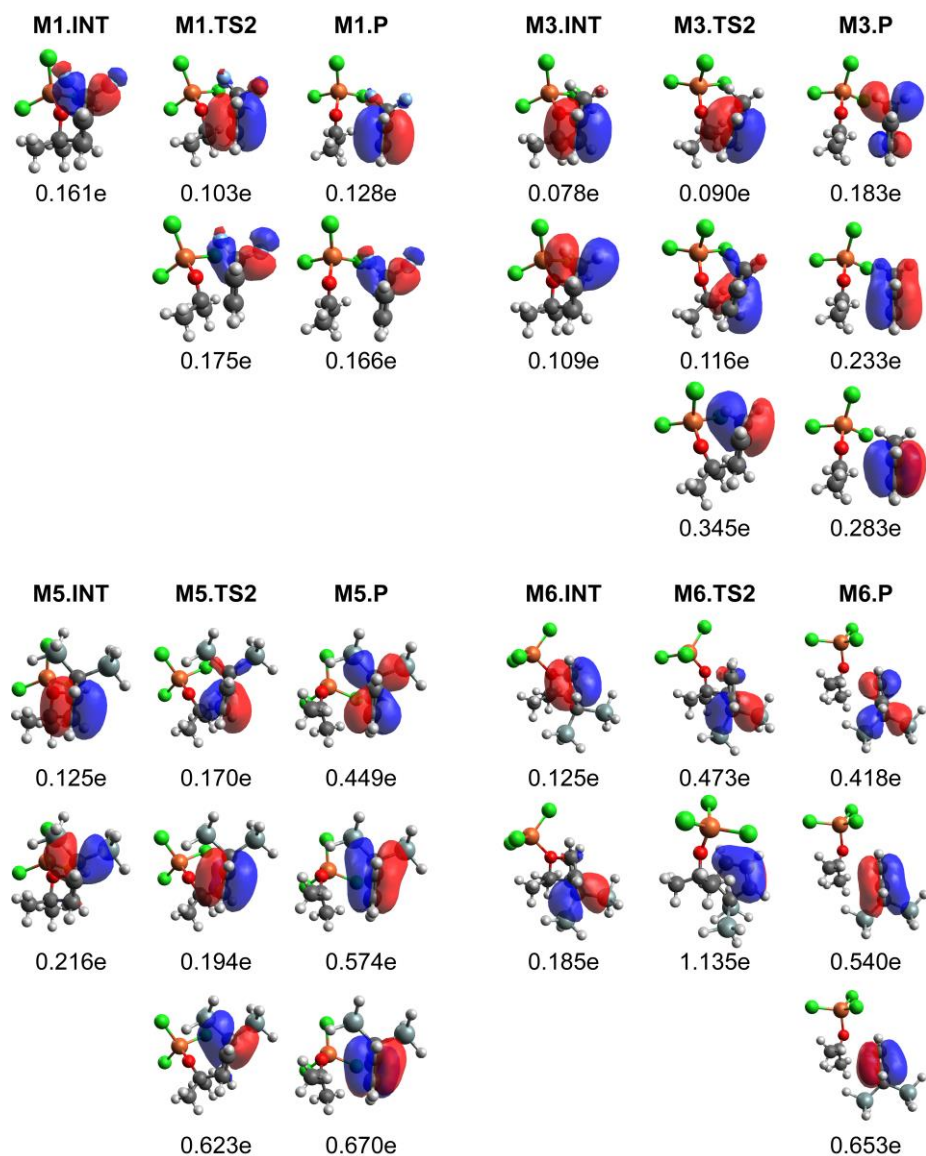


Fig. S7 Natural orbitals for bond delocalization (NOBDs) used in π -EDDB_{5MR} calculations. Substituents and hydrogens bound to the 5MRs are included in the computation of NOBDs. Contributions to EDDB are listed under the corresponding π NOBDs. Isosurface value: 0.030 a.u.

Table S5 Reaction barriers in FeCl₃ dimer models

	$\Delta G_1^\ddagger$ /(kcal mol ⁻¹)	$\Delta G_2^\ddagger$ /(kcal mol ⁻¹)	$\Delta G_3^\ddagger$ /(kcal mol ⁻¹)	$\Delta G_4^\ddagger$ /(kcal mol ⁻¹)
2Fe.M1	3.3 (INT0 → TS1) ^[b]	40.1 (-7.8) ^[a] (INT → TS2)	\	\
2Fe.M1Ph	5.4 (-6.9) (2FeCl₃/S → TS1)	18.1 (-7.4) (INT → TS2)	\	\
2Fe.M2	5.1 (-6.2) (2FeCl₃/S → TS1)	1.1 (INT0 → TS2) ^[c]	25.1 (-6.6) (INT → TS3)	26.4 (+5.4) (INT2 → TS4) ^[d]
2Fe.M2Ph	10.0 (-7.3) (2FeCl₃/S → TS1)	9.0 (-6.8) (INT → TS2)	6.7 (+1.5) (INT2 → TS3)	\
2Fe.M3	5.0 (-8.5) (2FeCl₃/S → TS1)	21.9 (-10.0) (INT → TS2)	\	\
2Fe.M3Ph	16.1 (-8.2) (2FeCl₃/S → TS1)	3.1 (INT → TS2)	3.0 (INT2 → TS3)	\
2Fe.M4	7.3 (-6.8) (2FeCl₃/S → TS1)	2.1 (INT0 → TS2) ^[c]	7.9 (-9.4) (INT → TS3)	4.6 (-14.1) (INT2 → TS4)
2Fe.M4Ph	12.7 (-4.5) (2FeCl₃/S → TS1)	4.8 (-3.9) (INT → TS2)	11.3 (+5.0) (INT2 → TS3)	\
2Fe.M5	10.2 (-5.1) (2FeCl₃/S → TS1)	8.2 (-5.8) (INT → TS2)	\	\
2Fe.M5Ph	18.4 (-2.2) (2FeCl₃/S → TS1)	1.3 (INT0 → TS2) ^[c]	4.6 (INT → TS3)	3.0 (INT2 → TS4)
2Fe.M6	15.6 (-3.3) (2FeCl₃/S → TS1)	0.7 (INT0 → TS2) ^[c]	5.9 (INT → TS3)	5.1 (INT2 → TS4)
2Fe.M6Ph	17.0 (-6.2) (2FeCl₃/S → TS1)	6.6 (INT → TS2)	7.7 (INT2 → TS3)	\

[a] Values in parentheses are the change of reaction barrier compared with FeCl₃ monomer models, not applicable if the mechanism is changed (e.g. from concerted to stepwise);

[b] Our calculations suggest that the **2FeCl₃/S** complex of model **2Fe.M1** directly transforms into a more stable intermediate (**INT0**, structurally similar to **TS1** and 1.1 kcal mol⁻¹ lower in energy compared with the **2FeCl₃/S**) via no transition state, followed by the oxetane (**INT**) formation via the **TS1** with a small barrier (3.3 kcal mol⁻¹);

[c] Similar to the **M5** computed in solvation model, the cycloadditions in **2Fe.M2**, **2Fe.M4**, **2Fe.M5Ph** and **2Fe.M6** should be considered as concerted instead of stepwise due to the **INT0** being considerably unstable (energetically close to the next transition state);

[d] The **TS4** of **M2** leads to the undesired product due to chloride migration, similar to the **P'** in the FeCl₃ monomer model (Fig. 7).

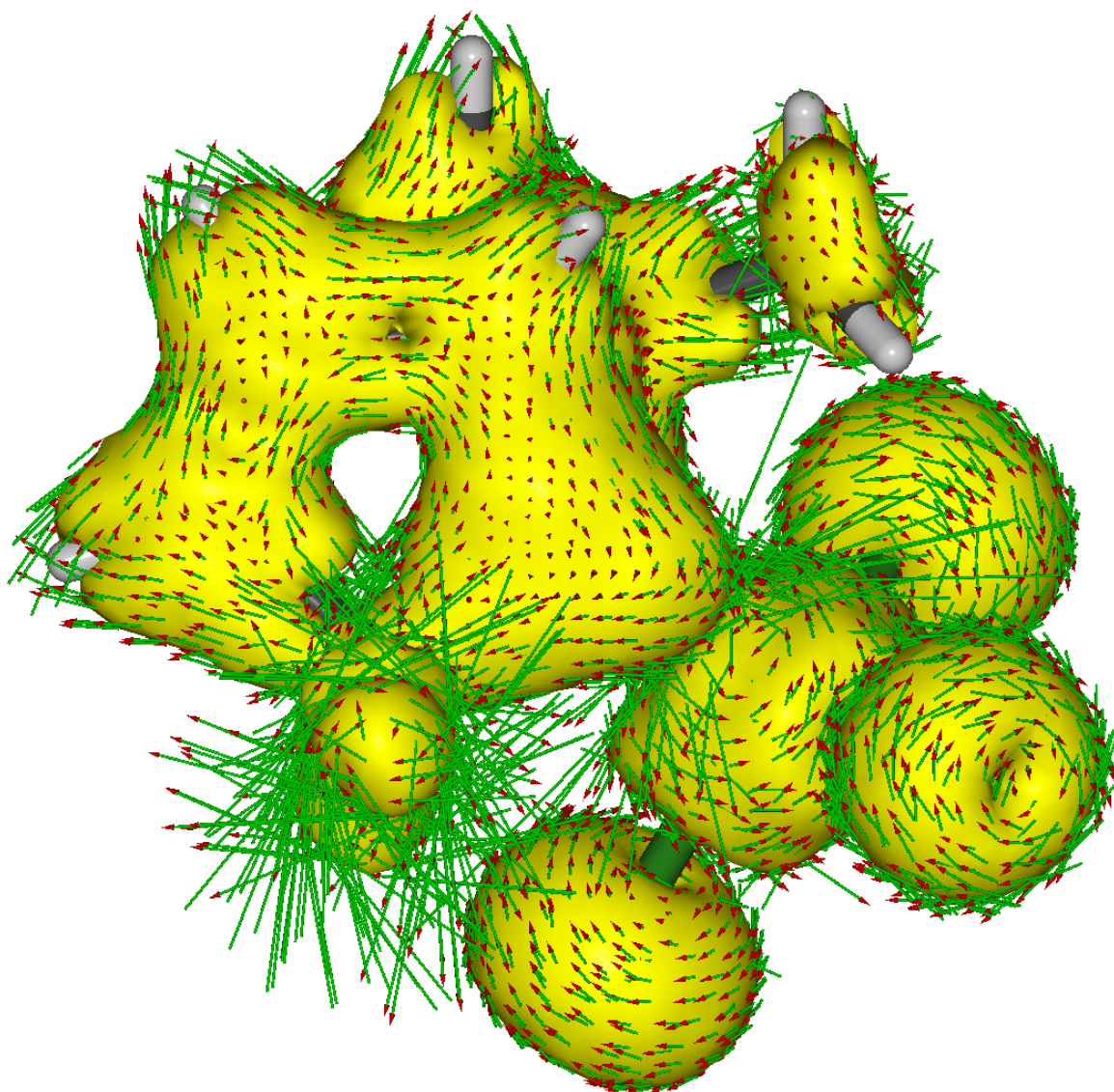


Fig. S8 ACID plot of **M1-TS2**. Isovalue: 0.035 a.u. The external magnetic field is perpendicular to the ring-plane and points out of the paper.

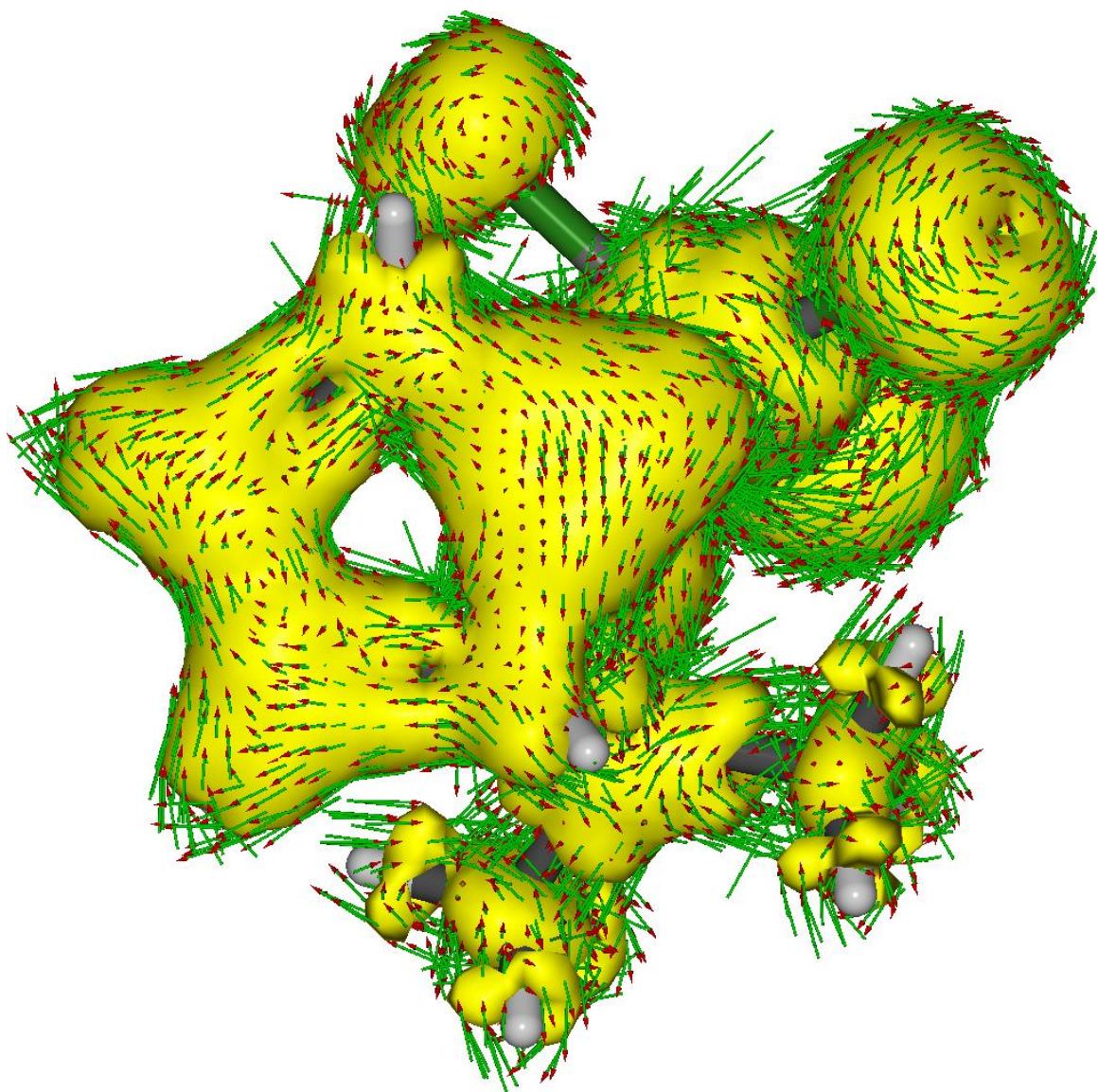


Fig. S9 ACID plot of **M3-TS2**. Isovalue: 0.035 a.u. The external magnetic field is perpendicular to the ring-plane and points out of the paper.

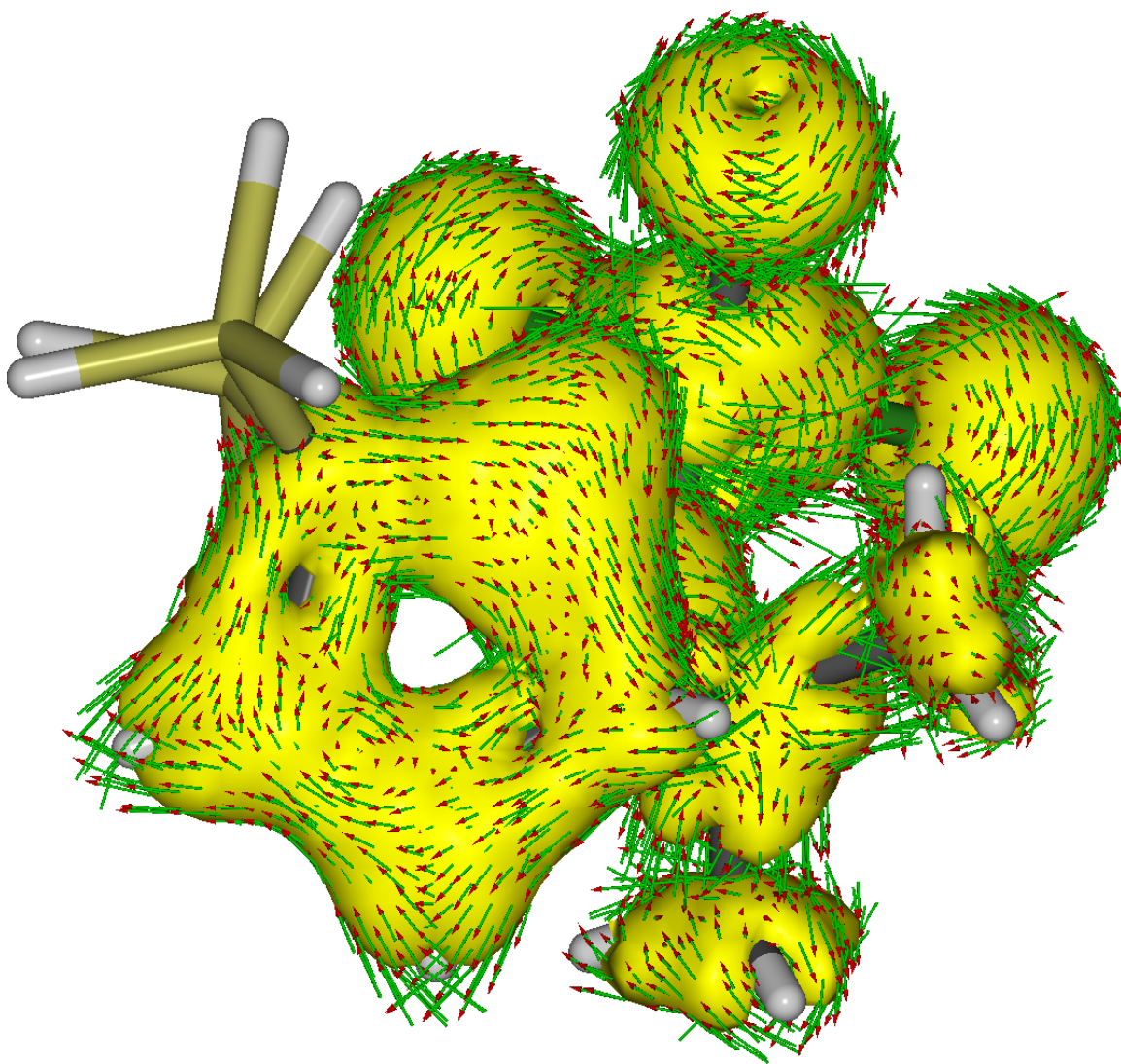


Fig. S10 ACID plot of **M5-TS2**. Isovalue: 0.035 a.u. The external magnetic field is perpendicular to the ring-plane and points out of the paper.

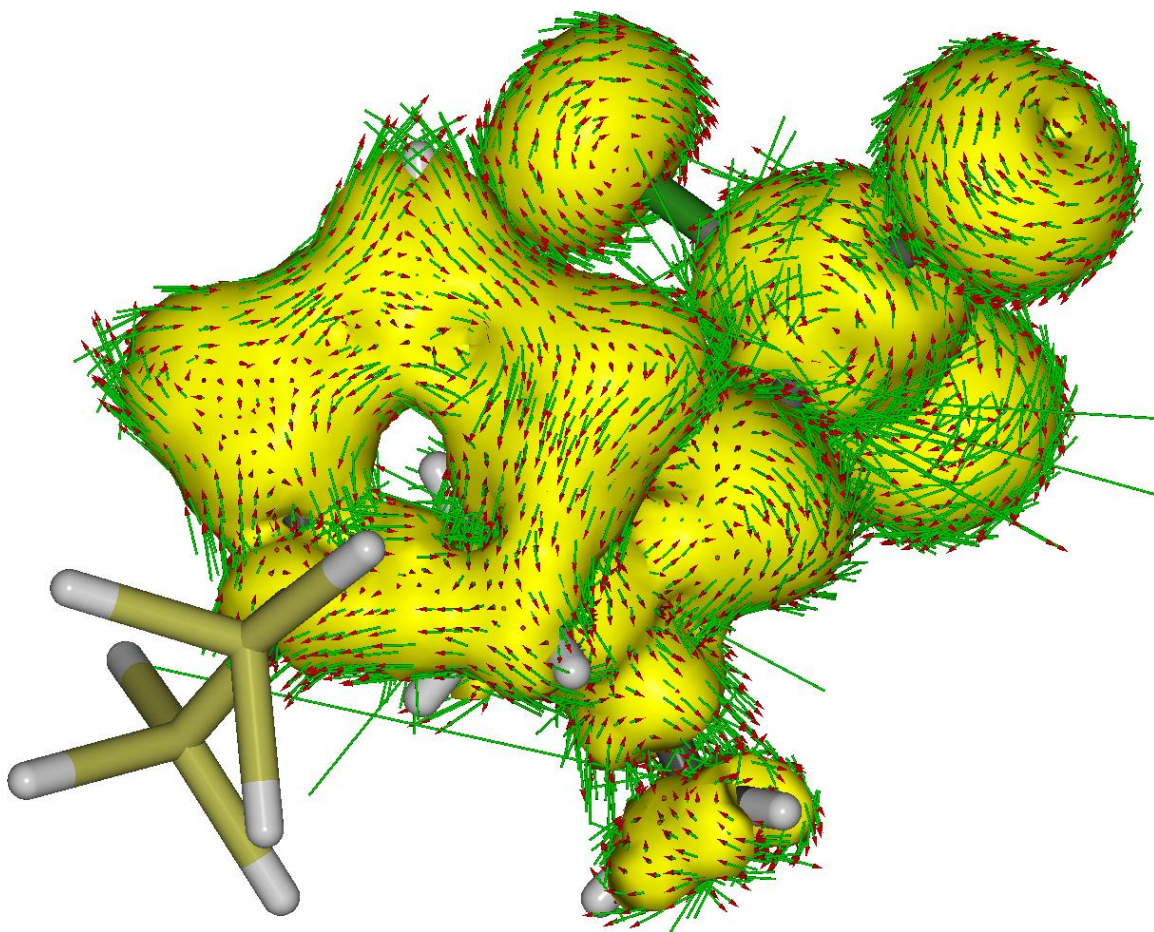


Fig. S11 ACID plot of **M6-TS2**. Isovalue: 0.035 a.u. The external magnetic field is perpendicular to the ring-plane and points out of the paper.

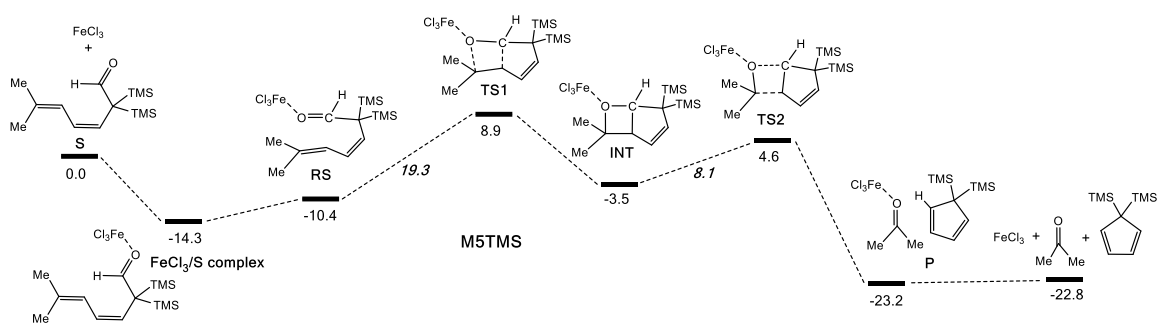


Fig. S12 Reaction profile for iron(III) catalyzed COM in **M5TMS**. Relative Gibbs energies (roman) and reaction barriers (italic) are given in kcal mol⁻¹. The trimethylsilyl (TMS) is commonly used in experiments. The cycloaddition barrier of **M5TMS** (23.2 kcal mol⁻¹) is higher than that of **M5** (15.3 kcal mol⁻¹). As for the cycloreversion, the activation barrier of **M5TMS** (8.1 kcal mol⁻¹) is smaller than that of **M5** (14.0 kcal mol⁻¹), indicating that the steric repulsion introduced by TMS groups might increase the cycloaddition barrier but decrease the cycloreversion barrier.

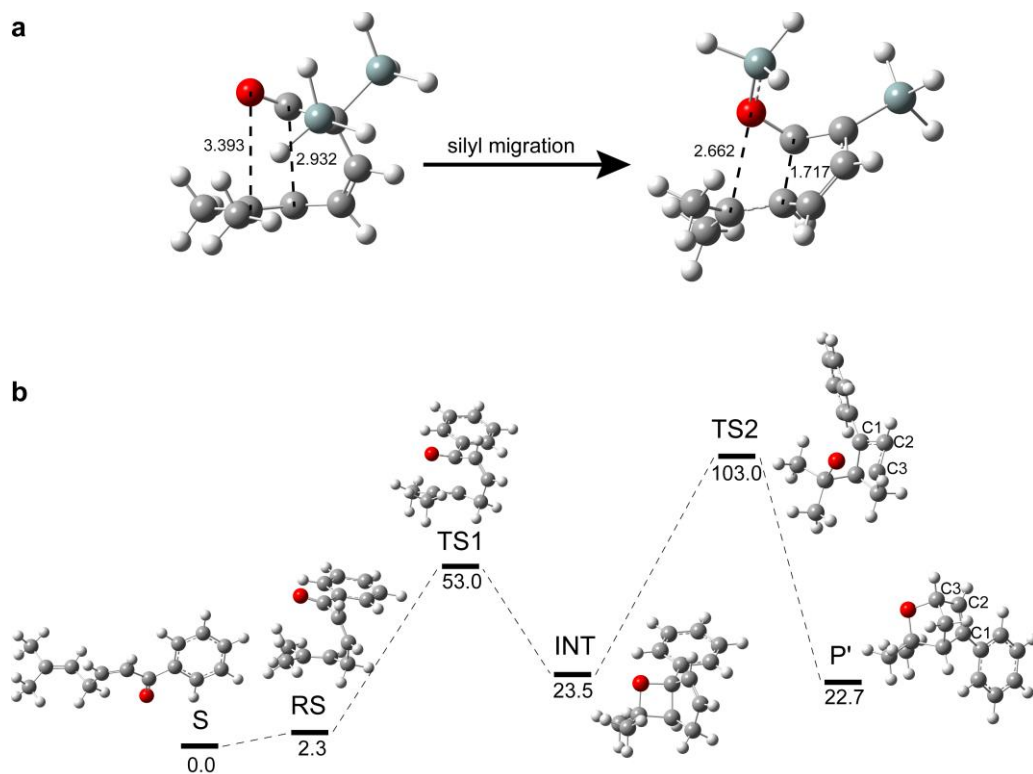
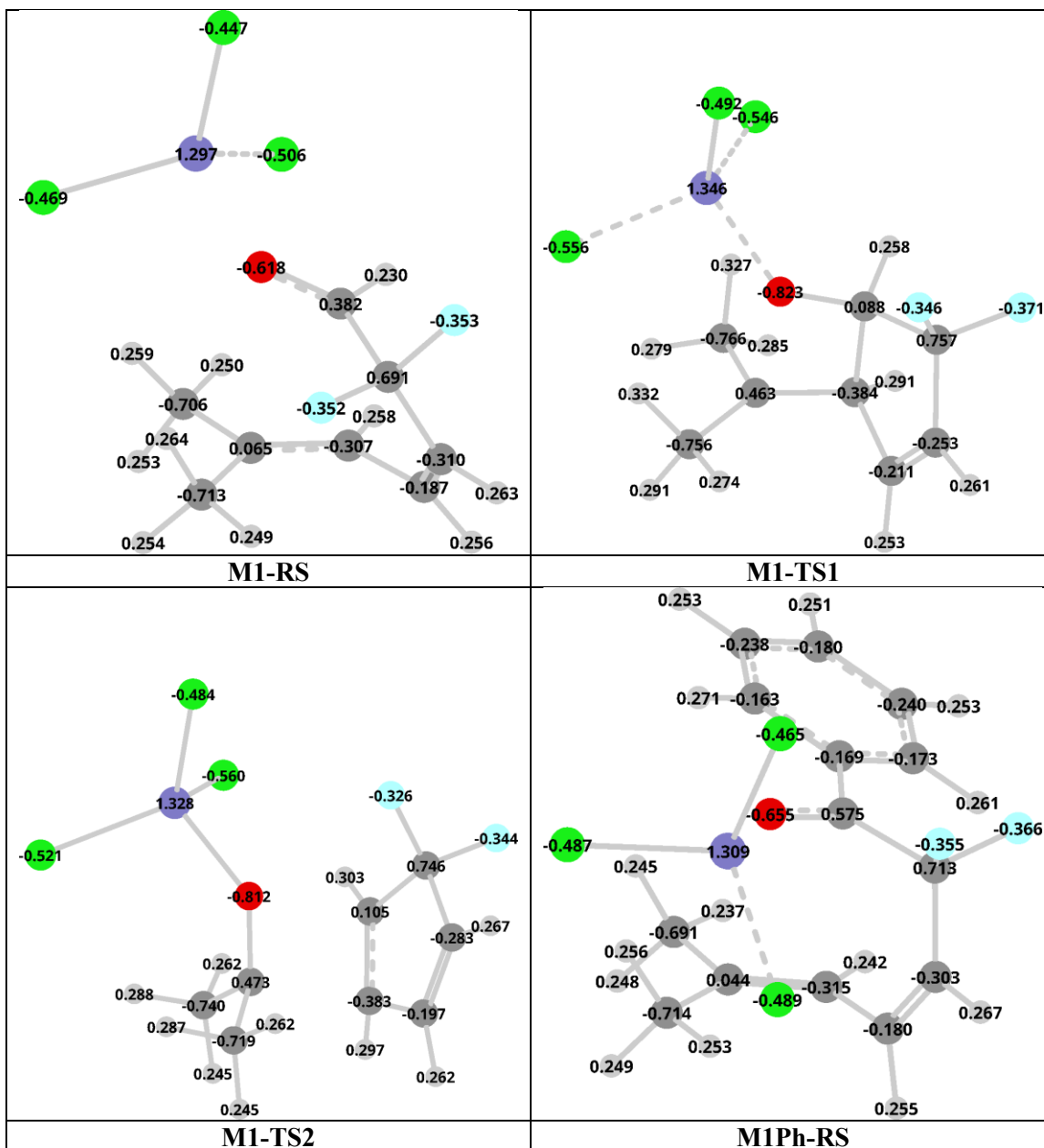
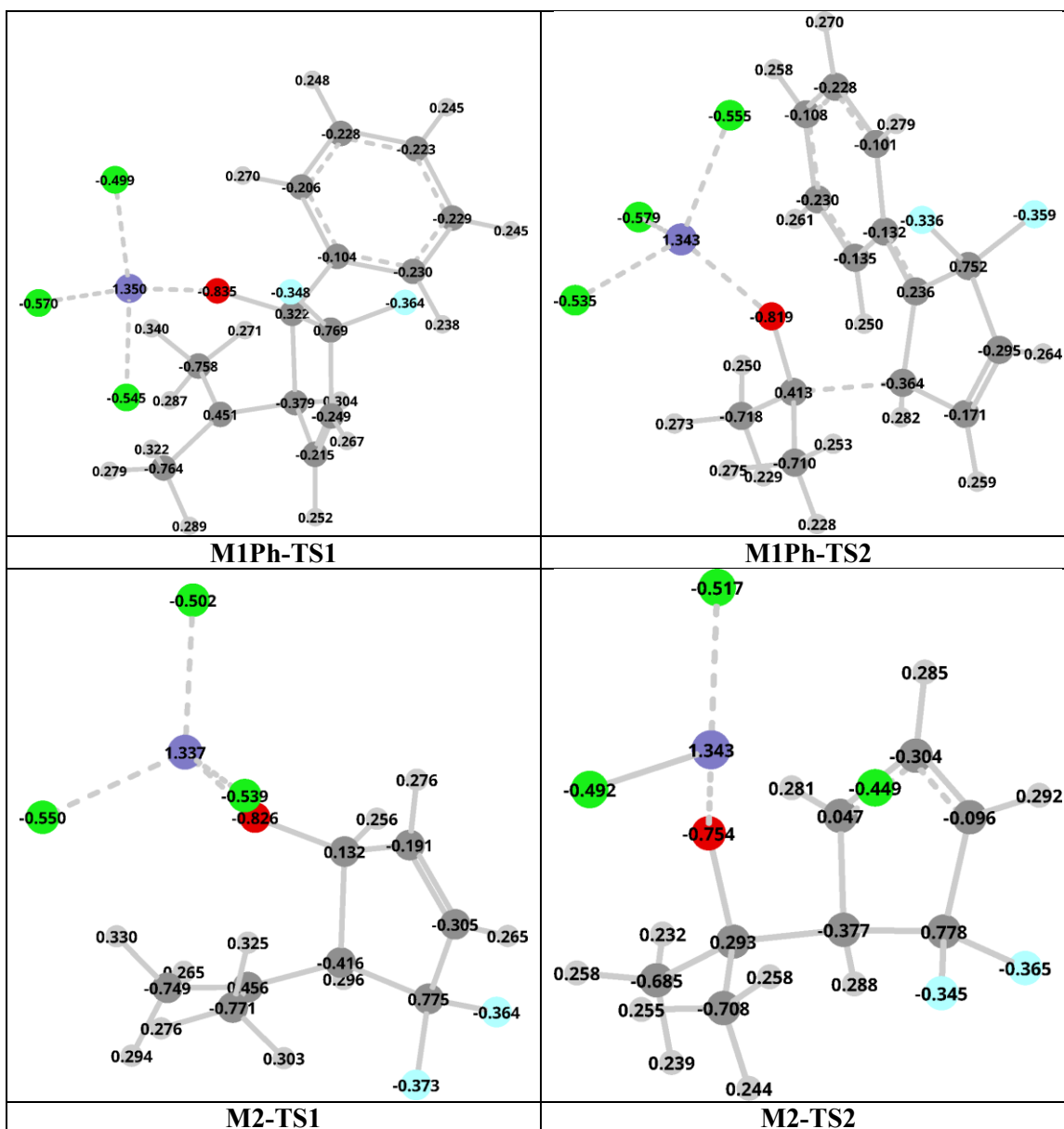
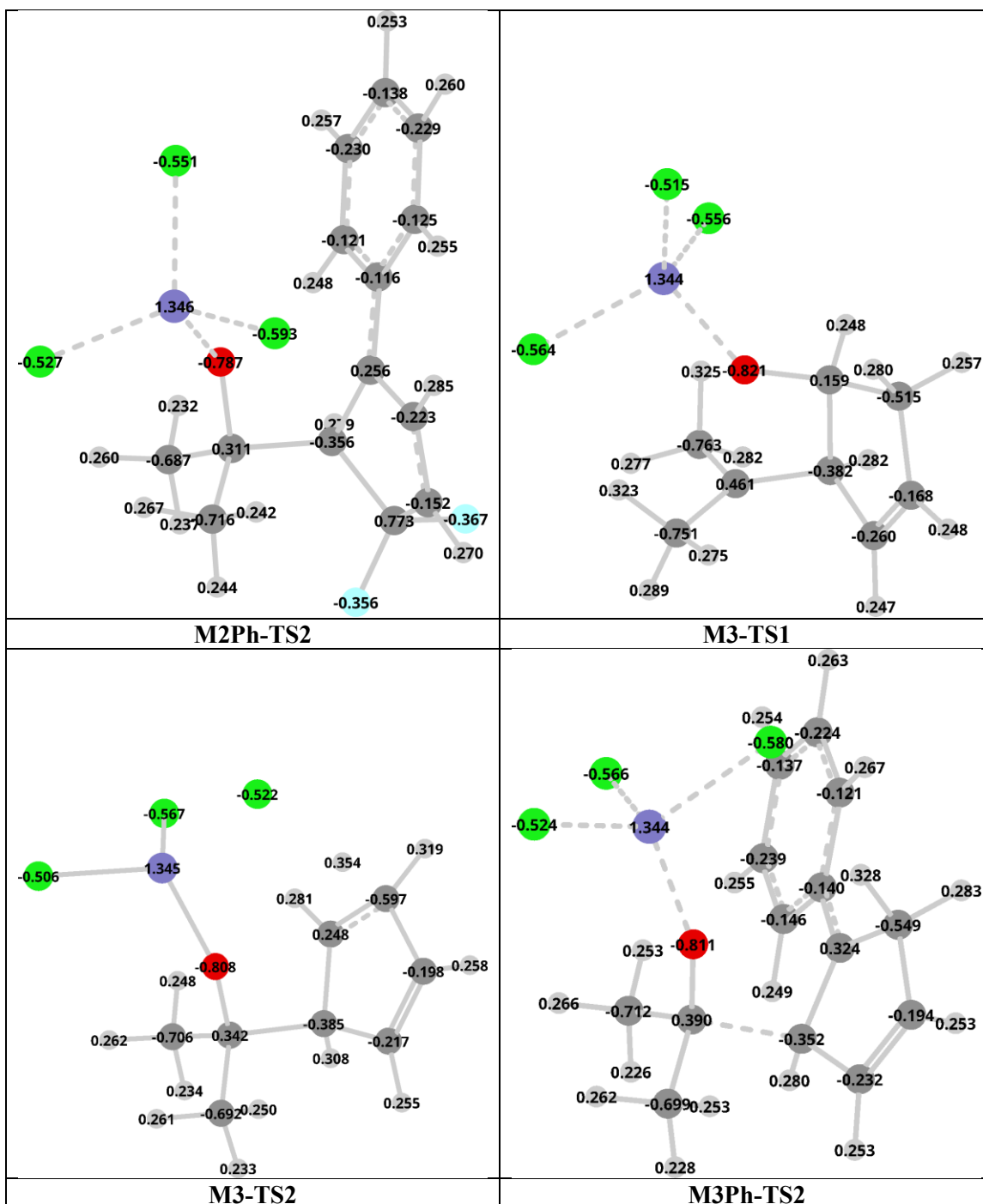


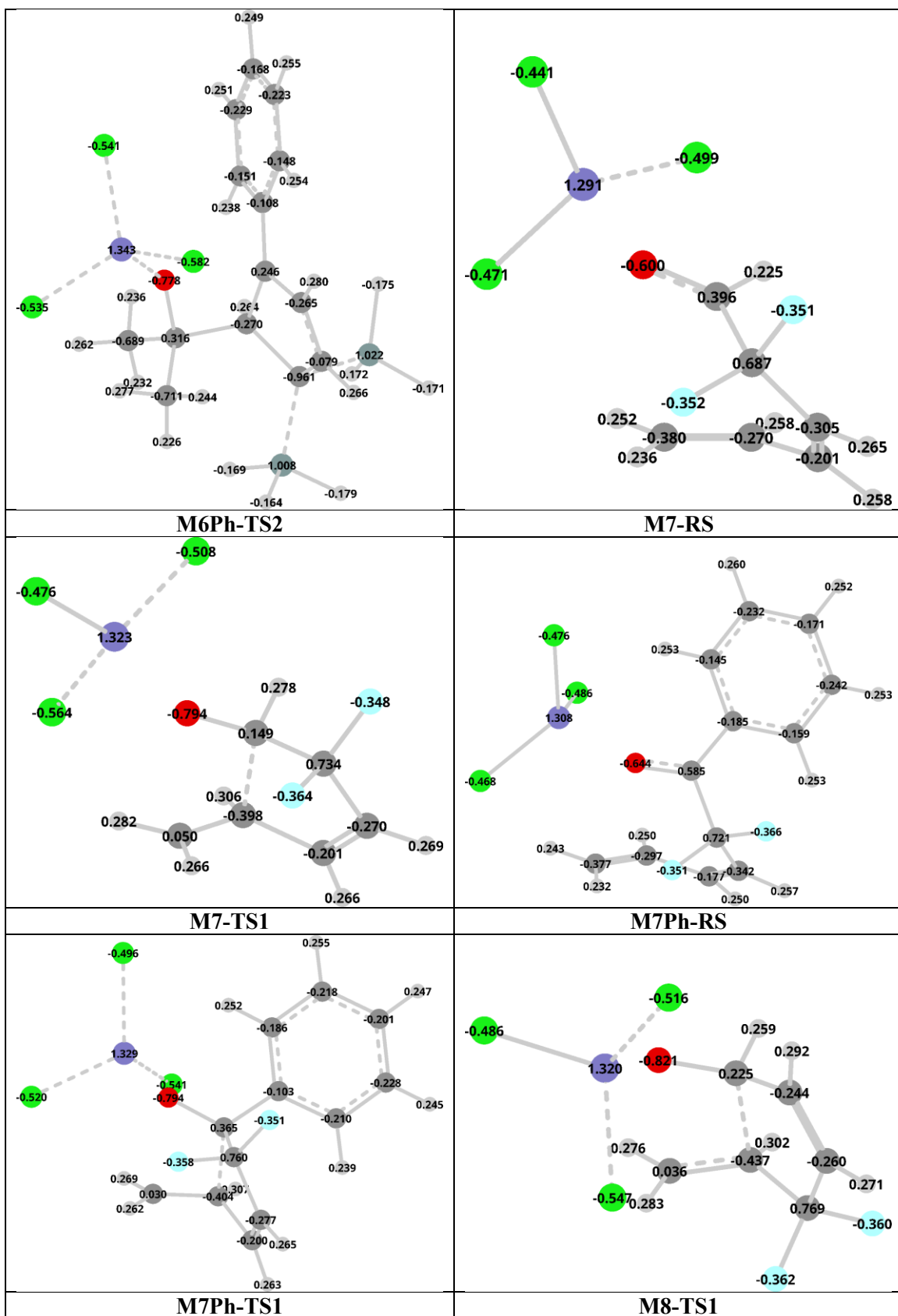
Fig. S13 Silyl migration in **M5** (a) and cycloaddition in **M4Ph** (b) without the presence of FeCl₃. Normal cycloreversion cannot be completed in **M4Ph** without FeCl₃ because it prefers the bonding of O-C3 rather than oxetane fragmentation after TS2. Distances of C5-C1 and O-C6 in **a** are given in Å. Relative Gibbs energies in **b** are given in kcal mol⁻¹.

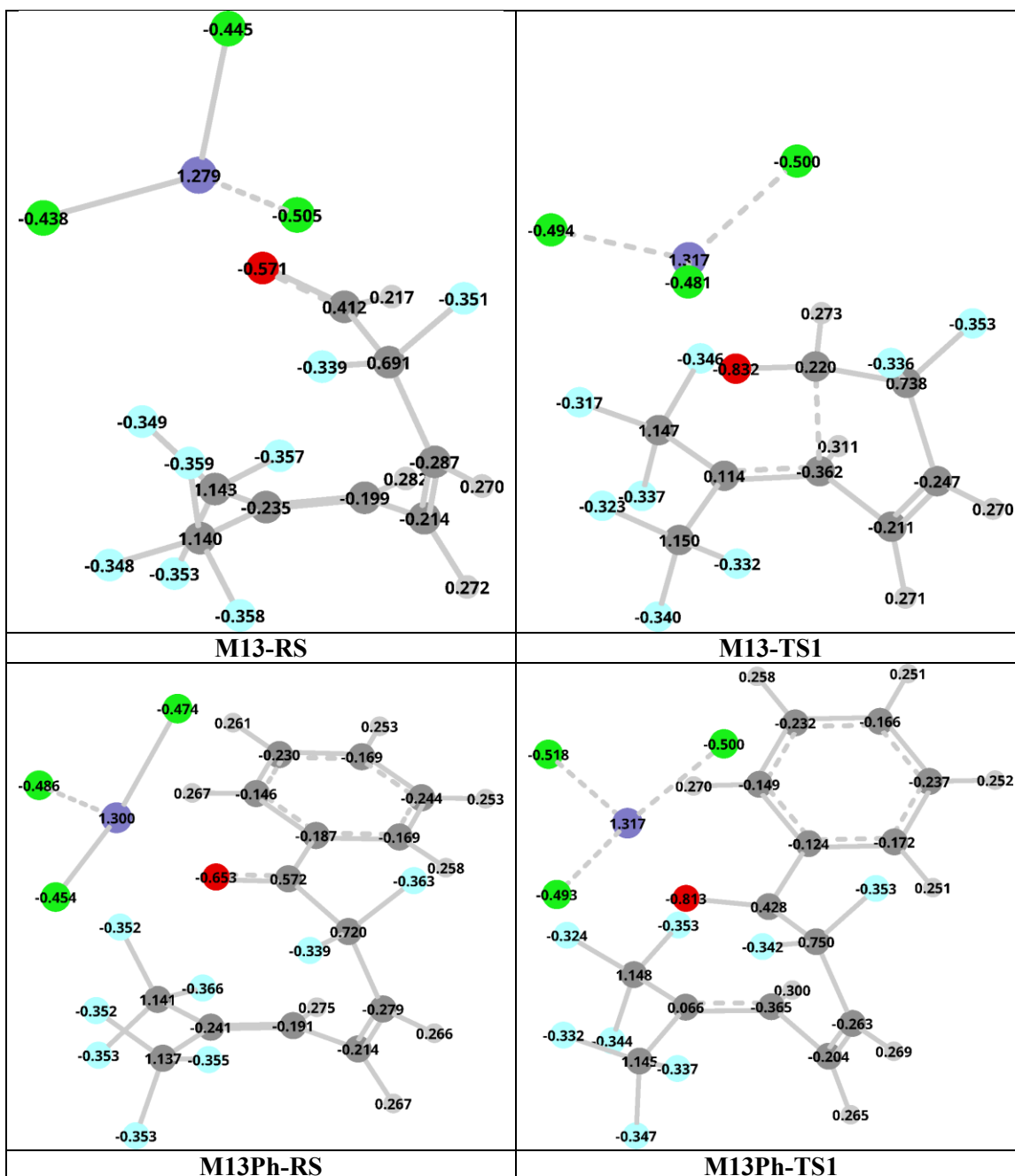
Table S6 Detailed NPA charges of atoms











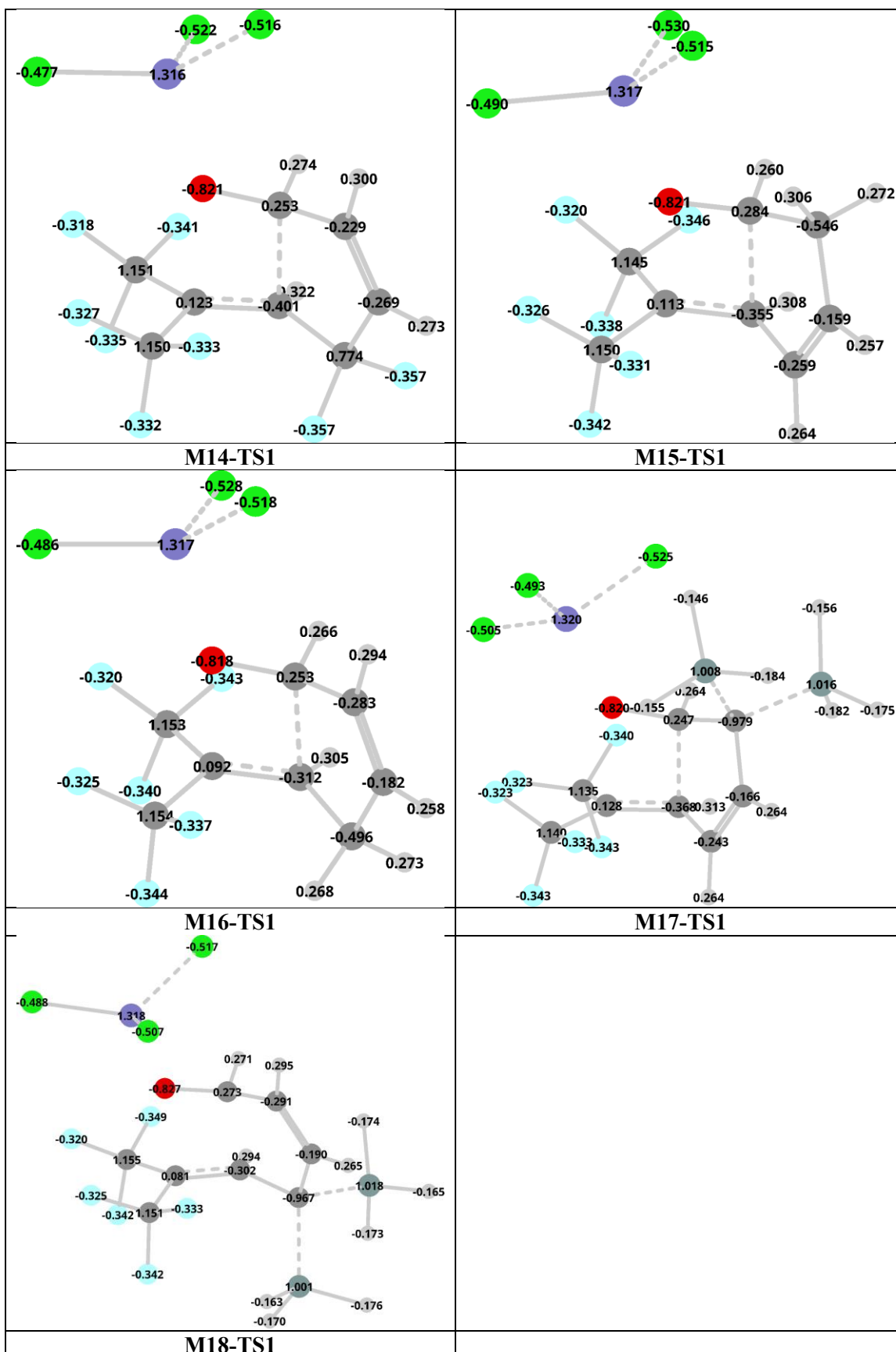


Table S7 Cartesian coordinates, thermal corrections, and electronic energies of key structures. All geometries were optimized in gas phase and in sextet state unless otherwise specified. The **FeCl₃/S** is the catalyst/substrate complex with the most stable conformation. Imaginary frequencies are given in cm⁻¹.

M1-S G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.125645 a.u. E (UωB97X-D/def2-tzvp) = -585.798109775 a.u.			
C	1.98852700	0.87313800	0.90119900
C	-1.15455200	-0.04715700	-0.10677100
C	-0.37617900	-1.21000000	0.26781500
C	0.96884400	-1.31716800	0.24334900
H	2.67729500	0.62799500	1.73568400
H	-0.59774100	0.82452200	-0.43395600
H	-0.91984400	-2.08832000	0.60655500
H	1.45682200	-2.22743800	0.57683100
C	1.90983600	-0.22687300	-0.16872700
C	-2.50306900	0.04846200	-0.06357200
O	1.33433700	1.88591200	0.86157000
C	-3.44007900	-1.04876300	0.36353600
H	-4.04408000	-0.72072400	1.22033100
H	-4.14801400	-1.27881500	-0.44408400
H	-2.93718300	-1.97638000	0.64263800
C	-3.18087100	1.33083900	-0.46536500
H	-3.78797600	1.72649200	0.36076900
H	-2.46004600	2.09820800	-0.76018800
H	-3.87078700	1.16206900	-1.30395100
F	3.17685500	-0.74785800	-0.29621800
F	1.56560200	0.34232800	-1.36177900
M1-RS (FeCl₃/S) G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.119456 a.u. E (UωB97X-D/def2-tzvp) = -3230.34975730 a.u.			
C	-0.97568700	0.80903000	0.27741400
C	-2.48132600	-1.27931400	0.99369300
C	-3.59179300	-0.32093500	0.93106500
C	-3.53007600	0.88268000	0.34835700
H	-0.85148200	0.72711800	1.36138500
H	-2.19927200	-1.60623600	1.99507800
H	-4.51558000	-0.60441600	1.43540200
H	-4.38364700	1.55312400	0.30877400
C	-2.27525300	1.43565400	-0.23620600
C	-1.85523100	-1.87297100	-0.05440500
O	-0.02933300	0.63522900	-0.49492000
Fe	1.86759700	0.09793300	0.03038600
Cl	3.00657800	1.95446800	-0.05224800
Cl	2.43186000	-1.43831400	-1.42351700
Cl	1.48270200	-0.63176900	2.08310700
C	-0.75221000	-2.86259900	0.19147900
H	-1.06526900	-3.85890300	-0.14911100
H	0.13860600	-2.60246200	-0.39173200
H	-0.46878900	-2.92012500	1.24440800
C	-2.20103300	-1.64988300	-1.49839600

H	-3.10888100	-1.06262400	-1.63866600
H	-1.37504700	-1.13365900	-2.00464400
H	-2.31935300	-2.61823600	-1.99877000
F	-2.14813500	2.75721800	0.14810600
F	-2.28051800	1.42209300	-1.59650800
M1-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.120670 a.u.			
E (UωB97X-D/def2-tzvp) = -3230.34398600 a.u.			
Imaginary frequency: 212.4059			
C	-1.34901900	0.27143700	0.49040000
C	-2.16832100	-1.09400300	0.46841200
C	-3.29539400	-0.80905800	-0.50152700
C	-3.40697700	0.48728500	-0.79012800
H	-1.04261400	0.52258500	1.51151400
H	-2.53582900	-1.32567800	1.47512700
H	-3.95259100	-1.59200600	-0.86735800
H	-4.15411200	0.95137400	-1.42355100
C	-2.38306700	1.29645100	-0.04714500
C	-1.14529800	-2.09292700	0.05654700
O	-0.27519700	0.13329400	-0.37407500
Fe	1.54418400	0.33148000	-0.06661800
Cl	2.37936900	2.27613800	-0.63502100
Cl	2.41805300	-1.45019100	-1.15096600
Cl	1.62972600	-0.07706900	2.17021000
C	-0.32294300	-2.71761700	1.08795800
H	0.31040700	-3.52420700	0.71790300
H	0.34971500	-1.91790500	1.48607100
H	-0.92205900	-3.02390500	1.95306600
C	-0.91414100	-2.42863200	-1.34405500
H	-1.55487600	-1.89249000	-2.04149000
H	0.15412800	-2.20192400	-1.54784100
H	-0.99679100	-3.51838900	-1.47356300
F	-2.97801800	1.93424000	1.01659600
F	-1.79455400	2.24677900	-0.80768100
M1-TS1 (optimized at the B3LYP-D3BJ/def2-TZVP level)			
Imaginary frequency: 235.8835			
C	-1.35655500	0.27544400	0.49106100
C	-2.15003400	-1.09819900	0.49225300
C	-3.30503100	-0.84302000	-0.44343800
C	-3.44934100	0.44046300	-0.74138000
H	-1.06597900	0.55257600	1.50724100
H	-2.48940900	-1.33684700	1.50278300
H	-3.95800200	-1.63622600	-0.78278200
H	-4.21942200	0.88257700	-1.35653200
C	-2.41554200	1.27443700	-0.04996900
C	-1.12077100	-2.07786100	0.06085400
O	-0.28147700	0.13602100	-0.36343200
Fe	1.56168500	0.33246300	-0.06370500
Cl	2.35877600	2.27874500	-0.61465200
Cl	2.41634800	-1.40686000	-1.18315100
Cl	1.67775500	-0.09378400	2.14478000
C	-0.28119300	-2.68966200	1.07192300
H	0.35475200	-3.48500300	0.69502300
H	0.38431400	-1.88062900	1.45872200
H	-0.86030800	-2.99386100	1.94621000
C	-0.92417800	-2.42455500	-1.33541400

H	-1.55997500	-1.87921400	-2.02363700
H	0.14249900	-2.24257700	-1.55984000
H	-1.05005100	-3.50959300	-1.44726400
F	-2.99046600	1.94354300	1.00968400
F	-1.86658600	2.21496800	-0.84858300
M1-INT			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.124868 a.u.			
E (UωB97X-D/def2-tzvp) = -3230.37569727 a.u.			
C	-1.43247800	0.15397700	0.73974100
C	-2.15380600	-1.20289800	0.72693600
C	-3.37881600	-0.95923600	-0.11335800
C	-3.46965900	0.30239700	-0.54198200
H	-1.05730200	0.56521800	1.67706200
H	-2.36233300	-1.67294800	1.69066200
H	-4.09036000	-1.74624900	-0.34168200
H	-4.24776400	0.72851300	-1.16472300
C	-2.32632600	1.13864300	-0.04125100
C	-0.89152700	-1.78901300	0.01123200
O	-0.34619100	-0.37631900	-0.07550600
Fe	1.55999800	0.29242900	-0.03147500
Cl	1.59759300	2.30361700	-0.86561000
Cl	2.64658200	-1.23023700	-1.18880700
Cl	1.90884900	0.26224800	2.14931600
C	-0.02770300	-2.64006800	0.91994000
H	0.94624100	-2.83291300	0.46280900
H	0.13114800	-2.15829600	1.88851500
H	-0.53216200	-3.59946100	1.08269500
C	-1.03158300	-2.33590800	-1.38947500
H	-1.64074400	-1.67712900	-2.01204000
H	-0.03996800	-2.43382800	-1.84141400
H	-1.49723300	-3.32723200	-1.35550000
F	-2.76388400	2.11959800	0.80956800
F	-1.65055400	1.75247900	-1.04822800
M1-TS2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.120320 a.u.			
E (UωB97X-D/def2-tzvp) = -3230.29484114 a.u.			
Imaginary frequency: 752.7503			
C	1.79804100	-0.01066300	0.86292600
C	2.41762500	1.21177600	0.55813500
C	3.38858800	0.92920300	-0.54608700
C	3.32139700	-0.34887100	-0.94073300
H	1.12395400	-0.25520400	1.68022500
H	2.59676400	1.97773300	1.30359400
H	4.02294800	1.69470400	-0.97689400
H	3.87317500	-0.83615100	-1.73370300
C	2.37968300	-1.10181800	-0.03914400
C	0.69872200	1.69660400	-0.11827600
O	0.14362600	0.48827100	-0.45381700
Fe	-1.56174900	-0.27525600	-0.05738600
Cl	-1.88211300	-2.01628900	-1.35204600
Cl	-3.06304200	1.33397900	-0.35070400
Cl	-1.30614100	-0.81203500	2.12319500
C	0.06368100	2.43419100	1.03925700
H	-0.94515900	2.71793200	0.71440600
H	-0.05421400	1.79901000	1.91992000
H	0.62067500	3.33973100	1.29418500

C	0.98789900	2.52719500	-1.33806000
H	1.54457300	1.95184600	-2.08014800
H	0.00288100	2.75769300	-1.77040600
H	1.50351200	3.46273700	-1.10400200
F	3.08135200	-1.88606000	0.85724500
F	1.48593300	-1.88965000	-0.65060900
M1-P			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.114484 a.u.			
E (UωB97X-D/def2-tzvp) = -3230.36395845 a.u.			
C	2.37715600	-0.09723500	1.15795700
C	3.13724200	0.95498600	0.82965700
C	3.72465000	0.75125700	-0.53086100
C	3.32194200	-0.42536600	-1.02379600
H	1.81526800	-0.28755300	2.06141600
H	3.32895500	1.82664700	1.44616700
H	4.38136600	1.46331500	-1.01803300
H	3.56038800	-0.88716100	-1.97270400
C	2.43422400	-1.09672600	0.01190800
C	0.18129700	2.03922600	-0.42702500
O	-0.24491400	0.94698900	-0.83073800
Fe	-1.59750900	-0.33806600	-0.03158600
Cl	-1.88455400	-2.02842400	-1.37728200
Cl	-3.34892700	1.01953900	-0.01864000
Cl	-0.98911400	-0.79050100	2.04626800
C	-0.23344000	2.60206700	0.89612900
H	-1.30833000	2.82238400	0.84633700
H	-0.11172700	1.84012100	1.67259200
H	0.31808900	3.50770500	1.15394100
C	1.08101600	2.83241500	-1.32262600
H	1.37666400	2.24594500	-2.19255900
H	0.54010400	3.73303600	-1.64451200
H	1.96234600	3.16992400	-0.76824500
F	2.95151200	-2.29249000	0.42070000
F	1.18971100	-1.37359300	-0.50083600
M2-S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.125513 a.u.			
E (UωB97X-D/def2-tzvp) = -585.793809552 a.u.			
C	-2.75524200	-0.92817200	0.40998100
C	0.70383800	-0.40293100	-0.41093000
C	-0.20770900	0.78903300	-0.36168000
C	-1.02830400	0.84954900	0.90791400
H	0.20170300	-1.26785400	-0.83096200
H	-0.64955600	1.57347700	1.62541700
C	-2.12115100	0.13638500	1.22025600
C	1.95621700	-0.51094200	0.05611400
O	-2.22575100	-1.54954900	-0.49139700
C	2.75270400	0.57413300	0.73486100
H	2.19588700	1.49853300	0.87273000
H	3.10400900	0.21941300	1.71298100
H	3.65228500	0.80409100	0.14819200
C	2.68563100	-1.82481700	-0.07894900
H	2.97777100	-2.20944800	0.90772900
H	2.07722600	-2.58348300	-0.57867900
H	3.61420000	-1.69446400	-0.65085300
H	-2.61846900	0.34762000	2.16551800
F	-1.03106000	0.77214800	-1.45693500

F	0.49023300	1.98107800	-0.43425100
H	-3.79751400	-1.16395300	0.71437600
M2-FeCl₃/S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.115961 a.u.			
E (UωB97X-D/def2-tzvp) = -3230.35576098 a.u.			
C	-0.03837700	1.40358000	-1.36458000
C	-2.13038500	-0.46729200	0.55189700
C	-2.47183000	0.99508900	0.58999900
C	-2.43359300	1.69782000	-0.75753500
H	-1.22142700	-0.72356100	1.08301100
H	-3.40273000	2.07549100	-1.07395200
C	-1.38075500	1.89621600	-1.58020800
C	-2.83237400	-1.41542400	-0.08737700
O	0.30516300	0.79657600	-0.33635200
C	-4.08851000	-1.16610700	-0.88179500
H	-4.49374900	-0.16261000	-0.74458800
H	-3.90069900	-1.32853300	-1.95154300
H	-4.86547300	-1.88288100	-0.58943600
C	-2.37054600	-2.84804300	-0.05187700
H	-2.23958800	-3.23274200	-1.07225300
H	-1.42444800	-2.96122800	0.48176600
H	-3.12683700	-3.48331700	0.42778800
H	-1.53898800	2.42540200	-2.51545000
Fe	2.02949400	-0.16247700	0.08328500
Cl	2.89949500	-0.27799200	-1.94072800
Cl	3.10664100	1.14765700	1.45580600
Cl	1.35798600	-2.07849900	0.92166800
F	-1.62751900	1.64284400	1.44935000
F	-3.75084500	1.19639000	1.07394900
H	0.69922900	1.54780500	-2.16546100
M2-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.118012 a.u.			
E (UωB97X-D/def2-tzvp) = -3230.35728039 a.u.			
C	-2.35191900	-1.66112900	0.17001000
C	-1.10553600	-1.66805700	-0.31801500
C	-0.60198300	-0.70935400	-1.30698800
C	-2.86259000	0.69808700	-0.67392200
H	-2.67914500	-2.44086100	0.85265100
H	-0.38391800	-2.40101700	0.03155300
H	-1.22773400	-0.46884200	-2.17146400
H	-3.23007700	0.91772500	-1.67310600
C	-3.38273300	-0.58741000	-0.09745600
C	-2.03411600	1.55859100	-0.04876500
O	0.55367400	-0.25142200	-1.31331700
Fe	2.06495900	-0.09582600	0.01531600
Cl	2.17363500	2.07760900	0.34014500
Cl	3.76655300	-0.99906800	-1.01119400
Cl	1.43564800	-1.19218200	1.82131500
C	-1.53609400	1.38844200	1.35940800
H	-1.92888800	2.20696600	1.97676200
H	-1.83754100	0.44953200	1.82158600
H	-0.44438800	1.47212700	1.39180800
C	-1.53094500	2.78084200	-0.76497800
H	-1.75031400	3.68653600	-0.18646700
H	-0.43842700	2.72833600	-0.85939300
H	-1.96803600	2.88760700	-1.76167000

F	-4.31515700	-1.11821800	-0.96047300
F	-4.03857400	-0.37105100	1.09555900
M2-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.120750 a.u.			
E (UωB97X-D/def2-tzvp) = -3230.34259953 a.u.			
Imaginary frequency: 228.9951			
C	-2.48243600	-1.61476800	0.50822700
C	-1.27493000	-1.74331100	-0.04140300
C	-0.97267200	-0.69791200	-1.09481800
C	-2.15462000	0.36369900	-0.84952200
H	-2.94683700	-2.26678500	1.23849300
H	-0.54759000	-2.51515400	0.18266700
H	-1.09748400	-1.12965500	-2.09921500
H	-2.56310400	0.72472800	-1.79528900
C	-3.21335400	-0.44993400	-0.07828900
C	-1.44653800	1.45927300	-0.14557900
O	0.25011500	-0.05626500	-1.00773200
Fe	1.83082600	-0.15240000	-0.04836500
Cl	2.41858200	2.01804400	0.12631200
Cl	3.30178200	-1.48205500	-1.00084600
Cl	1.20841800	-0.89940700	1.99741300
C	-1.24743700	1.46715200	1.30032000
H	-0.76104400	2.37565500	1.65583100
H	-2.18462300	1.26153300	1.82546600
H	-0.59105100	0.60453500	1.55597000
C	-0.88282100	2.55479900	-0.93386800
H	-1.25230100	3.51099600	-0.53403100
H	0.20871800	2.56673100	-0.73390000
H	-1.06906100	2.47979000	-2.00452100
F	-4.16778400	-0.85471200	-0.97727300
F	-3.89204500	0.29296200	0.86044300
M2-TS1 (optimized at the B3LYP-D3BJ/def2-TZVP level)			
Imaginary frequency: 226.9974			
C	-2.46989300	-1.61291300	0.51151000
C	-1.27003800	-1.72917000	-0.04044700
C	-0.97430200	-0.68130000	-1.08604600
C	-2.16194400	0.37011900	-0.83321900
H	-2.92695700	-2.26764700	1.23847900
H	-0.54040100	-2.49665500	0.17523400
H	-1.09972400	-1.11404300	-2.08698800
H	-2.57614900	0.72629300	-1.77469300
C	-3.20580500	-0.45099300	-0.06326200
C	-1.44633700	1.46558600	-0.14634100
O	0.23851600	-0.03478000	-0.99467700
Fe	1.84270800	-0.14817900	-0.04487900
Cl	2.55232600	1.95944600	-0.03529200
Cl	3.16648200	-1.65743700	-0.90386900
Cl	1.19333600	-0.70447400	2.04041100
C	-1.25359200	1.51471000	1.28486500
H	-0.82986400	2.45606100	1.62359500
H	-2.13716700	1.21879000	1.84566100
H	-0.50294200	0.71772900	1.52033300
C	-0.87759300	2.53366200	-0.96418000
H	-1.41259600	3.45826100	-0.70207600
H	0.16655200	2.69451500	-0.66341200
H	-0.94501800	2.35295800	-2.03188600

F	-4.16868200	-0.85993300	-0.95731100
F	-3.89395300	0.27863500	0.87747700
M2-INT			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.125259 a.u.			
E (UωB97X-D/def2-tzvp) = -3230.37902165 a.u.			
C	-2.46833000	-1.56205600	0.51110700
C	-1.31846100	-1.75324200	-0.14051200
C	-1.04911700	-0.64269100	-1.11339400
C	-2.14867100	0.40033600	-0.85468100
H	-2.91036500	-2.20967100	1.25965400
H	-0.63314500	-2.58230800	-0.00820100
H	-0.80953200	-0.95637000	-2.12980900
H	-2.64609900	0.82425600	-1.72650900
C	-3.15684000	-0.30235600	0.06115600
C	-1.04358000	1.33112700	-0.26559100
O	-0.00893600	0.29669300	-0.64730900
Fe	1.80360800	-0.15836000	0.05725700
Cl	2.81451900	1.78681900	0.13897600
Cl	2.39710000	-1.60366000	-1.48923100
Cl	1.48304000	-1.10271500	2.01719700
C	-0.98900100	1.59265300	1.22601500
H	-0.03282400	2.06691600	1.46835000
H	-1.79806200	2.27043500	1.51022700
H	-1.07885600	0.67489600	1.80739700
C	-0.78622300	2.57273300	-1.09513300
H	-1.57496500	3.30854300	-0.90269200
H	0.17859800	3.01091000	-0.82419400
H	-0.77691200	2.33835800	-2.16357300
F	-4.29010700	-0.60175100	-0.65656600
F	-3.57522800	0.46967000	1.11071400
M2-TS2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.126052 a.u.			
E (UωB97X-D/def2-tzvp) = -3230.32931940 a.u.			
Imaginary frequency: 225.1125			
C	-1.72472700	-1.68063200	0.26843500
C	-1.24059900	-1.74879600	-1.02905500
C	-1.36853400	-0.50500700	-1.63844000
C	-2.05776300	0.51096600	-0.74880700
H	-1.87990000	-2.51225000	0.94269300
H	-0.74170000	-2.60313300	-1.46669400
H	-1.13537300	-0.31244200	-2.67778500
H	-2.95346600	0.94945700	-1.19763200
C	-2.50019800	-0.38132800	0.43259600
C	-0.91722200	1.56642700	-0.58766800
O	0.22268500	0.76438700	-0.95284700
Fe	1.55014100	-0.08740000	0.01685400
Cl	2.95768100	1.29464800	0.97368800
Cl	2.36387800	-1.62512600	-1.34694100
Cl	0.32930200	-1.20246600	1.67699600
C	-0.74024300	2.22572200	0.77606900
H	0.07946900	2.94728800	0.71104900
H	-1.65228100	2.75672000	1.06731100
H	-0.50035900	1.50072600	1.55275400
C	-1.07875300	2.63393800	-1.67590800
H	-1.94006400	3.27612800	-1.46182000
H	-0.17721600	3.25176300	-1.70738700

H	-1.21477600	2.18217200	-2.66399400
F	-3.82473100	-0.72619000	0.24739000
F	-2.42703600	0.17654200	1.65695700
M2-INT2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.126167 a.u.			
E (UωB97X-D/def2-tzvp) = -3230.35341973 a.u.			
C	-1.50675000	-1.82708800	-0.12431200
C	-1.94657700	-1.47000700	-1.49642700
C	-2.35138600	-0.19626100	-1.56438000
C	-2.19001700	0.56788500	-0.27153500
H	-1.93203000	-2.73942600	0.29305100
H	-1.94903400	-2.18778500	-2.30781500
H	-2.75449800	0.26560400	-2.45809400
H	-3.12666800	1.04914900	0.03186400
C	-1.92102600	-0.59311400	0.71925100
C	-1.09806300	1.68318200	-0.36359800
O	0.12307400	1.05528700	-0.68296200
Fe	1.50444600	0.13410500	-0.04306000
Cl	2.18843400	0.47768500	2.00656000
Cl	3.07049400	-0.26431400	-1.52945200
Cl	0.31673600	-2.18272200	-0.03971900
C	-0.97936000	2.48443100	0.94066500
H	-0.21909000	3.26055300	0.81136000
H	-1.93227500	2.97195600	1.17523700
H	-0.68631700	1.85529800	1.77937500
C	-1.43164400	2.63769800	-1.52180100
H	-2.42487200	3.08281800	-1.39462300
H	-0.69182300	3.44266400	-1.54473500
H	-1.38963100	2.11881800	-2.48252000
F	-3.10255100	-0.93043600	1.32662900
F	-1.03426000	-0.32401600	1.71085500
M2-TS3			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.120321 a.u.			
E (UωB97X-D/def2-tzvp) = -3230.31416222 a.u.			
Imaginary frequency: 558.6499			
C	-1.60214800	-1.81117800	0.02317300
C	-2.00214700	-1.53763800	-1.38882400
C	-2.49308200	-0.27729500	-1.52190500
C	-2.38523900	0.48708700	-0.30741900
H	-2.08827300	-2.67938100	0.46995600
H	-1.92848000	-2.28495300	-2.16871700
H	-2.89407400	0.12328000	-2.44567200
H	-3.09342500	1.26781200	-0.04830000
C	-2.03435500	-0.51809300	0.77600600
C	-0.76315800	1.86113600	-0.62947600
O	0.19866800	1.03462700	-0.82085900
Fe	1.64034300	0.07957300	-0.01028700
Cl	2.13232700	0.80247000	2.01838000
Cl	3.04766900	-0.72929300	-1.50528700
Cl	0.17863800	-2.18892100	0.18527000
C	-0.80085300	2.66830000	0.65105300
H	-0.04451700	3.45939200	0.55491300
H	-1.77288100	3.14760100	0.79644300
H	-0.54026000	2.06641800	1.51904200
C	-1.28515800	2.55405100	-1.87540400
H	-2.29803800	2.94449600	-1.74196700

H	-0.62349600	3.40546100	-2.08300600
H	-1.24606500	1.88352600	-2.73554200
F	-3.17415100	-0.81492200	1.48269700
F	-1.11570300	-0.10398100	1.68194500
M2-P'			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.115388 a.u.			
E (UωB97X-D/def2-tzvp) = -3230.34705978 a.u.			
C	-1.76585800	-1.09125800	1.13187800
C	-1.48064300	-2.13546100	0.11576800
C	-1.88528100	-1.69376300	-1.14727600
C	-2.50774000	-0.46093500	-1.08268700
H	-2.29895200	-1.41557700	2.02491100
H	-0.95138600	-3.05142600	0.33477400
H	-1.71937600	-2.25721100	-2.05739700
H	-2.93089300	0.11547900	-1.89410100
C	-2.58677000	-0.02241600	0.34420600
C	0.12835600	2.16448200	-0.95326900
O	0.51552700	1.00906100	-1.15223700
Fe	1.67941400	-0.40351700	-0.16568900
Cl	3.20530900	0.65887600	1.06653800
Cl	1.55748300	-2.33218400	-1.26660300
Cl	-0.18577000	-0.40262900	1.80976600
C	0.55840800	2.95324200	0.24747800
H	0.45699000	4.02931300	0.08616500
H	-0.10290100	2.66517400	1.07474000
H	1.57863800	2.68918100	0.53729400
C	-0.83173000	2.79271200	-1.92280500
H	-1.73420900	3.10232300	-1.38302200
H	-0.38623900	3.69651700	-2.35556200
H	-1.09009900	2.08903500	-2.71548200
F	-3.87586800	-0.03996200	0.81255800
F	-2.14550700	1.26301400	0.53286600
M3-S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.143763 a.u.			
E (UωB97X-D/def2-tzvp) = -387.288621951 a.u.			
C	2.63933700	0.55654200	0.43839200
C	-0.63619900	-0.04948600	-0.18503600
C	0.06548100	-1.29422200	0.07346100
C	1.38295400	-1.50420900	-0.12220400
H	3.18861000	0.15725600	1.31962000
H	-0.02414300	0.79187700	-0.50085500
H	-0.51689500	-2.13036100	0.45315000
H	1.79874300	-2.47513900	0.13440400
C	2.35134000	-0.46442000	-0.64840100
C	-1.96167900	0.17194300	-0.04392000
O	2.27414600	1.71123600	0.40574600
C	-2.96615900	-0.85627600	0.40364000
H	-3.47879600	-0.51882500	1.31491300
H	-3.74590400	-0.98673400	-0.35937300
H	-2.52989800	-1.83611200	0.60676300
C	-2.54256200	1.52993700	-0.33720900
H	-3.04950400	1.93888400	0.54821600
H	-1.77517300	2.24330900	-0.65105000
H	-3.30307700	1.47004300	-1.12874700
H	3.29288600	-0.94891900	-0.93559900
H	1.95489900	0.06598700	-1.51975700

M3-FeCl₃/S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.135177 a.u.			
E (UωB97X-D/def2-tzvp) = -3031.84814093 a.u.			
C	-0.74744400	1.66820600	-0.02446200
C	-2.71222700	-0.12062900	0.68045600
C	-3.55188200	0.97873700	0.17694900
C	-3.14723200	2.25816400	0.16004300
H	-0.93647000	1.27160600	-1.03024600
H	-2.18845100	0.06630700	1.61847200
H	-4.55288800	0.74382400	-0.18054600
H	-3.81363700	3.04940900	-0.16892700
C	-1.73452400	2.64213300	0.54056100
C	-2.55726900	-1.33337300	0.10762200
O	0.28953200	1.34889600	0.57051600
C	-3.18588800	-1.70618700	-1.20578500
H	-2.39792100	-1.88621400	-1.94904300
H	-3.75368600	-2.64082400	-1.11445500
H	-3.84769500	-0.93039100	-1.59820000
C	-1.69725200	-2.38998600	0.74006100
H	-0.89603100	-2.69260900	0.05551000
H	-1.23568000	-2.04640500	1.66898300
H	-2.29139900	-3.28873400	0.95495000
Fe	1.64744200	-0.03106200	-0.02663800
Cl	0.63119200	-0.87293500	-1.80842100
Cl	1.79364900	-1.41823700	1.65736400
Cl	3.44639300	1.11657600	-0.48997300
H	-1.47922700	3.61742200	0.09587900
H	-1.56533000	2.73879200	1.62091800
M3-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.137822a.u.			
E (UωB97X-D/def2-tzvp) = -3031.78978596 a.u.			
C	1.00126700	1.28622400	0.19707200
C	2.87940200	-0.38701800	-0.91742700
C	3.75965300	0.75439500	-0.62575000
C	3.46489200	1.76668800	0.20290900
H	0.94957500	1.40983700	-0.89073200
H	2.65339100	-0.55038700	-1.97164300
H	4.70129500	0.79742600	-1.17339700
H	4.18412600	2.56651400	0.35667400
C	2.15322600	1.89134600	0.93599200
C	2.37703000	-1.27687100	-0.02987600
O	0.04406600	0.77889900	0.80235500
Fe	-1.64848400	0.04292800	-0.01798500
Cl	-3.12476700	1.62426900	0.30118100
Cl	-2.02406300	-1.83749800	1.04188400
Cl	-1.01008900	-0.16691800	-2.12482600
H	1.89334100	2.95819200	1.04241200
H	2.17375300	1.48218300	1.95399800
C	2.67336400	-1.25565100	1.44309800
H	2.93045200	-2.26342200	1.79013400
H	3.49265800	-0.57940800	1.69676700
H	1.77711300	-0.95557000	2.00570200
C	1.47842800	-2.39188100	-0.48861600
H	1.96080000	-3.36280100	-0.31158200
H	0.54351500	-2.40040600	0.08416800
H	1.22608500	-2.31037500	-1.54820600

M3-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.138522 a.u.			
E (UωB97X-D/def2-tzvp) = -3031.82998250 a.u.			
Imaginary frequency: 231.0452			
C	1.38369300	0.93015000	-0.56867100
C	2.56255400	-0.17239900	-0.55682500
C	3.61081700	0.46518600	0.32189000
C	3.34929100	1.75414500	0.55725000
H	0.97270900	0.99275400	-1.58146200
H	2.90779600	-0.33853700	-1.58472000
H	4.48384700	-0.07681200	0.67210800
H	3.99003200	2.41413900	1.13421500
C	2.08063900	2.22443400	-0.09942000
C	1.87709600	-1.37881400	-0.04894000
O	0.41031800	0.51958500	0.34361100
Fe	-1.38641900	0.16150200	0.08298700
Cl	-2.67504000	1.86373000	0.62663600
Cl	-1.72630600	-1.74047900	1.25013300
Cl	-1.42342300	-0.32191600	-2.13890500
H	2.29623100	2.89713600	-0.94050000
H	1.40679500	2.75439900	0.58372900
C	1.79398000	-1.67131100	1.38115100
H	2.27718500	-2.64510100	1.56267300
H	2.23140900	-0.89748500	2.00901700
H	0.72662300	-1.82562200	1.62516300
C	1.23715400	-2.28757300	-1.00152800
H	0.84779700	-3.19791500	-0.54486400
H	0.37649800	-1.73567300	-1.44503600
H	1.89714400	-2.50261100	-1.85000700
M3-TS1 (optimized at the B3LYP-D3BJ/def2-TZVP level)			
Imaginary frequency: 256.8175			
C	1.39366000	0.91863300	-0.57888300
C	2.56997900	-0.17845000	-0.56180400
C	3.61227700	0.46127000	0.31412300
C	3.35262100	1.74488700	0.54156400
H	0.99255900	0.98607500	-1.59214100
H	2.92072500	-0.34748200	-1.58280200
H	4.48201200	-0.07405400	0.67099800
H	3.99099400	2.40269700	1.11653600
C	2.08668700	2.21039800	-0.11151100
C	1.87718100	-1.37634700	-0.05851600
O	0.42359300	0.50094400	0.32690400
Fe	-1.39649800	0.15675900	0.08296700
Cl	-2.62717500	1.89338500	0.58459900
Cl	-1.74710000	-1.68230500	1.30043400
Cl	-1.46369000	-0.37710700	-2.10352900
H	2.29876800	2.88337100	-0.94778000
H	1.41725700	2.73620200	0.57286500
C	1.81640500	-1.68526200	1.36289500
H	2.38878500	-2.61212200	1.51829400
H	2.20331100	-0.89336700	1.99450300
H	0.77702000	-1.93278900	1.61802600
C	1.22951600	-2.26987300	-1.00571800
H	0.87627700	-3.19583600	-0.56080600
H	0.33905200	-1.72445200	-1.39070700
H	1.84889500	-2.44060500	-1.88783200

M3-INT			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.143474 a.u.			
E (UωB97X-D/def2-tzvp) = -3031.86333437 a.u.			
C	1.51961000	0.70981200	-0.83649100
C	2.58013300	-0.40670800	-0.70896400
C	3.61166200	0.20420000	0.20111300
C	3.31593500	1.46827900	0.52229200
H	1.04158700	0.87109000	-1.80301200
H	2.98489200	-0.83522300	-1.63031800
H	4.48053600	-0.34414400	0.55035600
H	3.91412500	2.10049900	1.17105200
C	2.04521300	1.96018000	-0.13381500
C	1.48161100	-1.29299000	-0.04147500
O	0.60000200	-0.06538000	0.02454200
Fe	-1.37459200	0.15953800	0.06979900
Cl	-1.64272600	2.13491100	0.99121000
Cl	-2.10393500	-1.56444600	1.22126200
Cl	-1.85792600	0.13234900	-2.08314100
H	2.24064500	2.76453900	-0.85528000
H	1.30421100	2.34512000	0.57675800
C	1.70950900	-1.80995300	1.35937700
H	2.40854300	-2.65334000	1.33152200
H	2.12306900	-1.02909500	2.00119600
H	0.76308000	-2.15835600	1.78385500
C	0.86856900	-2.31564000	-0.97906100
H	-0.04886100	-2.73024600	-0.55162200
H	0.63049800	-1.87304700	-1.95059800
H	1.58157200	-3.13367900	-1.13149700
M3-TS2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.137626 a.u.			
E (UωB97X-D/def2-tzvp) = -3031.80817612 a.u.			
Imaginary frequency: 264.7744			
C	1.78797000	-0.63323900	1.10295000
C	2.54282000	0.44650800	0.44541400
C	3.31530600	-0.28358400	-0.62680700
C	2.98189800	-1.57982800	-0.65814700
H	1.13033200	-0.50365000	1.95905300
H	3.15998100	1.01944700	1.15149800
H	4.01431700	0.21387500	-1.28712500
H	3.34818900	-2.32873000	-1.34919200
C	1.94094100	-1.86838800	0.39095800
C	1.37950500	1.43280500	-0.08867600
O	0.35763100	0.56426800	-0.50497500
Fe	-1.30447000	-0.08258600	-0.12292500
Cl	-1.07794600	-2.24833000	-0.85963200
Cl	-2.95139500	1.07610300	-1.00065000
Cl	-1.39316900	-0.22041800	2.14105300
H	2.01512600	-2.76888300	1.01559500
H	0.89941900	-2.02591600	-0.07805000
C	1.86657400	2.23497700	-1.29326000
H	2.73656600	2.85344600	-1.04550200
H	2.11471300	1.56861200	-2.12207900
H	1.05140300	2.89052700	-1.61662800
C	0.91866500	2.35327100	1.04342100
H	0.08422500	2.95967600	0.67724800
H	0.55557000	1.79033000	1.90643400

H	1.72592900	3.02418600	1.35637800
M3-P G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.131215 a.u. E (UωB97X-D/def2-tzvp) = -3031.81350698 a.u.			
C	2.34246700	-0.72927800	1.13217200
C	3.34384600	0.17033600	1.00653900
C	4.07974900	-0.09265500	-0.23954800
C	3.52098300	-1.14758700	-0.87101200
H	1.62701300	-0.80784600	1.94076100
H	3.59496500	0.95449400	1.71416200
H	4.93789500	0.47894500	-0.57804300
H	3.83911800	-1.58875100	-1.80821400
C	2.36818800	-1.66052000	-0.04961000
C	0.72672100	1.68607400	-0.47992100
O	0.12843700	0.64439800	-0.80106000
Fe	-1.48869300	-0.27306600	-0.03494800
Cl	-1.52744700	-2.19090700	-1.08767000
Cl	-3.07042000	1.17287300	-0.52855500
Cl	-1.17726000	-0.45528400	2.14237500
H	2.52909400	-2.70168500	0.26968300
H	1.42103400	-1.66887600	-0.60680400
C	1.82722800	2.18103300	-1.36044300
H	2.67475500	2.51676400	-0.75721200
H	2.14180900	1.40837000	-2.06113800
H	1.44729900	3.05492900	-1.90945900
C	0.30872700	2.48425400	0.71522600
H	-0.73768700	2.78796000	0.58165500
H	0.33698500	1.84251500	1.60216000
H	0.93594600	3.36419000	0.86463700
M4-S G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.144168 a.u. E (UωB97X-D/def2-tzvp) = -387.282487221 a.u.			
C	-2.98387300	0.44628300	-0.20274100
C	0.69868200	0.36656800	0.26029600
C	-0.26573100	-0.66615700	0.80343000
C	-1.09900400	-1.19754000	-0.33242500
H	0.23033400	1.32368300	0.03984300
H	0.26576500	-1.49567200	1.27912900
H	-0.67442300	-2.04695900	-0.86764300
C	-2.27211800	-0.70577400	-0.77822900
C	2.00391000	0.21106700	-0.00259100
O	-2.54527800	1.21627200	0.63819900
C	2.78251500	-1.06118200	0.21580100
H	2.18189600	-1.87121200	0.63650200
H	3.20860300	-1.41775800	-0.73219100
H	3.63205700	-0.88543900	0.88981500
C	2.81605100	1.35554600	-0.55719800
H	3.26601000	1.08778200	-1.52357000
H	2.20790500	2.25358900	-0.70091900
H	3.64828900	1.60964100	0.11398700
H	-0.90924900	-0.18709300	1.54462100
H	-2.76706400	-1.18852800	-1.61888900
H	-4.01048500	0.59491100	-0.60434500
M4-FeCl₃/S G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.134270 a.u. E (UωB97X-D/def2-tzvp) = -3031.84788412 a.u.			

C	0.08034200	2.02302400	-0.49539900
C	-2.57744800	-0.21068600	0.29692800
C	-2.37233600	1.04424500	1.13344600
C	-2.30226100	2.17906700	0.16069500
H	-1.66015800	-0.65904600	-0.07352000
H	-3.20283200	1.20617100	1.82498200
H	-3.24903500	2.67643700	-0.04789000
C	-1.22261900	2.61543800	-0.54693800
C	-3.75296300	-0.76044600	-0.04613400
O	0.35785700	1.02013900	0.20242800
C	-5.10295500	-0.22602200	0.35406100
H	-5.04987600	0.66178200	0.98966200
H	-5.69046500	0.03302700	-0.53693000
H	-5.67668900	-0.99269000	0.89101800
C	-3.78295100	-2.01510900	-0.88182800
H	-4.34419200	-1.85047300	-1.81185600
H	-2.77636500	-2.35477600	-1.14065700
H	-4.29425900	-2.82683900	-0.34726500
H	-1.44785300	0.95177400	1.70545800
H	-1.33751200	3.43951000	-1.24479500
Fe	1.85319400	-0.28914300	0.04777500
Cl	3.18183400	0.75098700	-1.37461500
Cl	2.65629900	-0.55226200	2.06370700
Cl	0.80950700	-2.03826200	-0.79448900
H	0.87260800	2.44678900	-1.12700600
M4-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.136421 a.u.			
E (UωB97X-D/def2-tzvp) = -3031.84501449 a.u.			
C	-2.53838600	-2.12336100	0.06850400
C	-1.31446500	-1.93702800	-0.45499100
C	-0.95541000	-0.84216000	-1.34948300
C	-3.38546300	0.18179600	-0.60452800
H	-2.69374400	-3.00947100	0.68215500
H	-0.49789800	-2.59722700	-0.17581300
H	-1.62655000	-0.58810700	-2.17381100
H	-3.74741400	0.36604100	-1.61461000
C	-3.70539100	-1.16997800	-0.00930300
C	-2.67720000	1.15232100	0.00732200
O	0.14508200	-0.25523000	-1.33921600
Fe	1.59998800	0.02276400	0.01077600
Cl	1.49518000	2.19551000	0.36279500
Cl	3.41513600	-0.69946300	-0.97307100
Cl	1.05835100	-1.13060000	1.81157000
H	-4.51079600	-1.65403400	-0.58068600
H	-4.10565600	-1.07167600	1.00924200
C	-2.13723600	1.03418000	1.40677700
H	-2.23869200	0.03319600	1.82977100
H	-1.07589300	1.30481400	1.43333400
H	-2.65512600	1.74308500	2.06715500
C	-2.34360000	2.43543400	-0.70372300
H	-2.66931800	3.30382100	-0.11693100
H	-1.25554300	2.52805600	-0.81881200
H	-2.80813800	2.49166800	-1.69286800
M4-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.138201 a.u.			
E (UωB97X-D/def2-tzvp) = -3031.82935638 a.u.			

Imaginary frequency: 316.4165			
C	-2.79129600	-1.91339700	0.26107100
C	-1.60418000	-1.91579000	-0.34052500
C	-1.36119300	-0.71397700	-1.22018100
C	-2.64585200	0.23703700	-0.83766700
H	-3.16799000	-2.70497200	0.90082200
H	-0.84583900	-2.68709700	-0.26440000
H	-1.46722300	-0.97728400	-2.28420000
H	-3.07287900	0.63245500	-1.76066100
C	-3.61132100	-0.68443500	-0.04980300
C	-1.98785900	1.30835100	-0.08465100
O	-0.17268300	-0.03144900	-1.04155500
Fe	1.37217900	-0.10024200	-0.02682600
Cl	1.69505300	2.10487300	0.44659300
Cl	3.02845700	-1.03368200	-1.14826300
Cl	0.88787500	-1.20317600	1.86242700
H	-4.47947700	-0.92338700	-0.67726600
H	-4.01274100	-0.20760900	0.85293900
C	-1.73032400	1.17319200	1.35765000
H	-1.54505100	0.13330200	1.64290700
H	-0.90421400	1.81106100	1.68033500
H	-2.64984000	1.49860300	1.87474100
C	-1.52203300	2.51710000	-0.75416600
H	-1.74082200	3.40749400	-0.15058600
H	-0.41091200	2.44357200	-0.72603000
H	-1.86738500	2.62700400	-1.78193000
M4-TS1 (optimized at the B3LYP-D3BJ/def2-TZVP level)			
Imaginary frequency: 351.7391			
C	-2.77902500	-1.92737200	0.25963700
C	-1.60929000	-1.92279400	-0.35887000
C	-1.36972000	-0.70898200	-1.21468800
C	-2.65427200	0.22795700	-0.81583300
H	-3.14308900	-2.72479400	0.89308200
H	-0.85558600	-2.69580200	-0.30691600
H	-1.46988100	-0.95896000	-2.27948800
H	-3.09748600	0.61444200	-1.73034300
C	-3.59715800	-0.69417100	-0.01349900
C	-1.98935500	1.30206800	-0.08327200
O	-0.19137900	-0.02531700	-1.01358600
Fe	1.38245200	-0.09487300	-0.01626000
Cl	1.72929200	2.09692000	0.37565600
Cl	2.97523600	-1.08644600	-1.14611500
Cl	0.90920800	-1.13956200	1.88853400
H	-4.48132600	-0.92278900	-0.61441300
H	-3.96792700	-0.22969900	0.90347000
C	-1.72936300	1.18853600	1.35199400
H	-1.58081800	0.15654300	1.66663900
H	-0.89117300	1.81140800	1.65944100
H	-2.63574500	1.56010900	1.85492100
C	-1.54259700	2.50406200	-0.76373400
H	-1.77028200	3.39246700	-0.16704100
H	-0.43482100	2.44611400	-0.73910400
H	-1.89342900	2.59886900	-1.78647800
M4-INT			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.142709 a.u.			
E (UωB97X-D/def2-tzvp) = -3031.86371948 a.u.			

C	-2.81499400	-1.70900000	0.48760700
C	-1.70645900	-1.83400100	-0.25051800
C	-1.50471900	-0.63341700	-1.11593600
C	-2.62655800	0.35130200	-0.72233500
H	-3.17391500	-2.45477700	1.19064100
H	-1.02034100	-2.67286900	-0.24758600
H	-1.27651100	-0.82990200	-2.16454100
H	-3.15845500	0.81870500	-1.55220900
C	-3.55494900	-0.41391200	0.24171400
C	-1.52383000	1.28390600	-0.13490500
O	-0.47211700	0.30951400	-0.60134800
Fe	1.35681200	-0.12617400	0.03547900
Cl	2.30346200	1.85006400	0.22751600
Cl	2.00093700	-1.44358400	-1.60383100
Cl	1.13876000	-1.18851300	1.95054100
H	-4.53415300	-0.59875600	-0.21860300
H	-3.75253600	0.13226500	1.17151200
C	-1.45006600	1.44877000	1.36942300
H	-1.49728600	0.48662700	1.88307800
H	-0.50921800	1.93684800	1.64207700
H	-2.27416200	2.08365000	1.71235000
C	-1.32133400	2.58368200	-0.88752700
H	-2.11905900	3.28812900	-0.62552100
H	-0.35793000	3.02823800	-0.62126700
H	-1.34284900	2.41682600	-1.96859200
M4-TS2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.142972 a.u.			
E (UωB97X-D/def2-tzvp) = -3031.83643352 a.u.			
Imaginary frequency: 172.4955			
C	-1.85041000	-1.93267000	0.72324900
C	-1.55075400	-1.99766400	-0.62915500
C	-1.90948300	-0.79327100	-1.22003800
C	-2.53452100	0.16117300	-0.23342300
H	-1.71670200	-2.74856500	1.42313200
H	-1.02741800	-2.80559000	-1.12269300
H	-1.83475500	-0.58655700	-2.28053000
H	-3.53559600	0.48361100	-0.54148400
C	-2.59032300	-0.67992800	1.06606500
C	-1.52213800	1.35423900	-0.29274300
O	-0.34495700	0.70005600	-0.78687300
Fe	1.21106900	0.01927800	-0.06356400
Cl	2.59867900	1.61931400	0.54473600
Cl	1.92355500	-1.45940500	-1.56115300
Cl	0.53693700	-1.16847300	1.81191500
H	-3.62502400	-0.94020800	1.33349200
H	-2.15993700	-0.18984500	1.93972000
C	-1.25775400	2.06762600	1.03006700
H	-0.80961900	1.39759100	1.76774900
H	-0.55392000	2.88761400	0.86000100
H	-2.18435200	2.48458200	1.44135900
C	-1.96542700	2.35794300	-1.36202100
H	-2.86266900	2.89972700	-1.04196500
H	-1.16053600	3.07804400	-1.53347700
H	-2.17865000	1.85882200	-2.31313400
M4-INT2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.144614 a.u.			

$E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -3031.84545224 \text{ a.u.}$			
C	-1.38736300	-2.04345200	0.56760000
C	-2.14123400	-1.98698700	-0.70768400
C	-2.70746100	-0.78611900	-0.87381500
C	-2.40305900	0.17749900	0.24753200
H	-1.50327200	-2.94956600	1.15987600
H	-2.19383300	-2.82499100	-1.39301800
H	-3.32080800	-0.51408800	-1.72599600
H	-3.33346100	0.59422300	0.65511700
C	-1.72385500	-0.74000400	1.30227300
C	-1.54468300	1.39785800	-0.21329600
O	-0.30374900	0.90382100	-0.68001200
Fe	1.24163400	0.21347100	-0.12602500
Cl	1.82681700	0.71208400	1.94473800
Cl	2.82113300	0.08935200	-1.64054600
Cl	0.48958600	-2.19749400	0.17672300
H	-2.44085100	-0.98856300	2.09201800
H	-0.85541500	-0.29864000	1.79371400
C	-1.32069000	2.37367000	0.94947700
H	-0.81510200	1.89541900	1.79107600
H	-0.69193500	3.20317800	0.61204600
H	-2.27712300	2.78215100	1.29393500
C	-2.21279000	2.12627000	-1.38756700
H	-3.22601200	2.45063300	-1.12424600
H	-1.62444300	3.00946600	-1.65256600
H	-2.26153800	1.48054200	-2.26787700
M4-TS3 $G_{\text{corr}}(\text{UB3LYP-D3BJ/6-31G}^*/\text{Lan2LDZ}) = 0.139561 \text{ a.u.}$ $E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -3031.81060059 \text{ a.u.}$ Imaginary frequency: 547.2394			
C	-1.36870200	-2.05322400	0.62501800
C	-2.16040500	-2.03066800	-0.64097300
C	-2.83798900	-0.86493200	-0.76495800
C	-2.54443100	0.04218600	0.32449100
H	-1.52728600	-2.94193900	1.23653100
H	-2.16887400	-2.85914400	-1.33914800
H	-3.50011900	-0.62246000	-1.58834900
H	-3.30504700	0.73443100	0.67598100
C	-1.73082900	-0.73562600	1.34396900
C	-1.36530700	1.56541300	-0.45538700
O	-0.28730500	0.93165500	-0.76762000
Fe	1.38457800	0.26671500	-0.08491600
Cl	1.62928000	0.88243500	2.05392500
Cl	2.88497900	-0.15003200	-1.64914700
Cl	0.44620100	-2.20075300	0.23280100
H	-2.35637100	-0.96531200	2.21572900
H	-0.85086500	-0.20967700	1.72485300
C	-1.32564900	2.49354400	0.74645200
H	-0.83073200	2.03109200	1.60160700
H	-0.72739700	3.37073000	0.46555100
H	-2.32483100	2.84019300	1.02442500
C	-2.20694400	2.03252300	-1.63104600
H	-3.24110100	2.24307700	-1.34226600
H	-1.77004500	2.96352100	-2.01547600
H	-2.18419100	1.29430400	-2.43489800
M4-P			

G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.133084 a.u.			
E (UωB97X-D/def2-tzvp) = -3031.85996888 a.u.			
C	-1.69394200	-1.86489900	0.23827600
C	-2.05759500	-1.48726200	-1.00985300
C	-3.11859200	-0.48090200	-0.91739400
C	-3.39002200	-0.23037700	0.38437500
H	-0.93974300	-2.59463900	0.50079400
H	-1.62857800	-1.85144600	-1.93558400
H	-3.60151100	-0.02135500	-1.77352400
H	-4.14185300	0.44700200	0.77358300
C	-2.52126000	-1.11117300	1.24377200
C	-0.90004100	1.88974500	-0.29068100
O	-0.28590300	0.91215600	-0.74313700
Fe	1.22963900	-0.21663000	-0.04581500
Cl	0.96820300	-0.73065300	2.09535200
Cl	2.78563500	1.35102600	-0.21281100
Cl	1.56758800	-1.91173200	-1.39366000
H	-3.12737300	-1.79123600	1.86160500
H	-1.89145700	-0.55263100	1.94925200
C	-0.66149000	2.38724600	1.10162000
H	-0.50463100	1.55272200	1.78950700
H	0.27612700	2.96149700	1.08436900
H	-1.46616200	3.03763600	1.45015200
C	-1.82129600	2.65191500	-1.19363300
H	-2.81463800	2.72432500	-0.74052700
H	-1.43735700	3.67544800	-1.30140200
H	-1.88501800	2.17515100	-2.17180300
M5-S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.168743 a.u.			
E (UωB97X-D/def2-tzvp) = -968.689373262 a.u.			
C	-0.96099300	-0.72700900	1.17176300
C	1.73773100	0.06424300	-0.01696600
C	0.92368200	1.24942600	-0.21768700
C	-0.42611100	1.31703100	-0.21765100
H	-0.44103200	-0.20654900	2.00431000
H	1.20936600	-0.88171400	0.07336200
H	1.44913100	2.18135800	-0.41148600
H	-0.87080600	2.28310700	-0.45002800
C	-1.38359000	0.17291300	0.03702700
C	3.08632700	0.01126300	0.04312400
O	-1.17786200	-1.92265600	1.22162900
C	4.00107600	1.20246200	-0.05684100
H	4.62284500	1.28189900	0.84534400
H	4.69402000	1.08396400	-0.90100100
H	3.47429800	2.15004200	-0.18337600
C	3.78909800	-1.30780400	0.22600000
H	4.40521300	-1.30160300	1.13610700
H	3.08414700	-2.14130200	0.29554600
H	4.47446600	-1.50601400	-0.61008600
Si	-1.63190300	-0.86184800	-1.54724300
H	-1.89488800	0.08303300	-2.65500900
H	-0.39209300	-1.61136000	-1.83096900
H	-2.77712800	-1.78855200	-1.44265700
Si	-3.06441000	0.90086800	0.57661300
H	-3.51308000	1.84440800	-0.46994200
H	-4.06217800	-0.17110900	0.75543700

H	-2.89432400	1.64021900	1.84761500
M5-FeCl₃/S G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.159435 a.u. E (UωB97X-D/def2-tzvp) = -3613.25184093 a.u.			
C	0.70600600	-0.88544700	-0.48372100
C	1.90335400	1.64916000	0.23689000
C	3.04171800	0.89724100	-0.26409000
C	3.12917300	-0.44807600	-0.36974800
H	0.68540500	-0.22489200	-1.36142100
H	1.17259700	1.09809900	0.82691500
H	3.91668700	1.46373500	-0.57355100
H	4.06970300	-0.88307100	-0.69776500
C	2.00244900	-1.40562400	-0.03898000
C	1.65908500	2.96574800	0.05670700
O	-0.37012700	-1.16087400	0.08380500
C	2.53585200	3.88924000	-0.74386700
H	1.97864000	4.27755000	-1.60695000
H	2.82381300	4.76071400	-0.14176300
H	3.44530700	3.41634500	-1.12028400
C	0.42134700	3.59724400	0.63135600
H	-0.22106600	3.97643600	-0.17440500
H	-0.16804000	2.89212800	1.22216300
H	0.68027000	4.45780600	1.26299300
Si	2.00044600	-1.85533400	1.82839900
H	3.37994500	-2.26488400	2.15691300
H	1.62612700	-0.64518700	2.58160200
H	1.07184900	-2.96437500	2.11738200
Si	2.26238600	-3.02432700	-1.05674400
H	3.59924300	-3.52566100	-0.68474400
H	1.21134500	-3.99830200	-0.71559700
H	2.22496400	-2.69625700	-2.49600300
Fe	-2.08868700	-0.12067800	-0.05629800
Cl	-1.60297000	1.27647200	-1.69984500
Cl	-2.14820400	0.86538400	1.90679800
Cl	-3.67844100	-1.55110500	-0.48652000
M5-RS G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.162083 a.u. E (UωB97X-D/def2-tzvp) = -3613.24878850 a.u.			
C	-0.91708200	-0.41204500	-0.38797500
C	-1.78688400	2.22440600	-0.99433000
C	-3.08919400	1.55211100	-0.80802100
C	-3.32186100	0.29737600	-0.39203900
H	-0.72220900	-0.04935100	-1.40248300
H	-1.52990300	2.44480400	-2.03209900
H	-3.96729700	2.13399000	-1.09369900
H	-4.35494600	-0.03717600	-0.31928800
C	-2.29161500	-0.73272400	0.02196100
C	-0.93805100	2.65684900	-0.04044200
O	0.05311300	-0.64280400	0.36330700
Fe	2.00526900	-0.37850000	-0.01930400
Cl	2.87408300	-2.38180100	0.05996800
Cl	2.66243300	1.01783800	1.54302800
Cl	1.91144700	0.48951600	-2.05038400
C	-1.17456900	2.48096100	1.43290600
H	-0.43312600	1.79166700	1.85790600
H	-1.04270700	3.43700700	1.95472800

H	-2.17430000	2.09980000	1.65216300
C	0.33008200	3.37839600	-0.41059000
H	1.20183800	2.89617200	0.04487100
H	0.48375400	3.41284800	-1.49202700
H	0.30233700	4.40717900	-0.02617400
Si	-2.70858300	-2.32576200	-1.00523900
H	-4.08667800	-2.69668600	-0.63070500
H	-2.63315500	-1.99152200	-2.44072400
H	-1.76204200	-3.40414300	-0.66818200
Si	-2.42355300	-1.19598600	1.88060500
H	-3.86548700	-1.38472200	2.14292600
H	-1.71234300	-2.46180600	2.14136600
H	-1.89604400	-0.11652900	2.72851100
M5-RS (quartet) G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.159733 a.u. E (UωB97X-D/def2-tzvp) = -3613.19674019 a.u.			
C	0.83097900	-0.37595000	0.22514000
C	1.55968300	2.18763100	1.29657600
C	2.88189300	1.53485300	1.21803300
C	3.19692100	0.34928400	0.67117400
H	0.50225400	-0.15051100	1.24696300
H	1.16538500	2.30177600	2.30807300
H	3.69737400	2.06459100	1.71386400
H	4.23697700	0.03063500	0.71155700
C	2.26467000	-0.62399800	-0.01743700
C	0.83801900	2.71284600	0.28741700
O	-0.01970500	-0.51643200	-0.66911800
Fe	-2.05131400	-0.53353300	-0.22331800
Cl	-2.17032400	-2.63026400	0.29500800
Cl	-2.70937100	1.00181600	-1.59776400
Cl	-2.27025700	0.41310000	1.75479600
C	1.27259400	2.69585900	-1.15097800
H	0.61446700	2.04473100	-1.74132000
H	1.18844400	3.70034800	-1.58453400
H	2.30204200	2.35162600	-1.27101600
C	-0.48439000	3.38140600	0.55218200
H	-1.28174600	2.91216800	-0.03564300
H	-0.76554600	3.33335200	1.60731300
H	-0.44452300	4.43606900	0.24748600
Si	2.56265400	-2.33342800	0.84934400
H	3.99614000	-2.63754500	0.67191100
H	2.24059300	-2.19454000	2.28315400
H	1.72496500	-3.37277700	0.22509600
Si	2.67104700	-0.85013900	-1.87702900
H	4.13993000	-1.00074400	-1.95258200
H	2.03631800	-2.07694500	-2.39610600
H	2.25389200	0.32036700	-2.66473500
M5-TS1 G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.163377 a.u. E (UωB97X-D/def2-tzvp) = -3613.23132214 a.u. Imaginary frequency: 246.9550			
C	-1.12346000	0.32347700	-0.38541600
C	-1.49087000	1.90155200	-0.28679100
C	-2.61092600	1.92994800	0.71515400
C	-3.09703000	0.70201000	0.93930700
H	-0.89262600	0.08652800	-1.42937900

H	-1.79194200	2.23600400	-1.28878600
H	-2.98536600	2.84782100	1.15597800
H	-3.93807900	0.48650800	1.59236100
C	-2.39381900	-0.37612600	0.16240400
C	-0.19837700	2.49025200	0.07169800
O	-0.00946600	0.08271700	0.42267200
Fe	1.67443500	-0.55888100	-0.06341500
Cl	1.99825300	-2.61507100	0.65849100
Cl	3.12595400	0.92764200	0.84573500
Cl	1.63681600	-0.37489900	-2.30125500
C	0.18776100	2.73641300	1.46097900
H	1.12175900	2.17017200	1.63372000
H	0.47363400	3.79266900	1.57923500
H	-0.57984500	2.45668100	2.18048100
C	0.74178500	2.86045000	-1.00119300
H	1.78137900	2.79906700	-0.66836600
H	0.59382200	2.26543000	-1.90642500
H	0.52181600	3.91341700	-1.25187800
Si	-3.51756700	-0.96808300	-1.25173900
H	-4.85377700	-1.30787600	-0.72075400
H	-3.65511300	0.13678700	-2.23017400
H	-2.92755300	-2.14356800	-1.92451400
Si	-1.89951500	-1.85317000	1.27755200
H	-3.18685400	-2.50309300	1.63046600
H	-1.07722100	-2.81024600	0.52289400
H	-1.25222600	-1.40787800	2.52381300
M5-TS1 (optimized at the B3LYP-D3BJ/def2-TZVP level)			
Imaginary frequency: 275.1038			
C	-1.13795500	0.32914600	-0.38571200
C	-1.52074800	1.89329100	-0.26456100
C	-2.62088000	1.89779000	0.75279700
C	-3.09180200	0.66838300	0.96363400
H	-0.92061000	0.09999300	-1.43156500
H	-1.84540500	2.23700500	-1.25186100
H	-2.99656800	2.80028700	1.21428300
H	-3.91755000	0.43899100	1.62515900
C	-2.39255600	-0.38652100	0.16450700
C	-0.22748700	2.48363100	0.06676900
O	-0.01519600	0.10441100	0.40863700
Fe	1.69074500	-0.54581900	-0.06534700
Cl	2.02182200	-2.56397400	0.70898800
Cl	3.11620800	0.94713000	0.81401300
Cl	1.65608100	-0.41300900	-2.28546300
C	0.17447500	2.76637500	1.43684900
H	1.13201100	2.24945500	1.60409300
H	0.41418700	3.83419000	1.52321800
H	-0.56601100	2.47692800	2.17451900
C	0.68482900	2.84022500	-1.02375000
H	1.72820200	2.79517000	-0.71555000
H	0.51751200	2.24168400	-1.91787400
H	0.44886700	3.88585100	-1.27674400
Si	-3.52617200	-0.97124700	-1.24308900
H	-4.86248600	-1.30604900	-0.70451300
H	-3.66175900	0.13853500	-2.21928000
H	-2.93983600	-2.14924300	-1.91876400
Si	-1.87696600	-1.88590900	1.23685800

H	-3.15720300	-2.56316800	1.57357100
H	-1.04422700	-2.80434100	0.44386700
H	-1.23013800	-1.46552000	2.49326100
M5-INT			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.168648 a.u.			
E (UωB97X-D/def2-tzvp) = -3613.25676404 a.u.			
C	-1.15977300	0.38688900	-0.66122200
C	-1.39033200	1.91686600	-0.69881500
C	-2.65047600	2.12185200	0.08747000
C	-3.15796900	0.95981200	0.51264200
H	-0.85900900	-0.10465000	-1.58783700
H	-1.39329300	2.39080900	-1.68444700
H	-3.07571200	3.10040200	0.28172800
H	-4.06329000	0.85616300	1.10326300
C	-2.35792200	-0.25446400	0.06924600
C	-0.03332400	2.09511400	0.04880600
O	0.06742700	0.57904100	0.15557900
Fe	1.72911800	-0.53056000	-0.04888600
Cl	1.23438200	-2.54765600	0.64070800
Cl	3.23720700	0.50922900	1.16560200
Cl	2.04595700	-0.50368100	-2.23475500
C	-0.04378200	2.65949200	1.45044400
H	0.91574000	2.45313800	1.93463900
H	-0.18564500	3.74519900	1.41145300
H	-0.84764400	2.22145900	2.04547000
C	1.06848000	2.66105000	-0.82398200
H	2.04558000	2.55613200	-0.34539200
H	1.09951800	2.16758800	-1.79859700
H	0.87125900	3.72817900	-0.97828600
Si	-3.38216200	-1.25361000	-1.18916500
H	-4.64330100	-1.69160100	-0.55516500
H	-3.69177400	-0.38492500	-2.34715500
H	-2.61108600	-2.42761300	-1.64767000
Si	-2.01399800	-1.36127100	1.58877700
H	-3.30186900	-1.39164200	2.31970700
H	-1.67356500	-2.73742100	1.19249300
H	-0.98388200	-0.77449400	2.46364300
M5-TS2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.165363 a.u.			
E (UωB97X-D/def2-tzvp) = -3613.23110756 a.u.			
Imaginary frequency: 110.9123			
C	1.71810300	0.57896600	0.75800300
C	1.47582900	1.92463000	0.23802900
C	2.41156000	2.03396300	-0.92686000
C	3.06579900	0.87492600	-1.10935600
H	1.19211400	0.14497200	1.60546900
H	1.60547300	2.70600600	0.99628200
H	2.51192400	2.92665600	-1.53086600
H	3.78532300	0.64327400	-1.88588600
C	2.62278200	-0.12514500	-0.07338700
C	-0.15235800	2.00622200	-0.11170600
O	-0.54135300	0.77182700	-0.60362500
Fe	-1.79621000	-0.45549900	-0.00975500
Cl	-1.79743100	-2.16024900	-1.45248100
Cl	-3.79408400	0.47693700	0.24280600
Cl	-0.92882200	-1.15286100	1.99525800

C	-0.35225200	3.06697200	-1.19559100
H	-1.42991200	3.18068700	-1.35238100
H	0.06449400	4.03815700	-0.90588100
H	0.09601600	2.73935800	-2.13622900
C	-0.86683500	2.39595300	1.18646900
H	-1.94375400	2.41590800	0.99627500
H	-0.69011500	1.66544000	1.98068400
H	-0.55039500	3.38777000	1.52748200
Si	4.01723400	-0.99295300	0.93695700
H	5.00271500	-1.45886200	-0.05379800
H	4.62543500	0.00128400	1.84113200
H	3.43451900	-2.11162900	1.69731900
Si	1.69203000	-1.65327600	-0.95299400
H	2.82816500	-2.46447900	-1.44277500
H	0.93753400	-2.35534000	0.08398400
H	0.94303100	-1.06762900	-2.06218000
M5-P			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.158943 a.u.			
E (UωB97X-D/def2-tzvp) = -3613.27418319 a.u.			
C	1.97211900	0.31577200	0.89686600
C	2.33663200	1.61728700	1.08925100
C	3.45804100	1.93235000	0.22728400
C	3.79408700	0.82117300	-0.49115000
H	1.17421900	-0.21992800	1.39639800
H	1.88237900	2.30592300	1.79335900
H	3.95831600	2.89384200	0.18364500
H	4.59917000	0.72929200	-1.21096000
C	2.89420000	-0.30498700	-0.10062100
C	-0.50047600	1.89179400	-0.70020800
O	-0.89219900	0.72750300	-0.90087400
Fe	-2.17489900	-0.45191300	0.10316600
Cl	-2.18706000	-2.33841000	-0.99446000
Cl	-4.02087600	0.74209700	-0.00282600
Cl	-1.38506600	-0.60199100	2.16325900
C	0.36374600	2.54741800	-1.72671800
H	0.08399600	3.59889000	-1.84898200
H	1.39876400	2.51944400	-1.35757500
H	0.31271800	2.01356600	-2.67599300
C	-0.91631400	2.65341100	0.51776000
H	-1.96707100	2.94560300	0.37829700
H	-0.88140700	2.00915100	1.40051900
H	-0.31081200	3.54901000	0.66512700
Si	3.96107400	-1.56211700	0.86068500
H	5.00549800	-2.11140000	-0.03168200
H	4.58778700	-0.86966800	2.00374500
H	3.11424700	-2.67578000	1.33932300
Si	2.03377500	-1.15831300	-1.55875900
H	3.05336200	-1.86916000	-2.36201900
H	1.03821000	-2.12154200	-1.05414900
H	1.37656400	-0.15566000	-2.41765100
M5-S (optimized with SMD (dichloroethane))			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.168307 a.u.			
E (UωB97X-D/def2-tzvp) = -968.689366759 a.u.			
C	-0.97172200	-0.74644200	1.15828100
C	1.74474000	0.05783100	-0.00962900
C	0.93018000	1.24371700	-0.20665400

C	-0.42026000	1.31449800	-0.20586700
H	-0.44416700	-0.25046700	1.99790100
H	1.21999000	-0.89053000	0.08498300
H	1.45535000	2.17678300	-0.39609800
H	-0.86321500	2.28249800	-0.43315600
C	-1.38194300	0.16989600	0.03821400
C	3.09533700	0.00782300	0.04652900
O	-1.21526100	-1.94165800	1.19590700
C	4.00909000	1.19842700	-0.05599800
H	4.63120200	1.27586600	0.84644100
H	4.70284300	1.07396700	-0.89891000
H	3.48490800	2.14747000	-0.18540800
C	3.80043900	-1.30917600	0.22871000
H	4.41661700	-1.29955600	1.13900600
H	3.09810800	-2.14578900	0.29689200
H	4.48820200	-1.50229100	-0.60682000
Si	-1.63813300	-0.83310200	-1.56207500
H	-1.88776000	0.12603900	-2.65935400
H	-0.40680400	-1.59469200	-1.85284200
H	-2.79057700	-1.75479600	-1.48137400
Si	-3.05988100	0.90225800	0.59293100
H	-3.52103900	1.83414900	-0.45668000
H	-4.04807500	-0.17665900	0.78550200
H	-2.87647200	1.64365000	1.85917300
M5-FeCl₃/S (optimized with SMD (dichloroethane))			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.160348 a.u.			
E (UωB97X-D/def2-tzvp) = -3613.25289596 a.u.			
C	0.40558700	-0.96372400	-0.45483200
C	2.46818100	1.11347800	0.07880600
C	3.24271800	-0.00948400	-0.41202900
C	2.85501100	-1.30600400	-0.45565200
H	0.52710000	-0.39011000	-1.38197500
H	1.52567700	0.88859400	0.57588400
H	4.25142800	0.19766500	-0.75981500
H	3.57834800	-2.04571800	-0.78829000
C	1.50019600	-1.81976900	-0.02036400
C	2.80459000	2.42219700	0.00674500
O	-0.68041700	-0.87747300	0.16949100
C	4.05034000	2.95496700	-0.64400200
H	3.78305400	3.63782400	-1.46196500
H	4.62874300	3.54797800	0.07728800
H	4.70256500	2.17971500	-1.05130000
C	1.89681000	3.47042500	0.58892700
H	1.57642400	4.17865200	-0.18778800
H	1.00361500	3.03499800	1.04707100
H	2.42503300	4.06250500	1.34922200
Si	1.48268100	-2.16334000	1.86860300
H	2.67947000	-2.97372900	2.15950400
H	1.55749300	-0.85803800	2.55048700
H	0.26902700	-2.89677400	2.27585300
Si	1.16480800	-3.49819700	-0.93787500
H	2.27774100	-4.38189400	-0.54734200
H	-0.13572700	-4.02893000	-0.49652800
H	1.17531200	-3.24995000	-2.39153900
Fe	-2.14867700	0.42295400	-0.05644100
Cl	-1.61636900	1.39927000	-1.97934100

Cl	-1.88905400	1.75499500	1.69612500
Cl	-3.96056600	-0.84784200	-0.07049100
M5-RS (optimized with SMD (dichloroethane))			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.161872 a.u.			
E (UωB97X-D/def2-tzvp) = -3613.24877905 a.u.			
C	0.89481400	-0.38342800	0.39907400
C	1.91769200	2.09411300	1.04662300
C	3.19421000	1.36115700	0.90657700
C	3.34595700	0.10075700	0.47250100
H	0.72180900	-0.07948800	1.43459100
H	1.56590900	2.22339700	2.07175400
H	4.09507100	1.88053300	1.23640900
H	4.34659600	-0.32371900	0.42947300
C	2.23416700	-0.80349300	-0.01580100
C	1.18258300	2.64829700	0.06055900
O	-0.09457100	-0.50342800	-0.36946500
Fe	-2.01064400	-0.28498300	0.01927000
Cl	-2.82699800	-2.32669500	-0.24099300
Cl	-2.78936200	1.16499900	-1.46112000
Cl	-1.99027700	0.42152000	2.12455200
C	1.55969300	2.60512800	-1.39266700
H	1.55428800	3.61954800	-1.81278900
H	2.54577100	2.16462500	-1.55725300
H	0.82053900	2.02805600	-1.96397800
C	-0.10171700	3.36635600	0.37237500
H	-0.94045700	2.91298600	-0.17037200
H	-0.33401600	3.35186700	1.44101300
H	-0.04516500	4.41185500	0.03946900
Si	2.46669500	-2.48994600	0.93479800
H	3.77957800	-3.00246300	0.50264900
H	2.45342200	-2.21213000	2.38295300
H	1.38177500	-3.41512100	0.56217400
Si	2.37171600	-1.19320500	-1.88946400
H	1.91548300	-0.05022000	-2.69484200
H	3.80039700	-1.46030000	-2.14607400
H	1.58298900	-2.39866600	-2.21208000
M5-TS1 (optimized with SMD (dichloroethane))			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.161924 a.u.			
E (UωB97X-D/def2-tzvp) = -3613.23136279 a.u.			
Imaginary frequency: 311.4400			
C	1.07413700	0.14868000	0.33465000
C	1.80605400	1.97512300	0.20366500
C	2.85249000	1.69626600	-0.81573200
C	3.16186400	0.40543200	-0.97041500
H	0.86257400	0.17414500	1.40606100
H	2.15375200	2.04818300	1.23659000
H	3.34119200	2.50537300	-1.35040800
H	3.94954500	0.04504600	-1.62633100
C	2.35085600	-0.56286600	-0.14289100
C	0.62229900	2.66162100	-0.07349200
O	0.01550500	-0.07680000	-0.42374500
Fe	-1.77847600	-0.42671700	0.04915800
Cl	-2.29246400	-2.46952100	-0.69228700
Cl	-3.13468400	1.11153000	-0.84689200
Cl	-1.82343100	-0.32818600	2.28197600
C	0.14359500	2.79154200	-1.46390800

H	-0.67080100	3.51157400	-1.56377100
H	0.95067500	3.00760100	-2.16909400
H	-0.25037700	1.79348100	-1.73333900
C	-0.26635200	3.11234000	1.02330400
H	-1.29499500	2.77632400	0.84172500
H	0.07442300	2.78786400	2.00854600
H	-0.30184900	4.21243500	1.00222800
Si	3.41690700	-1.11098900	1.34160500
H	4.71799300	-1.59074400	0.83685200
H	3.62738000	0.05066600	2.23259700
H	2.74381700	-2.19161500	2.09361700
Si	1.84875500	-2.08030800	-1.19333100
H	1.27830200	-1.67510300	-2.49155900
H	3.09609500	-2.83936700	-1.44248500
H	0.90953000	-2.93249100	-0.44383400
M5-INT' (optimized with SMD (dichloroethane)) G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.161526 a.u. E (UωB97X-D/def2-tzvp) = -3613.23663822 a.u.			
C	1.13223700	0.28036700	0.34653800
C	1.61103200	1.84017900	0.14205000
C	2.61861200	1.72571100	-0.96714200
C	3.05656700	0.46909800	-1.10243300
H	0.91151100	0.13906200	1.40863800
H	2.07040100	2.10339400	1.10478000
H	2.97466000	2.58574300	-1.52362400
H	3.84100600	0.15766500	-1.78594900
C	2.37647700	-0.49998500	-0.16646500
C	0.40627500	2.62825100	-0.03954200
O	0.02011900	-0.02086600	-0.42590600
Fe	-1.69416100	-0.48138700	0.04842400
Cl	-2.22806000	-2.48418600	-0.81891600
Cl	-3.11657000	1.09669100	-0.72766800
Cl	-1.73520700	-0.51684800	2.29800600
C	-0.06788000	2.93603400	-1.38693700
H	-0.99223600	3.51189300	-1.40612900
H	0.72186200	3.42648400	-1.97058700
H	-0.21626600	1.95686800	-1.87836400
C	-0.37887000	3.04019400	1.12508000
H	-1.44531900	2.84934200	0.94940200
H	-0.03536300	2.60430000	2.06393600
H	-0.28981700	4.14042600	1.18328700
Si	3.56832600	-0.93567800	1.24957200
H	4.85877400	-1.37895300	0.68461600
H	3.78943600	0.27019000	2.07929100
H	3.00541100	-2.00957300	2.09673400
Si	1.81524100	-2.08387300	-1.06694600
H	1.18181600	-1.79190300	-2.36628400
H	3.04581200	-2.87145100	-1.32430200
H	0.92613000	-2.88207100	-0.20504900
M5-TS2 (optimized with SMD (dichloroethane)) G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.162384 a.u. E (UωB97X-D/def2-tzvp) = -3613.23530890 a.u. Imaginary frequency: 121.6535			
C	1.17519000	0.35600700	0.43110700
C	1.60615700	1.87092700	0.27526700
C	2.67493700	1.82854300	-0.78216400

C	3.08863900	0.57468600	-1.00347800
H	0.94951300	0.11543400	1.47325400
H	1.97072000	2.25114000	1.23895500
H	3.06985600	2.72031400	-1.25615100
H	3.88521400	0.29717600	-1.68774900
C	2.36364600	-0.44636900	-0.15824200
C	0.31695000	2.52508600	-0.04858800
O	-0.00706700	0.20614700	-0.34664900
Fe	-1.66633000	-0.47341000	0.05238700
Cl	-2.06162700	-2.42671400	-0.98375700
Cl	-3.23522300	1.02266400	-0.60848600
Cl	-1.68745100	-0.70962600	2.29129700
C	-0.01395100	2.90043600	-1.42208400
H	-1.09180500	2.93499100	-1.59245200
H	0.37746500	3.92872300	-1.54210700
H	0.50542500	2.27736300	-2.15337300
C	-0.56625400	2.91297400	1.05405700
H	-1.62146500	2.86954800	0.77586900
H	-0.36076300	2.37100600	1.97966700
H	-0.32490900	3.97787200	1.23634700
Si	3.52567800	-1.03904000	1.22622700
H	4.80613600	-1.48959900	0.64388700
H	3.78085200	0.09014200	2.14855100
H	2.90836500	-2.15105300	1.98132200
Si	1.78418200	-1.93932400	-1.18601300
H	1.08747800	-1.53105600	-2.41964800
H	3.01410200	-2.67296400	-1.56982300
H	0.94815000	-2.83371800	-0.36757300
M5-INT (optimized with SMD (dichloroethane))			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.166767 a.u.			
E (UωB97X-D/def2-tzvp) = -3613.25718958 a.u.			
C	1.19003300	0.36064600	0.69634600
C	1.43700100	1.88512700	0.74493500
C	2.70924400	2.08454800	-0.02184800
C	3.20610800	0.92356700	-0.46191600
H	0.89132300	-0.13731800	1.61867100
H	1.42894800	2.34714200	1.73476900
H	3.14732900	3.06167100	-0.19331200
H	4.11827000	0.81402900	-1.04072200
C	2.37702800	-0.28567800	-0.04919900
C	0.09727300	2.10359600	-0.01936900
O	-0.05012500	0.57077700	-0.11481900
Fe	-1.70788400	-0.47769100	0.03784300
Cl	-1.26906400	-2.56337100	-0.54202600
Cl	-3.17250500	0.49098700	-1.31096600
Cl	-2.30102100	-0.43161300	2.17744100
C	0.14557400	2.65127100	-1.42344300
H	-0.82159200	2.50698800	-1.91532300
H	0.35395400	3.72610600	-1.38224900
H	0.92534000	2.16640500	-2.01446000
C	-1.00340500	2.69458500	0.83086500
H	-1.97752200	2.60827100	0.34051000
H	-1.04849200	2.22126500	1.81499900
H	-0.78625200	3.75963900	0.97053600
Si	3.37751400	-1.33970600	1.18252700
H	4.61730300	-1.81138600	0.53146500

H	3.72384000	-0.50848100	2.35618000
H	2.57373700	-2.49918800	1.62478200
Si	2.01050300	-1.33969900	-1.59494800
H	0.97625700	-0.72199300	-2.44500400
H	3.28397400	-1.38487200	-2.34652500
H	1.63822600	-2.72087300	-1.23967000
M5-TS3 (optimized with SMD (dichloroethane))			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.164877 a.u.			
E (UωB97X-D/def2-tzvp) = -3613.23477560 a.u.			
Imaginary frequency: 135.5862			
C	1.65283000	0.47724400	0.64657300
C	1.55606200	1.90607300	0.20572500
C	2.43539800	1.93529300	-1.01844800
C	2.98930800	0.73595300	-1.24177000
H	1.19148600	0.09053600	1.54947800
H	1.88810500	2.60790800	0.98269600
H	2.58449700	2.82848700	-1.61262600
H	3.66658100	0.46747200	-2.04425400
C	2.55382700	-0.25461800	-0.17944500
C	0.01295700	2.02624700	-0.02798600
O	-0.30427400	0.63497100	-0.32132100
Fe	-1.77819600	-0.40776200	0.02553200
Cl	-1.88406100	-2.05674700	-1.50461000
Cl	-3.70044000	0.75681200	-0.03687800
Cl	-1.43754400	-1.30280400	2.07806500
C	-0.37996900	2.87744800	-1.22390700
H	-1.47022200	2.86384100	-1.32703000
H	-0.05625900	3.91491100	-1.08660600
H	0.06277400	2.48444900	-2.14291200
C	-0.67918800	2.48795500	1.25210900
H	-1.76439900	2.44131000	1.12589600
H	-0.40304600	1.86299800	2.10751400
H	-0.39895300	3.52345900	1.47184700
Si	4.06664400	-0.69313000	0.98091800
H	5.12398900	-1.10629000	0.04474400
H	4.45362900	0.51579400	1.72890100
H	3.66432700	-1.78523400	1.88427800
Si	1.88979600	-1.95501800	-0.80383400
H	1.13215700	-1.67164200	-2.02898700
H	3.06259800	-2.80517900	-1.08875500
H	1.06727100	-2.53972400	0.26446700
M5-INT2' (optimized with SMD (dichloroethane))			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.163656 a.u.			
E (UωB97X-D/def2-tzvp) = -3613.23856772 a.u.			
C	1.74781900	0.56061800	0.67198100
C	1.39030500	1.77450200	-0.09355900
C	1.89333700	1.47716300	-1.47659000
C	2.44111100	0.25008900	-1.52610800
H	1.55884000	0.42221400	1.73045700
H	1.87779200	2.64814300	0.36780900
H	1.80107700	2.16663900	-2.30554900
H	2.88327500	-0.24082700	-2.38473400
C	2.40669900	-0.37226000	-0.15711200
C	-0.17625200	2.12902100	-0.02212100
O	-0.87342000	1.05302800	-0.57509700
Fe	-1.83162700	-0.38479300	-0.06356700

Cl	-1.85301100	-1.87745800	-1.75988000
Cl	-3.93582100	0.19886200	0.51794700
Cl	-0.79639200	-1.31463300	1.74973000
C	-0.43529700	3.36832700	-0.88601700
H	-1.49520300	3.62924700	-0.80177100
H	0.16334300	4.21922600	-0.54491500
H	-0.21675100	3.17295100	-1.93844100
C	-0.59269000	2.39869600	1.42740600
H	-1.64911200	2.68462400	1.43875600
H	-0.47702800	1.51476300	2.05849900
H	-0.00755800	3.22005000	1.85331900
Si	4.25614500	-0.04521700	0.55342800
H	5.08783600	-0.70995300	-0.46043300
H	4.47502700	1.40837600	0.58876700
H	4.36788800	-0.67381100	1.87885400
Si	2.15612900	-2.26968200	0.04075400
H	0.89766000	-2.60214600	-0.63926000
H	3.30584500	-2.89953500	-0.63829100
H	2.16348800	-2.60304500	1.47207600
M5-TS4 (optimized with SMD (dichloroethane)) G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.163069 a.u. E (UωB97X-D/def2-tzvp) = -3613.23542417 a.u. Imaginary frequency: 282.5297			
C	-2.10156000	0.68644800	-0.77210500
C	-1.79962800	1.88163600	-0.04812100
C	-2.20486400	1.62241600	1.35003700
C	-2.57739900	0.33106200	1.47868300
H	-1.96892100	0.54647200	-1.83917100
H	-1.97387200	2.84842500	-0.51571100
H	-2.14425400	2.35636500	2.14334600
H	-2.88546000	-0.17965000	2.38319200
C	-2.55409000	-0.33169600	0.13040100
C	0.04491400	1.91956900	-0.11238100
O	0.49775900	0.76946600	0.42087400
Fe	1.88601700	-0.37626600	0.06452500
Cl	2.10403700	-1.76366600	1.82017300
Cl	3.77130300	0.81908100	-0.23598600
Cl	1.42209300	-1.53016000	-1.82088000
C	0.37900300	3.11627600	0.76933700
H	1.46473400	3.26085500	0.70800300
H	-0.11558900	4.02747400	0.42321700
H	0.11959000	2.92395500	1.81172700
C	0.40013500	2.13406600	-1.57787900
H	1.47312900	2.35365300	-1.62736900
H	0.20960600	1.23963400	-2.17379200
H	-0.14414900	2.98210100	-2.00191700
Si	-4.45116500	-0.43272300	-0.38315300
H	-5.08899200	-1.19890500	0.69969400
H	-4.98200000	0.93804300	-0.46537300
H	-4.55565200	-1.13713700	-1.67379000
Si	-1.88735900	-2.12185700	-0.04334800
H	-2.88029200	-3.01003600	0.59472200
H	-1.78347400	-2.42889200	-1.47839500
H	-0.59901100	-2.21905600	0.65394300
M5-P (optimized with SMD (dichloroethane)) G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.157863 a.u.			

<i>E</i> (UωB97X-D/def2-tzvp) = -3613.27630736 a.u.			
C	-2.09618500	0.49110400	-0.81332000
C	-2.74578600	1.68434200	-0.94087000
C	-3.95115000	1.66156800	-0.13711100
C	-4.05545100	0.44967800	0.48054300
H	-1.17896600	0.18599500	-1.30084800
H	-2.42648500	2.52036700	-1.55389100
H	-4.65607700	2.48200500	-0.05424800
H	-4.84506000	0.11879800	1.14571100
C	-2.88383300	-0.39705300	0.09660000
C	0.50855900	2.07758500	0.47895600
O	0.94831300	0.95230900	0.81178700
Fe	2.11126100	-0.38210100	-0.05646300
Cl	2.40029900	-2.02246200	1.39731700
Cl	3.99539300	0.72642700	-0.41938100
Cl	1.17815600	-1.06857800	-1.94651500
C	-0.22814500	2.88363800	1.48640500
H	0.12120200	3.92186000	1.45167500
H	-1.28740000	2.89146500	1.19624400
H	-0.12449700	2.46505700	2.48786500
C	0.74740900	2.63580700	-0.87930300
H	1.71995500	3.14970600	-0.84595200
H	0.80511600	1.84849700	-1.63453900
H	-0.01169100	3.37482800	-1.14219200
Si	-3.47863000	-1.90338800	-0.88889100
H	-4.34742500	-2.75489900	-0.04676500
H	-4.23950500	-1.43583300	-2.06630400
H	-2.32016000	-2.70828600	-1.33396200
Si	-1.89831400	-0.90661300	1.63089000
H	-2.73387600	-1.77968700	2.48488400
H	-0.68182500	-1.64496100	1.23881000
H	-1.52332200	0.29965500	2.39369900
M5 silyl-migrated (without FeCl₃)			
<i>E</i> (B3LYP-D3BJ/6-31G*/Lan2LDZ) = -397.448133921 a.u.			
C	0.17307100	-0.21172600	-0.65758900
C	-1.02170200	-1.11943000	0.17779000
C	-0.43493600	-1.04743900	1.54988800
C	0.89998700	-0.73540500	1.49553600
H	0.20117600	-0.53008800	-1.70414000
H	-0.90764600	-2.11955900	-0.25996900
H	-1.00900300	-1.23142700	2.45102900
H	1.55697300	-0.75965200	2.36132000
C	1.35395000	-0.49245500	0.16615500
C	-2.29130200	-0.54491900	-0.12177200
O	-0.28671200	1.13077200	-0.63292100
C	-2.83363200	0.56623300	0.70438300
H	-3.34177100	1.31837300	0.08796900
H	-3.58026400	0.19078800	1.42449500
H	-2.03504700	1.03225900	1.29075000
C	-3.11473600	-1.05155300	-1.25625800
H	-4.02386900	-1.56003500	-0.89479600
H	-3.46372500	-0.22086400	-1.88557100
H	-2.56455000	-1.76429200	-1.87913000
Si	3.01279800	-0.96474300	-0.47709000
H	3.15274700	-2.40385900	-0.83933000
H	3.35258200	-0.18973500	-1.69449400

H	4.02590800	-0.68602300	0.56953800
Si	0.68505900	2.34995800	-0.00733500
H	-0.10523100	3.56376700	-0.31574700
H	0.87888500	2.28698100	1.45861300
H	2.00233100	2.45433100	-0.67403100
M6-S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.172433 a.u.			
E (UωB97X-D/def2-tzvp) = -968.677732892 a.u.			
C	-3.25687800	-0.13131400	-0.20838000
C	1.32317600	-0.64623000	-0.59141900
C	-0.09967300	-0.25154100	-0.21767400
C	-1.08216600	-1.09943400	-0.96168700
H	1.37939100	-1.52271200	-1.23918800
H	-0.63089200	-1.87944900	-1.57776600
C	-2.43983700	-1.07277300	-0.95807400
C	2.49711600	-0.11455200	-0.21283200
O	-2.81799000	0.79143100	0.47353700
C	2.68349800	1.07952100	0.68800900
H	1.75415100	1.48603300	1.08773300
H	3.31972200	0.81305400	1.54248900
H	3.19682800	1.88674600	0.14915600
C	3.78960600	-0.71590300	-0.70871300
H	4.41628400	-1.04762300	0.13058700
H	3.61864600	-1.57412300	-1.36559900
H	4.37881700	0.02715200	-1.26375100
H	-2.97377500	-1.80976000	-1.55200600
Si	-0.43649000	1.62534300	-0.53484300
H	-1.52420500	1.83706400	-1.50736500
H	-0.62675900	2.40863400	0.70062300
H	0.79203400	2.13611900	-1.18822600
Si	-0.26826200	-0.78446900	1.62632400
H	0.29245900	-2.15103600	1.71195200
H	0.53480400	0.10740500	2.48546300
H	-1.65396800	-0.82308100	2.12113000
H	-4.35214800	-0.28476400	-0.27964700
M6-RS (FeCl₃/S)			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.160973 a.u.			
E (UωB97X-D/def2-tzvp) = -3613.24617904a.u.			
C	-1.77889100	-1.07787600	0.55893100
C	-0.47079100	-0.92178200	0.20337500
C	-0.01511600	-0.17154600	-0.92579500
C	-2.99686200	0.81840000	-0.74352500
H	-1.93749400	-1.76691300	1.38998200
H	0.29185700	-1.42047800	0.79366100
H	-0.75038200	0.23030800	-1.62874800
H	-3.56490200	0.86549500	-1.67241900
C	-3.02872100	-0.51956900	-0.02100100
Si	-4.41545600	-0.38768900	1.29348500
H	-4.59854000	-1.69459100	1.96717600
H	-4.05119300	0.63272300	2.29514300
H	-5.66311400	-0.00282800	0.60767400
Si	-3.57030400	-1.88201900	-1.26841000
H	-3.58678600	-3.19803100	-0.60176500
H	-4.91757300	-1.55209700	-1.77765300
H	-2.59205800	-1.88216400	-2.37545000
C	-2.43106100	1.96459300	-0.31828100

O	1.18835800	0.04808400	-1.19464700
Fe	2.79203900	-0.08966000	0.00587500
Cl	2.12708300	1.16824400	1.69799700
Cl	4.48579600	0.69245000	-1.13124600
Cl	2.92819400	-2.22093300	0.55625100
C	-1.62728800	2.11131900	0.94482600
H	-0.54975700	2.14046400	0.72655100
H	-1.87155900	3.05682100	1.44232700
H	-1.78250900	1.29919100	1.65623900
C	-2.53133300	3.21238100	-1.15803800
H	-3.01110400	4.02214800	-0.59343900
H	-1.53101400	3.57356500	-1.43271700
H	-3.10097000	3.04735200	-2.07719400
M6-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.163218 a.u.			
E (UωB97X-D/def2-tzvp) = -3613.21830997 a.u.			
Imaginary frequency: 253.9406			
C	-2.11076500	-1.34043900	0.93415400
C	-0.89865600	-1.65131300	0.47424700
C	-0.55514600	-0.94751300	-0.82093300
C	-1.72193800	0.19180100	-0.89253200
H	-2.57325200	-1.78015800	1.81282800
H	-0.21161900	-2.36675900	0.90970600
H	-0.72330800	-1.62439400	-1.67444000
H	-2.04763400	0.29335800	-1.93025200
C	-2.84822100	-0.33727900	0.06294800
Si	-3.87008000	0.95692000	1.01807400
H	-5.24486300	0.44827600	1.21049200
H	-3.28995000	1.26319000	2.34155100
H	-3.92752700	2.20054600	0.21474900
Si	-4.08247700	-1.32878000	-1.01075400
H	-4.93633200	-2.14714700	-0.12804500
H	-4.92839100	-0.40378800	-1.80001100
H	-3.31706800	-2.19531300	-1.93146100
C	-1.00545800	1.41663300	-0.49903800
O	0.69294900	-0.37659500	-0.94204100
Fe	2.27197600	-0.20722800	0.00026100
Cl	2.72206900	2.01223100	-0.32233800
Cl	3.83222700	-1.56203100	-0.77054600
Cl	1.80877100	-0.53621400	2.16311400
C	-0.66690000	1.73149600	0.89588400
H	0.39337400	2.03156600	0.92920500
H	-1.23150000	2.62886900	1.19433400
H	-0.84943500	0.91879600	1.59426100
C	-0.48562700	2.31031800	-1.52517200
H	-0.46545700	3.35729200	-1.20632000
H	0.59349000	2.01992900	-1.57108100
M6-TS1 (optimized at the B3LYP-D3BJ/def2-TZVP level)			
Imaginary frequency: 289.7706			
C	-2.11967000	-1.35794400	0.91922300
C	-0.91374500	-1.66520000	0.46161000
C	-0.55991300	-0.94566400	-0.81746200
C	-1.72425000	0.18561700	-0.88709500
H	-2.58269900	-1.80653800	1.78855400
H	-0.23381300	-2.38610100	0.89070700
H	-0.71060900	-1.61843200	-1.67369000

H	-2.05104300	0.28899000	-1.92038700
C	-2.84588900	-0.33946300	0.06649200
Si	-3.86059400	0.94413300	1.03746400
H	-5.24467200	0.44408600	1.19780900
H	-3.29301800	1.21053700	2.37705400
H	-3.89071600	2.20710200	0.25914500
Si	-4.10215200	-1.29312100	-1.01423300
H	-4.95867700	-2.12109700	-0.14039700
H	-4.93937200	-0.33007700	-1.77078700
H	-3.35470200	-2.14585900	-1.96465500
C	-1.00255500	1.40302200	-0.49403100
O	0.67817100	-0.35923200	-0.91149500
Fe	2.28777100	-0.19632900	0.00836800
Cl	2.75669700	1.97920000	-0.38489300
Cl	3.78156400	-1.60084500	-0.75664400
Cl	1.84238500	-0.48058000	2.16539300
C	-0.67650600	1.71432400	0.89682700
H	0.36363900	2.05847300	0.94231000
H	-1.28181300	2.58136100	1.19424000
H	-0.83569200	0.89390200	1.58567600
C	-0.49744500	2.30315000	-1.51026500
H	-0.47175600	3.34191400	-1.17902100
H	0.57807000	2.01284000	-1.56647600
H	-0.95326500	2.18392200	-2.48826300
M6-INT			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.168436 a.u.			
E (UωB97X-D/def2-tzvp) = -3613.25554355 a.u.			
C	-2.07988400	-1.22407400	0.99834500
C	-0.91720700	-1.65564200	0.48898300
C	-0.62146300	-0.97328900	-0.80760500
C	-1.70509100	0.12267000	-0.93710800
H	-2.51299000	-1.58708600	1.92629000
H	-0.26375200	-2.40075400	0.92595300
H	-0.37815000	-1.62664000	-1.64702500
H	-2.10901100	0.25590400	-1.94320100
C	-2.79589000	-0.22068200	0.11702300
Si	-3.66723700	1.20092100	1.03523700
H	-5.05277800	0.77873700	1.34334700
H	-3.00532700	1.55444800	2.30609000
H	-3.72846000	2.38467300	0.15070600
Si	-4.17169900	-1.18771400	-0.79199300
H	-5.00420100	-1.91780300	0.18499200
H	-5.02201200	-0.25540000	-1.56724500
H	-3.52662800	-2.14414300	-1.71860200
C	-0.57349900	1.17589400	-0.67762400
O	0.44019200	0.06027400	-0.71606100
Fe	2.24449300	-0.15787900	0.09331300
Cl	3.26202100	1.71941600	-0.43590300
Cl	2.87319700	-2.00683500	-0.91434600
Cl	1.95020100	-0.42303100	2.25799200
C	-0.48728800	1.88349900	0.65874800
H	0.51089400	2.32040000	0.76527300
H	-1.21188600	2.70224600	0.70162900
H	-0.65110800	1.20270300	1.49473900
C	-0.30451500	2.09936700	-1.84818500
H	-1.08686900	2.86542700	-1.89586700

H	0.66460900	2.59157600	-1.72621900
H	-0.29867900	1.54468400	-2.79104000
M6-TS2 G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.167223 a.u. E (UωB97X-D/def2-tzvp) = -3613.23055529 a.u. Imaginary frequency: 216.2953			
C	-2.31374900	-1.13388500	1.14165500
C	-1.16683400	-1.81401600	0.75182800
C	-0.80777600	-1.35966100	-0.51680400
C	-1.60193700	-0.14553900	-0.87268800
H	-2.84754300	-1.33730500	2.06757500
H	-0.66828500	-2.59384200	1.30977500
H	-0.10292400	-1.84844200	-1.17472400
H	-1.91341100	-0.14815100	-1.92205600
C	-2.79124400	-0.18079000	0.13814300
Si	-3.64032200	1.39976100	0.82089600
H	-5.07524800	1.07465700	0.98265600
H	-3.10364000	1.79625900	2.13305800
H	-3.50397700	2.46650100	-0.18519400
Si	-4.24133700	-1.09379800	-0.77579300
H	-5.22312000	-1.59631900	0.20256500
H	-4.87274500	-0.12520500	-1.69251000
H	-3.62117300	-2.20800700	-1.51989200
C	-0.48020300	1.00428900	-0.72626100
O	0.70826900	0.26583400	-0.94705400
Fe	2.27692300	-0.07072800	-0.00351300
Cl	3.43906000	1.81445700	0.16135100
Cl	3.17856300	-1.75216800	-1.15393200
Cl	1.66761700	-0.82867900	2.04435600
C	-0.43582600	1.67293000	0.64524400
H	0.51521500	2.21213500	0.70663300
H	-1.23213600	2.41001100	0.77761800
H	-0.44428900	0.95126500	1.46541800
C	-0.62568600	2.04082600	-1.83726900
H	-1.57309800	2.58719600	-1.76214500
H	0.19999200	2.75498100	-1.75897900
H	-0.56606100	1.55674300	-2.81671000
M6-P G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.156589 a.u. E (UωB97X-D/def2-tzvp) = -3613.27382778 a.u.			
C	-3.07177000	-0.82906900	1.26696000
C	-1.83612600	-1.32545100	0.97470400
C	-1.53603100	-1.06435300	-0.41879300
C	-2.58367500	-0.40083100	-0.98755100
H	-3.58363500	-0.87193600	2.22134500
H	-1.17296600	-1.84210500	1.65744300
H	-0.62297400	-1.36938200	-0.91630900
H	-2.67532400	-0.08704500	-2.02117900
C	-3.66122500	-0.21625300	0.03554300
Si	-4.09854700	1.59876000	0.30632800
H	-5.14288600	1.73535500	1.34389500
H	-2.89037300	2.33466200	0.74128300
H	-4.58889300	2.20338400	-0.95254800
Si	-5.16500500	-1.25445400	-0.49004300
H	-6.21636100	-1.17629900	0.54816800
H	-5.71825500	-0.72679500	-1.75736100

H	-4.73333900	-2.65391200	-0.67098900
C	0.44997500	1.59480800	-0.51659200
O	1.31541600	0.80795800	-0.93767000
Fe	2.76134900	-0.25992700	-0.01606300
Cl	3.89166000	1.30381700	1.04523200
Cl	3.83257000	-1.25636900	-1.63717900
Cl	1.70199400	-1.62257200	1.34907500
C	0.20829500	1.79329100	0.94470900
H	1.16103100	1.85425700	1.48004800
H	-0.40317900	2.67605700	1.13922700
H	-0.32791500	0.90878400	1.31465000
C	-0.35389100	2.36862700	-1.51252400
H	-1.41692000	2.30470300	-1.26438200
H	-0.06746100	3.42669400	-1.43655200
H	-0.16833400	2.01023400	-2.52565800
M7-S $G_{\text{corr}}(\text{UB3LYP-D3BJ/6-31G}^*/\text{Lan2LDZ}) = 0.073507 \text{ a.u.}$ $E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -507.153479821 \text{ a.u.}$			
C	-1.24972100	1.03555300	-0.66217500
C	1.95908200	0.10367400	0.17835200
C	1.25964100	-0.97710000	-0.49938400
C	-0.07082700	-1.17752300	-0.54677300
H	-1.93742000	0.96893600	-1.52976400
H	1.36406500	0.84670300	0.69899300
H	1.89135300	-1.69393700	-1.02293700
H	-0.48690400	-2.00602400	-1.11116400
C	-1.09209300	-0.29077000	0.10064500
C	3.29651600	0.20805000	0.15467400
O	-0.65369000	2.04105900	-0.36635500
H	3.91651000	-0.51996800	-0.36419900
H	3.81269200	1.02252400	0.65306100
F	-2.31626700	-0.91498600	0.07027300
F	-0.78888400	-0.01368200	1.40248500
M7-FeCl₃/S $G_{\text{corr}}(\text{UB3LYP-D3BJ/6-31G}^*/\text{Lan2LDZ}) = 0.063669 \text{ a.u.}$ $E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -3151.70397019 \text{ a.u.}$			
C	1.03999200	-1.22264300	-0.12616800
C	2.24014200	1.86614500	0.32084500
C	2.97978400	1.10873000	-0.67013600
C	3.13942700	-0.23237500	-0.73249600
H	0.74257300	-1.77296100	-1.02896200
H	1.80793600	1.33876600	1.16326700
H	3.44394800	1.69496700	-1.46202200
H	3.66882500	-0.69283800	-1.56005600
C	2.51835100	-1.20609500	0.22254200
C	2.05734500	3.19118600	0.19690600
O	0.23305200	-0.55347800	0.51479500
Fe	-1.67968300	-0.00281300	-0.02885600
Cl	-1.72985700	-0.91312000	-2.03682400
Cl	-1.59173000	2.17944100	0.00290100
Cl	-2.97064900	-0.94618700	1.45039100
H	2.47535700	3.74900500	-0.63783200
H	1.47130000	3.75108600	0.91780300
F	3.01825600	-2.45905400	0.01338300
F	2.68343000	-0.87861700	1.53003800
M7-RS			

$G_{\text{corr}}(\text{UB3LYP-D3BJ/6-31G}^*/\text{Lan2LDZ}) = 0.064764 \text{ a.u.}$ $E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -3151.70118245 \text{ a.u.}$			
C	1.14412000	-0.54818200	0.29084600
C	2.47479500	1.94510000	0.33840500
C	3.63260900	1.08287300	0.58544300
C	3.67915000	-0.23109000	0.31719600
H	1.07010300	-0.18385300	1.32174100
H	2.22295200	2.66250700	1.11858400
H	4.50355200	1.54511200	1.04709300
H	4.57926000	-0.81333200	0.49032900
C	2.52023800	-1.02951500	-0.18597200
C	1.73704200	1.91037600	-0.78637400
O	0.14187500	-0.73318700	-0.39544700
Fe	-1.72831200	-0.00200400	0.03057400
Cl	-1.37437900	0.71708800	2.08903000
Cl	-3.10579600	-1.67305400	-0.15998100
Cl	-1.90750900	1.61723400	-1.43486200
H	2.00312500	1.27296800	-1.62406000
H	0.85759100	2.53442100	-0.90686100
F	2.51221500	-1.15546300	-1.54197300
F	2.60194300	-2.30221800	0.33790600
M7-TS1 $G_{\text{corr}}(\text{UB3LYP-D3BJ/6-31G}^*/\text{Lan2LDZ}) = 0.067831 \text{ a.u.}$ $E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -3151.65893902 \text{ a.u.}$ Imaginary frequency: 700.1715			
C	1.28466400	-0.08276700	0.25685100
C	1.85150300	1.54791700	0.29105500
C	3.31906600	1.31653700	0.49056100
C	3.72041800	0.06648100	0.25092100
H	1.06759600	-0.30360600	1.31146400
H	1.31196400	2.10537900	1.05730700
H	3.95787200	2.12515600	0.83083100
H	4.73343300	-0.31195600	0.31952800
C	2.58388600	-0.80600600	-0.18086000
C	1.29264100	1.65804900	-1.00939000
O	0.22631400	-0.23127300	-0.59478400
Fe	-1.58089300	-0.09624800	0.02047500
Cl	-1.43891800	-0.97373800	2.05158900
Cl	-2.94758300	-1.04112800	-1.39884700
Cl	-1.79565300	2.15136800	0.14980700
H	1.83670700	1.30197300	-1.88005400
H	0.30387400	2.09367500	-1.14401500
F	2.59197700	-0.97497800	-1.54176500
F	2.61522500	-2.04499900	0.37428900
M8-S $G_{\text{corr}}(\text{UB3LYP-D3BJ/6-31G}^*/\text{Lan2LDZ}) = 0.073902 \text{ a.u.}$ $E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -507.152271478 \text{ a.u.}$			
C	-2.41531500	0.25103700	-0.12595400
C	1.09636100	1.00818500	-0.20436100
C	0.66627700	-0.36711600	0.22008500
C	-0.31122900	-1.00269800	-0.74492600
H	0.31569200	1.75544900	-0.11397600
H	0.15127900	-1.74861300	-1.38619900
C	-1.62266400	-0.75273000	-0.87372400
C	2.31197800	1.27301700	-0.67735800
O	-1.96701900	1.22960600	0.43998700

H	-2.19176300	-1.34819900	-1.58576700
F	0.13027200	-0.32253900	1.48050300
F	1.75429300	-1.21041600	0.28496300
H	-3.50998600	0.06405900	-0.13849200
H	2.58746100	2.27776600	-0.98313400
H	3.06993600	0.50111000	-0.76409300
M8-RS (FeCl₃/S)			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.064639 a.u.			
E (UωB97X-D/def2-tzvp) = -3151.713534 a.u.			
C	-2.48786000	-0.88053500	0.61639500
C	-1.20664900	-0.93871700	0.21065000
C	-0.74861600	-0.37981100	-1.05122300
C	-3.65981700	1.27856700	-0.06063600
H	-2.75663200	-1.26861800	1.59476200
H	-0.44825800	-1.37582400	0.85397600
H	-1.48366400	-0.15283800	-1.82859700
H	-4.59083600	1.68832400	-0.44699400
C	-3.62740600	-0.22203300	-0.11956100
C	-2.68765500	2.06859600	0.39469500
O	0.44386800	-0.14038300	-1.30359200
H	-1.75532400	1.69667600	0.80842700
H	-2.80552600	3.14751300	0.37228900
Fe	2.01278400	0.01684200	-0.00877800
Cl	3.69997600	0.75382400	-1.16856300
Cl	2.23412600	-2.00070100	0.83737600
Cl	1.13759400	1.43950200	1.43713800
F	-4.79814500	-0.70927500	0.40104000
M8-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.067124 a.u.			
E (UωB97X-D/def2-tzvp) = -3151.661217 a.u.			
Imaginary frequency: 756.3576			
C	-2.37190000	-1.29910600	0.34868600
C	-1.29926200	-1.46921500	-0.41840900
C	-0.98321700	-0.38095300	-1.39906200
C	-2.34643400	0.71606700	-1.03107800
H	-2.72545100	-1.97973100	1.11422400
H	-0.59789200	-2.29777300	-0.36060100
H	-1.19968400	-0.63317700	-2.44473400
H	-2.91694700	0.85448900	-1.94626600
C	-3.08772200	-0.00977500	0.09326200
C	-1.35248700	1.65022000	-0.71622100
O	0.24028200	0.23842700	-1.28344500
H	-0.94219900	1.71503400	0.29369000
H	-0.96181800	2.33335800	-1.46377700
Fe	1.61477900	-0.00453400	0.02823400
Cl	3.27162700	1.29376300	-0.60191700
Cl	2.09922100	-2.16181000	0.15879900
Cl	0.61403500	0.75364700	1.89869800
F	-3.13616900	0.76181700	1.22320600
F	-4.38154100	-0.21519200	-0.29731700
M9-S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.091570 a.u.			
E (UωB97X-D/def2-tzvp) = -308.645186437 a.u.			
C	1.87274500	-0.38178700	-0.33512700
C	-1.48232600	-0.35057200	0.18284300
C	-1.01919800	0.95820500	-0.25613800

C	0.22181700	1.45375000	-0.09299200
H	2.37228700	-0.02263200	-1.26151500
H	-0.75302200	-1.01761100	0.63637000
H	-1.76023000	1.58262400	-0.75469300
H	0.44412900	2.44111100	-0.48953800
C	1.36008200	0.71563200	0.58245500
C	-2.74785100	-0.76799500	0.02751900
O	1.72587900	-1.56580800	-0.12712000
H	-3.50204100	-0.13691700	-0.43792900
H	-3.06899200	-1.75141400	0.35639900
H	2.17975600	1.41383500	0.79175900
H	1.04946800	0.25407300	1.52474200
M9-FeCl₃/S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.081912 a.u.			
E (UωB97X-D/def2-tzvp) = -2953.20531840 a.u.			
C	-1.01522000	-1.66381200	-0.34636600
C	-2.87394400	1.03789800	-0.37120900
C	-3.51214500	-0.07035600	0.31813800
C	-3.32153200	-1.38749100	0.09475200
H	-0.72337000	-2.17153500	0.58339300
H	-2.17192500	0.81801600	-1.16992200
H	-4.21675500	0.20523100	1.10198100
H	-3.83451900	-2.10974800	0.72229100
C	-2.35391000	-1.95612000	-0.93455000
C	-3.09186200	2.31729800	-0.02913900
O	-0.27478000	-0.79061700	-0.81502800
Fe	1.33221500	0.11347600	0.04468500
Cl	1.31883600	-0.88443200	2.01364500
Cl	0.76674300	2.22688100	0.07122800
Cl	3.02104000	-0.41437400	-1.23586000
H	-3.77326100	2.58281300	0.77591200
H	-2.58117500	3.13243700	-0.53053700
H	-2.49789000	-3.03713400	-1.02956500
H	-2.44129300	-1.48729200	-1.91811700
M9-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.082318 a.u.			
E (UωB97X-D/def2-tzvp) = -2953.203216 a.u.			
C	1.33013400	-1.06365800	-0.15567800
C	3.00411500	1.18368800	0.47033500
C	4.01617700	0.12381000	0.34963100
C	3.84412200	-1.06558300	-0.24759400
H	1.36451200	-0.96646500	0.93690600
H	2.89974200	1.64148400	1.45401300
H	4.97817900	0.31925700	0.82209700
H	4.67919000	-1.75980500	-0.28411100
C	2.55354800	-1.56173400	-0.85933900
C	2.22992500	1.62413000	-0.53300800
O	0.26639200	-0.86007700	-0.75227800
H	2.33351800	1.24564300	-1.54634300
H	1.47222400	2.38476000	-0.37669400
Fe	-1.39671300	0.01055800	0.02420200
Cl	-0.81927100	0.14451300	2.15250800
Cl	-3.02984500	-1.37219800	-0.40057400
Cl	-1.46760000	1.95201100	-0.99155900
H	2.46121000	-1.35680100	-1.93250900
H	2.51088600	-2.65943100	-0.75682400

M9-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.084720 a.u.			
E (UωB97X-D/def2-tzvp) = -2953.147727 a.u.			
Imaginary frequency: 715.6691			
C	1.55813700	-0.50155400	0.01074300
C	2.46264100	0.96383500	0.34992400
C	3.86216200	0.45642300	0.19500000
C	3.94614400	-0.76854700	-0.33091600
H	1.30115500	-0.83397500	1.02353700
H	2.15340700	1.35044500	1.32104700
H	4.70588100	1.05928700	0.51546600
H	4.88194800	-1.28360600	-0.52293700
C	2.61558200	-1.38474800	-0.66467000
C	1.74242800	1.49330600	-0.74480100
O	0.44654600	-0.23569500	-0.78241000
H	2.09422100	1.35404200	-1.76341900
H	0.83616800	2.07362600	-0.58350300
Fe	-1.28359000	-0.06366300	-0.00361500
Cl	-1.24385600	-1.63384700	1.56768600
Cl	-2.80716700	-0.23857100	-1.57048900
Cl	-1.13939200	1.99537400	0.91563300
H	2.42591200	-1.40634100	-1.74513000
H	2.51677200	-2.41522300	-0.30156900
M10-S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.091903 a.u.			
E (UωB97X-D/def2-tzvp) = -308.640588406 a.u.			
C	2.11540500	-0.33993200	-0.19420200
C	-1.55428300	-0.47242800	-0.17459600
C	-0.73677200	0.33604200	0.80844500
C	0.20019400	1.24989800	0.06174300
H	-0.98590400	-1.20404600	-0.74487900
H	-1.40337800	0.93408500	1.43984400
H	-0.18917400	2.24271700	-0.16182400
C	1.43523300	0.95127500	-0.38640500
C	-2.86318100	-0.32167600	-0.37371200
O	1.60179700	-1.36134900	0.23583400
H	-0.16264000	-0.34887200	1.43925400
H	2.00892600	1.71035400	-0.91480200
H	3.18931900	-0.34006100	-0.48226200
H	-3.40317600	-0.92817500	-1.09564000
H	-3.44792500	0.40571800	0.18600100
M10-RS (FeCl₃/S)			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.081712 a.u.			
E (UωB97X-D/def2-tzvp) = -2953.20673003 a.u.			
C	1.21081300	0.90557700	0.07600100
C	3.62396800	-0.87726000	-0.47200800
C	4.34051100	0.35735200	0.00338200
C	3.57647800	1.64843700	0.10670400
H	1.47129400	-0.15483500	0.03324000
H	3.19587900	-0.82421800	-1.47321400
H	5.19548100	0.56193900	-0.66036200
H	4.22369600	2.52160700	0.18930200
C	2.24671200	1.90471300	0.12874400
C	3.51718600	-2.00478600	0.23107500
O	0.00585600	1.23160400	0.09266700
H	3.93130200	-2.09548700	1.23305400

H	3.00137100	-2.87347300	-0.16547400
Fe	-1.56416000	-0.03978400	0.00027000
Cl	-2.70487600	0.59552500	-1.75343900
Cl	-2.56937500	0.15741400	1.93232900
Cl	-0.50136200	-1.96851100	-0.26982600
H	1.89985600	2.93184400	0.20683400
H	4.79384900	0.17468500	0.99080500
M10-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.084267 a.u.			
E (UωB97X-D/def2-tzvp) = -2953.14969225 a.u.			
Imaginary frequency: 689.7056			
C	1.51622700	0.38644200	-0.20498600
C	2.70057000	-0.95041900	-0.35803700
C	3.98173300	-0.39647700	0.25916700
C	3.70380200	1.06542600	0.52364500
H	1.15238400	0.49666400	-1.23154100
H	2.71456600	-1.17032400	-1.42303800
H	4.81917600	-0.53200600	-0.43495200
H	4.48088600	1.72716000	0.89258500
C	2.45421900	1.44659900	0.26912800
C	1.75371200	-1.64711600	0.40418200
O	0.49563700	0.09507800	0.70089300
H	1.83007700	-1.69701200	1.48656300
H	0.92281700	-2.17035300	-0.06886100
Fe	-1.29353000	0.05725900	0.04243600
Cl	-1.40031600	1.92773000	-1.14767900
Cl	-2.68390600	-0.18073900	1.72070800
Cl	-1.16359200	-1.73810800	-1.33053700
H	2.04308600	2.44326900	0.40467800
H	4.25494100	-0.92449700	1.18314500
M11-S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.116580 a.u.			
E (UωB97X-D/def2-tzvp) = -890.045769390 a.u.			
C	0.25235400	0.51956000	1.29628500
C	-2.51695800	0.00421000	0.09634700
C	-1.72410200	-1.12710800	-0.36220000
C	-0.37927000	-1.22019200	-0.42731200
H	-0.26291700	-0.12843900	2.03737100
H	-1.99596100	0.91358800	0.38622600
H	-2.29812100	-1.98615200	-0.70824800
H	0.02873700	-2.13273300	-0.85869100
C	0.61901100	-0.17032000	0.00540000
C	-3.85703200	-0.01690600	0.15537800
O	0.50806700	1.68007400	1.55347500
Si	0.85782100	1.13216800	-1.37070900
H	1.05514900	0.39983100	-2.64084600
H	-0.36653300	1.95133900	-1.46311900
H	2.03687800	1.98856900	-1.13414900
Si	2.29152300	-1.02795700	0.35052500
H	2.68584700	-1.76508500	-0.86905300
H	3.31977500	-0.03010600	0.69998800
H	2.12907500	-1.99049300	1.46290400
H	-4.42448000	-0.90051200	-0.12820000
H	-4.42680500	0.84517900	0.48720000
M11-FeCl₃/S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.106145 a.u.			

$E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -3534.60673733 \text{ a.u.}$			
C	0.88752900	-0.39931900	-0.46899500
C	1.63733200	2.43140400	-0.00876700
C	2.86280900	1.82692200	-0.50949800
C	3.18113200	0.51451800	-0.53271900
H	0.69958600	0.12560600	-1.41687800
H	0.91048800	1.80480100	0.50438000
H	3.60578500	2.52343200	-0.89559500
H	4.16878700	0.23424400	-0.89053800
C	2.27904700	-0.60406800	-0.05518500
C	1.35744500	3.73752900	-0.12701200
O	-0.08566900	-0.79908000	0.19892300
Si	2.43466600	-0.83887900	1.84593700
H	3.87993800	-0.89077500	2.13987200
H	1.81298100	0.33172500	2.48997000
H	1.79256200	-2.09142400	2.28680800
Si	2.81814500	-2.24231100	-0.92324200
H	4.23271800	-2.44570900	-0.55598800
H	1.97419100	-3.35119500	-0.44699600
H	2.69012600	-2.07234300	-2.38413200
Fe	-1.98264900	-0.12583500	-0.01133700
Cl	-2.00320100	0.38578000	-2.15510300
Cl	-1.90577300	1.64845900	1.29104000
Cl	-3.31310400	-1.73916100	0.60097300
H	2.03794600	4.42492400	-0.62423900
H	0.43330400	4.14948700	0.26456900
M11-RS $G_{\text{corr}}(\text{UB3LYP-D3BJ/6-31G}^*/\text{Lan2LDZ}) = 0.106920 \text{ a.u.}$ $E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -3534.60408319 \text{ a.u.}$			
C	-0.94586000	-0.17922100	-0.39351100
C	-1.60512700	2.60876100	-0.56479300
C	-2.93004300	1.98141700	-0.72223400
C	-3.26788600	0.70501700	-0.46777500
H	-0.74391000	0.27607600	-1.37041700
H	-1.21271800	3.11493600	-1.44757500
H	-3.71364300	2.62434100	-1.12361300
H	-4.30761500	0.41717700	-0.60921300
C	-2.34233100	-0.39564000	0.00932900
C	-0.88009200	2.62756600	0.56134300
O	0.01518400	-0.56779100	0.29736400
H	-1.23882100	2.18337700	1.48452300
H	0.10013400	3.09130300	0.59387500
Fe	1.96019400	-0.13939900	-0.02046500
Cl	1.83989400	0.84415300	-1.99875900
Cl	3.00167400	-2.05844900	-0.01361900
Cl	2.44359000	1.24059800	1.61398400
Si	-2.52147400	-0.74021400	1.88756200
H	-3.97026900	-0.72839500	2.17324800
H	-1.96207800	-2.05984300	2.23663400
H	-1.84456800	0.33012100	2.64031200
Si	-2.85217400	-2.00778600	-0.93785000
H	-4.25835000	-2.26135500	-0.56818700
H	-2.73939600	-1.75990000	-2.38853500
H	-1.98386200	-3.12365500	-0.52529700
M11-TS1 $G_{\text{corr}}(\text{UB3LYP-D3BJ/6-31G}^*/\text{Lan2LDZ}) = 0.110368 \text{ a.u.}$			

$E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -3534.54574613 \text{ a.u.}$ Imaginary frequency: 686.3686			
C	-0.97712400	0.49895400	-0.31956700
C	-1.45528300	2.19544200	-0.39422300
C	-2.93505400	2.08098700	-0.21112200
C	-3.35869100	0.83181400	0.01264300
H	-0.64621100	0.34079100	-1.35081300
H	-1.08432200	2.59382000	-1.33913200
H	-3.57796900	2.95171800	-0.28566900
H	-4.40055300	0.56991600	0.17163600
C	-2.27957400	-0.21357400	0.07245700
C	-0.57691300	2.36451800	0.69790600
O	0.05079900	0.29341700	0.60792600
H	-0.92344800	2.24233600	1.72035700
H	0.46689800	2.62664900	0.53383700
Fe	1.78770300	-0.16087000	-0.03323800
Cl	1.28478800	-1.56541900	-1.68656800
Cl	2.98617700	-0.93738600	1.62665200
Cl	2.44518000	1.83954800	-0.83767200
Si	-2.11915200	-0.89182100	1.85746700
H	-3.45634300	-1.43690600	2.19151400
H	-1.12077300	-1.96724900	1.96054600
H	-1.83738300	0.21528800	2.79636000
Si	-2.64562800	-1.64999600	-1.14021000
H	-4.04323900	-2.07298600	-0.90432000
H	-2.50795000	-1.14006900	-2.52047300
H	-1.72707700	-2.77608200	-0.90425300
M12-S $G_{\text{corr}}(\text{UB3LYP-D3BJ/6-31G}^*/\text{Lan2LDZ}) = 0.118996 \text{ a.u.}$ $E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -890.036947469 \text{ a.u.}$			
C	2.64681400	-0.11825400	0.14090500
C	-1.92084900	-0.29371500	0.87999700
C	-0.51520900	-0.11049400	0.33139300
C	0.49401600	-0.67082300	1.27848300
H	-1.98775600	-0.95421100	1.74646900
H	0.06207100	-1.16330000	2.15181500
C	1.84861100	-0.69815200	1.21048700
C	-3.05801000	0.19635300	0.37974700
O	2.19362500	0.51717900	-0.80652000
H	2.39671500	-1.19511000	2.00655000
Si	-0.14966000	1.72070400	-0.17367700
H	0.92970000	2.30664400	0.64271700
H	0.06842700	1.90121800	-1.61986800
H	-1.38574100	2.46599000	0.16321600
Si	-0.53104100	-1.23694500	-1.23133100
H	-1.08538500	-2.54380000	-0.81488500
H	-1.43307800	-0.62582400	-2.22842200
H	0.80211100	-1.45583900	-1.81728200
H	3.74058900	-0.28014500	0.21739400
H	-3.08596700	0.85136200	-0.48616600
H	-4.01311600	-0.04653500	0.83466300
M12-FeCl₃/S $G_{\text{corr}}(\text{UB3LYP-D3BJ/6-31G}^*/\text{Lan2LDZ}) = 0.109728 \text{ a.u.}$ $E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -3534.60407339 \text{ a.u.}$			
C	0.00492500	-1.93932300	0.49228900
C	-4.19358700	0.01996800	0.18675500

C	-2.70971500	-0.30102900	0.19401000
C	-2.47182400	-1.71216100	0.52905600
H	-4.85194900	-0.84763100	0.25491200
H	-3.38058200	-2.30038900	0.67349700
C	-1.31249500	-2.43979700	0.65701300
C	-4.75159000	1.22413200	0.03840400
O	0.24865200	-0.72724600	0.25256400
H	-1.39478000	-3.49785300	0.88301900
Fe	1.98724700	0.20420700	-0.07082100
Cl	3.35990600	-1.51337200	-0.25165100
Cl	1.61593500	1.32437700	-1.92089900
Cl	2.29426000	1.43061100	1.71999900
Si	-1.68483100	0.95042800	1.28052800
H	-0.99250000	0.23109400	2.36243800
H	-0.77246900	1.76270000	0.46302500
H	-2.69150100	1.84404300	1.88667800
Si	-2.23717100	-0.07092900	-1.68641300
H	-3.28283200	-0.78858000	-2.44337700
H	-2.29697500	1.37216800	-1.97082200
H	-0.92336900	-0.63700400	-2.01821600
H	0.85183300	-2.63132600	0.56663900
H	-4.16982900	2.13710900	-0.05067000
H	-5.83067600	1.33307200	0.00430100
M12-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.106463 a.u.			
E (UωB97X-D/def2-tzvp) = -3534.59868572 a.u.			
C	2.02350900	-0.55965000	-0.72961100
C	0.72821800	-0.74394400	-0.36716500
C	0.21395600	-0.51479700	0.95750800
C	2.88860000	1.12728300	1.03326400
H	2.26166900	-0.87132300	-1.74716900
H	0.01299400	-1.09272700	-1.10670600
H	0.91172800	-0.44197200	1.79639800
H	3.59172800	1.20683700	1.86223100
C	3.16968200	-0.01097500	0.06068700
Si	4.48953000	0.69381500	-1.13718500
H	5.00323800	-0.38775600	-2.00897200
H	3.85207300	1.74026500	-1.95992100
H	5.59535500	1.26069600	-0.34221100
Si	3.92987900	-1.50893700	0.98323000
H	4.17905900	-2.60609100	0.02863600
H	5.19776500	-1.08527300	1.61428000
H	2.97476600	-1.95411300	2.02019300
C	1.95468500	2.07403400	0.89827900
O	-0.99953600	-0.42967700	1.23594100
H	1.22536800	2.07798100	0.09252400
H	1.88373700	2.88186600	1.61983400
Fe	-2.52372200	-0.01060100	-0.02468800
Cl	-4.28056900	0.32779400	1.22395400
Cl	-2.64610100	-1.74676400	-1.37665900
Cl	-1.70980400	1.78159700	-1.02830400
M12-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.111688 a.u.			
E (UωB97X-D/def2-tzvp) = -3534.53975391 a.u.			
Imaginary frequency: 744.4868			
C	1.80962300	-1.06861700	-0.83138500

C	0.79146300	-1.68540300	-0.23213400
C	0.45694200	-1.21695600	1.14417500
C	1.84641000	-0.10173700	1.37464500
H	2.11467000	-1.27541400	-1.85264400
H	0.14387200	-2.42949800	-0.68596000
H	0.60230800	-1.94524200	1.95004100
H	2.39561100	-0.54315900	2.20599900
C	2.56388200	-0.06441300	0.01078000
Si	2.72899600	1.64895300	-0.85683800
H	2.23794700	1.56660200	-2.24129000
H	2.02616000	2.69498500	-0.08870700
H	4.16773200	2.00481600	-0.87765400
Si	4.33488800	-0.73410300	0.25666900
H	4.98692300	-0.87592800	-1.06017700
H	5.11050500	0.19235200	1.10860600
H	4.24369600	-2.05190000	0.92551500
C	0.84178700	0.80727200	1.74993200
O	-0.76329000	-0.56953500	1.31062600
H	0.39549200	1.49308600	1.03193600
H	0.50407200	0.87460300	2.77964300
Fe	-1.99719600	-0.01716400	-0.03243900
Cl	-3.68143600	0.88346300	1.06356400
Cl	-2.54264500	-1.72339000	-1.32906200
Cl	-0.81418800	1.57336600	-1.130419
M13-S G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.072457 a.u. E (UωB97X-D/def2-tzvp) = -1181.35043331 a.u.			
C	-3.26959000	-0.64386000	1.08783900
C	-0.14365300	0.06904300	-0.13836500
C	-0.92051400	1.29517500	-0.03721900
C	-2.26413100	1.35765500	-0.07482800
H	-4.07703900	-0.32332500	1.77571700
H	-0.68800800	-0.85821500	-0.26443600
H	-0.38116400	2.22838800	0.07980700
H	-2.76901000	2.31211000	0.03843300
C	-3.18888100	0.18224100	-0.21343200
C	1.19704800	-0.00283000	-0.06242900
O	-2.50162100	-1.53865300	1.33350600
C	2.07171900	1.21348500	0.13729000
C	1.90142100	-1.33083000	-0.17109000
F	-4.45340600	0.63494100	-0.48306400
F	-2.80727200	-0.64935000	-1.22709200
F	1.75100200	1.86355400	1.28037900
F	3.37444400	0.89915400	0.20150100
F	1.91360700	2.10282700	-0.87032400
F	2.76761400	-1.33959700	-1.20554200
F	2.60342200	-1.60374800	0.94772300
F	1.03144000	-2.34002700	-0.36182200
M13-FeCl₃/S G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.063566 a.u. E (UωB97X-D/def2-tzvp) = -3825.89804720 a.u.			
C	1.74401700	1.88292900	0.12300300
C	-1.45320000	1.03890800	0.40069700
C	-1.30409100	2.18853800	-0.47772600
C	-0.30434700	3.09082000	-0.40595600
H	2.48040100	2.08697400	-0.66731100

H	-0.80147100	0.97495000	1.26103500
H	-2.04332600	2.32771500	-1.25872300
H	-0.23548800	3.89785400	-1.12826900
C	0.84279600	3.03174300	0.56473700
C	-2.31126500	0.02414500	0.20585700
O	1.57974500	0.75765600	0.57782500
C	-3.26254800	-0.03297200	-0.97047400
C	-2.33470600	-1.14614100	1.16152400
Fe	2.23797500	-1.03776200	-0.24549500
Cl	0.47986800	-1.59379900	-1.41331600
Cl	2.77967300	-2.29770000	1.43567300
Cl	3.89042000	-0.22932500	-1.45589100
F	1.56907600	4.18251500	0.50090900
F	0.45017800	2.83087700	1.85071200
F	-2.58664000	-0.07773400	-2.13592100
F	-4.07312700	-1.09743000	-0.91536000
F	-4.04264500	1.07491500	-1.01111200
F	-3.52235000	-1.22030300	1.79490300
F	-2.13762200	-2.30601400	0.51549100
F	-1.37628100	-1.02913300	2.10189200
M13-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.064724 a.u.			
E (UωB97X-D/def2-tzvp) = -3825.891881 a.u.			
C	-0.23428300	1.61717600	-0.43684300
C	2.21921000	0.31220700	-1.33930200
C	2.72120100	1.69109900	-1.17501800
C	2.08840400	2.73704500	-0.63982400
H	-0.34481400	1.35602600	-1.49752100
H	1.97387100	0.00512800	-2.35457400
H	3.71707300	1.86020500	-1.58396400
H	2.58011900	3.70508600	-0.59402400
C	0.69642000	2.77966500	-0.09130800
C	2.12523800	-0.61637800	-0.38063000
O	-0.91316200	1.08132900	0.42457700
Fe	-2.40075100	-0.34483000	0.09599600
Cl	-1.81208700	-0.90588700	-1.95746200
Cl	-4.20722500	0.87156900	0.18699100
Cl	-2.17418900	-1.83892400	1.65332000
C	2.49781400	-0.34415200	1.06538700
C	1.66438700	-2.02011200	-0.71054100
F	2.62744800	-1.47814600	1.76539600
F	3.66295500	0.32832000	1.14505700
F	1.55515700	0.41057300	1.66970800
F	0.62819700	-2.37261800	0.06806100
F	2.65810800	-2.90564100	-0.51042700
F	1.28096300	-2.12054200	-1.99554400
F	0.70122100	2.98775700	1.24299800
F	0.04347700	3.84966700	-0.67662400
M13-TS1A			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.064708 a.u.			
E (UωB97X-D/def2-tzvp) = -3825.816576 a.u.			
Imaginary frequency: 776.7368			
C	0.21312000	1.10088300	-0.70409500
C	2.05803000	1.17881200	-0.67769200
C	2.26918000	2.43271600	0.10917100
C	1.17208100	3.15447000	0.32510300

H	0.04653100	0.93557800	-1.77063000
H	2.35012200	1.20968900	-1.72726300
H	3.26861900	2.72191200	0.41944800
H	1.13069300	4.10640100	0.84227100
C	-0.08218100	2.55804200	-0.23805300
C	1.97742800	-0.10722500	-0.13391600
O	-0.17318200	0.11513500	0.13603300
Fe	-1.98049300	-0.60144700	0.10041800
Cl	-2.68620600	0.57917100	-1.66831300
Cl	-3.00074900	-0.17266300	1.99144700
Cl	-1.81470600	-2.75148400	-0.34132500
C	2.11560400	-0.42032200	1.36184500
C	2.05314700	-1.30651700	-1.09104400
F	3.43556000	-0.69283700	1.50247500
F	1.80916200	0.62114800	2.12813900
F	1.41430100	-1.47345600	1.74709000
F	1.42728900	-2.38025800	-0.64840600
F	3.36940900	-1.57540900	-1.21462200
F	1.56985300	-0.97549900	-2.29644000
F	-1.08281500	2.53706700	0.67119500
F	-0.50363700	3.27951200	-1.31849900
M13-TS1B G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.065870 a.u. E (UωB97X-D/def2-tzvp) = -3825.79844706 a.u. Imaginary frequency: 203.5240			
C	0.21034900	1.15042700	-0.85029900
C	1.63752100	0.59924600	-1.19631800
C	2.51605500	1.82460200	-1.05781800
C	1.87284200	2.88500100	-0.57121100
H	-0.39958700	1.23918000	-1.75521300
H	1.64201300	0.22504400	-2.22490300
H	3.56220400	1.79975700	-1.34142500
H	2.28592900	3.87024900	-0.38957900
C	0.43983300	2.57470300	-0.26538200
C	1.98196100	-0.55441800	-0.29494600
O	-0.39914800	0.27811600	0.05695600
Fe	-2.05092400	-0.30689200	0.16685800
Cl	-3.08546500	1.49580800	0.77394300
Cl	-2.90992400	-1.87173100	1.34999400
Cl	-2.33234600	-0.92184300	-1.90337000
C	2.65986100	-0.32634300	1.02205700
C	1.54635100	-1.94751800	-0.64474200
F	3.91122800	0.15907600	0.83239300
F	1.98990400	0.58204100	1.75931100
F	2.76379800	-1.45477100	1.74000900
F	0.67686400	-2.44258400	0.26185100
F	2.59794500	-2.78936000	-0.69765100
F	0.93792700	-1.97126900	-1.84707700
F	0.17997900	2.61314600	1.06905100
F	-0.41214200	3.46459300	-0.86016600
M14-S G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.073195 a.u. E (UωB97X-D/def2-tzvp) = -1181.34393807 a.u.			
C	-3.39634800	1.27292500	-0.87019800
C	-0.37816600	0.34933800	0.57234100
C	-1.48587600	-0.67156900	0.68193800

C	-2.22322500	-0.94350300	-0.61352700
H	-0.68131200	1.34220800	0.87638500
H	-2.03762300	-1.93677100	-1.00862900
C	-3.06143100	-0.11846300	-1.25601100
C	0.86473200	0.14789200	0.13353900
O	-2.76233200	1.95752600	-0.09029200
C	1.41101600	-1.17725700	-0.35832000
C	1.84523400	1.29965200	0.12333300
H	-3.56824200	-0.48966800	-2.14438100
F	-2.36156300	-0.23721100	1.63919400
F	-0.98271200	-1.86784800	1.12722800
H	-4.29433900	1.68353700	-1.37529300
F	0.50204300	-1.83531900	-1.11500000
F	1.75801700	-1.98349100	0.65760800
F	2.50167200	-0.99581200	-1.12574400
F	2.98733200	0.95847500	0.75314800
F	2.16370800	1.66291700	-1.13425600
F	1.34534200	2.38566500	0.74178600
M14-FeCl₃/S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.063280 a.u.			
E (UωB97X-D/def2-tzvp) = -3825.90203868 a.u.			
C	1.10431200	1.95297100	-1.18404000
C	-1.20399500	0.43288100	0.76296400
C	-1.32621600	1.93981800	0.78791800
C	-1.16167100	2.71292200	-0.51304500
H	-0.37128000	0.05889200	1.34591500
H	-2.00855400	3.35749400	-0.72567600
C	-0.09312300	2.75699900	-1.33253800
C	-2.01828400	-0.43917500	0.17116000
O	1.18087900	1.02720700	-0.36338100
C	-3.26912200	-0.08479900	-0.60013800
C	-1.75262100	-1.92510000	0.31280200
H	-0.10289400	3.44481100	-2.17281200
Fe	2.65299000	-0.33111400	-0.00361200
Cl	4.39385300	0.79023100	-0.73948800
Cl	2.45936200	-0.61166400	2.15552000
Cl	2.04891500	-2.01478700	-1.25223100
F	-0.38629300	2.41584400	1.66296300
F	-2.55476600	2.28037100	1.29035800
H	1.96592300	2.16767700	-1.83024400
F	-3.18233400	1.14755100	-1.16164300
F	-4.34544400	-0.08385500	0.20105400
F	-3.49345800	-0.95580600	-1.59648600
F	-2.86489100	-2.55933700	0.73483000
F	-1.39242500	-2.46379400	-0.86408300
F	-0.77148400	-2.16996700	1.19619100
M14-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.063783 a.u.			
E (UωB97X-D/def2-tzvp) = -3825.89998926 a.u.			
C	-1.65601200	-2.54405000	0.81924700
C	-0.39752000	-2.39651100	1.26787600
C	0.60476500	-1.68272600	0.50168000
C	-1.84974500	-0.63092200	-0.92108100
H	-2.39742000	-3.05485700	1.42556900
H	-0.11048600	-2.74907300	2.25391800
H	0.42988000	-1.49430500	-0.56267700

H	-1.28524700	-0.57385300	-1.84685400
C	-2.19269200	-2.05108800	-0.51637500
C	-2.14675100	0.51082000	-0.30238200
O	1.65487100	-1.26609500	1.01284400
Fe	2.91037000	0.07839100	0.09521100
Cl	2.67777100	1.87215000	1.31031000
Cl	1.92306800	0.19051900	-1.88824200
Cl	4.87489300	-0.86251000	0.08940700
C	-2.96717700	0.65842100	0.95974500
C	-1.61707200	1.81956900	-0.86744500
F	-0.59191300	2.26009300	-0.11849400
F	-1.18045200	1.67183600	-2.12803600
F	-2.57265900	2.76555800	-0.86334900
F	-4.16533100	1.19456100	0.68603900
F	-2.34105100	1.45406600	1.84198900
F	-3.18578700	-0.52887800	1.56866200
F	-3.54465700	-2.22634500	-0.51819500
F	-1.67365500	-2.87323600	-1.48982600
M14-TS1 G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.066330 a.u. E (UωB97X-D/def2-tzvp) = -3825.81937752 a.u. Imaginary frequency: 759.8377			
C	-2.06436200	-2.60081200	0.24383100
C	-0.75422900	-2.40720500	0.12619500
C	-0.29196400	-1.14437700	-0.51907400
C	-1.95416400	-0.41985200	-0.86647700
H	-2.54442300	-3.46452800	0.68893000
H	0.03066800	-3.06459600	0.49356200
H	0.08849700	-1.21844700	-1.54530800
H	-2.00718500	-0.30842400	-1.94473500
C	-2.89964600	-1.48809900	-0.31306000
C	-1.42815000	0.66657400	-0.16749700
O	0.43465500	-0.30271600	0.28134900
Fe	2.36023900	-0.25814000	0.08951200
Cl	3.15317700	1.35661200	1.32868800
Cl	2.52180100	0.00123500	-2.11635800
Cl	2.90084500	-2.33651800	0.65405200
C	-1.66796800	0.95088200	1.32822500
C	-0.85019500	1.83561400	-0.99181300
F	0.22223200	2.39289000	-0.46176500
F	-0.57447700	1.44249200	-2.23847600
F	-1.85298900	2.73735500	-1.02933600
F	-2.86763700	1.56141200	1.36589900
F	-0.75314100	1.76752400	1.83272900
F	-1.71215300	-0.16141300	2.05277700
F	-3.76823000	-0.98261000	0.61037300
F	-3.66426400	-1.92760400	-1.35898200
M15-S G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.090975 a.u. E (UωB97X-D/def2-tzvp) = -982.846460453 a.u.			
C	3.84005400	0.48435700	0.56293900
C	0.61527700	-0.12595000	-0.25281200
C	1.34415800	-1.38100900	-0.20230400
C	2.67323000	-1.48532600	-0.39961200
H	4.50752300	0.01758400	1.31798000
H	1.19201800	0.77860400	-0.41375000

H	0.78462600	-2.28654900	0.00361900
H	3.12464200	-2.47042100	-0.31319700
C	3.60921300	-0.33547800	-0.70179200
C	-0.71271500	0.01970000	-0.08698000
O	3.31237800	1.55286500	0.77076900
C	-1.62892200	-1.15063300	0.17674000
C	-1.35446700	1.37909800	-0.15933700
H	4.56881100	-0.72640200	-1.05788300
H	3.19974900	0.33217300	-1.46551800
F	-1.97438400	1.69549000	0.99668400
F	-0.44797600	2.34456500	-0.40976000
F	-2.28167700	1.43281000	-1.13987300
F	-1.57680700	-2.05504000	-0.82943400
F	-2.91057300	-0.77371100	0.31565200
F	-1.27429000	-1.81038800	1.30468000
M15-RS (FeCl₃/S)			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.080935 a.u.			
E (UωB97X-D/def2-tzvp) = -3627.40424012 a.u.			
C	-1.64453000	2.24012500	-0.68149500
C	1.42814900	1.27726900	-0.57227300
C	1.37683200	2.49515900	0.22338800
C	0.45246300	3.45744300	0.06233100
H	-2.49963400	2.14789200	-1.36895800
H	0.88183900	1.26396800	-1.51051000
H	2.12867200	2.62379500	0.99409800
H	0.49127400	4.33249000	0.70392400
C	-0.70078900	3.38539600	-0.90242500
C	2.09017300	0.15320100	-0.25498400
O	-1.46418500	1.39487600	0.18943300
Fe	-2.17814500	-0.54394100	0.25208100
Cl	-4.25622300	-0.29176900	0.88170500
Cl	-0.84790400	-1.57712200	1.62534600
Cl	-1.93221500	-0.98100900	-1.89039100
H	-1.29661900	4.30836000	-0.90796100
H	-0.36958600	3.27087500	-1.95013900
C	2.84735200	0.00970700	1.04532700
C	2.10786300	-1.02691700	-1.19354100
F	3.87698400	0.89151900	1.10573500
F	2.05264700	0.27059300	2.10286900
F	3.35708700	-1.22005700	1.20236100
F	1.54906500	-2.11557100	-0.64086500
F	3.37628900	-1.34407600	-1.53202400
F	1.44148900	-0.75617500	-2.33487700
M15-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.084943 a.u.			
E (UωB97X-D/def2-tzvp) = -3627.31382092 a.u.			
Imaginary frequency: 778.1856			
C	0.22274100	1.32354100	-0.87151800
C	2.05686900	1.17782100	-0.87122200
C	2.41326800	2.46598700	-0.20453800
C	1.39564300	3.32628000	-0.12485200
H	-0.01521600	0.92439800	-1.86029600
H	2.31048700	1.07504500	-1.92659000
H	3.42301400	2.65839200	0.14272700
H	1.47917300	4.32243400	0.29749100
C	0.08154200	2.82270600	-0.66549700

C	1.84125700	-0.03242700	-0.20211400
O	-0.21674800	0.54193800	0.16558700
Fe	-2.00126300	-0.19286100	0.14407900
Cl	-3.29930000	1.56973900	0.50120300
Cl	-2.09612100	-1.78423500	1.64772500
Cl	-2.12888900	-0.84809300	-1.98575100
H	-0.74367000	2.95698600	0.04785500
H	-0.18909000	3.32971500	-1.60031800
C	2.04781800	-0.21382300	1.30831900
C	1.70755900	-1.33091000	-1.01553200
F	3.36672500	-0.50451100	1.41890000
F	1.79912600	0.89135400	2.00029700
F	1.34141400	-1.21852000	1.80546200
F	0.77005900	-2.14292200	-0.55711500
F	2.90737800	-1.93850900	-0.92586000
F	1.46143500	-1.06012600	-2.30433900
M16-S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.092157 a.u.			
E (UωB97X-D/def2-tzvp) = -982.843162389 a.u.			
C	4.07024600	0.65081600	0.16298900
C	0.57107100	0.25954200	-0.47768900
C	1.54609500	-0.85668800	-0.75066500
C	2.33918700	-1.11740900	0.50890700
H	0.99945100	1.25568100	-0.50846500
H	1.03280100	-1.76866000	-1.05789700
H	1.94642600	-1.90307100	1.15052900
C	3.43858200	-0.45229100	0.90848800
C	-0.72014400	0.12139500	-0.16194300
O	3.57615300	1.23414700	-0.79005800
C	-1.38352300	-1.23163900	-0.07101200
C	-1.58602000	1.32126200	0.11663300
H	2.21478800	-0.52600600	-1.54915200
H	3.93356400	-0.74624900	1.83159300
H	5.07451900	0.94621300	0.53250300
F	-0.70170600	-2.05817700	0.76353700
F	-1.42306200	-1.85059400	-1.27333600
F	-2.64788300	1.36366400	-0.71549200
F	-2.64351500	-1.15433300	0.38593000
F	-2.06537100	1.30415200	1.37849900
F	-0.90332200	2.47295400	-0.03834600
M16-FeCl3/S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.082549 a.u.			
E (UωB97X-D/def2-tzvp) = -3627.40430579 a.u.			
C	1.48094200	1.96666900	-1.00609300
C	-1.38482800	0.31790100	0.27245100
C	-1.04551200	1.71498500	0.75280500
C	-0.84453200	2.60459200	-0.44570300
H	-0.54084700	-0.32246500	0.03701200
H	-1.84875000	2.12049100	1.36880600
H	-1.71212400	3.19070600	-0.73873200
C	0.26985000	2.72125900	-1.20939300
C	-2.61923100	-0.16048100	0.09723100
O	1.59607800	1.09451900	-0.12111200
C	-3.85410500	0.66090700	0.38968000
C	-2.84325900	-1.57002900	-0.39468700
H	-0.13017600	1.65917200	1.34618300

H	0.27441200	3.40714500	-2.05125200
Fe	3.00766000	-0.32200700	0.15649400
Cl	4.39131900	0.15613100	-1.48802400
Cl	3.76672300	0.03085600	2.17258400
Cl	1.80226600	-2.13595000	-0.11417000
H	2.33402200	2.15062900	-1.67285000
F	-3.80703300	1.85771200	-0.25559200
F	-3.96106200	0.94142600	1.70739000
F	-3.59097500	-2.27182600	0.47980800
F	-4.98069600	0.04615300	0.00877600
F	-3.49141000	-1.57066000	-1.57801700
F	-1.68277000	-2.22415000	-0.56497500
M16-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.083237 a.u.			
E (UωB97X-D/def2-tzvp) = -3627.40345391 a.u.			
C	-1.29331900	-3.36358900	-0.94119800
C	0.03578000	-3.15308300	-0.82440200
C	0.59202700	-1.95950000	-0.22646400
C	-2.20220700	-1.00515800	-1.01946800
H	-1.60511600	-4.30218500	-1.39446100
H	0.74798600	-3.87583700	-1.21262900
H	-0.05545500	-1.30366300	0.36195700
H	-1.93749500	-0.89480000	-2.06721000
C	-2.41177200	-2.42274800	-0.54732700
C	-2.31934700	0.10825700	-0.29189400
O	1.79440700	-1.66672600	-0.35079900
Fe	2.51587500	0.19069700	0.11591800
Cl	1.20618200	0.72115500	1.80614500
Cl	2.02364300	1.27582800	-1.72374600
Cl	4.63020000	-0.05201800	0.58670300
C	-2.68209900	0.07606100	1.17650500
C	-2.09484500	1.46883100	-0.91142700
F	-1.08055800	2.11232100	-0.31499500
F	-1.80807900	1.36601800	-2.22370000
F	-3.20010900	2.23261300	-0.79231300
F	-3.90596200	-0.47059800	1.35871400
F	-2.68154800	1.28904300	1.73325300
F	-1.81016400	-0.70102000	1.87353900
H	-2.56606400	-2.46995400	0.53491700
H	-3.33978800	-2.79207900	-1.00122100
M16-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.085037 a.u.			
E (UωB97X-D/def2-tzvp) = -3627.31584801 a.u.			
Imaginary frequency: 741.6891			
C	-1.71306300	-3.17090600	-0.30288000
C	-0.47446300	-2.69902500	-0.42037400
C	-0.32518400	-1.26492300	-0.78970000
C	-2.12629700	-0.90419700	-1.04385600
H	-1.94576500	-4.19336100	-0.02389000
H	0.44682400	-3.24398100	-0.22917700
H	0.06966000	-1.03658700	-1.78576800
H	-2.18458300	-0.68187000	-2.10431300
C	-2.81895900	-2.17580900	-0.57274300
C	-1.78366600	0.18126300	-0.23355600
O	0.18814400	-0.43443300	0.19094900
Fe	2.05637500	0.05016000	0.14106100

Cl	2.41548200	1.57684600	1.66850400
Cl	2.24286100	0.71093200	-1.97960800
Cl	3.07213600	-1.90324600	0.42067800
C	-2.10285200	0.23078200	1.26881400
C	-1.45612800	1.53010200	-0.89719000
F	-0.52499600	2.23064600	-0.27564200
F	-1.10144700	1.35446600	-2.17438400
F	-2.62205400	2.21185000	-0.86066700
F	-3.41712500	0.55006400	1.32328000
F	-1.40877300	1.15490500	1.91427000
F	-1.93039400	-0.94983100	1.86085600
H	-3.44142600	-2.01830600	0.31319200
H	-3.48697700	-2.52423100	-1.36849600
M17-S G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.115951 a.u. E (UωB97X-D/def2-tzvp) = -1564.24672477 a.u.			
C	-2.24809200	0.82943500	-1.07386900
C	0.39932100	-0.07362700	0.06561000
C	-0.39704900	-1.28023900	0.18074900
C	-1.74806400	-1.32978100	0.15650800
H	-1.67451600	0.40826100	-1.92730800
H	-0.12305600	0.87678600	0.05236700
H	0.13195300	-2.21520200	0.32774300
H	-2.19440100	-2.30712300	0.33384600
C	-2.70375400	-0.18632700	-0.05263400
C	1.74321700	-0.01381800	0.00598000
O	-2.50196300	2.01587100	-1.01673900
C	2.60874000	-1.25008600	0.01654800
C	2.45374800	1.31040400	-0.06830500
F	3.16769800	1.42591200	-1.20734200
F	1.58570100	2.34227400	-0.03109300
F	3.31155000	1.46660200	0.96178900
F	2.47343400	-1.93614600	1.17620200
F	3.91152600	-0.95990700	-0.13232200
F	2.26437500	-2.10199400	-0.97691900
Si	-4.35817100	-0.87907200	-0.72750100
H	-4.83947000	-1.89813700	0.22868700
H	-5.34088900	0.21044000	-0.86562900
H	-4.11646400	-1.51670500	-2.03986600
Si	-3.03944200	0.69786500	1.61264500
H	-4.21168100	1.58884000	1.53181500
H	-3.30067000	-0.35332400	2.61880400
H	-1.82547200	1.44967400	1.98509800
M17-FeCl₃/S G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.106357 a.u. E (UωB97X-D/def2-tzvp) = -4208.80602680 a.u.			
C	1.08260200	1.28943400	-0.33270300
C	-1.68615700	0.77520600	0.33922800
C	-1.75537000	2.16011600	-0.10108900
C	-0.70081100	3.00138600	-0.16156800
H	0.56444800	0.89611900	-1.21947100
H	-0.80873600	0.46602500	0.89872500
H	-2.72817700	2.54723200	-0.38402500
H	-0.89777200	4.03507700	-0.43626700
C	0.73197800	2.63656700	0.13912300
C	-2.62263500	-0.16834600	0.14915800

O	1.94827000	0.58649400	0.21680400
C	-3.89523600	0.10756000	-0.61672300
C	-2.42985400	-1.56414700	0.68791700
Fe	2.35474200	-1.36694500	-0.19963600
Cl	0.74499700	-1.76464900	-1.65918300
Cl	2.11559600	-2.34575100	1.73481200
Cl	4.36803900	-1.34018000	-1.04505300
F	-2.41302100	-2.47160500	-0.30229800
F	-1.27098500	-1.67029000	1.36757800
F	-3.42893900	-1.89456200	1.53258500
F	-4.64324100	1.04860900	0.00935200
F	-4.65323100	-0.98833000	-0.75655800
F	-3.62537900	0.58711500	-1.85103700
Si	1.89846700	3.82534900	-0.85020700
H	1.55006900	5.18637100	-0.39996400
H	3.29742500	3.48928600	-0.54199000
H	1.61459900	3.67111100	-2.28997100
Si	1.11149700	2.85549000	2.01465000
H	2.56277800	2.81670800	2.26493000
H	0.56386800	4.17106800	2.39591000
H	0.41186600	1.77263800	2.72957600
M17-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.109284 a.u.			
E (UωB97X-D/def2-tzvp) = -4208.7992832 a.u.			
C	0.45746300	-1.25225900	-0.45752400
C	-2.28948800	-0.39932800	-1.40615400
C	-2.36634600	-1.87002000	-1.36979500
C	-1.49299400	-2.77190900	-0.89642700
H	0.25503200	-0.72753000	-1.40043300
H	-2.25572400	0.02296400	-2.40971500
H	-3.24186900	-2.26690900	-1.88405200
H	-1.77581400	-3.81680200	-1.00657900
C	-0.16292200	-2.55598800	-0.22175700
C	-2.32194800	0.49575700	-0.41030800
O	1.26593800	-0.74443600	0.33923800
Fe	2.24034200	1.01838900	0.09838000
Cl	1.38107100	1.64597600	-1.84376300
Cl	4.34187000	0.42197400	-0.02163700
Cl	1.68658900	2.24636200	1.80937000
C	-2.40753800	0.17235700	1.06086600
C	-2.27508400	1.97806000	-0.72454700
F	-3.25998900	0.99502000	1.69195800
F	-2.82211700	-1.09260800	1.28571400
F	-1.19800500	0.30877200	1.64898900
F	-1.36960500	2.59976300	0.04969100
F	-3.47219000	2.55683800	-0.50109300
F	-1.95445500	2.20142000	-2.01208400
Si	1.07296300	-3.77122600	-1.11800400
H	2.42516100	-3.58984300	-0.56824100
H	0.54639400	-5.12263700	-0.84628100
H	1.03502300	-3.48421800	-2.56483300
Si	-0.14757000	-3.08828400	1.63460100
H	-1.16680100	-4.14957900	1.74944400
H	1.17715200	-3.65324800	1.95964000
H	-0.45206700	-1.94786700	2.50472600
M17-TS1			

$G_{\text{corr}}(\text{UB3LYP-D3BJ/6-31G}^*/\text{Lan2LDZ}) = 0.109917 \text{ a.u.}$ $E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -4208.70957726 \text{ a.u.}$ Imaginary frequency: 722.1529			
C	0.45322900	-1.03404400	-0.45780900
C	-1.01993000	-1.99889500	-0.36941400
C	-0.60111700	-3.04588600	0.61000300
C	0.72818600	-3.08400200	0.77811400
H	0.49659800	-0.75254600	-1.51070900
H	-1.18281600	-2.35186900	-1.39079900
H	-1.31894200	-3.68858500	1.10665300
H	1.23508700	-3.80805100	1.40917800
C	1.49297000	-2.03328000	0.02503400
C	-1.80352000	-0.87666000	-0.03236900
O	0.22611800	0.04656300	0.37633500
Fe	0.89553700	1.81063500	-0.03591800
Cl	2.20702800	1.31184200	-1.78747300
Cl	1.98818500	2.53752000	1.73267300
Cl	-0.78256200	3.11253000	-0.62240900
C	-2.20663400	-0.48629900	1.38918300
C	-2.54241500	-0.16470400	-1.17305300
F	-3.49549600	-0.90000700	1.49050000
F	-1.48901200	-1.10949700	2.31917100
F	-2.15433300	0.82080100	1.59819900
F	-3.11463200	0.97169700	-0.81130800
F	-3.50349300	-1.02334500	-1.57946900
F	-1.71120400	0.05285000	-2.19944100
Si	2.49061600	-2.80454300	-1.40588000
H	3.52518200	-1.87027600	-1.88333400
H	3.10143500	-4.06196900	-0.93056600
H	1.53598200	-3.10472400	-2.49812700
Si	2.69942100	-1.19117000	1.29072500
H	3.65313800	-2.28971000	1.57792000
H	3.40366900	-0.07003600	0.66262500
H	1.99109900	-0.83330300	2.52806500
M18-S			
$G_{\text{corr}}(\text{UB3LYP-D3BJ/6-31G}^*/\text{Lan2LDZ}) = 0.120961 \text{ a.u.}$ $E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -1564.23631842 \text{ a.u.}$			
C	-4.33529400	0.52052200	-0.06193300
C	0.20584300	0.89425800	-0.06162500
C	-1.22342200	0.42413300	-0.03137500
C	-2.12199100	1.61654100	-0.17938900
H	0.30847900	1.97626200	-0.11006700
H	-1.60323800	2.56981300	-0.29002000
C	-3.47531500	1.68193900	-0.19661000
C	1.38468300	0.25338100	-0.03070800
O	-3.91464900	-0.62810900	0.07758300
C	1.60324200	-1.23282200	0.01643800
C	2.66481900	1.05604900	-0.03310800
H	-3.95530700	2.64878500	-0.31549400
Si	-1.60307800	-0.43948200	1.68289900
H	-2.67049200	0.31121400	2.36963800
H	-1.92919600	-1.86763400	1.58558900
H	-0.36777100	-0.28189600	2.48141200
Si	-1.59588600	-0.83425300	-1.47967300
H	-0.34724600	-0.88915200	-2.26965300
H	-1.94036600	-2.19254700	-1.04227500

H	-2.64162100	-0.26417900	-2.34881700
H	-5.42591600	0.70410500	-0.08874200
F	0.45161900	-1.90377500	0.28738200
F	2.06371100	-1.71282000	-1.15395500
F	3.27566300	1.02154400	1.16930200
F	2.44967500	2.35642500	-0.33024400
F	3.54256000	0.57506700	-0.93777500
F	2.49010200	-1.57439700	0.96889700
M18-FeCl₃/S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.112035 a.u.			
E (UωB97X-D/def2-tzvp) = -4208.79931109 a.u.			
C	1.99894300	-2.13561500	-0.16328800
C	-2.47540000	-1.07583600	-0.04260400
C	-0.96851900	-1.04084500	-0.06724800
C	-0.46139800	-2.42574700	-0.17998600
H	-2.88986400	-2.08164600	-0.03451000
H	-1.23442500	-3.19396900	-0.23666400
C	0.81639600	-2.91809600	-0.22565600
C	-3.41079700	-0.11581400	-0.01468100
O	1.97836900	-0.87859800	-0.06147500
C	-3.18349200	1.37126700	-0.04044400
C	-4.87065000	-0.50832100	0.05701600
H	0.95348400	-3.99066200	-0.31210100
Fe	3.57946300	0.35797800	0.03633300
Cl	5.22960900	-1.10594500	-0.04293700
Cl	3.40363700	1.62015800	-1.74329800
Cl	3.36668400	1.38439300	1.95752800
Si	-0.29856900	-0.24786300	1.61327800
H	0.55701200	-1.25080500	2.27050800
H	0.41031800	1.01481300	1.40064600
H	-1.50395600	-0.04318500	2.43859800
Si	-0.29416600	0.02139800	-1.58524800
H	-1.50217600	0.38927800	-2.34598500
H	0.44200800	1.21585500	-1.16860300
H	0.53332100	-0.86948400	-2.41654200
H	2.97398300	-2.63329100	-0.20223600
F	-1.87695600	1.68158300	0.18410500
F	-3.50935800	1.90500000	-1.23029000
F	-5.38471200	-0.26449600	1.27829600
F	-5.05312400	-1.82185600	-0.19822400
F	-5.60419600	0.18529200	-0.83476400
F	-3.90540000	1.99811200	0.90209600
M18-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.107782 a.u.			
E (UωB97X-D/def2-tzvp) = -4208.79493056 a.u.			
C	-0.56539900	-1.47260100	0.93902000
C	0.48375800	-0.63278100	0.74971400
C	0.64024200	0.25458700	-0.37229900
C	-2.47733200	-0.63677500	-0.62173200
H	-0.47143100	-2.12833800	1.80373400
H	1.30204700	-0.65025100	1.46292700
H	-0.21548200	0.46359600	-1.02144800
H	-2.87712700	-0.88522200	-1.60230200
C	-1.73852000	-1.76017500	0.05117600
C	-2.80956700	0.59061500	-0.18842900
O	1.71273700	0.81379100	-0.67270500

Fe	3.58650600	0.30763600	-0.08009800
Cl	4.95577200	1.51902900	-1.26812500
Cl	3.54517300	-1.84674300	-0.56167600
Cl	3.62357400	0.67554000	2.09113600
C	-2.42487200	1.20976000	1.13523000
C	-3.60967600	1.50449800	-1.09295300
F	-3.00942200	2.70711800	-1.19427600
F	-3.72597000	0.99961600	-2.33854200
F	-4.85452200	1.70430700	-0.62460100
F	-3.35130200	2.08821700	1.54692100
F	-1.25052800	1.87626500	1.04620200
F	-2.28861300	0.28329500	2.10866200
Si	-3.08120800	-2.79129300	0.96612600
H	-3.60594000	-2.01662300	2.10326800
H	-4.15662200	-3.09616000	0.00423900
H	-2.45100000	-4.04285100	1.43687800
Si	-0.97986200	-2.91006100	-1.30616500
H	-0.22274200	-3.98901400	-0.65104000
H	-2.08742400	-3.46101100	-2.11603400
H	-0.09576200	-2.06916700	-2.13583400
M18-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.108304 a.u.			
E (UωB97X-D/def2-tzvp) = -4208.69996338 a.u.			
Imaginary frequency: 736.1031			
C	-1.84972600	-2.08411900	0.57077300
C	-0.56311900	-2.03120100	0.22938600
C	-0.13839600	-0.91124600	-0.65533400
C	-1.81389300	-0.04260600	-0.74595900
H	-2.26283900	-2.85741200	1.21150500
H	0.21519700	-2.70658100	0.57197600
H	0.01706300	-1.13795300	-1.71501300
H	-1.97664800	0.08311000	-1.81278100
C	-2.74962500	-1.02372300	-0.02787300
C	-1.02996800	0.99179500	-0.21393300
O	0.78939500	-0.02511800	-0.14932900
Fe	2.63974100	-0.49278900	0.07119600
Cl	3.86662700	1.27961800	-0.31967000
Cl	2.64654800	-2.08274600	-1.51124800
Cl	2.83011800	-1.38468800	2.08046200
C	-0.94567900	1.37145000	1.27058000
C	-0.51275200	2.05248000	-1.20426700
F	0.61780400	2.63402000	-0.84928100
F	-0.36630100	1.52408700	-2.42786300
F	-1.49107300	2.98302700	-1.25157300
F	-2.03626100	2.14999900	1.48311500
F	0.13586700	2.07208100	1.57505700
F	-1.01449100	0.30889000	2.06801500
Si	-4.05823500	-0.30681800	1.17373100
H	-3.53316000	-0.05798800	2.52564000
H	-4.59867300	0.93101400	0.57906600
H	-5.13776700	-1.31528000	1.25830000
Si	-3.76245700	-1.92655000	-1.39024000
H	-4.34324700	-3.15383600	-0.81741500
H	-4.83522800	-1.04261900	-1.89614100
H	-2.83036200	-2.25491200	-2.49020900
M19-S			

G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.098852 a.u. E (UωB97X-D/def2-tzvp) = -883.580438043 a.u.			
C	-2.67763100	-0.92118900	0.96730400
C	0.29716100	0.50337400	-0.00459700
C	-0.70591700	1.52910700	0.21891400
C	-2.03934500	1.36161100	0.12920400
H	-3.49384000	-0.77955400	1.70451200
H	-0.05818200	-0.48699500	-0.26012200
H	-0.35767000	2.52342100	0.48440900
H	-2.71292400	2.18499200	0.34527500
C	-2.72763400	0.07159800	-0.20873200
C	1.62626300	0.69344300	0.10384000
O	-1.81160500	-1.75036400	1.08800000
C	2.34852800	1.96415300	0.45090100
H	2.98562100	1.80834100	1.32905500
H	3.00645600	2.26348500	-0.37306500
H	1.66777900	2.78912300	0.66347800
C	2.54845700	-0.47377900	-0.13853800
F	-4.05335900	0.32309000	-0.46308900
F	-2.18897300	-0.52794200	-1.30995200
F	3.27281700	-0.74944000	0.97396700
F	1.91101600	-1.60222600	-0.49454000
F	3.44031100	-0.18457200	-1.11830900
M19-FeCl₃/S G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.090696 a.u. E (UωB97X-D/def2-tzvp) = -3528.13024785 a.u.			
C	-1.58043000	1.65165300	-0.23353200
C	1.64363500	1.34492400	0.13640000
C	1.09235000	2.34706700	1.02419600
C	0.00830700	3.11713800	0.77454100
H	-2.46889900	1.65281500	0.41339100
H	1.31653900	1.35406600	-0.89388700
H	1.57562300	2.48932000	1.98680300
H	-0.36463900	3.81187800	1.51976600
C	-0.86715600	2.97859700	-0.43612800
C	2.49124900	0.36986200	0.52205400
O	-1.10345600	0.61157500	-0.68130700
C	3.03280000	0.11807400	1.89513300
H	2.55342300	-0.77297500	2.31720400
H	4.10936100	-0.07574000	1.84798400
H	2.85479600	0.95168200	2.57585700
C	2.92387900	-0.65363200	-0.50317100
Fe	-1.46321900	-1.27525800	0.07375100
Cl	-0.42503800	-1.13308400	2.00766300
Cl	-0.65663800	-2.67480000	-1.37352600
Cl	-3.64618500	-1.16035100	0.28395900
F	-1.79799000	3.97352500	-0.46639600
F	-0.19148100	2.97350700	-1.61529600
F	2.59039300	-1.89494400	-0.09336100
F	2.37460700	-0.45883000	-1.71515200
F	4.26902400	-0.62981900	-0.65632700
M19-RS G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.091901 a.u. E (UωB97X-D/def2-tzvp) = -3528.12704356 a.u.			
C	0.46348500	1.42271000	-0.26182200
C	2.71969000	-0.18884100	-0.87106100

C	3.39452100	1.11431100	-0.82660000
C	2.89869300	2.25322100	-0.32902100
H	0.40096900	1.22895900	-1.33928000
H	2.64945800	-0.65265500	-1.85258800
H	4.38250800	1.14956500	-1.28504700
H	3.48191600	3.16975100	-0.33364700
C	1.51810000	2.42575100	0.21499600
C	2.26818300	-0.88676200	0.18816200
O	-0.37101300	0.98424700	0.52075500
Fe	-2.08071900	-0.06798400	-0.03877600
Cl	-1.37996400	-0.82190700	-1.98820900
Cl	-3.50924500	1.57430300	-0.23019800
Cl	-2.52530400	-1.49090400	1.54275900
C	2.36178600	-0.51201600	1.63762400
C	1.63962700	-2.24167200	-0.05609300
F	0.41997900	-2.29732400	0.51948200
F	2.39182300	-3.21369400	0.50802300
F	1.49929400	-2.53993400	-1.35787700
F	1.50654500	2.48574400	1.57213900
F	1.01398700	3.62327600	-0.25060000
H	2.97947600	0.37288800	1.78865400
H	1.36501300	-0.31486000	2.04894600
H	2.78501600	-1.34821100	2.20349200
M19-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.092113 a.u.			
E (UωB97X-D/def2-tzvp) = -3528.08927989 a.u.			
Imaginary frequency: 611.9122			
C	0.77967500	0.92138800	-0.54758900
C	2.30134800	0.20517200	-0.86319100
C	3.22066900	1.38851900	-0.78897800
C	2.65525600	2.48708300	-0.28655100
H	0.37185100	1.13640000	-1.54555400
H	2.23244100	-0.29096900	-1.83216700
H	4.23885400	1.32157700	-1.15928200
H	3.12851400	3.45314400	-0.15310500
C	1.23420800	2.24835300	0.12347200
C	2.16967300	-0.69679900	0.23861000
O	0.01354000	0.10518300	0.21429600
Fe	-1.87890800	-0.09319400	0.00249300
Cl	-2.05068100	0.36578100	-2.18250500
Cl	-2.89408500	1.40765400	1.25676900
Cl	-2.36517900	-2.18112000	0.53045400
C	2.60134900	-0.45558000	1.61798000
C	1.62554800	-2.09848300	-0.05482700
F	0.92777800	-2.59484800	0.95478600
F	2.76210800	-2.83278500	-0.20942700
F	0.92533000	-2.16610300	-1.17981400
F	1.13809800	2.14776200	1.48530600
F	0.40014600	3.24742000	-0.26355700
H	2.99110000	0.54702400	1.77088200
H	1.76517200	-0.66048000	2.29589100
H	3.37690900	-1.20539300	1.84471700
M20-S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.098820 a.u.			
E (UωB97X-D/def2-tzvp) = -883.575956175 a.u.			
C	3.02820400	1.57410600	0.40427000

C	-0.00947100	-0.10302000	-0.38160200
C	1.25190300	-0.92133600	-0.35971600
C	2.06425000	-0.70874100	0.89979000
H	0.15460600	0.88859900	-0.78433700
H	1.98638800	-1.53443800	1.60255200
C	2.83486300	0.34391700	1.20955100
C	-1.20857100	-0.45438000	0.09130100
O	2.28740900	1.96728100	-0.47555900
C	-1.62507800	-1.74295900	0.74796300
H	-0.79036700	-2.42818800	0.87161300
H	-2.06970300	-1.53104200	1.72668900
H	-2.39554800	-2.23857400	0.14643200
C	-2.33095000	0.55097000	-0.01504100
H	3.39777600	0.31142800	2.14068900
F	1.99531800	-0.61796300	-1.46660000
F	0.98566600	-2.27303700	-0.43844700
H	3.92499600	2.16379200	0.68750300
F	-1.97468500	1.70241100	-0.61198300
F	-2.80905900	0.86528700	1.21393700
F	-3.36816300	0.03428300	-0.71532600
M20-FeCl₃/S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.087877 a.u.			
E (UωB97X-D/def2-tzvp) = -3528.13610283 a.u.			
C	-0.69273200	1.52976300	1.43538800
C	1.82048800	0.43957400	-0.57734100
C	1.67243400	1.93980500	-0.58594400
C	1.46215700	2.58465800	0.77610100
H	1.06923400	-0.10006500	-1.14048900
H	2.25791900	3.27147300	1.05250900
C	0.44085300	2.41319700	1.63853900
C	2.79362500	-0.20909500	0.06694100
O	-0.83929800	0.85098200	0.40837700
C	3.88336600	0.39340500	0.91091900
H	3.96854700	1.46945400	0.75950200
H	3.69942900	0.19194800	1.97282200
H	4.84563500	-0.06167100	0.65753300
C	2.82909100	-1.71803900	0.00406700
H	0.44544700	2.96297300	2.57522500
Fe	-2.37825900	-0.38918400	-0.08822500
Cl	-3.29984900	-0.63954200	1.89972600
Cl	-3.56185200	0.78848600	-1.49373200
Cl	-1.36719000	-2.13951200	-0.91067400
F	0.64466200	2.29314600	-1.41116600
F	2.81141600	2.52186700	-1.10183800
H	-1.44406700	1.45619200	2.23299200
F	1.88051200	-2.24425800	-0.78227800
F	2.67338500	-2.23285800	1.24693900
F	4.02807200	-2.14670900	-0.45340500
M20-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.089817 a.u.			
E (UωB97X-D/def2-tzvp) = -3528.13786046 a.u.			
C	0.04318400	-1.56610100	-0.32962300
C	2.53114900	-0.16565100	0.59429700
C	3.09476500	-1.50923200	0.21729400
C	2.34110600	-2.34664000	-0.80083300
H	0.30004300	-1.12336300	0.63659900

H	2.30714500	-0.04650900	1.64906600
H	2.99852500	-2.99564200	-1.37432800
C	1.02114600	-2.36288500	-1.05218900
C	2.32008500	0.83576700	-0.26384800
O	-1.09612700	-1.39010100	-0.78768300
Fe	-2.50640700	-0.13575700	0.01467600
Cl	-1.48146500	0.41625800	1.89317600
Cl	-4.28214400	-1.37557600	0.27236900
Cl	-2.63519800	1.45736100	-1.47129900
C	2.58317500	0.82878700	-1.74298000
C	1.70341600	2.11725500	0.25135700
F	0.50911800	2.31560500	-0.34662800
F	2.48631300	3.17609400	-0.05096500
F	1.50968300	2.11611000	1.57937000
H	3.15267600	-0.04630900	-2.05473800
H	1.63666800	0.86162200	-2.29591200
H	3.14898000	1.72371900	-2.02073100
H	0.62602700	-2.97981100	-1.85469600
F	4.36528400	-1.35799900	-0.29108400
F	3.20928000	-2.27178200	1.35282000
M20-TS1 $G_{\text{corr}}(\text{UB3LYP-D3BJ/6-31G}^*/\text{Lan2LDZ}) = 0.090640 \text{ a.u.}$ $E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -3528.08977765 \text{ a.u.}$ Imaginary frequency: 602.9094			
C	0.59046800	-0.91946000	0.40705100
C	2.16613200	-0.12250800	0.49418900
C	3.14043700	-1.22186800	0.05657600
C	2.32725800	-2.40731700	-0.35850600
H	0.30330500	-0.94355800	1.46723100
H	2.30396600	0.19718300	1.52408900
H	2.81230600	-3.29282400	-0.75281600
C	1.02063900	-2.23377800	-0.17019400
C	1.71461600	0.86933800	-0.40129900
O	-0.28544100	-0.22073800	-0.37479000
Fe	-2.15842000	-0.26548800	-0.03279900
Cl	-2.18435300	0.04450200	2.17624700
Cl	-2.72594700	-2.35615700	-0.54261300
Cl	-3.04610600	1.33155200	-1.25716800
C	1.81994700	0.83772200	-1.86397800
C	1.13492700	2.14867500	0.21567700
F	0.18553200	2.69298500	-0.53251600
F	2.19620200	2.99103100	0.26427400
F	0.68065100	1.95702300	1.45192000
H	1.98475400	-0.16799000	-2.24510900
H	0.94604200	1.30672500	-2.31872900
H	2.71000900	1.44118000	-2.11519500
H	0.23110600	-2.93727200	-0.42226100
F	3.96611300	-0.79350000	-0.95723300
F	3.95853900	-1.51175300	1.11098600
M21-S $G_{\text{corr}}(\text{UB3LYP-D3BJ/6-31G}^*/\text{Lan2LDZ}) = 0.116715 \text{ a.u.}$ $E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -685.073595963 \text{ a.u.}$			
C	-3.27761100	-0.88245300	0.44106400
C	-0.22167300	0.51343800	-0.10711800
C	-1.22739200	1.55032300	0.04512800
C	-2.54028700	1.39311800	-0.21420500

H	-4.00977200	-0.61637700	1.23422800
H	-0.57454000	-0.47501700	-0.38173500
H	-0.89857900	2.52752800	0.38852500
H	-3.20483700	2.23520100	-0.03830400
C	-3.18025600	0.11229600	-0.70649200
C	1.10160300	0.67051100	0.08986800
O	-2.59130800	-1.87493700	0.53421900
C	1.82092400	1.92652600	0.49550000
H	2.38594300	1.75964000	1.41987700
H	2.54510700	2.21707000	-0.27454700
H	1.13891400	2.76218300	0.65634600
C	2.01479300	-0.50975500	-0.10197400
H	-4.18892900	0.32457600	-1.08041800
H	-2.60165100	-0.35215600	-1.51037000
F	1.37991600	-1.62989100	-0.49334500
F	2.67786100	-0.80105100	1.04517800
F	2.96424600	-0.23874500	-1.03383000
M21-FeCl₃/S G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.109197 a.u. E (UωB97X-D/def2-tzvp) = -3329.63277598 a.u.			
C	-1.23994600	2.11436700	-0.84471600
C	1.81650500	1.33678500	-0.23070500
C	1.42742100	2.58515100	0.39478900
C	0.51127200	3.44669300	-0.09844400
H	-2.06744200	2.40440000	-0.18159600
H	1.52210200	1.18342400	-1.26164600
H	1.90216600	2.85026100	1.33554600
H	0.26219900	4.33957900	0.46643300
C	-0.32173400	3.17990300	-1.34608100
C	2.46665200	0.32950700	0.38246400
O	-1.01814400	0.91603900	-1.05912300
C	2.90120500	0.26767600	1.81525700
H	2.25251800	-0.42544400	2.36334600
H	3.92728500	-0.10771400	1.88764100
H	2.84694000	1.23934500	2.30841100
C	2.75579600	-0.92804700	-0.40011800
Fe	-1.70433300	-0.61622600	0.10498600
Cl	-0.72452500	-0.18201800	2.03002000
Cl	-1.11723500	-2.45802200	-0.89022700
Cl	-3.85165300	-0.14252300	0.15043500
H	-0.87608900	4.07472300	-1.64042000
H	0.26715900	2.80955100	-2.18896800
F	2.28344600	-0.89382000	-1.66118500
F	2.21438400	-2.00126600	0.21243500
F	4.09172500	-1.14526700	-0.47502600
M21-RS G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.109574 a.u. E (UωB97X-D/def2-tzvp) = -3329.63012476 a.u.			
C	-0.27350500	1.16233000	1.09883300
C	-3.04508500	1.14855000	0.46569400
C	-2.74567400	2.56085000	0.18593700
C	-1.51306100	3.05790000	-0.00024700
H	-0.91368500	1.30895400	1.97830000
H	-3.59157700	0.94312600	1.38402800
H	-3.58756000	3.25193400	0.19792700
H	-1.39573800	4.12140400	-0.18873600

C	-0.24301500	2.24850300	0.06902500
C	-2.70140700	0.10606700	-0.31255200
O	0.43999300	0.15572100	1.08129200
Fe	2.11237400	-0.27556200	-0.00516400
Cl	3.32212600	1.48172600	0.54346900
Cl	1.56687500	-0.24744000	-2.13935800
Cl	2.81270500	-2.19671100	0.73817900
C	-2.07477900	0.17385900	-1.67305100
C	-2.95298800	-1.29509500	0.18696500
F	-1.77683300	-1.95628100	0.30037100
F	-3.72343000	-1.99544800	-0.67255100
F	-3.55420900	-1.33308500	1.39290100
H	-2.04707200	1.19958300	-2.04379600
H	-1.05613300	-0.22900500	-1.66691800
H	-2.65147800	-0.43826900	-2.37475300
H	0.60472800	2.88861000	0.36603900
H	0.05517500	1.81926700	-0.89720800
M21-TS1 G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.111043 a.u. E (UωB97X-D/def2-tzvp) = -3329.57611649 a.u. Imaginary frequency: 144.8533			
C	-0.62830000	1.29708100	1.10395200
C	-2.19910100	1.07925700	0.68347200
C	-2.58451200	2.43834100	0.15859400
C	-1.52381600	3.22677000	-0.03659400
H	-0.64910600	1.53473700	2.17545300
H	-2.74366000	0.75473100	1.57463100
H	-3.61951200	2.70689000	-0.02829400
H	-1.57731400	4.24327900	-0.41430300
C	-0.22078000	2.55698900	0.29652700
C	-2.15909300	-0.01647100	-0.29090000
O	0.09492700	0.14458700	0.88602100
Fe	1.70404200	-0.22061300	0.08498300
Cl	3.20152700	1.31245500	0.60169800
Cl	1.11208000	0.08911800	-2.18969000
Cl	2.27609200	-2.31234200	0.42755800
C	-1.93658700	0.13885300	-1.67180800
C	-2.26036300	-1.44665000	0.23577900
F	-1.40470500	-2.25898200	-0.38587100
F	-3.52352700	-1.85046800	-0.04436600
F	-2.07962200	-1.53366800	1.55262400
H	-2.18358500	1.11999800	-2.07662700
H	-0.74170900	0.09874900	-1.74456600
H	-2.20954700	-0.71014400	-2.30048700
H	0.45928500	3.18403300	0.88219600
H	0.32177500	2.27309500	-0.61399100
M22-S G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.117661 a.u. E (UωB97X-D/def2-tzvp) = -685.069564953 a.u.			
C	-3.62197900	-0.85924500	0.15051900
C	-0.18206900	0.15975000	-0.40501900
C	-1.35622100	1.05206500	-0.72598500
C	-2.22528200	1.18599300	0.50035100
H	-0.43774400	-0.89064000	-0.31284300
H	-1.02988900	2.04388700	-1.05000600
H	-2.00586600	2.03766200	1.14324300

C	-3.20309200	0.34523600	0.88796500
C	1.08299700	0.54365700	-0.20403600
O	-3.03408900	-1.35200900	-0.79984300
C	1.63469600	1.94276300	-0.26865600
H	0.86438300	2.67731100	-0.50930100
H	2.08592300	2.22033600	0.69085400
H	2.42387000	2.01038800	-1.02619400
C	2.12029600	-0.49630200	0.12251700
H	-1.92612100	0.58370300	-1.53290100
H	-3.76088900	0.55940700	1.79738000
H	-4.55660200	-1.32785500	0.52659000
F	1.63132900	-1.74894300	0.19571600
F	2.71660400	-0.22869100	1.31273400
F	3.10979700	-0.50476900	-0.80556200
M22-FeCl₃/S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.107320 a.u.			
E (UωB97X-D/def2-tzvp) = -3329.63332239 a.u.			
C	1.02086700	2.04758400	-0.82401400
C	-1.94363600	0.61125500	0.50840500
C	-1.41623800	1.91576600	1.07824400
C	-1.18893500	2.86509000	-0.06409400
H	-1.18502700	-0.09154100	0.18108600
H	-2.12981900	2.35913000	1.77684000
H	-2.00323900	3.55864800	-0.26963700
C	-0.11770600	2.92495200	-0.89612100
C	-3.23505900	0.30062500	0.35500600
O	1.10766500	1.10841300	-0.00575700
C	-4.42542300	1.14657200	0.71401100
H	-4.13717900	2.09725000	1.16691800
H	-5.02322700	1.35909700	-0.17966900
H	-5.07627800	0.61290000	1.41525900
C	-3.59801800	-1.03472000	-0.24544700
H	-0.48225400	1.71706900	1.60821600
H	-0.09817100	3.65995100	-1.69525400
Fe	2.40114900	-0.43112700	0.08274700
Cl	3.80284800	0.11527800	-1.52889700
Cl	3.21846200	-0.36616700	2.10854200
Cl	1.06744300	-2.11338100	-0.36407800
H	1.84349100	2.19544900	-1.53664200
F	-2.53466100	-1.79156700	-0.55890600
F	-4.32311600	-0.86023000	-1.37884100
F	-4.37371400	-1.74777000	0.60518400
M22-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.106956 a.u.			
E (UωB97X-D/def2-tzvp) = -3329.63279788 a.u.			
C	0.18568200	1.85199200	0.25264700
C	-2.74476100	0.99141500	0.40945800
C	-2.86901500	2.42746300	-0.02564700
C	-1.75573400	3.36170400	0.38407800
H	-0.44286600	1.02863700	-0.09258400
H	-2.66035700	0.84492700	1.48303300
H	-3.79853200	2.83787900	0.39243500
H	-2.07944600	4.38528900	0.56780800
C	-0.43082000	3.12394100	0.52956400
C	-2.74113000	-0.08990800	-0.37818500
O	1.41334900	1.67181600	0.37704000

Fe	2.17161100	-0.17996900	-0.02472500
Cl	1.36298700	-1.33966000	1.64975400
Cl	4.33960600	0.01440300	-0.13572800
Cl	1.13803500	-0.60193600	-1.93531900
C	-2.80519200	-0.13308000	-1.87933900
C	-2.60634600	-1.45267800	0.26117800
F	-1.50688600	-2.08257900	-0.20044300
F	-3.67134800	-2.23019700	-0.04834200
F	-2.51854200	-1.40608700	1.60424200
H	-2.96320800	0.85337400	-2.31955200
H	-1.87240400	-0.54535000	-2.28040500
H	-3.62008000	-0.78825200	-2.20528200
H	0.23736000	3.92403600	0.83636100
H	-2.98495800	2.51104800	-1.11495100
M22-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.110685 a.u.			
E (UωB97X-D/def2-tzvp) = -3329.57582215 a.u.			
Imaginary frequency: 476.7003			
C	-0.74924600	1.41432400	0.71363700
C	-2.25935500	1.05609400	0.18545700
C	-2.72358400	2.31533400	-0.56907400
C	-1.77975800	3.39108000	-0.08129000
H	-0.62238900	0.99291500	1.71647100
H	-2.86232100	0.86758300	1.07634100
H	-3.77007000	2.52961200	-0.32289000
H	-1.94137800	4.43724200	-0.32042500
C	-0.75777900	2.91380100	0.62948900
C	-1.96648600	-0.18299000	-0.51258300
O	0.13350700	0.83770600	-0.19820700
Fe	1.73980400	-0.08201300	-0.02414600
Cl	1.51992100	-1.15104700	1.91289700
Cl	3.46786900	1.28409300	-0.08234600
Cl	1.54996200	-1.43470100	-1.84755300
C	-1.66941400	-0.37717300	-1.91175100
C	-2.04271400	-1.46486700	0.32603700
F	-1.18117000	-2.38858500	-0.07781400
F	-3.30579200	-1.91772900	0.12247000
F	-1.88131500	-1.24081000	1.63030300
H	-1.79591800	0.51209600	-2.52385800
H	-0.59850700	-0.72101800	-1.96673800
H	-2.22993600	-1.23503600	-2.30867000
H	0.05635900	3.48996400	1.05808700
H	-2.67608000	2.21596100	-1.65997200
M23-S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.141952 a.u.			
E (UωB97X-D/def2-tzvp) = -1266.47414378 a.u.			
C	1.60620300	-0.74829200	-1.09691200
C	-0.88191000	0.55031600	0.07943800
C	0.11367800	1.59938500	0.20260500
C	1.45478100	1.43904000	0.17250900
H	1.11793000	-0.21602700	-1.94113900
H	-0.52633100	-0.47376000	0.04266400
H	-0.25055600	2.61057900	0.36181400
H	2.05440600	2.33012300	0.35139400
C	2.21192100	0.15257600	-0.04702000
C	-2.21566400	0.73309200	0.03484500

O	1.66041500	-1.96190700	-1.07135200
C	-2.95816100	2.03951700	0.06607500
H	-3.60291100	2.12959100	-0.81578500
H	-3.60992600	2.08930700	0.94616200
H	-2.28629500	2.89843000	0.08531900
C	-3.11317700	-0.47031800	-0.06434100
Si	2.37770000	-0.80942900	1.59732800
H	2.81209300	0.15833900	2.62822700
H	1.05302100	-1.35017800	1.95870900
H	3.37871900	-1.89013200	1.51086300
Si	3.96038300	0.57510200	-0.69724000
H	4.59516800	1.49292600	0.27256600
H	4.76146100	-0.65384100	-0.84360800
H	3.84359000	1.25920500	-2.00412300
F	-2.44844400	-1.64190300	-0.06399700
F	-3.85461200	-0.42874100	-1.19964000
F	-3.99281900	-0.50498200	0.96733900
M23-FeCl₃/S G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.134259 a.u. E (UωB97X-D/def2-tzvp) = -3911.03447159 a.u.			
C	0.80863900	1.20637800	-0.36365500
C	-2.05892900	1.14809800	-0.04020900
C	-1.84472000	2.50169400	-0.52767000
C	-0.67754900	3.17868000	-0.46929800
H	0.35662500	0.87973700	-1.31059000
H	-1.32221700	0.74899900	0.65011700
H	-2.69716100	3.02192600	-0.95645500
H	-0.67019000	4.21464800	-0.79925000
C	0.62934600	2.60894000	0.04215300
C	-3.09471300	0.34563600	-0.34159400
O	1.46088900	0.38507900	0.30475000
C	-4.22937700	0.64541700	-1.27661400
H	-4.22487400	-0.06608600	-2.11048800
H	-5.18964400	0.53077400	-0.76115300
H	-4.17147800	1.65400000	-1.68857800
C	-3.16193400	-1.02243200	0.29110000
Si	0.77672200	2.83530700	1.93627900
H	0.44574800	4.23648700	2.20827800
H	-0.19790200	1.94484600	2.56727800
H	2.13505200	2.54752800	2.39778700
Si	2.08288300	3.54944800	-0.79621800
H	1.88801700	4.96278200	-0.46477600
H	3.35043400	3.04629200	-0.27137300
H	1.99900300	3.35248900	-2.24570400
Fe	1.61610000	-1.60804100	-0.08140400
Cl	0.11405200	-1.79774200	-1.69256800
Cl	1.07901400	-2.55397700	1.80888400
Cl	3.68364700	-1.86333900	-0.74614500
F	-2.11022000	-1.29533800	1.08607100
F	-3.22685100	-1.98451500	-0.65305300
F	-4.28185100	-1.13692500	1.04746800
M23-RS G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.134394 a.u. E (UωB97X-D/def2-tzvp) = -3911.03422210 a.u.			
C	1.83492500	-0.02136500	0.20507500
C	-0.55827600	1.90514100	-0.41866900

C	0.47753000	2.30286700	-1.35310600
C	1.79993900	2.05942300	-1.23218500
H	2.18023900	-0.54242800	1.11103000
H	-0.24360000	1.57936000	0.56555400
H	0.16713600	2.87377000	-2.22410400
H	2.45770900	2.49171500	-1.98280800
C	2.46575800	1.26180100	-0.13240800
C	-1.88261800	1.92093300	-0.65620600
O	0.95129800	-0.55051400	-0.48600500
Fe	-0.22881600	-2.11680200	-0.00372600
Cl	-0.33605100	-1.80011900	2.17632200
Cl	0.97573100	-3.86025300	-0.56541700
Cl	-2.06642600	-1.83397600	-1.15074800
C	-2.57014900	2.25863400	-1.94520900
C	-2.82507700	1.57188300	0.46922700
F	-3.76466500	0.69218400	0.07174300
F	-3.48262100	2.68619900	0.88328500
F	-2.20193800	1.05320100	1.54519400
H	-1.88159700	2.65911700	-2.69081600
H	-3.03529800	1.35648700	-2.35942900
H	-3.36899600	2.98916300	-1.77542100
Si	2.65973000	2.36845400	1.42050400
H	3.29025000	1.59319300	2.49489500
H	3.51903100	3.48944200	1.03812400
H	1.34313600	2.84480600	1.83924000
Si	4.25031600	0.77728200	-0.67430100
H	4.94477700	2.02962300	-0.97761400
H	4.91390500	0.06757300	0.42081300
H	4.15698100	-0.06742200	-1.86518000
M23-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.137644 a.u.			
E (UωB97X-D/def2-tzvp) = -3910.97543944 a.u.			
Imaginary frequency: 387.9624			
C	1.15689300	0.41433000	0.23117300
C	1.10072400	1.94012500	-0.32739700
C	2.13449600	1.93150400	-1.41525500
C	2.93921900	0.86497700	-1.30463700
H	0.94688200	0.41595500	1.30544700
H	1.34123800	2.61741300	0.50132600
H	2.22180100	2.72251400	-2.15202300
H	3.79582800	0.67669400	-1.94540700
C	2.57726100	-0.04435900	-0.16025200
C	-0.30460500	2.04143000	-0.68528900
O	0.15679400	-0.27086500	-0.46825200
Fe	-1.22904900	-1.40434400	0.09156300
Cl	-1.49702100	-0.85316900	2.22783000
Cl	-0.75870600	-3.53971700	-0.19936400
Cl	-2.93346300	-0.77424500	-1.26036500
C	-0.87633600	1.83207900	-1.99817200
C	-1.25095300	2.56201600	0.39775900
F	-2.47673700	2.06826600	0.28718000
F	-1.29357500	3.90261000	0.18644100
F	-0.78871000	2.34608600	1.63016800
H	-0.12897100	1.59177400	-2.75144700
H	-1.62051300	1.00329400	-1.90528500
H	-1.48492700	2.70201900	-2.28858900

Si	3.81248700	0.21682600	1.25226800
H	3.61842300	-0.79256200	2.29783300
H	5.17920400	0.14415600	0.72705200
H	3.58311000	1.55525800	1.81820700
Si	2.59106600	-1.87826400	-0.69450100
H	4.01760200	-2.16797300	-0.92029000
H	2.10021000	-2.71092300	0.39785000
H	1.86855100	-2.08165600	-1.94742300
M24-S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.145921 a.u.			
E (UωB97X-D/def2-tzvp) = -1266.46594541 a.u.			
C	-3.96965100	-0.54871400	-0.00021900
C	0.59132000	-0.60537600	-0.00007800
C	-0.88171000	-0.26244400	0.00003200
C	-1.69629500	-1.51655700	0.00002800
H	0.81597900	-1.66975100	-0.00027400
H	-1.11462100	-2.43958700	0.00024700
C	-3.04535600	-1.66538000	-0.00007300
C	1.63680600	0.23039800	0.00008500
O	-3.61947400	0.63328400	-0.00017700
C	1.60184700	1.73470200	0.00021200
H	0.58529500	2.13157600	0.00079700
H	2.11653800	2.12907200	0.88337900
H	2.11559800	2.12920500	-0.88344400
C	3.02761700	-0.33772100	-0.00009200
H	-3.46835900	-2.66550000	0.00006400
Si	-1.32194200	0.77050000	-1.59179600
H	-2.39082300	0.12133800	-2.37152300
H	-1.64362900	2.17911600	-1.30563700
H	-0.09557500	0.75018100	-2.42107900
Si	-1.32187500	0.77016700	1.59209800
H	-0.09561500	0.74917800	2.42151000
H	-1.64296700	2.17898600	1.30620700
H	-2.39120500	0.12129000	2.37145100
H	-5.04782900	-0.79692500	-0.00038200
F	3.06555900	-1.68680500	-0.00039400
F	3.72500100	0.08051700	1.08572000
F	3.72488200	0.08104000	-1.08571500
M24-RS (FeCl₃/S)			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.135889 a.u.			
E (UωB97X-D/def2-tzvp) = -3911.03001312 a.u.			
C	-0.23546800	-1.42650700	-0.45465000
C	2.29918500	0.25251300	0.41915600
C	2.88626300	-1.05481200	-0.07998700
C	2.11986000	-1.94690500	-0.99430200
H	0.04814500	-0.71609000	0.32579100
H	2.49108200	0.48609300	1.46310600
H	2.74920200	-2.61580000	-1.58316400
C	0.78126800	-2.13572200	-1.16849000
C	1.67348000	1.19925700	-0.29757700
O	-1.45177300	-1.59934700	-0.69297900
Fe	-2.84717300	-0.32322800	0.01077700
Cl	-1.92279800	0.27743200	1.92689900
Cl	-4.72586500	-1.41989500	0.17391300
Cl	-2.75866800	1.25737400	-1.51795000

C	1.29274700	1.15072800	-1.74852500
C	1.24245000	2.46830700	0.40123600
F	-0.08295000	2.65884400	0.26050600
F	1.86064600	3.54057100	-0.15070800
F	1.52505500	2.47775700	1.71835200
H	1.82851900	0.37120600	-2.29005900
H	0.21373800	0.97281900	-1.86009200
H	1.50321300	2.11443900	-2.22204800
H	0.43776800	-2.86714600	-1.89439300
Si	4.57328200	-0.58662000	-0.84347600
H	5.34615200	0.14443600	0.16086000
H	5.28155300	-1.81452800	-1.23210900
H	4.34753700	0.24800100	-2.02529300
Si	3.23370200	-2.18764800	1.42986700
H	3.79544100	-3.45652500	0.96075200
H	4.18395700	-1.50672200	2.31430900
H	1.95777200	-2.41090900	2.11332400
M24-TS1 G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.135752 a.u. E (UωB97X-D/def2-tzvp) = -3910.96649280 a.u. Imaginary frequency: 647.3692			
C	0.33419800	-0.81135600	0.18713000
C	1.81183100	0.15501300	0.41778300
C	2.94018900	-0.76428500	-0.10683500
C	2.21557400	-1.87800700	-0.84642500
H	0.09696900	-1.09595600	1.22156500
H	1.83630600	0.39348300	1.47910200
H	2.76606700	-2.61252900	-1.42695800
C	0.89374600	-1.89981000	-0.67468000
C	1.18435800	1.16681500	-0.35074800
O	-0.66387700	-0.06363900	-0.39612900
Fe	-2.49800400	-0.42817900	-0.05331700
Cl	-2.46309000	-0.67222800	2.16647100
Cl	-2.86364300	-2.38312800	-1.05325800
Cl	-3.65141400	1.27942000	-0.82990400
C	1.25258000	1.32441400	-1.81210800
C	0.46449000	2.28202900	0.41487000
F	-0.56434100	2.79068500	-0.24876600
F	1.41851000	3.24150800	0.54311500
F	0.07443300	1.90533000	1.63117300
H	1.53190200	0.39318600	-2.30311200
H	0.30301000	1.69866700	-2.19804700
H	2.02793600	2.08093400	-2.01701600
H	0.19141300	-2.60850300	-1.10327500
Si	4.31142500	0.08139700	-1.11019900
H	4.49226600	1.44319500	-0.59182200
H	5.55756800	-0.67565400	-0.94837600
H	3.98289600	0.14377800	-2.53869500
Si	3.77604200	-1.57364000	1.40437900
H	4.56391100	-2.71877400	0.94367000
H	4.65199700	-0.60097200	2.07141300
H	2.72162500	-2.00335300	2.32842900
M1Ph-S G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.200868 a.u. E (UωB97X-D/def2-tzvp) = -816.864741212 a.u.			
C	-0.69279800	0.38651100	-0.88993300

C	2.55591200	-0.08169700	0.09146300
C	1.76464200	0.42862200	1.19391200
C	0.64407600	1.17268300	1.10035600
H	2.21554600	0.17139600	-0.90696700
H	2.09720300	0.19018000	2.20103900
H	0.11244500	1.47643000	1.99642100
C	-0.00861000	1.58989900	-0.18340600
C	3.66176300	-0.85164700	0.20168100
O	-0.12918700	-0.10445500	-1.85180700
C	4.28043100	-1.30729000	1.49579300
H	4.31681200	-2.40450000	1.53458400
H	5.32060300	-0.96069200	1.56326100
H	3.75238600	-0.95778900	2.38489500
C	4.37893700	-1.32235600	-1.03551400
H	4.42418800	-2.41997400	-1.06751300
H	3.88956100	-0.97194500	-1.94833400
H	5.41975900	-0.96916700	-1.04262900
F	-0.94761800	2.56833600	0.07722900
F	0.88590500	2.13324900	-1.05764700
C	-1.94525700	-0.19244000	-0.32593100
C	-2.42201000	-1.36756500	-0.93091800
C	-2.64694700	0.35120700	0.76224400
C	-3.57126300	-1.99007200	-0.45795300
H	-1.86620300	-1.77268900	-1.76935000
C	-3.79713000	-0.27759600	1.23525800
H	-2.31200900	1.26777800	1.22850400
C	-4.26131000	-1.44609900	0.62932800
H	-3.93019900	-2.89878400	-0.93233300
H	-4.33476300	0.14973700	2.07658700
H	-5.15903600	-1.93157500	1.00175600
MlPh-FeCl₃/S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.193782 a.u.			
E (UωB97X-D/def2-tzvp) = -3461.41997675 a.u.			
C	-1.22503700	0.66019800	-0.80006600
C	2.03759200	1.95827900	0.09287500
C	0.86321900	2.57401700	0.65761400
C	-0.36367300	2.71943100	0.10167100
H	2.00804800	1.68623100	-0.95526800
H	0.96713900	2.99859800	1.65246500
H	-1.15437700	3.19837100	0.66940200
C	-0.83064100	2.10242100	-1.17493400
C	3.17707400	1.69992900	0.78485800
O	-0.33612900	-0.19240400	-1.01575100
C	3.35069900	1.90850300	2.26220900
H	3.34158300	0.92933900	2.75984300
H	4.32130200	2.37066100	2.47776500
H	2.56836800	2.51361000	2.72387000
C	4.36749000	1.10510500	0.09115200
H	4.61032400	0.12431300	0.51956500
H	4.19739100	0.96994700	-0.97830500
H	5.24901500	1.74451100	0.23665000
Fe	0.79118400	-1.59347000	-0.18884400
Cl	0.83635200	-0.98516700	1.93009800
Cl	2.72623900	-1.60103800	-1.22537800
Cl	-0.22280700	-3.53996300	-0.46631400
F	-1.90215000	2.78758300	-1.69118100

F	0.11663600	2.05837700	-2.14728000
C	-2.48690000	0.34084700	-0.13902900
C	-2.75057900	-1.00781800	0.17938700
C	-3.44305000	1.32554800	0.19645900
C	-3.92477900	-1.35912100	0.83165300
H	-2.04258900	-1.77866700	-0.09501700
C	-4.61044100	0.96451100	0.85568400
H	-3.27926600	2.36187800	-0.06150200
C	-4.85378700	-0.37453100	1.17701800
H	-4.11251100	-2.40066300	1.07131300
H	-5.33637100	1.72790500	1.11699300
H	-5.76963300	-0.64928500	1.69212500
M1Ph-RS G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.193402 a.u. E (UωB97X-D/def2-tzvp) = -3461.41638647 a.u.			
C	-0.77498800	-0.08126400	0.66932900
C	-1.71138700	2.12976500	-0.89272100
C	-0.77834000	2.88464100	-0.02628000
C	-0.21813500	2.41935200	1.09220500
H	-2.75561300	2.12654200	-0.58167900
H	-0.54216100	3.91126400	-0.30857400
H	0.44669300	3.03310200	1.69308600
C	-0.42111800	1.05215400	1.66966700
C	-1.37630400	1.48202400	-2.02291800
O	0.18233600	-0.55737700	0.03296500
Fe	2.19511800	-0.52591600	-0.07165400
Cl	2.90733700	-1.81390000	1.54970300
Cl	2.95985100	1.53580600	-0.05361800
Cl	2.46412400	-1.48097900	-2.04583300
C	-2.40747200	0.70470900	-2.79269800
H	-2.45021900	1.03401000	-3.83871000
H	-2.13979600	-0.36052100	-2.80905900
H	-3.40554900	0.79761800	-2.35460600
C	0.02491300	1.43208500	-2.55842200
H	0.05325400	1.81074700	-3.58861800
H	0.73116300	2.00692600	-1.95595100
H	0.38643800	0.39661800	-2.60023900
F	-1.34986700	1.09176700	2.68435400
F	0.74776100	0.65172600	2.26365500
C	-2.10061400	-0.68212300	0.52149400
C	-3.27393700	-0.14357300	1.08686200
C	-2.18302600	-1.85011300	-0.26534400
C	-4.49740100	-0.76122900	0.85826400
H	-3.22844200	0.75468000	1.68532600
C	-3.40926800	-2.46584100	-0.47871200
H	-1.27422300	-2.25542300	-0.69532600
C	-4.56872100	-1.92104000	0.08039500
H	-5.39954100	-0.33960100	1.28999500
H	-3.46375700	-3.36765200	-1.08011900
H	-5.52858000	-2.39994600	-0.08933100
M1Ph-TS1 G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.194106 a.u. E (UωB97X-D/def2-tzvp) = -3461.40076462 a.u. Imaginary frequency: 120.8411			
C	-0.97626800	0.45776000	0.14956100
C	-0.95936800	1.82621300	-0.81928400

C	-0.49889300	2.92193700	0.10087200
C	-0.38426500	2.54334300	1.37041800
H	-1.98696800	1.95385500	-1.17734600
H	-0.28613300	3.92349500	-0.26103800
H	-0.06954600	3.15854800	2.20511200
C	-0.82127500	1.13033300	1.58162900
C	-0.10636400	1.50125400	-1.96223500
O	0.09870800	-0.31677700	-0.14106800
Fe	1.86848500	-0.72566600	0.18226600
Cl	2.14698000	-2.41060900	1.56485700
Cl	2.94022200	1.17562100	0.76704700
Cl	2.51517500	-1.22339400	-1.94112600
C	-0.50710600	0.44869900	-2.89294700
H	-0.30654500	0.73784800	-3.93151000
H	0.21397200	-0.37236000	-2.67980400
H	-1.52538200	0.08743600	-2.75574000
C	1.21093100	2.11241700	-2.10082000
H	1.13340500	3.20802800	-2.06975200
H	1.79035600	1.87038700	-1.17972500
H	1.76638600	1.77351200	-2.97425300
F	-2.00833800	1.11932300	2.26842300
F	0.05391500	0.41258500	2.32992100
C	-2.27216700	-0.31273300	-0.03770400
C	-3.52603700	0.31003000	0.04438800
C	-2.20604300	-1.68428500	-0.30219400
C	-4.69172200	-0.42657600	-0.14129300
H	-3.59625900	1.36908500	0.27561400
C	-3.37727500	-2.42243200	-0.48494300
H	-1.23555700	-2.16189300	-0.35665000
C	-4.62052200	-1.79747100	-0.40889200
H	-5.65691400	0.06658300	-0.07226400
H	-3.31217200	-3.48751300	-0.68659600
H	-5.53126100	-2.37108600	-0.55408200
MIPh-INT			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.200389 a.u.			
E (UωB97X-D/def2-tzvp) = -3461.43407950 a.u.			
C	-1.06380800	0.77746700	-0.04935100
C	-1.00356900	1.91459700	-1.10026500
C	-0.61503400	3.13204300	-0.30844400
C	-0.47935400	2.88683300	0.99664300
H	-1.88196900	2.04687200	-1.73541800
H	-0.43794300	4.09393300	-0.77866100
H	-0.18827500	3.58836900	1.76962300
C	-0.82493200	1.46738900	1.32765600
C	0.16478700	1.13776500	-1.77487400
O	0.20337300	0.23732700	-0.55668000
Fe	1.79093000	-0.71775000	0.27307600
Cl	1.08882400	-2.25364400	1.66550900
Cl	3.22215800	0.75698700	1.05241300
Cl	2.59448000	-1.64829400	-1.57419100
C	-0.25680800	0.30323700	-2.96816300
H	-0.36321000	0.95299800	-3.84407700
H	0.50462400	-0.45194800	-3.18013800
H	-1.21036600	-0.19846700	-2.78505100
C	1.48219100	1.85276500	-1.96923000
H	1.36493300	2.60036900	-2.76218200

H	1.80878700	2.35158800	-1.05525600
H	2.25622600	1.14463100	-2.27695300
F	-1.94195100	1.40654300	2.11099900
F	0.16309300	0.82362100	2.02138100
C	-2.19056800	-0.21173200	-0.11293800
C	-3.50650500	0.26234800	-0.03066200
C	-1.95597700	-1.58008200	-0.26517200
C	-4.57608300	-0.62606000	-0.09904800
H	-3.69189300	1.32496800	0.09514300
C	-3.03142000	-2.46744200	-0.33159400
H	-0.94308800	-1.95565900	-0.32811100
C	-4.34051600	-1.99488200	-0.25020300
H	-5.59288700	-0.25011100	-0.03509400
H	-2.83863500	-3.52968700	-0.44678400
H	-5.17502300	-2.68771700	-0.30454600
M1Ph-TS2 G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.196192 a.u. E (UωB97X-D/def2-tzvp) = -3461.38930591 a.u. Imaginary frequency: 371.4685			
C	-2.02887700	0.03311600	-0.27676200
C	-2.02743900	1.12597900	-1.21781400
C	-2.92556100	2.16090200	-0.59538400
C	-3.21619900	1.87920600	0.67759000
H	-2.19770200	0.89047700	-2.26688700
H	-3.23741000	3.05040900	-1.12956200
H	-3.78733900	2.46831800	1.38323700
C	-2.62101300	0.55794100	1.05045500
C	-0.30049900	1.66181100	-1.20686500
O	0.27550500	1.16404600	-0.09391100
Fe	1.82837600	0.27457900	0.39362100
Cl	1.46034100	-0.62706200	2.40889100
Cl	3.46104600	1.78431600	0.29682200
Cl	2.25418400	-1.39606700	-1.05939600
C	0.28872000	1.13108000	-2.50719000
H	1.33649300	1.44985600	-2.55332600
H	0.29703900	0.04011700	-2.52947600
H	-0.23844000	1.52589100	-3.38192100
C	-0.34120900	3.18552700	-1.15616200
H	-0.78247100	3.53237500	-0.21975200
H	0.70195400	3.52201500	-1.17715200
H	-0.87312800	3.62252500	-2.00777000
F	-3.57178900	-0.33700400	1.47708800
F	-1.69561700	0.64078100	2.04106600
C	-1.53514900	-1.26713500	-0.43276100
C	-1.15863700	-2.02068600	0.71995000
C	-1.30677400	-1.81725400	-1.72956900
C	-0.51724400	-3.23605700	0.56628900
H	-1.29916500	-1.60069000	1.70534900
C	-0.70827000	-3.05032600	-1.86248000
H	-1.63156500	-1.26864700	-2.60588600
C	-0.29026600	-3.74674900	-0.71518200
H	-0.16596500	-3.77317400	1.43967600
H	-0.53294000	-3.47164800	-2.84615600
H	0.22127600	-4.69756200	-0.82869700
M1Ph-P G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.190062 a.u.			

$E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -3461.43139187 \text{ a.u.}$			
C	-2.48953800	-0.29530900	-0.39860400
C	-2.97591400	0.36673300	-1.47312500
C	-4.00905000	1.34305000	-1.05529700
C	-4.17211700	1.30605800	0.27602900
H	-2.67813100	0.21082800	-2.50326900
H	-4.54327800	1.98433800	-1.74774300
H	-4.83699900	1.88521200	0.90264500
C	-3.22297500	0.26379900	0.83110000
C	-0.11012200	2.05974300	-0.25984400
O	0.50698300	1.27245100	0.47794700
Fe	2.22222500	0.26139200	0.16437400
Cl	2.72873300	-0.79351000	2.01407100
Cl	3.51690800	2.01880200	-0.22791000
Cl	2.08868900	-0.95184100	-1.66230200
C	0.10417200	2.06058800	-1.74126500
H	1.08001000	2.53100100	-1.92936800
H	0.17054300	1.03442100	-2.11212300
H	-0.67148700	2.61994900	-2.26722300
C	-1.01486800	3.07797900	0.35172500
H	-1.00345600	3.00810100	1.43813700
H	-0.68361700	4.07222200	0.02445400
H	-2.03657400	2.93948300	-0.01953600
F	-3.87416700	-0.72426800	1.50793900
F	-2.34665300	0.83092900	1.73616100
C	-1.54544500	-1.40231500	-0.32424500
C	-0.86248600	-1.69391400	0.87218400
C	-1.31522800	-2.21701200	-1.44911100
C	0.02411000	-2.76694200	0.93403200
H	-1.01938200	-1.07465800	1.74637800
C	-0.43170500	-3.28708600	-1.38011400
H	-1.85579900	-2.02193600	-2.37045700
C	0.24109300	-3.56625700	-0.18763700
H	0.55726400	-2.96473600	1.85734300
H	-0.26559200	-3.90542800	-2.25699800
H	0.93699100	-4.39790200	-0.13701500
M2Ph-S			
$G_{\text{corr}}(\text{UB3LYP-D3BJ/6-31G}^*/\text{Lan2LDZ}) = 0.200131 \text{ a.u.}$			
$E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -816.862888302 \text{ a.u.}$			
C	-1.02471500	0.39315400	-0.32099400
C	2.58531200	0.51384500	0.26382500
C	1.77475500	-0.72536600	0.51201000
C	0.95737000	-1.12668600	-0.69207200
H	1.98956000	1.40689600	0.42396000
H	1.45486300	-1.85661300	-1.32579400
C	-0.25616100	-0.67692300	-1.02909700
C	3.84220500	0.61689500	-0.19095300
O	-0.47136800	1.40029300	0.10406700
C	4.76384800	-0.52412800	-0.53999600
H	4.29366400	-1.50114700	-0.45285000
H	5.13896900	-0.39791400	-1.56439600
H	5.64514800	-0.51120700	0.11562900
C	4.44384700	1.98547800	-0.39742700
H	4.74249900	2.12369600	-1.44560000
H	3.74809500	2.78512900	-0.12896100
H	5.35475000	2.10295100	0.20508400

C	-2.50302700	0.22209300	-0.20520000
C	-3.13739000	-1.00023100	-0.46853900
C	-3.27051200	1.32142500	0.20843500
C	-4.51928100	-1.11921300	-0.32749600
H	-2.55041200	-1.86490200	-0.76177400
C	-4.64982700	1.20429800	0.34083000
H	-2.75896200	2.25436700	0.41947700
C	-5.27671400	-0.01660400	0.07147800
H	-5.00384900	-2.07073600	-0.52585300
H	-5.23980800	2.06035100	0.65530100
H	-6.35413400	-0.10845500	0.17659100
H	-0.73010300	-1.09643000	-1.91378200
F	0.95572600	-0.51359400	1.59349900
F	2.56232000	-1.81269000	0.84445700
M2Ph-RS (FeCl₃/S) G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.194024 a.u. E (UωB97X-D/def2-tzvp) = -3461.43145969 a.u.			
C	0.53512200	-0.58475500	-0.64437300
C	2.03778800	1.37113300	0.86655600
C	2.25985100	2.02159800	-0.46603300
C	1.32326900	1.61977500	-1.58446900
H	2.83179200	0.69906500	1.17344100
H	1.25218700	2.35127800	-2.38540300
C	0.58697700	0.50789000	-1.64652900
C	0.96140200	1.55514600	1.64880300
O	-0.56724900	-0.88482500	-0.12288400
Fe	-2.47354800	-0.33118700	-0.15448900
Cl	-3.46563300	-2.01800500	-1.14336600
Cl	-2.63377600	1.53956700	-1.30693800
Cl	-2.96039200	-0.08944000	1.98216900
C	-0.16161200	2.50802400	1.34397800
H	-1.13051800	2.01410100	1.46547600
H	-0.13758300	3.33213500	2.06977000
H	-0.10943400	2.94302400	0.34665900
C	0.81196300	0.77263300	2.92451200
H	0.67601100	1.44284300	3.78260300
H	-0.09131100	0.15067600	2.86863700
H	1.67449700	0.12804500	3.11686900
C	1.69763900	-1.41935800	-0.33935800
C	2.89726400	-1.30122500	-1.06428900
C	1.59430800	-2.36489000	0.70012100
C	3.98183400	-2.10959800	-0.74093300
H	2.97900900	-0.57575500	-1.86310000
C	2.68422500	-3.16149000	1.02118400
H	0.66116800	-2.44503100	1.24582800
C	3.87871600	-3.03412700	0.30152400
H	4.90753800	-2.01836500	-1.29984700
H	2.60927100	-3.88276000	1.82881300
H	4.72957700	-3.66016000	0.55382200
H	-0.11876400	0.38525500	-2.46503900
F	3.54635400	1.73735800	-0.89167500
F	2.18708300	3.39536400	-0.37550300
M2Ph-TS1 G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.194417 a.u. E (UωB97X-D/def2-tzvp) = -3461.40428399 a.u. Imaginary frequency: 289.425			

C	0.88311200	-0.01220000	-0.13514100
C	1.51552700	1.33941600	0.71001900
C	2.11335000	2.21213200	-0.40638500
C	1.57533600	1.69778500	-1.69908300
H	2.27921200	0.99360200	1.40312400
H	1.74494800	2.23040300	-2.62747100
C	0.93026100	0.54475900	-1.54442100
C	0.31808000	1.79816100	1.38031700
O	-0.37978700	-0.26855700	0.32703800
Fe	-2.14210100	-0.46253400	-0.22540200
Cl	-2.49821100	-2.59444800	-0.68750900
Cl	-2.42126200	0.89912200	-1.97229400
Cl	-3.26576600	0.28553200	1.58678100
C	-0.65626000	2.70913800	0.75345900
H	-1.65446900	2.56538800	1.17340200
H	-0.31587300	3.73298400	0.97919800
H	-0.68222000	2.61597300	-0.33396900
C	0.00418600	1.28794000	2.72002300
H	-0.31076900	2.11178200	3.37453000
H	-0.89970400	0.66163900	2.59745900
H	0.80765100	0.70848200	3.17482000
C	1.79605300	-1.20707800	0.05191500
C	3.15000300	-1.15889900	-0.31519400
C	1.26001000	-2.39196600	0.57111300
C	3.95571400	-2.28219800	-0.15594800
H	3.57621500	-0.24437300	-0.71240700
C	2.06996900	-3.51843000	0.71486700
H	0.20988000	-2.42962400	0.83076300
C	3.41723700	-3.46624300	0.35753200
H	5.00341400	-2.23675100	-0.43816600
H	1.64254300	-4.43745600	1.10448100
H	4.04670900	-4.34366100	0.47407900
H	0.45159200	-0.02886900	-2.33035400
F	3.48507900	2.10991700	-0.35214200
F	1.84685400	3.54868700	-0.22590100
M2Ph-INT			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.200385 a.u.			
E (UωB97X-D/def2-tzvp) = -3461.43906842 a.u.			
C	-2.89534200	0.00181500	1.67487900
C	-1.60597000	-0.34226200	1.69900000
C	-1.05246300	-0.54516800	0.31328600
C	-2.17138800	-0.02541100	-0.61918500
H	-3.53694500	0.19140900	2.52779300
H	-0.99214900	-0.44944500	2.58447000
H	-2.39222700	-0.61463600	-1.50684400
C	-3.41327300	0.08145700	0.26724000
C	-1.29589700	1.22752600	-0.91782900
O	-0.21018900	0.65688100	-0.05097600
Fe	1.74063200	0.95022200	0.16858100
Cl	1.99771100	3.05605800	-0.42866400
Cl	2.79149000	-0.43353600	-1.16765300
Cl	2.02844500	0.55310900	2.32093800
C	-1.70387700	2.58188700	-0.37348000
H	-0.85171500	3.26233500	-0.45230400
H	-2.53575300	2.98261500	-0.95887600
H	-2.00824100	2.52397800	0.67213200

C	-0.80870600	1.29057600	-2.35373000
H	-1.64634500	1.55620300	-3.00825700
H	-0.02973300	2.05122100	-2.45770400
H	-0.39862900	0.32893200	-2.67358400
C	-0.31237100	-1.82023200	0.04602300
C	-0.30116500	-2.39003200	-1.23386600
C	0.45566600	-2.41140100	1.05887200
C	0.46090600	-3.52464600	-1.49707500
H	-0.87967300	-1.94641500	-2.03652100
C	1.22345500	-3.54314000	0.79288600
H	0.48714800	-1.97533600	2.04968100
C	1.22770800	-4.10258600	-0.48421500
H	0.46235600	-3.95198000	-2.49505500
H	1.82323800	-3.98118100	1.58452000
H	1.82957000	-4.98215700	-0.69192700
F	-4.14910600	1.21351700	0.04030600
F	-4.25639500	-0.97044900	-0.00344200
M2Ph-TS2 G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.199057 a.u. E (UωB97X-D/def2-tzvp) = -3461.41262212 a.u. Imaginary frequency: 141.4902			
C	-2.87487400	-0.01782500	1.61314000
C	-1.63841600	-0.55982500	1.66395200
C	-1.21551700	-0.93713500	0.32781400
C	-2.11223200	-0.18898100	-0.64481500
H	-3.48582100	0.28922300	2.45446500
H	-1.06689400	-0.73992800	2.56196000
H	-2.34378700	-0.74987500	-1.55052100
C	-3.37872900	0.01018900	0.19226600
C	-1.24621300	1.09121100	-0.99257000
O	0.05494100	0.58839000	-0.73163600
Fe	1.63580200	1.07035000	0.10434500
Cl	2.18125900	3.14381600	-0.46576800
Cl	3.10701700	-0.48746400	-0.51835400
Cl	1.22310100	0.86347700	2.32816500
C	-1.49539800	2.33303900	-0.12999500
H	-0.71152100	3.05388000	-0.37950100
H	-2.46911900	2.78460200	-0.32452600
H	-1.39930600	2.11560600	0.93684300
C	-1.37045200	1.43492700	-2.47506200
H	-2.39310000	1.74588900	-2.71773000
H	-0.68504800	2.25300400	-2.71514600
H	-1.10295200	0.57224400	-3.09401000
C	-0.29632500	-1.98040800	0.03325400
C	-0.08437900	-2.40211700	-1.30406700
C	0.47817000	-2.56360700	1.06854900
C	0.85003400	-3.38004400	-1.58750800
H	-0.64110200	-1.93652300	-2.10740300
C	1.41835700	-3.53618400	0.77344300
H	0.37164200	-2.21611000	2.08782800
C	1.60321200	-3.94661400	-0.55023100
H	1.01664100	-3.69193600	-2.61296700
H	2.02531800	-3.96010700	1.56590700
H	2.35124900	-4.69929200	-0.77995100
F	-4.09221000	1.12549300	-0.11064200
F	-4.23594800	-1.05146200	0.00365500

M2Ph-INT2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.199504 a.u.			
E (UωB97X-D/def2-tzvp) = -3461.41854369 a.u.			
C	-3.27138100	-0.40306100	1.42216300
C	-2.10078700	-1.05749800	1.57143400
C	-1.41760200	-1.13284100	0.29450200
C	-2.05720300	-0.18046300	-0.64447400
H	-4.01575500	-0.19671500	2.18212400
H	-1.73179500	-1.48679800	2.49246200
H	-2.13291400	-0.56942500	-1.65960100
C	-3.46405300	-0.03175900	-0.02711700
C	-1.17984700	1.20297600	-0.76401300
O	0.13232400	0.81302900	-0.95839900
Fe	1.65359100	1.00488100	0.08435000
Cl	2.16394900	3.16742200	0.22725100
Cl	3.29292100	-0.20656600	-0.82637700
Cl	1.14733200	0.19213500	2.16249800
C	-1.33777700	2.09908500	0.47161200
H	-0.66615500	2.95223500	0.33865600
H	-2.35640700	2.47227100	0.58118200
H	-1.03041400	1.58801600	1.38647800
C	-1.67156900	1.91833900	-2.03030900
H	-2.73828700	2.15095500	-1.97575900
H	-1.10706400	2.84913800	-2.13851900
H	-1.47802200	1.29905100	-2.91178300
C	-0.32555900	-1.96538000	-0.01999700
C	0.18935900	-2.00742800	-1.34796300
C	0.32098200	-2.73733400	0.98986100
C	1.30180400	-2.77221400	-1.64201100
H	-0.27285900	-1.41420200	-2.12307200
C	1.43283000	-3.49395300	0.68444600
H	-0.03526300	-2.69720700	2.01048700
C	1.92851300	-3.50481200	-0.62820900
H	1.70907800	-2.77464600	-2.64622800
H	1.94024800	-4.05436500	1.46189800
H	2.81987700	-4.08050300	-0.85784600
F	-4.05943500	1.18027400	-0.18535400
F	-4.30877900	-0.94380000	-0.61723000
M2Ph-TS3			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.197473 a.u.			
E (UωB97X-D/def2-tzvp) = -3461.40823596 a.u.			
Imaginary frequency: 380.6558			
C	3.35592300	0.32577300	1.43775400
C	2.20691900	1.01103300	1.56717900
C	1.54997900	1.12626800	0.25806200
C	2.19215900	0.24493300	-0.65317000
H	4.06776700	0.06165800	2.21005000
H	1.81386700	1.42116800	2.48713900
H	2.22139900	0.50344300	-1.70557900
C	3.55149300	-0.04519400	-0.01471300
C	1.02458200	-1.33279600	-0.78298700
O	-0.18604300	-0.84409000	-0.97119000
Fe	-1.74968100	-0.92750100	0.10819200
Cl	-2.28217800	-3.08292900	0.19251700
Cl	-3.33073400	0.30123600	-0.83764100
Cl	-1.23822000	-0.18423300	2.17379600

C	1.23916000	-2.12559400	0.49318300
H	0.57207000	-2.99451600	0.43315900
H	2.26482600	-2.47597100	0.59320100
H	0.94480900	-1.55683400	1.37686800
C	1.60062200	-1.96877400	-2.04120000
H	2.67042700	-2.16187100	-1.94842200
H	1.07829600	-2.92234300	-2.18831700
H	1.40351000	-1.34062500	-2.91359400
C	0.42973800	1.95788100	-0.03703500
C	-0.08438500	2.02455200	-1.35739800
C	-0.20858200	2.71477900	0.97884300
C	-1.19250500	2.80397700	-1.64246400
H	0.37845000	1.44749400	-2.14590100
C	-1.31332300	3.49338500	0.68499900
H	0.14899400	2.66237900	1.99891900
C	-1.81048200	3.53409800	-0.62334200
H	-1.59515900	2.82529700	-2.64880700
H	-1.80775400	4.05121800	1.47302700
H	-2.69171800	4.12772300	-0.84572700
F	4.02691500	-1.31778000	-0.16680200
F	4.49883300	0.76826100	-0.59021600
M2Ph-P			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.191893 a.u.			
E (UωB97X-D/def2-tzvp) = -3461.43410068 a.u.			
C	3.25158900	-0.26190100	1.56760700
C	2.15208600	0.49581500	1.61517600
C	1.86535900	1.08029200	0.25653800
C	2.82202700	0.64962200	-0.59481200
H	3.71766300	-0.83246100	2.36019500
H	1.52176700	0.65297800	2.47981800
H	2.96894600	0.91880700	-1.63186300
C	3.79204700	-0.23095900	0.15261800
C	0.51801200	-1.65222300	-1.15420700
O	-0.45818500	-0.87982600	-1.11980200
Fe	-1.98082500	-0.75077500	0.18577200
Cl	-2.78276100	-2.80138200	-0.02384300
Cl	-3.33379300	0.79680500	-0.54491100
Cl	-1.18910800	-0.43004400	2.22438200
C	0.86007400	-2.53473400	0.00214400
H	0.14223600	-3.36719300	0.00262900
H	1.87624000	-2.92020200	-0.06871100
H	0.72275200	-1.99506100	0.94297900
C	1.30260200	-1.76493500	-2.42268500
H	2.37235800	-1.72526200	-2.20495800
H	1.09586800	-2.75353300	-2.85745000
H	1.00840000	-0.99177300	-3.13358200
C	0.73640000	1.96426600	-0.03526400
C	0.34473500	2.21175300	-1.36466200
C	0.02820200	2.59793300	0.99991400
C	-0.70763500	3.07244800	-1.64746500
H	0.85952800	1.70819800	-2.17657800
C	-1.02431100	3.46414700	0.71469500
H	0.30197400	2.41854100	2.03289500
C	-1.39510100	3.70476800	-0.60733300
H	-1.00569700	3.24013600	-2.67788100
H	-1.56354800	3.93920200	1.52821900

H	-2.22757000	4.36533800	-0.82855600
F	3.84691900	-1.51218500	-0.38957200
F	5.07483000	0.23572100	0.09200700
M3Ph-S G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.219168 a.u. E (UωB97X-D/def2-tzvp) = -618.357151073 a.u.			
C	0.69104100	0.34153800	-1.12227200
C	-2.55358800	-0.13598700	-0.15792900
C	-1.77052900	-1.32263500	0.13792800
C	-0.63976800	-1.69033600	-0.49658900
H	-2.14755600	0.52960800	-0.91544400
H	-2.12114400	-1.97214600	0.93665500
H	-0.12763800	-2.58802700	-0.15909600
C	0.00468600	-0.92746300	-1.63433400
C	-3.70983100	0.23539000	0.43413000
O	0.18459200	1.43621600	-1.32203300
C	-4.41231200	-0.53694500	1.51888800
H	-4.51248900	0.07748100	2.42437100
H	-5.43359600	-0.79445300	1.20567700
H	-3.90405300	-1.46253500	1.79572800
C	-4.39869700	1.51104400	0.02588100
H	-4.51275400	2.18760100	0.88480800
H	-3.84582900	2.04121100	-0.75491900
H	-5.41370700	1.30963700	-0.34565800
C	1.95868500	0.21679600	-0.33834800
C	2.51761100	1.38656200	0.19863400
C	2.60568400	-1.00890600	-0.12716700
C	3.69763300	1.33247300	0.93269500
H	2.00188100	2.32474500	0.02464100
C	3.78906900	-1.06343600	0.60782000
H	2.19088300	-1.92527200	-0.53264000
C	4.33627400	0.10588400	1.13867800
H	4.12208400	2.24289900	1.34614400
H	4.28359600	-2.01743400	0.76626300
H	5.25827700	0.06202300	1.71172800
H	0.72732800	-1.56679000	-2.15235200
H	-0.73776500	-0.60215700	-2.36772900
M3Ph-FeCl₃/S G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.211483 a.u. E (UωB97X-D/def2-tzvp) = -3262.92041146 a.u.			
C	-1.20081900	-0.82130800	1.07761200
C	2.11367500	-1.99236900	0.37739000
C	0.99039100	-2.69817400	-0.19497000
C	-0.23839100	-2.84246800	0.34828800
H	2.01555400	-1.64838500	1.40410300
H	1.15121400	-3.18897100	-1.15100000
H	-0.99253100	-3.39516300	-0.20434500
C	-0.71606000	-2.14900700	1.60750700
C	3.28017200	-1.72064800	-0.25618000
O	-0.39065500	0.13814700	1.12187300
C	3.54771600	-2.00818400	-1.70664900
H	3.54412200	-1.06216500	-2.26444700
H	4.53994700	-2.45701300	-1.83799100
H	2.80694600	-2.66038600	-2.17255600
C	4.40377800	-1.03573100	0.46773400
H	4.65264600	-0.08392600	-0.01774200

H	4.15461600	-0.82347600	1.50983600
H	5.30974900	-1.65718600	0.43871500
Fe	0.61710000	1.44066700	0.04702600
Cl	0.73029600	0.50153500	-1.94346100
Cl	2.53845300	1.79540500	1.05757500
Cl	-0.55371200	3.32376000	-0.00943000
C	-2.52568800	-0.67648100	0.46952900
C	-2.93468100	0.58214000	-0.01128600
C	-3.41032100	-1.76995500	0.37425300
C	-4.19060200	0.73668500	-0.58581700
H	-2.27392900	1.43542700	0.07482300
C	-4.66274400	-1.60958500	-0.20499900
H	-3.11952400	-2.74731900	0.74100200
C	-5.05434600	-0.35661900	-0.68709300
H	-4.49403700	1.71129000	-0.95440400
H	-5.33519200	-2.45820300	-0.28147300
H	-6.03450100	-0.23375500	-1.13855900
H	-1.50555000	-2.71238700	2.10971000
H	0.09299500	-1.96258500	2.31512800
M3Ph-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.213195 a.u.			
E (UøB97X-D/def2-tzvp) = -3262.91456139 a.u.			
C	1.03497800	0.21764500	-1.04976900
C	1.30360100	2.61647800	0.94918500
C	2.35704100	2.88041700	-0.03907200
C	2.48547700	2.36164600	-1.26936200
H	1.65342100	2.30255500	1.93341200
H	3.14856600	3.55784000	0.28818000
H	3.32012000	2.68806900	-1.88591900
C	1.58111100	1.33533300	-1.92032100
C	-0.01640400	2.84611600	0.79658800
O	-0.21141700	0.09732700	-1.02836400
Fe	-1.76137700	-0.70571800	-0.09630800
Cl	-2.13028800	-2.62198500	-1.12548300
Cl	-3.40776000	0.73340300	-0.35981500
Cl	-1.16932800	-0.97667600	2.00396300
C	-0.63266900	3.38662900	-0.46436100
H	-1.22912400	2.61063900	-0.96052400
H	-1.32758100	4.20104000	-0.22563400
H	0.11603800	3.76277500	-1.16549600
C	-0.97428300	2.62730600	1.93688100
H	-1.38048400	3.59144200	2.27384300
H	-1.83034400	2.02221300	1.62117400
H	-0.49783000	2.13213100	2.78664500
C	1.91265400	-0.76494800	-0.40602600
C	3.27664400	-0.49427800	-0.17393300
C	1.39695400	-2.02895400	-0.05599300
C	4.08561700	-1.44719000	0.43203700
H	3.68590200	0.47298200	-0.43339400
C	2.21550600	-2.98216800	0.53729100
H	0.37402300	-2.28900900	-0.29290500
C	3.55660800	-2.69002800	0.79345000
H	5.12992200	-1.22221800	0.62491100
H	1.80491500	-3.95276700	0.79562500
H	4.19292700	-3.43281100	1.26578300
H	0.71183200	1.81005900	-2.38752700

H	2.14322300	0.84048200	-2.72411600
M3Ph-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.213613 a.u.			
E (UωB97X-D/def2-tzvp) = -3262.88382018 a.u.			
Imaginary frequency: 217.5850			
C	1.06821300	0.75082000	-0.53939800
C	1.20218900	1.98498300	0.51055800
C	2.01186600	3.01441700	-0.24086700
C	2.21000800	2.67547900	-1.51768700
H	1.67647500	1.63827300	1.43197400
H	2.37044600	3.92105400	0.23671600
H	2.76816100	3.27817400	-2.22847000
C	1.57781000	1.36912600	-1.89012300
C	-0.19841100	2.37917700	0.79670900
O	-0.28263300	0.42084900	-0.64157100
Fe	-1.65325300	-0.70430400	-0.15204300
Cl	-1.93411700	-2.36583100	-1.58998100
Cl	-3.44968300	0.67165400	-0.03137000
Cl	-1.19306300	-1.42990200	1.93768200
C	-1.00819400	3.13472600	-0.15762300
H	-1.91540700	2.53081300	-0.35404900
H	-1.37739000	4.04530600	0.33826100
H	-0.48921200	3.38290300	-1.08119600
C	-0.78012100	2.00088400	2.08200700
H	-1.80032400	2.35368800	2.23211900
H	-0.77683200	0.88904100	2.14028200
H	-0.11324400	2.31136800	2.89847600
C	1.96281200	-0.40480300	-0.11701000
C	3.24101800	-0.16455700	0.40881900
C	1.56217800	-1.72600300	-0.33960600
C	4.08518500	-1.22355500	0.73576900
H	3.58838700	0.85364400	0.55752700
C	2.40897700	-2.78538400	-0.01277000
H	0.59998000	-1.94250700	-0.78569900
C	3.66827800	-2.54073700	0.53263500
H	5.06772500	-1.01871300	1.15141000
H	2.07245600	-3.80351400	-0.18334200
H	4.32177400	-3.36745800	0.79534400
H	0.71526100	1.50410700	-2.55454100
H	2.27321500	0.69084900	-2.39521800
M3Ph-INT			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.218788 a.u.			
E (UωB97X-D/def2-tzvp) = -3262.92228090 a.u.			
C	0.77685800	-1.34560200	0.40180200
C	0.44451500	-2.55190200	-0.52101300
C	0.20506700	-3.68507100	0.43539400
C	0.31514200	-3.30135900	1.71013300
H	1.15098400	-2.79015800	-1.31880700
H	-0.05366100	-4.68424600	0.10021600
H	0.16976400	-3.94833800	2.56967000
C	0.69364600	-1.84987400	1.85691800
C	-0.81903500	-1.78588600	-1.02178000
O	-0.54949300	-0.72946900	0.01408500
Fe	-1.18603800	1.15564300	0.15084100
Cl	-0.98932000	1.60514600	2.30427500
Cl	-3.27670200	1.05359700	-0.54786900

Cl	0.03213600	2.40558500	-1.17871500
C	-0.69716800	-1.18423900	-2.40996500
H	-1.51489700	-0.47981800	-2.59059800
H	0.24867300	-0.65317300	-2.53687600
H	-0.75971700	-1.98346900	-3.15724500
C	-2.17067900	-2.41698000	-0.76869000
H	-2.24471300	-2.79355500	0.25329200
H	-2.96343700	-1.68386700	-0.93682800
H	-2.31596200	-3.25315100	-1.46236300
C	1.90748200	-0.40506200	0.09854100
C	2.21670800	0.60134700	1.02548400
C	2.62922400	-0.46424900	-1.09870600
C	3.20707000	1.54005900	0.74934700
H	1.65820300	0.67338900	1.95208100
C	3.62836100	0.46940900	-1.37124700
H	2.42151900	-1.24070000	-1.82633400
C	3.91532700	1.47740500	-0.45108900
H	3.41930900	2.32318000	1.47059600
H	4.17944900	0.40930600	-2.30501300
H	4.68726900	2.20963200	-0.66827100
H	-0.04362900	-1.26435800	2.41945800
H	1.65474000	-1.73319400	2.37096400
M3Ph-TS2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.215825 a.u.			
E (UωB97X-D/def2-tzvp) = -3262.89642388 a.u.			
Imaginary frequency: 171.2999			
C	1.55438500	-1.23931900	0.57808200
C	1.18409500	-2.31931200	-0.33249000
C	0.83900400	-3.46637000	0.57261800
C	0.71463100	-3.04666100	1.83555200
H	1.86195200	-2.52049600	-1.16298500
H	0.64384400	-4.46573800	0.20505100
H	0.39840400	-3.63816700	2.68625600
C	1.05066000	-1.58395200	1.93884100
C	-0.25532400	-1.75164200	-1.14230500
O	-0.99287400	-1.02899200	-0.25741600
Fe	-1.61614400	0.67385900	0.07203400
Cl	-1.28199000	0.99416200	2.30413000
Cl	-3.75351600	0.77932100	-0.50567100
Cl	-0.41170300	2.21772400	-1.02525800
C	0.18718700	-0.95648100	-2.36721000
H	-0.71458500	-0.65376700	-2.91009100
H	0.71210900	-0.03966200	-2.09955700
H	0.80628100	-1.56390100	-3.03633000
C	-1.02591100	-3.01080600	-1.55109900
H	-1.40541300	-3.52897700	-0.66923600
H	-1.88447200	-2.68776600	-2.14918400
H	-0.41531400	-3.69425600	-2.15121000
C	2.19649000	-0.01842900	0.25395800
C	2.09129800	1.08916100	1.13747100
C	2.91788200	0.13783800	-0.95977800
C	2.65378400	2.30782600	0.79791900
H	1.49708700	1.00237500	2.03885200
C	3.49388500	1.35404200	-1.27884500
H	3.03747900	-0.70938000	-1.62475300
C	3.35304400	2.44129700	-0.40554700

H	2.52753400	3.16191100	1.45402100
H	4.04814100	1.46812800	-2.20451400
H	3.78931700	3.39990800	-0.66996800
H	0.15645100	-0.96004500	2.14983200
H	1.77581300	-1.33222500	2.72284800
M3Ph-P			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.208679 a.u.			
E (UωB97X-D/def2-tzvp) = -3262.93106047 a.u.			
C	2.75350400	-0.75775700	0.38822000
C	3.83374600	-1.28540500	-0.25286900
C	3.79045000	-2.74348300	-0.19204300
C	2.68770900	-3.12844500	0.48850300
H	4.62371000	-0.72610400	-0.74283200
H	4.54046100	-3.39480200	-0.62760400
H	2.37768800	-4.14227000	0.71081000
C	1.93115800	-1.90840500	0.93007000
C	0.12762300	0.15829500	-1.83750100
O	-0.55050000	-0.52513400	-1.05048100
Fe	-2.16615100	-0.29465800	0.12606900
Cl	-1.64201800	-1.37799100	1.96848700
Cl	-3.72311300	-1.25123300	-1.08383600
Cl	-2.56729700	1.84264000	0.47418400
C	-0.14637500	1.60539600	-2.07651400
H	-1.20931600	1.83120900	-1.97345100
H	0.38275100	2.17422100	-1.29848900
H	0.23441400	1.92623300	-3.04898200
C	1.24506700	-0.50401400	-2.57960700
H	1.47884500	-1.48091200	-2.15721900
H	0.93055800	-0.61768000	-3.62666100
H	2.13045900	0.13790800	-2.57133000
C	2.37095100	0.64709200	0.51680900
C	1.25851600	1.02065200	1.29629900
C	3.07257200	1.66835900	-0.15773200
C	0.86289700	2.35297600	1.39628100
H	0.68963300	0.26072800	1.82086700
C	2.68100200	2.99953300	-0.05330800
H	3.93226900	1.41275200	-0.77003200
C	1.57008500	3.35121600	0.72177300
H	-0.00992800	2.60563300	1.98893200
H	3.23992200	3.76662000	-0.58238000
H	1.25995200	4.38907400	0.79742100
H	0.90065200	-1.89811400	0.55163400
H	1.83969900	-1.86642100	2.02488400
M4Ph-S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.217826 a.u.			
E (UωB97X-D/def2-tzvp) = -618.349173788 a.u.			
C	1.01891700	0.62670600	-0.22002200
C	-3.10011500	-0.10694000	0.55151700
C	-2.13341100	0.76594600	-0.21157400
C	-1.24166100	-0.08370400	-1.07673300
H	-2.63916200	-0.69088500	1.34848900
H	-2.66976200	1.46824900	-0.86241300
H	-1.77690800	-0.74176100	-1.76257500
C	0.10074400	-0.17001100	-1.07046600
C	-4.41631200	-0.26194800	0.34734300
O	0.67238600	1.66683200	0.33738800

C	-5.21206100	0.44652700	-0.71866800
H	-4.61316700	1.12941200	-1.32515900
H	-5.68064100	-0.28055600	-1.39616900
H	-6.03168500	1.02365700	-0.26940000
C	-5.22518100	-1.19505800	1.21408200
H	-5.70989000	-1.97394700	0.60896500
H	-4.60698000	-1.68652700	1.97132400
H	-6.03156300	-0.65499500	1.72937700
C	2.42983700	0.13933600	-0.06467700
C	2.82745300	-1.17011400	-0.37098800
C	3.37907600	1.03799200	0.44516400
C	4.14933500	-1.56928200	-0.17764500
H	2.10371800	-1.89097400	-0.73624400
C	4.70013700	0.64364000	0.62614800
H	3.05138300	2.04212200	0.69167900
C	5.08866800	-0.66237600	0.31401400
H	4.44490500	-2.58851800	-0.40949500
H	5.42914100	1.35019400	1.01272800
H	6.12002400	-0.97256300	0.45732900
H	-1.52635000	1.36467900	0.46944200
H	0.56529400	-0.87652700	-1.75194800
M4Ph-FeCl₃/S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.210500 a.u.			
E (UωB97X-D/def2-tzvp) = -3262.91630019 a.u.			
C	0.64287300	-1.17827700	-0.91720400
C	-2.88409700	-0.67185100	-0.00048500
C	-2.44871100	-0.80862500	-1.44888900
C	-1.62318500	-2.05701000	-1.49335000
H	-2.11507900	-0.28099300	0.66061000
H	-3.30835000	-0.91779800	-2.11466900
H	-2.19204200	-2.97198100	-1.65757800
C	-0.29950600	-2.22816800	-1.23930200
C	-4.06717800	-1.01591100	0.53064300
O	0.32724800	0.03906500	-1.09194000
C	-5.22162100	-1.60403300	-0.23710400
H	-5.02088400	-1.72170700	-1.30486000
H	-5.48717100	-2.59081000	0.16611700
H	-6.11472500	-0.97448000	-0.12909800
C	-4.32436900	-0.80002000	2.00088800
H	-4.58886100	-1.74512500	2.49538500
H	-3.45260000	-0.37639600	2.50734000
H	-5.17316000	-0.11944000	2.15151500
C	1.97530700	-1.51782500	-0.40048300
C	2.21656700	-2.73575400	0.26331300
C	3.02126200	-0.58720100	-0.54135700
C	3.47663200	-3.00815600	0.78347400
H	1.41054600	-3.44516300	0.41375200
C	4.28243800	-0.87245700	-0.03275400
H	2.83984500	0.35077800	-1.05139100
C	4.51118600	-2.08024000	0.63199900
H	3.65213700	-3.93864100	1.31413900
H	5.08412000	-0.15029400	-0.14876900
H	5.49506500	-2.29749600	1.03737500
H	-1.88402400	0.07309700	-1.74843800
H	0.09316300	-3.23851900	-1.24225600
Fe	0.32678100	1.65514500	0.02461100

Cl	2.11876800	2.87773700	-0.37831800
Cl	-1.53638300	2.68941200	-0.53820200
Cl	0.24715300	0.78531300	2.05476300
M4Ph-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.212612 a.u.			
E (UωB97X-D/def2-tzvp) = -3262.91774445 a.u.			
C	0.75476200	0.34916200	0.57498600
C	1.48788000	-2.35630400	0.30764200
C	0.46537100	-2.63859000	1.37077600
C	0.17120500	-1.44516800	2.24693000
H	2.50609700	-2.24889700	0.67944000
H	0.82004300	-3.45594400	2.01366300
H	-0.25311300	-1.65498900	3.22670300
C	0.33725600	-0.16382100	1.90756300
C	1.29755500	-2.20820700	-1.01685400
O	-0.12896100	0.57031100	-0.29468500
Fe	-2.11450700	0.51765300	-0.11458300
Cl	-2.90312000	-1.44878900	0.51038400
Cl	-2.74935600	1.04710700	-2.15045500
Cl	-2.47354600	2.07662200	1.40473100
C	-0.03243200	-2.28824700	-1.70974900
H	-0.28445400	-1.31261600	-2.14835200
H	0.01094600	-3.00206800	-2.54225400
H	-0.85476100	-2.57252000	-1.05311200
C	2.46235600	-1.88448500	-1.91413900
H	2.57411900	-2.64148200	-2.70137300
H	2.29678900	-0.92505400	-2.42290600
H	3.40331000	-1.81614200	-1.36061300
H	-0.48868700	-2.97818300	0.94973300
H	0.03429300	0.62899900	2.59108200
C	2.12359900	0.79854100	0.31243900
C	3.14350400	0.57796500	1.25356900
C	2.41268500	1.46335200	-0.89288900
C	4.43908200	1.00491600	0.98540100
H	2.90975500	0.06591600	2.18088400
C	3.70943600	1.89070900	-1.15370000
H	1.61028500	1.63624200	-1.60130600
C	4.72264800	1.65881100	-0.21807600
H	5.22815900	0.83210900	1.71051300
H	3.93374000	2.40489100	-2.08299000
H	5.73528700	1.99248300	-0.42509200
M4Ph-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.212902 a.u.			
E (UωB97X-D/def2-tzvp) = -3262.89122621 a.u.			
Imaginary frequency: 366.4250			
C	0.90680800	-0.45389800	0.41801700
C	1.01379600	-2.08753000	-0.01433300
C	0.31485900	-2.84823600	1.12404600
C	0.20041800	-1.83876600	2.23649500
H	2.07855300	-2.31492100	-0.07030300
H	0.91016900	-3.72384600	1.41024100
H	-0.16745600	-2.11544000	3.21884000
C	0.53091500	-0.60253100	1.87302200
C	0.42280100	-1.98814400	-1.33579200
O	-0.09086700	0.10209300	-0.37698200
Fe	-1.79476700	0.74386800	0.04371000

Cl	-2.99226200	-0.92292700	0.97919200
Cl	-2.59697600	1.19822900	-1.99147300
Cl	-1.56697700	2.46078400	1.42911300
C	-0.99172000	-2.25537500	-1.63107000
H	-1.37842700	-1.51952000	-2.34480200
H	-1.02010100	-3.23813400	-2.13649800
H	-1.63470500	-2.28765700	-0.75201900
C	1.31865500	-1.62202000	-2.45393400
H	0.77960100	-1.38309200	-3.37150300
H	1.95476100	-0.77612500	-2.15472200
H	2.00717500	-2.46070700	-2.63481600
H	-0.67952400	-3.21885500	0.85150400
H	0.47767300	0.28941200	2.48826000
C	2.22462900	0.24435100	0.18764700
C	3.36706100	-0.13724300	0.90814900
C	2.31213200	1.29557300	-0.73456600
C	4.57818000	0.51412200	0.70163400
H	3.29526300	-0.93673900	1.64104100
C	3.53047800	1.94829900	-0.93916000
H	1.41614900	1.60239100	-1.26115600
C	4.66333800	1.55841400	-0.22710800
H	5.45640700	0.21556500	1.26663900
H	3.58748100	2.76701800	-1.65033700
H	5.60941500	2.06777600	-0.38539700
M4Ph-INT			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.218650 a.u.			
E (UωB97X-D/def2-tzvp) = -3262.92377579 a.u.			
C	0.10789600	-3.27836000	1.66569000
C	0.44036800	-1.98444400	1.70902600
C	0.60473900	-1.41469000	0.33199100
C	0.11385100	-2.54729600	-0.60884300
H	-0.04727700	-3.90326600	2.54017700
H	0.57409600	-1.39191300	2.60514000
H	0.71677300	-2.71489400	-1.50038200
C	-0.02380000	-3.81025100	0.25892700
C	-1.15561900	-1.69981300	-0.91631800
O	-0.63614200	-0.60599500	-0.03373200
Fe	-1.00017100	1.32464700	0.17101100
Cl	-3.12657600	1.49097200	-0.40906800
Cl	0.31430100	2.43122200	-1.19486400
Cl	-0.61139200	1.67753800	2.31509100
C	-2.48804500	-2.17674900	-0.37416300
H	-3.20589100	-1.35257800	-0.41019300
H	-2.87130900	-2.99944000	-0.98777500
H	-2.40095900	-2.51157100	0.66173400
C	-1.24272400	-1.19870200	-2.34635100
H	-1.47709000	-2.03772400	-3.01152500
H	-2.03143400	-0.44701500	-2.44352000
H	-0.29687600	-0.75059600	-2.66236900
H	-0.97310800	-4.33470500	0.09840700
H	0.77050800	-4.53318300	0.03090800
C	1.83777100	-0.60711100	0.05323900
C	2.39323700	0.19376700	1.06127800
C	2.40064800	-0.56482400	-1.22900000
C	3.47847600	1.02373900	0.78852200
H	1.96129200	0.20073600	2.05436000

C	3.49046100	0.25841400	-1.49959200
H	1.98350600	-1.16564200	-2.02961500
C	4.03019300	1.05828100	-0.49156900
H	3.88572300	1.64895300	1.57710500
H	3.91060600	0.28340000	-2.50050100
H	4.87264000	1.70936200	-0.70512000
M4Ph-TS2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.216934 a.u.			
E (UωB97X-D/def2-tzvp) = -3262.90827749 a.u.			
Imaginary frequency: 147.8441			
C	0.18614400	-3.15183700	1.69971200
C	0.67354600	-1.88665200	1.72643000
C	1.06768800	-1.49607200	0.39833500
C	0.45085700	-2.50011700	-0.56691100
H	-0.11364800	-3.70850800	2.58265300
H	0.80428700	-1.28292200	2.61177200
H	1.10067700	-2.73666300	-1.41096400
C	0.16887000	-3.73312700	0.31770700
C	-0.82520300	-1.70042400	-1.06571000
O	-0.51640000	-0.38677900	-0.61729500
Fe	-1.20888900	1.16821600	0.09461700
Cl	-3.32101100	1.40423900	-0.55941800
Cl	0.15265200	2.79214500	-0.60447600
Cl	-1.01016300	0.92209100	2.33936800
C	-2.14585100	-2.15321100	-0.44220300
H	-2.91178300	-1.42147000	-0.71351400
H	-2.45931600	-3.13701500	-0.80784800
H	-2.08815900	-2.17094200	0.65033800
C	-0.91815700	-1.69193700	-2.59022400
H	-1.09329800	-2.70050600	-2.98347700
H	-1.74549500	-1.04490800	-2.89722900
H	0.00336100	-1.29408800	-3.02696600
H	-0.76849500	-4.24401000	0.08510500
H	0.96657800	-4.48369600	0.21971300
C	2.05206900	-0.49661200	0.10302500
C	2.42932500	0.44032600	1.09361400
C	2.60037100	-0.37866900	-1.19474100
C	3.32276800	1.45665300	0.79102000
H	1.96931000	0.40948900	2.07301500
C	3.50361600	0.62991500	-1.48488400
H	2.30251800	-1.07413700	-1.97027900
C	3.86379500	1.55070600	-0.49337500
H	3.57964700	2.19104500	1.54677600
H	3.91677800	0.71750000	-2.48441800
H	4.55521700	2.35371200	-0.73016900
M4Ph-INT2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.217219 a.u.			
E (UωB97X-D/def2-tzvp) = -3262.91886347 a.u.			
C	-3.81493400	0.19824200	1.04802800
C	-2.82341700	-0.70301200	1.27700000
C	-2.01404400	-0.83193900	0.09999300
C	-2.38074500	0.24672100	-0.84824500
H	-4.57088500	0.48679300	1.77145200
H	-2.67982000	-1.25620200	2.19509600
H	-2.40168200	-0.09989100	-1.88212800
C	-3.75604300	0.73257200	-0.34479400

C	-1.24873100	1.44577100	-0.84860700
O	-0.01486800	0.84652800	-0.97467100
Fe	1.45605300	0.77551700	0.15366100
Cl	2.26490000	2.84726300	0.35630900
Cl	2.95252900	-0.63341800	-0.71637300
Cl	0.72976500	0.03059800	2.17749900
C	-1.35600900	2.31284000	0.41357900
H	-0.54332700	3.04404900	0.38219700
H	-2.29962700	2.86376200	0.46220200
H	-1.22965000	1.72468500	1.32456800
C	-1.51515200	2.28563800	-2.10728500
H	-2.52759200	2.70549100	-2.11887700
H	-0.79479700	3.10856600	-2.13215800
H	-1.36835900	1.67781300	-3.00526300
H	-3.91305300	1.81240000	-0.39841200
H	-4.55690700	0.27608300	-0.94585600
C	-1.02391000	-1.82258400	-0.13317200
C	-0.61913700	-2.70537400	0.90529200
C	-0.39198200	-1.92884800	-1.40066700
C	0.37704200	-3.63636800	0.68534400
H	-1.06120100	-2.61963500	1.88944500
C	0.60409100	-2.86644600	-1.61187800
H	-0.66887500	-1.25609600	-2.19914700
C	0.99306400	-3.71414300	-0.57147600
H	0.70078300	-4.28617700	1.49121900
H	1.10295000	-2.91892000	-2.57261400
H	1.79073800	-4.43233200	-0.73457900
M4Ph-TS3			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.215563 a.u.			
E (UωB97X-D/def2-tzvp) = -3262.90710659 a.u.			
Imaginary frequency: 390.7226			
C	3.74505800	-0.14478700	1.22257600
C	2.70572500	0.70643900	1.40296200
C	2.02577400	0.91169700	0.14028000
C	2.55446800	-0.00830800	-0.81104900
H	4.41531700	-0.49596000	1.99942500
H	2.41932600	1.16110900	2.34131400
H	2.55168800	0.26522400	-1.86012500
C	3.84287300	-0.55789100	-0.21305900
C	1.19694900	-1.44526900	-0.95059000
O	0.03017100	-0.83958000	-1.03225700
Fe	-1.44464500	-0.79897500	0.16570900
Cl	-2.19647500	-2.89567400	0.18515400
Cl	-2.95684100	0.62564700	-0.59485500
Cl	-0.70640500	-0.24207700	2.21692600
C	1.41859400	-2.33270700	0.26129600
H	0.63627200	-3.10099500	0.23673800
H	2.38708600	-2.83582200	0.23824700
H	1.30361400	-1.78438800	1.19808400
C	1.62373200	-2.06405200	-2.27639500
H	2.67560700	-2.36432800	-2.27678300
H	1.00615000	-2.95656300	-2.43591300
H	1.43475900	-1.37289500	-3.10145400
H	4.00672600	-1.63154500	-0.34400200
H	4.70445300	-0.06179600	-0.68713500
C	0.96859900	1.85434600	-0.10532200

C	0.42944600	2.63501400	0.94455800
C	0.43383100	2.01238300	-1.40548700
C	-0.60180700	3.52736700	0.70234900
H	0.80159900	2.51425300	1.95380900
C	-0.59832000	2.90727700	-1.64208400
H	0.82042800	1.42071300	-2.22433200
C	-1.12008900	3.66279600	-0.58991100
H	-1.02103900	4.10353800	1.52055200
H	-1.01513000	3.00056300	-2.63903700
H	-1.94119000	4.34881600	-0.77333900
M4Ph-P G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.209954 a.u. E (UωB97X-D/def2-tzvp) = -3262.92708429 a.u.			
C	3.52701200	-1.06631300	1.49333100
C	2.61368800	-0.07863800	1.57629600
C	2.37992000	0.50431800	0.23734000
C	3.16718600	-0.16499500	-0.65060200
H	3.88916400	-1.68183700	2.30814400
H	2.09752400	0.23351700	2.47438000
H	3.28163400	0.06263100	-1.70295400
C	3.98498100	-1.20379500	0.06636300
C	0.54903200	-1.76215700	-1.26115400
O	-0.28250800	-0.84115700	-1.16513600
Fe	-1.69776100	-0.45668300	0.20957200
Cl	-2.89157200	-2.31323400	-0.02160900
Cl	-2.77521900	1.33609100	-0.41378600
Cl	-0.80543900	-0.39259300	2.22422500
C	0.78972000	-2.71615500	-0.13665900
H	-0.16841600	-3.17675500	0.13571400
H	1.51292600	-3.48916600	-0.40080500
H	1.14157800	-2.16219400	0.74203200
C	1.20781700	-1.98308700	-2.58951400
H	2.25387200	-2.27437000	-2.47381900
H	0.68376500	-2.81861200	-3.07708600
H	1.11379700	-1.09778700	-3.21983800
H	3.83306300	-2.22292100	-0.32239400
H	5.06359700	-1.00774200	-0.03532300
C	1.45888400	1.61368000	-0.04333700
C	0.93381900	2.39694700	0.99872400
C	1.08589300	1.93090600	-1.36273000
C	0.07861600	3.46297800	0.73134400
H	1.19598100	2.17351600	2.02619400
C	0.23200300	2.99447900	-1.62973800
H	1.45868300	1.32813800	-2.18448400
C	-0.27501400	3.76734100	-0.58246600
H	-0.32125200	4.04849900	1.55358700
H	-0.05271200	3.21261500	-2.65474600
H	-0.95479100	4.58795400	-0.78966700
M4Ph-S (optimized with SMD (dichloroethane)) G_{corr} (B3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.217664 a.u. E (ωB97X-D/def2-tzvp) = -618.349006467 a.u.			
C	1.02429200	0.68762700	-0.21342400
C	-3.07490600	-0.13173800	0.56017500
C	-2.13375700	0.81157900	-0.15170800
C	-1.24685700	0.04281100	-1.09262900
H	-2.59666200	-0.75427200	1.31717800

H	-2.69300500	1.55122800	-0.73849100
H	-1.78630800	-0.56137200	-1.82277800
C	0.09704000	-0.04040100	-1.10944300
C	-4.38887000	-0.30471500	0.34716100
O	0.69786700	1.71186100	0.39164800
C	-5.20208300	0.44667400	-0.67438800
H	-4.62304100	1.18425900	-1.23533800
H	-5.64679300	-0.25154300	-1.39720000
H	-6.04083500	0.96759000	-0.19224400
C	-5.17326600	-1.30976200	1.15318900
H	-5.63790000	-2.06064900	0.49854700
H	-4.54382300	-1.83226400	1.88075400
H	-5.99477500	-0.82242100	1.69693000
C	2.41892200	0.15685500	-0.06765400
C	2.77884500	-1.14987300	-0.43261000
C	3.39181700	1.00092900	0.49172300
C	4.08602600	-1.59890100	-0.24460300
H	2.03933700	-1.82907400	-0.84309100
C	4.69847800	0.55688200	0.66714600
H	3.10225800	2.00608600	0.77950600
C	5.04862500	-0.74620000	0.29894700
H	4.35182000	-2.61487200	-0.52208200
H	5.44517700	1.22210400	1.09146800
H	6.06800300	-1.09541600	0.43774400
H	-1.52565200	1.36339200	0.56737300
H	0.55342800	-0.69826300	-1.84275800
M4Ph-RS (FeCl₃/S) (optimized with SMD (dichloroethane))			
G_{corr} (B3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.211438 a.u.			
E (ω B97X-D/def2-tzvp) = -3262.91716371 a.u.			
C	0.80988100	0.34431900	0.58403400
C	1.41310700	-2.37555700	0.31488800
C	0.39641100	-2.62670500	1.39068700
C	0.14631300	-1.41898900	2.25920000
H	2.43647700	-2.28500000	0.67597300
H	0.74474500	-3.43900200	2.04274700
H	-0.26428900	-1.60783000	3.24896600
C	0.37647900	-0.14687400	1.91732500
C	1.20930700	-2.23793500	-1.00973500
O	-0.08598000	0.57465100	-0.28772200
Fe	-2.02381600	0.50062600	-0.10610600
Cl	-3.06798900	-1.32557200	0.61560000
Cl	-2.70491000	0.98685600	-2.17136000
Cl	-2.48148700	2.19364500	1.27024800
C	-0.13271300	-2.29938400	-1.67938300
H	-0.35448500	-1.33560800	-2.15837900
H	-0.12822700	-3.04844000	-2.48237000
H	-0.95228800	-2.53360100	-0.99800800
C	2.36315500	-1.94480200	-1.92888400
H	2.43849400	-2.70463800	-2.71853600
H	2.21170400	-0.98168600	-2.43596200
H	3.31648300	-1.90307700	-1.39389200
H	-0.56728700	-2.96002800	0.98631800
H	0.16937400	0.66007200	2.62008800
C	2.17324600	0.77354400	0.31436800
C	3.18844900	0.55273300	1.26500100
C	2.47710800	1.41044400	-0.90574700

C	4.48921000	0.95881500	0.99413600
H	2.94947600	0.05818900	2.20025200
C	3.78001400	1.81513500	-1.16755900
H	1.68650000	1.57967400	-1.62788700
C	4.78528200	1.58782200	-0.22072000
H	5.27362600	0.78795300	1.72444500
H	4.01657300	2.30671800	-2.10588900
H	5.80324100	1.90361300	-0.42930600
M4Ph-TS1 (optimized with SMD (dichloroethane)) G_{corr} (B3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.211615 a.u. E (ω B97X-D/def2-tzvp) = -3262.89612759 a.u. Imaginary frequency: 59.8522			
C	0.92978500	-0.52459600	0.42438800
C	1.23034400	-2.10316400	-0.01940400
C	0.69322000	-2.96987900	1.13377600
C	0.43704400	-1.99237600	2.24757500
H	2.31416400	-2.17946800	-0.11017800
H	1.44214600	-3.72162000	1.40760600
H	0.14749400	-2.32121600	3.24098000
C	0.58427300	-0.71988600	1.88341300
C	0.60862400	-2.16191600	-1.33444700
O	-0.15604700	-0.05197800	-0.32731700
Fe	-1.78740100	0.67232200	0.03635100
Cl	-3.21996800	-0.92486200	0.76051100
Cl	-2.53715500	1.49484400	-1.92890400
Cl	-1.63162800	2.31990900	1.56394100
C	-0.76046900	-2.63831400	-1.54144400
H	-1.23355600	-2.14818300	-2.39559900
H	-0.65781800	-3.70989800	-1.79952000
H	-1.38426200	-2.57606500	-0.64904400
C	1.40634300	-1.73594800	-2.49023500
H	0.79842200	-1.44729000	-3.34899200
H	2.12783800	-0.95664300	-2.21974000
H	2.01286900	-2.61636200	-2.77110100
H	-0.21955700	-3.51901900	0.87777500
H	0.44032300	0.15540500	2.50838300
C	2.14887900	0.34104400	0.18346600
C	3.31687300	0.12265000	0.92943600
C	2.12793000	1.35894400	-0.77739900
C	4.44525500	0.91010300	0.71618300
H	3.33679700	-0.66369100	1.67889500
C	3.26146200	2.14840800	-0.98895300
H	1.22387600	1.53092100	-1.34946000
C	4.42079500	1.92624100	-0.24572000
H	5.34368000	0.73453200	1.30097900
H	3.23359300	2.93762700	-1.73487500
H	5.30140000	2.54041400	-0.41083200
M4Ph-INT (optimized with SMD (dichloroethane)) G_{corr} (B3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.216942 a.u. E (ω B97X-D/def2-tzvp) = -3262.92591830 a.u.			
C	1.01220000	-0.98538300	0.21704500
C	0.92814900	-2.26072900	-0.67349300
C	0.92392100	-3.46108800	0.28778300
C	0.75607300	-2.82606600	1.64539500
H	1.69517800	-2.32205400	-1.44478600
H	1.87072500	-4.01243800	0.22954300

H	0.62750200	-3.41517600	2.54881300
C	0.80453700	-1.48959500	1.61269900
C	-0.42322200	-1.75241900	-1.24002700
O	-0.28851800	-0.49347300	-0.38612800
Fe	-1.53318400	0.86311000	0.24011300
Cl	-3.18176100	-0.06405300	1.40386500
Cl	-2.29124100	1.87237600	-1.58851300
Cl	-0.33941400	2.20073800	1.53455900
C	-1.68674200	-2.49233900	-0.86452800
H	-2.56549100	-1.90801800	-1.15531200
H	-1.71804000	-3.44198000	-1.40909800
H	-1.74022000	-2.69523000	0.20678900
C	-0.38572500	-1.34396400	-2.69616300
H	-1.25989100	-0.73673000	-2.94999900
H	0.52229900	-0.78132800	-2.92836600
H	-0.39955100	-2.24900700	-3.31413700
H	0.13009900	-4.18303900	0.06731600
H	0.73322600	-0.81636600	2.45996200
C	2.10390500	0.02383600	0.00794200
C	3.24981100	-0.03968300	0.81148400
C	2.02535400	0.99688300	-0.99701200
C	4.30195200	0.85445800	0.61165500
H	3.31803200	-0.79027700	1.59295900
C	3.07538300	1.89435600	-1.18966400
H	1.13922400	1.06595700	-1.61692200
C	4.21687700	1.82593000	-0.38781600
H	5.18394500	0.79560500	1.24297300
H	2.99754900	2.65053700	-1.96566400
H	5.03259000	2.52726100	-0.53827000
M4Ph-TS2 (optimized with SMD (dichloroethane)) G_{corr} (B3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.216399 a.u. E (ω B97X-D/def2-tzvp) = -3262.91174528 a.u. Imaginary frequency: 321.4317			
C	0.55271200	2.73059000	-1.95238200
C	0.83927400	1.41747000	-1.83884300
C	1.23751600	1.11006300	-0.47328000
C	0.90513100	2.34664000	0.37572100
H	0.29669300	3.22148000	-2.88646300
H	0.84647800	0.70160400	-2.64996000
H	1.67172700	2.60105800	1.10653400
C	0.68966100	3.47291300	-0.65622400
C	-0.36209500	1.75303900	1.06280300
O	-0.30188500	0.43828900	0.39914500
Fe	-1.53435400	-0.88090000	-0.04738200
Cl	-3.06226500	-1.07348400	1.58131200
Cl	-0.39229200	-2.79031500	-0.29669600
Cl	-2.50866500	-0.32381000	-1.99413000
C	-1.68716900	2.42653200	0.74369000
H	-2.50384200	1.84217900	1.17927400
H	-1.71847000	3.43090300	1.17833100
H	-1.85323600	2.49798300	-0.33413000
C	-0.18488300	1.54187600	2.55822300
H	-0.17058200	2.51002500	3.07142600
H	-1.01616900	0.94897100	2.95260300
H	0.75021500	1.01682400	2.77144300
H	-0.17339100	4.10906700	-0.44273400

H	1.56342300	4.13702600	-0.69531900
C	2.25243600	0.10811200	-0.15901200
C	2.97469900	0.15809400	1.04925700
C	2.51881800	-0.93349900	-1.07018000
C	3.94053800	-0.80142700	1.33217500
H	2.78535800	0.94951800	1.76449500
C	3.48204400	-1.89379000	-0.78063100
H	1.96244800	-1.00034900	-1.99719200
C	4.19544300	-1.82943100	0.41917900
H	4.49529300	-0.74935600	2.26384700
H	3.67363000	-2.69460900	-1.48790000
H	4.94872000	-2.57896300	0.64326500
M4Ph-INT2 (optimized with SMD (dichloroethane))			
G_{corr} (B3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.217362 a.u.			
E (ω B97X-D/def2-tzvp) = -3262.92625370 a.u.			
C	4.11032100	-1.64333000	0.33377600
C	3.72689600	-0.36427500	0.61685100
C	2.56441900	-0.03900700	-0.13664700
C	2.06563500	-1.26705100	-0.83846200
H	4.98759400	-2.13133200	0.74669800
H	4.26414700	0.31922800	1.26089200
H	1.87506500	-1.06825100	-1.89627700
C	3.19999800	-2.29440200	-0.63810300
C	0.66447700	-1.76534800	-0.25567200
O	-0.27323800	-0.77105600	-0.55872000
Fe	-1.85060700	-0.16412700	0.07680200
Cl	-3.16155800	-1.94328800	0.60648400
Cl	-2.84533700	1.04633400	-1.56262200
Cl	-1.58048400	1.10302200	1.93704200
C	0.72983400	-1.99135800	1.25909200
H	-0.22424500	-2.40648700	1.59861100
H	1.52270500	-2.69473000	1.53293200
H	0.89714000	-1.04634000	1.78349700
C	0.24409900	-3.04185000	-0.99743600
H	0.89491500	-3.88948900	-0.76336000
H	-0.77558800	-3.29441200	-0.69183500
H	0.25021700	-2.87611600	-2.07965700
H	2.87183000	-3.27477300	-0.27948100
H	3.73327700	-2.48494700	-1.58060700
C	1.97073500	1.25851900	-0.20116600
C	1.06049800	1.59722100	-1.23524500
C	2.27777200	2.23295600	0.78649800
C	0.47653300	2.85482000	-1.27032100
H	0.83196700	0.87829400	-2.00905900
C	1.67274900	3.47751700	0.75417100
H	2.95444700	1.98907800	1.59716100
C	0.77367900	3.79074600	-0.27488400
H	-0.21906800	3.10435700	-2.06361200
H	1.89170300	4.20750800	1.52644500
H	0.30515700	4.77004700	-0.29951900
M4Ph-TS3 (optimized with SMD (dichloroethane))			
G_{corr} (B3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.213256 a.u.			
E (ω B97X-D/def2-tzvp) = -3262.90932671 a.u.			
Imaginary frequency: 224.1182			
C	4.22014800	-0.98816000	0.68181600
C	3.50413900	0.12932800	0.95365000

C	2.52636100	0.34777700	-0.10262400
C	2.56406500	-0.75040800	-0.97734000
H	5.00943900	-1.40483000	1.29743600
H	3.63957600	0.77181500	1.81404200
H	2.20486800	-0.70033400	-1.99705300
C	3.75737500	-1.60019000	-0.60186500
C	0.74294700	-1.83365700	-0.38585900
O	-0.19035500	-0.98421800	-0.69956600
Fe	-1.76662600	-0.36350300	0.10440300
Cl	-2.85531600	-2.25989000	0.65952000
Cl	-2.98014400	0.73973800	-1.41682600
Cl	-1.46975200	0.80969100	1.98068200
C	0.98866900	-2.11235400	1.07029700
H	0.23546900	-2.84728000	1.38766600
H	1.97301800	-2.55051600	1.24828000
H	0.86711400	-1.21005500	1.67219400
C	0.88677400	-2.98051300	-1.35647000
H	1.77841300	-3.57965900	-1.16828100
H	0.00577500	-3.62013000	-1.20391900
H	0.87431600	-2.63121500	-2.39113700
H	3.56105400	-2.67404600	-0.50726200
H	4.53420400	-1.50971300	-1.37751600
C	1.65876600	1.50752700	-0.20306300
C	0.82261200	1.69122500	-1.32581200
C	1.63196000	2.47823800	0.82124200
C	-0.01086500	2.80151000	-1.41513100
H	0.83246700	0.96792600	-2.13132200
C	0.80015200	3.58652700	0.72616100
H	2.25761300	2.35957400	1.69824800
C	-0.02457400	3.75138900	-0.39134400
H	-0.65248400	2.92285100	-2.28124000
H	0.78792800	4.32154400	1.52526200
H	-0.67622100	4.61731600	-0.46269700
M4Ph-P (optimized with SMD (dichloroethane))			
G_{corr} (B3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.212580 a.u.			
E (ω B97X-D/def2-tzvp) = -3262.92584512 a.u.			
C	4.26444100	-0.67830500	0.94733500
C	3.36373000	0.30327000	1.15926200
C	2.59008700	0.54484700	-0.07515100
C	3.03070400	-0.32986100	-1.02628700
H	4.96525000	-1.08106800	1.66961200
H	3.20497200	0.83184800	2.09195000
H	2.70520200	-0.37301000	-2.05822300
C	4.15254600	-1.15964100	-0.47264500
C	0.62753900	-2.10244100	-0.49705900
O	-0.25660900	-1.27311600	-0.81459900
Fe	-1.72206500	-0.36279800	0.12182100
Cl	-2.73858800	-2.24414900	0.85248000
Cl	-3.12181300	0.51679200	-1.37157600
Cl	-1.40336700	0.83319000	1.95860600
C	1.00577600	-2.34149800	0.92197400
H	0.54603000	-3.29327900	1.22554200
H	2.08806600	-2.45822100	1.02331400
H	0.64838300	-1.54614000	1.57790700
C	1.16651900	-2.98571600	-1.57250300
H	2.18784200	-3.30823700	-1.36680100

H	0.52829500	-3.88274500	-1.58199300
H	1.09088900	-2.50563300	-2.54976200
H	3.96272100	-2.24140800	-0.53173500
H	5.08495200	-0.99518300	-1.03523700
C	1.55832100	1.57920600	-0.22398400
C	0.67261100	1.57094900	-1.32080100
C	1.44243300	2.62076500	0.71262000
C	-0.28572900	2.57254300	-1.47448200
H	0.73964300	0.78158600	-2.06118900
C	0.48362600	3.62010500	0.55680500
H	2.11472300	2.66038300	1.56320200
C	-0.38568100	3.60109900	-0.53549500
H	-0.95802700	2.54311800	-2.32549100
H	0.41551500	4.41647000	1.29266700
H	-1.13536800	4.37810200	-0.65352700
M4Ph-RS (without FeCl₃) G_{corr} (B3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.220774 a.u. E (ω B97X-D/def2-tzvp) = -618.348474539 a.u.			
C	-0.21079200	0.46508100	-1.32992100
C	-1.24185000	-0.08923700	1.36985500
C	-1.76556500	1.32542300	1.35974000
C	-1.65846700	2.06720800	0.04462300
H	-0.30529900	-0.25459400	1.89605200
H	-2.82632500	1.34510900	1.65124100
H	-2.22451900	2.99902600	0.01008200
C	-1.01252100	1.70769600	-1.07032200
C	-1.80546000	-1.12891900	0.73618400
O	-0.58713500	-0.32090400	-2.19345000
C	-3.06262600	-1.02277100	-0.08424600
H	-2.80021500	-1.00539100	-1.15076200
H	-3.71267200	-1.89082600	0.08126900
H	-3.63622500	-0.11718800	0.13004300
C	-1.13549700	-2.47609900	0.71507400
H	-0.88734900	-2.75060500	-0.31978700
H	-0.20989900	-2.48150400	1.29839000
H	-1.79918400	-3.26122800	1.10166700
C	1.08875500	0.26176200	-0.62046100
C	1.63885000	1.23389200	0.22542600
C	1.77708100	-0.94255600	-0.82590900
C	2.84981800	0.99611100	0.87364200
H	1.11270300	2.17070600	0.37382900
C	2.98182800	-1.18242700	-0.17310400
H	1.34278200	-1.67426300	-1.49824900
C	3.51963600	-0.21392400	0.68065700
H	3.27132800	1.75347700	1.52847000
H	3.50610700	-2.12117300	-0.32832200
H	4.46107900	-0.40093500	1.18975900
H	-1.25221000	1.91646300	2.13193700
H	-1.12216800	2.33271200	-1.95543400
M4Ph-TS1 (without FeCl₃) G_{corr} (B3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.221758 a.u. E (ω B97X-D/def2-tzvp) = -618.268609546 a.u. Imaginary frequency: 1014.8801			
C	-0.32617500	0.10182300	-0.67855000
C	-1.27459600	0.24495200	1.01162800
C	-1.87775400	1.63567700	0.97637300

C	-1.57739800	2.20714400	-0.39241600
H	-0.57294700	0.02294800	1.80926400
H	-2.96122800	1.64087900	1.17012100
H	-1.97693200	3.17193900	-0.69691600
C	-0.81505300	1.44655600	-1.17497400
C	-1.94656500	-0.88227000	0.45303400
O	-0.80204700	-0.97711000	-1.28768900
C	-3.27101000	-0.76095100	-0.22550200
H	-3.44035700	-1.59754100	-0.90441500
H	-4.04755100	-0.77503100	0.55645600
H	-3.35959200	0.17616200	-0.77549100
C	-1.51549800	-2.24086700	0.89311000
H	-1.76727200	-3.00389000	0.15561100
H	-0.44194100	-2.26331500	1.09383600
H	-2.04047100	-2.46090000	1.83649100
C	1.13426500	0.06085300	-0.31502900
C	1.81305400	1.16746800	0.21707900
C	1.82672200	-1.13949100	-0.51390000
C	3.16053200	1.06990800	0.55154700
H	1.27653900	2.10024300	0.36501800
C	3.17875400	-1.23525600	-0.18351100
H	1.27622400	-1.96815800	-0.94525300
C	3.84705200	-0.13347900	0.35285100
H	3.68110700	1.93037000	0.96343600
H	3.71231100	-2.16814200	-0.34572500
H	4.89952300	-0.20733700	0.61318800
H	-1.43286900	2.25647000	1.76563200
H	-0.52614900	1.70978600	-2.19017800
M4Ph-INT (without FeCl₃)			
G_{corr} (B3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.244407 a.u.			
E (ω B97X-D/def2-tzvp) = -618.338318186 a.u.			
C	1.58434400	2.33777000	0.26452700
C	0.67328900	1.68907700	1.00167300
C	0.28410800	0.33038500	0.37942200
C	1.24184900	0.21669700	-0.87563800
H	2.01928400	3.31716300	0.50481500
H	0.23724200	2.03911300	1.94517200
H	0.76285400	-0.11974300	-1.80909300
C	1.98073300	1.58374900	-1.01757000
C	1.94279900	-0.95769000	-0.08096300
O	0.94712500	-0.84448700	1.04803700
C	3.39597700	-0.70099800	0.42580800
H	3.68903100	-1.50378200	1.11906800
H	4.10299700	-0.69052300	-0.41780000
H	3.45399400	0.25983200	0.95699100
C	1.82885800	-2.34908500	-0.78086500
H	2.48366400	-2.38224300	-1.66538800
H	2.13089200	-3.14866700	-0.08760000
H	0.79158800	-2.53017300	-1.09984500
H	3.07470800	1.46204900	-1.10481200
H	1.63705500	2.12650700	-1.91786800
C	-1.23169200	0.11413800	0.18953600
C	-1.78109600	-1.16733000	0.40601000
C	-2.07212500	1.17045100	-0.22775800
C	-3.15612700	-1.39393800	0.21193300
H	-1.10428300	-1.96694000	0.73757400

C	-3.44618200	0.94286500	-0.42672200
H	-1.64437100	2.16823000	-0.39341600
C	-3.99033100	-0.33868100	-0.20709700
H	-3.57871900	-2.39236600	0.38650000
H	-4.09606800	1.76616600	-0.75169600
H	-5.06328600	-0.51319900	-0.36066400
M4Ph-TS2 (without FeCl₃)			
G_{corr} (B3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.243368 a.u.			
E (ω B97X-D/def2-tzvp) = -618.210597229 a.u.			
Imaginary frequency: 817.1599			
C	2.07449000	1.72652000	0.11245900
C	0.70709400	2.10670300	-0.13446900
C	0.25055400	0.73836700	-0.24831700
C	1.34314000	-0.16813200	-1.02424100
H	2.83133200	2.33047500	0.64859900
H	0.15255500	2.87358700	0.40691300
H	1.05789800	-0.71077900	-1.94102100
C	2.49577800	0.87253700	-1.12957400
C	1.72473000	-0.96359200	0.28282300
O	1.38715000	0.26240700	1.08768700
C	3.19261500	-1.45371600	0.49853800
H	3.23948400	-2.08918100	1.39512500
H	3.52609200	-2.04845800	-0.36589200
H	3.88628300	-0.61382900	0.63986400
C	0.74138200	-2.12944200	0.62366400
H	0.93581300	-2.97934500	-0.04844400
H	0.89999200	-2.46046800	1.66082200
H	-0.30433800	-1.81845900	0.50683700
H	3.49636100	0.42064600	-1.08640100
H	2.42959200	1.49435200	-2.03720800
C	-1.20518200	0.33004900	-0.15429300
C	-2.01595200	0.87626100	0.87326200
C	-1.79637000	-0.55836800	-1.08817500
C	-3.37781200	0.54022700	0.96684800
H	-1.56222100	1.56082100	1.60187800
C	-3.16093000	-0.88664500	-0.99799500
H	-1.18440900	-0.98564500	-1.89209600
C	-3.95422400	-0.34156500	0.03068000
H	-3.99239900	0.96628700	1.77086800
H	-3.60706100	-1.57105700	-1.73160200
H	-5.01804100	-0.60342800	0.10300600
M4Ph-P' (without FeCl₃)			
G_{corr} (B3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.246314 a.u.			
E (ω B97X-D/def2-tzvp) = -618.341561128 a.u.			
C	2.13575500	1.60947400	0.04322400
C	0.62615900	1.74087000	0.34709700
C	0.00858600	0.67428800	-0.22355600
C	1.13129600	-0.16146800	-0.89847900
H	2.76218000	2.50656900	0.20990400
H	0.18589100	2.50194600	0.99990700
H	0.81795600	-0.91728200	-1.63495800
C	2.07239300	0.98913600	-1.39404700
C	2.03029800	-0.73538900	0.29327900
O	2.68379000	0.48310300	0.87616400
C	3.14283000	-1.70763900	-0.23319800
H	3.80842900	-1.99207000	0.59540700

H	2.68172200	-2.61962400	-0.64162000
H	3.74741600	-1.23393200	-1.01893100
C	1.20000000	-1.45895000	1.40694800
H	0.70282200	-2.34910200	0.99286500
H	1.86904800	-1.77573300	2.22068100
H	0.43615300	-0.78552000	1.81897900
H	3.04998000	0.64705100	-1.76710400
H	1.58865700	1.64874300	-2.13093600
C	-1.42455600	0.27097500	-0.14727800
C	-2.40478700	1.16984200	0.35583800
C	-1.84915600	-1.01584600	-0.57210700
C	-3.75524600	0.79340200	0.43220300
H	-2.09802700	2.17127600	0.68300500
C	-3.20160200	-1.39085300	-0.49268600
H	-1.11114400	-1.72808900	-0.96019600
C	-4.15995500	-0.48906200	0.00875700
H	-4.49783500	1.50212000	0.82210300
H	-3.50948400	-2.39164400	-0.82323700
H	-5.21617100	-0.78222300	0.06884600
M5Ph-S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.244622 a.u.			
E (UωB97X-D/def2-tzvp) = -1199.75437237 a.u.			
C	0.90654000	-0.43231200	0.80561900
C	-1.18986100	1.65918600	-0.06856600
C	-0.32540300	1.62919500	-1.23337300
C	0.91423200	1.09728000	-1.30172400
H	-0.74566900	1.35402700	0.87450500
H	-0.70852000	2.07464500	-2.14817800
H	1.44194800	1.19942100	-2.24921600
C	1.68513000	0.43070600	-0.18223100
C	-2.48556600	2.03738400	-0.03211200
O	1.13345500	-0.29834400	2.00656500
C	-3.28730300	2.48008000	-1.22650700
H	-4.15618000	1.82227300	-1.36632500
H	-3.68642300	3.49149400	-1.06933500
H	-2.71805200	2.48189400	-2.15807900
C	-3.24496300	2.02179100	1.26795200
H	-4.11711600	1.35588500	1.20465200
H	-2.61972100	1.68745200	2.10099800
H	-3.63449100	3.02099000	1.50917600
C	-0.08007500	-1.46140000	0.35067800
C	-0.80386500	-2.13736700	1.34635300
C	-0.30213300	-1.78814300	-0.99470200
C	-1.73075700	-3.11618200	1.00555500
H	-0.61663200	-1.87528800	2.38169100
C	-1.22616600	-2.77429400	-1.33477700
H	0.22958300	-1.26499100	-1.77836700
C	-1.94349600	-3.43764600	-0.33800700
H	-2.28687100	-3.63063700	1.78394200
H	-1.38890500	-3.02139600	-2.37976800
H	-2.66688100	-4.20251000	-0.60664100
Si	3.10729200	-0.62529900	-0.89214500
H	4.13776300	0.28356900	-1.44187100
H	3.69707200	-1.45392000	0.17739400
H	2.63070000	-1.49715100	-1.98801300
Si	2.50914700	1.81789300	0.85443800

H	3.57697100	1.31762500	1.74555100
H	3.13473900	2.74517800	-0.11686900
H	1.48100700	2.55219800	1.61517100
M5Ph-FeCl₃/S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.237105 a.u.			
E (UωB97X-D/def2-tzvp) = -3844.27376445 a.u.			
C	0.77108600	-0.65972600	0.59746700
C	1.23271900	2.24414200	-0.50988000
C	2.55710600	1.81643800	-0.10863800
C	2.86628400	0.80498900	0.73455300
H	0.39165200	1.80222100	0.01400300
H	3.40101000	2.37028800	-0.51272000
H	3.91724000	0.64883200	0.96963700
C	1.87332200	-0.09836400	1.44932200
C	0.93817300	3.17646500	-1.44446500
O	-0.40595700	-0.47305700	1.01203600
C	1.95537300	3.89036400	-2.29274500
H	1.75021200	3.70782500	-3.35616400
H	1.88113900	4.97591400	-2.14523600
H	2.98642700	3.58990200	-2.09571100
C	-0.49096000	3.56310300	-1.70970300
H	-0.78111900	3.29753000	-2.73509800
H	-1.18656200	3.07359300	-1.02518400
H	-0.61647900	4.65076000	-1.61820900
Fe	-2.19144400	-0.10698500	0.23018900
Cl	-1.87933000	0.16593300	-1.93197700
Cl	-2.76096600	1.78534400	1.20108000
Cl	-3.43225900	-1.85398200	0.72609800
C	0.99666600	-1.50995000	-0.57945200
C	0.00485900	-2.45764600	-0.90710400
C	2.17341400	-1.45179400	-1.35111200
C	0.18348200	-3.31689800	-1.98353200
H	-0.88787200	-2.54054200	-0.29818700
C	2.33600700	-2.30324100	-2.43703600
H	2.93147500	-0.71618500	-1.11872800
C	1.34403900	-3.23528900	-2.75583600
H	-0.58512700	-4.04509100	-2.22102500
H	3.23582400	-2.23737600	-3.04055800
H	1.47737100	-3.89839800	-3.60560100
Si	2.80561100	-1.60547300	2.18573400
H	3.61276900	-1.12002600	3.32385600
H	1.82884300	-2.61118500	2.64529800
H	3.69416500	-2.18923200	1.16093500
Si	1.12499800	0.88841400	2.92387600
H	0.36901000	-0.00332300	3.82786300
H	2.28400100	1.43743200	3.65830100
H	0.27668100	1.98239400	2.42734100
M5Ph-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.237996 a.u.			
E (UωB97X-D/def2-tzvp) = -3844.31157853 a.u.			
C	0.75211900	-0.32841900	0.30143300
C	2.58240900	-0.04665700	-1.95125300
C	3.17397600	-1.24871200	-1.33076500
C	2.71547900	-1.90401100	-0.25118300
H	3.11509900	0.88193600	-1.73795400
H	4.12777400	-1.59011400	-1.73641200

H	3.28906300	-2.75861200	0.10490400
C	1.43341300	-1.65262500	0.51049900
C	1.48662400	0.03643000	-2.72687500
O	-0.46150200	-0.39910900	-0.03231800
Fe	-2.31404900	0.23059400	0.14940900
Cl	-2.36098600	1.07522600	2.17745400
Cl	-3.54196300	-1.57004200	-0.11205100
Cl	-2.61658200	1.73097200	-1.44816400
C	0.67537600	-1.14850500	-3.16613500
H	-0.33301100	-1.10847600	-2.73519200
H	0.55093800	-1.13633800	-4.25660700
H	1.13776900	-2.09536400	-2.88060500
C	0.97720300	1.37442400	-3.19049500
H	-0.03813700	1.54393800	-2.80756300
H	1.61372100	2.19654100	-2.85010500
H	0.90917000	1.41455500	-4.28552800
Si	1.70286400	-1.87453900	2.41459200
H	1.65979600	-3.32359000	2.69847400
H	3.01930400	-1.35363000	2.83251200
H	0.61738200	-1.18064700	3.13024100
Si	0.19076200	-3.08083900	0.10882300
H	0.99564000	-4.31666000	0.21702000
H	-0.87018300	-3.11076600	1.13280600
H	-0.37251800	-2.97880800	-1.24136300
C	1.36551700	0.97689900	0.58456800
C	2.67422600	1.08128000	1.09556100
C	0.63200900	2.15379500	0.34292300
C	3.22017000	2.32621200	1.37995000
H	3.27660800	0.19454200	1.23594600
C	1.18517900	3.39725200	0.62494400
H	-0.35722800	2.10290600	-0.09010300
C	2.47577800	3.48747400	1.15044900
H	4.22884800	2.39304600	1.77526400
H	0.60646000	4.29481200	0.43238200
H	2.90520600	4.45979300	1.37320700
M5Ph-TS1 G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.239320 a.u. E (UωB97X-D/def2-tzvp) = -3844.28438824 a.u. Imaginary frequency: 199.1761			
C	0.92336700	-0.50447500	-0.27799400
C	0.98295300	-1.39289900	-1.69150200
C	1.88264000	-2.54584300	-1.35913700
C	2.28407800	-2.53752600	-0.08261300
H	1.36580100	-0.73417500	-2.47546100
H	2.15677100	-3.29338600	-2.09667200
H	2.93919100	-3.28991300	0.34896800
C	1.75969200	-1.39900600	0.73037000
C	-0.41567400	-1.69956800	-2.00226900
O	-0.39039200	-0.44791600	0.16370100
Fe	-1.93517300	0.56029900	0.36609800
Cl	-1.99828800	1.39940900	2.41718800
Cl	-3.56547700	-0.96978400	-0.01429900
Cl	-2.05171400	2.15354400	-1.19402800
C	-1.09916300	-2.87550700	-1.48676500
H	-1.80955700	-2.46466200	-0.73186400
H	-1.75694000	-3.31786100	-2.24510400

H	-0.44313300	-3.60972500	-1.02314900
C	-1.16992300	-0.75981400	-2.84550400
H	-2.24879200	-0.83017000	-2.68834100
H	-0.82986400	0.27237200	-2.71416600
H	-0.94981600	-1.04315300	-3.89053100
Si	3.20250100	-0.53383000	1.63639000
H	3.81661700	-1.56476100	2.50379500
H	4.23146600	-0.05342300	0.69423300
H	2.71746200	0.57293700	2.48042300
Si	0.55299300	-2.05432600	2.07667400
H	1.37747200	-2.94168900	2.93446700
H	0.01617400	-0.96517700	2.90669300
H	-0.51265800	-2.88663700	1.48893800
C	1.53946600	0.86911000	-0.49375600
C	2.61633200	1.07355900	-1.36948800
C	1.09960600	1.94364900	0.29074000
C	3.21067100	2.32810300	-1.48717900
H	3.02170800	0.24735200	-1.94545300
C	1.69742700	3.19745800	0.17551100
H	0.30777700	1.80431100	1.01574000
C	2.74681100	3.39814500	-0.72009300
H	4.03868700	2.46675700	-2.17607300
H	1.33130500	4.01638200	0.78679600
H	3.20447100	4.37816500	-0.81685700
M5Ph-INT			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.245343 a.u.			
E (UωB97X-D/def2-tzvp) = -3844.31419891 a.u.			
C	-1.16952500	-0.31497300	0.51494900
C	-1.26483000	-1.13338300	1.83690600
C	-2.26918200	-2.20585200	1.55757200
C	-2.72710500	-2.13767800	0.30485100
H	-1.45796300	-0.57860800	2.75708500
H	-2.54816300	-2.95654400	2.28877200
H	-3.45004800	-2.82070600	-0.13081300
C	-2.18035400	-0.96005700	-0.48322300
C	0.23069300	-1.52625300	1.67893800
O	0.24891200	-0.83679900	0.32957200
Fe	1.90139800	0.03454000	-0.45308800
Cl	1.61930600	0.39216300	-2.60654600
Cl	3.44707400	-1.51405800	-0.13092300
Cl	2.39500400	1.86118400	0.66606900
C	1.14858900	-0.82560300	2.66336200
H	2.19924800	-0.97794200	2.40289300
H	0.94996900	0.24789000	2.70150100
H	0.97745200	-1.25205600	3.65869200
C	0.56386000	-2.98939600	1.48900800
H	-0.10483200	-3.45540800	0.76311200
H	1.59520600	-3.09243300	1.14297300
H	0.46353400	-3.51394500	2.44605400
C	-1.12538200	1.18808700	0.53524500
C	-0.89760200	1.87171700	-0.66899200
C	-1.25632400	1.92699300	1.71562400
C	-0.78174200	3.25894400	-0.68764000
H	-0.78199900	1.32058500	-1.59439400
C	-1.15139100	3.31729400	1.69485600
H	-1.44391300	1.42730700	2.65901900

C	-0.90795700	3.98627900	0.49546000
H	-0.58478400	3.76547800	-1.62709000
H	-1.25465100	3.87610700	2.62010600
H	-0.81552800	5.06802300	0.48385700
Si	-3.69907100	0.15558000	-0.83022100
H	-3.45492200	1.17879100	-1.86459200
H	-4.77167900	-0.74576000	-1.30743200
H	-4.13553500	0.79610100	0.42673300
Si	-1.50023000	-1.61149300	-2.14274800
H	-0.32718600	-2.47903000	-1.94057700
H	-2.60531700	-2.41784200	-2.70989600
H	-1.20031200	-0.51551300	-3.07843300
M5Ph-TS2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.241658 a.u.			
E (UωB97X-D/def2-tzvp) = -3844.29926539 a.u.			
Imaginary frequency: 229.7653			
C	-1.75040000	-0.03523200	0.63322100
C	-1.49015500	-0.94798100	1.75073200
C	-2.41068600	-2.09652400	1.54047700
C	-3.00279600	-2.00228100	0.34127900
H	-1.47892800	-0.51043000	2.74786700
H	-2.51903700	-2.91302500	2.24305600
H	-3.67955700	-2.71847000	-0.11022000
C	-2.58446700	-0.72594800	-0.36154500
C	0.21453100	-1.40190400	1.53152500
O	0.59242500	-1.02943400	0.27870600
Fe	2.07845200	-0.22843800	-0.48391300
Cl	1.46454800	0.22945800	-2.59963700
Cl	3.73459900	-1.70802200	-0.27074100
Cl	2.60569800	1.67426800	0.57906200
C	0.98080400	-0.67620700	2.63299200
H	2.03885500	-0.94455500	2.53553400
H	0.91537400	0.40727200	2.51976100
H	0.63253500	-0.97406700	3.62771900
C	0.30421200	-2.91909200	1.67782200
H	-0.24970300	-3.41908000	0.88140900
H	1.36282300	-3.18232500	1.57514900
H	-0.05536600	-3.26583500	2.65207600
C	-1.24032500	1.30207700	0.56184900
C	-0.96432300	1.92695000	-0.67829500
C	-0.97608000	2.02092700	1.75495800
C	-0.40849200	3.19502900	-0.71785700
H	-1.10511600	1.38497300	-1.60162300
C	-0.45495600	3.30321700	1.70512600
H	-1.22006300	1.57870600	2.71367000
C	-0.15626900	3.88648100	0.46972500
H	-0.14416600	3.63305400	-1.67393000
H	-0.26435300	3.84616700	2.62486100
H	0.28370600	4.87812700	0.43409000
Si	-4.14311200	0.33522800	-0.72868600
H	-3.78966000	1.49602800	-1.56568100
H	-5.10273300	-0.53907600	-1.43033900
H	-4.71318100	0.78737900	0.55574500
Si	-1.82614600	-1.28717000	-2.06287500
H	-0.63791900	-2.10559400	-1.82012000
H	-2.92503100	-2.10357500	-2.62509500

H	-1.60396700	-0.13768100	-2.94963400
M5Ph-P			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.234352 a.u.			
E (UωB97X-D/def2-tzvp) = -3844.33600804 a.u.			
C	-2.17602700	0.13370500	0.62884100
C	-2.52830200	-0.45350600	1.82436400
C	-3.44076200	-1.54322500	1.60104100
C	-3.68350300	-1.65115700	0.26495700
H	-2.19160900	-0.12909300	2.80238300
H	-3.86795100	-2.16515100	2.37985100
H	-4.32877100	-2.37039800	-0.22541200
C	-2.91212700	-0.59659800	-0.47121900
C	0.47910100	-1.52099900	1.55179400
O	0.86388000	-1.26849600	0.39568800
Fe	2.39104500	-0.26299400	-0.41600600
Cl	1.88251800	0.09589400	-2.52305000
Cl	3.93582700	-1.81577500	-0.13303700
Cl	2.89595000	1.50107200	0.79427300
C	0.83667000	-0.62254300	2.69283200
H	1.92327400	-0.66278100	2.84264000
H	0.60028600	0.41363500	2.42774800
H	0.33168000	-0.90941700	3.61608200
C	-0.24449400	-2.81001800	1.78701100
H	-0.81574800	-3.09956900	0.90416800
H	0.52749400	-3.57491600	1.96104300
H	-0.89025700	-2.76657100	2.66414200
C	-1.34734500	1.33639100	0.47960600
C	-0.70739200	1.66280000	-0.72912500
C	-1.18010100	2.21802200	1.56841000
C	0.07018500	2.81271800	-0.84524100
H	-0.79834300	1.01142900	-1.58702800
C	-0.39748500	3.36263300	1.45266200
H	-1.69961800	2.01957600	2.50061600
C	0.23166200	3.66708300	0.24336600
H	0.57026600	3.01965700	-1.78566700
H	-0.28697100	4.02495000	2.30647900
H	0.84775200	4.55621300	0.15493900
Si	-4.19945200	0.60663800	-1.20260800
H	-3.52153000	1.70340700	-1.92268100
H	-5.06718500	-0.12680400	-2.15005500
H	-5.01171400	1.14970100	-0.09552600
Si	-1.96414800	-1.47601400	-1.87252100
H	-0.88016000	-2.30196400	-1.31620300
H	-2.95096100	-2.34717800	-2.54744100
H	-1.42123200	-0.53975700	-2.87258900
M6Ph-S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.247219 a.u.			
E (UωB97X-D/def2-tzvp) = -1199.74659724 a.u.			
C	-1.42756200	0.12901500	0.04556300
C	3.07529500	0.92716200	0.14159900
C	1.67249200	0.35042700	0.06268200
C	0.66082100	1.43133400	0.25863400
H	3.11181800	2.00365600	0.31719300
H	1.08452200	2.42090600	0.43752000
C	-0.69508100	1.36949000	0.25194100
C	4.25238300	0.29626500	0.02482000

O	-0.81115300	-0.94380100	-0.10374000
C	4.41671500	-1.18145200	-0.21876600
H	3.47258300	-1.72529100	-0.29991200
H	4.97756600	-1.35837500	-1.14608600
H	4.99200300	-1.64351500	0.59451100
C	5.54757600	1.06046200	0.13478900
H	6.14459600	0.95776000	-0.78218900
H	5.37905300	2.12701400	0.31287600
H	6.16641800	0.67119500	0.95536000
C	-2.91799700	0.11999700	0.02429300
C	-3.69511600	1.28794500	-0.01667500
C	-3.56255400	-1.12772300	0.03134000
C	-5.08617000	1.20816800	-0.04509300
H	-3.22386800	2.26398700	-0.04575100
C	-4.95067900	-1.20610700	0.01026400
H	-2.94743700	-2.02032200	0.05419600
C	-5.71647600	-0.03722000	-0.02744600
H	-5.67780800	2.11816100	-0.08284800
H	-5.43879800	-2.17633200	0.02184400
H	-6.80103500	-0.09721600	-0.04582700
H	-1.24379400	2.28566800	0.43170700
Si	1.40105000	-0.97734100	1.45538400
H	0.26170200	-0.64194400	2.33150400
H	1.30380600	-2.36284600	0.96023100
H	2.61743800	-0.90701000	2.30110200
Si	1.37135600	-0.46521900	-1.67403000
H	2.56732700	-0.12417000	-2.48107000
H	1.27793100	-1.93624300	-1.64349100
H	0.20964500	0.12459200	-2.36757500
M6Ph-RS (FeCl₃/S)			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.236827 a.u.			
E (UωB97X-D/def2-tzvp) = -3844.31246838 a.u.			
C	0.15393600	-0.85893400	-0.58351600
C	2.11296000	0.66200200	0.92009400
C	2.12304400	1.65106500	-0.23403800
C	1.21239900	1.30776900	-1.37674100
H	2.93412800	-0.05419100	0.92714400
H	1.17507100	2.04689200	-2.17772400
C	0.37944800	0.26262200	-1.51579300
C	1.22039000	0.53626800	1.92035600
O	-0.97209600	-0.97763200	-0.03105600
Fe	-2.69995500	-0.01554600	-0.18495400
Cl	-3.62738100	-1.06020900	-1.88522600
Cl	-2.39449200	2.12400100	-0.63838200
Cl	-3.61736100	-0.35929600	1.78472700
C	-0.01765200	1.37036400	2.09660800
H	-0.86935000	0.73444000	2.36499600
H	0.11070800	2.08339900	2.92232500
H	-0.30329800	1.92665800	1.20429400
C	1.40619100	-0.54018000	2.95660500
H	1.42643000	-0.10804800	3.96579400
H	0.55911200	-1.23861900	2.93417900
H	2.32656600	-1.11027100	2.80265600
C	1.12769800	-1.93959800	-0.40328100
C	2.30749600	-1.98179700	-1.16521800
C	0.85888500	-2.96051400	0.52681800

C	3.22088100	-3.01314000	-0.97654100
H	2.49522400	-1.20912000	-1.90072900
C	1.77702000	-3.98639100	0.71356000
H	-0.06619000	-2.92632300	1.09054400
C	2.96015400	-4.01096500	-0.03298600
H	4.13220000	-3.04305100	-1.56543100
H	1.57364000	-4.76971800	1.43699700
H	3.67509200	-4.81512700	0.11466200
H	-0.32109400	0.26789200	-2.34950400
Si	1.78270500	3.47556200	0.28075000
H	2.28349200	3.67295000	1.65463000
H	2.53714400	4.36072200	-0.63895200
H	0.35690100	3.83258300	0.17885900
Si	3.90649800	1.70207700	-0.93087700
H	4.37507000	0.31632700	-1.15442300
H	3.93343100	2.44168100	-2.20898800
H	4.80235000	2.36136200	0.04311600
M6Ph-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.239140 a.u.			
E (UωB97X-D/def2-tzvp) = -3844.27776257 a.u.			
Imaginary frequency: 253.9406			
C	0.47995300	-0.47445900	-0.15714900
C	1.63537700	0.51254900	0.78626600
C	2.53070500	1.19335900	-0.28064500
C	1.82156800	0.92994100	-1.59125400
H	2.15637100	-0.19102900	1.43399800
H	2.16003700	1.38805300	-2.51641000
C	0.77848100	0.10557100	-1.51546200
C	0.61805700	1.22495000	1.51359200
O	-0.77534000	-0.21917900	0.34147200
Fe	-2.46903800	0.24050200	-0.27868200
Cl	-3.48645000	-1.55345800	-1.06648000
Cl	-2.17408700	1.81473200	-1.83707700
Cl	-3.37542700	1.10600200	1.59889600
C	-0.02086500	2.46533800	1.02741900
H	-1.07105800	2.49954900	1.33278300
H	0.48652100	3.31391800	1.51443500
H	0.05073500	2.58523100	-0.05322600
C	0.16413900	0.69731400	2.81825100
H	0.48920400	1.40655200	3.59656200
H	-0.93212600	0.67380900	2.84475400
H	0.58108400	-0.28588800	3.04330000
C	0.83462900	-1.92608000	0.00850200
C	1.79561800	-2.54454700	-0.80407500
C	0.18113100	-2.67987600	0.99600100
C	2.10810400	-3.88989900	-0.62388200
H	2.27942700	-1.97625900	-1.59018900
C	0.50025900	-4.02257600	1.17806300
H	-0.59192300	-2.20826900	1.59060000
C	1.46705700	-4.62970900	0.37233300
H	2.84552200	-4.36259800	-1.26576200
H	-0.01545400	-4.60036700	1.93921600
H	1.71073400	-5.67890300	0.51177100
H	0.15064400	-0.19445800	-2.34750300
Si	2.96836000	3.04276000	-0.06480400
H	3.12670500	3.34376900	1.37532900

H	4.26197800	3.28155900	-0.74228400
H	1.96530400	3.94714700	-0.65924600
Si	4.24119900	0.32855600	-0.28192400
H	4.08005100	-1.12041300	-0.05822400
H	4.90352000	0.57613000	-1.57808600
H	5.07269600	0.88949500	0.80781800
M6Ph-INT			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.243452 a.u.			
E (UωB97X-D/def2-tzvp) = -3844.31735279 a.u.			
C	2.38976700	-0.41673100	1.60844200
C	1.16355900	0.12245900	1.63034900
C	0.68393200	0.44158400	0.24443900
C	1.73203200	-0.26120700	-0.67525000
H	2.94772400	-0.70662400	2.49464800
H	0.56013700	0.33354500	2.50493600
H	1.96676500	0.29822800	-1.58307700
C	2.97182100	-0.54368500	0.21464000
Si	3.97770200	-2.12730300	-0.11148200
H	5.40042300	-1.85354400	0.19461900
H	3.54685300	-3.26560000	0.72430000
H	3.87213400	-2.48490100	-1.54275400
Si	4.19945300	0.90430700	-0.02215400
H	5.17947700	0.90416200	1.08337600
H	4.91310800	0.74564600	-1.31016600
H	3.44719900	2.17451000	-0.03106700
C	0.65300900	-1.34970600	-0.98193800
O	-0.35025300	-0.54221400	-0.20493000
Fe	-2.28283300	-0.70215600	0.25991900
Cl	-2.62974100	-2.79804600	0.84137200
Cl	-3.35904100	-0.19190400	-1.59659400
Cl	-2.49256400	0.71545200	1.92270000
C	0.77182900	-2.72387200	-0.35660200
H	-0.19775100	-3.22689200	-0.40493300
H	1.49339700	-3.33074000	-0.91165400
H	1.06811500	-2.66922800	0.69179900
C	0.22287300	-1.40948700	-2.43491000
H	0.99444900	-1.92416000	-3.01859500
H	-0.71698900	-1.96047300	-2.53728800
H	0.08357700	-0.40808400	-2.85031000
C	0.24378200	1.85132700	-0.02164200
C	0.67709700	2.88902700	0.81104800
C	-0.56955700	2.15075600	-1.12182700
C	0.30477200	4.20644800	0.54771600
H	1.30645200	2.66538900	1.66622800
C	-0.94999200	3.46628300	-1.37690800
H	-0.94198600	1.35538400	-1.75607200
C	-0.51172200	4.49832300	-0.54538500
H	0.64488800	5.00216900	1.20383700
H	-1.59776400	3.68108200	-2.22141700
H	-0.81105100	5.52317600	-0.74412400
M6Ph-TS2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.242653 a.u.			
E (UωB97X-D/def2-tzvp) = -3844.29955083 a.u.			
Imaginary frequency: 216.2953			
C	2.48503200	-0.03535300	1.64862100
C	1.23225700	0.50170900	1.68503100

C	0.83999100	0.88076000	0.35650400
C	1.78213600	0.14403900	-0.59467200
H	3.04639300	-0.31054300	2.53776200
H	0.66155400	0.69339900	2.58122200
H	2.00232600	0.70870800	-1.50293400
C	3.05746400	-0.11131800	0.27473700
Si	4.20653500	-1.59556500	-0.07896600
H	5.59767900	-1.14328000	0.15490200
H	3.94688000	-2.74076600	0.81222800
H	4.07795700	-1.98013200	-1.49777300
Si	4.17997000	1.43573000	0.06354000
H	5.17882700	1.49928700	1.14851100
H	4.86353900	1.35544800	-1.24491200
H	3.30356300	2.62530000	0.10456700
C	0.85381200	-1.08602300	-0.97785700
O	-0.40895700	-0.54702100	-0.58776000
Fe	-2.05507300	-1.04896400	0.11220100
Cl	-2.52733600	-3.11343100	-0.56852900
Cl	-3.49557200	0.49417100	-0.59387900
Cl	-1.77659700	-0.89219500	2.34949100
C	1.09837500	-2.38434700	-0.21219100
H	0.22454900	-3.02332100	-0.36925400
H	1.97152300	-2.92861900	-0.58167800
H	1.18954200	-2.21882700	0.86407100
C	0.84445100	-1.33499700	-2.48341700
H	1.82551700	-1.67462800	-2.83547200
H	0.10050600	-2.10260700	-2.71751600
H	0.56976300	-0.42030400	-3.01820700
C	-0.03504000	1.98256000	0.04999800
C	-0.87919900	2.51223400	1.05079200
C	-0.10822900	2.51098600	-1.25673300
C	-1.76250000	3.53904500	0.75044300
H	-0.88051800	2.07965900	2.04331300
C	-0.98399200	3.54487700	-1.54701300
H	0.51449300	2.09876400	-2.04188500
C	-1.81373500	4.05964800	-0.54447400
H	-2.42614700	3.92065400	1.51906000
H	-1.03723000	3.94284900	-2.55518600
H	-2.51158900	4.85770600	-0.77901700
M6Ph-P			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.243894 a.u.			
E (UωB97X-D/def2-tzvp) = -3844.31040424 a.u.			
C	2.82818000	0.44194400	1.58354700
C	1.61113900	1.06044400	1.70857100
C	0.99496900	1.13712200	0.43372600
C	1.74035100	0.26762700	-0.51430400
H	3.52428800	0.29341400	2.40471000
H	1.21813600	1.47963900	2.62388500
H	1.83846100	0.72699300	-1.49971000
C	3.12011300	0.04498900	0.19212400
Si	4.22035100	-1.52393500	0.11330100
H	5.61497700	-1.04456400	0.25301600
H	3.94788200	-2.43862200	1.23616000
H	4.09821600	-2.21170100	-1.18076100
Si	4.25374100	1.44119500	-0.51290300
H	5.41731600	1.65948700	0.36707200

H	4.71106900	1.03275100	-1.85747500
H	3.43466100	2.66737900	-0.59460600
C	0.81212300	-1.09020500	-0.85716500
O	-0.49135800	-0.67418600	-0.95856400
Fe	-2.01026700	-1.02045000	0.05314100
Cl	-2.50649000	-3.18982900	-0.15006500
Cl	-3.66027200	0.28618400	-0.67336700
Cl	-1.48343900	-0.55517000	2.21611800
C	0.99579100	-2.16448000	0.21655900
H	0.21862000	-2.91931000	0.06477700
H	1.95749600	-2.67452700	0.13100200
H	0.87614400	-1.76793100	1.22722900
C	1.25198000	-1.58618600	-2.24144200
H	2.32341800	-1.79414900	-2.29962900
H	0.70185800	-2.50513800	-2.46626400
H	0.98926600	-0.84163200	-2.99902800
C	-0.13540000	1.94102300	0.09506800
C	-0.91682700	2.55294900	1.10878700
C	-0.49771400	2.15023000	-1.25913700
C	-2.01421900	3.32685600	0.77824400
H	-0.68888000	2.36691600	2.15000300
C	-1.59098600	2.93551300	-1.58224800
H	0.07674300	1.68695800	-2.04945500
C	-2.35354600	3.51858000	-0.56634600
H	-2.62584000	3.76162500	1.56146300
H	-1.87001500	3.07474800	-2.62095100
H	-3.22558800	4.11261700	-0.82171700
M7Ph-S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.148889 a.u.			
E (UωB97X-D/def2-tzvp) = -738.220433522 a.u.			
C	0.01955100	0.04248400	-0.87100700
C	3.07225600	-1.03072500	0.33505600
C	2.39010900	-0.19234200	1.31010500
C	1.47657000	0.76356000	1.06145000
H	2.83481400	-0.88642800	-0.71366000
H	2.65292300	-0.37121300	2.35222400
H	1.01135100	1.30402000	1.87966100
C	0.97074700	1.13355900	-0.30214000
C	3.95773400	-1.96959500	0.70147500
O	0.46835600	-0.71353100	-1.71376600
F	0.30652500	2.34079800	-0.23136800
F	1.99053700	1.30071700	-1.19046800
C	-1.35327800	-0.11282300	-0.31493700
C	-2.09990600	-1.20746100	-0.78312300
C	-1.91936000	0.74343300	0.64369000
C	-3.38185100	-1.44578500	-0.30221200
H	-1.64598800	-1.85823100	-1.52234100
C	-3.20380700	0.49873600	1.12573300
H	-1.37348500	1.60615800	1.00088000
C	-3.93644100	-0.59248900	0.65633600
H	-3.94972500	-2.29539300	-0.66985600
H	-3.63501200	1.16586500	1.86626300
H	-4.93771900	-0.77766900	1.03497000
H	4.45637600	-2.59790200	-0.02991300
H	4.21212400	-2.13791600	1.74587600
M7Ph-FeCl₃/S			

G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.140608 a.u.			
E (UωB97X-D/def2-tzvp) = -3382.77599127 a.u.			
C	1.02005700	-0.54603500	-0.68913700
C	-1.31846000	-2.65945500	0.73917400
C	0.04645000	-2.98103100	1.10976100
C	1.17138300	-2.75535600	0.40027600
H	-1.51019900	-2.26677500	-0.25214500
H	0.17164300	-3.44485600	2.08732800
H	2.14053100	-3.00574600	0.81895300
C	1.23189400	-2.06025500	-0.92566400
C	-2.33671300	-2.80692500	1.60191800
O	-0.15128000	-0.15820100	-0.86964600
Fe	-1.61924700	0.95743000	-0.09646500
Cl	-1.05422300	1.01900900	2.02567300
Cl	-3.51282800	-0.06848900	-0.53230600
Cl	-1.50545200	2.93073000	-1.07484200
F	2.44761000	-2.27857800	-1.52097300
F	0.27647100	-2.48891000	-1.79248800
C	2.08698300	0.32246700	-0.21020700
C	1.83543100	1.70787100	-0.11828800
C	3.35066800	-0.17534300	0.17819700
C	2.81187700	2.56712100	0.36607500
H	0.88674400	2.11141500	-0.44701700
C	4.31611500	0.69081900	0.67271600
H	3.57731100	-1.22842600	0.09248100
C	4.04961100	2.06029400	0.77018100
H	2.60569500	3.63043700	0.42981000
H	5.28107100	0.30046800	0.97974000
H	4.81041400	2.73248000	1.15601000
H	-3.34679500	-2.52090300	1.33003400
H	-2.18172700	-3.19454900	2.60629300
M7Ph-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.139860 a.u.			
E (UωB97X-D/def2-tzvp) = -3382.77083454 a.u.			
C	-0.98283800	-0.34947000	-0.65846200
C	-0.49914800	-2.38102200	1.86195400
C	-1.85336700	-2.62532900	1.35971100
C	-2.36142700	-2.37804800	0.14129400
H	-0.43554300	-1.99430200	2.87812800
H	-2.54442800	-3.05845000	2.08370000
H	-3.38644500	-2.66035000	-0.08403400
C	-1.68726400	-1.68890300	-1.01086100
C	0.62997500	-2.67890400	1.20593700
O	0.25148900	-0.34146900	-0.78950900
Fe	1.96477500	0.37948700	-0.05256600
Cl	2.41967000	2.16488200	-1.26305500
Cl	3.47475000	-1.19539300	-0.26047000
Cl	1.46142900	0.88442000	2.02939500
H	0.62102700	-3.11431100	0.21305700
H	1.60069700	-2.49630200	1.65332600
F	-0.77701200	-2.49043100	-1.63137900
F	-2.64760000	-1.37975900	-1.94773000
C	-1.75853600	0.81181600	-0.24574700
C	-1.11449700	2.06419000	-0.15844000
C	-3.13381600	0.72161600	0.06114700
C	-1.82116500	3.18823000	0.24648800

H	-0.07422000	2.16328000	-0.43840800
C	-3.83009700	1.84895100	0.47325400
H	-3.65098800	-0.22494400	-0.01170100
C	-3.17589100	3.08163800	0.57076800
H	-1.31503900	4.14595700	0.30698300
H	-4.88449400	1.77065800	0.71788300
H	-3.72613900	3.96052600	0.89380100
M7Ph-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.142335 a.u.			
E (UωB97X-D/def2-tzvp) = -3382.71045236 a.u.			
Imaginary frequency: 663.9730			
C	-0.96599800	-0.63135800	-0.12736700
C	-1.05287900	-1.51394300	1.38252000
C	-2.32777800	-2.28907400	1.20794700
C	-2.76477100	-2.34976700	-0.04907800
H	-0.98931100	-0.81069100	2.21116300
H	-2.81550200	-2.74450800	2.06417600
H	-3.64002400	-2.87747700	-0.40924900
C	-1.85905900	-1.61770700	-0.98635700
C	0.17338500	-2.16641800	1.07541100
O	0.33572700	-0.64640900	-0.56301100
Fe	1.95632400	0.20994900	-0.04562400
Cl	2.60736700	1.80281200	-1.42142400
Cl	3.39303800	-1.48746500	0.11555200
Cl	1.45591800	0.89827500	2.02992900
H	0.19926800	-3.01172100	0.39459900
H	1.11650000	-1.85901600	1.51705800
F	-1.04630000	-2.50691800	-1.63804300
F	-2.52950000	-0.92975200	-1.94559300
C	-1.58529400	0.72628200	0.03191000
C	-0.93989500	1.82544400	-0.55079700
C	-2.80745500	0.92625500	0.69639700
C	-1.50694900	3.09572200	-0.47681800
H	-0.00923000	1.69671500	-1.08621200
C	-3.35822800	2.19908500	0.78674300
H	-3.32636000	0.09274300	1.15433400
C	-2.71042600	3.29003400	0.19887300
H	-0.99261700	3.93225300	-0.93910400
H	-4.29476400	2.34146200	1.31738800
H	-3.14140600	4.28393600	0.27361200
M13Ph-S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.148432 a.u.			
E (UωB97X-D/def2-tzvp) = -1412.41835039 a.u.			
C	2.05140100	0.52956400	0.84057900
C	-1.23538700	0.53688600	-0.03824800
C	-0.42394100	0.80206400	-1.21674900
C	0.80243300	1.35434800	-1.19504600
H	-0.83115100	0.82850400	0.92334500
H	-0.83114600	0.52923200	-2.18362800
H	1.35166700	1.48701000	-2.12201600
C	1.55145100	1.77052500	0.04003700
C	-2.43923100	-0.06304900	-0.05048100
O	1.40082300	0.20535200	1.81737800
F	2.61323400	2.56714900	-0.32066100
F	0.76706500	2.51278300	0.86999300
C	3.20969300	-0.26013900	0.35053200

C	3.51962900	-1.42979000	1.06687500
C	3.97311500	0.07606600	-0.78004600
C	4.56728500	-2.24743600	0.66192800
H	2.91738900	-1.67619100	1.93435600
C	5.01948200	-0.75007300	-1.18484400
H	3.76942100	0.98286100	-1.33333400
C	5.31897800	-1.90933800	-0.46760100
H	4.79824400	-3.14932500	1.22077300
H	5.60565800	-0.48407300	-2.05928400
H	6.13684400	-2.54878300	-0.78719000
C	-3.18997800	-0.30266100	1.23336300
C	-3.10473700	-0.53265500	-1.32278500
F	-3.41164300	-1.61926200	1.43129400
F	-2.51179300	0.15956700	2.29988700
F	-4.39228300	0.31059900	1.21957900
F	-2.33437600	-1.43428500	-1.97616800
F	-4.29525400	-1.10884400	-1.09379200
F	-3.30658000	0.49474600	-2.18092500
M13Ph-FeCl₃/S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.141168 a.u.			
E (UωB97X-D/def2-tzvp) = -4056.96963885 a.u.			
C	-1.99218700	-0.68585700	0.95482800
C	1.70864800	-1.09992300	0.50548200
C	0.80938000	-2.08846900	-0.06907600
C	-0.39538400	-2.46123800	0.40230500
H	1.43398500	-0.64349700	1.44649400
H	1.15263300	-2.60556700	-0.95758100
H	-0.95984800	-3.21494300	-0.13744400
C	-1.15705300	-1.85175600	1.54134700
C	2.87954000	-0.73603000	-0.04593900
O	-1.45805800	0.43312500	1.07483600
Fe	-0.72796400	1.94427300	-0.02214300
Cl	-0.38202900	0.86013700	-1.90418900
Cl	1.07098200	2.64563700	0.99186900
Cl	-2.28066000	3.50132200	-0.17210000
F	-1.96951800	-2.78809000	2.12604700
F	-0.35790600	-1.35575500	2.51950400
C	-3.23226100	-0.90526600	0.22708800
C	-3.89603200	0.22112000	-0.30768900
C	-3.77542600	-2.19303900	0.01296200
C	-5.05618500	0.06188800	-1.05107400
H	-3.50228600	1.21448200	-0.13476000
C	-4.93297800	-2.34074600	-0.73880700
H	-3.30375700	-3.06797300	0.43667900
C	-5.57304100	-1.21807100	-1.27329300
H	-5.55485200	0.93425600	-1.46026000
H	-5.34147000	-3.33203300	-0.90633100
H	-6.47808000	-1.34173200	-1.86071200
C	3.80811800	0.21461700	0.67005700
C	3.35972000	-1.27223800	-1.37766600
F	3.99818500	1.34575400	-0.02890900
F	3.33668400	0.54581700	1.88482400
F	5.01681400	-0.36357000	0.85088400
F	2.43574700	-1.08139800	-2.34220200
F	4.49790900	-0.68945000	-1.77960500
F	3.58375900	-2.60771600	-1.31021600

M13Ph-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.139614 a.u.			
E (UωB97X-D/def2-tzvp) = -4056.96539951 a.u.			
C	0.27313300	1.12798400	0.79635400
C	2.60059800	-0.74412300	0.69650500
C	2.67199500	-0.32046700	2.10670300
C	1.85264300	0.48934500	2.78090700
H	3.38157100	-0.31933600	0.06837600
H	3.57435500	-0.65109800	2.62165900
H	2.07930100	0.74437800	3.81314600
C	0.57633100	1.12919800	2.31737500
C	1.76937400	-1.60302200	0.09694800
O	-0.68463800	0.42678900	0.44946300
Fe	-2.49773600	0.17764900	-0.35715800
Cl	-3.28982300	2.20835000	-0.07989100
Cl	-3.55052200	-1.36375900	0.77184000
Cl	-2.20307600	-0.29995000	-2.48806700
C	0.69311600	-2.42424900	0.77604300
C	1.91383100	-1.86131200	-1.38838400
F	1.13641200	-3.67899400	0.98740300
F	0.33032900	-1.91510100	1.96391600
F	-0.40585400	-2.50391800	0.00344100
F	0.88154400	-1.33157000	-2.07131000
F	1.94875400	-3.17892200	-1.65135900
F	3.04331000	-1.31098500	-1.88285400
F	-0.47135300	0.55479500	2.95602700
F	0.59787800	2.45334600	2.70964500
C	1.07492500	1.89392300	-0.14406900
C	0.78740600	1.76277100	-1.52007100
C	2.14952200	2.70940900	0.27261500
C	1.56581900	2.42827300	-2.45623900
H	-0.02941100	1.12964100	-1.84297900
C	2.92178300	3.36870200	-0.67442700
H	2.36630600	2.83420200	1.32457700
C	2.63339400	3.22813500	-2.03620400
H	1.34343400	2.32146600	-3.51276500
H	3.74587400	3.99812600	-0.35438700
H	3.24259800	3.74526000	-2.77173900
M13Ph-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.142479 a.u.			
E (UωB97X-D/def2-tzvp) = -4056.87891888 a.u.			
Imaginary frequency: 810.1315			
C	-0.68490400	0.69693400	0.55367800
C	0.29370500	2.34459000	0.27344800
C	0.38177400	2.84148800	1.67097000
C	-0.07567200	2.02646300	2.61920000
H	-0.29673800	2.94120000	-0.41590700
H	0.76761100	3.83774200	1.86920600
H	-0.08603100	2.23497700	3.68331100
C	-0.58757700	0.70922000	2.13354200
C	1.26781800	1.53735900	-0.34587000
O	0.15929900	-0.18868200	-0.06572500
Fe	0.11335800	-2.14129700	-0.02644600
Cl	-1.74382200	-2.63058400	1.06472500
Cl	1.97267300	-2.88136800	0.88129700
Cl	-0.05960500	-2.66840900	-2.17878000

C	2.57711300	1.10210000	0.31817900
C	1.26519300	1.45797200	-1.87683900
F	3.39745100	2.17562400	0.21326100
F	2.43837300	0.80702500	1.60652000
F	3.14282600	0.07479300	-0.30654700
F	1.60115100	0.27232400	-2.35930100
F	2.16357000	2.37374500	-2.30065100
F	0.06134700	1.79734400	-2.36868000
F	0.23132300	-0.30649600	2.51188400
F	-1.80786100	0.44189200	2.68624300
C	-1.99760800	0.86926900	-0.05584500
C	-2.25728000	0.22774000	-1.28676600
C	-2.99437100	1.68777000	0.52559800
C	-3.50201500	0.35835100	-1.88938300
H	-1.49263300	-0.38528500	-1.74544200
C	-4.22099500	1.83420600	-0.09981900
H	-2.80259500	2.19917600	1.46022300
C	-4.48216800	1.16123200	-1.30263100
H	-3.70380400	-0.16334800	-2.81905500
H	-4.98487300	2.46108100	0.34892900
H	-5.45150800	1.26938500	-1.78032300
M5TMS-S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.333627 a.u.			
E (UωB97X-D/def2-tzvp) = -1204.69321166 a.u.			
C	0.06737300	-0.39672700	1.47164300
C	-2.63601100	-0.30820100	0.03748300
C	-1.73329900	-0.83999200	-0.96801100
C	-0.38222300	-0.78569600	-0.97421900
H	-0.55032600	-1.30779400	1.62877100
H	-2.18310400	0.24037200	0.85877100
H	-2.19334200	-1.31470300	-1.83156200
H	0.10201200	-1.18686900	-1.86300100
C	0.54017100	-0.19558200	0.06432200
C	-3.98415400	-0.39527700	0.04484500
O	0.35139500	0.31529300	2.42187300
C	-4.80770700	-1.11154700	-0.99229700
H	-5.40989600	-1.90181800	-0.52303800
H	-5.51914600	-0.41961200	-1.46391000
H	-4.21149400	-1.57191000	-1.78244900
C	-4.78316800	0.24659100	1.14846800
H	-5.38192600	-0.50089700	1.68819500
H	-4.14240700	0.75831200	1.87279100
H	-5.49576100	0.97928100	0.74376400
Si	0.79358200	1.68032800	-0.31871200
Si	2.18791900	-1.22284200	0.00874800
C	-0.71245100	2.62914300	0.28620000
H	-1.62743400	2.30577800	-0.21990300
H	-0.84995600	2.50457300	1.36471800
H	-0.58049700	3.69942800	0.08510300
C	2.32949400	2.39693900	0.49581800
H	3.25854900	2.01933000	0.05557200
H	2.33206300	3.48737200	0.37560500
H	2.33505700	2.17317600	1.56636100
C	0.91441700	1.90204700	-2.18510400
H	0.99939700	2.96908600	-2.42448400
H	1.78333600	1.39713300	-2.61787800

H	0.01810600	1.51876500	-2.68376600
C	3.33008200	-0.79189300	1.43476000
H	4.09516500	-1.57053900	1.54067700
H	3.84249500	0.16167000	1.28345600
H	2.78086200	-0.72551100	2.37882100
C	3.06218000	-0.93399100	-1.63204700
H	3.47911800	0.07626400	-1.69420600
H	3.89430300	-1.64138500	-1.73299000
H	2.40080400	-1.07915000	-2.49291700
C	1.70395800	-3.03795900	0.15090400
H	0.98090400	-3.32993600	-0.61792500
H	2.58531600	-3.68196100	0.04642000
H	1.25364800	-3.25274300	1.12692200
M5TMS-FeCl₃/S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.325206 a.u.			
E (UωB97X-D/def2-tzvp) = -3849.26550969 a.u.			
C	0.32506200	-0.07819500	-0.47193800
C	-0.01116100	2.77692100	-0.09988100
C	1.36628900	2.67992700	-0.55102500
C	2.13881800	1.56899100	-0.55438400
H	-0.11140600	0.43292600	-1.33990200
H	-0.39981100	1.93339600	0.46583600
H	1.83558000	3.59457900	-0.90586200
H	3.17655200	1.67813700	-0.85874100
C	1.70577200	0.18718300	-0.12681200
C	-0.86893400	3.80237200	-0.29103700
O	-0.39626300	-0.90037900	0.14603000
C	-0.54446600	5.05487000	-1.05854400
H	-1.21640900	5.15282500	-1.92182000
H	-0.71189500	5.94153900	-0.43273500
H	0.48207700	5.08769600	-1.42964300
C	-2.27125100	3.72593700	0.25014000
H	-3.00233900	3.77049500	-0.56847800
H	-2.44903800	2.80290400	0.80869400
H	-2.48443000	4.57995600	0.90774000
Si	2.07769000	-0.08999300	1.76475900
Si	2.62641200	-1.10694700	-1.31177200
Fe	-2.35966400	-1.10886700	-0.01168100
Cl	-2.78363800	0.01939700	-1.86639000
Cl	-3.08685800	-0.06852100	1.79215100
Cl	-2.71931900	-3.26467500	-0.12738400
C	0.74671900	0.80110500	2.74051400
H	0.75392900	1.87772700	2.54291200
H	-0.25624600	0.41774600	2.52830500
H	0.93334900	0.66094500	3.81247800
C	2.10042800	-1.90588600	2.23902700
H	2.93749200	-2.45411600	1.79435400
H	2.19997400	-1.98874000	3.32821600
H	1.16830400	-2.40147400	1.95153600
C	3.73700100	0.70596200	2.14311800
H	3.93014800	0.64342900	3.22089900
H	4.57438100	0.22429600	1.63060600
H	3.73342400	1.76588900	1.86925800
C	1.88448500	-2.81837100	-1.15195400
H	2.35595400	-3.47775000	-1.89104200
H	2.04436000	-3.25652900	-0.16422500

H	0.80736000	-2.82392300	-1.34622700
C	4.44628600	-1.10957700	-0.85437000
H	4.62185500	-1.58293200	0.11620500
H	4.99778100	-1.68396500	-1.60865100
H	4.87586900	-0.10315600	-0.82698300
C	2.38991800	-0.48601500	-3.06806000
H	2.73895000	0.54323400	-3.19537800
H	2.94897900	-1.11966600	-3.76696000
H	1.33624800	-0.52150800	-3.36791500
M5TMS-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.324557 a.u.			
E (UωB97X-D/def2-tzvp) = -3849.26551124 a.u.			
C	-0.30493400	0.01276200	-0.46386100
C	-0.23388300	2.63121500	-1.50553500
C	-1.69917900	2.48016300	-1.32985400
C	-2.33293600	1.41745600	-0.80639000
H	0.08825200	0.23409000	-1.45828600
H	0.19408100	2.16660000	-2.39476100
H	-2.32826700	3.29397600	-1.69454500
H	-3.42019400	1.44176800	-0.77764000
C	-1.71521600	0.19537200	-0.17293200
C	0.60372000	3.31352500	-0.70271900
O	0.48410500	-0.51168700	0.36262800
Fe	2.41482300	-0.84538400	0.12862700
Cl	2.66718400	-2.96780300	0.61199600
Cl	3.35480500	0.59370600	1.50342900
Cl	2.67749200	-0.36119600	-2.02077500
C	0.14602600	4.06323900	0.51747800
H	0.64612200	3.68266500	1.41644100
H	0.42008400	5.12329400	0.43206500
H	-0.93483200	3.99492200	0.66449000
C	2.08077100	3.36613300	-0.98558800
H	2.64517100	2.93065000	-0.15150900
H	2.34471000	2.81431700	-1.89149100
H	2.41871200	4.40568000	-1.09282300
Si	-2.44804100	-1.36234400	-1.16719800
Si	-2.08417400	0.13993800	1.73419900
C	-1.92065900	-1.59051400	2.44659400
H	-0.91624600	-1.99172700	2.28047000
H	-2.08504200	-1.54457400	3.53004300
H	-2.64860600	-2.29895300	2.03838300
C	-0.88653000	1.29010900	2.60484600
H	-1.04168900	1.22626500	3.68878300
H	0.15698700	1.03420000	2.40048300
H	-1.05217100	2.32927600	2.30905300
C	-3.82960700	0.78789100	2.00642200
H	-4.59874100	0.18182400	1.51875300
H	-4.04848500	0.79258700	3.08105000
H	-3.93094300	1.81797100	1.64854500
C	-1.41899000	-2.89129300	-0.83113800
H	-1.33488500	-3.12283700	0.23306500
H	-1.88061500	-3.75395700	-1.32694200
H	-0.40270000	-2.79361100	-1.22713600
C	-4.23661500	-1.60043800	-0.65281200
H	-4.68325400	-2.37343700	-1.29010700
H	-4.33202500	-1.93114600	0.38528600

H	-4.82853300	-0.68823100	-0.77891100
C	-2.34710600	-0.93059100	-2.99116800
H	-2.78189400	-1.73955300	-3.59034400
H	-2.88456200	-0.00751600	-3.22746900
H	-1.30800400	-0.80757300	-3.31737300
M5TMS-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.328924 a.u.			
E (UωB97X-D/def2-tzvp) = -3849.23226714 a.u.			
Imaginary frequency: 245.6426			
C	0.40018900	0.85566700	0.09624300
C	0.45832900	2.35400700	-0.50895200
C	1.38965200	2.20185300	-1.67721100
C	2.07396600	1.05079800	-1.59356000
H	0.30713400	0.90261000	1.18513100
H	0.84091200	3.02867900	0.26554900
H	1.51047100	2.96048200	-2.44329900
H	2.84431800	0.75390500	-2.29942500
C	1.71820000	0.21209400	-0.39957500
C	-0.95989000	2.62367700	-0.74072600
O	-0.76096300	0.26684000	-0.44794100
Fe	-2.21247400	-0.55185200	0.37691500
Cl	-2.58752200	-2.60424900	-0.36489700
Cl	-4.06443000	0.67898200	-0.11145900
Cl	-1.67624000	-0.36822300	2.54539500
C	-1.57628200	2.42283600	-2.06126700
H	-2.60272500	2.05623000	-1.95158500
H	-1.62532700	3.40914900	-2.55426800
H	-0.97320800	1.75852700	-2.68183600
C	-1.77522500	3.16750900	0.35493800
H	-2.67963200	2.54890400	0.47094400
H	-1.23295600	3.24732000	1.29814700
H	-2.14420900	4.16031300	0.05307400
Si	3.10422900	0.43569200	0.92050500
Si	1.46489100	-1.63507900	-0.93557800
C	0.79444500	-2.68694600	0.47022600
H	0.19433600	-2.12238300	1.18893400
H	0.14688100	-3.47216500	0.06933200
H	1.60948200	-3.16565900	1.02258300
C	0.40591700	-1.71320800	-2.48692100
H	0.58787600	-2.65637600	-3.01639100
H	-0.65685800	-1.66168200	-2.24448800
H	0.64344400	-0.89474200	-3.17658100
C	3.16304900	-2.31764500	-1.40732600
H	3.82789500	-2.43967400	-0.54593400
H	3.02374400	-3.31228700	-1.84905200
H	3.68150900	-1.70382600	-2.15288000
C	2.97527200	-0.84867300	2.28335300
H	3.27256200	-1.84550900	1.94434900
H	3.63244800	-0.57145600	3.11626900
H	1.95422100	-0.92048500	2.67338700
C	4.80310500	0.40383500	0.11181400
H	5.57278700	0.57101600	0.87497700
H	5.02861800	-0.54410200	-0.38265800
H	4.90184700	1.20394700	-0.63062600
C	2.93076600	2.14214300	1.71240500
H	3.74927400	2.28827300	2.42757800

H	3.00507600	2.94472800	0.97003100
H	1.99472900	2.26275100	2.26919100
M5TMS-INT			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.334558 a.u.			
E (UωB97X-D/def2-tzvp) = -3849.25763269 a.u.			
C	0.55311500	0.97296400	0.21994400
C	0.52336900	2.37334300	-0.43679900
C	1.47539500	2.23927200	-1.59131600
C	2.10439600	1.05830700	-1.56466300
H	0.43342700	0.90647700	1.29998600
H	0.72463300	3.23260700	0.20927800
H	1.61629800	3.01587500	-2.33523600
H	2.84239800	0.73841700	-2.29394000
C	1.73556000	0.19911700	-0.36841800
C	-0.98122300	2.17314100	-0.72751800
O	-0.83367100	0.70563800	-0.35027900
Fe	-2.31103900	-0.43938900	0.39500700
Cl	-2.42345800	-2.44444700	-0.48869900
Cl	-4.25158500	0.51590600	-0.05820100
Cl	-1.72869200	-0.40763800	2.53278600
C	-1.47887500	2.25289200	-2.15121500
H	-2.49552100	1.85159000	-2.21335800
H	-1.50460400	3.29883500	-2.47695000
H	-0.82533600	1.69018500	-2.82161900
C	-1.84072500	2.92889000	0.27199400
H	-2.89622400	2.67162400	0.18382700
H	-1.51517400	2.73389700	1.29879100
H	-1.72479300	4.00096700	0.07469900
Si	3.18042000	0.39686100	0.90436100
Si	1.44034600	-1.61930600	-0.90599300
C	0.78336000	-2.66647100	0.50857700
H	0.09958500	-2.13518100	1.17493900
H	0.23779200	-3.52958400	0.11492200
H	1.61167300	-3.04099700	1.11847400
C	0.34048700	-1.59407000	-2.43125000
H	0.08686800	-2.61478400	-2.73850400
H	-0.59435000	-1.05620400	-2.26801600
H	0.86843700	-1.11415800	-3.26415400
C	3.08128200	-2.37329400	-1.44959600
H	3.76351000	-2.54541400	-0.61096300
H	2.88367700	-3.34865400	-1.91123600
H	3.60410500	-1.76297000	-2.19445900
C	3.06892200	-0.86448600	2.29298400
H	3.36339200	-1.86722900	1.96822100
H	3.73867000	-0.57190500	3.11048700
H	2.05509400	-0.93157700	2.70273100
C	4.84167800	0.29322000	0.02919000
H	5.64356800	0.45422600	0.75991300
H	5.02063500	-0.67165200	-0.45123000
H	4.93408400	1.07455000	-0.73302600
C	3.07996900	2.12088600	1.66482600
H	3.95056700	2.27897800	2.31265300
H	3.09921200	2.90042100	0.89574300
H	2.18725300	2.26769600	2.28241800
M5TMS-TS2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.331270 a.u.			

$E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -3849.24139756 \text{ a.u.}$ Imaginary frequency: 325.7680			
C	0.96070500	0.95404900	0.35940400
C	0.60875000	2.16661200	-0.33013000
C	1.50051100	2.20749300	-1.51370200
C	2.23991400	1.08064100	-1.56227000
H	0.48346100	0.61506800	1.27444200
H	0.50785300	3.07214300	0.26568600
H	1.51451200	3.01511700	-2.23509400
H	2.95618600	0.80725200	-2.32757800
C	1.94165000	0.21642000	-0.36888900
C	-1.19078800	1.98366900	-0.73496200
O	-1.52246500	0.68472600	-0.81562700
Fe	-2.61097700	-0.39971600	0.25702300
Cl	-2.54419200	-2.45728700	-0.56944200
Cl	-4.66739600	0.43976800	0.28847100
Cl	-1.67651000	-0.31734900	2.33341300
C	-1.33544700	2.66585500	-2.08942700
H	-2.40766400	2.69813800	-2.31690300
H	-0.94819500	3.68919600	-2.08310300
H	-0.83643900	2.08276000	-2.86555500
C	-1.86968900	2.74232700	0.40190400
H	-2.95243900	2.65845100	0.25881700
H	-1.63266400	2.29955100	1.37266800
H	-1.59170600	3.80072200	0.39966000
Si	3.49547900	0.41286500	0.87446900
Si	1.57087200	-1.66041900	-0.79433600
C	5.04875300	0.22288000	-0.15826500
H	5.91454900	0.29135300	0.51262400
H	5.10903400	-0.73113500	-0.68502200
H	5.13458300	1.03140100	-0.89083000
C	3.39252900	-0.84937600	2.25120100
H	3.58475700	-1.86740400	1.90127700
H	4.15018100	-0.60862000	3.00703300
H	2.41613100	-0.84047000	2.74612100
C	3.47562500	2.15019600	1.58569300
H	2.69595300	2.28292500	2.34268100
H	4.44072600	2.36020600	2.06234800
H	3.32603000	2.89913900	0.80093900
C	3.16992100	-2.51199300	-1.30044400
H	3.69236300	-1.98140900	-2.10394600
H	3.86795800	-2.65690800	-0.46994600
H	2.91426500	-3.50716600	-1.68536500
C	0.81627500	-2.54804800	0.66424500
H	0.28559900	-3.43227900	0.29447700
H	1.57532000	-2.88415200	1.37717200
H	0.07836900	-1.94825000	1.20200600
C	0.45494100	-1.55573100	-2.29165100
H	0.05714800	-2.54716200	-2.53416200
H	-0.39091500	-0.89045200	-2.10485400
H	1.00701500	-1.18466200	-3.16281000
M5TMS-P $G_{\text{corr}}(\text{UB3LYP-D3BJ/6-31G}^*/\text{Lan2LDZ}) = 0.322639 \text{ a.u.}$ $E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -3849.27712152 \text{ a.u.}$			
C	1.29065600	1.05395400	0.48510300
C	1.31414300	2.38001200	0.15534200

C	2.35954000	2.60779100	-0.82099500
C	2.98838100	1.42182100	-1.07365700
H	0.62944000	0.57806900	1.19923200
H	0.68682000	3.15554500	0.58207500
H	2.60715700	3.56980700	-1.25804300
H	3.81797700	1.26440800	-1.75303500
C	2.38503500	0.34378100	-0.23948000
C	-1.82649600	1.95202500	-0.93151000
O	-2.07244200	0.73232300	-0.96556900
Fe	-2.97143400	-0.50370000	0.34438500
Cl	-3.01671800	-2.45290100	-0.63622700
Cl	-4.94075900	0.45323900	0.58597200
Cl	-1.76324200	-0.40094500	2.19417600
C	-1.25622600	2.60263900	-2.14854700
H	-1.70053100	3.59137800	-2.30158700
H	-0.18110500	2.74129800	-1.96874500
H	-1.38813700	1.96982100	-3.02645800
C	-2.12568200	2.76179100	0.28916900
H	-3.21868600	2.82162700	0.38763300
H	-1.75905700	2.24071700	1.17904900
H	-1.70888800	3.76796200	0.23030400
Si	3.71513300	-0.10286500	1.09561400
Si	1.75049700	-1.13553500	-1.27802300
C	5.38253600	-0.43194900	0.28547000
H	6.10808600	-0.73801300	1.04933900
H	5.34426100	-1.22273800	-0.46851700
H	5.77230200	0.47265400	-0.19414300
C	3.18401400	-1.61087700	2.08508600
H	3.27420000	-2.53770400	1.50954000
H	3.82072300	-1.71219600	2.97249200
H	2.14722900	-1.52827300	2.42804100
C	3.90245600	1.36177000	2.25839900
H	3.05510500	1.44337100	2.94594700
H	4.81498800	1.25382200	2.85714900
H	3.97299000	2.30073900	1.70015000
C	3.19624100	-2.07418000	-2.03680700
H	3.87551800	-1.41838000	-2.59298600
H	3.78316900	-2.60373800	-1.27935800
H	2.81551700	-2.82532600	-2.73946700
C	0.72340300	-2.31263500	-0.23655800
H	0.10036000	-2.93224700	-0.89141500
H	1.33929000	-2.98271600	0.36962500
H	0.04561700	-1.78445500	0.44015900
C	0.67664700	-0.46823700	-2.67221300
H	0.51731000	-1.24678800	-3.42792100
H	-0.30660400	-0.17294100	-2.29763100
H	1.13729700	0.39360200	-3.16663800
2Fe.M1-2FeCl3/S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.108295 a.u.			
E (UωB97X-D/def2-tzvp) = -5874.88667167 a.u.			
C	-2.75769000	0.70514100	0.10530800
C	-2.82072200	-1.93907000	0.53624400
C	-4.27490500	-1.71459300	0.53360700
C	-4.82446300	-0.53213600	0.84549900
H	-2.94873000	0.44876300	-0.94312800
H	-2.27507100	-1.54782800	1.39335500

H	-4.93049900	-2.54885900	0.29210000
H	-5.89531800	-0.37022600	0.91068400
C	-3.95926200	0.66661100	1.06195700
C	-2.12755000	-2.63157300	-0.39817400
O	-1.66827700	1.12616500	0.47589600
C	-2.76181000	-3.20114200	-1.63457500
H	-2.37244200	-2.67685000	-2.51764000
H	-2.49494600	-4.25820100	-1.75493800
H	-3.85036500	-3.10811000	-1.64268300
C	-0.64758300	-2.84266200	-0.26865500
H	-0.12090200	-2.45555800	-1.14886500
H	-0.23574100	-2.36008600	0.61944100
H	-0.41835500	-3.91533900	-0.21671000
Fe	0.12015800	1.23696900	-0.62222200
Cl	-0.74322500	0.22494100	-2.38911000
Cl	0.17210400	3.40473200	-0.70992000
F	-4.65969300	1.81058600	0.75335300
F	-3.51142400	0.79065800	2.34024900
Fe	2.95977400	-0.45546300	0.43292400
Cl	0.89830700	0.10795700	1.43437000
Cl	4.63082600	0.27528600	1.58967100
Cl	2.49737200	0.85065800	-1.42570000
Cl	2.97957500	-2.57009200	-0.05264600
2Fe.M1-INT0			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.111271 a.u.			
E (UωB97X-D/def2-tzvp) = -5874.89882721 a.u.			
C	1.62051800	-0.86083400	-0.88176400
C	1.49049100	-2.38767800	-0.45611100
C	2.94360400	-2.86680000	-0.49220500
C	3.81919100	-1.87534100	-0.65627800
H	1.38903200	-0.85364400	-1.95556700
H	0.87596400	-2.93316500	-1.17578200
H	3.18559900	-3.92148200	-0.41739000
H	4.89571700	-1.97386100	-0.74014400
C	3.13790800	-0.54339800	-0.73294700
C	0.94628400	-2.59337500	0.90318800
O	0.80014200	-0.02670100	-0.18673000
Fe	0.63484000	1.74586200	0.22304200
Cl	1.87640800	3.13483400	-0.90421000
Cl	0.68953700	1.92069000	2.41985300
C	-0.11687800	-3.57847400	1.08507200
H	-0.20551900	-3.95440500	2.10572600
H	-1.03422500	-2.97792400	0.88547400
H	-0.10493200	-4.37587700	0.33824500
C	1.34151700	-1.74245600	2.00786600
H	2.30187800	-1.24431600	1.88489000
H	0.58597100	-0.91902100	1.93415600
H	1.20998800	-2.20144100	2.98924900
F	3.58509400	0.20880700	-1.77069600
F	3.37090600	0.18480000	0.41074200
Fe	-2.46822900	-0.15640500	-0.32149400
Cl	-1.61154500	-1.67131700	-1.71570300
Cl	-2.09454300	-0.81154500	1.77981500
Cl	-4.60674400	0.04789800	-0.68440500
Cl	-1.63736700	2.04947200	-0.55514800
2Fe.M1-TS1			

$G_{\text{corr}}(\text{UB3LYP-D3BJ/6-31G}^*/\text{Lan2LDZ}) = 0.113049 \text{ a.u.}$ $E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -5874.89532851 \text{ a.u.}$ Imaginary frequency: -117.0606			
C	1.65984700	-0.93738100	-0.81561900
C	1.82092600	-2.32638700	-0.12245100
C	3.26607700	-2.70279400	-0.38004800
C	3.95942900	-1.71332900	-0.94594200
H	1.13657300	-1.04793400	-1.77051500
H	1.11106900	-3.05404600	-0.52103700
H	3.65351300	-3.68885100	-0.14512600
H	5.00110900	-1.73646300	-1.24566400
C	3.12056600	-0.47922700	-1.11016300
C	1.47238900	-2.01905800	1.31231600
O	0.95019300	-0.13522800	0.07467900
Fe	0.51714500	1.63922100	0.24470900
Cl	1.66317400	3.09098300	-0.90571900
Cl	0.43526100	1.99319000	2.41741200
C	0.23317300	-2.51779500	1.87400000
H	0.26804700	-2.63904400	2.96022100
H	-0.51022300	-1.69857800	1.70393500
H	-0.17488100	-3.38600300	1.35360200
C	2.40436500	-1.29028000	2.18809100
H	3.17876900	-0.75070200	1.64901500
H	1.84553800	-0.60996300	2.84205400
H	2.87574600	-2.04656900	2.83963700
F	3.22106400	0.06640000	-2.35010500
F	3.52527500	0.48760700	-0.22018800
Fe	-2.62313100	-0.37189600	-0.34308700
Cl	-1.51968400	-2.04286800	-1.30854300
Cl	-2.46656300	-0.53675400	1.87063500
Cl	-4.68078500	-0.24828800	-1.03281500
Cl	-1.64133400	1.72732300	-0.83945300
2Fe.M1-INT $G_{\text{corr}}(\text{UB3LYP-D3BJ/6-31G}^*/\text{Lan2LDZ}) = 0.116721 \text{ a.u.}$ $E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -5874.91592429 \text{ a.u.}$			
C	1.53572500	-1.44221000	-0.07136800
C	2.19788000	-1.87516900	1.24458900
C	3.64792700	-2.05230000	0.87359300
C	3.88397700	-1.83678400	-0.42390100
H	0.58238000	-1.87354900	-0.36940900
H	1.75974800	-2.72666100	1.76920800
H	4.40353100	-2.31776000	1.60584500
H	4.83702900	-1.89830200	-0.93619800
C	2.61552900	-1.51949600	-1.16123700
C	1.78716200	-0.49368500	1.84749500
O	1.34795000	-0.08176500	0.44241100
Fe	0.64007700	1.56433300	-0.37683700
Cl	1.92413200	2.66857700	-1.72861100
Cl	0.09656800	2.83368200	1.30521100
C	0.57244000	-0.55591500	2.74559500
H	0.87938700	-0.94230200	3.72427100
H	0.14056200	0.43795400	2.88326000
H	-0.19493000	-1.21631900	2.33440900
C	2.87037300	0.44391900	2.32428300
H	3.68918100	0.50795600	1.60397800
H	2.45513400	1.44334500	2.48520100

H	3.26715000	0.08309200	3.27968400
F	2.29001000	-2.50876600	-2.04601200
F	2.68336100	-0.35631000	-1.87346600
Fe	-2.68363300	-0.51309300	-0.06521700
Cl	-1.77545300	-2.49058300	0.35484600
Cl	-2.77896800	0.71667700	1.73210900
Cl	-4.51908100	-0.61580100	-1.21993500
Cl	-1.11759300	0.62862000	-1.58627500
2Fe.M1-TS2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.112054 a.u.			
E (UωB97X-D/def2-tzvp) = -5874.84738162 a.u.			
Imaginary frequency: -628.2953			
C	1.72321600	-1.99002300	0.55346800
C	2.70725300	-1.50884900	1.43641200
C	3.88457500	-1.13716800	0.57352700
C	3.59921400	-1.27187000	-0.72626800
H	0.75540400	-2.43388000	0.77269800
H	2.83747200	-1.93962400	2.42491700
H	4.81224500	-0.75954400	0.98548300
H	4.21937300	-1.02692600	-1.57771500
C	2.24698500	-1.91176600	-0.87786300
C	1.64798600	-0.05225800	1.77225300
O	0.94620600	0.11176800	0.59775200
Fe	0.55248300	1.51897200	-0.54532500
Cl	2.25518100	1.86940900	-1.90371100
Cl	0.08924600	3.34609400	0.56912600
C	0.75479000	-0.44375700	2.93043600
H	1.33442200	-0.65120500	3.83427400
H	0.09187100	0.40828000	3.11813300
H	0.11207600	-1.29265800	2.68847200
C	2.61259000	1.07293400	2.05960500
H	3.25199400	1.27548700	1.19723500
H	1.99773700	1.96751300	2.23234700
H	3.21773900	0.88246500	2.95028900
F	2.36560200	-3.24718400	-1.21030900
F	1.41142100	-1.34732500	-1.76163400
Fe	-2.52847000	-0.47811500	0.00349800
Cl	-1.60690400	-2.47858200	0.37735100
Cl	-2.39677800	0.80713100	1.77507800
Cl	-4.54697500	-0.66881300	-0.78330500
Cl	-1.31595800	0.67892400	-1.73469000
2Fe.M1-P			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.105216 a.u.			
E (UωB97X-D/def2-tzvp) = -5874.90516712 a.u.			
C	2.15445000	-2.77287100	-0.08600300
C	2.85729500	-2.65874500	1.04651000
C	3.72783500	-1.44466300	0.98014400
C	3.54645300	-0.81773500	-0.18899400
H	1.42933000	-3.52200100	-0.37049000
H	2.82425000	-3.33391300	1.89387800
H	4.41429900	-1.14976700	1.76663100
H	4.02815100	0.06939300	-0.57544500
C	2.53693600	-1.61962100	-0.99746000
C	1.02997800	0.28482300	2.15504000
O	0.71066200	0.30591200	0.95437900
Fe	0.50524600	1.57527100	-0.52532900

Cl	2.29366600	2.17237300	-1.61741900
Cl	-0.25710100	3.36117900	0.48971600
C	0.60476300	-0.87177200	2.98994200
H	1.44805600	-1.23741600	3.58576000
H	-0.15739700	-0.50455200	3.69209200
H	0.17464300	-1.66032200	2.37324400
C	1.79435600	1.42309400	2.75065300
H	2.68825400	1.61076400	2.14539200
H	1.16917400	2.32320300	2.68319700
H	2.07242600	1.24120300	3.78958100
F	3.07039800	-2.05080900	-2.17449200
F	1.42430000	-0.87051100	-1.34766400
Fe	-2.43255100	-0.64653900	-0.08989600
Cl	-1.32430600	-2.52937900	0.17739300
Cl	-2.44161200	0.56221100	1.75446300
Cl	-4.40537700	-0.92410400	-0.95985200
Cl	-1.25534400	0.69453900	-1.77504300
2Fe.M1Ph-2FeCl₃/S (RS)			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.185117 a.u.			
E (UωB97X-D/def2-tzvp) = -6105.95653217 a.u.			
C	1.26565100	0.51702500	0.18434100
C	3.80677100	-0.23663700	1.33129500
C	2.94437900	-0.60840200	2.47406900
C	1.64072400	-0.34879700	2.60964700
H	4.32589100	0.71631800	1.43536100
H	3.42929900	-1.10065100	3.31872200
H	1.10227600	-0.63754200	3.50872700
C	0.75518800	0.36463600	1.63579800
C	4.03959900	-0.96881000	0.22746100
O	0.97784700	-0.42483800	-0.58883000
Fe	-0.28904600	-1.94642100	-0.49896200
Cl	0.15188800	-2.82212000	-2.45800500
Cl	0.10464800	-3.43012900	1.05716100
C	3.43583800	-2.32047400	-0.01792100
H	2.85572200	-2.32219000	-0.94989000
H	4.22675200	-3.07114600	-0.14618700
H	2.78046900	-2.64459600	0.79145100
C	4.91511300	-0.42974800	-0.86958700
H	5.73138500	-1.12520700	-1.10213700
H	4.32986200	-0.31197900	-1.79191900
H	5.34437800	0.54326000	-0.61418600
C	1.97528400	1.68142100	-0.30977000
C	2.41348200	2.72527400	0.53029900
C	2.22727600	1.74458400	-1.69632600
C	3.10520400	3.79922700	-0.01288600
H	2.21842400	2.69114700	1.59319400
C	2.91068800	2.82755800	-2.22971800
H	1.86563900	0.94410400	-2.33085700
C	3.35335200	3.85373900	-1.38881600
H	3.44519200	4.60188600	0.63335600
H	3.09461600	2.87886700	-3.29788500
H	3.88743000	4.70182900	-1.80687200
Fe	-3.05871100	0.84217400	-0.00412200
Cl	-2.58073700	-1.49505800	-0.56743800
Cl	-3.30891700	0.99165500	2.15764700
Cl	-1.33841500	1.98569300	-0.79832200

Cl	-4.89703800	1.22851200	-1.10952600
F	-0.42111900	-0.36941600	1.52487900
F	0.37845400	1.57453200	2.13699100
2Fe.M1Ph-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.185304 a.u.			
E (UωB97X-D/def2-tzvp) = -6105.94818970 a.u.			
Imaginary frequency:			
C	1.72217700	0.62752900	0.44782500
C	3.25364800	0.14836500	0.88811500
C	3.09562800	-0.35906300	2.29397100
C	1.88335400	-0.15515600	2.80198200
H	3.89173100	1.03492100	0.81236500
H	3.91634400	-0.82761000	2.82887400
H	1.53929300	-0.42290900	3.79413400
C	0.97846600	0.56272000	1.85187600
C	3.63674800	-0.80966800	-0.14942200
O	1.20943600	-0.31492600	-0.40998700
Fe	0.20062300	-1.81538300	-0.60836800
Cl	1.21854700	-2.75340100	-2.37615300
Cl	0.39644600	-3.20110700	1.11321800
C	3.69508200	-2.24212900	0.14577600
H	3.86067300	-2.86348500	-0.73362500
H	4.48947600	-2.40675200	0.89256400
H	2.77047400	-2.55368100	0.66269400
C	3.91206700	-0.34370500	-1.51164400
H	4.89668400	-0.71377300	-1.83362500
H	3.18279300	-0.85781200	-2.16388500
H	3.84045700	0.73617300	-1.63517800
C	1.76438000	1.99053600	-0.20304700
C	2.35028200	3.08691300	0.44691300
C	1.23028200	2.15646600	-1.48537100
C	2.39723100	4.32846800	-0.17690600
H	2.75228300	2.97699300	1.44982400
C	1.27836200	3.40432000	-2.10841200
H	0.76147900	1.31503500	-1.97807300
C	1.86174100	4.49023400	-1.45953100
H	2.84548500	5.17304100	0.33759000
H	0.84882100	3.52365100	-3.09815300
H	1.89748400	5.46120800	-1.94434800
Fe	-3.08866100	0.35697700	0.05293400
Cl	-1.99587100	-1.40636400	-1.26081400
Cl	-3.33516100	-0.42485500	2.07919000
Cl	-1.81449900	2.13915800	-0.10905600
Cl	-4.98470900	0.59351700	-1.01260300
F	-0.20705300	-0.08852100	1.70395700
F	0.68733700	1.80517600	2.32526300
2Fe.M1Ph-INT			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.191590 a.u.			
E (UωB97X-D/def2-tzvp) = -6105.97224151 a.u.			
C	1.75418900	1.00245300	0.56361200
C	3.23087800	0.88736600	1.01603900
C	3.14269400	0.33568700	2.41402800
C	1.88716400	0.14159100	2.82613400
H	3.85359300	1.77790600	0.91069200
H	4.02716300	0.09342000	2.99407500
H	1.55975100	-0.26367200	3.77612900

C	0.90464400	0.63003700	1.80923700
C	3.42641500	-0.17669700	-0.10470200
O	1.91412400	-0.20473900	-0.26523300
Fe	0.66026000	-1.72969100	-0.61460800
Cl	1.67874400	-2.47114600	-2.42420400
Cl	0.68570700	-3.30650700	0.88264500
C	3.95560700	-1.53791600	0.28311300
H	3.86679900	-2.23521500	-0.55419800
H	5.01687300	-1.44475700	0.54003100
H	3.42003800	-1.94826800	1.14157100
C	4.01853100	0.37102500	-1.38679600
H	5.10257400	0.47610300	-1.26778800
H	3.82156800	-0.31844300	-2.21230300
H	3.59489500	1.34777900	-1.63275500
C	1.28275500	2.18419100	-0.22530200
C	1.38904000	3.45949100	0.34326200
C	0.70647100	2.03124900	-1.48821400
C	0.91344200	4.57058800	-0.34687700
H	1.82432500	3.57974400	1.33094200
C	0.22989700	3.14767300	-2.17520100
H	0.61805500	1.04885100	-1.93414800
C	0.33036400	4.41632100	-1.60698700
H	0.99156800	5.55616500	0.10173900
H	-0.22858400	3.01833900	-3.15045100
H	-0.04718600	5.28327800	-2.14044300
Fe	-3.00276100	-0.06710800	0.14811700
Cl	-1.38550300	-1.07378100	-1.45405200
Cl	-2.95712700	-1.25369300	1.97994500
Cl	-2.36511400	2.01839700	0.31968200
Cl	-4.85579900	-0.29329700	-0.98705900
F	-0.01895000	-0.33665100	1.43689200
F	0.18812900	1.67726700	2.27768600
2Fe.M1Ph-TS2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.187257 a.u.			
E (UωB97X-D/def2-tzvp) = -6105.93905582 a.u.			
C	2.40288800	0.57282800	0.92942000
C	2.85339500	-0.75338100	1.27138000
C	1.97899600	-1.14725800	2.44146700
C	0.91041700	-0.35628800	2.55668900
H	3.92879300	-0.90865600	1.36189200
H	2.17917000	-2.02648000	3.04022400
H	0.06210000	-0.45228800	3.21982900
C	1.02270600	0.77003400	1.58449500
C	2.43879000	-1.79860800	-0.09527800
O	1.19135700	-1.47979200	-0.49396300
Fe	-0.50335100	-2.17859100	-0.55618800
Cl	-0.42096300	-3.85491400	-1.99489700
Cl	-1.20388600	-2.87060000	1.41265100
C	2.54931000	-3.21913500	0.46262400
H	2.37209500	-3.90899300	-0.37017800
H	3.53898800	-3.42043000	0.88491400
H	1.77797600	-3.40722000	1.21214000
C	3.44748500	-1.53124100	-1.20682600
H	4.47905300	-1.69043900	-0.87572100
H	3.23115500	-2.23535800	-2.01705300
H	3.34002200	-0.52410800	-1.61423700

C	2.99016700	1.55909300	0.11775200
C	4.36470300	1.48075000	-0.25445100
C	2.19709700	2.64136100	-0.37362700
C	4.91809800	2.43826000	-1.08026800
H	4.97813400	0.67769000	0.13711000
C	2.76272900	3.57853500	-1.22205800
H	1.14464200	2.70862300	-0.12752000
C	4.11490500	3.48298700	-1.56976700
H	5.96719200	2.38671100	-1.35143900
H	2.14978600	4.38204700	-1.61570300
H	4.55343200	4.22834600	-2.22690800
Fe	-2.71176600	1.29290900	-0.09997000
Cl	-1.94132300	-0.53747900	-1.49896600
Cl	-2.64610900	0.74552900	2.03137900
Cl	-1.52179900	3.09212500	-0.65352900
Cl	-4.77787000	1.54019000	-0.77358400
F	0.07550100	0.76334800	0.60115000
F	0.96368500	1.99182300	2.18698500
2Fe.M1Ph-P			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.184134 a.u.			
E (UωB97X-D/def2-tzvp) = -6105.96905837 a.u.			
C	-2.34415000	-1.41495200	1.09458000
C	-2.55459100	-1.31148800	2.42513000
C	-1.31033700	-1.61248900	3.17447500
C	-0.31573400	-1.90115600	2.32536800
H	-3.48981600	-1.05350900	2.90795400
H	-1.24159200	-1.58034000	4.25499200
H	0.71885800	-2.14452700	2.51998800
C	-0.87579000	-1.81073100	0.93110800
C	-2.30949000	1.96415500	-0.82266500
O	-1.12487500	1.60390200	-0.81423300
Fe	0.51391600	1.47264700	0.39507000
Cl	1.29374500	3.48642000	-0.00172500
Cl	-0.44502800	1.64273600	2.40076200
C	-3.05874200	2.28815300	0.43322800
H	-2.69017200	3.24868200	0.81598500
H	-4.13190200	2.35865200	0.24901000
H	-2.84315500	1.54286000	1.20044100
C	-3.00509200	2.11853100	-2.13696700
H	-3.86359100	1.43780800	-2.16970700
H	-3.39882300	3.14014300	-2.21536600
H	-2.32581000	1.90765300	-2.96336100
C	-3.24337000	-1.23566300	-0.03901400
C	-4.58829500	-0.85962200	0.15471200
C	-2.79468600	-1.44762600	-1.35846600
C	-5.45469400	-0.72173800	-0.92395500
H	-4.95661600	-0.68403400	1.16087500
C	-3.66935800	-1.31764700	-2.43552800
H	-1.76468600	-1.72388700	-1.54175300
C	-5.00196700	-0.95888700	-2.22717900
H	-6.48911500	-0.43993400	-0.74937200
H	-3.30357400	-1.49773800	-3.44201300
H	-5.68278600	-0.86445900	-3.06797400
Fe	3.04562500	-0.72514900	-0.58249300
Cl	2.49426500	0.34205300	1.42846700
Cl	2.57165700	-2.84637700	-0.41084300

Cl	1.53668500	0.46692500	-1.83714300
Cl	5.09835600	-0.30370800	-1.14810700
F	-0.20490600	-0.82427400	0.17639700
F	-0.71432400	-2.95166000	0.21518600
2Fe.M2-2FeCl₃/S (RS)			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.108230 a.u.			
E (UωB97X-D/def2-tzvp) = -5874.89587235 a.u.			
C	-3.27903500	-1.69451600	-1.23892500
C	-2.04370300	-1.20787600	-1.40516700
C	-1.63477200	0.12207500	-0.95218300
C	-3.84892500	0.05425000	0.52559000
H	-3.56165800	-2.65995400	-1.64924300
H	-1.25276500	-1.79681400	-1.86445400
H	-2.25403500	0.99476400	-1.17465100
H	-4.26053300	1.04516900	0.35122300
C	-4.34723200	-0.99855900	-0.42553700
C	-3.00803100	-0.16263300	1.56048200
O	-0.49234500	0.29949700	-0.47576000
Fe	0.65747700	1.87549100	-0.26191400
Cl	-0.16602800	3.18714900	-1.80686600
Cl	0.66307800	2.84024000	1.67520000
C	-2.43693000	-1.50519200	1.92185700
H	-2.53690700	-1.66732200	3.00133300
H	-2.92072600	-2.33395300	1.40684600
H	-1.36050500	-1.52037300	1.70480900
C	-2.55004000	0.98128800	2.41873000
H	-2.85968100	0.82306100	3.45938800
H	-1.45460100	1.03335700	2.42514400
H	-2.94444300	1.94348900	2.08100300
F	-5.23371200	-0.42085900	-1.30389900
F	-5.04417300	-1.98281000	0.24111000
Fe	2.49938800	-1.22221900	0.02922300
Cl	2.70887700	1.01956500	-0.95994800
Cl	1.39079000	-2.43548800	-1.43127000
Cl	4.53893500	-1.88386700	0.36233400
Cl	1.37370600	-0.79480300	1.88117900
2Fe.M2-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.111589 a.u.			
E (UωB97X-D/def2-tzvp) = -5874.89111147 a.u.			
Imaginary frequency: -258.6008			
C	-3.25841000	-1.29363100	-1.56918200
C	-2.13854200	-0.58302200	-1.66896400
C	-1.90349500	0.47702600	-0.63402100
C	-3.22711700	-0.13670000	0.60737500
H	-3.60879700	-2.03606400	-2.27680200
H	-1.39518700	-0.68374800	-2.45269800
H	-2.39934100	1.43332500	-0.84515200
H	-3.71002400	0.78103900	0.93587400
C	-4.07870700	-0.95130500	-0.36418800
C	-2.36435900	-0.73997900	1.53925600
O	-0.68024300	0.59372600	-0.16486400
Fe	0.53074100	2.02048700	-0.13022500
Cl	-0.29378000	3.48132600	-1.54172700
Cl	0.77436600	2.81541600	1.88904400
C	-1.82012500	-2.10345200	1.35994500
H	-1.35862600	-2.48188400	2.27314700

H	-2.55369400	-2.80476300	0.96456100
H	-1.00986200	-2.01804500	0.61091300
C	-1.76756900	0.10059400	2.59220800
H	-1.68326200	-0.44287400	3.53888200
H	-0.72801300	0.29496000	2.27050100
H	-2.27085400	1.05805300	2.73401600
F	-5.16253300	-0.18994600	-0.72066900
F	-4.59098700	-2.07983400	0.22933400
Fe	2.28666500	-1.22077200	-0.14022800
Cl	2.49496900	1.03256000	-0.99648000
Cl	0.77815300	-2.30903400	-1.34202100
Cl	4.27768800	-2.07141300	-0.32387400
Cl	1.61793600	-0.99777000	1.95299200
2Fe.M2-INT0 G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.111710 a.u. E (UωB97X-D/def2-tzvp) = -5874.89713587 a.u.			
C	-3.20472200	-1.32402600	-1.61714900
C	-2.13842300	-0.53476500	-1.72880200
C	-1.99095900	0.46086500	-0.60051600
C	-3.03711900	-0.16217200	0.51880800
H	-3.55731300	-2.06009300	-2.32967800
H	-1.42327000	-0.52224200	-2.54299500
H	-2.42185500	1.43291700	-0.88063100
H	-3.59148100	0.65776100	0.97697200
C	-3.96851600	-1.02102200	-0.36713000
C	-2.19248500	-0.84241800	1.49951600
O	-0.71385100	0.60233800	-0.13170800
Fe	0.43943800	2.02919200	-0.11875700
Cl	-0.38768200	3.52061700	-1.49968300
Cl	0.64595800	2.73685900	1.95816100
C	-1.64209800	-2.17313500	1.25831200
H	-1.12650500	-2.58723300	2.12365100
H	-2.37812700	-2.86170800	0.84103000
H	-0.88336700	-2.03414900	0.45439200
C	-1.70698600	-0.06006100	2.62983400
H	-1.39463800	-0.66774000	3.48100900
H	-0.77488800	0.40147600	2.22641700
H	-2.35932000	0.76630200	2.91753100
F	-5.09171300	-0.28338000	-0.63272400
F	-4.41294500	-2.15080000	0.27546900
Fe	2.28350000	-1.14944800	-0.16153000
Cl	2.46278000	1.10152900	-0.96782100
Cl	0.76671400	-2.24824800	-1.36310400
Cl	4.27158400	-1.99867900	-0.38480500
Cl	1.63211400	-1.01615600	1.94733900
2Fe.M2-TS2 G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.113399 a.u. E (UωB97X-D/def2-tzvp) = -5874.89711267 a.u. Imaginary frequency: -87.8495			
C	-3.15893100	-1.45443400	-1.56443000
C	-2.15005600	-0.59864000	-1.72785200
C	-2.06918200	0.44445300	-0.63820600
C	-3.05289000	-0.14535200	0.47113500
H	-3.45891700	-2.25571100	-2.22908900
H	-1.43863900	-0.58246200	-2.54535300
H	-2.44854300	1.41201600	-0.99155600

H	-3.66091800	0.64222100	0.92208400
C	-3.93506400	-1.12980200	-0.32626500
C	-2.09510200	-0.68666100	1.46727700
O	-0.79196700	0.58102700	-0.08637500
Fe	0.37330200	1.99494800	-0.14351400
Cl	-0.48168500	3.41011800	-1.59429200
Cl	0.63882800	2.83919200	1.86893100
C	-1.53899800	-2.03088900	1.37728900
H	-0.84854700	-2.02340500	0.50560700
H	-0.95432100	-2.30899500	2.25359900
H	-2.30345100	-2.76829500	1.12284100
C	-1.69414700	0.17655600	2.58189800
H	-1.99998000	1.21655600	2.47440700
H	-2.15926300	-0.25477800	3.48699900
H	-0.60984400	0.10400100	2.73550700
F	-5.11193600	-0.49291800	-0.62145300
F	-4.29247000	-2.24245500	0.39707700
Fe	2.31074200	-1.13006100	-0.14386200
Cl	2.39270000	1.08306200	-1.03623200
Cl	0.77948400	-2.30330400	-1.25612800
Cl	4.30820200	-1.94563900	-0.39898100
Cl	1.72946500	-0.91575000	1.98152900
2Fe.M2-INT			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.116097 a.u.			
E (UωB97X-D/def2-tzvp) = -5874.91775517 a.u.			
C	-2.43080600	-2.20480900	-1.18348500
C	-1.76329200	-1.14676300	-1.65071700
C	-2.24519900	0.11941900	-1.01779900
C	-3.23480700	-0.30724100	0.07231700
H	-2.28645900	-3.24097900	-1.46548400
H	-0.95829600	-1.16543700	-2.37558900
H	-2.49331000	0.93736600	-1.69442200
H	-4.18092600	0.23168200	0.11484300
C	-3.47376300	-1.80312500	-0.17676500
C	-2.21173200	0.17738000	1.14242300
O	-1.28478300	0.62687900	0.00822400
Fe	0.11838300	1.94159200	-0.29762600
Cl	-0.79141400	3.23016700	-1.81587800
Cl	0.65649200	3.00706900	1.50321300
C	-1.47153800	-0.82086600	2.00102000
H	-1.05437300	-1.63788800	1.41203200
H	-0.65143800	-0.31358600	2.51535400
H	-2.15540900	-1.23500200	2.74695400
C	-2.68368200	1.40014200	1.90069900
H	-3.12802900	2.14043000	1.22824000
H	-3.44272000	1.09061000	2.62782200
H	-1.85487600	1.86482900	2.44121600
F	-4.73536100	-1.97536100	-0.69195100
F	-3.42540200	-2.56272900	0.95788100
Fe	2.41945300	-1.09576700	0.04819900
Cl	1.75795400	0.74518500	-1.44619500
Cl	1.02085500	-2.73159000	-0.39486900
Cl	4.48576700	-1.50602000	-0.47748700
Cl	2.10776700	-0.23425500	2.03997000
2Fe.M2-TS3			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.116068 a.u.			

$E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -5874.87773571 \text{ a.u.}$ Imaginary frequency: -122.0299			
C	-1.95067700	-2.19049500	-1.23368700
C	-1.85394400	-1.00452300	-1.94829200
C	-2.40821900	0.02648200	-1.20667200
C	-2.89285200	-0.41454800	0.14883700
H	-1.79693200	-3.18984600	-1.61964000
H	-1.40033100	-0.89344000	-2.92471600
H	-2.52002100	1.04125000	-1.57472300
H	-3.94070100	-0.15627100	0.32762300
C	-2.79856400	-1.95159700	0.01012700
C	-1.96208900	0.38598800	1.13111800
O	-0.80726800	0.63545300	0.32443500
Fe	0.19881100	2.02686300	-0.26537000
Cl	-0.98621000	3.11802900	-1.80954300
Cl	1.01622900	3.34038500	1.26794100
C	-1.53664500	-0.33081000	2.40808300
H	-0.90578300	-1.19064700	2.19095600
H	-0.95983900	0.37014400	3.01797100
H	-2.41014900	-0.66071300	2.97964400
C	-2.64874600	1.71836900	1.46206200
H	-2.95524000	2.25135600	0.55613300
H	-3.53033400	1.54967000	2.08952900
H	-1.94898300	2.35625000	2.00998200
F	-4.04614100	-2.43658000	-0.32580600
F	-2.40511400	-2.63232500	1.10004400
Fe	2.00729400	-1.08462500	0.00640500
Cl	1.79956000	0.71764800	-1.51825600
Cl	0.34630600	-2.64862400	-0.24774000
Cl	3.85781800	-2.07110600	-0.56911500
Cl	2.07450000	-0.27236800	2.02302300
2Fe.M2-INT2 $G_{\text{corr}}(\text{UB3LYP-D3BJ/6-31G}^*/\text{Lan2LDZ}) = 0.121869 \text{ a.u.}$ $E(\text{U}\omega\text{B97X-D/def2-tzvp}) = -5874.90661585 \text{ a.u.}$			
C	-2.19262200	1.77834000	-0.98410900
C	-1.31320000	2.97938900	-0.88033200
C	-0.75643300	3.08856700	0.32838100
C	-1.15953500	1.98884200	1.28172100
H	-3.18859500	1.95727500	-1.39003500
H	-1.15134700	3.64180800	-1.72163500
H	-0.08572600	3.88640200	0.62345300
H	-1.59400900	2.40828700	2.19690500
C	-2.30685600	1.32403000	0.49381000
C	-0.01123900	1.04029500	1.73298500
O	0.32795400	0.16701600	0.62356500
Fe	1.95946500	0.20218900	-0.38028100
Cl	2.21356700	1.98095400	-1.62521500
Cl	3.73601000	-0.33400000	0.76607200
C	-0.43870500	0.20255200	2.94153700
H	-1.35967100	-0.35404200	2.76029100
H	0.34878200	-0.51037100	3.19239900
H	-0.60205300	0.86358700	3.79921900
C	1.22809400	1.86111100	2.10695300
H	1.63577800	2.39976400	1.24555700
H	0.97217300	2.60026600	2.87350200
H	2.00417200	1.20588500	2.50930500

F	-3.50401800	1.75840100	0.96593700
F	-2.35117900	-0.06434300	0.63212400
Fe	-0.61849600	-1.52739700	-0.00326800
Cl	1.24049600	-1.68334900	-1.59455000
Cl	-1.45563700	0.53147100	-2.08122300
Cl	-2.15810000	-2.65768400	-1.07578200
Cl	-0.05095700	-2.88473700	1.63343800
2Fe.M2-TS4			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.114404 a.u.			
E (UωB97X-D/def2-tzvp) = -5874.85713128 a.u			
Imaginary frequency: -456.0955			
C	3.29246800	-0.11616600	-0.83024700
C	2.21901700	-0.34517100	-1.84929300
C	1.38339300	-1.35940100	-1.45899800
C	1.76637500	-1.91017500	-0.19146500
H	4.29647800	-0.00517500	-1.23953000
H	2.15994800	0.20275600	-2.77831400
H	0.51274100	-1.67995300	-2.01936300
H	1.62757300	-2.96752900	0.00947500
C	3.17892200	-1.38580900	0.04688200
C	0.26307300	-1.31256600	1.13523200
O	-0.44290000	-0.39716000	0.46225500
Fe	-2.33349800	-0.53301600	-0.16499900
Cl	-2.25651300	-1.63909300	-2.05701000
Cl	-3.64254900	-1.40423400	1.35272100
C	0.98155900	-0.78584300	2.34768500
H	1.55059600	0.11946100	2.14312100
H	0.19463400	-0.51861500	3.06797400
H	1.62800300	-1.54292500	2.79046100
C	-0.41273200	-2.65576200	1.29425200
H	-0.80587800	-3.02846500	0.34344300
H	0.27237800	-3.39042700	1.72273000
H	-1.25860500	-2.53475100	1.98135900
F	4.05013400	-2.31492300	-0.47450300
F	3.54213600	-1.20804900	1.33582000
Fe	-0.15390000	1.62608800	0.06725700
Cl	-2.68472600	1.70663500	-0.28832500
Cl	2.96876400	1.38738200	0.12880500
Cl	0.25818700	1.97548900	-2.10121300
Cl	0.27888400	2.74059300	1.91241800
2Fe.M2-P			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.105589 a.u.			
E (UωB97X-D/def2-tzvp) = -5874.89357052 a.u			
C	4.06713500	0.21997200	-0.64860100
C	2.91193600	0.59533800	-1.52114700
C	1.96298400	-0.42526600	-1.52805200
C	2.32915200	-1.46867700	-0.69090900
H	4.99699900	0.07380600	-1.20214000
H	2.85906600	1.52626900	-2.06829500
H	1.05384700	-0.40814800	-2.11675400
H	1.80817700	-2.40632300	-0.55045000
C	3.63188100	-1.14760800	-0.02626800
C	0.26742700	-0.22465800	1.41607800
O	-0.65798000	-0.06708700	0.57181000
Fe	-2.13223300	-1.30813900	-0.22577500
Cl	-0.99851300	-2.60089500	-1.58595600

Cl	-3.16160200	-2.14184700	1.50435200
C	1.09601600	0.94982600	1.78112300
H	1.38011500	1.49833800	0.87660300
H	0.46039400	1.62760300	2.37067700
H	1.98409400	0.67201800	2.34471500
C	0.43365900	-1.53746200	2.08916800
H	-0.05726700	-2.34329400	1.54216100
H	1.49219800	-1.74780400	2.24681000
H	-0.04757100	-1.45273500	3.07610400
F	4.58612600	-2.09618400	-0.25366000
F	3.49466400	-1.08269000	1.34626100
Fe	-1.53498200	1.67933800	-0.23263800
Cl	-3.27883400	0.44748100	-1.27387700
Cl	4.44342300	1.49426300	0.58260100
Cl	-0.07828300	2.47153100	-1.66715300
Cl	-2.11718400	2.72281200	1.60256800
2Fe.M2Ph-2FeCl₃/S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.185105 a.u.			
E (UωB97X-D/def2-tzvp) = -6105.97040557 a.u.			
C	-0.32349300	1.71927900	-0.09840100
C	-3.73317800	0.32107900	0.24821500
C	-3.40541700	1.68258900	-0.30258000
C	-2.41629300	1.75420700	-1.44675800
H	-3.62678000	0.25458300	1.32672900
H	-2.87210000	1.81144000	-2.42983800
C	-1.08354000	1.84326800	-1.35160100
C	-4.24425100	-0.70761000	-0.45395100
O	-0.66061300	0.83534500	0.74596100
C	-4.44890900	-0.68594800	-1.94577900
H	-4.59411500	0.32240500	-2.33798400
H	-3.58064500	-1.13933800	-2.44167300
H	-5.32407400	-1.28377200	-2.21999000
C	-4.64541600	-1.98499400	0.22825300
H	-4.13503000	-2.83704000	-0.23669900
H	-4.41169000	-1.98038500	1.29386600
H	-5.72372300	-2.14687300	0.10128800
C	0.81903100	2.56177900	0.18332300
C	1.11814300	3.67462900	-0.62998900
C	1.65341900	2.24301800	1.27507700
C	2.23461000	4.45012400	-0.35422600
H	0.47064400	3.93038200	-1.46145400
C	2.77358500	3.01757500	1.53648500
H	1.42636300	1.37276100	1.87843500
C	3.06398100	4.11834800	0.72414100
H	2.46722500	5.30786800	-0.97672500
H	3.43215200	2.75492600	2.35691500
H	3.94593600	4.71853500	0.92702100
H	-0.49510100	1.99740000	-2.24899900
Fe	-0.94298200	-1.05854200	0.80661400
Cl	-1.97683100	-1.65334600	2.63819200
Cl	-1.26298500	-2.27020800	-0.96692200
F	-2.93715600	2.45742600	0.73316500
F	-4.55474900	2.30037700	-0.76078800
Fe	2.74155000	-1.19604100	-0.46258200
Cl	1.31310100	-1.56118300	1.45627800
Cl	3.38080900	-3.16050600	-1.14319200

Cl	1.52757100	-0.10872300	-1.96372800
Cl	4.35931300	0.04744900	0.34007400
2Fe.M2Ph-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.186093 a.u.			
E (UωB97X-D/def2-tzvp) = -6105.96974015 a.u.			
C	2.17400800	2.32145800	-1.41643200
C	1.41144100	1.23485300	-1.57833600
C	1.38289600	0.03988400	-0.71042200
C	2.84543900	1.87544800	1.01455200
H	2.09271900	3.13895800	-2.12810800
H	0.65939500	1.22063200	-2.36314700
H	3.63627400	1.20985500	1.34376900
C	3.13210900	2.58871800	-0.27306300
C	1.71031400	1.99975900	1.72345900
O	0.23757000	-0.31950100	-0.30855400
Fe	-0.78149800	-1.93748400	-0.05110900
Cl	-0.80739900	-2.71635100	1.98069700
Cl	0.15911700	-3.35022100	-1.42880100
C	0.58217600	2.92201900	1.34828600
H	-0.26540200	2.34937900	0.95731200
H	0.21786900	3.44477800	2.24021800
H	0.87231100	3.66916100	0.61015600
C	1.48606800	1.15301200	2.94592800
H	1.30613500	1.77917000	3.82849200
H	0.58619000	0.53828200	2.81327500
H	2.33513300	0.49492300	3.15269800
C	2.56628300	-0.76224800	-0.43585300
C	2.55345300	-1.69080800	0.62555300
C	3.71657000	-0.63227700	-1.23806400
C	3.67357100	-2.46643700	0.88047900
H	1.68475400	-1.77183400	1.26820800
C	4.82879100	-1.42705700	-0.98564900
H	3.72735500	0.07746900	-2.05471800
C	4.81033800	-2.33930100	0.07215800
H	3.66563600	-3.16991200	1.70659400
H	5.70985000	-1.33501900	-1.61212400
H	5.68350700	-2.95382400	0.26998800
F	3.15118000	3.95733300	-0.10048800
F	4.39949600	2.24548700	-0.70526500
Fe	-3.14045500	0.80410600	-0.18843000
Cl	-2.87339200	-1.47070900	-1.01215300
Cl	-2.21968000	0.61089700	1.80962400
Cl	-5.27485500	1.20348100	-0.16972600
Cl	-1.98604500	2.11139000	-1.52787600
2Fe.M2Ph-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.186320 a.u.			
E (UωB97X-D/def2-tzvp) = -6105.95566052 a.u.			
Imaginary frequency: -152.5953			
C	2.16166600	2.27697600	-1.72532600
C	1.88862900	0.98300700	-1.57887800
C	1.96172200	0.46986100	-0.15392100
C	2.15770200	1.88683500	0.67668000
H	2.18347200	2.84399200	-2.64869500
H	1.62906900	0.28028700	-2.36352000
H	2.96592100	1.78354200	1.39802700
C	2.53165400	2.90412400	-0.41996100

C	0.85906900	2.01519200	1.33333600
O	0.73798200	-0.08117200	0.25013300
Fe	-0.11029400	-1.60672000	-0.36533100
Cl	-0.50549800	-3.01969600	1.26101100
Cl	1.09398100	-2.48568800	-1.99013200
C	-0.29778800	2.65937400	0.70274500
H	-1.23717700	2.27777400	1.10409500
H	-0.22579400	3.72982200	0.96237800
H	-0.28264900	2.60187900	-0.38558700
C	0.69836300	1.48172700	2.69332900
H	0.20437600	2.22810400	3.33052100
H	-0.02318500	0.65154700	2.62108500
H	1.62823000	1.13617100	3.14516500
C	3.13286300	-0.44362000	0.12255100
C	3.00471200	-1.47763700	1.05919500
C	4.36126100	-0.24053000	-0.52172300
C	4.08294200	-2.32104400	1.31906800
H	2.06164100	-1.63785000	1.56823600
C	5.43708000	-1.08333400	-0.25463300
H	4.47507100	0.57263000	-1.23026800
C	5.29928800	-2.12874700	0.66196900
H	3.96760200	-3.13242300	2.03114800
H	6.38133800	-0.92836700	-0.76775300
H	6.13687300	-2.79023300	0.86207900
F	1.93773000	4.12562700	-0.22970100
F	3.88300000	3.13190300	-0.34658300
Fe	-3.47975900	0.23926100	-0.03026300
Cl	-2.08749800	-0.96513700	-1.55357000
Cl	-2.47109200	0.06249800	1.94701100
Cl	-5.45685800	-0.65901900	-0.07718000
Cl	-3.42531700	2.32442700	-0.74258300
2Fe.M2Ph-INT			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.190477 a.u.			
E (UωB97X-D/def2-tzvp) = -6105.97879251 a.u.			
C	2.41087800	2.48722000	-1.58877100
C	2.32635200	1.15574300	-1.58409000
C	2.37421200	0.59378200	-0.18675000
C	2.28960600	1.84089200	0.73010300
H	2.41124300	3.14009200	-2.45422300
H	2.23408000	0.50590000	-2.44665700
H	2.96826500	1.84789800	1.58191400
C	2.55778500	3.03155700	-0.19394300
C	0.83939600	1.43702100	1.10633000
O	0.99908700	0.18005700	0.24758000
Fe	-0.06095700	-1.33999300	-0.40562300
Cl	-0.47096900	-2.72674800	1.20594500
Cl	1.17366200	-2.20937000	-1.98190500
C	-0.32573500	2.25239000	0.59342400
H	-1.25984800	1.73742800	0.81911300
H	-0.34266700	3.21939000	1.10218200
H	-0.26513800	2.42703400	-0.48130800
C	0.68576000	1.01049400	2.55072500
H	0.64659700	1.90669000	3.17995600
H	-0.24443800	0.45360900	2.68915500
H	1.52819600	0.39488200	2.87716500
C	3.39078500	-0.47580800	0.07852400

C	3.17679100	-1.45716600	1.05410000
C	4.59353900	-0.46594400	-0.63750600
C	4.14821700	-2.42710600	1.29465400
H	2.24630100	-1.48624000	1.60866100
C	5.56798400	-1.43003300	-0.38478600
H	4.76890000	0.29620500	-1.39046300
C	5.34562400	-2.41580100	0.57791300
H	3.96381900	-3.19419700	2.04050200
H	6.49630500	-1.41533200	-0.94766100
H	6.10018900	-3.17354400	0.76600500
F	1.74562100	4.10499600	0.03958000
F	3.84176600	3.47691000	0.00948700
Fe	-3.70808400	0.14490500	0.00326200
Cl	-1.89831700	-0.48633400	-1.54221700
Cl	-2.84536700	-0.17603300	2.00516300
Cl	-5.38405900	-1.14416400	-0.49003400
Cl	-3.97631000	2.26684900	-0.45370200
2Fe.M2Ph-TS2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.190755 a.u.			
E (UωB97X-D/def2-tzvp) = -6105.96471939 a.u.			
Imaginary frequency: -55.3484			
C	0.95022500	2.60962100	-1.66885900
C	1.48985700	1.37720900	-1.76334600
C	2.26068900	1.08203400	-0.57688700
C	1.88835200	2.09915400	0.49497600
H	0.35032600	3.11883800	-2.41310700
H	1.38166300	0.70256800	-2.60107100
H	2.72204400	2.45966100	1.09775200
C	1.36601700	3.26152600	-0.37644000
C	0.86645600	1.25839300	1.36214600
O	0.60320600	0.16170000	0.47857700
Fe	0.13121700	-1.57727000	0.29426500
Cl	1.46301900	-2.81493000	1.54935000
Cl	0.26315200	-2.13966300	-1.84824800
C	-0.45824300	1.92575800	1.71362500
H	-1.06256300	1.20165700	2.26722100
H	-0.30250000	2.80555300	2.34459000
H	-1.01733600	2.21536200	0.82615700
C	1.55557800	0.74390200	2.62780200
H	1.83827600	1.58078700	3.27621600
H	0.86246700	0.09867800	3.17464100
H	2.43960400	0.14699900	2.39605300
C	3.32338400	0.13075900	-0.49720100
C	4.27653200	0.18826600	0.54992700
C	3.41871700	-0.91115400	-1.45401800
C	5.27417900	-0.76780500	0.64259300
H	4.23881100	0.99242300	1.27388500
C	4.40269100	-1.87937800	-1.33649400
H	2.68001000	-0.99511400	-2.23943100
C	5.32953600	-1.81017300	-0.29108800
H	6.00394100	-0.71428600	1.44348100
H	4.44323100	-2.69491500	-2.05036400
H	6.09840900	-2.57160900	-0.20164800
F	0.39313300	4.02008400	0.17833900
F	2.41834100	4.11701300	-0.62993600
Fe	-3.34745900	-0.07461600	-0.14670700

Cl	-2.08604200	-1.74648100	1.09267200
Cl	-4.05178700	1.30664300	1.40448100
Cl	-4.94565600	-1.17341600	-1.13823000
Cl	-1.98661600	0.93409900	-1.57505600
2Fe.M2Ph-INT2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.191302 a.u.			
E (UωB97X-D/def2-tzvp) = -6105.96832692 a.u.			
C	0.61171900	2.12117000	-1.58329700
C	1.58838300	1.18912300	-1.74600800
C	2.39696300	1.13750800	-0.57578700
C	1.72018000	1.84793000	0.55645700
H	-0.07594800	2.48958700	-2.33147800
H	1.79098800	0.65190100	-2.66068500
H	2.39894600	2.46709600	1.14649100
C	0.72021900	2.75026800	-0.21821100
C	1.05349000	0.78092100	1.55516800
O	0.18820200	0.00356500	0.78932300
Fe	-0.09121900	-1.68205500	0.21139600
Cl	0.82109700	-3.20859400	1.51948200
Cl	0.66920100	-1.96112600	-1.87742200
C	0.27016300	1.50595700	2.66289400
H	-0.08937600	0.74963100	3.36606200
H	0.92279800	2.20125500	3.20279900
H	-0.59256700	2.03716700	2.27374500
C	2.13859600	-0.07823800	2.22138000
H	2.86393400	0.54735000	2.75271300
H	1.65456000	-0.73516100	2.94689000
H	2.66613400	-0.71671700	1.51254900
C	3.67143700	0.49436900	-0.51656500
C	4.65100100	0.89967400	0.42480900
C	3.96259400	-0.57709100	-1.39972700
C	5.87995500	0.26405000	0.47032200
H	4.44567100	1.72828300	1.09235700
C	5.18162700	-1.23301800	-1.31719400
H	3.19664000	-0.93754500	-2.07620200
C	6.14241400	-0.80902400	-0.39259300
H	6.63422800	0.58952300	1.17896200
H	5.38385200	-2.07830000	-1.96632500
H	7.09938200	-1.31932900	-0.33854000
F	-0.48661900	2.95320100	0.34071400
F	1.29958900	3.99198900	-0.37533400
Fe	-3.33405000	0.09597000	-0.16946300
Cl	-2.44373800	-2.05762600	0.36880400
Cl	-3.25489100	1.36680400	1.61272600
Cl	-5.38015600	-0.27871900	-0.82981200
Cl	-2.05839800	0.80200600	-1.85510200
2Fe.M2Ph-TS3			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.186407 a.u.			
E (UωB97X-D/def2-tzvp) = -6105.95275198 a.u.			
Imaginary frequency: -290.0739			
C	0.75882500	2.04732700	-1.62718400
C	1.74822000	1.14079800	-1.74007800
C	2.60022000	1.19743400	-0.55763700
C	1.97006800	1.97206500	0.43881500
H	-0.02749200	2.27237600	-2.33362800
H	1.92419100	0.49894500	-2.59063400

H	2.53483300	2.46986900	1.21950400
C	0.89916600	2.77752800	-0.31249600
C	1.03723000	0.54522000	1.58929800
O	0.18809100	-0.01896300	0.76280700
Fe	-0.20534700	-1.69835200	0.06760600
Cl	0.64087900	-3.25431900	1.37457600
Cl	0.54515800	-1.99551700	-1.98756100
C	0.40210500	1.41393400	2.65916500
H	-0.07025700	0.72388400	3.37061400
H	1.15395500	2.00030000	3.19383700
H	-0.37494500	2.05594300	2.25669400
C	2.19066700	-0.29887200	2.08712600
H	2.97340600	0.31652200	2.53733200
H	1.79069800	-0.96638300	2.85906300
H	2.61997400	-0.92395800	1.30517200
C	3.86351300	0.50385500	-0.45130500
C	4.86967800	0.96202500	0.42637400
C	4.08589500	-0.67271200	-1.19965700
C	6.06294600	0.26472000	0.54948900
H	4.71628900	1.87893200	0.98588000
C	5.27339900	-1.38025100	-1.05094400
H	3.30392100	-1.06055200	-1.84310000
C	6.26346300	-0.91135700	-0.18322500
H	6.83870800	0.63066300	1.21448400
H	5.42589200	-2.29856200	-1.60855700
H	7.19329100	-1.46172400	-0.07597600
F	-0.29535500	2.93073000	0.30516700
F	1.38860600	4.04572700	-0.52613700
Fe	-3.43565600	0.20314700	-0.10817200
Cl	-2.53112700	-2.00995300	0.28454000
Cl	-3.10120100	1.37919500	1.71246700
Cl	-5.54737800	-0.13262500	-0.53431600
Cl	-2.29060900	0.87982900	-1.86830300
2Fe.M2Ph-P			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.180606 a.u.			
E (UωB97X-D/def2-tzvp) = -6105.97788676 a.u.			
C	2.11188200	2.77973200	-1.40027500
C	2.14024300	1.44436000	-1.38590900
C	3.13980500	0.96439900	-0.36944100
C	3.73111300	2.03671100	0.19376400
H	1.48152900	3.43593300	-1.98540700
H	1.51396400	0.78198000	-1.96969100
H	4.51334800	2.06278100	0.94122200
C	3.11114800	3.29256400	-0.38081500
C	0.40192700	0.08924800	1.62865000
O	0.14498400	-0.26042300	0.45571800
Fe	-0.50101500	-1.77518700	-0.57867700
Cl	-0.04584500	-3.69985600	0.33423300
Cl	0.00065400	-1.58955500	-2.68790700
C	0.67415900	1.52604800	1.89501400
H	0.25871100	1.81915800	2.86216500
H	1.76418300	1.65684100	1.93717700
H	0.28737800	2.14997800	1.09011100
C	0.43777600	-0.90931100	2.73582800
H	0.75562200	-1.88778500	2.37105900
H	1.07490000	-0.56916300	3.55492300

H	-0.58954600	-0.99418600	3.11767500
C	3.32019200	-0.44787900	-0.02128800
C	3.71190400	-0.82174300	1.27627000
C	3.04342200	-1.45957800	-0.95696100
C	3.82290200	-2.16593100	1.62689300
H	3.91240400	-0.05089500	2.01515000
C	3.15389900	-2.80309100	-0.60477400
H	2.74737400	-1.19378200	-1.96492600
C	3.53772400	-3.16160600	0.68966900
H	4.12178800	-2.43680700	2.63545900
H	2.92715700	-3.56968300	-1.33866100
H	3.60733500	-4.20885800	0.96633800
F	2.47312000	4.01093400	0.61084200
F	4.03580400	4.13691300	-0.92578600
Fe	-3.13968300	0.84047200	0.11983200
Cl	-2.82454300	-1.53635400	-0.34480000
Cl	-2.65659700	0.97789700	2.27635700
Cl	-5.22032900	1.23829700	-0.35140100
Cl	-1.69373900	1.89641200	-1.14845900
2Fe.M3-2FeCl₃/S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.126080 a.u.			
E (UωB97X-D/def2-tzvp) = -5676.38750477 a.u.			
C	-1.84582700	0.09806000	1.54831600
C	-2.81066400	-1.79274100	-0.10173000
C	-3.74745600	-1.98552100	1.02024700
C	-3.40125500	-1.67446300	2.27801400
H	-2.71038700	0.65354300	1.16599600
H	-1.80420100	-2.18084200	0.04983200
H	-4.72783500	-2.41561300	0.82463100
H	-4.06253100	-1.86883100	3.11625100
C	-2.08178400	-0.98876900	2.54697900
C	-3.09276100	-1.23996700	-1.30320700
O	-0.70038500	0.46197400	1.22858200
C	-4.43472000	-0.65696800	-1.64371700
H	-4.32894800	0.41213600	-1.87063100
H	-4.84431000	-1.12915100	-2.54599900
H	-5.16080200	-0.76246200	-0.83378800
C	-2.04702300	-1.16534700	-2.37938200
H	-1.89459400	-0.12831700	-2.70215900
H	-1.08829400	-1.57073900	-2.04738100
H	-2.37335300	-1.72680800	-3.26551500
Fe	-0.10389200	1.79175500	-0.09359900
Cl	-2.00147000	2.34410600	-1.05746600
Cl	0.85335100	3.50271400	0.80923000
H	-2.09553500	-0.48877000	3.52933900
H	-1.21127700	-1.65801200	2.55198500
Fe	2.26453100	-0.96103800	-0.05184200
Cl	1.15905000	0.57555500	-1.62420300
Cl	4.06865200	-1.61085600	-1.06894100
Cl	0.79829200	-2.56326700	0.32461600
Cl	2.56315100	0.34020200	1.68659500
2Fe.M3-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.128199 a.u.			
E (UωB97X-D/def2-tzvp) = -5676.38474593 a.u.			
C	1.27207400	-1.57414200	-0.51268300
C	2.25410900	-2.23924400	0.46997000

C	3.39978300	-2.65595000	-0.41375600
C	3.17680000	-2.35624200	-1.69817000
H	0.21325300	-1.78034300	-0.39756500
H	1.85367200	-3.03305300	1.10621900
H	4.29340900	-3.13491200	-0.02740500
H	3.86498600	-2.56185800	-2.51202500
C	1.82950900	-1.70872300	-1.92642800
C	2.39152700	-0.87406200	1.21238200
O	1.56230500	-0.23869900	0.09257000
Fe	0.77628600	1.51942900	-0.13601500
Cl	0.74767900	2.02929400	-2.24188500
Cl	1.96142100	2.89572600	1.07507000
H	1.16672600	-2.32761500	-2.54400700
H	1.88785700	-0.73072700	-2.41920500
C	3.75917500	-0.23604300	1.25950300
H	4.38183200	-0.79082700	1.97064500
H	4.23986400	-0.26713900	0.27960300
H	3.69190600	0.80081200	1.59763200
C	1.61259100	-0.76995700	2.50619800
H	1.53361700	0.27439100	2.82475700
H	0.60786500	-1.18815700	2.40254200
H	2.14356800	-1.32550800	3.28731300
Fe	-2.51477800	-0.42440200	0.08339800
Cl	-1.32411600	1.52742000	0.91454800
Cl	-1.73035100	-0.63963600	-1.96153100
Cl	-4.62816800	0.03362200	0.24325400
Cl	-1.81173500	-2.08230800	1.36330300
2Fe.M3-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.129411 a.u.			
E (UωB97X-D/def2-tzvp) = -5676.38293203 a.u.			
Imaginary frequency: -114.3021			
C	1.32485600	-1.22379700	-0.89335500
C	2.51950600	-2.14378600	-0.30403200
C	3.66630900	-1.86633100	-1.24322000
C	3.28715100	-1.14549200	-2.30155200
H	0.41007800	-1.81859400	-0.92883900
H	2.17857500	-3.18722500	-0.33070000
H	4.66432400	-2.25615800	-1.06849800
H	3.94571100	-0.85816900	-3.11543300
C	1.82662200	-0.79448700	-2.28890500
C	2.66757100	-1.71786400	1.10346100
O	1.13291300	-0.16025400	-0.01242700
Fe	0.62393700	1.55523800	0.19190900
Cl	0.72420600	2.79572900	-1.60627600
Cl	1.92006500	2.30671800	1.86393200
H	1.27891300	-1.32625200	-3.07671100
H	1.63446500	0.27410100	-2.43435000
C	3.62353400	-0.69471400	1.49288600
H	4.08497000	-0.91896500	2.46151300
H	4.35528900	-0.44794400	0.72492800
H	3.00983200	0.22062900	1.68448100
C	1.78073600	-2.30233100	2.11820400
H	1.93468900	-1.89162900	3.11677400
H	0.73400800	-2.14296500	1.80346400
H	1.90712300	-3.39430500	2.12965100
Fe	-2.43725600	-0.45762100	0.00018500

Cl	-1.58815900	1.46861500	1.12028700
Cl	-1.70301600	-0.30076100	-2.07266800
Cl	-4.60313700	-0.36428800	0.17443500
Cl	-1.58717600	-2.26929000	0.99309900
2Fe.M3-INT			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.135015 a.u.			
E (UωB97X-D/def2-tzvp) = -5676.40501815 a.u.			
C	1.07538100	-0.84247400	-1.20058400
C	3.38101900	-1.94411700	-0.63113700
C	3.91741200	-0.58846600	-0.90020500
C	3.24625900	0.24691700	-1.70163800
H	0.62695000	-1.82894600	-1.33990500
H	3.42175700	-2.64330500	-1.46952000
H	4.87134500	-0.29020200	-0.46895300
H	3.61626400	1.23347000	-1.96134600
C	1.90787900	-0.19682100	-2.26653000
C	2.85910500	-2.38854900	0.53610500
O	0.73062700	-0.22197100	-0.17153800
Fe	0.57630000	1.59925900	0.45057400
Cl	0.72280300	3.00121500	-1.20815600
Cl	1.91751200	2.05906600	2.09336900
H	2.02686100	-0.89415800	-3.10413000
H	1.33291300	0.66624200	-2.62599300
C	2.74083000	-1.52230900	1.75228800
H	3.16991900	-2.02511800	2.62772500
H	3.22201400	-0.55072900	1.63027900
H	1.67978700	-1.34990200	1.97818800
C	2.29783600	-3.77736600	0.65586500
H	2.79510500	-4.32618200	1.46570400
H	1.23180800	-3.73289500	0.91467100
H	2.40973700	-4.35005600	-0.26941300
Fe	-2.42542700	-0.51895000	-0.05413100
Cl	-1.62878400	1.40478600	1.23752600
Cl	-1.83088800	-0.12087500	-2.15210600
Cl	-4.57524900	-0.47491700	0.25331400
Cl	-1.47166100	-2.34818000	0.73031800
2Fe.M3-TS2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.128626 a.u.			
E (UωB97X-D/def2-tzvp) = -5676.36377386 a.u.			
Imaginary frequency: -364.6615			
C	-1.12180100	-2.41492800	0.18824500
C	-2.40185500	-2.37105400	-0.46610500
C	-3.39985700	-2.29435100	0.65291700
C	-2.77010300	-2.15472800	1.82673000
H	-0.15873600	-2.52009000	-0.30788800
H	-2.57267500	-3.07247900	-1.28460700
H	-4.47020800	-2.29815200	0.49086900
H	-3.22831800	-2.01626600	2.79773500
C	-1.27925600	-2.18487900	1.61993100
C	-2.20201900	-0.86646300	-1.30085000
O	-1.33540400	-0.11370600	-0.53285100
Fe	-0.95589700	1.52091100	0.15115900
Cl	-1.12728300	1.37885500	2.35180800
Cl	-2.12809700	3.12869900	-0.76748700
H	-0.71170400	-2.93746400	2.19418300
H	-0.75932500	-1.24133200	1.88893100

C	-3.57682600	-0.22387900	-1.40555200
H	-4.28331600	-0.86413200	-1.94262000
H	-3.97129700	0.01621500	-0.41643100
H	-3.45618700	0.71468500	-1.95820300
C	-1.58773800	-1.18396700	-2.65883300
H	-1.40580600	-0.23129000	-3.16774500
H	-0.62624500	-1.69103200	-2.56302300
H	-2.26852700	-1.78469400	-3.26980800
Fe	2.47685000	-0.21511800	-0.09515700
Cl	1.34036400	1.84733900	-0.47722300
Cl	1.89159000	-0.94047400	1.90464200
Cl	4.59124100	0.26507200	-0.25367700
Cl	1.84909800	-1.73534100	-1.60474000
2Fe.M3-P G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.125029 a.u. E (UωB97X-D/def2-tzvp) = -5676.40246527 a.u.			
C	-1.93659700	-2.34130000	0.15632600
C	-3.00696700	-2.85281500	-0.49901700
C	-4.21906900	-2.61944000	0.29052500
C	-3.88607900	-1.97261700	1.43441400
H	-0.90079200	-2.37311900	-0.15490500
H	-2.98608200	-3.36890400	-1.45291500
H	-5.21556300	-2.93044100	-0.00481600
H	-4.55915100	-1.66813600	2.22715800
C	-2.39829500	-1.76215700	1.46568000
C	-2.08115000	0.24983700	-1.41220700
O	-0.94593600	0.57274500	-0.99607600
Fe	-0.15969900	1.90500500	0.17467300
Cl	-0.92534400	1.76176300	2.20543100
Cl	-0.72309000	3.79266600	-0.76234400
H	-1.93269600	-2.29456800	2.30858900
H	-2.10755600	-0.71217600	1.60610700
C	-3.32247400	0.71137700	-0.73375900
H	-3.99620900	1.16193200	-1.47208200
H	-3.84683800	-0.16168800	-0.31622500
H	-3.10981100	1.41965200	0.06839100
C	-2.15500000	-0.50751400	-2.69897600
H	-2.07653000	0.23399200	-3.50818900
H	-1.30490700	-1.18633800	-2.78574700
H	-3.10171400	-1.03857800	-2.80249200
Fe	2.29551500	-0.87671300	-0.03668000
Cl	2.12597100	1.56951000	-0.12496200
Cl	1.08803600	-1.34010500	1.73693700
Cl	4.42016900	-1.28280900	0.15532200
Cl	1.37942900	-1.66757800	-1.87803200
2Fe.M3Ph-2FeCl3/S G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.202974 a.u. E (UωB97X-D/def2-tzvp) = -5907.46712424 a.u.			
C	-0.35253000	1.59394000	0.45727300
C	-3.81962600	0.62120300	0.87473900
C	-3.45702700	2.02334200	0.89661700
C	-2.29545700	2.52953400	1.36542200
H	-3.26083400	-0.03937100	1.53080000
H	-4.19429800	2.73817800	0.53813000
H	-2.13755500	3.60434500	1.34550200
C	-1.09613100	1.69244600	1.76119100

C	-4.81278800	0.06055400	0.13989100
O	-0.62729100	0.64488600	-0.33488700
C	-5.61736400	0.79812500	-0.89103900
H	-5.33600300	0.43489300	-1.88958200
H	-6.68812400	0.59271500	-0.77087700
H	-5.46491700	1.87939600	-0.87820000
C	-5.14455400	-1.39710200	0.28484900
H	-5.08192000	-1.90560300	-0.68509600
H	-4.47428400	-1.90512300	0.98149800
H	-6.17773200	-1.51487100	0.64022200
Fe	-1.10069000	-1.19395900	-0.44866900
Cl	-2.48287200	-1.51391200	-2.11200100
Cl	-1.58711900	-2.20675500	1.42358100
C	0.56567800	2.62480600	-0.00388900
C	1.13193400	2.50393300	-1.28891600
C	0.92036900	3.71917600	0.81098700
C	2.02674500	3.45983800	-1.74939300
H	0.87103400	1.65002300	-1.90128600
C	1.81477300	4.67207300	0.34316200
H	0.50505400	3.82267100	1.80648300
C	2.36821400	4.54313800	-0.93571800
H	2.47102300	3.35275900	-2.73315800
H	2.08952000	5.51147300	0.97367800
H	3.07418200	5.28641800	-1.29415600
H	-0.49517000	2.16451600	2.53876500
H	-1.36202300	0.68825400	2.09257100
Fe	2.69851600	-1.17468200	0.19169100
Cl	0.94831100	-2.10233900	-1.21527000
Cl	3.69824800	0.30553700	-1.07852000
Cl	3.95540500	-2.86350300	0.73992800
Cl	1.68823100	-0.24285900	1.92899800
2Fe.M3Ph-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.204327 a.u.			
E (UωB97X-D/def2-tzvp) = -5907.46166334 a.u.			
C	1.92544100	-0.12954400	0.76305100
C	3.45637200	-0.27699200	-1.59630600
C	3.57669900	-1.69263600	-1.17808900
C	3.30971400	-2.13632400	0.05359400
H	4.28498600	0.37669100	-1.32044000
H	3.92594400	-2.41712700	-1.91434500
H	3.44217500	-3.18654200	0.29611500
C	2.82567000	-1.26141300	1.19599000
C	2.43446500	0.25807200	-2.29282000
O	0.77378000	-0.42814600	0.32890600
Fe	-0.38839000	-1.96249600	0.35036000
Cl	0.37995000	-3.68983300	-0.74102300
Cl	-0.64645700	-2.47963800	2.45223200
C	1.23982900	-0.53553800	-2.73614400
H	0.32412400	-0.11378800	-2.30101400
H	1.11689200	-0.47050300	-3.82508800
H	1.30837500	-1.58837800	-2.45590400
C	2.40548600	1.72456500	-2.61817600
H	2.31138800	1.88459700	-3.70000900
H	1.52712800	2.19533800	-2.15752300
H	3.30172800	2.24306300	-2.26488300
C	2.25585000	1.27857700	0.94054300

C	3.53452100	1.70134600	1.35906800
C	1.26318200	2.24174000	0.67272000
C	3.80557800	3.05475700	1.50535200
H	4.32142000	0.98110900	1.54954600
C	1.54002900	3.59406700	0.82652300
H	0.28564400	1.91844900	0.34922600
C	2.80909100	4.00282200	1.24222400
H	4.79199200	3.37600300	1.82428000
H	0.76526800	4.32467700	0.61829300
H	3.02660900	5.06014800	1.36143700
H	2.22199300	-1.86870000	1.88460500
H	3.67131400	-0.89061200	1.78125200
Fe	-2.70744900	0.93982200	-0.17512800
Cl	-2.34839700	-1.37754700	-0.79996200
Cl	-1.88660200	1.05393400	1.86133200
Cl	-1.50920200	2.11241100	-1.61349300
Cl	-4.84911400	1.27768800	-0.32014400
2Fe.M3Ph-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.206387 a.u.			
E (UωB97X-D/def2-tzvp) = -5907.44483716 a.u.			
Imaginary frequency: -123.8238			
C	2.41592000	-0.17954000	-0.41008200
C	2.40014900	-0.11707700	-2.03504800
C	2.87365000	-1.48768600	-2.43866200
C	3.36905400	-2.17284600	-1.40561600
H	3.05942700	0.68897300	-2.37451700
H	2.82983900	-1.83767100	-3.46510600
H	3.78799600	-3.17167000	-1.46824200
C	3.34119100	-1.39328700	-0.12435200
C	0.99658200	0.24224200	-2.31904900
O	1.07650800	-0.45464900	-0.07482700
Fe	0.04765200	-1.57574800	0.92565800
Cl	0.68933400	-3.66608700	0.58809000
Cl	0.00167500	-1.00559600	3.03848600
C	0.04828200	-0.77711400	-2.77986400
H	-0.98865500	-0.52018200	-2.55556400
H	0.14468200	-0.77777800	-3.88262200
H	0.32000300	-1.77635700	-2.43305600
C	0.56468600	1.63291500	-2.18136300
H	-0.25273100	1.88518400	-2.86324300
H	0.10880900	1.69400700	-1.17034400
H	1.38373100	2.35197200	-2.21589300
C	2.88364200	1.11186600	0.22413400
C	4.11750000	1.67065100	-0.14290800
C	2.11081900	1.74262600	1.20279300
C	4.56313800	2.84811000	0.45007400
H	4.73687600	1.18245600	-0.89227900
C	2.56196600	2.92276200	1.79912300
H	1.16795500	1.30831300	1.50407100
C	3.78209900	3.48052000	1.42333200
H	5.51835900	3.27285700	0.15551800
H	1.94976200	3.40168800	2.55707800
H	4.12858100	4.40051900	1.88470600
H	2.94043100	-1.96242800	0.72052800
H	4.34698900	-1.06045700	0.15881800
Fe	-2.96478900	0.70121600	-0.14886000

Cl	-2.15941500	-1.54601500	-0.04190900
Cl	-1.41802900	1.96286200	0.80396600
Cl	-3.04302400	1.13800400	-2.32481200
Cl	-4.90116600	0.77275800	0.82835200
2Fe.M3Ph-INT			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.211147 a.u.			
E (UωB97X-D/def2-tzvp) = -5907.45696024 a.u.			
C	2.60590100	-0.35466800	-0.35395700
C	2.58004300	-0.83163600	-1.83499200
C	3.00410000	-2.27075700	-1.75145800
C	3.31369200	-2.63518500	-0.50343200
H	3.14425900	-0.22900000	-2.55217300
H	3.03478100	-2.92024600	-2.62016200
H	3.63442200	-3.62790300	-0.20529200
C	3.20438300	-1.49959200	0.48122200
C	1.05562100	-0.54837500	-1.86107300
O	1.10717700	-0.36707600	-0.34511300
Fe	-0.22365400	-0.94151600	1.00579300
Cl	0.21515700	-3.11846200	1.12336200
Cl	0.36249500	-0.14942300	2.95224600
C	0.12089700	-1.67732300	-2.22911700
H	-0.91790400	-1.41572700	-2.00263400
H	0.18202200	-1.84774200	-3.30966500
H	0.38550200	-2.60056100	-1.71130700
C	0.68997300	0.77679000	-2.49963200
H	0.80478100	0.68053500	-3.58544800
H	-0.34666600	1.04457600	-2.28746800
H	1.34417700	1.57858700	-2.14917400
C	3.14861500	1.01285400	-0.04978100
C	4.47141400	1.29018400	-0.42204100
C	2.40126600	1.98981300	0.61062200
C	5.03742700	2.53055600	-0.13717700
H	5.05839300	0.53336900	-0.93712800
C	2.97181400	3.23189500	0.89525900
H	1.38009400	1.78705300	0.90071400
C	4.28706400	3.50671500	0.52317000
H	6.06180600	2.73588100	-0.43390200
H	2.37959700	3.98339600	1.40867800
H	4.72644600	4.47492100	0.74391300
H	2.58015400	-1.72912800	1.34997800
H	4.18455300	-1.20049900	0.87254400
Fe	-3.14263800	0.68398200	-0.28206100
Cl	-2.57704700	-1.43326800	0.61466200
Cl	-1.20282400	1.63294200	0.38573500
Cl	-3.18101000	0.47951800	-2.46088900
Cl	-4.92991800	1.48618400	0.63528000
2Fe.M3Ph-TS2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.208631 a.u.			
E (UωB97X-D/def2-tzvp) = -5907.44944721 a.u.			
Imaginary frequency: -108.6202			
C	2.73999600	-0.88045600	0.20203200
C	2.91034500	-0.29855200	1.59841900
C	4.04534700	0.67953800	1.40794600
C	4.37893500	0.82156900	0.12436400
H	3.10498900	-1.04819700	2.37295300
H	4.47184100	1.23028200	2.23775000

H	5.12730200	1.49987800	-0.26851500
C	3.59085100	-0.10491200	-0.76576800
C	1.51405100	0.40461600	1.83304400
O	1.07004400	0.53626200	0.47193600
Fe	0.37372900	1.70986400	-0.72099500
Cl	1.27794700	3.70902100	-0.51576500
Cl	0.75640100	0.87478100	-2.75027500
C	1.62335800	1.76620700	2.50794600
H	0.62466400	2.20899900	2.57857100
H	2.02166600	1.66075700	3.52360300
H	2.25768900	2.44611900	1.93754200
C	0.52232700	-0.48558900	2.57748300
H	0.89979700	-0.72127100	3.57937400
H	-0.43069100	0.03860000	2.68163100
H	0.31536400	-1.40857500	2.03578500
C	2.10885200	-2.10430800	-0.13992700
C	1.77990800	-3.07100700	0.84455900
C	1.80210500	-2.37446500	-1.50016400
C	1.16798600	-4.25809000	0.48000600
H	2.03823900	-2.89419700	1.88132300
C	1.16707500	-3.55323700	-1.85048800
H	2.00592800	-1.62426100	-2.25448600
C	0.85156200	-4.49413200	-0.86357300
H	0.92680000	-4.99935300	1.23434800
H	0.89835600	-3.73674600	-2.88497400
H	0.35214600	-5.41717700	-1.14201500
H	2.97440900	0.40760500	-1.51885500
H	4.22831900	-0.80015000	-1.33100200
Fe	-2.87458400	-0.15627300	0.19797300
Cl	-1.93645100	2.01587600	-0.26449700
Cl	-1.39170700	-1.64896800	-0.47122800
Cl	-3.18062700	-0.21484200	2.37560300
Cl	-4.73562700	-0.25403600	-0.93708700
2Fe.M3Ph-INT2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.207258 a.u.			
E (UωB97X-D/def2-tzvp) = -5907.45217409 a.u.			
C	2.87617000	-0.84732700	0.16310400
C	2.92880200	-0.19334300	1.50775500
C	3.91862200	0.92732300	1.30448100
C	4.23120100	1.07862700	0.01618700
H	3.18204300	-0.87963200	2.32317700
H	4.25740000	1.55454400	2.11915900
H	4.86630500	1.84791500	-0.40592900
C	3.56747900	0.02521400	-0.82901600
C	1.42572500	0.35630400	1.81911100
O	0.83813100	0.61276000	0.57219700
Fe	0.28602000	1.76946200	-0.67705000
Cl	1.13711600	3.77992000	-0.36447800
Cl	0.81924600	0.97101500	-2.71316100
C	1.49774200	1.63362600	2.65669000
H	0.47460700	1.95292200	2.87849900
H	2.01851000	1.45737000	3.60444600
H	1.99156800	2.43712800	2.10791400
C	0.59421900	-0.70860500	2.53304000
H	1.07717700	-1.02188000	3.46574200
H	-0.38502800	-0.28552100	2.76903700

H	0.41071900	-1.57458900	1.89682800
C	2.28198700	-2.08395200	-0.16195600
C	2.02432800	-3.06907900	0.83096800
C	1.90618500	-2.34758700	-1.50991400
C	1.41363300	-4.26109700	0.48801900
H	2.34518700	-2.89696900	1.85104800
C	1.26795000	-3.53075700	-1.83413400
H	2.04416300	-1.58271500	-2.26460000
C	1.02357400	-4.48553200	-0.83956400
H	1.22848600	-5.01614500	1.24438500
H	0.93614200	-3.70623600	-2.85136500
H	0.52059200	-5.41216200	-1.09898200
H	2.83560400	0.43960900	-1.54856100
H	4.26402300	-0.56511900	-1.44140700
Fe	-2.84189900	-0.22930500	0.17341500
Cl	-2.08556800	1.93665300	-0.53549800
Cl	-1.36763400	-1.75106800	-0.47084200
Cl	-3.02920100	-0.11085300	2.36548500
Cl	-4.77192200	-0.51140700	-0.81098200
2Fe.M3Ph-TS3			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.206177 a.u.			
E (UωB97X-D/def2-tzvp) = -5907.44629107 a.u.			
Imaginary frequency: -295.2419			
C	-3.10536600	0.32449100	0.20259000
C	-2.98272200	-0.26329400	1.51561200
C	-3.52896800	-1.64601800	1.39307400
C	-3.74054000	-1.95016400	0.10647000
H	-3.23093300	0.33736200	2.38884800
H	-3.64661600	-2.31259700	2.23757900
H	-4.05607100	-2.90719100	-0.28921200
C	-3.46027600	-0.75760500	-0.76441900
C	-1.16787000	-0.35491900	1.74853100
O	-0.58872300	-0.58382400	0.54890000
Fe	0.05728800	-1.74922100	-0.67705800
Cl	-0.51754400	-3.82604400	-0.21849400
Cl	-0.58765000	-1.14845900	-2.73495700
C	-0.96265900	-1.50332600	2.72801000
H	0.10519100	-1.51616500	2.97694300
H	-1.53365100	-1.36036000	3.65031500
H	-1.21784400	-2.45964600	2.26943600
C	-0.75300000	0.99289400	2.31126000
H	-1.29172100	1.22280300	3.23573900
H	0.31691400	0.93459800	2.53160300
H	-0.88131300	1.79634700	1.58725100
C	-2.83911300	1.67113700	-0.17365400
C	-2.99138900	2.73681600	0.74911300
C	-2.35363500	1.95052400	-1.47654700
C	-2.67254300	4.03293700	0.37882300
H	-3.38797100	2.53426600	1.73802300
C	-2.00185900	3.24576100	-1.82361600
H	-2.17668000	1.13814400	-2.17175500
C	-2.16539400	4.28555400	-0.90255800
H	-2.80447800	4.84796300	1.08280100
H	-1.58109100	3.44542500	-2.80302000
H	-1.89090000	5.29855800	-1.18077500
H	-2.65084200	-0.93105000	-1.49375200

H	-4.32281100	-0.44414000	-1.37180900
Fe	2.82182800	0.62164300	0.16743800
Cl	2.42556400	-1.61540200	-0.62822800
Cl	1.22499800	1.93264200	-0.61520100
Cl	2.81247800	0.42311500	2.36993000
Cl	4.78660100	1.16206400	-0.61337200
2Fe.M3Ph-P			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.201711 a.u.			
E (UωB97X-D/def2-tzvp) = -5907.47162123 a.u.			
C	-3.43173900	0.25521400	0.09117900
C	-3.72784500	-0.30249900	1.33715200
C	-3.97828600	-1.68527600	1.20708400
C	-3.84918000	-2.05558600	-0.12907800
H	-3.70777700	0.22899200	2.28069000
H	-4.19447900	-2.36187800	2.02485000
H	-4.08370200	-3.02345900	-0.54816700
C	-3.59988800	-0.82989200	-0.94668200
C	-0.24224100	-0.28028400	2.22895800
O	-0.45071900	-0.11833200	1.01932700
Fe	-0.06678900	-1.12613000	-0.73207000
Cl	-1.35719500	-3.02726900	-0.00487000
Cl	-0.66557600	-0.93863800	-2.89376500
C	0.32442400	-1.55487900	2.77068300
H	1.31775400	-1.71286100	2.33880500
H	0.39757400	-1.54305600	3.85943800
H	-0.30105400	-2.38720900	2.42778900
C	-0.57649300	0.83705500	3.16926400
H	-1.21632900	0.47374000	3.98248100
H	0.35938600	1.18447200	3.62453700
H	-1.04908300	1.66122900	2.63320900
C	-2.95669400	1.58543200	-0.17193300
C	-3.02125500	2.59452900	0.82161600
C	-2.34107700	1.89204100	-1.40796800
C	-2.47394900	3.84594000	0.59225900
H	-3.51791200	2.39038200	1.76480200
C	-1.78069800	3.14471400	-1.62376100
H	-2.23933400	1.12883200	-2.17030500
C	-1.84165700	4.12273000	-0.62878900
H	-2.53192300	4.61176400	1.35960200
H	-1.27514600	3.34870800	-2.56148800
H	-1.39553400	5.09793800	-0.79781300
H	-2.75509600	-0.94205500	-1.63687800
H	-4.47245400	-0.61446100	-1.58378300
Fe	2.97756600	0.29090000	-0.00466700
Cl	2.23298500	-1.92464100	-0.23456000
Cl	1.29706400	1.38425600	-1.01635100
Cl	2.96262800	0.74918200	2.16718200
Cl	4.91657300	0.56335100	-0.95040800
2Fe.M4-2FeCl₃/S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.125201 a.u.			
E (UωB97X-D/def2-tzvp) = -5676.39071488 a.u.			
C	-1.05560600	0.93626000	2.03755100
C	-3.20493200	-0.67080000	-0.33390000
C	-2.37206000	-1.50574400	0.62827300
C	-2.66282700	-0.94658000	1.97727100
H	-2.69568300	0.20696300	-0.72134100

H	-2.65337700	-2.56071900	0.59519700
H	-3.47597800	-1.42456700	2.52294500
C	-2.07331400	0.12085500	2.59851600
C	-4.47722200	-0.90602900	-0.69622500
O	-0.66835700	0.85219000	0.83848100
C	-5.30720100	-2.06001400	-0.19978300
H	-4.76595600	-2.72423400	0.47857000
H	-6.19771700	-1.69191400	0.32705300
H	-5.67194100	-2.66104400	-1.04277200
C	-5.16582400	-0.00088200	-1.68466000
H	-6.08051800	0.42654600	-1.25152800
H	-4.51918800	0.82033600	-2.00618300
H	-5.47483900	-0.56341300	-2.57566500
H	-1.31910600	-1.41684400	0.36972400
H	-2.39268000	0.39525200	3.59930200
Fe	0.57865600	1.94640300	-0.17048000
Cl	0.77252000	3.73316200	1.08152200
Cl	-0.26606900	2.33038600	-2.12850000
H	-0.60554700	1.71352100	2.66649700
Fe	1.96042600	-1.43692300	-0.14243400
Cl	2.66955600	0.89790400	-0.11335600
Cl	1.14747900	-1.81579400	1.87088300
Cl	3.71395800	-2.60978600	-0.65349500
Cl	0.38003600	-1.38212300	-1.67447400
2Fe.M4-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.128085 a.u.			
E (UωB97X-D/def2-tzvp) = -5676.39165130 a.u.			
C	-0.30046400	-1.77819300	-0.46769700
C	-3.30417200	-2.32212900	-0.33442600
C	-2.83927800	-2.80930400	1.01244200
C	-1.41263600	-3.24962500	1.14925900
H	-3.16046100	-3.03717000	-1.14511600
H	-3.46519700	-3.65453300	1.33489500
H	-1.24668700	-3.98829200	1.93310800
C	-0.29312700	-2.81583900	0.51232500
C	-3.91025700	-1.15774700	-0.62047700
O	0.74529800	-1.23608600	-0.91307100
Fe	2.42822300	-0.58336100	-0.24379700
Cl	2.81638300	-1.38716100	1.74079000
Cl	3.98119000	-1.01164900	-1.69502800
C	-4.19253600	-0.05900400	0.36858500
H	-3.72180000	0.87144400	0.03058800
H	-5.27238000	0.13086500	0.42343600
H	-3.82873500	-0.26383800	1.37689800
C	-4.36652900	-0.86476600	-2.02722800
H	-5.44860100	-0.68035700	-2.05160000
H	-3.88034600	0.04280900	-2.40497200
H	-4.14385600	-1.68817300	-2.71253800
H	-2.98425700	-2.03992200	1.78586400
H	0.67887300	-3.19158100	0.81833600
Fe	-0.35408000	1.89258000	0.19051800
Cl	2.04218500	1.74174000	-0.15346200
Cl	-1.31901500	1.34665700	-1.71236300
Cl	-0.74760400	3.93472500	0.81482900
Cl	-0.79996200	0.38193200	1.74777700
H	-1.24669200	-1.41875900	-0.87901300

2Fe.M4-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.129180 a.u.			
E (UωB97X-D/def2-tzvp) = -5676.38302494 a.u.			
Imaginary frequency: -113.9142			
C	-1.65017000	0.93201500	-1.12434900
C	-2.50324800	2.35686900	-0.35740600
C	-3.90369900	1.78917500	-0.14267000
C	-4.04640500	0.72462200	-1.20117800
H	-2.46912100	3.03820100	-1.20861000
H	-4.64638500	2.58862200	-0.25120000
H	-5.01434100	0.31841000	-1.47632500
C	-2.88999700	0.32505500	-1.72507200
C	-1.59570700	2.69824500	0.66880700
O	-1.00202500	0.14622500	-0.26000300
Fe	-0.83565600	-1.63751900	0.19853600
Cl	-1.25766900	-1.82733600	2.34272900
Cl	-1.99130300	-2.99200800	-1.07241900
C	-1.61282300	2.01120800	1.96553100
H	-1.16409600	1.01976300	1.74174200
H	-0.97840500	2.48634400	2.71456400
H	-2.61369800	1.81549200	2.35450200
C	-0.43961600	3.57429400	0.36932000
H	-0.40712800	4.39552600	1.09817200
H	0.48388000	2.99745600	0.52947300
H	-0.45121200	3.97775500	-0.64407400
H	-4.04253200	1.35827900	0.85545400
H	-2.76207000	-0.47127900	-2.45153700
Fe	2.36953300	0.20230000	-0.19058600
Cl	1.46636000	-2.02004200	-0.28497800
Cl	1.65946200	1.46813000	-1.86834700
Cl	4.52200100	-0.10967400	-0.31515500
Cl	1.77767400	1.05256500	1.76823000
H	-0.95045700	1.43461200	-1.79776800
2Fe.M4-INT0			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.128807 a.u.			
E (UωB97X-D/def2-tzvp) = -5676.38424849 a.u.			
C	-1.63462900	0.96167400	-1.13119400
C	-2.42946800	2.35316200	-0.37977600
C	-3.84137600	1.81709100	-0.12785500
C	-4.02226100	0.75955100	-1.18808900
H	-2.41544400	3.04576100	-1.22329100
H	-4.56973200	2.63192500	-0.21368700
H	-4.99996600	0.36464300	-1.44401800
C	-2.87728400	0.35310700	-1.73169000
C	-1.51718800	2.72545600	0.64454600
O	-0.99350100	0.16107800	-0.25793100
Fe	-0.87794300	-1.62006100	0.20268800
Cl	-1.35660800	-1.77831700	2.34137500
Cl	-2.02563500	-2.96911300	-1.08214700
C	-1.52674800	2.05929600	1.94706100
H	-1.07985600	1.06607000	1.71533100
H	-0.88408500	2.53521200	2.68800000
H	-2.52343400	1.85736300	2.34274500
C	-0.36949100	3.60074400	0.32371300
H	-0.32183000	4.42402600	1.04924200
H	0.55404500	3.01977600	0.47649900

H	-0.39230200	3.99635500	-0.69230900
H	-3.96280100	1.38204300	0.87078100
H	-2.76029700	-0.44000100	-2.46281400
Fe	2.36523600	0.16037700	-0.18621500
Cl	1.43130400	-2.04665600	-0.22562000
Cl	1.68357000	1.42073000	-1.88071500
Cl	4.51212500	-0.19055000	-0.31147600
Cl	1.80616000	1.06852600	1.75912100
H	-0.92078800	1.42097400	-1.82077100
2Fe.M4-TS2 G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.131309 a.u. E (UωB97X-D/def2-tzvp) = -5676.38337390 a.u. Imaginary frequency: -102.8282			
C	-2.83917100	-2.56923500	-1.61334000
C	-2.15249000	-1.44060900	-1.78780700
C	-2.40934200	-0.42946300	-0.69907900
C	-3.17047900	-1.30356400	0.40387500
H	-2.84130200	-3.41269800	-2.29574600
H	-1.49536000	-1.19727100	-2.61447400
H	-3.05997000	0.38328200	-1.04857500
H	-3.96240800	-0.70768600	0.86487500
C	-3.68631300	-2.54482000	-0.36045600
C	-2.08821500	-1.52139900	1.39653100
O	-1.24156400	0.10326900	-0.12347700
Fe	-0.57762500	1.80396500	-0.15565400
Cl	-1.78999800	2.90814200	-1.62487500
Cl	-0.62868700	2.67891300	1.86529200
C	-1.15056700	-2.63292700	1.28765600
H	-0.40554400	-2.30920700	0.52737700
H	-0.59486200	-2.81603700	2.20828100
H	-1.59691500	-3.54101700	0.87761800
C	-1.96299100	-0.59813900	2.52950500
H	-2.50440600	0.33774400	2.39437900
H	-2.38688800	-1.13794700	3.39699100
H	-0.90949600	-0.40979000	2.76374800
Fe	2.27641100	-0.53423000	-0.11318400
Cl	1.65641600	1.59257200	-0.99051500
Cl	1.21579000	-2.12392300	-1.25075500
Cl	4.43597100	-0.66598800	-0.33476000
Cl	1.61957300	-0.56100300	2.00237800
H	-3.62689600	-3.46890400	0.22690400
H	-4.74855600	-2.40689700	-0.60009000
2Fe.M4-INT G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.133645 a.u. E (UωB97X-D/def2-tzvp) = -5676.40469671 a.u.			
C	-1.27581600	-3.15093100	-1.27659900
C	-1.42172200	-1.91557600	-1.77048500
C	-2.41706100	-1.15048100	-0.97593500
C	-2.86990500	-2.08073000	0.16580800
H	-0.59730200	-3.89680100	-1.67697900
H	-0.89027900	-1.49416300	-2.61551200
H	-3.14650700	-0.55688000	-1.52817000
H	-3.94903300	-2.18479200	0.28714100
C	-2.15779300	-3.42776900	-0.08295500
C	-2.26076600	-1.07612100	1.18794900
O	-1.76577100	-0.22507800	0.02660800

Fe	-1.00687400	1.51582700	-0.31737000
Cl	-2.34828900	2.31806700	-1.84697100
Cl	-0.92491700	2.67003700	1.51169000
C	-1.08155100	-1.50402500	2.02756100
H	-0.31080800	-1.99195400	1.42823200
H	-0.63190300	-0.63360600	2.51286000
H	-1.42150700	-2.19439000	2.80753800
C	-3.29550400	-0.27662100	1.95449400
H	-4.09349200	0.07541200	1.29324100
H	-3.73993100	-0.91393300	2.72707800
H	-2.83395800	0.58753600	2.44061000
Fe	2.45944500	-0.21939700	0.06363900
Cl	1.00163500	1.08013000	-1.42644700
Cl	1.91665600	-2.33106000	-0.23614100
Cl	4.46744200	0.27639000	-0.60807800
Cl	1.95299700	0.50319700	2.06784200
H	-1.57596300	-3.77304400	0.77872000
H	-2.88322900	-4.22136100	-0.30185300
2Fe.M4-TS3 G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.133067 a.u. E (UωB97X-D/def2-tzvp) = -5676.39148489 a.u. Imaginary frequency: -98.2305			
C	-0.71899900	-3.39696200	-0.98477600
C	-1.28468700	-2.43094100	-1.78610300
C	-2.23557900	-1.73498500	-1.03452300
C	-2.35603100	-2.27786700	0.36335800
H	0.02177900	-4.11724300	-1.31479400
H	-1.01680000	-2.21485200	-2.81227200
H	-2.87897600	-0.96014600	-1.43861400
H	-3.34976300	-2.70053500	0.55597800
C	-1.26709800	-3.37742200	0.39834200
C	-2.10906000	-0.98563400	1.19890400
O	-1.26007100	-0.27686500	0.27172500
Fe	-1.05509400	1.42634300	-0.35343500
Cl	-2.57521200	1.63393000	-1.97527700
Cl	-1.21660900	2.98008700	1.16945600
C	-1.37934600	-1.17551000	2.52255100
H	-0.36147000	-1.54021800	2.37114300
H	-1.30342700	-0.21240000	3.03421800
H	-1.92672000	-1.87165900	3.16858400
C	-3.41949000	-0.21912400	1.40267400
H	-3.95171300	-0.06422600	0.45887600
H	-4.07510000	-0.76214000	2.09208000
H	-3.20242100	0.76364900	1.83104900
Fe	2.32840200	-0.03093200	0.04975300
Cl	1.04626100	1.29305400	-1.48340200
Cl	1.92848900	-2.19445600	-0.35524200
Cl	4.40513700	0.46340100	-0.38169800
Cl	1.69084400	0.57183900	2.05611500
H	-0.45235200	-3.14496000	1.09236900
H	-1.64823100	-4.36388200	0.69157300
2Fe.M4-INT2 G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.133339 a.u. E (UωB97X-D/def2-tzvp) = -5676.40014566 a.u.			
C	-0.30326200	-3.09512100	-0.98373000
C	-1.25709600	-2.59231500	-1.86062200

C	-2.29679700	-2.06054000	-1.11611000
C	-2.08632600	-2.23160000	0.34458700
H	0.59255700	-3.62680000	-1.28174300
H	-1.18320000	-2.58095600	-2.93979000
H	-3.18989200	-1.62274400	-1.54419900
H	-2.86044100	-2.93036800	0.70090700
C	-0.69292600	-2.88574100	0.42499700
C	-2.26259900	-0.93168000	1.21891900
O	-1.25943500	-0.03136500	0.84480300
Fe	-1.11619500	1.41433400	-0.21185000
Cl	-1.75476900	0.71764900	-2.25447400
Cl	-2.31918500	3.12229600	0.47087100
C	-2.05158300	-1.29014700	2.69675200
H	-1.04535000	-1.67973700	2.86826600
H	-2.16279800	-0.38194800	3.29535300
H	-2.78963500	-2.02628700	3.03436700
C	-3.65528400	-0.32169600	1.00805500
H	-3.79936200	-0.00145400	-0.02790800
H	-4.44293300	-1.03489100	1.27572800
H	-3.75608900	0.56342800	1.64112500
Fe	2.40266100	0.07476200	0.13571500
Cl	1.18273400	2.09314400	-0.09886800
Cl	1.78334700	-1.17423500	-1.60774200
Cl	4.50633900	0.61756100	0.04798000
Cl	1.86741700	-0.94363500	2.02469000
H	0.04578100	-2.22424000	0.90540600
H	-0.66605900	-3.82377600	0.99469900
2Fe.M4-TS4			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.130594 a.u.			
E (UωB97X-D/def2-tzvp) = -5676.39009633 a.u.			
Imaginary frequency: -366.7604			
C	1.13886400	2.13778000	-1.43286000
C	2.38113500	1.68275200	-1.81302000
C	3.28306500	1.92884400	-0.75285100
C	2.59709200	2.41811600	0.38001000
H	0.21367200	2.02469200	-1.98504700
H	2.62113200	1.17084400	-2.73487500
H	4.34118900	1.69079800	-0.78024300
H	3.12199500	2.98023600	1.14666400
C	1.22170700	2.83616300	-0.12327000
C	2.15562400	0.76891600	1.35235800
O	1.22379500	0.22881700	0.59776000
Fe	0.93137600	-1.36489800	-0.31474600
Cl	2.53873100	-1.69999100	-1.79747400
Cl	0.83711100	-3.01232300	1.11098900
C	1.62363400	1.33781300	2.66032900
H	0.72377500	1.93405000	2.50902700
H	1.34462500	0.48212000	3.28686200
H	2.38369400	1.92370100	3.18359000
C	3.45098100	-0.01680300	1.48880000
H	3.77054900	-0.42570700	0.52845000
H	4.24911600	0.59532300	1.91839900
H	3.25918500	-0.85735700	2.16731400
Fe	-2.48355100	0.23017900	0.03159300
Cl	-1.06233700	-0.97999400	-1.52696400
Cl	-2.23434600	2.36303400	-0.51516300

Cl	-4.49385700	-0.51537900	-0.33483000
Cl	-1.71284500	-0.21180900	2.03768900
H	0.36570500	2.62742800	0.51805000
H	1.22717500	3.92441200	-0.29749200
2Fe.M4-P			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.127153 a.u.			
E (UωB97X-D/def2-tzvp) = -5676.39814108 a.u.			
C	0.49870400	2.31298400	-0.30400400
C	1.30046100	2.10456400	-1.38827100
C	2.68406700	2.42625900	-1.03566500
C	2.72424100	2.85301000	0.24684800
H	-0.58058600	2.26893300	-0.28461700
H	0.96766400	1.80315500	-2.37290500
H	3.52220100	2.32450900	-1.71478600
H	3.60519000	3.16806400	0.79451400
C	1.33660500	2.83443700	0.83019900
C	3.23042600	-0.64026200	1.27237300
O	2.16475000	-0.12323500	0.90659300
Fe	0.74335500	-0.63735400	-0.46475900
Cl	2.10346900	-0.83900500	-2.23268600
Cl	0.36936500	-2.75173100	0.14058300
C	4.03614000	0.05324600	2.32805400
H	3.54094400	0.96420100	2.66449500
H	4.19213100	-0.62897000	3.17290100
H	5.02947000	0.28895600	1.92554500
C	3.73135900	-1.92378100	0.69496200
H	3.84039300	-1.80302600	-0.38972500
H	4.67626000	-2.23675900	1.14182000
H	2.96501000	-2.69614500	0.83204400
Fe	-2.58602200	0.07900300	0.22197900
Cl	-1.32525800	-0.22578800	-1.74638400
Cl	-3.41657500	2.09876000	0.14124400
Cl	-4.01652100	-1.51476900	0.53500000
Cl	-0.81306500	0.04867100	1.66657700
H	1.25605900	2.21164300	1.72911100
H	1.00054400	3.84136100	1.12048200
2Fe.M4Ph-2FeCl₃/S (RS)			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.201103 a.u.			
E (UωB97X-D/def2-tzvp) = -5907.45948899 a.u.			
C	-1.89365300	-0.22665800	-0.72302200
C	-3.79976900	0.10322700	1.52946900
C	-4.44984700	-1.15055700	1.01235700
C	-3.86754600	-1.75089500	-0.24038600
H	-4.25217700	1.03752000	1.20653800
H	-5.51860400	-0.96818400	0.82721300
H	-4.35692700	-2.66702000	-0.57089600
C	-2.78635800	-1.37699500	-0.94027400
C	-2.71971300	0.17080300	2.32700600
O	-0.66363200	-0.46094000	-0.51120900
Fe	0.58626100	-1.91545500	-0.55825400
Cl	0.64283200	-3.13365200	1.23552200
Cl	0.02101300	-3.11688200	-2.30958700
C	-1.96130500	-1.02907400	2.82292600
H	-0.90797000	-0.95840800	2.53133600
H	-1.97670100	-1.06739600	3.92015400
H	-2.34745200	-1.97622900	2.43969500

C	-2.16964000	1.50519100	2.75246200
H	-2.10911200	1.57200300	3.84662600
H	-1.14697900	1.63552900	2.37704800
H	-2.78144800	2.33481100	2.38650300
H	-4.43277900	-1.94628900	1.77046000
H	-2.41824900	-2.03990600	-1.72269700
C	-2.29201700	1.15930900	-0.91375100
C	-3.55212400	1.48375500	-1.45357000
C	-1.38048700	2.18145200	-0.58514200
C	-3.89772400	2.81489700	-1.64321800
H	-4.23932400	0.68998300	-1.72382500
C	-1.73737700	3.51013900	-0.77311800
H	-0.41088100	1.92281800	-0.18105800
C	-2.99406000	3.82771800	-1.29789500
H	-4.86513300	3.06908000	-2.06463300
H	-1.03293100	4.29464900	-0.51724000
H	-3.26933800	4.86761300	-1.44766000
Fe	2.82050800	0.99253300	0.19601100
Cl	2.67624000	-1.01390000	-1.15860300
Cl	2.11909600	2.64763400	-1.06404800
Cl	4.89338700	1.15955800	0.82673000
Cl	1.40088900	0.54836300	1.83394800
2Fe.M4Ph-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.206338 a.u.			
E (UωB97X-D/def2-tzvp) = -5907.44452873 a.u.			
Imaginary frequency: -47.3310			
C	-2.20757900	-0.12506000	0.36233000
C	-2.47730300	-0.13675600	2.05020800
C	-3.67332000	-1.09850200	2.25684500
C	-3.93300700	-1.71045300	0.90710400
H	-2.69887000	0.88867100	2.33830800
H	-4.53828900	-0.52557300	2.61338500
H	-4.68612700	-2.47950000	0.76599500
C	-3.18460800	-1.19911500	-0.06536500
C	-1.20281900	-0.57195700	2.58328100
O	-0.88499800	-0.46377700	0.10429600
Fe	-0.04333300	-1.32293600	-1.27061800
Cl	0.54322900	-3.33986600	-0.60835400
Cl	-1.27895000	-1.33755500	-3.09149400
C	-0.79115000	-1.98277500	2.55409000
H	0.20314800	-2.05189700	2.09050900
H	-0.65119500	-2.31742600	3.59453800
H	-1.48692200	-2.63958000	2.03493700
C	-0.25182200	0.43168900	3.06198100
H	0.58713600	0.01591000	3.62103000
H	0.18118000	0.88371900	2.14420600
H	-0.74015600	1.25446600	3.59229100
H	-3.47329700	-1.85663100	3.02382900
H	-3.21991600	-1.46661800	-1.11600300
C	-2.53529000	1.25241600	-0.15954900
C	-3.86879400	1.68630100	-0.21742200
C	-1.51006700	2.11413100	-0.56845000
C	-4.17038700	2.96184500	-0.68488700
H	-4.66718300	1.01635200	0.08793900
C	-1.81649700	3.39139000	-1.03532000
H	-0.47997600	1.78823400	-0.52288400

C	-3.14361000	3.81837500	-1.09472700
H	-5.20530100	3.28685700	-0.73751500
H	-1.01301500	4.04911400	-1.35216100
H	-3.38024700	4.81288800	-1.46137200
Fe	2.87162300	0.65802600	0.22272900
Cl	1.86039300	0.02814600	-1.83723600
Cl	1.75508200	2.43093200	0.96577100
Cl	4.95367600	1.10343600	-0.21730900
Cl	2.60251100	-1.04099200	1.61174000
2Fe.M4Ph-INT			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.209866 a.u.			
E (UωB97X-D/def2-tzvp) = -5907.46646418 a.u.			
C	-2.57229200	0.31042600	0.54169600
C	-2.65184200	-0.20685100	2.00499700
C	-4.11616300	-0.60642900	2.24610400
C	-4.69062700	-0.64289300	0.84996700
H	-2.25579700	0.48792900	2.74607400
H	-4.63104800	0.13705700	2.86802800
H	-5.68849000	-1.01708900	0.64097000
C	-3.85263900	-0.16442600	-0.07590800
C	-1.62512300	-1.32302300	1.65889700
O	-1.43757700	-0.69406000	0.28744400
Fe	-0.41798400	-0.96077200	-1.33301100
Cl	0.21159100	-3.03613200	-1.40132600
Cl	-1.75678700	-0.38344500	-2.95929900
C	-2.13512400	-2.74014600	1.48412400
H	-1.36875700	-3.34622900	0.99343700
H	-2.33834400	-3.17999700	2.46621100
H	-3.04392500	-2.77608900	0.88082500
C	-0.32319200	-1.26827100	2.42654500
H	0.43853100	-1.89703600	1.95783700
H	0.07105000	-0.25315500	2.50321700
H	-0.49807700	-1.64414700	3.44132500
H	-4.21774500	-1.56735300	2.76376400
H	-4.03944300	-0.09927600	-1.14026800
C	-2.10207900	1.68938000	0.20028900
C	-2.86549600	2.53236700	-0.61689400
C	-0.87423200	2.14799300	0.69596300
C	-2.40279400	3.80830700	-0.93641200
H	-3.82155900	2.19692400	-1.00337200
C	-0.40766200	3.41714200	0.36978500
H	-0.26072300	1.50907300	1.31810300
C	-1.17232700	4.25097600	-0.44886400
H	-3.00118500	4.45211300	-1.57390800
H	0.55622300	3.74133300	0.74883600
H	-0.80880500	5.24087200	-0.70826900
Fe	3.00909400	0.18188400	0.35940600
Cl	1.37353900	0.53759300	-1.42050300
Cl	2.34232200	1.42634300	2.05787000
Cl	4.88124000	0.86195000	-0.51520500
Cl	2.93570600	-1.95976100	0.80961800
2Fe.M4Ph-TS2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.209146 a.u.			
E (UωB97X-D/def2-tzvp) = -5907.45813403 a.u.			
Imaginary frequency: -251.3899			
C	2.59616700	0.91836700	-0.50324700

C	2.65114600	0.38670000	-1.94290500
C	4.15481000	0.15293200	-2.20150200
C	4.72701500	0.11452600	-0.81147600
H	2.20168300	1.05713000	-2.67575700
H	4.59265500	0.98389500	-2.77133300
H	5.75416000	-0.16960300	-0.60310500
C	3.84621700	0.51863200	0.12690100
C	1.76970500	-0.89301600	-1.73233100
O	1.38852400	-0.61424000	-0.35245600
Fe	0.56219200	-1.23803000	1.16455300
Cl	0.04790800	-3.35085500	1.06737200
Cl	1.93605700	-0.75446300	2.83838600
C	2.49503200	-2.23320500	-1.76252000
H	1.81064600	-3.00422700	-1.39668200
H	2.79489700	-2.49640100	-2.78214400
H	3.37499800	-2.23279300	-1.11349600
C	0.53266500	-0.91113400	-2.61591200
H	-0.12591400	-1.73606500	-2.33138800
H	-0.03775300	0.01555900	-2.52460400
H	0.82659100	-1.04398400	-3.66359500
H	4.36358100	-0.75779500	-2.76972300
H	4.03963000	0.58828200	1.18777900
C	1.76064900	1.98832500	-0.00229200
C	1.92899600	2.46151300	1.31859800
C	0.72574700	2.52705800	-0.79311100
C	1.08746200	3.44198200	1.82366200
H	2.69513400	2.04031900	1.95621700
C	-0.11060000	3.51053600	-0.28403900
H	0.55309000	2.15405300	-1.79431800
C	0.06824800	3.96814800	1.02400400
H	1.21497100	3.78797400	2.84414600
H	-0.91974500	3.89371100	-0.89485400
H	-0.59643000	4.72716800	1.42540700
Fe	-2.84802100	0.02251000	-0.35181900
Cl	-1.26854600	0.26215700	1.46250100
Cl	-2.32782500	1.45559900	-1.96211600
Cl	-4.77221100	0.49308700	0.56290100
Cl	-2.65175800	-2.04658300	-1.04357000
2Fe.M4Ph-INT2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.209406 a.u.			
E (UωB97X-D/def2-tzvp) = -5907.47834784 a.u.			
C	2.93817600	-1.02182400	-0.83639300
C	1.91787700	-2.02553300	-0.41445500
C	2.71924800	-3.33543900	-0.26104400
C	4.14049400	-2.89794900	-0.33303400
H	1.09397200	-2.10975800	-1.12738600
H	2.49405300	-4.02928800	-1.08411000
H	4.98183100	-3.56420000	-0.16820000
C	4.24567100	-1.58056800	-0.65070600
C	1.18457300	-1.57538900	0.95268100
O	0.47637600	-0.42396100	0.63990000
Fe	-0.04768300	1.12990600	1.39311100
Cl	-0.79884200	0.82792200	3.43518400
Cl	1.57636600	2.64323900	1.31268600
C	2.19461900	-1.28910400	2.07199200
H	1.64288200	-1.06290500	2.98913600

H	2.84550300	-2.14754000	2.26895100
H	2.81277500	-0.42100400	1.82628300
C	0.18912300	-2.67044100	1.35883500
H	-0.41162100	-2.28918100	2.18824800
H	-0.48736300	-2.90689000	0.53462700
H	0.69662900	-3.58236200	1.68967900
H	2.50954700	-3.89055600	0.65832200
H	5.17613300	-1.04967400	-0.80428700
C	2.67477600	0.28346100	-1.33115500
C	3.70471300	1.26601300	-1.36413600
C	1.38042500	0.63432500	-1.79984200
C	3.43741600	2.54327100	-1.81347900
H	4.69298400	1.02929200	-0.98713900
C	1.12984100	1.91437300	-2.26914800
H	0.58954200	-0.10159700	-1.81281300
C	2.14883900	2.86883600	-2.26640500
H	4.21590200	3.29860700	-1.80247400
H	0.13494100	2.17160600	-2.61360200
H	1.94296200	3.87669400	-2.61407400
Fe	-2.72217500	-0.37014000	-0.72042200
Cl	-1.75409600	1.76198100	-0.18636800
Cl	-1.39471400	-1.60114900	-2.04195800
Cl	-4.52899500	0.18250300	-1.81933900
Cl	-3.14443400	-1.35965000	1.18141000
2Fe.M4Ph-TS3			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.206830 a.u.			
E (UωB97X-D/def2-tzvp) = -5907.45780265 a.u.			
C	-3.02663900	-1.02927200	0.83798800
C	-2.13915700	-2.10877400	0.63403000
C	-2.97676900	-3.33047200	0.30615800
C	-4.34899700	-2.76311300	0.11252900
H	-1.21417300	-2.20115600	1.19055500
H	-2.96318300	-4.03064600	1.15586600
H	-5.19816500	-3.34083300	-0.23530300
C	-4.35924900	-1.44578500	0.42128300
C	-1.07276200	-1.52315900	-1.09876300
O	-0.42493300	-0.47499000	-0.66996800
Fe	0.05276400	1.21129800	-1.28238800
Cl	0.78948300	0.94731700	-3.33001700
Cl	-1.54517000	2.71155600	-1.24288800
C	-2.14485700	-1.27750800	-2.13295100
H	-1.63822600	-1.14221000	-3.09811800
H	-2.83410600	-2.12030300	-2.22402500
H	-2.70341200	-0.36636000	-1.90943400
C	-0.21417100	-2.75725300	-1.26822500
H	0.47174000	-2.54479800	-2.09788000
H	0.39559600	-2.94218300	-0.38312700
H	-0.80410900	-3.64003700	-1.52098300
H	-2.63730300	-3.91226200	-0.55802000
H	-5.22708300	-0.80042600	0.38657500
C	-2.69329700	0.27989200	1.34944800
C	-3.64083200	1.32847900	1.33102900
C	-1.41023100	0.53889300	1.88283300
C	-3.31313200	2.58478000	1.81685000
H	-4.62880400	1.16379500	0.91638200
C	-1.08771500	1.80087800	2.36713000

H	-0.66912000	-0.24716700	1.92818900
C	-2.03504600	2.82496900	2.33425700
H	-4.04530100	3.38512800	1.78304100
H	-0.09376100	1.98284200	2.76054000
H	-1.77958100	3.81231000	2.70675300
Fe	2.75848500	-0.43176900	0.67172800
Cl	1.78053400	1.74567400	0.25606200
Cl	1.45254000	-1.67165200	1.98463700
Cl	4.62162300	0.06731400	1.68988900
Cl	3.05705500	-1.34484700	-1.29448800
2Fe.M4Ph-P			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.202101 a.u.			
E (UωB97X-D/def2-tzvp) = -5907.46946795 a.u.			
C	-3.22727400	-0.91350700	0.86498100
C	-2.64605600	-2.13072500	1.08467000
C	-3.53312700	-3.22103300	0.55082500
C	-4.66538200	-2.45888500	-0.08319300
H	-1.75477700	-2.31447400	1.67122600
H	-3.89234100	-3.86492700	1.36887300
H	-5.49219200	-2.92447000	-0.60638200
C	-4.47917300	-1.13845300	0.11475000
C	-0.83609200	-1.64650000	-1.17091900
O	-0.26675400	-0.63922300	-0.69460800
Fe	0.05774600	1.19740800	-1.22190400
Cl	0.80601500	0.91617200	-3.26404100
Cl	-1.58095800	2.61780000	-1.30453100
C	-1.92005700	-1.49369300	-2.18535700
H	-1.46809400	-1.65673100	-3.17455100
H	-2.70906200	-2.23651000	-2.04575400
H	-2.34640700	-0.48938200	-2.15571500
C	-0.24700100	-2.98584000	-0.87158100
H	0.57930700	-3.12114600	-1.58487200
H	0.19523700	-2.99900100	0.12571000
H	-0.96499200	-3.79499200	-1.00773600
H	-3.03247000	-3.90166100	-0.15313100
H	-5.13263700	-0.34773400	-0.23358900
C	-2.74756300	0.39745300	1.31355300
C	-3.59682000	1.51574800	1.30457100
C	-1.43236400	0.56266600	1.79306000
C	-3.15136600	2.75357500	1.76217100
H	-4.61784500	1.41909700	0.95132200
C	-0.98943700	1.80242800	2.25081500
H	-0.75340800	-0.28014700	1.82336800
C	-1.84657200	2.90295300	2.23646300
H	-3.82506200	3.60506900	1.74585100
H	0.02840500	1.90179300	2.61235900
H	-1.50001900	3.87032400	2.58685000
Fe	2.82467900	-0.45442400	0.64623900
Cl	1.84402400	1.74054200	0.20209500
Cl	1.54828400	-1.54377800	2.09365800
Cl	4.76326000	0.05614400	1.49451600
Cl	2.95978900	-1.47782100	-1.29161000
2Fe.M5-2FeCl₃/S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.153321 a.u.			
E (UωB97X-D/def2-tzvp) = -6257.79444408 a.u.			
C	-1.00151500	0.94977000	-0.18419600

C	-3.81048600	0.38965500	-0.12785600
C	-3.76549500	1.75443100	-0.62759700
C	-2.74724000	2.63036200	-0.46379700
H	-1.23276000	0.59899200	-1.19579300
H	-3.12475500	0.14756000	0.68213700
H	-4.63799400	2.12001700	-1.16381900
H	-2.87520700	3.64886600	-0.82048900
C	-1.42719500	2.28730800	0.19703000
C	-4.62484500	-0.60414100	-0.54549000
O	-0.40637300	0.16919100	0.60142100
C	-5.61868400	-0.47057400	-1.66588200
H	-5.36060100	-1.16245800	-2.47882500
H	-6.62259800	-0.75313500	-1.32359500
H	-5.66887100	0.53485300	-2.08860500
C	-4.55060500	-1.96691300	0.08680100
H	-4.25631200	-2.71916200	-0.65696900
H	-3.82802200	-2.00457500	0.90623800
H	-5.53276400	-2.27106900	0.47292400
Si	-1.47984000	2.53725800	2.10120200
H	-2.05901800	3.87528100	2.32641400
H	-2.36280100	1.49676300	2.66199900
H	-0.12985200	2.45754300	2.68511800
Si	-0.10474900	3.51925100	-0.53258000
H	-0.63431000	4.83999500	-0.13513300
H	1.21141400	3.26727000	0.06228500
H	-0.11396600	3.39510500	-1.99944100
Fe	-0.10779500	-1.74371900	0.34381900
Cl	-1.06824600	-2.23215700	-1.55104900
Cl	-1.04807900	-2.70415900	2.05373900
Fe	3.01642600	0.07844300	-0.26494800
Cl	2.18558000	-2.14495000	0.33307000
Cl	1.68369300	0.68996700	-1.93023800
Cl	5.09097300	-0.19396700	-0.83822700
Cl	2.70405900	1.28298800	1.53439700
2Fe.M5-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.153875 a.u.			
E (UωB97X-D/def2-tzvp) = -6257.78964499 a.u.			
C	1.28075200	-0.53252800	-0.33997000
C	2.02082600	-1.25404000	2.27148700
C	2.85717800	-2.20079400	1.50604700
C	3.00707700	-2.26427300	0.17442900
H	0.52361200	-1.00160800	0.29047500
H	1.13094100	-1.69254800	2.72427000
H	3.36629700	-2.96956800	2.08921100
H	3.65191000	-3.03678600	-0.23872100
C	2.38673700	-1.33881400	-0.85153700
C	2.26545500	0.05095400	2.50519900
O	1.13155100	0.66341300	-0.69704700
Fe	-0.21253400	2.03752100	-0.38293300
Cl	-1.14414200	2.74668200	-2.19793900
Cl	0.85911500	3.62239100	0.67356400
C	3.46995000	0.78326800	1.98385500
H	3.16724400	1.55150100	1.26042300
H	3.97693200	1.31042900	2.80181600
H	4.18646000	0.11446100	1.50232500
C	1.31723100	0.86830300	3.34135100

H	0.99260800	1.76542100	2.80241600
H	0.43031000	0.29893600	3.63166400
H	1.82117700	1.21807100	4.25251900
Si	1.53701400	-2.53580800	-2.14452000
H	2.64505500	-3.40146600	-2.59570500
H	0.50512100	-3.31877200	-1.44744800
H	0.99524000	-1.75850700	-3.26920500
Si	3.70000500	-0.30723100	-1.79680000
H	4.75658100	-1.26056200	-2.19227200
H	3.10418100	0.29593300	-3.00355200
H	4.26428900	0.73241800	-0.92125100
Fe	-2.46686700	-0.96791700	0.22745700
Cl	-1.69981900	1.12516700	1.20301700
Cl	-1.69213800	-0.82033300	-1.83547300
Cl	-4.62054400	-1.05153000	0.42907000
Cl	-1.34102700	-2.49498100	1.34923500
2Fe.M5-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.155478 a.u.			
E (UωB97X-D/def2-tzvp) = -6257.78037691 a.u.			
Imaginary frequency: -167.3573			
C	1.34477100	-0.83934000	0.34119300
C	1.96957100	-0.95496600	1.83350500
C	3.34315600	-1.51689400	1.59638400
C	3.50010700	-1.91747300	0.32872000
H	0.32237600	-1.20887600	0.38007200
H	1.30371600	-1.61711500	2.40279900
H	4.08435400	-1.60517600	2.38354800
H	4.39928100	-2.39015900	-0.05575300
C	2.28383300	-1.71286900	-0.53062400
C	1.86488700	0.41566100	2.34640100
O	1.34751300	0.51181700	-0.04019800
Fe	0.23265300	1.84325000	-0.58512000
Cl	-0.04409600	2.13458500	-2.72358800
Cl	1.01105000	3.67980700	0.44614900
C	2.96890700	1.36871800	2.22788200
H	2.59824100	2.20365900	1.60360600
H	3.17483200	1.82577700	3.20645500
H	3.87061400	0.93878300	1.79517600
C	0.62343000	0.85018400	3.00539500
H	0.43576500	1.91781100	2.86010600
H	-0.24005100	0.24431100	2.72087000
H	0.78601800	0.68817800	4.08673800
Si	1.51951900	-3.42801300	-0.89882100
H	2.63214600	-4.37922800	-1.10927200
H	0.73674500	-3.84285500	0.28500000
H	0.66451200	-3.39885600	-2.09837700
Si	2.71376900	-0.84057000	-2.17610000
H	3.53489700	-1.82004900	-2.92779200
H	1.49281700	-0.53880900	-2.93533400
H	3.52893100	0.36705200	-1.94078500
Fe	-2.55705500	-0.66056800	0.18164600
Cl	-1.87197200	1.59539500	0.57804600
Cl	-1.47425400	-1.18738700	-1.66106000
Cl	-4.72159200	-0.69952800	0.04474800
Cl	-1.74201000	-1.79503100	1.92221300
2Fe.M5-INT			

G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.161009 a.u. E (UωB97X-D/def2-tzvp) = -6257.79762719 a.u.			
C	1.38068800	-0.96001500	0.51520900
C	1.97918600	-0.84933300	1.93278300
C	3.39249700	-1.33005900	1.77314500
C	3.64142600	-1.70607000	0.51367500
H	0.37363300	-1.34998800	0.42452300
H	1.41450900	-1.33824000	2.73092300
H	4.10922700	-1.34594700	2.58668000
H	4.59293900	-2.08550900	0.15357900
C	2.42776600	-1.61307300	-0.39654100
C	1.75265000	0.68943000	1.89249100
O	1.27458400	0.54484800	0.43570100
Fe	0.11147000	1.79824100	-0.52237200
Cl	0.11215600	1.68350600	-2.67926700
Cl	0.73496500	3.79519200	0.12331200
C	2.97149200	1.58102500	1.91626100
H	2.69869500	2.60521100	1.65077000
H	3.38884700	1.58641200	2.92949600
H	3.73708200	1.21880300	1.22749800
C	0.61537500	1.17381400	2.76547200
H	0.34879800	2.20824000	2.53191100
H	-0.26646400	0.53769400	2.66035800
H	0.94405500	1.13582100	3.81032800
Si	1.87513200	-3.40538900	-0.79042000
H	3.08955100	-4.18392200	-1.11171300
H	1.23889100	-3.96030900	0.42339200
H	0.93532500	-3.45373800	-1.92520300
Si	2.86207500	-0.73367100	-2.02551600
H	4.02205500	-1.47228300	-2.57278900
H	1.74450000	-0.80281300	-2.97824800
H	3.26299600	0.66514500	-1.77429000
Fe	-2.61103000	-0.74545600	0.16606500
Cl	-2.06850700	1.61002900	0.36338800
Cl	-1.38242700	-1.35436100	-1.56105900
Cl	-4.75803500	-0.88415200	-0.09102100
Cl	-1.82227800	-1.65393400	2.01872500
2Fe.M5-TS2 G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.157184 a.u. E (UωB97X-D/def2-tzvp) = -6257.78067885 a.u. Imaginary frequency: -84.7280			
C	3.01404400	0.71500500	0.59508900
C	2.42560900	2.06301900	0.39343600
C	3.06740000	2.52598600	-0.88733300
C	3.89330800	1.58683800	-1.37088900
H	2.78004900	0.06270600	1.43444800
H	2.61861200	2.73782000	1.23893500
H	2.86024500	3.48841700	-1.33751400
H	4.47930000	1.63833700	-2.28100700
C	3.90555800	0.38496900	-0.45372700
C	0.85673300	1.76748900	0.34249600
O	0.78797800	0.43310400	-0.16836100
Fe	0.01636500	-1.12527000	0.38052400
Cl	1.29033200	-1.74585200	2.16040400
Cl	0.16492700	-2.71978600	-1.12667300
C	0.14531700	2.70916500	-0.62199800

H	-0.92804600	2.51126600	-0.59250100
H	0.31008900	3.75454900	-0.33668300
H	0.49785000	2.54844000	-1.64308700
C	0.27596000	1.85226900	1.75400400
H	-0.78222200	1.57942000	1.72789800
H	0.78729900	1.17218900	2.44225500
H	0.34898400	2.87508300	2.13820400
Si	5.64640400	0.16093000	0.40246400
H	6.60074700	0.16692100	-0.71816300
H	5.88137300	1.30740000	1.29867900
H	5.65502700	-1.11277200	1.14057900
Si	3.56158600	-1.34032400	-1.30095000
H	4.82990100	-1.69589500	-1.97106400
H	3.23339400	-2.29256100	-0.23652000
H	2.49464200	-1.08257300	-2.27202500
Fe	-3.37119800	0.25241200	-0.21284600
Cl	-2.07496900	0.12523500	-1.99133600
Cl	-5.33030400	-0.66753900	-0.42682300
Cl	-3.40616700	2.29414100	0.62388400
Cl	-2.12386800	-1.02421200	1.40920000
2Fe.M5-P			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.147622 a.u.			
E (UωB97X-D/def2-tzvp) = -6257.81547046 a.u.			
C	3.51302900	0.33393800	0.80809700
C	3.63472300	1.54460800	1.42798000
C	4.29071700	2.47516800	0.53294500
C	4.58682600	1.83510100	-0.63642200
H	3.08052900	-0.56950000	1.22062600
H	3.32002600	1.77418200	2.43998200
H	4.52444200	3.50712800	0.77070900
H	5.09031900	2.25544300	-1.49925800
C	4.14274300	0.41231400	-0.54392400
C	0.42152700	1.43605000	0.55289300
O	0.28557000	0.32620000	-0.01000600
Fe	-0.29641400	-1.46383600	0.52003100
Cl	0.91326700	-2.05050400	2.25173000
Cl	-0.20034100	-2.92112100	-1.07087700
C	0.68646100	2.62658200	-0.30045800
H	0.22496300	3.51806200	0.13134700
H	1.77540200	2.78039100	-0.32693200
H	0.32623300	2.45108000	-1.31477400
C	0.26945900	1.58192500	2.02876300
H	-0.80508600	1.71732500	2.21720100
H	0.60140600	0.68448000	2.55421100
H	0.79128300	2.46809000	2.39406300
Si	5.72489700	-0.65596200	-0.46498600
H	6.49466200	-0.49316400	-1.71701200
H	6.53096500	-0.21543600	0.69003400
H	5.35426500	-2.08017900	-0.31698600
Si	3.04773500	-0.16181700	-1.98335500
H	3.88150500	-0.28800000	-3.19839000
H	2.45691600	-1.47181100	-1.65056300
H	1.98224900	0.82274600	-2.23891700
Fe	-3.32119400	0.51637500	-0.34474300
Cl	-2.12777600	0.04521500	-2.12139600
Cl	-5.44668300	0.11849100	-0.49386900

Cl	-2.80040500	2.50477500	0.47104900
Cl	-2.45256800	-1.04166000	1.34129000
2Fe.M5Ph-2FeCl₃/S			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.227372 a.u.			
E (UωB97X-D/def2-tzvp) = -6488.85716213 a.u.			
C	-1.20716400	0.91280600	0.44769000
C	-3.81367800	-0.67391000	0.07969200
C	-4.28672700	0.53550300	0.72170200
C	-3.53328100	1.44567600	1.37973400
H	-2.80474000	-0.99256900	0.32265000
H	-5.35315700	0.74179800	0.67542200
H	-4.04552300	2.28203900	1.85028500
C	-2.03397300	1.36923500	1.60670900
C	-4.50954900	-1.46750100	-0.76533900
O	-0.37705400	-0.02420000	0.68706700
C	-5.91474000	-1.19625200	-1.22859400
H	-5.93891800	-1.10013800	-2.32242200
H	-6.56817800	-2.04209500	-0.97766200
H	-6.35162800	-0.29007100	-0.80437600
C	-3.88288300	-2.71288000	-1.33056200
H	-3.82320700	-2.65416600	-2.42594400
H	-2.87663600	-2.88371300	-0.94216400
H	-4.49693800	-3.59366100	-1.09841900
Fe	0.26843900	-1.72891200	0.09859700
Cl	0.00376800	-1.98252200	-2.04479600
Cl	-0.85112100	-3.25807600	1.19024100
C	-1.20149800	1.54492000	-0.86931100
C	-0.05952600	1.37829200	-1.68055200
C	-2.25510400	2.36377500	-1.33319600
C	0.02731600	1.99963400	-2.91870500
H	0.78112100	0.80460000	-1.32558800
C	-2.16725700	2.97092600	-2.57730900
H	-3.14531700	2.48861200	-0.73293300
C	-1.02907900	2.79080600	-3.37296000
H	0.92322600	1.86571000	-3.51522900
H	-2.98833600	3.58504500	-2.93338300
H	-0.96754000	3.27257100	-4.34443300
Si	-1.39428400	3.12703100	2.08495700
H	-2.07382700	3.47193100	3.35024500
H	0.06518700	3.10083800	2.26009300
H	-1.78630100	4.08328700	1.03147300
Si	-1.75981400	0.24033100	3.14244000
H	-0.35430800	0.26875600	3.59275100
H	-2.62287400	0.80005200	4.20214200
H	-2.19053900	-1.12654100	2.81223000
Fe	3.55494800	0.19451400	0.02298700
Cl	2.49397400	-1.87847100	0.77532100
Cl	3.28160700	0.17920600	-2.15636900
Cl	2.37411500	1.78757900	0.97628000
Cl	5.61454200	0.05207400	0.70226400
2Fe.M5Ph-RS			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.229849 a.u.			
E (UωB97X-D/def2-tzvp) = -6488.83561956 a.u.			
C	-1.34432200	1.24558100	-0.11535300
C	-2.80902300	-1.65402600	0.81560200
C	-3.84216500	-0.71184000	0.45408200

C	-3.76377400	0.63807800	0.39551300
H	-1.84938200	-1.24840200	1.10911200
H	-4.82386800	-1.12266400	0.23177000
H	-4.69085200	1.16759100	0.18716700
C	-2.56907000	1.54076100	0.65344700
C	-2.93717400	-3.00184100	0.84998400
O	-1.32470100	0.23927600	-0.87658900
Fe	0.05795600	-0.68768000	-1.87257700
Cl	-0.05589700	-2.82434600	-1.52144400
Cl	-0.23787200	-0.12581800	-3.96459300
C	-4.16868100	-3.76266900	0.44210100
H	-5.00177500	-3.12849400	0.13341800
H	-3.92951200	-4.43350400	-0.39389900
H	-4.51255900	-4.40273500	1.26533300
C	-1.79208600	-3.86005000	1.31214300
H	-2.09087000	-4.45784600	2.18480600
H	-1.50057600	-4.57158700	0.52891400
H	-0.91352200	-3.26804800	1.57790500
Si	-2.44210700	1.53979700	2.58463300
H	-3.75054400	2.05726800	3.02892500
H	-2.22882200	0.16611000	3.05543600
H	-1.39335200	2.44329800	3.09328200
Si	-3.05130000	3.35895900	0.19317800
H	-4.40873200	3.57555200	0.72911000
H	-2.10595300	4.32004900	0.78488200
H	-3.06381200	3.48157100	-1.27768000
C	-0.19837500	2.18785000	-0.19996300
C	0.57527100	2.58910000	0.89675300
C	0.12061000	2.65340300	-1.48986800
C	1.66772400	3.42919100	0.69811900
H	0.37681500	2.19535400	1.88307100
C	1.19289500	3.52119800	-1.67149400
H	-0.47518100	2.34041100	-2.34115800
C	1.97365300	3.90187800	-0.57940800
H	2.29408200	3.69313500	1.54310000
H	1.42804000	3.88035400	-2.66822900
H	2.82786000	4.55607300	-0.72386100
Fe	2.56374200	-0.70103800	0.97105000
Cl	2.24824600	-0.01375000	-1.32788700
Cl	0.54387300	-0.67885300	1.90421600
Cl	3.88743200	0.81884600	1.81742200
Cl	3.40955700	-2.70156700	0.90768200
2Fe.M5Ph-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.229296 a.u.			
E (UωB97X-D/def2-tzvp) = -6488.82976257 a.u.			
Imaginary frequency: -243.4330			
C	-2.16523500	0.21854800	0.44053600
C	-1.94196600	0.71828500	2.23247200
C	-2.95265600	-0.19542000	2.84316700
C	-3.88241100	-0.61956300	1.98238100
H	-2.26306900	1.75888300	2.20990800
H	-2.94203700	-0.42572200	3.90353400
H	-4.74315500	-1.21905800	2.26497400
C	-3.67412200	-0.16406900	0.56512500
C	-0.55898300	0.54478000	2.45546100
O	-1.41705800	-0.87305800	0.22348700

Fe	-0.01452600	-1.68493700	-0.66843100
Cl	0.94957900	-3.20323100	0.57217000
Cl	-0.69905100	-2.49058400	-2.59872400
C	-0.05311800	-0.76426900	2.90642600
H	-0.75357700	-1.57112200	2.68026700
H	0.94517900	-0.97742300	2.51617900
H	0.05220000	-0.71153200	4.00448600
C	0.41113300	1.60754200	2.12649800
H	1.36161900	1.47988300	2.64849400
H	0.64396600	1.50276200	1.05104600
H	0.01630200	2.61622400	2.26186000
Si	-4.89800600	1.26130300	0.22292100
H	-6.24341300	0.76146600	0.57438300
H	-4.58371200	2.41249900	1.09455300
H	-4.87433900	1.67191300	-1.19399900
Si	-4.04788000	-1.61401900	-0.63754400
H	-5.52081500	-1.76631400	-0.61886200
H	-3.61644900	-1.27115900	-2.00096000
H	-3.43283600	-2.86422700	-0.16183500
C	-1.83943400	1.37308800	-0.48822800
C	-1.84681200	2.72918400	-0.13137800
C	-1.59653400	1.04370900	-1.83263600
C	-1.59826900	3.71970200	-1.08024900
H	-2.03264300	3.03870300	0.88890900
C	-1.35997300	2.03389600	-2.78193700
H	-1.60671800	0.00914300	-2.15111000
C	-1.35246600	3.37727400	-2.40935300
H	-1.58986200	4.76072400	-0.77250500
H	-1.17060100	1.74641900	-3.81128500
H	-1.15261200	4.15010700	-3.14499800
Fe	3.54623200	0.44813500	0.07970600
Cl	1.53073300	0.04575800	-1.20244000
Cl	3.37289400	2.61975200	0.42098100
Cl	5.22248700	-0.13533300	-1.17490100
Cl	3.43077900	-0.64571100	1.98943800
2Fe.M5Ph-INT0			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.230534 a.u.			
E (UωB97X-D/def2-tzvp) = -6488.83482229 a.u.			
C	-2.16151200	0.23969700	0.53230800
C	-1.91843400	0.62430800	2.15742900
C	-2.91012500	-0.27516000	2.83853000
C	-3.86238400	-0.69204000	1.99832500
H	-2.19742300	1.67549800	2.25735600
H	-2.87082500	-0.48197700	3.90236800
H	-4.72572200	-1.28062600	2.29518000
C	-3.66405500	-0.22491200	0.58488100
C	-0.50792500	0.43696900	2.41769600
O	-1.36388600	-0.84634300	0.23954100
Fe	-0.02307200	-1.63087700	-0.71927700
Cl	0.97463300	-3.17760800	0.47211900
Cl	-0.68819400	-2.36099700	-2.68770300
C	-0.02426200	-0.85633300	2.90614800
H	-0.72743200	-1.66435000	2.69616400
H	0.98593200	-1.07999900	2.55041100
H	0.05690800	-0.75604600	4.00534900
C	0.45386900	1.49847300	2.10911000

H	1.42209500	1.35868200	2.59196300
H	0.64368100	1.40407100	1.01942300
H	0.06051600	2.50651600	2.25314500
Si	-4.93339800	1.15899200	0.23974400
H	-6.26646000	0.62037900	0.58275100
H	-4.65668700	2.31532600	1.11813200
H	-4.91459600	1.57673600	-1.17474200
Si	-3.96851100	-1.67694500	-0.62894800
H	-5.43148500	-1.90741600	-0.58602500
H	-3.58659100	-1.30055000	-1.99788800
H	-3.28609100	-2.90194700	-0.17996300
C	-1.89131900	1.40795800	-0.40885600
C	-1.91146900	2.75679100	-0.02751500
C	-1.68049800	1.10796000	-1.76422300
C	-1.70836100	3.77025900	-0.96423000
H	-2.08359800	3.04641900	1.00252700
C	-1.48557200	2.11879000	-2.70095000
H	-1.67586400	0.07935000	-2.10062000
C	-1.49230500	3.45601200	-2.30490300
H	-1.71352500	4.80579400	-0.63814600
H	-1.31802700	1.85316800	-3.73995500
H	-1.32658400	4.24508900	-3.03177600
Fe	3.55303400	0.44389300	0.06929200
Cl	1.52149600	0.14570100	-1.19704500
Cl	3.42477200	2.60437200	0.50474900
Cl	5.21743500	-0.12786400	-1.20406400
Cl	3.42966400	-0.69790200	1.95688600
2Fe.M5Ph-TS2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.231420 a.u.			
E (UωB97X-D/def2-tzvp) = -6488.83361418 a.u.			
Imaginary frequency: -160.8658			
C	-2.18873200	0.26157800	0.61163900
C	-1.96870500	0.50019100	2.17869800
C	-2.94622400	-0.44258900	2.82163900
C	-3.83891700	-0.89695700	1.93570000
H	-2.16996200	1.53932500	2.45731800
H	-2.93914400	-0.66302300	3.88345000
H	-4.67510600	-1.54467200	2.18290700
C	-3.62230800	-0.36841900	0.54280700
C	-0.52121600	0.21965300	2.35300100
O	-1.19989900	-0.72180700	0.32325800
Fe	0.00665300	-1.50333400	-0.80326900
Cl	0.98095000	-3.15650500	0.26036700
Cl	-0.69931500	-2.08988600	-2.80211400
C	-0.06189800	-1.05097800	2.91291900
H	-0.80620700	-1.84234300	2.82318700
H	0.90907300	-1.34400500	2.50115000
H	0.11433100	-0.85106300	3.98745500
C	0.45171600	1.27643100	2.05036900
H	1.43264700	1.09395600	2.48997300
H	0.59350500	1.26896700	0.95380900
H	0.07322000	2.27503600	2.28254400
Si	-4.99953900	0.91580400	0.20547900
H	-6.29106300	0.24112900	0.45599800
H	-4.86652800	2.03976500	1.15548900
H	-4.96082300	1.41045200	-1.18329500

Si	-3.80141800	-1.78344100	-0.73083900
H	-5.20556900	-2.23257200	-0.59243100
H	-3.59347800	-1.28099600	-2.09739600
H	-2.91020500	-2.91240700	-0.41595400
C	-1.99598400	1.48580300	-0.27196600
C	-2.12368600	2.80022600	0.19588100
C	-1.73189800	1.28825900	-1.63510400
C	-1.97466500	3.88548500	-0.66851900
H	-2.34653400	3.00213900	1.23788400
C	-1.58530600	2.37001600	-2.49908100
H	-1.64454900	0.28695700	-2.03781100
C	-1.70103900	3.67490100	-2.01878200
H	-2.06731500	4.89475000	-0.27908200
H	-1.37151500	2.18676500	-3.54735900
H	-1.57555800	4.51923500	-2.68950200
Fe	3.58708200	0.44195900	0.08635200
Cl	1.60215300	0.23098200	-1.27337400
Cl	3.45947400	2.56596900	0.67027700
Cl	5.29124600	-0.05199800	-1.16708200
Cl	3.39663500	-0.82749700	1.88753000
2Fe.M5Ph-INT			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.237152 a.u.			
E (UωB97X-D/def2-tzvp) = -6488.85587633 a.u.			
C	-2.15389400	0.41534200	0.72851800
C	-1.97972700	0.08406900	2.24113000
C	-3.35885900	-0.22180500	2.73232200
C	-4.25829600	-0.15009700	1.74829600
H	-1.44437000	0.81467300	2.85036000
H	-3.56895600	-0.50244900	3.75833900
H	-5.31954100	-0.35002000	1.85904000
C	-3.67641200	0.30831700	0.42173300
C	-1.09941500	-1.14364700	1.87483100
O	-1.38783300	-0.88002000	0.39948200
Fe	-0.13110500	-1.26259900	-1.07313700
Cl	0.66410400	-3.24397800	-0.63592500
Cl	-1.15576100	-1.28015100	-2.99859600
C	-1.60714500	-2.52430900	2.22252800
H	-2.65891700	-2.64304700	1.95651700
H	-1.01481400	-3.27877400	1.69769600
H	-1.49626200	-2.69041600	3.29979300
C	0.36906000	-0.95014200	2.17977500
H	0.98780000	-1.71998900	1.71375300
H	0.72417700	0.03285900	1.86610600
H	0.51473500	-1.02238100	3.26348200
Si	-4.48462000	2.02147500	0.10465800
H	-5.92080400	1.85747200	0.41765100
H	-3.89510800	3.01296400	1.02543700
H	-4.35744200	2.47840800	-1.29207200
Si	-4.24124000	-0.90613200	-0.93536300
H	-5.71085400	-0.98909600	-0.78439300
H	-3.93857300	-0.39834500	-2.28389900
H	-3.65760500	-2.24376400	-0.72921100
C	-1.40815700	1.54728500	0.07952200
C	-0.51272000	2.35669000	0.78702900
C	-1.55669200	1.75023600	-1.30366800
C	0.22059500	3.34306600	0.12890200

H	-0.36650000	2.22247100	1.85172200
C	-0.82146000	2.73397800	-1.96004600
H	-2.23584000	1.13100800	-1.87632300
C	0.07003400	3.53309600	-1.24440300
H	0.92581400	3.94507100	0.69146100
H	-0.94046100	2.86487600	-3.03084600
H	0.65214700	4.29387400	-1.75505500
Fe	3.49177300	0.28110900	0.30101800
Cl	1.62419500	0.25042200	-1.28155100
Cl	2.89080400	1.71017400	1.87178800
Cl	5.13936900	1.00974300	-0.92398400
Cl	3.73418500	-1.76172400	1.03831000
2Fe.M5Ph-TS3			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.236059 a.u.			
E (UωB97X-D/def2-tzvp) = -6488.84748818 a.u.			
Imaginary frequency: -181.2494			
C	-2.32420200	0.62565400	0.72607800
C	-2.03844800	0.13144900	2.15529900
C	-3.38746100	-0.29653800	2.65815500
C	-4.31288600	-0.21539200	1.70127700
H	-1.56444200	0.88020400	2.79636000
H	-3.54440300	-0.67015700	3.66287000
H	-5.35700000	-0.49299400	1.79675700
C	-3.75691100	0.35697000	0.40336200
C	-1.05665400	-1.04928800	1.83121800
O	-1.23554000	-1.05311200	0.37798200
Fe	-0.04141200	-1.53400400	-0.95992800
Cl	0.92188800	-3.43382200	-0.47902700
Cl	-1.14242100	-1.50096900	-2.86956400
C	-1.47453500	-2.41277100	2.36369000
H	-2.48751700	-2.66735200	2.04522100
H	-0.78386100	-3.16680200	1.97494800
H	-1.42840400	-2.43287600	3.45807300
C	0.38058100	-0.72730400	2.20577900
H	1.05626200	-1.50751400	1.84409400
H	0.70495200	0.22744700	1.79122200
H	0.48452100	-0.67730900	3.29520500
Si	-4.68079800	2.02106700	0.08666000
H	-6.11117500	1.74136100	0.32274300
H	-4.19399500	3.02032100	1.05690600
H	-4.48109900	2.50179300	-1.29222800
Si	-4.22126900	-0.86516500	-1.00691000
H	-5.69127900	-0.97413500	-0.88063300
H	-3.90380300	-0.31700100	-2.33298200
H	-3.59398800	-2.16865400	-0.75605600
C	-1.51039400	1.59698700	0.02215800
C	-0.55112800	2.37327100	0.70516600
C	-1.66398700	1.77980100	-1.37206600
C	0.21247400	3.31213200	0.02195300
H	-0.40759300	2.25737800	1.77170200
C	-0.88298300	2.70154100	-2.05074500
H	-2.35325800	1.15716100	-1.92605400
C	0.05171200	3.47510500	-1.35419400
H	0.95318800	3.89102300	0.56080800
H	-0.98853900	2.80639300	-3.12536700
H	0.66643600	4.19294100	-1.88830700

Fe	3.45469400	0.39828400	0.25897900
Cl	1.57247000	0.18768600	-1.24589600
Cl	2.87276700	1.91794700	1.76732100
Cl	5.05814900	1.11569800	-1.03790800
Cl	3.81607800	-1.56536000	1.14779600
2Fe.M5Ph-INT2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.235292 a.u.			
E (UωB97X-D/def2-tzvp) = -6488.86310803 a.u.			
C	-2.54230500	0.75185500	-0.05934100
C	-1.59175400	1.47223700	0.82253900
C	-2.45315600	2.27670200	1.73949300
C	-3.74559200	1.97059000	1.56630800
H	-0.82178000	2.03847400	0.28978900
H	-2.05471500	2.97157900	2.46685700
H	-4.58765100	2.36787800	2.12119300
C	-3.92059300	0.99840200	0.41942800
C	-0.64877900	0.39472900	1.67525900
O	0.18014700	-0.19763900	0.75420400
Fe	0.98069500	-1.79974600	0.47536600
Cl	1.87236900	-2.57471000	2.32477600
Cl	-0.42758300	-3.25134000	-0.43525700
C	-1.51065700	-0.65459400	2.38264900
H	-1.97205900	-1.32480100	1.65299400
H	-0.86270300	-1.25761700	3.02635500
H	-2.28447000	-0.19063000	3.00118900
C	0.17694500	1.22070800	2.66719000
H	0.91202800	0.55342700	3.12477800
H	0.72058500	2.01958500	2.15832700
H	-0.45330800	1.64095800	3.45608900
Si	-4.79781900	2.02238300	-0.97089200
H	-6.06954500	2.50186200	-0.39407000
H	-3.92048200	3.15293400	-1.32258000
H	-5.04762700	1.16080300	-2.14035400
Si	-5.07669800	-0.46354400	0.89461800
H	-5.92228700	0.03179300	1.99678500
H	-5.94095800	-0.83375800	-0.24453200
H	-4.28173100	-1.62829400	1.31430400
C	-2.15922000	-0.00928600	-1.20125700
C	-0.87462400	0.17866400	-1.78007000
C	-3.03530400	-0.95503600	-1.80388700
C	-0.48568200	-0.55645200	-2.89091500
H	-0.20123100	0.92206800	-1.38043100
C	-2.63238300	-1.69330300	-2.89814600
H	-4.02028000	-1.13048600	-1.39086700
C	-1.35367900	-1.49739100	-3.44311900
H	0.50215200	-0.40356800	-3.30967200
H	-3.29916200	-2.43369700	-3.32709100
H	-1.04011000	-2.08439100	-4.30094700
Fe	3.16924400	1.07456100	-0.37191400
Cl	2.58044900	-1.11689800	-1.18206800
Cl	1.55521900	2.58605000	-0.73857300
Cl	4.91852800	1.57311600	-1.58181000
Cl	3.63099800	0.85149400	1.75231600
2Fe.M5Ph-TS4			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.233908 a.u.			
E (UωB97X-D/def2-tzvp) = -6488.85688234 a.u.			

Imaginary frequency: -347.3533			
C	-2.54909400	0.80729600	-0.17403200
C	-1.67075100	1.69056000	0.55368500
C	-2.51947800	2.52170300	1.42335500
C	-3.79261600	2.08671400	1.37316500
H	-0.81312300	2.12733700	0.04955700
H	-2.14289200	3.32752100	2.03964700
H	-4.63425100	2.46767900	1.93941900
C	-3.93302300	0.99162600	0.34378600
C	-0.59272800	0.57931700	1.66127700
O	0.18948000	-0.05942600	0.79740200
Fe	0.92246300	-1.73402100	0.58865600
Cl	1.79743900	-2.37185000	2.49389900
Cl	-0.52770200	-3.22473600	-0.13863400
C	-1.50539600	-0.33017200	2.46331900
H	-1.91818100	-1.11614400	1.82827700
H	-0.89679400	-0.80994400	3.23906800
H	-2.30969600	0.22885800	2.94749900
C	0.16590300	1.61062000	2.48301400
H	0.90391800	1.05860700	3.07541700
H	0.71107900	2.30491200	1.84152000
H	-0.49758000	2.15287300	3.16007000
Si	-4.91041700	1.84522100	-1.09088300
H	-6.20293200	2.28181200	-0.52497100
H	-4.12242400	3.00136600	-1.55351900
H	-5.13114100	0.88294800	-2.18560200
Si	-4.97780100	-0.49035300	0.96835500
H	-5.79615900	0.01223900	2.08891300
H	-5.87981300	-0.96982100	-0.09966900
H	-4.11239800	-1.59686700	1.40649300
C	-2.14126700	-0.06041800	-1.24320400
C	-0.86537200	0.10074100	-1.83990100
C	-2.98717400	-1.08235100	-1.74352000
C	-0.45474500	-0.73277600	-2.87253500
H	-0.20387500	0.89004000	-1.51275900
C	-2.57021000	-1.90993200	-2.77064500
H	-3.96947600	-1.24073100	-1.31665700
C	-1.29990100	-1.73991900	-3.33669900
H	0.53020900	-0.59665200	-3.30424700
H	-3.22425500	-2.69902800	-3.12674600
H	-0.97357100	-2.39587800	-4.13787100
Fe	3.22150900	0.99141300	-0.42471100
Cl	2.55117000	-1.23898900	-1.08112800
Cl	1.67619500	2.51107000	-0.96709000
Cl	5.02927200	1.30907800	-1.60567100
Cl	3.60035500	0.91577300	1.72764600
2Fe.M5Ph-P			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.228955 a.u.			
E (UωB97X-D/def2-tzvp) = -6488.88078538 a.u.			
C	-2.85409400	0.11419200	-1.12975400
C	-2.41169400	1.15409000	-1.92076100
C	-3.26083100	2.30288900	-1.75841700
C	-4.24433600	2.00821000	-0.85889900
H	-1.57361800	1.10210500	-2.60436500
H	-3.14087200	3.24364800	-2.28491700
H	-5.05153800	2.65557500	-0.53710300

C	-4.10740500	0.57671700	-0.42678500
C	-0.10923900	2.18001500	-0.06570300
O	0.24671300	1.00509600	0.15300400
Fe	0.58705900	-0.25257500	1.60291000
Cl	1.22039300	1.07133300	3.23163900
Cl	-0.94411100	-1.59304500	2.34906600
C	-0.94155200	2.94245800	0.90704100
H	-0.94338700	2.47399600	1.89145200
H	-0.58610400	3.97567400	0.97612200
H	-1.96736200	2.97460200	0.51228700
C	0.36184800	2.85315800	-1.31087100
H	1.24215500	3.44795500	-1.02791000
H	0.68305800	2.12542900	-2.05611100
H	-0.39781300	3.53418500	-1.70298300
Si	-5.65185300	-0.22287600	-1.23155200
H	-6.85480900	0.49886500	-0.76511800
H	-5.51329500	-0.10319600	-2.69515900
H	-5.79909100	-1.64322200	-0.85406900
Si	-4.13917400	0.43245300	1.46592500
H	-5.32845400	1.17184000	1.94306400
H	-4.23559700	-0.96964200	1.90684800
H	-2.92687900	1.05111300	2.03170000
C	-2.19428300	-1.18581300	-0.97902900
C	-0.85199000	-1.34104800	-1.39066400
C	-2.83362500	-2.30089700	-0.41004200
C	-0.18405200	-2.55379400	-1.23891000
H	-0.31641700	-0.51060700	-1.83076400
C	-2.16395900	-3.51249100	-0.25803400
H	-3.86050500	-2.22918000	-0.07852900
C	-0.83580300	-3.64654600	-0.66770100
H	0.84812400	-2.62979300	-1.56288100
H	-2.68324000	-4.35469200	0.18942500
H	-0.31405900	-4.58958500	-0.53784000
Fe	3.49423500	0.03106200	-0.74480000
Cl	2.43394600	-1.48456000	0.83145300
Cl	2.31975700	-0.05747300	-2.61508800
Cl	5.49932500	-0.77717800	-0.97919900
Cl	3.44085700	2.01813400	0.20106600
2Fe.M6-2FeCl₃/S (RS)			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.153284 a.u.			
E (UωB97X-D/def2-tzvp) = -6257.79204139 a.u.			
C	-3.46563200	0.45646000	-1.43510800
C	-2.21914700	0.96400700	-1.70300900
C	-1.16337100	1.08394500	-0.76408600
C	-3.25746100	-0.61712900	0.93433300
H	-4.15713300	0.52293500	-2.27666300
H	-2.02236900	1.36922600	-2.69123500
H	-1.24636700	0.59973700	0.21194300
H	-3.53508200	-0.29832300	1.93845800
C	-4.08927400	-0.03380700	-0.19041500
Si	-5.48802700	-1.30162200	-0.53558500
H	-6.21519200	-1.53017800	0.72602300
H	-6.41382500	-0.75830200	-1.55691700
H	-4.89709000	-2.56105000	-1.02468000
Si	-4.95457000	1.56200800	0.47315700
H	-5.78199500	2.16541100	-0.58892800

H	-5.79584700	1.18601300	1.62677500
H	-3.88317600	2.48928000	0.88654200
C	-2.31911600	-1.58381500	0.84132000
O	-0.12846300	1.75666000	-1.02807500
Fe	1.42518500	2.04480800	0.10635900
Cl	0.89774700	3.68522100	1.44130400
Cl	1.41454800	0.10509700	1.45444400
C	-1.83826000	-2.17049200	-0.45483400
H	-0.89267700	-1.70622300	-0.76717200
H	-1.62621300	-3.23774900	-0.33976700
H	-2.54548000	-2.03625800	-1.27654300
C	-1.65892000	-2.11648700	2.08472600
H	-1.83745900	-3.19512900	2.17826200
H	-0.57216300	-1.98993000	2.02971200
H	-2.02425600	-1.62098300	2.98870900
Fe	2.35305000	-1.56312200	-0.07744600
Cl	3.27093900	2.27663900	-0.98741200
Cl	4.51244200	-1.40547800	0.04173400
Cl	1.52438500	-3.45164100	0.66537500
Cl	1.46837200	-0.94613700	-2.00340000
2Fe.M6-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.154518 a.u.			
E (UωB97X-D/def2-tzvp) = -6257.76835694 a.u.			
Imaginary frequency: -149.7894			
C	-3.63553800	-0.34997600	-1.75739700
C	-2.56634500	0.43090800	-1.90378600
C	-1.92592200	0.87396800	-0.61723400
C	-2.73505700	-0.23244500	0.50622700
H	-4.25254100	-0.70392200	-2.57802300
H	-2.15443700	0.79033500	-2.84046900
H	-2.31730300	1.82311700	-0.22609800
H	-2.96171800	0.38431100	1.37711600
C	-3.97932500	-0.67389600	-0.31765000
Si	-4.55310300	-2.47429500	-0.03280300
H	-4.07951400	-2.90574300	1.30140700
H	-6.02994600	-2.53304400	-0.07078200
H	-4.02319100	-3.39027700	-1.06430900
Si	-5.44329900	0.45831100	0.17395300
H	-6.53392700	0.27558700	-0.80297500
H	-5.91771600	0.10265500	1.52972400
H	-4.97208100	1.85904900	0.16517100
C	-1.65101100	-1.12519200	0.78491900
O	-0.57593600	0.85240200	-0.63398500
Fe	0.65284500	1.99345300	0.12736700
Cl	-0.54266500	2.91501700	1.76932700
Cl	2.36417700	0.76652300	1.25754300
C	-1.17580200	-2.12193400	-0.17289700
H	-0.36607500	-1.57822200	-0.71091800
H	-0.67184800	-2.96288300	0.31036700
H	-1.90431500	-2.43919600	-0.91547300
C	-0.84196500	-0.88488300	1.99546000
H	-1.31706600	-1.48127200	2.79526900
H	0.18567500	-1.23898700	1.89659800
H	-0.87877900	0.16078000	2.31612700
Fe	2.93878600	-1.14092700	-0.09424800
Cl	1.49789200	3.42816900	-1.27704700

Cl	5.09658000	-1.15968000	-0.32529200
Cl	2.14534800	-2.86153600	1.05945100
Cl	1.81721400	-0.87806200	-1.97538800
2Fe.M6-INT0			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.154041 a.u.			
E (UωB97X-D/def2-tzvp) = -6257.77015727 a.u.			
C	-3.64973100	-0.44208400	-1.80049800
C	-2.65744500	0.42199700	-2.02294100
C	-2.01622400	0.90870600	-0.74350400
C	-2.58616100	-0.12261800	0.34683500
H	-4.28842700	-0.86950600	-2.56794800
H	-2.34616800	0.81845400	-2.98277400
H	-2.39448300	1.90209400	-0.46460800
H	-2.79479200	0.42318700	1.26945200
C	-3.87575200	-0.72955000	-0.32657900
Si	-4.29889400	-2.54481600	0.08355200
H	-3.77351500	-2.85531200	1.43309600
H	-5.76620900	-2.71833200	0.08650500
H	-3.70905600	-3.48543600	-0.89112600
Si	-5.36221400	0.33074300	0.24955400
H	-6.51606900	0.03368700	-0.62151300
H	-5.69619400	-0.00159500	1.65245100
H	-4.99139200	1.75668500	0.14936400
C	-1.49763000	-1.08906600	0.61049800
O	-0.62340000	0.92677400	-0.78043000
Fe	0.53126000	2.01121900	0.12086200
Cl	-0.73681300	2.73142800	1.82216800
Cl	2.19683500	0.71427400	1.29148100
C	-1.01438500	-2.01390200	-0.39585400
H	-0.14559100	-1.45476500	-0.82810600
H	-0.57220700	-2.92022200	0.02551200
H	-1.69159200	-2.19388900	-1.22775600
C	-0.84642900	-1.04940900	1.92402200
H	-1.55631500	-1.55197800	2.60855300
H	0.10569100	-1.58099400	1.95639400
H	-0.76251900	-0.01976300	2.29329800
Fe	2.94726400	-1.09211900	-0.07745000
Cl	1.45325500	3.57750600	-1.08434400
Cl	5.10794100	-0.99866800	-0.23343900
Cl	2.19323600	-2.90163200	0.96761300
Cl	1.87745600	-0.82293700	-1.99827100
2Fe.M6-TS2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.155358 a.u.			
E (UωB97X-D/def2-tzvp) = -6257.77037156 a.u.			
Imaginary frequency: -94.9549			
C	-3.64211100	-0.43145900	-1.79243400
C	-2.64891900	0.43901800	-1.99170400
C	-2.03077000	0.90928900	-0.69604000
C	-2.61922000	-0.11566700	0.36350800
H	-4.26375100	-0.85765900	-2.57439900
H	-2.32278600	0.84252800	-2.94364500
H	-2.37168400	1.92022700	-0.43534300
H	-2.83500100	0.40870700	1.29740300
C	-3.89409700	-0.72560400	-0.32366800
Si	-4.32381900	-2.54016800	0.08459600
H	-3.76232500	-2.86732300	1.41574300

H	-5.79177500	-2.70224700	0.13201800
H	-3.77352800	-3.47851800	-0.91510200
Si	-5.38974800	0.33473400	0.22761600
H	-6.53125200	0.03698300	-0.65932400
H	-5.74424300	0.00533900	1.62623300
H	-5.01651700	1.76050100	0.13056300
C	-1.49891300	-1.06499300	0.61114800
O	-0.62823200	0.85811400	-0.68241800
Fe	0.54942300	1.98971800	0.12867500
Cl	-0.67729100	2.77755700	1.82929500
Cl	2.25656800	0.74405800	1.28828700
C	-1.05071700	-2.03951000	-0.37140500
H	-0.14199600	-1.56798300	-0.81200300
H	-0.68097500	-2.95878100	0.09317400
H	-1.73917400	-2.21310800	-1.19493400
C	-0.82997800	-1.00409100	1.91391100
H	-1.51135900	-1.54912300	2.59622400
H	0.14047200	-1.50268400	1.92979300
H	-0.78180200	0.02207800	2.29573000
Fe	2.95291500	-1.08654300	-0.07999000
Cl	1.40457100	3.51912600	-1.17011600
Cl	5.11263700	-1.02764700	-0.26576200
Cl	2.18556600	-2.87907700	0.98345200
Cl	1.85742100	-0.81473700	-1.98512400
2Fe.M6-INT			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.161248 a.u.			
E (UωB97X-D/def2-tzvp) = -6257.78938722 a.u.			
C	-3.84561300	-0.03537700	-1.63883600
C	-2.88861200	0.90540500	-1.64439900
C	-2.29347300	1.05525100	-0.28471000
C	-2.88340900	-0.10205800	0.54407700
H	-4.44150600	-0.30808900	-2.50558200
H	-2.58012600	1.50438700	-2.49311700
H	-2.25857700	2.06353000	0.12946100
H	-3.14114000	0.15840200	1.57281900
C	-4.09077900	-0.64396500	-0.27368900
Si	-4.45152400	-2.51327300	-0.24966100
H	-4.01931600	-3.06843100	1.05057800
H	-5.91332100	-2.70799600	-0.38011800
H	-3.79356400	-3.23962000	-1.35349000
Si	-5.65765100	0.20563400	0.42242600
H	-6.76396000	0.08997000	-0.54873800
H	-6.04998300	-0.42954000	1.70071600
H	-5.33741200	1.63040800	0.65810700
C	-1.46910400	-0.77405300	0.51225000
O	-0.92681900	0.46075100	-0.19961000
Fe	0.68981700	1.55476200	0.10807500
Cl	-0.14027800	2.69456900	1.84079300
Cl	2.65596900	0.86558900	1.33360700
C	-1.21931400	-1.96873000	-0.38154000
H	-0.14333400	-2.10415900	-0.51189300
H	-1.61117900	-2.87515600	0.08986500
H	-1.67226200	-1.83998900	-1.36547600
C	-0.82925900	-0.91715200	1.87808400
H	-1.32399500	-1.73732200	2.41062300
H	0.23168800	-1.17052300	1.79321500

H	-0.93450800	-0.00300700	2.46717400
Fe	3.15384300	-0.97412300	-0.08741200
Cl	0.83775100	3.02524300	-1.49526400
Cl	5.23119400	-0.97382400	-0.68522400
Cl	2.42665100	-2.78357800	0.90690900
Cl	1.68740300	-0.33120500	-1.68556300
2Fe.M6-TS3			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.158582 a.u.			
E (UωB97X-D/def2-tzvp) = -6257.77732545 a.u.			
Imaginary frequency: -228.6296			
C	3.93442000	-0.42090700	1.71129900
C	3.07370200	0.62301800	2.00648200
C	2.48684500	1.05603800	0.80818300
C	2.76823800	0.05963400	-0.27782300
H	4.58372300	-0.88990000	2.44768900
H	2.95218100	1.09133800	2.97471100
H	2.07824000	2.04387300	0.64461600
H	2.95903700	0.54140300	-1.24035500
C	3.97460000	-0.76018500	0.28375000
Si	4.24747300	-2.61240500	-0.14337000
H	3.61620300	-2.87489400	-1.44766800
H	5.70811300	-2.81673300	-0.26028700
H	3.73433700	-3.50140200	0.91229100
Si	5.56900300	0.09961100	-0.41425100
H	6.74099000	-0.28612000	0.39292700
H	5.73190500	-0.33589500	-1.81397800
H	5.32240900	1.55282600	-0.32914900
C	1.34284900	-0.64788700	-0.35821000
O	0.52818700	0.34758400	0.30259700
Fe	-0.55661400	1.72324800	-0.24602300
Cl	0.66040700	2.77516100	-1.80296700
Cl	-2.52128400	0.94715700	-1.29797500
C	1.17657200	-1.90632300	0.48657400
H	0.10332200	-2.07189800	0.60650600
H	1.58964700	-2.79097200	-0.00430800
H	1.60418800	-1.79720200	1.48716000
C	0.90837700	-0.88234900	-1.79826800
H	1.55315100	-1.63104900	-2.27220900
H	-0.11761500	-1.26099800	-1.81117700
H	0.95637000	0.04325600	-2.37746900
Fe	-3.14983000	-0.93500300	0.09693700
Cl	-0.83134200	3.07077800	1.46245900
Cl	-5.32660100	-0.97282500	0.10546600
Cl	-2.23709700	-2.70702400	-0.86002200
Cl	-2.23810800	-0.51547000	2.05074100
2Fe.M6-INT2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.157561 a.u.			
E (UωB97X-D/def2-tzvp) = -6257.79723482 a.u.			
C	4.35685800	-0.58418900	1.61792200
C	3.43208400	-0.00542200	2.49416500
C	2.28872700	0.29141200	1.77381900
C	2.41014400	-0.13086600	0.37402400
H	5.35358700	-0.90790000	1.90878500
H	3.59643400	0.18995700	3.54631200
H	1.39948400	0.78488300	2.15418900
H	2.26852000	0.75307800	-0.27279300

C	3.85345900	-0.67958000	0.26401400
Si	4.38751600	-2.32571100	-0.58196000
H	4.36726400	-2.16527100	-2.04452700
H	5.77442900	-2.54143700	-0.12347800
H	3.53828300	-3.44627000	-0.15182800
Si	4.82860800	0.66932800	-0.77933400
H	6.24890500	0.27296100	-0.81990300
H	4.22946300	0.67042200	-2.12050700
H	4.64306700	1.94954800	-0.07662600
C	1.10812900	-0.98949500	-0.07519500
O	0.05428900	-0.09842300	0.07908000
Fe	-0.39592400	1.60302300	-0.31832000
Cl	1.08296800	2.27153700	-1.87413500
Cl	-2.61122500	1.41806600	-1.07166200
C	0.86560000	-2.17523000	0.86454200
H	0.01620000	-2.74875000	0.48535300
H	1.73615400	-2.83341500	0.92849700
H	0.60759200	-1.81548900	1.86375900
C	1.22229800	-1.40995300	-1.54086300
H	1.93957500	-2.22352600	-1.68329300
H	0.23959500	-1.77556900	-1.85031800
H	1.49289200	-0.56333900	-2.17679800
Fe	-3.18394800	-0.67865500	0.04491400
Cl	-0.13923900	2.87367400	1.48465800
Cl	-5.36795400	-0.66214800	-0.02371300
Cl	-2.36087800	-2.35964800	-1.13422300
Cl	-2.43064700	-0.57423300	2.10923000
2Fe.M6-TS4			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.156332 a.u.			
E (UωB97X-D/def2-tzvp) = -6257.78792106 a.u.			
Imaginary frequency: -298.0723			
C	4.29398300	-0.93313400	1.63260900
C	3.37439700	-0.32182300	2.47311800
C	2.39883500	0.29359400	1.68013500
C	2.60331100	-0.00777900	0.29596400
H	5.15941000	-1.50138700	1.96138700
H	3.41085800	-0.31306000	3.55516100
H	1.56261000	0.88071800	2.04472300
H	2.38776000	0.77504300	-0.43083400
C	3.95658900	-0.71228000	0.22482900
Si	4.38266000	-2.21467000	-0.88197100
H	4.30418900	-1.83095000	-2.30150100
H	5.77369000	-2.56836800	-0.53371100
H	3.50378600	-3.36190400	-0.59849400
Si	5.15748900	0.69396300	-0.39018800
H	6.54658000	0.20217000	-0.31744500
H	4.79288500	1.00225800	-1.78348100
H	4.94848700	1.84817100	0.50034500
C	1.02812000	-0.94777300	-0.13738300
O	0.09108700	-0.03340100	0.11877600
Fe	-0.45182000	1.66228200	-0.30612800
Cl	0.89466900	2.39403400	-1.91746900
Cl	-2.66072800	1.37697900	-1.04200600
C	0.92222200	-2.14679600	0.78814200
H	0.12398300	-2.78855300	0.39900800
H	1.84746100	-2.72653900	0.82619600

H	0.64170900	-1.82656000	1.79220800
C	1.15741500	-1.27254600	-1.61599300
H	1.88139100	-2.06582600	-1.80766100
H	0.17118400	-1.63448900	-1.92868500
H	1.39990400	-0.38675100	-2.20590100
Fe	-3.20247600	-0.73189700	0.06720900
Cl	-0.25818800	2.92665100	1.48830100
Cl	-5.38229500	-0.77084400	0.01282900
Cl	-2.31558100	-2.36875400	-1.13103800
Cl	-2.40400700	-0.61957600	2.11009300
2Fe.M6-P			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.155414 a.u.			
E (UωB97X-D/def2-tzvp) = -6257.81094984 a.u.			
C	2.97414700	-0.86666500	1.80433900
C	1.99543200	-0.09787100	2.36698200
C	1.84048200	1.10176900	1.58728200
C	2.69965200	1.05382400	0.49973000
H	3.33474500	-1.82251000	2.16785300
H	1.42041600	-0.33199300	3.25365600
H	1.20749100	1.94035400	1.84562800
H	2.86918300	1.85208400	-0.21216400
C	3.53402600	-0.17859200	0.60145500
Si	3.82731900	-1.28184500	-0.91977800
H	4.34549300	-0.47432400	-2.03574400
H	4.85152500	-2.27248200	-0.51594400
H	2.61942000	-2.02292800	-1.31693200
Si	5.26550300	0.46707600	1.15951800
H	6.10358200	-0.68701300	1.54244000
H	5.90447300	1.18392600	0.03674600
H	5.06624900	1.36950700	2.30837000
C	0.09679500	-2.20435300	-0.47211200
O	0.29308300	-1.05680300	-0.04782200
Fe	0.20698500	0.89046100	-0.66396000
Cl	1.37971500	0.61988400	-2.55023200
Cl	-2.07860500	0.49146800	-1.65099200
C	0.31726300	-3.35631000	0.45901700
H	-0.60453600	-3.94597000	0.51927300
H	1.09889500	-4.00951200	0.05186100
H	0.59889000	-2.99877600	1.44955400
C	-0.36998500	-2.47634000	-1.86535600
H	-0.07926200	-3.47804200	-2.19131000
H	-1.46621800	-2.42448300	-1.85599900
H	-0.00126100	-1.71380500	-2.55323500
Fe	-3.03224200	-0.06530700	0.41256800
Cl	0.07198000	3.07493500	-0.42625500
Cl	-4.94461200	0.92413600	0.67158800
Cl	-3.14359600	-2.27247100	0.50072900
Cl	-1.40155400	0.71442300	1.75988700
2Fe.M6Ph-FeCl₃/S (RS)			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.228422 a.u.			
E (UωB97X-D/def2-tzvp) = -6488.85645250 a.u.			
C	1.01815400	-0.03398700	0.96246600
C	3.47891700	0.79800300	-1.04928100
C	4.10576000	-0.35165100	-0.27810900
C	3.28634900	-1.16724900	0.65792600
H	3.94791300	1.77098700	-0.90514500

H	3.79178700	-2.07977600	0.98048900
C	2.01575300	-1.07334300	1.13502900
C	2.45820300	0.75300200	-1.92366300
O	-0.19608300	-0.37892100	0.77945000
Fe	-1.17749100	-2.00603100	0.56192000
Cl	-0.73882000	-3.22950600	2.32882700
Cl	-0.65675900	-3.03708000	-1.27937400
C	1.64284000	-0.46573200	-2.25702700
H	0.58328200	-0.27378000	-2.05391700
H	1.70944400	-0.69215900	-3.32883700
H	1.92999000	-1.35785600	-1.70364100
C	2.01283800	2.00849900	-2.62877700
H	2.60132800	2.88074400	-2.33012800
H	2.09451600	1.88842000	-3.71711700
H	0.95639800	2.21353100	-2.41621000
C	1.29325900	1.38970400	1.07483900
C	2.39473900	1.84725700	1.82014900
C	0.41647000	2.31246900	0.47347500
C	2.63643900	3.21007700	1.93245000
H	3.02750900	1.13227400	2.33073400
C	0.67468300	3.67286100	0.57686400
H	-0.43476100	1.95031900	-0.08679300
C	1.78375100	4.12220500	1.30087100
H	3.48013000	3.56435000	2.51618400
H	0.00696100	4.38301400	0.10027200
H	1.97675200	5.18760200	1.38631300
H	1.62840800	-1.94658200	1.65698700
Si	4.93590700	-1.54283200	-1.55037200
H	5.75938100	-0.72723000	-2.46067800
H	5.80165700	-2.49728800	-0.81808800
H	3.92889700	-2.30484900	-2.30826300
Si	5.61933700	0.28839200	0.72108700
H	5.22301400	1.45183100	1.53671300
H	6.12256500	-0.78713200	1.59807800
H	6.67818500	0.70220900	-0.22227000
Fe	-3.51252100	0.78299900	-0.33739700
Cl	-3.44903600	-1.43264500	0.66196000
Cl	-5.53066200	1.02143100	-1.11108400
Cl	-2.98696600	2.19723500	1.25205100
Cl	-1.95462500	0.70415600	-1.91127400
2Fe.M6Ph-TS1			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.230260 a.u.			
E (UωB97X-D/def2-tzvp) = -6488.83120037 a.u.			
Imaginary frequency: -181.3025			
C	1.65017700	0.38100300	0.27190600
C	2.41521400	-0.64564900	-0.97183700
C	3.78416600	-1.04909000	-0.33699000
C	3.69865000	-0.59276500	1.09804900
H	2.51477200	-0.00572800	-1.84759000
H	4.48750600	-0.82583800	1.80825100
C	2.61783200	0.12215100	1.40208000
C	1.39926200	-1.64023700	-1.18212800
O	0.37795100	-0.07590800	0.52203600
Fe	-0.77422800	0.15211500	1.92667700
Cl	-0.00824300	1.72076600	3.26810500
Cl	-1.08273200	-1.77561700	2.93266400

C	1.10206100	-2.69512200	-0.19807400
H	0.02982700	-2.64390900	0.03980600
H	1.25086200	-3.67746600	-0.67087600
H	1.67890000	-2.62159900	0.72110100
C	0.50617600	-1.51006600	-2.34040500
H	1.01991100	-1.13740800	-3.23057200
H	-0.06762100	-2.41497700	-2.54767700
H	-0.24056200	-0.73752000	-2.06761700
C	1.63744600	1.78854800	-0.25729500
C	2.73064700	2.64560700	-0.06551900
C	0.50716500	2.25605500	-0.94442400
C	2.69318900	3.94914800	-0.55484600
H	3.59510300	2.29988800	0.48951000
C	0.47737700	3.55537700	-1.44120900
H	-0.35199300	1.61245800	-1.07711500
C	1.56990500	4.40506900	-1.24891300
H	3.53718400	4.61135400	-0.38686100
H	-0.40525100	3.90367900	-1.96862300
H	1.54247100	5.42180200	-1.62961200
H	2.38830800	0.55551800	2.36985600
Si	4.32321000	-2.88040000	-0.48702600
H	3.84538300	-3.41521000	-1.78073100
H	5.80121100	-2.92388500	-0.46314500
H	3.81624400	-3.71662300	0.61842200
Si	5.17335500	-0.08471000	-1.24170200
H	4.74394300	1.30286400	-1.49526300
H	6.38613200	-0.10308800	-0.40017800
H	5.45680300	-0.75043500	-2.53305000
Fe	-3.33032000	-0.27713000	-0.90096900
Cl	-2.81109700	1.03694100	1.01660400
Cl	-5.49412900	-0.25990000	-1.10567400
Cl	-2.29459300	0.67321300	-2.62441400
Cl	-2.48697100	-2.28863000	-0.54451600
2Fe.M6Ph-INT			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.234784 a.u.			
E (UωB97X-D/def2-tzvp) = -6488.85958937 a.u.			
C	2.00064200	0.47153200	0.29401700
C	2.48463200	-0.31404400	-0.95827500
C	4.01276400	-0.50930900	-0.78060500
C	4.17291500	-0.29990400	0.70892100
H	2.21026700	0.15615900	-1.90457100
H	5.09999300	-0.52501400	1.22890700
C	3.08934500	0.22895300	1.29558200
C	1.46132400	-1.44619800	-0.61808600
O	0.87026800	-0.54198700	0.45328700
Fe	-0.54905900	-0.53429400	1.77313300
Cl	0.28290600	0.50490400	3.50395300
Cl	-1.11941200	-2.58944800	2.17563000
C	1.93408400	-2.72250300	0.04789600
H	1.07768000	-3.21080900	0.52205700
H	2.33336800	-3.41133400	-0.70219400
H	2.68982800	-2.53548300	0.81136100
C	0.43121100	-1.70632700	-1.69390500
H	0.91184300	-2.25777300	-2.51034100
H	-0.39585300	-2.31105400	-1.31273300
H	0.01980200	-0.78100200	-2.10249500

C	1.42715500	1.85074200	0.20115300
C	1.93489900	2.89998100	0.97642400
C	0.36293600	2.09868000	-0.67525200
C	1.37907200	4.17491900	0.87979800
H	2.76527800	2.72368000	1.65131800
C	-0.19817000	3.36850600	-0.76493500
H	-0.05119500	1.29872300	-1.27615800
C	0.30964100	4.41038200	0.01405000
H	1.77747800	4.98180300	1.48734600
H	-1.03536200	3.53214800	-1.43592300
H	-0.12802900	5.40205300	-0.05179200
H	2.98325200	0.48217500	2.34255000
Si	4.78547900	-2.10132900	-1.48527800
H	3.95331800	-2.57743800	-2.61067000
H	6.13959900	-1.79302900	-1.99627800
H	4.91017100	-3.16434100	-0.46781900
Si	4.88877000	0.95270700	-1.65235900
H	4.16985300	2.19780600	-1.31564000
H	6.28816300	1.03054900	-1.18601000
H	4.86572900	0.74171800	-3.11706900
Fe	-3.39519200	-0.10774900	-0.97817300
Cl	-2.35118400	0.76402000	1.05026000
Cl	-5.45751300	0.56661700	-0.83056400
Cl	-2.29912600	0.80316200	-2.66564200
Cl	-3.12925900	-2.27880200	-0.87968900
2Fe.M6Ph-TS2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.234958 a.u.			
E (UωB97X-D/def2-tzvp) = -6488.84920954 a.u.			
Imaginary frequency: -278.8643			
C	2.06324300	0.70872000	0.47843600
C	2.47702500	0.15987400	-0.89596200
C	4.02109400	-0.04520600	-0.76668300
C	4.17099300	-0.16641700	0.71869000
H	2.20948300	0.81875600	-1.72357700
H	5.09814200	-0.47852300	1.19210500
C	3.07395700	0.23636000	1.40704700
C	1.52334000	-1.09250500	-0.90320400
O	0.72877700	-0.69019300	0.25279800
Fe	-0.53500800	-1.22737700	1.48036700
Cl	0.32961800	-0.76564300	3.46833600
Cl	-1.11451800	-3.31918200	1.29418800
C	2.12593700	-2.45592700	-0.58948300
H	1.30664700	-3.13035500	-0.32264100
H	2.63264800	-2.88312800	-1.45876500
H	2.81289500	-2.41787200	0.25905100
C	0.65053600	-1.14616000	-2.14662900
H	1.27178400	-1.36400600	-3.02319900
H	-0.10438200	-1.93056800	-2.04864900
H	0.12873900	-0.20027400	-2.31068100
C	1.21144900	1.85193500	0.73840600
C	1.10796500	2.38068000	2.04296500
C	0.43128400	2.41415200	-0.29087200
C	0.25004800	3.44049000	2.30218900
H	1.68147500	1.95006000	2.85353100
C	-0.42488500	3.47372100	-0.02681600
H	0.46054400	1.99729800	-1.28911100

C	-0.51669800	3.98815600	1.26930600
H	0.16862400	3.83335500	3.31042800
H	-1.04043700	3.87443500	-0.82413200
H	-1.19560300	4.80968100	1.47729200
H	2.98329700	0.27635200	2.48298600
Si	4.89290800	-1.37720900	-1.82080500
H	4.09663800	-1.61778200	-3.04038300
H	6.21570600	-0.84506500	-2.21813200
H	5.10962900	-2.63342100	-1.07889900
Si	4.84904600	1.61408100	-1.27236000
H	4.06220400	2.70791300	-0.66612000
H	6.24032800	1.65012100	-0.78042600
H	4.83122700	1.73154300	-2.74574600
Fe	-3.19951700	0.14862100	-1.01274900
Cl	-2.27928800	0.37192600	1.21088600
Cl	-5.28650100	0.73816800	-0.78163400
Cl	-2.10783800	1.49376100	-2.39783200
Cl	-2.89919300	-1.95330900	-1.55543900
2Fe.M6Ph-INT2			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.235693 a.u.			
E (UωB97X-D/def2-tzvp) = -6488.87319137 a.u.			
C	2.63685300	0.77463700	-0.73256900
C	2.18655500	-0.50265700	-0.10045500
C	3.50424000	-1.32024800	0.08293200
C	4.54926400	-0.32449100	-0.17688100
H	1.44224700	-1.02454800	-0.70972100
H	5.61020300	-0.53608400	-0.07116100
C	4.04367500	0.87335600	-0.62207400
C	1.30867600	-0.17136700	1.22724300
O	0.18231700	0.46354600	0.72829900
Fe	-1.21420100	1.48967300	1.21164800
Cl	-0.78956000	3.64010700	0.90060200
Cl	-1.84143700	1.02901900	3.26767500
C	2.04805400	0.76127300	2.19310900
H	1.45179600	0.86396600	3.10496100
H	3.03341100	0.37440300	2.46720300
H	2.16478700	1.75369600	1.74990100
C	0.86532400	-1.47431100	1.89942200
H	1.66181300	-1.93555400	2.48717400
H	0.05242800	-1.22919300	2.58762900
H	0.48185100	-2.18862400	1.16811700
C	1.79482100	1.74659400	-1.35983700
C	2.22928700	3.09194500	-1.48181600
C	0.52976900	1.38558900	-1.88507900
C	1.41410400	4.03946200	-2.07357200
H	3.18246600	3.39198500	-1.05968400
C	-0.26785700	2.33794200	-2.50222600
H	0.19091600	0.36076600	-1.82765700
C	0.16497400	3.66269800	-2.58696600
H	1.73474700	5.07448200	-2.12845000
H	-1.23742900	2.05012900	-2.89245100
H	-0.47367100	4.41006600	-3.04772700
H	4.64088000	1.71726100	-0.94179700
Si	3.99138600	-2.42631300	1.57123300
H	3.15803600	-3.63810800	1.62477600
H	5.39025400	-2.80992700	1.28108700

H	3.96318400	-1.70041400	2.85297100
Si	3.51377600	-2.54354700	-1.42827500
H	3.25540800	-1.72125700	-2.62494800
H	4.83542600	-3.19537100	-1.51982400
H	2.45155400	-3.53800200	-1.21144600
Fe	-2.52527500	-1.54152800	-0.65747800
Cl	-2.81388800	0.82519400	-0.47726700
Cl	-4.22881300	-2.17504900	-1.86772900
Cl	-0.61144300	-2.06529700	-1.71541100
Cl	-2.55845700	-2.34481600	1.37374300
2Fe.M6Ph-TS3			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.232826 a.u.			
E (UωB97X-D/def2-tzvp) = -6488.85807068 a.u.			
Imaginary frequency: -266.0936			
C	2.70572200	0.76526900	-0.68173700
C	2.37698600	-0.54459700	-0.20397000
C	3.69448300	-1.24271700	0.11000000
C	4.67717200	-0.13767700	0.03829300
H	1.56604300	-1.10674000	-0.65540900
H	5.72742600	-0.25141900	0.28816300
C	4.09015200	1.01341200	-0.40858800
C	1.16164400	-0.08954200	1.37838700
O	0.15822000	0.47502500	0.74369300
Fe	-1.31115000	1.53128700	1.07381900
Cl	-0.94879600	3.67328900	0.77504100
Cl	-1.94200700	1.09799200	3.12946500
C	1.96322500	0.83178700	2.27132600
H	1.40550600	0.94134200	3.21121300
H	2.95092300	0.42910600	2.50477800
H	2.06381700	1.81782600	1.81422000
C	0.82153600	-1.45780000	1.92692100
H	1.65411800	-1.91124000	2.46252600
H	0.00349700	-1.30517800	2.64190000
H	0.45273500	-2.12655600	1.14872600
C	1.81309100	1.69661100	-1.33477200
C	2.12764200	3.07305800	-1.38686600
C	0.62198200	1.24979400	-1.94758600
C	1.27676000	3.96741700	-2.01802000
H	3.02489300	3.44211200	-0.90134600
C	-0.22111900	2.15006100	-2.58822500
H	0.36400400	0.19906100	-1.93348000
C	0.10152700	3.50732400	-2.62294600
H	1.51665200	5.02572900	-2.03059100
H	-1.13646800	1.79139400	-3.04591800
H	-0.56528000	4.21063200	-3.11214900
H	4.60768000	1.94386600	-0.60173600
Si	4.04352700	-2.39396500	1.58784000
H	3.17939200	-3.58667600	1.54695100
H	5.45575400	-2.80323200	1.43623600
H	3.90017900	-1.69594700	2.88008700
Si	3.99290400	-2.32557700	-1.46793400
H	3.84317700	-1.43930300	-2.63659200
H	5.35332100	-2.89955400	-1.42138600
H	2.99104400	-3.40732900	-1.48521700
Fe	-2.55991800	-1.62915100	-0.62508000
Cl	-2.84548900	0.76418600	-0.58368100

Cl	-4.23243300	-2.32050300	-1.84020700
Cl	-0.60819300	-2.18075800	-1.56452000
Cl	-2.64374600	-2.27799700	1.46039100
2Fe.M6Ph-P			
G_{corr} (UB3LYP-D3BJ/6-31G*/Lan2LDZ) = 0.227220 a.u.			
E (UωB97X-D/def2-tzvp) = -6488.88098297 a.u.			
C	2.92162800	0.67550200	-0.52468700
C	3.38163200	-0.55554200	-0.92661400
C	4.56976500	-0.94200300	-0.10497600
C	4.66356200	0.16101900	0.89947100
H	3.04057300	-1.11367300	-1.79080100
H	5.40578900	0.19914800	1.68847800
C	3.71078700	1.09624000	0.62529700
C	0.57807000	-1.28504400	1.11295100
O	-0.15861600	-0.37183900	0.69040900
Fe	-1.14709900	1.17417500	1.34371900
Cl	-0.00099100	3.00598700	1.47646600
Cl	-1.84849000	0.62109100	3.33829900
C	1.33586400	-1.11873500	2.38539100
H	1.61917800	-2.08045400	2.81635900
H	2.25600200	-0.56294000	2.14856500
H	0.75462500	-0.52877900	3.09961400
C	0.63182400	-2.55407400	0.33550400
H	1.58460100	-3.06984100	0.45782500
H	-0.16387400	-3.19114200	0.75184800
H	0.38623400	-2.38177400	-0.71284200
C	1.88572400	1.49821800	-1.17000100
C	1.98832400	2.89811900	-1.15441100
C	0.78611500	0.91625500	-1.81986000
C	1.01518900	3.69141000	-1.76024500
H	2.84014100	3.36784600	-0.67256400
C	-0.19421300	1.70945300	-2.41516600
H	0.67912500	-0.16178600	-1.84445000
C	-0.08405200	3.10056300	-2.38480300
H	1.11236900	4.77271000	-1.73482100
H	-1.04519600	1.23265600	-2.88944500
H	-0.85142800	3.71808000	-2.84159700
H	3.54897800	2.02025000	1.16859700
Si	4.61092600	-2.69208000	0.60061600
H	4.35275900	-3.66829400	-0.47912100
H	5.93426300	-2.96209400	1.20104100
H	3.58420900	-2.86574500	1.64956800
Si	6.07114500	-0.68790700	-1.27113400
H	6.00767300	0.68280400	-1.81037700
H	7.32785200	-0.89009000	-0.51700100
H	6.02122000	-1.67932900	-2.36825000
Fe	-3.25481200	-1.05584400	-0.76247900
Cl	-2.91589300	1.29422300	-0.18016500
Cl	-5.31816900	-1.11711300	-1.44423600
Cl	-1.80972300	-1.57146800	-2.34641300
Cl	-2.89301600	-2.19553900	1.08805000