Supporting Information for

Electronic Effects on the Reaction Mechanism of the Metalloenzyme Peptide Deformylase

Jason S. Fell, Darren M. Steele, Tommy C. Hatcher III, Benjamin F. Gherman*

Department of Chemistry,

California State University, Sacramento,

6000 J Street

Sacramento, CA 95819-6057

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* Corresponding author: e-mail: ghermanb@csus.edu; phone: 916-278-6600; fax: 916-278-4986.

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Table S1. Bond indices for coordination to the Fe^{II} metal center through the course of the deformylation reaction.

substituent	Fe-OH bond index in the FeL(OH) reactant complex	Fe-$O_{formamide}$ bond index in the transition state complex	sum of Fe-$O_{formate}$ bond indices in the FeL(formate) product complex
NO_2	0.482	0.214	0.361
CN	0.463	0.194	0.351
$CClF_2$	0.444	0.205	0.338
F	0.441	0.185	0.336
H	0.428	0.172	0.319
i-Pr	0.401	0.180	0.302
CH_3	0.403	0.181	0.301
OCH_3	0.434	0.188	0.319
$OCH(CH_3)_2$	0.419	0.180	0.298
$N{=}CHC_6H_5$	0.383	0.183	0.314
$NHCH_3$	0.377	0.177	0.290
$N(CH_3)_2$	0.387	0.184	0.306

Table S2. Changes in IEF-PCM solvation energy (kcal/mol) between reactants and transition state ($\Delta G^{\ddagger}_{,solv}$) and reactants and products ($\Delta G_{rxn,solv}$), and changes in the dipole moment (Debye) of the iron-coordination complex between reactant and transition state ($\Delta dipole^{\ddagger}$) and reactant and product ($\Delta dipole_{rxn}$).

substituent	$\Delta G^{\ddagger}_{,solv}$	$\Delta G_{rxn,solv}$	$\Delta dipole^{\ddagger}$	$\Delta dipole_{rxn}$
NO_2	7.60	6.93	-3.38	0.01
CN	9.69	7.67	-2.51	-1.56
$CClF_2$	7.29	6.88	-4.03	-0.29
F	7.66	8.57	-5.22	-0.61
H	8.48	9.85	-4.92	-0.72
i-Pr	7.89	7.85	-3.96	-0.39
CH_3	7.79	8.11	-4.03	-0.44
OCH_3	7.66	8.42	-3.72	-0.25
$OCH(CH_3)_2$	7.01	6.38	-3.06	-0.26
$N{=}CHC_6H_5$	-1.17	-1.44	1.23	4.54
$NHCH_3$	6.36	7.20	-2.33	-1.43
$N(CH_3)_2$	6.03	1.59	-2.68	0.06

Table S3. Changes in CPCM solvation energy (kcal/mol) between reactants and transition state ($\Delta G^{\ddagger}_{,solv}$) and reactants and products ($\Delta G_{rxn,solv}$).

substituent	$\mathbf{\Delta G^{\ddagger}_{,solv}}$	$\mathbf{\Delta G_{rxn,solv}}$
NO_2	7.99	7.29
CN	10.10	8.02
$CClF_2$	7.66	7.23
F	8.03	8.94
H	8.86	10.23
i-Pr	8.27	8.21
CH_3	8.17	8.48
OCH_3	8.01	8.80
$OCH(CH_3)_2$	7.01	6.73
$N{=}CHC_6H_5$	-0.99	-1.68
$NHCH_3$	6.70	7.60
$N(CH_3)_2$	6.90	2.47

Figure S1. Initial plot of ΔG_{rxn} versus substituent σ_p value. Outlying point at σ_p = -0.70 (R = $NHCH_3$) is shown in red.

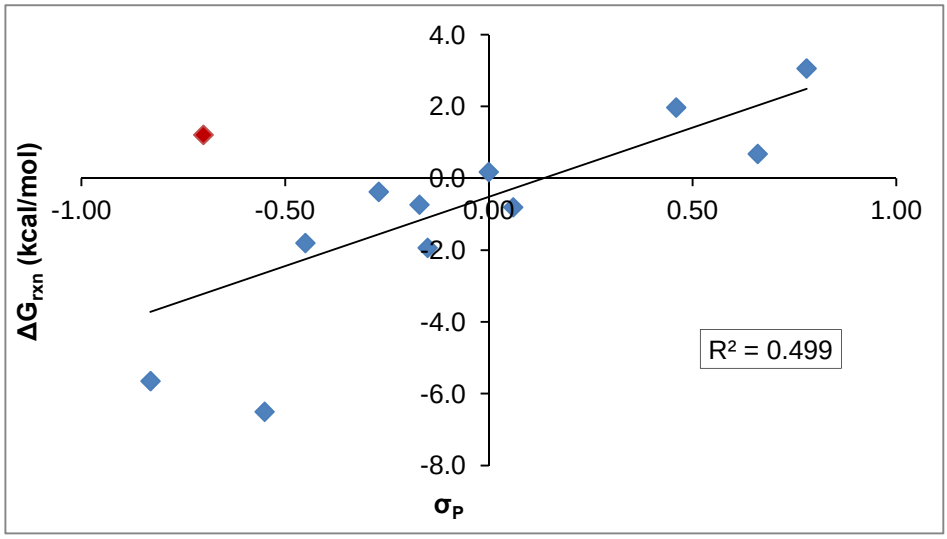
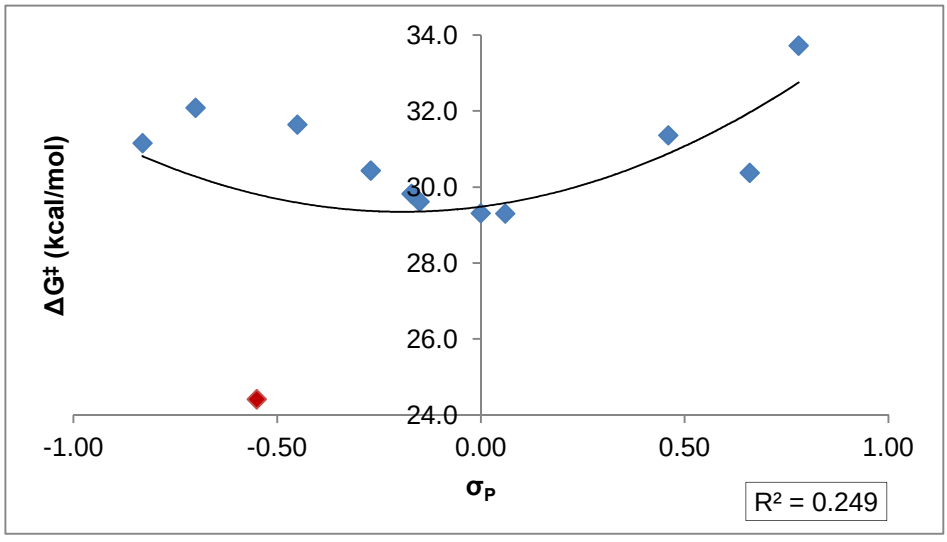


Figure S2. Initial plot of $\Delta G^{\ddagger}$ versus substituent σ_p value. Outlying point at σ_p = -0.55 (R = N=CHC_6H_5) is shown in red.



Solvation energy analysis for the outlying points in Hammett plots for ΔG_{rxn} and $\Delta G^{\ddagger}$.

The $NHCH_3$ substituent point is omitted from the Hammett plot for ΔG_{rxn} (Figure 3), while the $N{=}CHC_6H_5$ substituent point is omitted from the Hammett plot for $\Delta G^{\ddagger}$ (Figure 4). Based on an analysis of solvation energies, these two points are shown to be anomalous and therefore were not included in the reaction energetics analyses.

An initial Hammett plot for ΔG_{rxn} containing points for all substituents (Figure S1) with a linear fit gives an R^2 value of 0.499. An initial Hammett plot for $\Delta G^{\ddagger}$ containing points for all substituents (Figure S2) with a quadratic fit gives an R^2 value of 0.249. It would appear that there is no correlation between the σ_p parameters and the reaction energetics. However, one significantly outlying point (shown in red in Figures S1 and S2) can be identified in each plot.

In the Hammett plot for ΔG_{rxn}, the outlying point corresponds to the $NHCH_3$ substituent. From the correlation line in Figure S1, it might be expected that $R{=}NHCH_3$ would give a ΔG_{rxn} of ~ -3.0 kcal/mol. Alternatively, comparing to the other nitrogen-based substituents (Table 2), ΔG_{rxn} = ~ -6.0 kcal/mol might be expected. From either viewpoint, the actual calculated value of ΔG_{rxn} = 1.21 kcal/mol for $NHCH_3$ appears too high by ~4-7 kcal/mol. Table S2 shows the change in dipole moment between the reactant FeL(OH) and product FeL(formate) complexes, $\Delta dipole_{rxn}$, for $NHCH_3$ is much lower than for the other N-based substituents. The change in solvation energy between reactants and products ($\Delta G_{rxn,solv}$) is then much higher (by ~7 kcal/mol) compared to that for the other N-based substituents. This difference matches the deviation seen in ΔG_{rxn} for $NHCH_3$.

In the Hammett plot for $\Delta G^{\ddagger}$, the outlying point corresponds to the $N{=}CHC_6H_5$ substituent. Table S2 also examines the change in dipole moment of the coordination complex between the reactant FeL(OH) and the transition state complexes ($\Delta dipole^{\ddagger}$). With virtually all substituents, there is a decrease in the dipole moment (average change of -3.6 Debye) between the reactant and transition state complexes, except for the $N{=}CHC_6H_5$ case, where the transition state is actually more polar than the reactant complex. Whereas then with all other substituents the change in solvation energy between reactant and transition state complexes is on average +7.6 kcal/mol, the transition state complex with $N{=}CHC_6H_5$ is actually better solvated than the reactant complex by 1.2 kcal/mol. This difference in solvation energies largely accounts for the difference between the calculated activation free energy with $N{=}CHC_6H_5$ (24.41 kcal/mol, Table 2) and what might be expected from the correlation curve in Figure S2 (~30 kcal/mol).

In order to confirm that the aforementioned anomalies in solvation energies were not due to the IEF-PCM solvation model [1-4], solvation energies were also computed using the CPCM polarizable conductor solvation model [5,6]. Differences in solvation energies between reactant, transition state, and product complexes with the various substituents were consistent between IEF-PCM (Table S2) and CPCM (Table S3), with the same anomalies being observed.

Based upon this analysis, the $NHCH_3$ and $N{=}CHC_6H_5$ points were removed from the ΔG_{rxn} and $\Delta G^{\ddagger}$ Hammett plots, respectively. The resulting final Hammett plots involving ΔG_{rxn} and $\Delta G^{\ddagger}$ (Figures 3 and 4, respectively) show significantly higher R^2 values of 0.767 and 0.596 (cf. Figures S1 and S2), respectively, for the current purpose of *qualitatively* understanding the effect of ligand substituents on the reaction energetics.

References

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Table S4. Raw computational data used to calculate the thermodynamics of the deformylation reactions.

a) small molecules

	E (gas phase, 6-311G(d,p) basis, a.u.)	E (gas phase, a.u.)[a]	E (water, IEF-PCM, a.u.)[a]	E (water, CPCM, a.u.)[a]	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)
ammonia	-56.55477	-56.53786	-56.54468	-56.54480	21.695	2.308	48.151
formamide	-169.88802	-169.84236	-169.85838	-169.85905	28.502	2.938	62.248

[a] 6-31G(d,p) basis.

b) H substituent

	E (gas phase, 6-311G(d,p) basis, a.u.)	E (gas phase, a.u.)[a]	E (water, IEF-PCM, a.u.)[a]	E (water, CPCM, a.u.)[a]	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)
FeL(OH)	-1284.57310	-1284.38313	-1284.41582	-1284.41615	185.727	13.697	153.745
transition state	-1454.44961	-1454.21430	-1454.24950	-1454.24990	216.373	15.663	167.950
intermediate	-1454.45774	-1454.22358	-1454.25755	-1454.25793	217.797	15.848	171.533
FeL(formate) - bidentate	-1397.92593	-1397.70768	-1397.73386	-1397.73414	192.797	14.569	160.782
FeL(formate) - monodentate	n/a	n/a	n/a	n/a	n/a	n/a	n/a

[a] 6-31G(d,p) basis.

c) CH_3 substituent

	E (gas phase, 6-311G(d,p) basis, a.u.)	E (gas phase, a.u.)[a]	E (water, IEF-PCM, a.u.)[a]	E (water, CPCM, a.u.)[a]	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)
FeL(OH)	-1363.20354	-1362.99925	-1363.02683	-1363.02716	220.032	15.541	166.763
transition state	-1533.07828	-1532.82892	-1532.86009	-1532.86049	251.346	17.804	183.923
intermediate	-1533.08774	-1532.83917	-1532.86765	-1532.86800	252.466	18.126	187.633
FeL(formate) - bidentate	-1476.55365	-1476.32127	-1476.34512	-1476.34541	227.366	16.934	179.383
FeL(formate) - monodentate	-1476.55326	-1476.32024	-1476.34445	n/a	227.240	16.435	173.940

[a] 6-31G(d,p) basis.

d) iPr substituent

	E (gas phase, 6-311G(d,p) basis, a.u.)	E (gas phase, a.u.)[a]	E (water, IEF-PCM, a.u.)[a]	E (water, CPCM, a.u.)[a]	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)
FeL(OH)	-1520.43150	-1520.19780	-1520.22450	-1520.22485	291.623	18.806	191.106
transition state	-1690.30541	-1690.02664	-1690.05678	-1690.05719	322.782	21.214	211.013
intermediate	-1690.31498	-1690.03705	-1690.06426	-1690.06463	323.906	21.538	215.149
FeL(formate) - bidentate	-1633.78086	-1633.51905	-1633.54244	-1633.54276	298.674	20.386	208.151
FeL(formate) - monodentate	-1633.77993	-1633.51747	-1633.54018	n/a	298.630	19.832	200.640

[a] 6-31G(d,p) basis.

e) OCH_3 substituent

	E (gas phase, 6-311G(d,p) basis, a.u.)	E (gas phase, a.u.)[a]	E (water, IEF-PCM, a.u.)[a]	E (water, CPCM, a.u.)[a]	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)
FeL(OH)	-1513.59103	-1513.34468	-1513.38264	-1513.38308	226.256	16.769	176.182
transition state	-1683.46265	-1683.17117	-1683.21295	-1683.21349	257.221	19.152	196.619
intermediate	-1683.47258	-1683.18195	-1683.22266	-1683.22319	258.408	19.469	200.560
FeL(formate) - bidentate	-1626.93658	-1626.66197	-1626.69589	n/a	233.301	17.662	184.591
FeL(formate) - monodentate	-1626.94026	-1626.66458	-1626.69832	-1626.69869	233.020	17.843	187.525

[a] 6-31G(d,p) basis.

f) $OCH(CH_3)_2$ substituent

	E (gas phase, 6-311G(d,p) basis, a.u.)	E (gas phase, a.u.)[a]	E (water, IEF-PCM, a.u.)[a]	E (water, CPCM, a.u.)[a]	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)
FeL(OH)	-1670.83085	-1670.55537	-1670.58541	-1670.58577	296.837	20.051	206.005
transition state	-1840.70273	-1840.38175	-1840.41663	-1840.41767	328.077	22.360	220.332
intermediate	-1840.71281	-1840.39270	-1840.42698	-1840.42746	329.365	22.568	222.844
FeL(formate) - bidentate	-1784.17927	-1783.87541	-1783.90265	n/a	303.733	21.067	211.419
FeL(formate) - monodentate	-1784.18132	-1783.87614	-1783.90520	-1783.90557	303.651	21.203	213.105

[a] 6-31G(d,p) basis.

g) $N{=}CHC_6H_5$ substituent

	E (gas phase, 6-311G(d,p) basis, a.u.)	E (gas phase, a.u.)[a]	E (water, IEF-PCM, a.u.)[a]	E (water, CPCM, a.u.)[a]	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)
FeL(OH)	-1933.49732	-1933.17674	-1933.20757	-1933.20794	314.146	21.708	219.854
transition state	-2103.36192	-2102.99715	-2103.04587	-2103.04662	344.375	24.385	244.147
intermediate	-2103.37382	-2103.00917	-2103.05662	-2103.05561	345.570	24.121	240.032
FeL(formate) - bidentate	-2046.83961	-2046.49190	-2046.53428	n/a	320.430	22.932	231.028
FeL(formate) - monodentate	-2046.84041	-2046.49113	-2046.53345	-2046.53476	320.424	22.903	230.351

[a] 6-31G(d,p) basis.

h) $NHCH_3$ substituent

	E (gas phase, 6-311G(d,p) basis, a.u.)	E (gas phase, a.u.)[a]	E (water, IEF-PCM, a.u.)[a]	E (water, CPCM, a.u.)[a]	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)
FeL(OH)	-1473.87589	-1473.64357	-1473.67998	-1473.68047	242.585	17.299	179.353
transition state	-1643.74494	-1643.46744	-1643.50973	-1643.51036	273.594	19.185	193.799
intermediate	-1643.75617	-1643.47901	-1643.51572	-1643.51621	274.603	19.620	199.651
FeL(formate) - bidentate	-1587.22201	-1586.96128	-1586.99695	n/a	249.192	18.608	192.985
FeL(formate) - monodentate	-1587.22050	-1586.95925	-1586.99338	-1586.99378	249.066	18.611	190.832

[a] 6-31G(d,p) basis.

i) $N(CH_3)_2$ substituent

	E (gas phase, 6-311G(d,p) basis, a.u.)	E (gas phase, a.u.)[a]	E (water, IEF-PCM, a.u.)[a]	E (water, CPCM, a.u.)[a]	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)
FeL(OH)	-1552.46920	-1552.22504	-1552.25092	-1552.25211	277.601	19.014	192.261
transition state	-1722.33775	-1722.04707	-1722.07935	-1722.07983	308.202	21.072	208.986
intermediate	-1722.35024	-1722.05965	-1722.08896	-1722.08937	309.498	21.375	213.557
FeL(formate) - bidentate	-1665.81484	-1665.53473	-1665.56726	-1665.56761	283.985	20.272	205.287
FeL(formate) - monodentate	-1665.81503	-1665.54015	-1665.56726	n/a	284.020	20.396	206.865

[a] 6-31G(d,p) basis.

j) F substituent

	E (gas phase, 6-311G(d,p) basis, a.u.)	E (gas phase, a.u.)[a]	E (water, IEF-PCM, a.u.)[a]	E (water, CPCM, a.u.)[a]	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)
FeL(OH)	-1483.03310	-1482.78019	-1482.81308	-1482.81341	175.310	14.381	158.200
transition state	-1652.90646	-1652.60841	-1652.64511	-1652.64551	206.014	16.892	178.323
intermediate	-1652.91620	-1652.61927	-1652.65436	-1652.65474	207.403	17.162	185.713
FeL(formate) - bidentate	-1596.38192	-1596.10097	-1596.12939	-1596.12969	182.390	15.832	174.677
FeL(formate) - monodentate	n/a	n/a	n/a	n/a	n/a	n/a	n/a

[a] 6-31G(d,p) basis.

k) $CClF_2$ substituent

	E (gas phase, 6-311G(d,p) basis, a.u.)	E (gas phase, a.u.)[a]	E (water, IEF-PCM, a.u.)[a]	E (water, CPCM, a.u.)[a]	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)
FeL(OH)	-2679.33706	-2678.94971	-2678.98139	-2678.98174	188.942	18.376	191.082
transition state	-2849.20672	-2848.77506	-2848.81114	-2848.81157	219.942	20.777	211.455
intermediate	-2849.21609	-2848.78552	-2848.81958	-2848.82000	220.950	20.638	211.852
FeL(formate) - bidentate	-2792.67925	-2792.26610	-2792.29602	-2792.29637	195.820	19.917	206.116
FeL(formate) - monodentate	n/a	n/a	n/a	n/a	n/a	n/a	n/a

[a] 6-31G(d,p) basis.

l) CN substituent

	E (gas phase, 6-311G(d,p) basis, a.u.)	E (gas phase, a.u.)[a]	E (water, IEF-PCM, a.u.)[a]	E (water, CPCM, a.u.)[a]	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)
FeL(OH)	-1469.02788	-1468.79414	-1468.83583	-1468.83621	183.427	15.531	166.416
transition state	-1638.90209	-1638.62374	-1638.66600	-1638.66640	214.136	18.094	188.180
intermediate	-1638.90964	-1638.63213	-1638.67660	-1638.67703	215.605	18.194	190.488
FeL(formate) - bidentate	-1582.37267	-1582.11077	-1582.14942	-1582.14981	190.367	17.059	183.169
FeL(formate) - monodentate	n/a	n/a	n/a	n/a	n/a	n/a	n/a

[a] 6-31G(d,p) basis.

m) NO_2 substituent

	E (gas phase, 6-311G(d,p) basis, a.u.)	E (gas phase, a.u.)[a]	E (water, IEF-PCM, a.u.)[a]	E (water, CPCM, a.u.)[a]	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)
FeL(OH)	-1693.55080	-1693.24940	-1693.29124	-1693.29166	188.453	16.449	175.456
transition state	-1863.41769	-1863.07158	-1863.11733	-1863.11780	219.271	18.456	192.863
intermediate	-1863.42717	-1863.08105	-1863.12740	-1863.12788	220.399	19.351	202.412
FeL(formate) - bidentate	-1806.89147	-1806.56246	-1806.60245	-1806.60285	195.447	17.992	190.616
FeL(formate) - monodentate	n/a	n/a	n/a	n/a	n/a	n/a	n/a

[a] 6-31G(d,p) basis.

Cartesian coordinates of optimized geometries from DFT calculations

ammonia

N	-6.193659	1.108616	-0.002386
H	-5.985305	1.510656	-0.911576
H	-5.304737	0.769805	0.355490
H	-6.436900	1.895123	0.593673

formamide

N	12.620103	2.178491	-5.165207
C	12.084423	2.787800	-6.257182
H	11.016335	2.517113	-6.396681
O	12.683467	3.539219	-7.002876
H	13.586563	2.347853	-4.935881
H	12.078209	1.564724	-4.581774

FeL(OH) – H substituent

H	8.469673	7.950472	-4.048306
H	6.794868	8.283939	-3.619926
H	2.611951	8.895289	-2.466861
H	4.303634	8.711036	-2.918182
H	8.073906	8.450819	-2.405770
H	3.867441	9.116285	-1.250086
C	2.337677	6.244483	-1.903359
C	3.447757	7.067065	-1.803552
C	7.586487	6.402559	-2.905900
C	7.730229	7.848508	-3.252367
C	5.850825	6.643755	-1.048387
C	7.723716	4.188720	-2.765028
C	6.248642	6.619480	0.475834
C	2.766943	4.975535	-1.484477
C	8.227798	5.303418	-3.453029
C	5.296601	7.579640	1.214220
C	7.689086	7.154728	0.583626
C	3.576859	8.521028	-2.121064
H	5.936026	7.684408	-1.357963
H	1.352197	6.535206	-2.235238
H	8.962958	5.317992	-4.243696
H	5.354171	8.601627	0.813957
H	4.261943	7.236048	1.168886
H	5.581381	7.619003	2.267106
H	7.783623	8.165753	0.162971
H	8.402406	6.494202	0.088374
H	7.968493	7.205942	1.637472
H	4.912211	1.482144	-1.527901
H	7.959346	3.140153	-2.882094
H	2.214419	4.049329	-1.409871
N	4.464597	6.274376	-1.335904
N	6.830941	4.562323	-1.851853
N	6.752211	5.909041	-1.935609
N	4.053574	5.000862	-1.146007
O	5.187325	1.765911	-0.651117
S	6.178208	4.974250	1.328986
Fe	5.530878	3.557669	-0.393887

transition state – H substituent

C	-4.080149	0.244759	-0.677992
H	3.843084	2.340987	0.132073
H	3.793261	3.232479	-1.387560
H	3.951869	1.479095	-1.411202
H	-5.139576	0.973864	0.887840
H	4.044117	-2.930593	-1.509167
H	-3.540929	-1.665809	0.485808
H	4.023503	-2.112869	0.052076

H	4.057832	-1.170933	-1.447326
H	-4.333599	-0.110195	-1.687364
H	-6.064888	-0.001473	-0.173852
N	-5.159562	0.248664	0.188016
O	-3.135080	-1.332102	-0.323629
O	-3.151466	1.115704	-0.509826
C	1.291440	-0.018315	1.810802
C	1.073396	3.115919	-1.528945
C	2.152070	-2.107388	-1.033805
C	1.875124	1.243395	2.474044
C	1.956899	-1.263091	2.426933
C	3.466866	2.314881	-0.895201
C	3.644428	-2.067836	-0.973616
C	0.013981	-2.594284	-1.398041
C	1.323596	-3.042740	-1.632826
C	1.679014	0.024932	0.287944
C	-0.194937	2.552710	-1.314658
C	1.976236	2.234224	-0.956875
H	2.767007	0.069249	0.251486
H	3.049915	-1.246663	2.309894
H	1.566136	-2.185204	1.993580
H	1.738042	-1.286959	3.496148
H	1.655706	1.213751	3.543011
H	-1.174321	2.906883	-1.602281
H	1.424310	2.153308	2.074516
H	1.313193	4.039275	-2.034920
H	1.637265	-3.926356	-2.168486
H	-0.933043	-3.021968	-1.694667
H	2.966793	1.302164	2.357862
N	1.225504	1.216288	-0.427580
N	1.321637	-1.172277	-0.472351
N	-0.092205	1.405070	-0.651030
N	0.023240	-1.462988	-0.698771
S	-0.523555	-0.081534	2.165570
Fe	-1.557278	-0.105076	0.086646

intermediate – H substituent

C	4.084528	-0.176442	-0.632244
H	-4.194137	-1.729738	-0.045114
H	-4.270223	-2.548546	-1.603830
H	-4.120066	-0.795407	-1.548081
H	4.630561	-1.295890	0.940145
H	-3.499972	3.533122	-1.493062
H	4.093186	1.285844	0.675480
H	-3.625129	2.656541	0.030659
H	-3.800247	1.798429	-1.508900
H	4.596212	0.089189	-1.574289
H	5.792332	-1.185521	-0.191713
N	5.092435	-0.646775	0.307063
O	3.538605	1.068216	-0.084189
O	3.027857	-0.999593	-0.832962
C	-1.283264	0.123263	1.745431
C	-1.569822	-2.913301	-1.691608
C	-1.771300	2.392731	-1.053691
C	-2.037049	-1.070482	2.361252
C	-1.788495	1.426863	2.392692
C	-3.798556	-1.724710	-1.065661
C	-3.250413	2.594552	-0.995484
C	0.419113	2.539935	-1.402569
C	-0.800708	3.196011	-1.629586
C	-1.658314	0.180053	0.216950
C	-0.227176	-2.595869	-1.428423
C	-2.316015	-1.904709	-1.104623
H	-2.738043	0.318625	0.180650

H	-2.872531	1.553966	2.263824
H	-1.275562	2.301914	1.990304
H	-1.582911	1.392778	3.464098
H	-1.843136	-1.094409	3.435119
H	0.678296	-3.111973	-1.714852
H	-1.696154	-2.019861	1.945715
H	-1.956339	-3.761962	-2.236034
H	-0.965416	4.131174	-2.143570
H	1.423301	2.824326	-1.683174
H	-3.123675	-0.986624	2.219273
N	-1.409075	-1.054385	-0.524597
N	-1.106170	1.320584	-0.516416
N	-0.140535	-1.471821	-0.723705
N	0.225738	1.407415	-0.732332
S	0.518302	-0.051051	2.146289
Fe	1.497676	-0.200248	0.030487

FeL(formate), bidentate – H substituent

C	-0.050772	-4.582273	1.545150
H	3.345646	-4.930289	8.879758
H	4.672035	-5.446944	7.825191
H	6.064921	-3.676315	6.472809
H	6.948290	-2.495226	5.511306
H	5.682397	-1.952047	6.609988
H	-0.480085	-4.964817	0.601866
H	3.696671	-6.644325	8.670459
O	-0.398714	-5.116779	2.638364
O	0.776967	-3.625957	1.498773
C	3.982419	-2.942376	2.796269
C	1.230494	-6.448623	5.469359
C	2.701297	-5.796913	7.005407
C	1.826131	-2.304200	6.465743
C	1.952702	-6.886522	6.590744
C	4.999578	-2.867805	4.772957
C	5.223175	-2.718563	3.413828
C	2.558507	-0.952113	6.551424
C	1.228909	-2.646162	7.843534
C	5.962583	-2.743473	5.908093
C	3.653940	-5.685881	8.150632
C	2.900141	-3.404656	6.128188
H	3.711707	-2.926707	1.750111
H	6.164556	-2.479250	2.942254
H	1.938918	-7.864878	7.047338
H	3.631211	-3.363860	6.934485
H	2.001785	-2.692671	8.623115
H	0.683809	-3.590941	7.823572
H	0.519526	-1.866145	8.125792
H	1.843376	-0.179359	6.839096
H	3.355943	-0.967138	7.307142
H	2.983005	-0.661703	5.589341
H	0.530039	-6.979603	4.840544
N	3.666983	-3.162624	4.906330
N	2.398356	-4.778616	6.138396
N	1.507131	-5.175331	5.203232
N	3.049637	-3.210977	3.705188
S	0.423740	-2.120922	5.262975
Fe	0.927044	-3.728013	3.672243

FeL(OH) – CH_3 substituent

H	8.016710	8.289177	-3.769232
H	7.877621	8.563454	-2.034132
H	3.897272	9.386030	-2.281908
H	5.324471	9.249936	-1.262152
H	9.398242	8.003388	-2.709773

H	3.759786	9.587117	-0.534327
H	7.439196	2.710085	-4.332317
H	2.463452	3.493469	-0.779420
H	1.540396	4.292277	-2.066389
H	1.156809	4.622963	-0.376581
H	7.167641	2.187237	-2.657408
H	8.812677	2.481448	-3.248977
C	2.727666	6.929718	-1.286701
C	3.958128	7.554831	-1.182180
C	7.908401	6.471689	-2.641618
C	8.311204	7.905828	-2.787103
C	6.299861	6.667384	-0.661327
C	7.677707	4.257817	-2.864776
C	6.754978	6.358660	0.815039
C	2.957565	5.557778	-1.066438
C	8.329418	5.389253	-3.393544
C	5.950335	7.286689	1.745036
C	8.250775	6.716168	0.912927
C	4.262083	9.013870	-1.319899
H	6.530629	7.718253	-0.811255
H	1.783731	7.412123	-1.495369
H	9.027056	5.417597	-4.218043
H	4.539829	1.889387	-1.818789
C	7.775741	2.829299	-3.296962
C	1.979116	4.426774	-1.071749
H	4.886891	7.043593	1.730859
H	6.077864	8.346027	1.481289
H	6.303166	7.152787	2.769164
H	8.440567	7.764650	0.643068
H	8.861494	6.071152	0.279243
H	8.583458	6.571616	1.942406
N	4.862061	6.562438	-0.905688
N	6.897906	4.625550	-1.844982
N	4.257745	5.351685	-0.839219
N	7.041889	5.965912	-1.706655
O	4.930483	1.955366	-0.942179
S	6.543187	4.616111	1.416211
Fe	5.554794	3.624415	-0.432150

transition state – CH_3 substituent

C	-4.078550	0.397382	-0.174461
H	4.162655	2.952742	-1.237233
H	4.179259	1.192813	-1.244697
H	4.086664	2.074116	0.288356
H	-4.623003	0.932831	1.697849
H	4.109918	-1.350436	-1.260868
H	-3.328598	-1.470669	1.014653
H	3.995486	-3.105924	-1.321626
H	3.964060	-2.283377	0.236909
H	-4.540955	0.008622	-1.092883
H	-5.693956	-0.152607	0.950632
H	-1.421476	-2.829456	-2.983593
H	-1.996528	2.683851	-1.609636
H	-1.051313	3.412961	-2.931289
H	-1.231030	4.265027	-1.397607
H	-2.150919	-2.712784	-1.370284
H	-1.297050	-4.191571	-1.869559
N	-5.011233	0.581374	0.832995
O	-3.157549	-1.177971	0.110680
O	-3.102484	1.233685	-0.254187
C	3.626961	-2.219759	-0.802136
C	-0.014461	-2.549464	-1.391123
C	1.290726	-3.050145	-1.571730
C	1.745830	-0.031951	0.390778

C	0.129452	2.615368	-1.336454
C	2.256214	2.111261	-0.868740
C	1.350162	-0.038645	1.910547
C	1.462219	3.046756	-1.501533
C	2.138064	-2.173694	-0.920752
C	1.999120	1.192481	2.570184
C	1.936777	-1.314273	2.543592
C	3.745423	2.069159	-0.751198
H	1.608684	2.123447	2.156069
H	1.804228	3.929564	-2.021747
H	1.581778	-3.939044	-2.112095
C	-1.297009	-3.099395	-1.928232
H	2.834682	-0.060871	0.373231
H	3.093448	1.185291	2.467337
H	3.030656	-1.356717	2.444601
H	1.504719	-2.215912	2.106259
H	1.699900	-1.321151	3.609283
H	1.765986	1.185467	3.636733
C	-1.111986	3.273184	-1.846779
N	1.398062	1.181947	-0.343377
N	1.335249	-1.210346	-0.371751
N	0.105293	1.478902	-0.632190
N	0.028957	-1.431099	-0.659512
S	-0.465556	0.002042	2.241888
Fe	-1.462769	0.032632	0.158579

intermediate – CH_3 substituent

C	-4.000038	-0.472893	-0.334426
H	4.012762	3.185157	-1.227682
H	4.130288	1.428778	-1.209664
H	3.999333	2.326528	0.311129
H	-4.557090	0.843208	1.078212
H	4.214820	-1.151369	-1.222938
H	-3.883412	-1.684173	1.197314
H	4.198858	-2.911497	-1.243437
H	4.122747	-2.057288	0.296031
H	-4.529320	-0.931777	-1.188703
H	-5.721254	0.555592	-0.017802
H	-1.402269	-2.758279	-2.769705
H	-2.121127	2.496018	-1.540739
H	-1.265664	3.468842	-2.756626
H	-1.530559	4.120352	-1.138579
H	-1.915954	-3.077680	-1.109973
H	-0.944488	-4.277323	-1.991087
N	-5.008600	0.102908	0.545034
O	-3.352970	-1.546482	0.403049
O	-3.014109	0.366579	-0.744310
C	3.781739	-2.035775	-0.743392
C	0.161566	-2.581105	-1.310636
C	1.491981	-3.009408	-1.490157
C	1.777982	0.058696	0.430608
C	-0.002984	2.623689	-1.247887
C	2.160888	2.240374	-0.827963
C	1.363119	0.038549	1.949492
C	1.299109	3.136074	-1.431562
C	2.292652	-2.075002	-0.859657
C	1.918769	1.319650	2.599358
C	2.035429	-1.186910	2.597320
C	3.650864	2.286364	-0.725555
H	1.459334	2.215762	2.179676
H	1.578500	4.045872	-1.942622
H	1.830069	-3.890966	-2.014699
C	-1.096653	-3.209210	-1.818721
H	2.866771	0.089526	0.427657

H	3.010049	1.393013	2.492668
H	3.129143	-1.153903	2.495756
H	1.665076	-2.121027	2.172090
H	1.800983	-1.197807	3.663334
H	1.690009	1.302467	3.666548
C	-1.306095	3.203741	-1.695525
N	1.369150	1.249738	-0.308608
N	1.439571	-1.144441	-0.329342
N	0.058810	1.476864	-0.567015
N	0.146286	-1.447325	-0.603822
S	-0.452583	-0.055400	2.304699
Fe	-1.371593	-0.061878	0.164817

FeL(formate), monodentate – CH_3 substituent

C	-0.294215	0.042320	4.936435
H	5.883304	-5.194521	4.024761
H	-0.900642	0.944868	5.157342
H	4.896640	-5.369590	2.564174
H	6.308163	-4.318338	2.556198
H	1.238975	-7.706873	2.517191
H	2.200551	-7.656693	3.992838
H	2.748111	-6.801574	2.541367
H	3.642408	0.467149	4.892944
H	2.521737	0.255697	3.542375
H	4.244426	0.555248	3.231642
H	-1.551987	-2.467848	3.509667
H	-2.187211	-3.428975	4.850284
H	-2.484338	-3.943771	3.183906
O	-0.063865	-0.288177	3.772157
O	0.112417	-0.576786	6.002935
C	3.804673	-1.425627	3.893780
C	-0.491525	-4.297561	3.861600
C	2.871918	-4.691481	4.919198
C	1.075569	-5.863301	3.543471
C	2.930354	-4.797148	6.489306
C	4.656933	-3.469810	3.572117
C	4.852758	-2.133567	3.273357
C	-0.230957	-5.531417	3.233712
C	4.413358	-4.762138	6.903324
C	2.324315	-6.155934	6.887275
C	1.866478	-7.063461	3.136055
C	5.469169	-4.656304	3.166603
H	3.443211	-5.541822	4.550263
H	-0.910729	-6.109961	2.625822
H	5.653794	-1.722410	2.677022
H	4.483793	-4.881229	7.986043
H	4.983513	-5.578637	6.439671
H	4.881412	-3.810359	6.647213
H	1.268511	-6.220730	6.619647
H	2.395954	-6.274472	7.969975
C	-1.748231	-3.487805	3.848778
C	3.536660	0.045226	3.887945
H	2.864098	-6.992582	6.423203
N	3.010015	-2.282525	4.541741
N	3.531914	-3.518995	4.350114
N	0.597074	-3.895764	4.524311
N	1.542489	-4.848716	4.334676
S	2.039704	-3.472907	7.434655
Fe	1.189303	-2.183698	5.724907

FeL(formate), bidentate – CH_3 substituent

C	-4.064810	0.113437	-0.039494
H	3.880688	-2.845867	-1.610641
H	3.956929	-1.943850	-0.099166

H	3.686365	2.364334	-0.054732
H	3.690370	1.472135	-1.584716
H	3.525087	3.224668	-1.584064
H	-5.144092	0.056568	-0.271659
H	3.818070	-1.086782	-1.642995
H	-2.286106	-2.772121	-1.356101
H	-1.527091	-4.268370	-0.797545
H	-1.403386	-3.811076	-2.497055
H	-2.561586	2.757434	-0.871585
H	-2.094163	2.778913	-2.580020
H	-1.787850	4.194863	-1.572054
O	-3.332233	-0.867312	-0.415659
O	-3.602791	1.106014	0.563011
C	-0.453508	2.566031	-1.215836
C	-0.147025	-2.680975	-1.186720
C	2.000257	-2.077107	-1.015639
C	1.304538	0.031041	1.852074
C	1.170494	-3.060613	-1.518197
C	1.748045	2.230220	-1.007934
C	0.811106	3.101483	-1.531162
C	1.923083	1.312879	2.441697
C	2.040748	-1.195713	2.422528
C	3.239105	2.315860	-1.052106
C	3.488993	-1.971739	-1.087921
C	1.553619	0.054688	0.297686
H	1.934021	-1.198972	3.508859
H	1.803770	1.298423	3.526523
H	2.997874	1.383358	2.225076
H	1.423377	2.208974	2.070206
C	-1.415955	-3.415863	-1.477227
H	1.017963	4.012965	-2.072394
C	-1.801951	3.101991	-1.574026
H	1.479607	-3.942842	-2.059386
H	2.634560	0.119368	0.182262
H	3.114866	-1.170923	2.192741
H	1.617433	-2.129424	2.049294
N	1.036679	1.227779	-0.406163
N	-0.126675	-1.524480	-0.516989
N	-0.300234	1.427178	-0.532183
N	1.177131	-1.165347	-0.409906
S	-0.462517	-0.048292	2.409053
Fe	-1.574390	-0.083459	0.386017

FeL(OH) – iPr substituent

H	3.081423	2.858251	-2.707310
H	1.322189	2.910546	-2.758539
H	-3.068441	2.855366	-2.721273
H	-1.308944	2.902903	-2.768450
H	2.192445	3.603069	-1.380455
H	-2.180801	3.602830	-1.395068
C	4.565155	-1.829090	0.364535
H	-2.539606	-2.483157	0.285547
C	-3.385831	-2.815570	-1.657818
C	-4.573749	-1.816869	0.361099
C	3.384417	-2.816634	-1.664152
H	2.530121	-2.490769	0.276822
H	4.083473	-2.357103	-2.370743
H	4.433874	-1.265282	1.292224
H	5.316749	-1.313608	-0.242511
H	4.963091	-2.815408	0.622307
H	-2.424925	-2.944416	-2.165128
H	-5.321644	-1.303062	-0.251905
H	-4.445821	-1.248809	1.286665
H	-4.974651	-2.801221	0.621797

H	-4.081219	-2.357894	-2.369214
H	-3.771987	-3.808888	-1.409316
H	2.425421	-2.941796	-2.175992
H	3.767965	-3.811607	-1.418262
C	-3.097740	0.417110	-1.511521
C	-2.170518	1.438926	-1.428941
C	2.176716	1.439356	-1.422396
C	2.182472	2.773825	-2.094438
C	0.001037	1.699781	-0.117765
C	2.621778	-0.625605	-0.682165
C	-0.000370	2.112500	1.403493
C	-2.623067	-0.621919	-0.681848
C	3.101725	0.415610	-1.506040
C	-1.257995	2.966722	1.650361
C	1.251503	2.975077	1.650458
C	-2.171175	2.770883	-2.105944
H	0.001642	2.635903	-0.674346
H	-4.002114	0.429728	-2.101169
H	4.007980	0.428319	-2.092795
C	3.230422	-1.972897	-0.387218
C	-3.235820	-1.966648	-0.383810
H	-2.172315	2.390938	1.499324
H	-1.283759	3.855832	1.004808
H	-1.255136	3.309402	2.686703
H	1.270096	3.865485	1.006450
H	-0.004641	-3.508192	0.653655
H	2.169783	2.406120	1.497457
H	1.247455	3.315931	2.687398
N	1.199645	0.996230	-0.570111
N	-1.197255	0.996864	-0.571773
N	1.465337	-0.255725	-0.125901
N	-1.467497	-0.252616	-0.123295
O	-0.003164	-2.974369	1.453626
S	0.004678	0.729486	2.640924
Fe	-0.000869	-1.132956	1.258452

transition state – iPr substituent

C	1.422987	3.581878	0.695887
H	5.224059	-0.998476	-1.121389
H	-0.063346	-4.397833	-1.391419
H	0.795850	-4.712904	0.124313
H	-4.910236	2.130460	-1.476102
H	1.217048	4.273964	-0.132826
H	-0.641760	3.231407	1.751506
H	-4.129889	-3.034859	-1.462708
H	-3.347373	-3.424555	0.067430
H	-2.467353	-3.613108	-1.457543
C	-2.472237	2.360731	-2.884492
C	-4.095528	2.633106	-0.944045
H	-1.960969	2.672315	-0.820613
C	3.527273	0.309622	-2.967454
C	4.763341	-0.067208	-0.774356
H	3.006162	1.118962	-1.049471
H	2.011627	3.648116	2.628946
H	1.309437	5.090572	2.071183
H	-1.473295	2.028007	-3.181862
H	-2.553249	3.428089	-3.114094
H	-3.201885	1.829364	-3.504908
H	-4.249264	2.481374	0.128257
H	-4.180474	3.705078	-1.147589
H	1.635384	-4.857019	-1.418478
H	2.558096	0.518462	-3.430624
H	3.928149	-0.601421	-3.424608
H	4.204253	1.131986	-3.219502

H	4.663231	-0.121949	0.313111
H	5.450135	0.752422	-1.007689
N	1.820863	4.251592	1.840526
O	-0.363271	3.112783	0.834757
O	1.948354	2.432101	0.454821
C	0.892944	-4.272466	-0.872482
C	-2.746490	-1.556264	-0.846421
C	-0.616855	-1.913131	0.491216
C	-2.534107	0.661934	-1.033862
C	1.337674	-2.846363	-0.829410
C	-0.554146	-1.712998	2.047096
C	-3.352434	-0.434649	-1.378127
C	2.411589	-0.899063	-1.066284
C	-3.184293	-2.983184	-0.920319
C	0.431851	-2.750018	2.616704
C	-1.958290	-1.994186	2.614412
C	-2.715501	2.116990	-1.384104
C	3.397789	0.177940	-1.439939
C	2.468031	-2.274652	-1.377649
H	-0.941820	-2.942353	0.343236
H	0.461143	-2.649323	3.703386
H	-2.298587	-3.013642	2.383411
H	-2.694757	-1.280935	2.240682
H	1.445287	-2.587719	2.246480
H	0.125613	-3.779873	2.385202
H	-1.927396	-1.893866	3.701113
H	-4.271426	-0.419668	-1.944329
H	3.233497	-2.792565	-1.935629
N	-1.621695	-1.111190	-0.205060
N	-1.485054	0.232910	-0.322815
N	0.663035	-1.829104	-0.208279
N	1.306718	-0.642633	-0.356031
S	-0.020808	-0.031559	2.591534
Fe	0.321836	1.157238	0.640590

intermediate – iPr substituent

C	-2.428803	2.927091	0.657209
H	3.961526	3.635203	-0.890240
H	3.478632	-2.642289	-1.569390
H	4.293675	-2.223646	-0.054333
H	-4.651639	-2.511936	-1.636027
H	-3.191385	3.252783	-0.072842
H	-3.223559	1.959755	2.160653
H	-0.098313	-5.055804	-1.658499
H	0.708251	-4.744646	-0.122912
H	1.374888	-4.092653	-1.628469
C	-3.343249	-0.269422	-2.743962
C	-4.569755	-1.637390	-0.981936
H	-3.322715	0.061650	-0.624023
C	1.875736	3.196301	-2.749359
C	2.943776	3.784920	-0.514223
H	0.937594	3.091813	-0.827677
H	-1.436965	3.883884	2.121044
H	-2.412561	4.863083	1.267539
H	-2.475556	0.365635	-2.943544
H	-4.244233	0.328076	-2.915441
H	-3.339880	-1.088046	-3.471476
H	-4.558633	-1.988708	0.053747
H	-5.472598	-1.035609	-1.123344
H	4.874090	-1.569743	-1.584495
H	1.124071	2.580313	-3.251398
H	2.840326	3.017219	-3.236407
H	1.611699	4.245959	-2.911582
H	2.948301	3.580936	0.560452

H	2.688581	4.839887	-0.656083
N	-2.360348	3.945277	1.697129
O	-2.914172	1.708536	1.281775
O	-1.255486	2.610052	0.049906
C	3.974488	-1.831550	-1.024894
C	-0.415704	-3.088047	-0.945854
C	1.198130	-1.667183	0.413956
C	-2.052288	-1.564165	-1.020342
C	3.112481	-0.617670	-0.898073
C	1.101355	-1.541441	1.980397
C	-1.690275	-2.864996	-1.430379
C	2.211135	1.429325	-0.989894
C	0.445331	-4.300896	-1.088017
C	2.536391	-1.411114	2.524607
C	0.478126	-2.846434	2.511819
C	-3.321013	-0.799090	-1.298091
C	1.927888	2.887949	-1.243420
C	3.333477	0.661255	-1.371141
H	1.813050	-2.547743	0.232875
H	2.499033	-1.369130	3.614722
H	1.071966	-3.727190	2.230120
H	-0.544790	-2.977977	2.155749
H	3.018236	-0.495727	2.177611
H	3.159132	-2.272033	2.244122
H	0.442694	-2.804702	3.602022
H	-2.279508	-3.562723	-2.005924
H	4.200261	0.990507	-1.924352
N	-0.061507	-1.948930	-0.273137
N	-1.050827	-1.021577	-0.320682
N	1.902168	-0.577519	-0.256721
N	1.352416	0.659612	-0.315421
S	0.100458	-0.124042	2.630326
Fe	-0.631554	0.898726	0.673098

FeL(formate), monodentate – iPr substituent

C	3.271606	-1.697413	-0.472622
C	-3.269916	-1.700303	-0.472986
C	-3.366260	-2.517826	-1.772114
C	3.366247	-2.515900	-1.771299
H	5.357218	-1.020269	-0.422586
H	4.553570	-0.995168	1.155076
H	2.375816	-2.674678	-2.203410
H	5.058619	-2.533456	0.439794
H	-2.376464	-2.675796	-2.205988
H	3.802942	-3.497730	-1.565024
H	-3.802124	-3.500021	-1.565854
H	-3.999443	-2.021425	-2.514969
H	-5.054996	-2.538209	0.441640
H	-5.355855	-1.024439	-0.418995
H	-4.549704	-1.000212	1.157418
H	3.997975	-2.019749	-2.515563
H	-2.609033	-2.244168	0.207465
H	2.612183	-2.241133	0.209384
C	4.640091	-1.547711	0.214961
C	-4.637435	-1.552016	0.216980
C	0.002866	-3.703833	0.725521
C	-2.634655	-0.354752	-0.711057
C	2.635050	-0.352464	-0.710806
C	-0.000853	1.933625	-0.058397
C	2.168053	1.732381	-1.379789
C	-0.000956	2.278658	1.478867
C	-2.169768	1.730743	-1.379503
C	-3.101702	0.718197	-1.500183
C	3.101067	0.720795	-1.500148

C	-1.256277	3.122380	1.768371
C	1.254607	3.121882	1.768733
C	2.161183	3.088396	-2.006883
C	-2.164345	3.087003	-2.006088
H	-2.171561	3.892137	-1.264972
H	-0.001197	2.894399	-0.571323
H	0.004652	-4.748939	1.099243
H	4.004578	0.759614	-2.089572
H	-4.005299	0.756295	-2.089527
H	-1.251120	3.418859	2.818914
H	-1.279456	4.039067	1.163335
H	-2.172379	2.556800	1.592329
H	2.170516	2.555792	1.593350
H	1.249034	3.418727	2.819170
H	1.278553	4.038339	1.163381
H	-1.301593	3.239208	-2.663190
H	-3.060923	3.197567	-2.618164
H	3.057478	3.199554	-2.619266
H	2.167877	3.893833	-1.266083
H	1.298093	3.239542	-2.663781
N	-1.476260	-0.013509	-0.139345
N	-1.198968	1.252275	-0.540357
N	1.476430	-0.012169	-0.139030
N	1.197784	1.253180	-0.540442
O	0.000491	-3.469336	-0.481498
O	0.003583	-2.820518	1.680982
S	-0.001559	0.834560	2.646943
Fe	0.000380	-0.934921	1.168296

FeL(formate), bidentate – iPr substituent

C	-0.676296	-3.596813	1.199301
C	3.323826	-2.482501	-2.237322
C	-3.318241	-1.963523	-2.339351
H	2.556730	3.801429	-0.717716
H	1.675329	3.448892	-2.213198
H	-1.715229	4.199052	-0.770100
H	-0.873657	3.694016	-2.244483
H	-2.629339	3.822033	-2.228412
H	-0.754824	-4.696982	1.274140
H	3.422623	3.247123	-2.148114
H	2.426401	-2.527746	-0.294758
C	4.486703	-2.009466	-0.022103
H	-2.870980	-1.982761	-0.238537
C	-4.815127	-1.127290	-0.456280
H	-3.810005	-1.340094	-3.093532
H	3.645944	-3.527509	-2.196675
H	4.069098	-1.927834	-2.817320
H	2.375783	-2.444489	-2.781842
H	-3.827021	-2.932446	-2.323915
H	-2.286266	-2.130434	-2.662346
H	-5.390159	-0.473785	-1.120826
H	4.357270	-1.641356	0.999673
H	5.284853	-1.426286	-0.493587
H	4.822658	-3.049481	0.035205
H	-4.837702	-0.696763	0.548527
H	-5.325715	-2.094119	-0.418758
O	0.387635	-3.122441	0.665087
O	-1.599517	-2.869832	1.621438
C	3.169668	-1.920020	-0.814040
C	-3.368961	-1.313651	-0.944706
C	-2.609656	-0.012133	-0.921779
C	2.647152	-0.506332	-0.833800
C	2.377399	1.690532	-1.166689
C	0.198360	1.997298	1.713946

C	3.221618	0.632381	-1.439174
C	-1.920706	2.094334	-1.232214
C	-2.938528	1.212523	-1.540105
C	-0.970962	2.921160	2.104263
C	1.525067	2.652382	2.141117
C	-1.765334	3.525968	-1.631270
C	2.502795	3.122652	-1.574277
C	0.207017	1.879118	0.143920
H	0.307074	2.900588	-0.220085
H	-0.971483	3.055555	3.187456
H	4.137926	0.683590	-2.007621
H	-3.809831	1.434708	-2.137374
H	1.659886	3.641411	1.681933
H	-0.876524	3.914555	1.644415
H	2.382456	2.024829	1.893965
H	-1.934672	2.490443	1.828342
H	1.520103	2.788199	3.224186
N	-1.035326	1.395576	-0.456416
N	1.508852	-0.161406	-0.222060
N	-1.448565	0.115245	-0.269804
N	1.352084	1.171871	-0.421330
S	0.007184	0.414064	2.659351
Fe	-0.132488	-1.129612	0.948469

FeL(OH) – OCH_3 substituent

H	8.549667	7.860147	-3.986684
H	6.884461	8.255130	-3.573771
H	2.664192	8.930958	-2.528579
H	3.907344	9.212751	-1.311645
H	4.359466	8.710456	-2.948917
H	0.368144	2.924646	-1.268577
H	0.185947	4.646454	-0.841840
H	0.546806	4.172195	-2.530755
H	8.166891	8.435910	-2.365643
H	9.922643	2.866666	-3.274996
H	8.700248	2.686353	-4.571412
H	9.002325	1.347523	-3.432172
O	2.113415	3.918463	-1.173750
O	7.936202	2.854616	-2.635542
C	7.709938	4.175895	-2.560006
C	5.871147	6.733972	-0.969513
C	6.262668	6.794180	0.555004
C	5.299264	7.783656	1.238088
C	7.696651	7.351415	0.639192
C	3.622565	8.570903	-2.150744
C	7.807785	7.809864	-3.187980
C	8.256040	5.256018	-3.285428
C	2.775676	5.076604	-1.323978
C	0.727466	3.933231	-1.475132
C	8.949392	2.431946	-3.533482
C	2.355259	6.331723	-1.813029
C	3.480952	7.137785	-1.752234
C	7.624907	6.383147	-2.783359
H	4.269401	7.424225	1.212863
H	5.583105	7.885521	2.287084
H	7.780114	8.343900	0.173731
H	8.417841	6.676833	0.175157
H	7.974843	7.452906	1.689734
H	4.918899	1.469597	-0.964308
H	1.379661	6.624484	-2.166229
H	8.999103	5.235801	-4.066249
H	5.965054	7.754571	-1.338493
H	5.343622	8.782588	0.781112
N	4.060999	5.100577	-0.980286

N	6.768795	5.947548	-1.812253
N	4.484333	6.364030	-1.241802
N	6.812977	4.597594	-1.672151
O	5.191302	1.855908	-0.126433
S	6.208654	5.196232	1.489005
Fe	5.520837	3.664075	-0.129600

transition state – OCH_3 substituent

C	-4.033387	-0.151094	0.182065
O	-1.373639	2.816337	-1.675224
O	-0.705817	-3.148219	-1.574943
C	-0.556252	-4.345479	-2.317978
H	-4.486622	-0.661046	-0.680230
H	-5.494054	-0.826140	1.438383
H	-2.993467	-1.831039	1.448409
H	4.458533	-2.529760	-1.216235
H	4.350801	-1.708249	0.339648
H	4.063233	1.798287	-1.023869
H	3.785911	2.690057	0.480102
H	-0.036759	-5.118132	-1.737591
H	-4.537370	0.433701	2.047515
H	4.315942	-0.775756	-1.165607
H	3.749445	3.529485	-1.069572
H	-1.233533	4.897667	-1.715842
C	-1.508915	4.050636	-2.356481
H	-0.017581	-4.173600	-3.258586
H	-1.568493	-4.684354	-2.540890
H	-2.564207	4.128604	-2.620030
H	-0.905079	4.076863	-3.272903
N	-4.932401	-0.013181	1.230664
O	-3.172174	0.783012	-0.004977
O	-2.911115	-1.599095	0.514910
C	-0.153330	2.511837	-1.213222
C	0.421744	-2.547434	-1.166803
C	2.003938	2.386323	-0.708656
C	1.081262	3.177852	-1.371377
C	1.984215	1.441381	2.730332
C	2.190413	-1.057225	2.707565
C	2.496320	-1.873779	-0.762422
C	3.476132	2.601164	-0.565143
C	1.775393	-2.870945	-1.398977
C	1.835042	0.191958	0.557452
C	3.979355	-1.702822	-0.689520
C	1.460735	0.146143	2.081280
H	1.494240	2.324277	2.316108
H	2.184516	-3.701896	-1.950670
H	3.073045	1.548000	2.620386
H	1.287903	4.097766	-1.894119
H	3.280896	-0.991478	2.582204
H	1.840153	-2.001742	2.287993
H	1.980622	-1.077591	3.778747
H	2.916911	0.315549	0.520769
H	1.759197	1.416080	3.798296
N	0.308101	-1.443276	-0.430555
N	1.582203	-1.041030	-0.184691
N	-0.014498	1.398081	-0.494962
N	1.308146	1.333497	-0.186768
S	-0.343177	0.000384	2.434962
Fe	-1.399548	-0.207220	0.371752

intermediate – OCH_3 substituent

C	-3.964284	0.389062	0.150770
O	-0.439891	3.374446	-1.253977
O	-1.703038	-2.620290	-1.590099

C	-2.005391	-3.827211	-2.269624
H	-4.600434	-0.030275	-0.649212
H	-5.516779	1.661107	0.468878
H	-3.910167	-0.675161	1.787113
H	3.358472	-3.839671	-1.269968
H	3.546744	-3.037138	0.288394
H	4.282244	0.409549	-1.458747
H	4.551152	1.241876	0.082011
H	-1.781497	-4.704504	-1.650453
H	-4.228293	1.917330	1.420453
H	3.843105	-2.148394	-1.213896
H	4.627189	2.136082	-1.434354
H	0.452525	5.245654	-1.500941
C	-0.228653	4.553156	-2.011605
H	-1.461688	-3.902564	-3.219880
H	-3.076527	-3.793810	-2.470885
H	-1.208461	5.021442	-2.110385
H	0.165030	4.325904	-3.010230
N	-4.816762	1.185182	1.028349
O	-2.879724	1.035124	-0.347594
O	-3.470707	-0.735754	0.930236
C	0.635497	2.609633	-1.015557
C	-0.430909	-2.448196	-1.202226
C	2.644551	1.680054	-0.844496
C	1.994166	2.791416	-1.354924
C	2.384236	0.878271	2.605985
C	2.011395	-1.603877	2.640106
C	1.752639	-2.537845	-0.811384
C	4.097969	1.339034	-0.909492
C	0.722651	-3.228266	-1.430070
C	1.855006	-0.343208	0.476447
C	3.201054	-2.898722	-0.740208
C	1.546302	-0.272932	2.018272
H	2.062705	1.846013	2.218427
H	0.810942	-4.158927	-1.967036
H	3.458089	0.751231	2.407133
H	2.450555	3.607100	-1.892236
H	3.083944	-1.781396	2.476331
H	1.443120	-2.448829	2.247328
H	1.840628	-1.570601	3.717611
H	2.918332	-0.567228	0.399576
H	2.246774	0.896866	3.688739
N	-0.143170	-1.361477	-0.489652
N	1.193003	-1.424902	-0.251989
N	0.453698	1.472969	-0.347081
N	1.687212	0.915325	-0.241287
S	-0.224564	-0.020827	2.492182
Fe	-1.297425	0.288903	0.429325

FeL(formate), monodentate – OCH_3 substituent

C	1.011515	-0.620896	4.144272
C	4.711723	-0.931383	0.963961
C	-3.313770	-2.735985	3.076283
H	-0.243066	-6.770856	-0.418110
H	-0.558207	-7.864613	0.939026
H	-3.450726	-2.467923	2.021966
H	-1.897472	-7.099155	0.086887
O	-1.955904	-3.032519	3.362566
H	0.926808	0.357052	4.662318
O	3.922054	-1.728341	1.832847
H	2.171472	-6.131886	-1.120899
H	3.838796	-5.730263	-1.519061
H	3.505821	-6.897590	-0.242112
H	4.890880	0.001199	1.499400

H	4.182468	-0.715542	0.028364
H	5.673259	-1.410550	0.741281
H	-3.567231	-1.879380	3.701197
H	-3.971791	-3.576130	3.331008
O	1.396346	-1.589126	4.921072
O	0.753337	-0.722502	2.945128
C	3.511422	-7.005388	3.092130
C	-0.882805	-6.938683	0.454722
C	3.164631	-5.960358	-0.692501
C	-1.393902	-4.031432	2.670460
C	1.589656	-5.797219	2.016493
C	3.528044	-2.921156	1.370320
C	3.175501	-4.822398	0.275768
C	1.151670	-7.592564	3.717348
C	2.105325	-6.436641	3.360229
C	3.875833	-3.629325	0.199512
C	-0.882652	-5.774632	1.391490
C	-1.944909	-4.970292	1.771818
H	3.868806	-7.507457	3.993008
H	3.505795	-7.743560	2.277790
H	4.225726	-6.216466	2.852628
H	-2.966522	-5.064006	1.440666
H	0.144200	-7.232281	3.930883
H	1.517866	-8.090352	4.617086
H	4.541630	-3.329894	-0.593718
H	1.579554	-6.606316	1.287247
H	1.103147	-8.343099	2.916015
N	2.671288	-3.618988	2.112006
N	0.215218	-5.306739	2.055279
N	2.468884	-4.783245	1.443498
N	-0.088483	-4.234672	2.830606
S	2.211857	-5.307266	4.829445
Fe	1.525908	-3.273181	3.936380

FeL(formate), bidentate – OCH_3 substituent

C	-0.076576	-3.908867	1.831034
C	5.131041	-3.155036	0.607764
C	-0.001786	-9.176502	3.639288
C	6.702392	-4.746523	5.634069
C	4.141810	-8.006064	7.054571
O	4.144635	-3.630135	1.509743
O	0.468493	-7.839954	3.697053
H	4.084081	-9.080585	7.235402
H	5.885045	-3.922944	0.393580
H	4.596887	-2.908895	-0.310211
H	-0.770912	-3.695718	0.996940
H	6.716986	-5.796205	5.946202
H	6.562973	-4.130657	6.526909
H	3.996535	-7.502672	8.015096
H	7.687517	-4.516691	5.225041
H	5.157711	-7.788398	6.708504
H	5.624834	-2.254257	0.991488
H	-0.807842	-9.173313	2.905237
H	-0.396078	-9.506711	4.608121
H	0.784817	-9.867362	3.310512
O	0.925668	-3.153336	1.992129
O	-0.320506	-4.900721	2.580446
C	1.459631	-7.583514	4.557390
C	3.609329	-5.141121	5.931065
C	4.557008	-3.963610	2.737788
C	5.667264	-4.477290	4.590321
C	2.183563	-8.442179	5.411822
C	5.852586	-4.031903	3.291068
C	2.768551	-4.080500	6.728422

C	3.105197	-7.625933	6.047127
C	3.735610	-2.981496	7.209814
C	2.163466	-4.787565	7.955995
H	4.393599	-5.468454	6.613252
H	2.067898	-9.504652	5.552682
H	6.796295	-3.799850	2.824541
H	1.451787	-5.561015	7.663337
H	1.620573	-4.053166	8.553887
H	2.936238	-5.234402	8.597429
H	4.525886	-3.385746	7.857916
H	4.194085	-2.452067	6.372768
H	3.174890	-2.246488	7.790307
N	3.633426	-4.323609	3.630493
N	2.894672	-6.363068	5.577711
N	4.323196	-4.632758	4.761149
N	1.891679	-6.325277	4.659585
S	1.404086	-3.271298	5.783736
Fe	1.434760	-4.349491	3.739476

FeL(OH) – $OCH(CH_3)_2$ substituent

C	-4.149149	-2.073254	-0.643303
C	3.964667	-2.099650	0.862030
C	5.434669	-1.400861	-1.106297
H	-3.035671	3.629928	-1.965183
H	-5.488253	-1.385867	-2.207144
H	3.044837	-2.620699	1.134729
H	5.494859	-1.374908	-2.197814
H	4.143514	-3.107356	-1.020886
C	-5.435560	-1.399745	-1.115028
H	3.928091	-1.090434	1.281533
H	4.807920	-2.623788	1.322325
H	6.294965	-1.964776	-0.733237
H	5.518107	-0.380273	-0.722785
H	-3.063433	-2.598672	1.156008
H	-1.278224	3.719685	-1.917650
H	-2.219731	3.948581	-0.435363
H	1.297970	3.732197	-1.901253
C	-3.979922	-2.078415	0.870863
H	3.055728	3.640401	-1.927995
H	2.221470	3.949110	-0.405943
H	-4.147994	-3.107367	-1.001604
H	-4.827629	-2.594880	1.331608
H	-3.943249	-1.064514	1.278831
H	-5.519850	-0.374829	-0.743495
H	-6.299322	-1.958101	-0.741609
C	-2.145122	1.900768	-1.128558
C	-1.265611	2.468461	2.301968
C	2.172323	3.383375	-1.341273
C	2.552797	-0.284199	-1.074721
C	1.241796	2.486494	2.310055
C	-2.159775	3.375992	-1.365977
C	-3.035514	0.940501	-1.572513
C	-0.004974	1.727287	1.817567
C	4.144010	-2.077391	-0.650767
C	-0.000399	1.779198	0.245661
C	2.153138	1.906540	-1.114504
C	3.043031	0.947407	-1.561779
C	-2.550470	-0.288605	-1.074187
H	-1.265186	2.491717	3.393246
H	-1.293587	3.507789	1.945113
H	1.255691	3.526828	1.955316
H	2.163301	1.991819	1.999247
H	1.235262	2.507667	3.401366
H	-0.001238	2.836817	-0.015466

H	3.911804	1.113169	-2.178599
H	-2.177711	1.959304	1.986915
H	-3.901118	1.103948	-2.194380
H	0.000486	-3.543201	-0.339444
N	-1.194930	1.235245	-0.398856
N	-1.437093	-0.097104	-0.363646
N	1.198547	1.238020	-0.393211
N	1.437159	-0.095238	-0.367204
O	0.006877	-3.201908	0.560703
O	2.973597	-1.536393	-1.334124
O	-2.973303	-1.541878	-1.325113
S	0.005452	0.039733	2.580883
Fe	0.001470	-1.365902	0.717798

transition state – $OCH(CH_3)_2$ substituent

C	0.412978	3.808002	0.445255
C	-4.194597	1.572546	-1.386917
C	4.218103	1.310639	-1.385841
H	5.526433	-0.361151	-1.917363
H	1.072574	-4.425604	-1.155891
H	-3.219594	-4.193894	-1.119144
C	-4.552572	1.594020	0.093781
C	4.496073	1.273930	0.111622
H	2.075540	-4.380454	0.302793
H	-0.057503	4.347450	-0.388633
H	2.827026	-4.400768	-1.291673
H	-2.372139	-4.220949	0.426705
H	-1.307492	2.910214	1.749497
H	-1.466652	-4.348337	-1.089730
C	-5.272399	0.957613	-2.278563
C	5.313453	0.664105	-2.232724
H	-5.475239	2.164481	0.238133
H	-0.031218	5.306590	1.756455
H	4.114269	2.355502	-1.693414
H	-6.164341	1.591820	-2.264177
H	-4.025611	2.602074	-1.717328
H	-3.752194	2.069602	0.662615
H	-4.718230	0.586291	0.486255
H	1.100252	4.171945	2.308161
H	5.431425	1.802760	0.319208
H	6.241398	1.236543	-2.135960
H	4.604557	0.249323	0.479649
H	3.690306	1.764321	0.659517
H	-5.573626	-0.036794	-1.938897
H	-4.923346	0.887934	-3.312299
H	5.028417	0.655796	-3.288249
N	0.693415	4.646924	1.513316
O	1.219471	2.837144	0.209026
O	-1.174219	2.878145	0.793567
O	2.904176	0.785587	-1.725795
O	-2.886062	0.986132	-1.629755
C	2.471043	-0.374651	-1.207804
C	-2.549326	-0.207542	-1.113493
C	-0.063741	-2.056584	0.599022
C	2.015343	-2.511852	-0.787058
C	2.905846	-1.695712	-1.458168
C	-2.239652	-2.368443	-0.681977
C	-3.088976	-1.494119	-1.335236
C	-0.006151	-1.726819	2.131290
C	1.985357	-4.004819	-0.720918
C	-2.317618	-3.858999	-0.604176
C	1.250464	-2.402138	2.711366
C	-1.254423	-2.343021	2.790167
H	3.732712	-2.015657	-2.071409

H	-3.953513	-1.762191	-1.919919
H	-0.102220	-3.143428	0.532337
H	-2.172583	-1.895997	2.405423
H	-1.220830	-2.148035	3.863799
H	2.163285	-1.988700	2.279643
H	1.242416	-3.490859	2.558893
H	-1.299451	-3.432397	2.649273
H	1.284979	-2.217829	3.786881
N	-1.453752	-0.284243	-0.354739
N	1.392180	-0.374449	-0.420422
N	1.120467	-1.679682	-0.169243
N	-1.267758	-1.602441	-0.098107
S	0.047655	0.073546	2.532443
Fe	-0.005243	1.189535	0.488846

intermediate – $OCH(CH_3)_2$ substituent

C	-0.731337	3.713927	0.220806
C	-4.348477	1.116341	-1.124249
C	4.120939	1.797688	-1.128564
H	5.631224	0.218229	-1.083789
H	1.638412	-4.291902	-1.306752
H	-2.674480	-4.488232	-1.319267
C	-4.613355	0.975159	0.369434
C	4.021408	1.994931	0.378910
H	2.570140	-4.194143	0.196317
H	-1.421715	4.019743	-0.590240
H	3.386501	-4.094843	-1.362475
H	-1.842392	-4.495540	0.234474
H	-1.169462	3.214792	2.028612
H	-0.915465	-4.443452	-1.273790
C	-5.395444	0.439911	-2.007533
C	5.439625	1.173498	-1.580484
H	-5.590893	1.405989	0.606601
H	-0.721828	5.663432	0.853387
H	4.013388	2.770934	-1.617367
H	-6.357049	0.949160	-1.889979
H	-4.327064	2.181237	-1.375615
H	-3.852084	1.505315	0.944067
H	-4.627613	-0.073676	0.679846
H	0.741804	5.072354	0.409256
H	4.836324	2.642153	0.717748
H	6.268074	1.844946	-1.334591
H	4.100381	1.047185	0.918831
H	3.072525	2.465246	0.642132
H	-5.547072	-0.609145	-1.740206
H	-5.107428	0.498839	-3.060532
H	5.441228	1.015610	-2.662491
N	-0.116999	4.848598	0.898573
O	0.221663	2.863566	-0.236623
O	-1.601343	3.061762	1.175493
O	2.971294	1.085978	-1.669482
O	-2.994218	0.719338	-1.487717
C	2.629626	-0.123277	-1.191314
C	-2.487950	-0.455600	-1.077209
C	0.227255	-2.086445	0.505139
C	2.373610	-2.308757	-0.847582
C	3.197254	-1.387485	-1.466275
C	-1.912936	-2.587010	-0.783065
C	-2.882537	-1.783575	-1.355216
C	0.230888	-1.766047	2.044650
C	2.486889	-3.798570	-0.820456
C	-1.820616	-4.078582	-0.777116
C	1.528971	-2.347123	2.636393
C	-0.975129	-2.490454	2.672267

H	4.070862	-1.601962	-2.060834
H	-3.735904	-2.119276	-1.921118
H	0.296275	-3.170961	0.430740
H	-1.919986	-2.101158	2.290059
H	-0.965608	-2.324890	3.751169
H	2.413035	-1.857826	2.224740
H	1.607377	-3.430392	2.468438
H	-0.937574	-3.575402	2.499802
H	1.533717	-2.176712	3.714544
N	-1.354082	-0.444323	-0.374295
N	1.531197	-0.255780	-0.444352
N	1.381293	-1.586568	-0.237677
N	-1.006256	-1.743433	-0.200559
S	0.132898	0.024109	2.504022
Fe	-0.015052	1.099339	0.429520

FeL(formate), monodentate – $OCH(CH_3)_2$ substituent

C	0.012025	-3.210261	1.720352
C	-3.750994	-2.427867	-0.479614
C	3.766342	-2.407506	-0.479222
H	3.070063	2.718939	-3.082112
H	1.310946	2.748256	-3.150593
C	2.906666	-2.898967	-1.637363
h	2.170927	3.720711	-1.945301
C	-2.882992	-2.913225	-1.634007
H	0.017490	-4.151907	2.309359
H	5.290214	-1.403468	-1.698797
H	-3.092188	2.709906	-3.073597
H	-2.193425	3.713785	-1.938367
H	-1.333400	2.746096	-3.147463
H	-3.761850	-3.205114	0.290686
H	5.725002	-3.016334	-1.138375
C	-5.199068	-2.123371	-0.859701
H	3.780128	-3.185323	0.290465
C	5.213612	-2.091723	-0.853204
H	-1.876401	-3.140849	-1.278572
H	3.350442	-3.808759	-2.053045
H	2.843554	-2.162190	-2.443114
H	1.900305	-3.133638	-1.285898
H	-3.318685	-3.826073	-2.051564
H	-2.821939	-2.175909	-2.439431
H	-5.702558	-3.052171	-1.145326
H	-5.277388	-1.437144	-1.706815
H	-5.736139	-1.694350	-0.009832
H	5.744179	-1.660122	-0.000567
O	-3.143867	-1.327271	0.254252
O	3.147960	-1.312379	0.252872
O	0.005558	-2.148063	2.464650
O	0.012498	-3.247059	0.489502
C	-1.264073	3.692788	1.203602
C	2.168276	2.759906	-2.469052
C	-2.188683	2.753629	-2.463281
C	2.620765	-0.248733	-0.366729
C	-0.006053	2.118479	-0.297676
C	-2.622452	-0.260377	-0.364715
C	-2.177463	1.589289	-1.526765
C	1.247423	3.696996	1.202736
C	-0.006877	2.806749	1.119876
C	2.164491	1.596806	-1.530949
C	3.104071	0.589780	-1.397919
C	-3.112272	0.577872	-1.392967
H	-1.260300	4.226574	2.155697
H	-1.288184	4.442406	0.400499
H	-2.178467	3.098916	1.165424

H	4.018566	0.498940	-1.959591
H	2.163765	3.106156	1.164337
H	1.242295	4.231162	2.154614
H	-4.028090	0.484189	-1.952016
H	-0.007985	2.933052	-1.020858
H	1.268699	4.446333	0.399293
N	-1.459030	0.204535	0.094615
N	1.192425	1.343871	-0.603924
N	-1.201769	1.338923	-0.602957
N	1.456590	0.211788	0.094916
S	-0.004682	1.677159	2.593167
Fe	0.000160	-0.408609	1.583501

FeL(formate), bidentate – $OCH(CH_3)_2$ substituent

C	-0.015416	-3.715362	0.765475
C	-4.250423	-1.787792	-0.899668
C	4.257615	-1.784589	-0.866554
C	-2.192528	3.636166	-1.115396
C	2.104885	3.599517	-1.307565
H	-4.625081	-0.439877	0.773685
H	-6.293551	-1.912164	-1.582127
H	2.977066	3.878154	-1.901169
C	-5.393096	-1.331132	-1.804534
H	-4.112027	-2.864917	-1.031640
H	-0.010194	-4.819763	0.803137
H	-1.328418	4.020564	-1.667600
H	-2.229629	4.146862	-0.148521
H	2.153946	4.159260	-0.368508
H	-3.085669	3.922218	-1.673219
H	1.218361	3.935450	-1.855880
C	-4.485962	-1.507379	0.579070
H	4.139910	-2.865720	-0.984961
C	4.461258	-1.478362	0.611943
C	5.408938	-1.319779	-1.756048
H	-5.138133	-1.489916	-2.855715
H	-5.639102	-0.275960	-1.656596
H	-5.392936	-2.025810	0.904385
H	-3.649230	-1.870055	1.177851
H	5.364431	-1.985582	0.964397
H	3.614522	-1.835785	1.199831
H	4.590647	-0.406938	0.791813
H	6.318114	-1.873715	-1.502291
H	5.625428	-0.255883	-1.624686
H	5.180868	-1.505937	-2.808921
O	-2.966828	-1.281427	-1.370560
O	2.975106	-1.306437	-1.368256
O	-1.122255	-3.105868	0.759474
O	1.090005	-3.099942	0.724337
C	2.550903	-0.063403	-1.093987
C	0.013950	1.952166	0.330657
C	-2.559479	-0.041286	-1.060535
C	-2.165262	2.148709	-0.973802
C	3.008256	1.182424	-1.578511
C	-3.059186	1.216450	-1.466594
C	0.051072	1.839829	1.897251
C	-1.148221	2.633740	2.449323
C	1.355866	2.497601	2.383939
C	2.115971	2.120366	-1.094266
H	0.016925	3.019043	0.110789
H	3.853804	1.371546	-2.219945
H	-3.933157	1.419981	-2.063807
H	2.234601	1.953883	2.034444
H	1.374091	2.483460	3.475305
H	1.432153	3.545783	2.062192

H	-1.110176	3.690823	2.150702
H	-2.098698	2.205935	2.126277
H	-1.127818	2.595837	3.540105
N	-1.438070	0.108337	-0.352094
N	1.192236	1.428867	-0.356478
N	-1.200320	1.443054	-0.305471
N	1.454867	0.098382	-0.348643
S	-0.031300	0.122339	2.581283
Fe	-0.001704	-1.225638	0.696454

FeL(OH) – N=CHC$_6$H$_5$ substituent

C	4.540605	4.255115	0.094855
C	5.630487	-4.462983	-0.000563
C	2.167711	3.943245	-0.329464
C	3.095593	-3.298533	-0.290510
C	2.024873	5.335038	-0.483078
C	4.389146	5.634038	-0.063831
C	3.279110	-4.673307	-0.530163
C	4.537121	-5.247564	-0.386938
C	4.199366	-2.518663	0.098354
C	3.128503	6.170512	-0.352532
C	3.437474	3.413422	-0.038198
C	5.458726	-3.098858	0.242805
C	1.036638	3.022075	-0.464957
C	-4.664190	1.627523	-1.781735
C	-3.913021	-1.877674	1.799822
C	-4.383221	0.588474	1.863020
C	-4.025641	-2.588905	-2.004529
C	-2.651900	-2.467800	-1.429913
C	-3.051449	-0.386511	-0.036075
C	-3.274730	1.822904	-1.268499
C	1.790091	-2.648410	-0.433723
C	-1.232633	2.577655	-0.762397
C	-3.331149	-0.480814	1.514202
C	-2.437652	2.905352	-1.424060
C	-0.507223	-2.726569	-0.854463
C	-1.564697	-3.294637	-1.601163
H	1.042049	5.736506	-0.705910
H	5.248586	6.291116	0.037936
H	6.305104	-2.488831	0.545729
H	6.611838	-4.916099	0.110896
H	1.780149	-1.572062	-0.240617
H	1.284554	1.961906	-0.368366
H	-4.741763	0.773120	-2.462376
H	4.054172	-1.459816	0.294256
H	-5.393985	1.488423	-0.978753
H	-4.959171	2.515887	-2.342452
H	-4.069813	-3.487112	-2.622480
H	-4.798890	-2.682097	-1.235791
H	-4.008615	1.597921	1.685687
H	-4.627240	0.512609	2.924264
H	-4.024941	-0.512481	-0.506865
H	-2.644077	3.822940	-1.952722
H	-4.171508	-1.943058	2.858287
H	-1.512812	-4.197017	-2.190290
H	5.517022	3.837020	0.323022
H	2.054563	0.261045	2.017805
H	-3.189815	-2.666665	1.589316
H	-4.827409	-2.065905	1.220680
H	-5.313178	0.444484	1.296328
H	-4.284917	-1.739708	-2.645569
H	3.542979	2.340473	0.095961
H	2.422586	-5.268601	-0.828082
H	3.011982	7.243895	-0.474863

H	4.671980	-6.309201	-0.575103
N	-0.161936	3.444171	-0.678007
N	-1.330919	1.349166	-0.213088
N	-2.577375	0.908154	-0.518673
N	-0.931477	-1.600414	-0.242997
N	-2.236064	-1.461814	-0.593018
N	0.736566	-3.315461	-0.759171
O	1.665694	0.224979	1.138516
S	-1.875430	-0.224998	2.632665
Fe	-0.186820	-0.004997	1.095245

transition state – N=CHC$_6$H$_5$ substituent

C	0.433788	1.954706	2.657963
H	-3.844784	5.136877	0.947992
H	2.961092	2.845105	0.154191
H	-3.056715	2.803243	0.563388
H	-6.144974	2.264182	-2.381344
H	-5.781843	6.023381	-0.331360
H	4.850997	0.028182	-1.523446
H	-4.714441	0.434550	-1.885120
H	6.504833	1.673485	-1.978997
H	6.100735	5.711879	-0.567091
H	-0.093276	2.298028	4.601833
H	0.085233	2.950354	2.348267
H	-1.595914	0.759716	2.980672
H	7.418469	3.965563	-1.747036
H	-6.935119	4.581087	-1.995102
H	0.914622	0.958131	4.345244
H	3.874712	5.153968	0.386443
N	0.620802	1.872771	4.028651
O	1.216738	1.283655	1.894333
O	-1.207109	1.176272	2.201569
C	-4.343825	4.507760	0.216015
C	-4.538582	2.388098	-0.942600
C	-5.640155	2.895141	-1.653487
C	-5.436281	5.007557	-0.502924
C	-6.085159	4.198078	-1.437445
C	6.441752	3.726928	-1.335661
C	5.927003	2.438332	-1.465349
C	-3.893429	3.209303	0.003352
C	4.662095	2.117474	-0.943337
C	3.923632	3.110440	-0.270708
C	4.444895	4.393133	-0.139397
C	5.700254	4.707332	-0.673351
C	-1.320328	-4.446294	1.571455
C	4.142688	0.757953	-1.103188
C	-2.620599	-0.753480	-0.869879
C	-0.101270	-3.159724	-0.209192
C	2.474413	-0.840307	-0.950967
C	-2.272110	-2.865748	-1.505836
C	-0.077568	-3.576287	1.304201
C	2.019517	-2.930815	-1.589727
C	1.186641	-4.424507	1.538570
C	-2.326450	-4.225923	-2.122494
C	1.993821	-4.283351	-2.224764
C	2.927199	-1.909764	-1.766586
C	-3.144515	-1.810485	-1.659393
C	-4.087785	1.018267	-1.194573
H	1.109148	-4.434232	-2.852631
H	-2.357031	-5.023542	-1.374614
H	2.868760	-4.387785	-2.868546
H	-2.244887	-3.886448	1.420467
H	1.210189	-5.319154	0.900058
H	-1.338382	-5.346855	0.941062

H	-0.125615	-4.090683	-0.773841
H	3.783668	-1.930373	-2.422563
H	-4.036238	-1.813222	-2.266828
H	-1.304426	-4.772050	2.613304
H	2.096485	-3.845040	1.374307
H	1.197031	-4.759291	2.577619
H	-1.477087	-4.417726	-2.786896
H	-3.232629	-4.304844	-2.725366
H	2.028258	-5.092298	-1.489059
N	2.944279	0.442117	-0.766951
N	-3.030753	0.541291	-0.642015
N	1.092746	-2.467246	-0.687875
N	-1.294102	-2.433023	-0.642733
N	-1.494232	-1.158020	-0.258481
N	1.350396	-1.198305	-0.308317
S	-0.075912	-2.167635	2.491303
Fe	-0.047890	-0.214670	1.221031

intermediate – N=CHC$_6$H$_5$ substituent

C	-0.398775	2.508678	1.307296
H	-4.890532	4.567907	1.580804
H	3.025267	3.142053	-0.734636
H	-3.722169	2.435787	1.103693
H	-6.319422	1.773632	-2.263199
H	-6.776989	5.306194	0.138974
H	5.064280	-0.054791	-0.698112
H	-4.770540	0.093176	-1.696886
H	6.927842	1.371555	-0.401691
H	6.512020	5.648425	-0.406557
H	0.640278	4.108591	0.651766
H	-1.303176	3.053346	1.640256
H	-1.504325	1.751050	-0.129759
H	7.951662	3.625141	-0.298191
H	-7.492271	3.900090	-1.782675
H	1.563796	2.884246	1.238442
H	4.048465	5.407803	-0.626115
N	0.714665	3.418558	1.393289
O	-0.185399	1.403437	2.075416
O	-0.613283	2.129834	-0.079750
C	-5.197436	3.960611	0.734201
C	-4.923457	1.969119	-0.625441
C	-6.003878	2.388253	-1.423627
C	-6.260942	4.374638	-0.075735
C	-6.664041	3.584846	-1.154685
C	6.874309	3.523315	-0.391596
C	6.297645	2.256202	-0.450968
C	-4.532802	2.769101	0.466048
C	4.904080	2.108632	-0.562906
C	4.098142	3.260542	-0.632161
C	4.677220	4.523496	-0.574575
C	6.064730	4.659388	-0.451933
C	-1.206170	-4.367055	1.679296
C	4.332863	0.762478	-0.618095
C	-2.610025	-0.902637	-0.698907
C	0.073085	-3.146164	-0.109402
C	2.612550	-0.758461	-0.740825
C	-2.090536	-2.946376	-1.434693
C	0.075668	-3.555675	1.410720
C	2.258532	-2.869981	-1.377538
C	1.299950	-4.461304	1.645595
C	-2.039465	-4.279235	-2.107342
C	2.309538	-4.228825	-1.996877
C	3.151377	-1.827301	-1.500555
C	-3.049188	-1.962734	-1.533580

C	-4.258351	0.708233	-0.945423
H	1.463752	-4.413762	-2.667944
H	-2.029553	-5.108718	-1.393858
H	3.219468	-4.310703	-2.593645
H	-2.102708	-3.758526	1.552113
H	1.269458	-5.364638	1.020236
H	-1.277457	-5.252510	1.032009
H	0.093421	-4.080471	-0.668158
H	4.049252	-1.823133	-2.099009
H	-3.945570	-2.018252	-2.130991
H	-1.192299	-4.713816	2.714201
H	2.235986	-3.930661	1.463975
H	1.306164	-4.781117	2.689208
H	-1.166140	-4.382061	-2.760014
H	-2.926606	-4.394663	-2.732147
H	2.331555	-5.029513	-1.252019
N	3.067645	0.534964	-0.568215
N	-3.155041	0.330690	-0.394807
N	1.252010	-2.414522	-0.562731
N	-1.139039	-2.469090	-0.565930
N	-1.442793	-1.234105	-0.119348
N	1.446646	-1.129770	-0.188858
S	0.154615	-2.158506	2.612206
Fe	-0.013218	-0.267289	1.260683

FeL(formate), monodentate – N=CHC$_6$H$_5$ substituent

H	2.718806	3.052920	-0.043419
H	-5.961097	5.883525	-0.038712
H	-3.547577	5.372473	0.271528
H	-6.711703	1.757969	-0.975134
H	4.956192	0.161203	-1.077758
H	-2.712977	3.055976	-0.041445
H	-4.956590	0.170060	-1.078437
H	-7.542727	4.071754	-0.666434
H	3.558897	5.367499	0.269328
H	6.715091	1.744594	-0.972941
H	5.973924	5.872408	-0.038982
H	7.551607	4.056423	-0.664525
C	-4.240427	4.579707	0.004178
C	-3.766582	3.283238	-0.164805
C	-4.658394	2.250199	-0.515406
C	-5.598765	4.867875	-0.172508
C	-6.019842	2.550547	-0.699771
C	6.024958	2.539011	-0.698544
C	4.249996	4.572883	0.002941
C	5.609202	4.857599	-0.172659
C	-6.488454	3.851043	-0.526020
C	6.496666	3.838401	-0.524938
C	4.662602	2.242095	-0.515246
C	3.773080	3.277523	-0.165896
C	0.004980	2.547812	1.583081
C	-1.255742	-4.460306	1.598813
C	4.200159	0.867648	-0.704167
C	-2.569152	-0.772149	-0.709057
C	-0.002759	-3.152886	-0.145326
C	2.566642	-0.775508	-0.709734
C	-2.175708	-2.846026	-1.447384
C	-0.002158	-3.596846	1.363977
C	2.168292	-2.847545	-1.450561
C	1.254291	-4.455993	1.599311
C	-2.196882	-4.174524	-2.130810
C	2.186114	-4.175089	-2.135925
C	3.067931	-1.806890	-1.545859
C	-3.073509	-1.803804	-1.543010

C	-4.199081	0.874706	-0.704435
H	0.008417	3.389461	2.309394
H	1.322635	-4.315438	-2.795082
H	-2.222351	-5.008896	-1.423480
H	3.081249	-4.241288	-2.756340
H	-2.173454	-3.888253	1.453583
H	1.276884	-5.337279	0.943293
H	-1.274508	-5.342104	0.943357
H	-0.003379	-4.072519	-0.728407
H	3.951124	-1.787712	-2.165411
H	-3.957670	-1.783978	-2.161158
H	-1.252777	-4.815034	2.631107
H	2.170042	-3.880529	1.455263
H	1.251627	-4.811429	2.631362
H	-1.335172	-4.316893	-2.791863
H	-3.093608	-4.240510	-2.748947
H	2.212283	-5.010536	-1.429863
N	2.993210	0.507082	-0.446027
N	-2.993044	0.511406	-0.445911
N	1.192408	-2.432114	-0.577807
N	-1.197794	-2.431129	-0.576648
N	-1.422525	-1.174950	-0.139331
N	1.420098	-1.177017	-0.138893
O	0.004824	1.389683	2.175995
O	0.001977	2.766160	0.375454
S	-0.005051	-2.222430	2.600817
Fe	-0.001077	-0.315807	1.281398

FeL(formate), bidentate – N=CHC$_6$H$_5$ substituent

C	0.538037	2.157353	2.083698
H	-3.546661	5.421835	0.692201
H	3.642536	2.367358	1.056622
H	-2.784750	3.084632	0.300455
H	-6.594316	2.158350	-1.473872
H	-5.829840	6.120577	0.002224
H	4.432557	0.307100	-2.035470
H	-4.971311	0.438041	-1.318538
H	7.087796	4.181596	-2.039592
H	6.508266	5.418884	0.037042
H	4.788211	4.510572	1.584053
H	5.945628	2.046805	-2.565300
H	-7.354674	4.483885	-1.081043
H	0.582540	3.231860	2.346482
O	1.372375	1.359461	2.544657
O	-0.410050	1.806651	1.287652
C	-4.211128	4.706949	0.214983
C	-4.635231	2.471389	-0.618415
C	-5.926218	2.874919	-1.001749
C	-5.497468	5.100910	-0.172537
C	-6.355138	4.182307	-0.781057
C	5.691369	2.588348	-1.657219
C	5.037210	3.972233	0.673918
C	6.334212	3.788908	-1.362952
C	6.007348	4.483348	-0.196380
C	-3.776708	3.404108	-0.003088
C	4.711482	2.070269	-0.792202
C	4.390683	2.775450	0.384846
C	-1.529462	-4.261717	1.646455
C	4.055524	0.807798	-1.131498
C	-2.648631	-0.622316	-0.790800
C	-0.190566	-3.081619	-0.121254
C	2.541357	-0.900116	-0.728762
C	-2.339207	-2.735747	-1.450588
C	-0.238765	-3.455601	1.405931

C	1.989199	-2.946988	-1.436763
C	0.978951	-4.351098	1.703848
C	-2.418585	-4.090291	-2.076635
C	1.923116	-4.292767	-2.082398
C	2.960402	-1.975381	-1.554269
C	-3.197939	-1.665541	-1.582057
C	-4.213389	1.091083	-0.860542
H	1.050649	-4.399356	-2.735613
H	-2.477846	-4.891992	-1.334577
H	2.810535	-4.432160	-2.701827
H	-2.421704	-3.662943	1.456537
H	0.988800	-5.253267	1.076091
H	-1.567563	-5.170185	1.029265
H	-0.231189	-4.026863	-0.660461
H	3.862260	-2.050279	-2.141796
H	-4.090497	-1.641618	-2.187986
H	-1.561899	-4.570905	2.692772
H	1.917355	-3.811002	1.569871
H	0.935005	-4.672709	2.745958
H	-1.565682	-4.298064	-2.731676
H	-3.319041	-4.144245	-2.690592
H	1.900943	-5.106345	-1.351136
N	3.098816	0.321118	-0.423986
N	-3.039369	0.674812	-0.546086
N	1.048552	-2.448514	-0.569309
N	-1.338542	-2.320227	-0.605762
N	-1.510416	-1.042514	-0.214658
N	1.379605	-1.215470	-0.133295
S	-0.210294	-2.037915	2.594256
Fe	0.006797	-0.181669	1.210382

FeL(OH) – $NHCH_3$ substituent

H	10.002926	3.388861	-3.647735
C	8.391806	2.304066	-2.929604
C	9.575580	8.293466	-2.122725
C	6.655574	7.519868	1.991762
C	9.093343	7.405009	1.413762
C	5.400256	9.012450	-1.637649
C	5.077864	7.607214	-1.244974
C	7.364151	6.960163	-0.359120
C	9.229812	6.839795	-2.077597
C	3.204606	3.668039	0.384111
C	9.093859	4.636363	-2.411247
C	7.714190	6.763380	1.168181
C	9.794551	5.806328	-2.794364
C	4.099570	5.650086	-0.799894
C	3.868395	6.947281	-1.321063
H	2.244557	4.978490	-0.900204
H	3.159860	4.145325	1.373874
H	8.725911	8.916325	-2.421578
H	9.944187	8.667190	-1.163759
H	10.364361	8.446361	-2.861212
H	6.143097	9.058130	-2.440789
H	4.493921	9.498033	-2.003120
H	2.342749	3.005576	0.274353
H	7.961294	2.100788	-1.948204
H	8.894158	1.395290	-3.269605
H	7.571135	2.531180	-3.629003
H	9.875701	6.909909	0.835832
H	9.352450	7.297353	2.468698
H	7.517187	8.021637	-0.550014
H	10.602463	5.883805	-3.506919
H	6.934335	7.482738	3.046650
H	2.937156	7.351784	-1.689564

H	5.720181	2.064047	-1.148422
H	5.670595	7.062565	1.893992
H	6.588429	8.577532	1.699749
H	9.091170	8.478162	1.177568
H	5.773557	9.606974	-0.797211
H	4.107007	3.056418	0.333238
N	9.381915	3.365299	-2.854265
N	8.144973	4.934342	-1.512176
N	8.246598	6.286714	-1.308399
N	5.381518	5.519816	-0.435220
N	5.967866	6.725829	-0.701757
N	3.172958	4.631662	-0.713168
O	6.229251	2.185248	-0.340641
S	7.813726	5.013190	1.774832
Fe	6.840252	3.914919	-0.007400

transition state – $NHCH_3$ substituent

C	3.928677	-0.265933	0.662025
C	2.004916	2.728309	-2.089626
H	0.416333	4.012607	-2.432417
C	2.036420	-2.156829	-2.630847
H	0.730138	-3.758776	-2.671601
C	-3.687911	-2.381336	-0.479180
C	-2.432647	2.025093	-0.767473
C	-1.855498	-0.070740	0.512153
C	-0.339923	2.615864	-1.261247
C	-2.219425	-2.245418	-0.724476
C	-1.502904	-0.053104	2.042515
C	-1.697421	2.985575	-1.425947
C	-0.116619	-2.484477	-1.431222
C	-1.408570	-3.062366	-1.481281
C	-3.919464	1.920232	-0.652508
C	-2.103515	-1.315227	2.688377
C	-2.160327	1.190017	2.669874
H	4.694319	0.138194	-0.016139
H	5.033183	0.218222	2.311734
H	-4.056293	-3.253683	-1.021715
H	3.756692	-0.864361	2.583018
H	-4.310104	1.014222	-1.127896
H	1.643252	-1.412931	-3.341942
H	2.498151	2.358148	-1.190253
H	2.639522	3.503627	-2.525911
H	1.912511	1.906728	-2.817317
H	2.586545	-1.650957	-1.838047
H	2.737800	-2.804838	-3.162167
H	-4.256028	-1.515489	-0.835361
H	-3.924454	-2.525299	0.578532
H	-2.084597	3.839751	-1.961679
H	-2.943405	-0.121283	0.478319
H	-1.669749	-2.224306	2.268375
H	-3.196558	-1.352597	2.581603
H	-1.875583	-1.307390	3.756132
H	-1.709294	-3.951570	-2.015721
H	-1.757677	2.112726	2.249203
H	-1.950433	1.197680	3.741373
H	-3.252274	1.185787	2.545134
H	2.898669	1.633840	1.570509
H	-4.374370	2.773211	-1.158905
H	-4.262842	1.932361	0.385947
N	4.439190	-0.503170	1.929545
N	0.726103	3.335338	-1.753483
N	0.994189	-3.000696	-2.062080
N	-1.537174	1.147129	-0.227137
N	-0.243102	1.496109	-0.529082

N	-1.422196	-1.250406	-0.234370
N	-0.125268	-1.384348	-0.662565
O	2.971815	1.306564	0.665247
O	3.041108	-1.080787	0.206875
S	0.300993	-0.016673	2.399847
Fe	1.314629	0.073819	0.333847

intermediate – $NHCH_3$ substituent

C	-4.035832	0.230661	0.347472
C	-2.427844	-2.825171	-1.334912
H	-1.002236	-3.826671	-2.487607
C	-1.660686	2.672852	-2.442831
H	-0.306655	4.192552	-2.099815
C	3.980788	2.101263	-0.190118
C	2.219081	-2.099072	-1.128033
C	1.916007	-0.160368	0.457662
C	0.055518	-2.609871	-1.318948
C	2.510409	2.134478	-0.457982
C	1.543272	-0.302570	1.982279
C	1.359281	-2.988869	-1.731043
C	0.446086	2.650617	-1.134765
C	1.778652	3.124292	-1.080913
C	3.710519	-2.050149	-1.209637
C	2.411178	0.689994	2.778402
C	1.890611	-1.737488	2.419199
H	-4.870373	-0.015823	-0.336715
H	-4.886512	2.048759	0.631687
H	4.431886	3.014109	-0.582790
H	-3.707605	1.696686	1.691475
H	4.070374	-1.114786	-1.650758
H	-1.253884	2.143149	-3.318854
H	-2.533184	-2.636981	-0.266354
H	-3.130492	-3.617414	-1.604874
H	-2.706087	-1.907237	-1.867921
H	-2.216414	1.967203	-1.825963
H	-2.361310	3.434622	-2.794446
H	4.476609	1.257350	-0.681776
H	4.213132	2.049204	0.876545
H	1.630135	-3.820795	-2.363940
H	3.001896	-0.241444	0.424631
H	2.201845	1.723295	2.495831
H	3.483734	0.488199	2.651720
H	2.178487	0.591026	3.840453
H	2.159128	4.058433	-1.467399
H	1.255252	-2.470527	1.921410
H	1.725056	-1.831167	3.494326
H	2.943192	-1.982817	2.219741
H	-4.338124	-0.794863	1.954824
H	4.058795	-2.865973	-1.845198
H	4.188921	-2.170449	-0.232063
N	-4.516624	1.302997	1.213788
N	-1.088962	-3.290379	-1.640207
N	-0.627805	3.343893	-1.658766
N	1.448558	-1.240056	-0.397348
N	0.110334	-1.532356	-0.521844
N	1.628789	1.137493	-0.153441
N	0.359228	1.439942	-0.564659
O	-3.765620	-0.896842	1.185327
O	-2.910478	0.496676	-0.378560
S	-0.222410	0.041077	2.413485
Fe	-1.196735	0.079313	0.326011

FeL(formate), monodentate – $NHCH_3$ substituent

C	-0.023760	-0.342716	5.001012

H	-0.262350	0.529176	5.647481
O	0.634597	-1.266851	5.630470
O	-0.380164	-0.357947	3.823658
C	3.060699	-0.256012	3.329220
C	1.418164	-7.043463	5.479463
H	4.690639	-0.871209	2.181158
C	-1.246242	-4.666628	3.352848
C	2.170538	-5.597584	3.556246
C	3.687187	-2.543551	2.557213
C	0.052718	-6.138043	2.289246
C	2.404760	-5.931578	5.080449
C	4.079727	-4.702705	2.151528
C	3.843935	-6.459497	5.230456
C	0.604958	-7.228680	1.430065
C	4.606951	-6.010437	1.654462
C	4.536416	-3.437783	1.858857
C	-2.391274	-3.014995	4.836551
C	-1.245778	-5.690704	2.370193
H	-3.119775	-4.006505	3.145427
H	4.981543	-6.644818	2.462111
H	-0.204509	-7.660008	0.839044
H	3.330641	0.759172	3.029561
H	3.855845	-6.581456	1.099219
H	-1.759396	-3.317520	5.674029
H	-3.414896	-2.925230	5.210575
H	-2.057223	-2.040116	4.470341
H	1.985256	-0.364722	3.186047
H	3.292675	-0.375801	4.396117
H	0.385558	-6.696317	5.445489
H	4.005694	-7.370310	4.637961
H	1.517660	-7.925409	4.831759
H	2.470263	-6.500029	3.024962
H	5.360924	-3.183029	1.209881
H	-2.095804	-6.072283	1.824728
H	1.629888	-7.356763	6.503762
H	4.580937	-5.707586	4.943284
H	4.024610	-6.708994	6.277859
H	1.050402	-8.040563	2.014454
H	1.361181	-6.858465	0.730452
H	5.436773	-5.819333	0.972161
N	3.779524	-1.179941	2.476346
N	-2.370288	-4.043576	3.816257
N	3.017589	-4.549745	2.995465
N	0.781260	-5.398898	3.177237
N	-0.001772	-4.466665	3.817703
N	2.759798	-3.223245	3.252387
S	2.223341	-4.507880	6.254465
Fe	1.238576	-2.965759	4.870339

FeL(formate), bidentate – $NHCH_3$ substituent

C	0.003630	-3.613388	1.664481
H	0.406524	-9.100036	3.839152
C	4.802594	-3.766669	2.737271
C	-0.737662	-7.381683	3.688342
C	1.606570	-7.660123	4.449453
C	3.669150	-5.121182	5.820434
C	3.455982	-7.639338	5.700136
C	2.709854	-4.169083	6.631055
C	2.540492	-8.489757	5.118702
C	5.762104	-4.241440	4.695208
C	6.036899	-3.763323	3.433885
C	3.589479	-3.123791	7.343989
C	6.711865	-4.437811	5.832940
C	4.641505	-7.984398	6.541602

H	5.507068	-3.298067	0.941061
C	1.979279	-5.017023	7.687527
C	3.458123	-3.571973	0.648630
H	-0.621406	-6.435508	3.163051
H	6.462216	-3.812308	6.694157
H	-1.143801	-7.191691	4.692819
H	-1.455495	-7.986491	3.129404
H	6.753748	-5.477137	6.174319
H	7.716134	-4.164309	5.505359
H	4.598479	-7.528770	7.536282
H	5.582584	-7.683142	6.070407
H	3.650345	-3.194963	-0.358155
H	4.677328	-9.066130	6.680396
H	2.683223	-5.565698	8.328520
H	4.298047	-3.595203	8.038955
H	4.140047	-2.508204	6.630386
H	1.391322	-4.356574	8.328067
H	1.293564	-5.727861	7.226015
H	6.996824	-3.437188	3.062182
H	4.430954	-5.426242	6.536350
H	2.532106	-9.567924	5.182032
H	2.950213	-2.455044	7.923486
H	2.604916	-3.024205	1.049141
H	3.197612	-4.637359	0.577229
H	-0.785264	-3.645760	0.886644
N	4.640546	-3.328241	1.451160
N	0.528461	-8.106512	3.718889
N	1.941185	-6.369148	4.597935
N	3.819383	-4.227234	3.527782
N	3.066703	-6.371167	5.379042
N	4.421724	-4.499320	4.734595
O	0.393556	-4.772457	2.091212
O	0.456228	-2.534206	2.059649
S	1.465676	-3.228795	5.629728
Fe	1.609385	-4.364126	3.639096

FeL(OH) – $N(CH_3)_2$ substituent

C	4.416001	-2.453082	-1.024227
C	2.138636	-3.278233	-0.654842
C	-3.867430	-1.617602	0.680260
C	-4.454306	-1.621618	-1.688430
H	-1.277851	3.690725	-1.866418
H	-3.038084	-1.493816	1.373708
H	-4.887213	-2.610260	-1.515438
H	-5.274554	-0.883989	-1.660684
H	-4.017124	-1.619654	-2.689754
H	-4.680843	-0.934959	0.975607
H	2.075134	3.125300	-2.063880
H	2.887708	3.418240	-0.521114
H	3.790266	2.771791	-1.890193
H	-0.310403	2.712613	-2.983645
H	-2.029723	2.958777	-3.281739
H	-4.228619	-2.645713	0.768273
H	1.267820	-3.144536	-0.013044
H	2.624241	-4.208319	-0.349747
H	1.804523	-3.389581	-1.700161
H	5.141002	-1.752094	-0.603456
H	4.473116	-2.398395	-2.124857
H	4.717315	-3.457984	-0.720628
C	2.829960	2.735256	-1.373021
C	-1.256392	2.786828	1.671201
C	1.235058	2.917051	1.905587
C	-1.288223	2.796034	-2.497893
C	-1.646847	1.562963	-1.734313

C	0.224384	1.656781	-0.023926
C	2.557488	1.324153	-0.960798
C	2.649445	-0.880540	-0.589395
C	0.059702	2.004216	1.506257
C	3.376105	0.222991	-1.105510
C	-2.604864	-0.284066	-0.919034
C	-2.710543	0.701973	-1.930534
H	2.194835	2.409865	1.793936
H	1.131741	3.186286	2.958417
H	0.366220	2.615919	-0.520425
H	4.356543	0.223778	-1.552514
H	-1.338937	3.126905	2.705331
H	-3.473439	0.799768	-2.686096
H	-1.174626	-3.309955	0.558317
H	-2.125684	2.164498	1.457535
H	-1.288728	3.674162	1.023053
H	1.246161	3.847763	1.321728
N	3.091365	-2.186587	-0.497204
N	1.443498	-0.471572	-0.153539
N	1.406844	0.876727	-0.381417
N	-1.525585	-0.044404	-0.159018
N	-0.964090	1.091866	-0.651116
N	-3.425711	-1.382294	-0.693305
O	-0.592941	-2.995017	1.257471
S	0.069224	0.568560	2.681735
Fe	-0.208775	-1.178413	1.193126

transition state – $N(CH_3)_2$ substituent

C	-0.598650	2.585953	-2.615443
C	1.130702	4.274064	-2.284199
C	-2.607318	-3.262159	-2.661230
C	-3.263455	-2.599744	-0.410254
H	-1.032911	1.691968	-2.178036
H	-1.965182	-2.981806	-3.499593
H	-1.383480	3.345272	-2.655313
H	1.731870	4.121327	-3.198197
H	-2.500765	-4.346760	-2.484443
H	-3.642611	-3.072540	-2.955941
H	-3.231980	-3.610109	0.031126
H	-3.090224	-1.853441	0.360820
H	-4.267519	-2.428279	-0.807338
H	1.772555	4.706065	-1.512997
H	0.351931	5.005943	-2.515334
H	-0.269953	2.358617	-3.644172
N	0.501472	3.066920	-1.793610
C	-3.254525	2.107915	0.668354
C	1.410559	-0.874988	2.154707
C	2.729008	2.154775	-1.091105
C	1.256759	-2.679048	-1.082324
C	2.635657	-0.316397	2.902847
C	1.171376	-2.327345	2.607470
C	4.457397	0.527634	-0.067057
C	2.665352	-3.139270	-1.276302
C	-0.952648	-2.375169	-1.160669
C	0.112438	-3.130327	-1.708057
C	1.741592	-0.892234	0.620537
C	1.314297	2.148144	-1.158114
C	3.082234	1.027255	-0.375262
H	2.025974	-2.977107	2.370295
H	2.423295	-0.314546	3.973877
H	-4.092227	1.931293	-0.022175
H	-4.524436	2.530958	2.211491
H	4.681611	0.550043	1.002357
H	2.715461	-1.374813	0.540971

H	0.273901	-2.745955	2.151290
H	5.185116	1.164631	-0.572761
H	1.032536	-2.342662	3.690503
H	2.842759	0.715703	2.614777
H	3.412038	2.858934	-1.538368
H	0.059466	-3.923069	-2.436643
N	-2.299525	-2.448678	-1.499073
H	3.534238	-0.927834	2.740152
H	4.623332	-0.496162	-0.418565
H	-2.909290	2.987408	2.452741
H	2.674069	-3.967113	-1.987365
H	-3.134533	0.243290	2.058124
H	3.120622	-3.500239	-0.348070
H	3.306340	-2.350752	-1.684514
N	-3.654459	2.821210	1.789325
N	1.916436	0.413719	-0.021000
N	0.862247	-1.720166	-0.195649
N	0.825900	1.089111	-0.486386
N	-0.484431	-1.503153	-0.250516
O	-3.134718	0.313256	1.094815
O	-2.076218	2.326178	0.202041
S	-0.038807	0.172077	2.595466
Fe	-1.125835	0.527921	0.583614

intermediate – $N(CH_3)_2$ substituent

C	-0.366177	3.009529	-2.273985
C	1.571145	4.435031	-1.863346
C	-2.891877	-3.274586	-2.452971
C	-3.394568	-2.072512	-0.383979
H	-1.028235	2.289447	-1.800148
H	-2.268948	-3.212214	-3.348541
H	-0.933138	3.936911	-2.391015
H	2.109784	4.280754	-2.814618
H	-2.894895	-4.319583	-2.098457
H	-3.913213	-3.015556	-2.742232
H	-3.564050	-2.968379	0.235294
H	-3.061918	-1.263291	0.258587
H	-4.347629	-1.767225	-0.822830
H	2.296057	4.709893	-1.093547
H	0.892135	5.280842	-1.996805
H	-0.080256	2.650876	-3.276980
N	0.799368	3.282692	-1.436456
C	-3.522506	1.873338	0.541280
C	1.409942	-0.997546	2.071678
C	2.948344	2.062274	-0.983503
C	1.097605	-2.798470	-1.133346
C	2.660317	-0.493823	2.816889
C	1.122286	-2.448713	2.499207
C	4.543744	0.175766	-0.215620
C	2.460133	-3.376812	-1.337570
C	-1.089340	-2.332989	-1.161810
C	-0.096895	-3.191917	-1.700824
C	1.739001	-1.009305	0.530754
C	1.539234	2.202595	-0.975305
C	3.215607	0.834291	-0.410233
H	1.950241	-3.122934	2.238318
H	2.456618	-0.492898	3.889372
H	-4.386339	1.948415	-0.147075
H	-3.418380	3.897034	0.574278
H	4.796972	0.042579	0.839544
H	2.680403	-1.551058	0.446532
H	0.204811	-2.824416	2.045966
H	5.316319	0.802495	-0.664343
H	0.994879	-2.481130	3.583054

H	2.912033	0.529885	2.534378
H	3.681226	2.743661	-1.384093
H	-0.229543	-4.012274	-2.387126
N	-2.438836	-2.325553	-1.455598
H	3.529296	-1.143019	2.642100
H	4.600945	-0.804909	-0.699413
H	-2.563765	3.171078	1.749191
H	2.388867	-4.221728	-2.024453
H	-4.289726	1.288220	2.208754
H	2.902479	-3.748024	-0.407106
H	3.154652	-2.654178	-1.778717
N	-3.455447	3.145488	1.256970
N	2.007644	0.294766	-0.077715
N	0.806972	-1.764075	-0.293028
N	0.974188	1.118984	-0.413988
N	-0.523891	-1.456124	-0.313771
O	-3.777336	0.859576	1.513089
O	-2.411186	1.520534	-0.167901
S	-0.006917	0.077782	2.588326
Fe	-0.966723	0.542123	0.545716

FeL(formate), monodentate – $N(CH_3)_2$ substituent

C	-1.367485	3.602048	0.222847
C	2.269787	3.143279	-0.054026
C	4.352360	2.497376	-1.236948
C	-4.012347	0.982477	0.593158
C	-4.620692	0.611028	-1.742814
H	4.427431	3.573718	-1.399374
H	-0.794128	-4.280493	-1.265596
H	-0.103803	-3.394631	-2.636713
H	3.988047	-2.803104	-1.890967
H	-1.969376	4.483604	0.531707
H	3.141558	-3.414220	-0.471497
H	-1.784265	-3.920861	-2.677050
H	5.091603	2.211617	-0.471463
H	2.634501	4.142692	-0.297192
H	2.294675	-3.264239	-2.018078
H	-5.131100	1.576735	-1.698944
H	-3.173588	0.998583	1.284510
H	-5.378796	-0.179017	-1.602450
H	-4.188375	0.510176	-2.740665
H	-4.782400	0.298569	0.987163
H	-4.431598	1.991415	0.555824
H	1.207871	3.123882	-0.297986
H	2.408550	2.977691	1.024735
H	4.622279	2.009844	-2.177561
N	2.987062	2.176301	-0.867294
N	-3.572795	0.593677	-0.741968
O	-1.095762	2.805923	1.216149
O	-1.021633	3.462733	-0.946907
C	-0.743367	-2.893717	2.048934
C	-2.619256	-0.400691	-0.857636
C	0.480455	-1.819041	0.129260
C	2.648423	0.848670	-0.795713
C	-1.472785	-2.231030	-1.438939
C	0.426057	-1.955453	1.699665
C	2.681604	-1.375145	-1.034747
C	1.748045	-2.600756	2.155596
C	-1.004055	-3.522045	-2.026741
C	3.032952	-2.790567	-1.363373
C	3.412520	-0.237982	-1.297479
C	-2.648233	-1.549649	-1.686331
H	-1.705238	-2.450789	1.788662
H	1.890949	-3.595227	1.710972

H	-0.651506	-3.864946	1.542907
H	0.724334	-2.817181	-0.231965
H	4.371905	-0.206413	-1.786305
H	-3.434694	-1.863924	-2.353613
H	-0.743658	-3.077342	3.125126
H	2.606382	-1.972119	1.912624
H	1.729505	-2.721934	3.240350
N	1.545162	-0.972810	-0.397341
N	-0.794938	-1.505456	-0.502708
N	-1.470020	-0.373940	-0.161191
N	1.505511	0.391181	-0.245268
S	0.232835	-0.375487	2.656767
Fe	-0.247579	1.068114	0.929720

FeL(formate), bidentate – $N(CH_3)_2$ substituent

C	-0.150231	-3.689977	1.102165
C	4.466181	-1.284154	-1.962801
C	3.767744	-1.753988	0.330454
C	-4.439265	-1.803843	-1.536670
C	-2.152988	-2.626331	-1.744009
H	-1.125604	-2.442476	-1.441851
H	-2.199479	-2.601704	-2.845700
H	-4.721402	-2.853830	-1.422687
H	-0.062101	-4.793013	1.125845
H	-4.636241	-1.511640	-2.582688
H	4.832730	-2.313835	-1.972485
H	2.938812	-1.651423	1.024419
H	-2.711766	3.814244	0.121917
H	5.328081	-0.619695	-1.779226
H	4.063224	-1.067022	-2.954845
H	4.658489	-1.275060	0.769262
H	3.966187	-2.821339	0.206707
H	-1.858275	3.836578	-1.425465
H	-3.589861	3.523563	-1.379589
H	1.513651	4.100628	-1.279759
H	0.499815	3.364875	-2.533683
H	-2.425709	-3.630310	-1.407455
H	-5.083684	-1.215224	-0.880251
H	2.229872	3.571535	-2.799642
N	-3.052831	-1.650694	-1.146548
N	3.426076	-1.171608	-0.961215
O	0.744152	-3.057207	0.427635
O	-1.079412	-3.119946	1.701311
C	-2.605089	-0.365970	-0.911251
C	2.642446	-0.035578	-0.995407
C	-0.086425	1.876848	0.212919
C	1.775436	1.963154	-1.496707
C	0.085706	1.925195	1.779232
C	2.799064	1.099464	-1.832152
C	-2.437804	1.858469	-0.762303
C	-3.288436	0.847095	-1.166494
C	-1.020797	2.836334	2.344811
C	-2.649695	3.335235	-0.858576
C	1.480075	3.320396	-2.047670
C	1.457068	2.555583	2.083510
H	1.568812	3.538683	1.605202
H	-0.956840	3.855408	1.939531
H	-2.014183	2.429316	2.148274
H	1.550582	2.697240	3.162054
H	2.275733	1.912219	1.760837
H	-4.256791	0.979926	-1.621179
H	-0.161054	2.918167	-0.099217
H	3.573135	1.287845	-2.558366
H	-0.907553	2.901414	3.428604

N	1.564966	0.120700	-0.206571
N	-1.405620	-0.108152	-0.359372
N	1.062892	1.353090	-0.506824
N	-1.315077	1.252057	-0.282287
S	-0.063668	0.303364	2.663168
Fe	0.061208	-1.164885	0.886715

FeL(OH) – F substituent

H	5.725236	10.329392	-0.243175
H	4.369370	10.416992	-1.366054
H	8.413819	9.462224	-2.841513
H	9.984162	8.958717	-3.458744
H	9.785159	9.274116	-1.735374
H	5.986515	10.086189	-1.979056
C	7.373568	7.636924	-0.456093
C	5.299204	9.889012	-1.149424
C	8.959688	7.408056	-2.445606
C	8.778815	5.220094	-2.580216
C	7.852026	7.379188	1.021794
C	5.005389	8.433291	-0.990749
C	9.411610	6.318888	-3.174651
C	4.101617	6.431813	-0.867410
C	3.791342	7.775265	-1.112444
C	9.296016	8.852870	-2.618836
C	7.072462	8.346396	1.932876
C	9.351863	7.723676	1.087789
F	3.273608	5.400737	-0.879795
F	8.879489	3.948880	-2.930201
H	7.572480	8.688806	-0.656727
H	10.094032	6.321435	-4.009710
H	2.828822	8.203930	-1.342325
H	5.740531	2.598257	-1.297517
H	6.002323	8.133909	1.925522
H	7.233704	9.396456	1.650744
H	7.420738	8.221589	2.959640
H	9.549676	8.761298	0.784067
H	9.947722	7.049800	0.470559
H	9.694563	7.608783	2.117562
N	8.118019	6.911702	-1.484926
N	5.382624	6.241188	-0.610865
N	5.937831	7.477010	-0.683088
N	8.000958	5.562648	-1.569514
O	6.128866	2.802345	-0.441802
S	7.625404	5.660647	1.676923
Fe	6.687748	4.515478	-0.114664

transition state – F substituent

C	-4.085665	-0.026806	-0.356014
H	-4.394974	-0.446164	-1.323525
H	3.774747	3.400111	-1.238877
H	4.016638	1.656431	-1.224731
H	3.810155	2.538148	0.298231
H	-3.316892	-1.851712	0.841598
H	4.348403	-2.694524	-1.223557
H	4.211687	-1.868538	0.327974
H	-6.003242	-0.363171	0.326494
H	-5.053211	0.715373	1.264550
H	4.268164	-0.936318	-1.177484
N	-5.090280	-0.033093	0.590890
O	-3.016217	-1.529909	-0.017034
O	-3.194742	0.898618	-0.304843
C	1.993315	2.323046	-0.855608
C	3.881023	-1.850090	-0.714687
C	3.475183	2.476429	-0.741272

C	1.756631	0.141535	0.436152
C	1.338494	0.106454	1.948467
C	2.397067	-1.967365	-0.843164
C	-0.150695	2.523274	-1.301121
C	1.086678	3.150759	-1.497016
C	0.328954	-2.555566	-1.302768
C	1.660698	-2.947370	-1.489449
C	1.831650	1.413322	2.598169
C	2.063328	-1.083364	2.605628
H	2.841249	0.243926	0.425485
F	-1.321983	2.934808	-1.749679
H	1.290124	4.066493	-2.029083
H	2.031454	-3.811033	-2.018322
F	-0.748232	-3.168842	-1.758815
H	1.589638	1.389980	3.662351
H	1.336744	2.287528	2.171887
H	2.920403	1.535308	2.505558
H	1.815762	-1.102378	3.668580
H	3.156192	-1.000430	2.518843
H	1.742697	-2.035767	2.180005
N	1.267419	1.292844	-0.319028
N	0.215148	-1.441839	-0.600505
N	1.492722	-1.086149	-0.313393
N	-0.056125	1.408108	-0.598085
S	-0.473986	-0.060567	2.260747
Fe	-1.508000	-0.189800	0.190676

intermediate – F substituent

C	-0.675394	-4.735374	1.727067
H	-0.736592	-5.765030	1.334403
H	6.961297	-2.458924	5.543630
H	6.090156	-3.661647	6.489451
H	5.684294	-1.943403	6.643194
H	-1.979043	-4.228860	3.093228
H	3.764641	-6.595677	8.748496
H	3.322696	-4.898016	8.922898
H	-1.740102	-4.279717	0.044376
H	-1.069461	-3.000895	0.803488
H	4.715284	-5.360242	7.930194
N	-1.560950	-3.876532	0.956661
O	-1.201411	-4.801503	3.094974
O	0.602166	-4.289362	1.821850
C	5.019855	-2.850632	4.795611
C	3.697613	-5.644976	8.217379
C	5.977920	-2.724095	5.934905
C	2.928271	-3.424092	6.138135
C	1.826259	-2.352380	6.473545
C	2.799235	-5.811513	7.035579
C	4.014219	-2.921540	2.840028
C	5.257655	-2.683155	3.440962
C	1.448337	-6.538124	5.459324
C	2.133747	-6.949967	6.608889
C	2.515775	-0.975176	6.506128
C	1.282365	-2.676002	7.878454
H	3.658947	-3.362802	6.943586
F	3.732896	-2.884312	1.550237
H	6.188986	-2.427213	2.961130
H	2.146196	-7.929486	7.059812
F	0.678417	-7.276511	4.680135
H	1.783942	-0.222538	6.804816
H	2.894341	-0.690202	5.523451
H	3.341152	-0.944979	7.231388
H	0.545196	-1.920023	8.154477
H	2.076096	-2.662482	8.638529

H	0.778480	-3.643737	7.902128
N	3.691486	-3.162928	4.920844
N	1.646031	-5.263602	5.175540
N	2.476284	-4.815781	6.151457
N	3.069674	-3.211568	3.715950
S	0.383539	-2.262432	5.316465
Fe	0.901503	-3.830571	3.659204

FeL(formate), bidentate – F substituent

C	-4.093683	-0.038913	-0.072315
H	3.772213	2.239606	-0.090163
H	3.756224	-1.263725	-1.609177
H	3.829064	-2.148117	-0.075036
H	3.708624	-3.023494	-1.599772
F	-1.514576	3.090238	-1.489851
F	-1.434215	-3.144780	-1.465125
H	-5.178778	-0.051113	-0.275382
H	3.721493	1.341769	-1.617442
H	3.630133	3.099886	-1.621662
O	-3.473524	-1.138725	0.026095
O	-3.501925	1.072688	0.051760
C	1.548609	0.018371	0.305356
C	1.877237	-2.145460	-1.005119
C	1.289113	0.020410	1.856096
C	0.998556	-3.083846	-1.521321
C	1.821189	2.180692	-1.020111
C	0.918939	3.092442	-1.543207
C	1.945865	1.287208	2.436043
C	3.313443	2.205719	-1.082709
C	3.369637	-2.133366	-1.067752
C	1.981489	-1.223137	2.444867
C	-0.336071	2.575493	-1.197244
C	-0.269224	-2.597221	-1.177882
H	2.630894	0.032200	0.185045
H	1.135697	3.995053	-2.092097
H	1.238393	-3.983932	-2.064736
H	3.059620	-1.230932	2.232518
H	1.536476	-2.147222	2.072968
H	1.857529	-1.216236	3.529224
H	1.822581	1.284130	3.520483
H	3.023216	1.324461	2.223055
H	1.474326	2.195586	2.058257
N	1.079256	1.206542	-0.405516
N	-0.253163	1.445440	-0.516370
N	-0.215156	-1.460469	-0.505315
N	1.110612	-1.186603	-0.396890
S	-0.485807	-0.002489	2.387307
Fe	-1.666258	-0.021263	0.401160

FeL(OH) – $CClF_2$ substituent

C	-2.180727	-2.974775	-1.250721
C	2.142790	-2.973985	-1.282670
H	-1.323625	-3.326010	-1.834794
H	-2.178899	-3.501075	-0.291887
H	3.035197	-3.271779	-1.835114
H	1.275956	-3.324578	-1.852579
H	-3.082219	-3.273594	-1.787748
H	2.156840	-3.501780	-0.324673
C	3.082190	-0.570962	-1.561563
C	2.150196	-1.489728	-1.118668
C	-2.185311	-1.490313	-1.088711
C	-0.008251	-1.273328	0.212824
C	-2.635686	0.679138	-1.107830
C	0.002083	-1.146108	1.781935

C	2.602741	0.679151	-1.139995
C	-3.122206	-0.571223	-1.520252
C	1.261014	-1.871305	2.295033
C	-1.248474	-1.873978	2.311525
C	-3.280433	2.011361	-1.347687
C	3.245114	2.011143	-1.386593
F	4.564011	1.835334	-1.607897
F	-3.117088	2.839466	-0.308652
F	-4.603075	1.836020	-1.547048
H	-0.009397	-2.341007	0.000724
H	3.987237	-0.776574	-2.110950
H	-4.034762	-0.776753	-2.057130
H	0.016045	4.054765	-0.585856
H	2.176271	-1.382595	1.957310
H	1.280939	-2.926869	1.990299
H	1.262294	-1.841277	3.385936
H	-1.270015	-2.929626	2.007224
H	-2.169096	-1.387272	1.985652
H	-1.235609	-1.843712	3.402342
Cl	-2.620962	2.827687	-2.822880
F	3.099405	2.837028	-0.343035
Cl	2.562173	2.832624	-2.848667
N	1.183883	-0.763831	-0.466335
N	-1.474182	0.558170	-0.464039
N	1.449677	0.558338	-0.481304
N	-1.209510	-0.764309	-0.450476
O	-0.007717	3.705781	0.309915
S	0.004522	0.572299	2.459783
Fe	-0.007331	1.900039	0.560249

transition state – $CClF_2$ substituent

C	0.345130	-3.486119	1.522066
H	-3.312776	3.689247	-2.213599
H	-1.575593	3.920823	-2.055297
H	-2.639246	4.170408	-0.658583
H	-0.386262	-3.761010	3.388059
H	2.633148	4.522928	-1.434534
H	1.702863	-1.975379	2.699963
H	1.670423	4.673159	0.035338
H	0.877806	4.445315	-1.531758
H	0.989918	-3.999709	0.797381
H	1.028851	-4.647596	3.055212
Cl	4.101167	-0.732128	-2.609480
F	-3.217850	-2.156249	-0.060311
Cl	-2.071874	-2.460383	-2.337796
F	-4.344190	-1.442138	-1.777950
F	2.295273	-1.782349	-1.137167
F	4.041108	-1.027859	-0.073263
N	0.200585	-4.200383	2.692689
O	1.616691	-2.133354	1.751355
O	-0.659017	-2.790575	1.108144
C	1.741577	4.155009	-0.924545
C	2.456156	0.542616	-0.827245
C	2.859745	1.833137	-1.202047
C	-0.385891	2.263864	0.371131
C	-2.603617	-0.098578	-1.032117
C	-2.358703	2.094412	-1.204835
C	-0.542439	2.277309	1.930382
C	-3.137474	1.044926	-1.648193
C	1.854648	2.674352	-0.764797
C	-1.962640	2.775069	2.258315
C	0.483669	3.279376	2.493639
C	-2.466239	3.546013	-1.540283
C	3.166860	-0.764743	-1.057512

C	-3.112429	-1.499713	-1.219308
H	3.749484	2.115613	-1.741547
H	-2.726176	2.079092	1.908114
H	-3.977248	1.097179	-2.322471
H	-2.161873	3.769748	1.835590
H	0.321970	4.296200	2.109536
H	1.508463	2.970795	2.277723
H	0.379651	3.314934	3.579543
H	-2.064443	2.849862	3.342564
H	-0.500516	3.298940	0.053217
N	-1.426847	1.542708	-0.360433
N	0.932768	1.871988	-0.140853
N	-1.563258	0.203415	-0.254054
N	1.293348	0.574883	-0.172307
S	-0.265322	0.651035	2.746955
Fe	0.098625	-0.912314	1.088390

intermediate – $CClF_2$ substituent

C	-1.067645	-3.925370	2.501009
H	6.695764	-1.517622	6.322848
H	5.887819	-2.787295	7.235107
H	5.375809	-1.099294	7.412015
H	-1.089166	-2.174801	1.521602
H	3.747448	-5.835406	9.430835
H	-2.372947	-3.049858	3.657972
H	3.217372	-4.164455	9.612008
H	4.627279	-4.551322	8.610134
H	-1.345306	-4.951346	2.205060
H	-1.646109	-3.409096	0.625531
Cl	0.553746	-8.510381	5.769721
F	2.346570	-1.600575	1.789996
Cl	3.834432	-3.619053	1.250751
F	4.462449	-1.160635	1.522460
F	1.092953	-6.770327	3.976436
F	-0.679127	-6.355964	5.161176
N	-1.677748	-3.004162	1.555146
O	-1.653042	-3.675941	3.801509
O	0.282308	-3.797931	2.649940
C	3.627289	-4.888520	8.902288
C	1.413631	-5.927129	6.144861
C	2.140523	-6.275235	7.292556
C	2.732504	-2.719845	6.842512
C	3.831254	-2.107268	3.546153
C	4.796114	-2.014038	5.538191
C	1.599614	-1.691293	7.200530
C	5.038284	-1.802145	4.195324
C	2.732893	-5.104172	7.725889
C	2.246332	-0.295170	7.280165
C	1.053547	-2.072916	8.590425
C	5.725233	-1.848543	6.695634
C	0.589398	-6.790865	5.223698
C	3.584697	-2.033352	2.067420
H	2.228082	-7.248258	7.747446
H	2.629479	0.029691	6.311622
H	5.960499	-1.469464	3.745962
H	3.057456	-0.256312	8.020531
H	1.838476	-2.057699	9.359140
H	0.577434	-3.054814	8.581442
H	0.292045	-1.346735	8.879861
H	1.485304	0.425156	7.585375
H	3.464872	-2.642832	7.644543
N	3.487701	-2.421396	5.625741
N	2.335760	-4.130386	6.844907
N	2.895024	-2.487916	4.415685

N	1.535422	-4.622680	5.878786
S	0.177374	-1.616513	6.028044
Fe	0.709902	-3.170517	4.379015

FeL(formate), bidentate – $CClF_2$ substituent

C	-0.451181	-3.103400	2.125379
H	3.759016	-5.864591	9.321754
H	3.409677	-4.147188	9.498493
H	5.342776	-0.881685	7.253327
H	5.836317	-2.579808	7.352774
H	6.705317	-1.468733	6.300313
H	-1.053586	-3.290242	1.219186
H	4.677269	-4.691698	8.383481
F	0.640554	-6.821558	4.210358
F	-1.010572	-5.925954	5.308853
Cl	-0.212794	-8.185546	6.196521
F	2.811172	-3.582621	1.808347
Cl	5.211942	-3.018795	1.133171
F	3.219334	-1.465197	1.513123
O	-0.343397	-4.071772	2.964178
O	0.094743	-1.997610	2.309943
C	3.968692	-2.454098	3.509084
C	1.130324	-5.790168	6.261514
C	2.667950	-5.075963	7.690383
C	1.629150	-1.632858	7.150524
C	1.930316	-6.191533	7.341780
C	4.832940	-2.053077	5.510732
C	5.139087	-2.042402	4.162884
C	2.340193	-0.293342	7.426863
C	0.907726	-2.093870	8.430895
C	5.713831	-1.730436	6.672661
C	3.681713	-4.922983	8.776213
C	2.738541	-2.693762	6.814398
C	0.148110	-6.587749	5.440315
C	3.704803	-2.602005	2.033905
H	3.037282	-0.367622	8.272779
H	2.875028	0.070799	6.547622
H	0.193563	-1.322995	8.725578
H	6.088492	-1.790829	3.718289
H	1.590226	0.458091	7.679800
H	1.964389	-7.160333	7.812760
H	3.463519	-2.636477	7.624782
H	1.604835	-2.240218	9.267434
H	0.345335	-3.014528	8.270002
N	3.520386	-2.442796	5.598957
N	1.353427	-4.510530	5.948389
N	2.987731	-2.684526	4.384098
N	2.284356	-4.084063	6.824597
S	0.387070	-1.336482	5.819554
Fe	0.781400	-3.026848	4.297007

FeL(OH) – CN substituent

H	2.286612	-3.517751	-0.740902
H	3.149947	-3.055815	-2.206139
H	1.393923	-3.171911	-2.233228
H	-2.104046	-3.637624	-0.792650
H	-1.201276	-3.241442	-2.266258
H	-2.961234	-3.222396	-2.275334
C	3.096284	-0.416889	-1.568264
C	2.201578	-1.420602	-1.257579
C	-2.124273	-1.538392	-1.307597
C	3.143286	2.057349	-1.018476
C	-3.260109	1.882661	-1.090371
C	2.571408	0.754489	-0.983459

C	-2.618858	0.612897	-1.042435
C	0.022396	-1.456091	0.068406
C	0.006555	-1.533661	1.641064
C	1.278225	-2.286700	2.076607
C	-1.231774	-2.355255	2.048032
C	2.248938	-2.868283	-1.620335
C	-2.084183	-2.986073	-1.671133
C	-3.065127	-0.584692	-1.639177
H	0.054500	-2.486656	-0.280174
H	4.007336	-0.508026	-2.139060
H	-3.956365	-0.725067	-2.230887
H	1.329189	-3.292605	1.637919
H	2.184389	-1.735991	1.818820
H	1.265616	-2.398878	3.162004
H	-1.217856	-3.362103	1.608760
H	-2.160480	-1.854525	1.769445
H	-1.237621	-2.467440	3.133481
H	-0.136667	4.076619	1.150596
N	1.209007	-0.826266	-0.514278
N	-1.183258	-0.891532	-0.541533
N	1.420356	0.491896	-0.346340
N	-1.470247	0.412849	-0.378724
N	-3.848009	2.887641	-1.160800
N	3.676509	3.093030	-1.078561
O	-0.111199	3.408087	0.461447
S	-0.047777	0.081786	2.539866
Fe	-0.070156	1.629691	0.819853

transition state – CN substituent

N	2.850927	-3.427094	-1.129848
N	2.035899	3.998570	-1.252143
C	3.738833	0.506803	-0.120578
C	-1.947794	-0.178300	1.725096
C	-0.717007	-3.154025	-1.537171
C	-2.259386	1.964482	-1.193511
C	-2.543309	-1.522573	2.186972
C	-2.875569	0.965223	2.181174
C	-3.227584	-2.500978	-1.511119
C	-3.717286	1.817837	-1.481423
C	-0.139688	2.611518	-1.037154
C	-1.396053	2.974647	-1.566637
C	-1.942122	-0.179133	0.151941
C	0.424429	-2.535672	-0.985137
C	-1.777790	-2.341517	-1.190914
H	-3.895916	0.846882	1.790939
H	-2.610109	-1.519600	3.276220
H	4.125253	1.532920	-0.062225
H	5.691965	-0.158521	-0.162601
H	-3.846140	-2.597037	-0.613939
H	-2.979827	-0.296854	-0.156153
H	-2.488819	1.942148	1.886761
H	-3.361028	-3.409329	-2.100571
H	-2.934047	0.955939	3.270872
C	1.769849	-2.994933	-1.055694
H	-1.909508	-2.364318	1.903791
H	-0.754473	-4.067816	-2.109720
H	-1.632716	3.856013	-2.142344
C	1.078792	3.340855	-1.142363
H	-3.555733	-1.683228	1.790926
H	-3.615497	-1.667786	-2.106039
H	4.508373	-1.304354	-0.666121
H	-4.050484	2.677754	-2.064361
H	3.518689	-0.220009	2.014839
H	-4.320797	1.783084	-0.569883

H	-3.936530	0.921367	-2.070722
N	4.729466	-0.447703	-0.183711
N	-1.238331	-1.307751	-0.461252
N	-1.504287	1.071266	-0.469679
N	0.092699	-1.411871	-0.334460
N	-0.220695	1.450668	-0.373214
O	3.116792	0.545727	1.585631
O	2.624213	0.280015	-0.743252
S	-0.306403	0.049657	2.535223
Fe	1.268928	0.201704	0.787576

intermediate – CN substituent

N	-1.817465	4.086329	-1.593973
N	-2.456709	-3.393678	-1.978684
C	-3.885758	-0.138576	0.056414
C	1.646114	-0.126100	1.931555
C	1.609428	3.067512	-1.348366
C	2.051119	-2.254985	-0.994549
C	2.427994	1.054313	2.539867
C	2.217036	-1.446929	2.483763
C	3.897918	1.925970	-0.916857
C	3.538571	-2.383166	-1.019985
C	-0.143769	-2.494272	-1.241971
C	1.099557	-3.073910	-1.567746
C	1.908201	-0.113397	0.380278
C	0.286766	2.683815	-1.041993
C	2.410978	2.053701	-0.864957
H	3.288962	-1.554354	2.267969
H	2.304686	1.033308	3.623991
H	-4.325831	-0.808733	-0.701708
H	-5.821280	0.341709	0.539094
H	4.349078	1.876070	0.078381
H	2.986126	-0.202577	0.258258
H	1.681740	-2.313713	2.092730
H	4.309463	2.802171	-1.420014
H	2.095181	-1.454834	3.568123
C	-0.898209	3.417583	-1.333137
H	2.048887	2.015885	2.189966
H	1.926972	3.965621	-1.855090
H	1.270565	-3.969037	-2.145339
C	-1.432228	-2.961541	-1.626068
H	3.503780	0.990236	2.325387
H	4.219957	1.045665	-1.482707
H	-4.800380	1.620206	0.378393
H	3.805961	-3.279940	-1.580755
H	-3.584059	-0.671760	1.898394
H	3.965205	-2.481258	-0.017651
H	4.020989	-1.534239	-1.515370
N	-4.882150	0.673408	0.729917
N	1.557749	1.135045	-0.299719
N	1.356835	-1.251084	-0.361335
N	0.269119	1.503651	-0.405274
N	0.026026	-1.385630	-0.505880
O	-3.304732	-1.045141	1.050124
O	-2.881642	0.621016	-0.455213
S	-0.117891	0.002366	2.460722
Fe	-1.291290	0.119143	0.447099

FeL(formate), bidentate – CN substituent

C	3.925589	0.233385	0.540355
H	-3.871760	2.861927	-1.724406
H	-4.031732	1.968814	-0.213703
H	-3.768602	-2.384879	-0.432252
H	-3.588040	-1.444128	-1.924661

H	-3.439184	-3.197487	-1.960547
H	5.025214	0.299683	0.504051
H	-3.846298	1.102815	-1.749301
O	3.238754	1.298384	0.513544
O	3.373156	-0.904341	0.605490
C	0.462251	-2.574957	-1.113394
C	0.113284	2.608399	-1.120061
C	-2.038446	2.057001	-1.045616
C	-1.590927	-0.131527	1.807322
C	-1.175323	3.028394	-1.508705
C	-1.734662	-2.242245	-1.151684
C	-0.753040	-3.104420	-1.594084
C	-2.161512	-1.476544	2.296078
C	-2.471717	1.014980	2.340702
C	-3.210477	-2.309187	-1.370072
C	-3.523653	1.981773	-1.181919
C	-1.690368	-0.114306	0.239715
C	1.757994	-3.116533	-1.347965
H	-0.884483	-3.996391	-2.186667
H	-1.430319	3.920916	-2.058637
H	-2.751187	-0.187507	0.006352
H	-3.521179	0.899575	2.037512
H	-2.108453	1.992067	2.017440
H	-2.439337	1.003989	3.431539
H	-2.165309	-1.479293	3.387412
H	-3.195636	-1.631439	1.959168
H	-1.548397	-2.318807	1.971969
C	1.333626	3.281016	-1.412795
N	-1.085634	-1.263437	-0.437750
N	-1.253568	1.125758	-0.408110
N	0.053571	1.448621	-0.447490
N	0.247595	-1.453276	-0.408019
S	0.106295	0.076640	2.499806
Fe	1.478125	0.097471	0.650364
N	2.772836	-3.628967	-1.607752
N	2.276877	3.895008	-1.718185

FeL(OH) – NO_2 substituent

O	9.520753	3.220830	-3.886596
O	2.105806	5.111407	-1.274648
O	3.822113	3.773108	-1.002421
H	4.361298	10.039650	-1.243971
H	5.658492	9.931444	-0.054590
H	6.013812	9.758434	-1.782953
H	9.878200	8.860589	-1.558719
H	10.094035	8.579836	-3.286039
H	8.529074	9.113820	-2.680835
O	7.949357	2.723066	-2.439020
C	9.009580	7.037958	-2.328038
C	8.726381	4.864194	-2.535181
C	7.845903	7.018372	1.120798
C	9.413627	5.955688	-3.084029
C	4.153874	6.028092	-0.924347
C	3.825121	7.378354	-1.106756
C	9.390734	8.475173	-2.458738
C	7.042236	7.970527	2.027562
C	9.341848	7.376344	1.213504
C	5.288296	9.519932	-0.997832
C	7.388637	7.277429	-0.360435
C	5.012119	8.055664	-0.910459
H	10.095421	5.946237	-3.918631
H	7.583397	8.328955	-0.566624
H	6.016431	1.818437	-0.428599
H	5.974165	7.747789	2.004783

H	7.199221	9.023825	1.757571
H	7.376900	7.839621	3.058012
H	9.532015	8.420918	0.931095
H	9.955583	6.718613	0.595790
H	9.670088	7.247739	2.246298
H	2.860248	7.788297	-1.356658
N	7.960277	5.214802	-1.503660
N	8.138671	6.541809	-1.379466
N	5.438786	5.856016	-0.619737
N	5.957556	7.096542	-0.609769
N	8.734267	3.499040	-2.984289
N	3.296611	4.883310	-1.074830
O	6.368682	2.374752	0.273071
S	7.612345	5.295606	1.720573
Fe	6.694037	4.117779	-0.067187

transition state – NO_2 substituent

C	-0.980539	-4.203680	1.767815
H	-2.088067	-2.523834	1.560394
H	-2.984491	-3.975988	1.473886
H	4.490328	-4.999456	8.243521
H	2.992567	-4.592288	9.100267
H	-1.035632	-5.275921	1.551248
H	-1.637812	-3.922961	4.044538
H	3.527686	-6.268655	8.992562
H	5.888959	-3.108398	6.978249
H	5.391729	-1.409554	6.890517
H	6.812460	-1.966747	6.008175
N	0.967776	-7.252980	4.509293
N	-2.094405	-3.515087	1.367682
N	4.146806	-3.083950	1.623955
O	-1.091109	-4.618793	3.656676
O	0.152693	-3.594592	1.762688
O	3.137753	-3.608458	1.175342
O	0.695280	-8.384791	4.901881
O	0.831728	-6.832071	3.364543
O	5.116344	-2.696468	0.974810
C	4.997195	-2.544140	5.091794
C	4.241672	-2.906383	3.059581
C	3.464975	-5.328183	8.443298
C	1.689648	-2.112562	6.471234
C	5.379386	-2.493535	3.766931
C	2.372993	-0.746639	6.675674
C	5.801976	-2.242716	6.313159
C	0.924945	-2.490507	7.753910
C	2.686339	-5.554124	7.189687
C	2.821177	-3.179017	6.257236
C	1.552657	-6.365556	5.486200
C	2.135800	-6.725541	6.708623
H	6.338138	-2.215562	3.361071
H	2.931985	-0.437342	5.790749
H	2.165172	-7.705831	7.155398
H	3.042759	-0.747875	7.546716
H	1.603533	0.007440	6.850348
H	0.400945	-3.441657	7.646494
H	3.485261	-3.094930	7.116267
H	0.171931	-1.725375	7.950232
H	1.586971	-2.538613	8.629519
N	3.679738	-2.954072	5.091775
N	1.691420	-5.069028	5.222683
N	2.384367	-4.577387	6.263777
N	3.212085	-3.182921	3.852771
S	0.496484	-1.964429	5.081558
Fe	0.808393	-3.801843	3.656276

intermediate – NO_2 substituent

C	-1.188148	-4.373930	2.067597
H	-2.031191	-2.631434	1.551744
H	-1.885415	-3.674190	0.310816
H	4.485206	-4.994409	8.320610
H	2.972834	-4.623217	9.166867
H	-1.173246	-5.396915	1.649647
H	-2.565783	-4.679519	3.399570
H	3.534202	-6.290352	9.038083
H	5.987912	-3.262701	6.878962
H	5.521465	-1.552224	6.922614
H	6.890678	-2.075492	5.943229
N	0.925247	-7.217138	4.570099
N	-2.143502	-3.609583	1.291667
N	3.971312	-2.828369	1.633516
O	-1.639589	-4.412478	3.419817
O	0.083585	-3.859074	2.086382
O	2.875341	-3.196569	1.226660
O	0.696416	-8.365511	4.943360
O	0.665459	-6.747137	3.466175
O	4.934577	-2.499935	0.944057
C	5.024748	-2.562558	5.076695
C	4.165240	-2.772875	3.062420
C	3.462859	-5.341711	8.504143
C	1.744026	-2.129796	6.560957
C	5.346209	-2.443178	3.739971
C	2.405696	-0.739123	6.623765
C	5.889801	-2.353908	6.275665
C	1.115218	-2.447236	7.931943
C	2.701761	-5.558925	7.238507
C	2.879057	-3.185685	6.304525
C	1.578297	-6.355008	5.521292
C	2.128720	-6.719113	6.757076
H	6.292256	-2.166046	3.304946
H	2.857429	-0.459533	5.670792
H	2.118215	-7.694668	7.214997
H	3.165404	-0.679082	7.415245
H	1.637107	0.002679	6.846541
H	0.627083	-3.423366	7.938049
H	3.567115	-3.109231	7.145014
H	0.346196	-1.702751	8.145204
H	1.854643	-2.404465	8.743608
N	3.697782	-2.933905	5.120288
N	1.764694	-5.066042	5.241292
N	2.448598	-4.585321	6.294862
N	3.165733	-3.070022	3.891316
S	0.407439	-2.106704	5.301670
Fe	0.999315	-3.675251	3.678746

FeL(formate), bidentate – NO_2 substituent

C	-0.039376	-3.277710	2.138237
H	5.384548	-7.747436	6.903747
H	4.375124	-9.099982	7.403867
H	-0.806516	-2.884694	1.449293
H	6.606772	-3.999043	6.577607
H	4.137064	-7.517589	8.142847
H	6.854466	-5.662049	6.014807
H	7.753602	-4.337913	5.281767
N	4.178123	-3.749531	1.455518
N	0.866811	-8.265314	3.579101
O	-0.110901	-4.521843	2.450165
O	0.857483	-2.534709	2.586942
O	0.542203	-9.447421	3.649417

O	0.468958	-7.448809	2.759545
O	3.034261	-4.073519	1.146460
O	5.019043	-3.253834	0.713266
C	2.536063	-8.621041	5.466755
C	5.886149	-3.976052	3.343463
C	6.782860	-4.617680	5.693244
C	4.369302	-8.027636	7.203761
C	5.739151	-4.416772	4.645016
C	2.298253	-4.954875	8.047800
C	1.829811	-7.816069	4.563960
C	3.364408	-7.743108	6.136700
C	2.784918	-4.234375	6.775617
C	3.717810	-5.222290	5.994099
C	3.632712	-3.013561	7.184038
C	4.590050	-4.006723	2.814268
H	6.793889	-3.689480	2.838012
H	2.454464	-9.687969	5.594246
H	3.009938	-2.335689	7.770155
H	3.134097	-5.261809	8.691203
H	4.523418	-5.492609	6.675044
H	4.491373	-3.299663	7.806878
H	1.684229	-5.826257	7.814431
H	1.675449	-4.266529	8.621655
H	3.985324	-2.454833	6.315463
N	4.392708	-4.658021	4.821201
N	2.159937	-6.531481	4.652936
N	3.095831	-6.494178	5.618197
N	3.689131	-4.406249	3.705748
S	1.325612	-3.638376	5.830489
Fe	1.498448	-4.489280	3.672033