Electronic Supplementary Material (ESI) for RSC Advances.

Modeling study on the catalytic activities by 2-imino-1, 10-phenanthrolinylmetal (Fe, Co, and Ni) precatalysts in ethylene oligomerization

Wenhong Yang,[1,2]* Zhifeng Ma,[1,2] Wen-Hua Sun[1,2]*

[1]*Key laboratory of Engineering Plastics and Beijing National Laboratory for Molecular Science, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China*

[2]*University of Chinese Academy of Sciences, Beijing 100049, China*

E-mail addresses:
whyang@iccas.ac.cn; mazhifeng@iccas.ac.cn; whsun@iccas.ac.cn.

*Author to whom correspondence should be addressed;
Key laboratory of Engineering Plastics and Beijing National Laboratory for Molecular Science, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China
E-Mail: whyang@iccas.ac.cn, Tel.: +86-10-6255-7955; Fax: +86-10-6261-8239.

Key laboratory of Engineering Plastics and Beijing National Laboratory for Molecular Science, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China
E-Mail: whsun@iccas.ac.cn, Tel.: +86-10-6255-7955; Fax: +86-10-6261-8239.

Received data:

Table **S1**. Different catalytic activities stem from experimental data.

Activity/10^4 g mol^{-1} h^{-1} atm^{-1}											
Fe–1a [a]	**Act.**	**Fe–1b** [a]	**Act.**	**Fe–2** [b]	**Act.**	**Fe–3** [c]	**Act.**	**Co–3** [d]	**Act.**	**Ni–3** [e]	**Act.**
1	389	**7**	389	**13**	93.3	**Fe19**	4.78	**Co19**	68.5	**Ni19**	37.4
2	491	**8**	491	**14**	91.0	**Fe20**	1.63	**Co20**	67.1	**Ni20**	32.9
3	94.2	**9**	94.2	**15**	87.2	**Fe21**	0.199	**Co21**	52.3	**Ni21**	33.3
4	389	**10**	127	**16**	41.1	**Fe22**	26.4	**Co22**	55.8	**Ni22**	34.7
5	196	**11**	230	**17**	92.4	**Fe23**	5.13	**Co23**	64.2	**Ni23**	33.1
6	222	**12**	13.1	**18**	26.3	**Fe24**	0.275	**Co24**	28.5	**Ni24**	58.8

Condition: [a] **Fe–1** oligomers, 10 atm and temperature: 40°C, 1000 of Al/Fe, MAO; [b] **Fe–2**: oligomers, 1 atm and temperature: 20°C, 500 of Al/Fe, MAO; [c] **Fe–3**: oligomers, 1 atm and temperature: 20°C, 500 of Al/Fe, MMAO; [d] **Co–3**: oligomers, 1 atm and temperature: 20°C, 500 of Al/Co, MAO; [e] **Ni–3**: oligomers, 1 atm and temperature: 20°C, 300 of Al/Ni, Et_2AlCl.

Table **S2.** The original fitting coefficients of multiple linear regression equation (m) for combined system of **Fe–1a** and **Fe–2** along with correlation coefficient (R^2)

m_0	m_1	m_2	m_3	m_4	R^2
27168.89	73.66	–236.12	479.52	–67.36	0.627

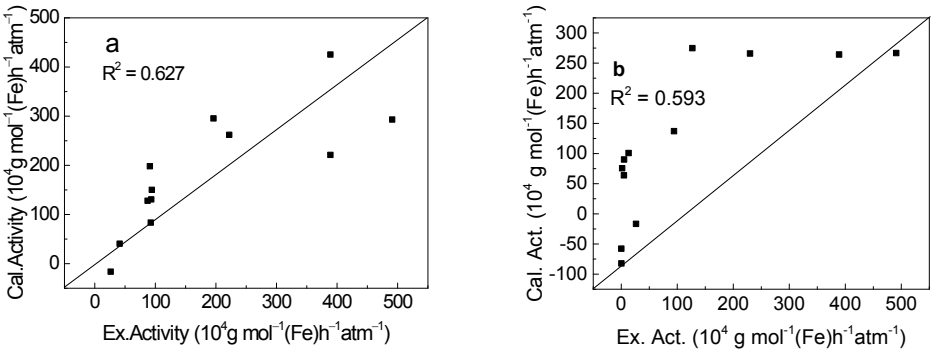

Figure **S1**. The plot of calculated activities versus experimental activities for combined system of **Fe–1a** and **Fe–2** (a) as well as **Fe–1b** and **Fe–3** (b) systems.

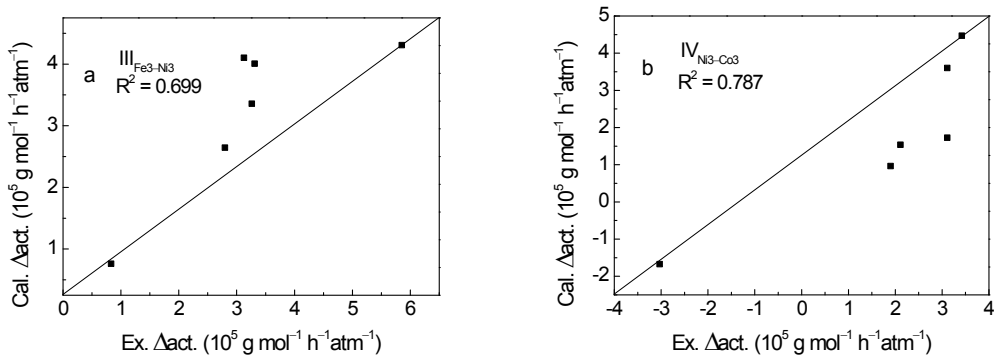

Figure S2. The plot of calculated activities versus experimental activities for **III$_{Fe3–Ni3}$** (a) and **IV$_{Ni3–Co3}$** (b) systems.

Table **S3**. The all coordinates of the optimize structures for complexes **1**–**Ni24**.

Complex 1			
	X	Y	Z
Fe	-0.2800	4.1810	5.1580
Cl	-1.8510	2.5140	5.0660
Cl	-1.1630	6.0810	4.2270
N	1.2240	3.5430	3.5670
N	-0.5290	4.7550	7.3420
N	1.6260	3.9870	6.0600
C	-0.4110	2.2370	0.5720
H	-0.8750	1.3940	0.2230
C	0.8970	4.5840	1.4580
C	3.5520	2.8180	3.0650
H	3.2180	2.6450	2.0420
H	3.9420	1.8720	3.4450
H	4.3600	3.5500	3.0300
C	0.1470	2.2640	1.8710
C	-1.7820	5.4740	9.2190
H	-2.6760	5.7650	9.6230
C	2.4630	3.3090	3.9620
C	0.7680	3.4620	2.3310
C	3.9500	3.4350	5.9750
H	4.7820	3.1240	5.4700
C	2.9920	4.4820	9.4580
H	3.8690	4.4090	9.9800
C	4.0730	3.7340	7.3460
H	4.9840	3.6350	7.8020
C	1.8230	4.9010	10.1310
H	1.8710	5.1260	11.1280

C	2.9510	4.1640	8.0800
C	-0.6210	5.4100	10.0180
H	-0.6710	5.6560	11.0090
C	2.6950	3.5700	5.3270
C	-1.6890	5.1290	7.8530
H	-2.5160	5.1660	7.2550
C	0.6000	5.0050	9.4330
C	1.7250	4.2750	7.3820
C	0.5730	4.6850	8.0530
C	-0.3370	3.3580	-0.2680
H	-0.7510	3.3250	-1.2020
C	0.3200	4.5170	0.1680
H	0.3800	5.3120	-0.4730
C	0.0720	1.0080	2.6650
H	0.5120	1.1020	3.6580
H	-0.9690	0.7040	2.7830
H	0.6080	0.2140	2.1410
C	1.6520	5.8080	1.8490
H	1.5920	6.5960	1.0960
H	1.2720	6.2140	2.7830
H	2.7050	5.5580	1.9840
Complex 2			
	X	Y	Z
Fe	-0.3450	3.9850	5.2030
Cl	-1.7400	2.1710	5.2960
Cl	-1.4520	5.7280	4.2040
N	1.1680	3.4230	3.5880
N	-0.5750	4.6830	7.3530
N	1.5940	3.9920	6.0530
C	-0.2100	2.1650	0.4430
H	-0.5480	1.3080	0.0000
C	0.8060	4.5710	1.5480
C	-1.1360	0.1160	2.5270
H	-1.1260	-0.6780	3.2760
H	-1.3290	-0.3420	1.5550
H	-1.9540	0.8010	2.7540
C	3.5210	2.7900	3.0730
H	3.1780	2.5480	2.0670
H	3.9760	1.8890	3.4870
H	4.2820	3.5680	2.9840
C	0.2370	2.1600	1.7850
C	0.2260	0.8570	2.5260
H	0.9710	0.2000	2.0700
H	0.5250	0.9890	3.5670

C	-1.8260	5.4320	9.2200
H	-2.7270	5.6850	9.6310
C	2.4220	3.2570	3.9720
C	0.7320	3.3800	2.3410
C	3.9450	3.5740	5.9370
H	4.7810	3.2830	5.4280
C	3.0100	4.7790	9.3750
H	3.9030	4.7960	9.8740
C	4.0830	3.9650	7.2830
H	5.0090	3.9490	7.7180
C	1.8330	5.1630	10.0550
H	1.8910	5.4540	11.0340
C	2.9550	4.3730	8.0210
C	-0.6420	5.4990	9.9840
H	-0.6830	5.8030	10.9600
C	2.6680	3.5970	5.3160
C	-1.7450	5.0070	7.8760
H	-2.5880	4.9480	7.3020
C	0.5880	5.1420	9.3890
C	1.7070	4.3640	7.3530
C	0.5480	4.7350	8.0320
C	1.4610	5.8160	2.0830
H	1.1170	5.9940	3.1020
H	2.5360	5.6260	2.1400
C	1.2660	7.1530	1.3260
H	1.7240	7.9670	1.8930
H	0.2030	7.3720	1.2070
H	1.7430	7.1150	0.3450
C	-0.1980	3.3360	-0.3220
H	-0.5450	3.3220	-1.2840
C	0.3050	4.5230	0.2240
H	0.3150	5.3470	-0.3780
Complex 3			
	X	Y	Z
Fe	-0.1980	4.5960	4.8890
Cl	-1.9130	3.2500	4.1750
Cl	-0.6840	6.7480	4.2670
N	1.4960	3.8610	3.5390
N	-0.8500	4.7180	7.0640
N	1.5200	4.2260	6.0640
C	0.6780	1.5170	0.8460
H	0.5490	0.5220	0.6420
C	1.0090	4.2940	1.2550
C	3.9740	3.8630	3.2580

H	3.7920	3.7150	2.1950
H	4.6070	3.0430	3.5970
H	4.5230	4.7980	3.3770
C	1.0570	1.9590	2.1410
C	-2.4400	5.0260	8.7930
H	-3.4040	5.2080	9.0800
C	2.7110	3.9340	4.0550
C	1.1910	3.3790	2.3460
C	3.8810	3.9280	6.2740
H	4.8100	3.8030	5.8680
C	2.2910	4.2010	9.6750
H	3.0790	4.0880	10.3180
C	3.7610	3.9680	7.6770
H	4.5990	3.8700	8.2550
C	0.9980	4.4200	10.1990
H	0.8670	4.4560	11.2130
C	2.4970	4.1450	8.2760
C	-1.4250	4.8450	9.7570
H	-1.6540	4.8970	10.7520
C	2.7240	4.0390	5.4590
C	-2.0990	4.9570	7.4250
H	-2.8150	5.0920	6.7090
C	-0.1010	4.5980	9.3300
C	1.3880	4.2920	7.4110
C	0.1180	4.5360	7.9320
C	0.4790	2.4040	-0.2140
H	0.2130	2.0510	-1.1370
C	0.6580	3.7730	-0.0130
H	0.5280	4.3880	-0.8190
C	0.4520	0.8980	4.4430
C	1.3210	0.8580	3.1600
C	2.8240	0.6500	3.4960
H	-0.6000	0.7900	4.1790
H	0.5950	1.8220	4.9990
H	0.7080	0.0650	5.1030
H	1.0370	-0.1030	2.7160
H	3.0030	-0.3830	3.8060
H	3.1390	1.2850	4.3210
H	3.4510	0.8480	2.6240
C	-0.0790	6.5800	0.9390
C	1.1950	5.7880	1.3600
C	2.4360	6.2810	0.5640
H	-0.9670	6.1640	1.4180
H	-0.2310	6.5500	-0.1410

H	0.0120	7.6270	1.2350
H	1.3930	6.0630	2.3970
H	2.6030	7.3450	0.7470
H	2.3040	6.1360	-0.5100
H	3.3320	5.7430	0.8770
Complex 4			
	X	Y	Z
Fe	-0.2070	4.2690	5.0810
Cl	-1.8010	2.6310	4.9060
Cl	-0.9990	6.2000	4.1310
N	1.3190	3.5920	3.5320
N	-0.5100	4.8140	7.2670
N	1.6740	4.0500	6.0290
C	-0.1710	2.0450	0.5860
H	-0.5470	1.1370	0.2990
C	0.8940	4.5190	1.3940
C	3.6760	2.9500	3.0570
H	3.3680	2.7950	2.0240
H	4.0810	2.0060	3.4240
H	4.4670	3.7020	3.0550
C	0.3570	2.1890	1.8830
C	-1.8070	5.5110	9.1210
H	-2.7100	5.7990	9.5060
C	2.5600	3.3970	3.9430
C	0.8690	3.4380	2.3050
C	4.0030	3.5130	5.9890
H	4.8470	3.2150	5.4980
C	2.9580	4.5070	9.4640
H	3.8230	4.4280	10.0050
C	4.0920	3.7930	7.3670
H	4.9930	3.6920	7.8420
C	1.7740	4.9170	10.1130
H	1.7970	5.1290	11.1140
C	2.9510	4.2070	8.0810
C	-0.6660	5.4330	9.9470
H	-0.7400	5.6660	10.9400
C	2.7610	3.6480	5.3140
C	-1.6820	5.1840	7.7540
H	-2.4930	5.2330	7.1350
C	0.5670	5.0320	9.3870
C	1.7410	4.3240	7.3560
C	0.5740	4.7290	8.0030
C	-0.1830	3.1300	-0.3170
C	0.3630	4.3640	0.0990

H	0.3820	5.1600	-0.5430
Br	0.3950	0.6880	2.9910
Br	1.6550	6.1620	1.8430
C	-0.7520	2.9510	-1.6740
H	-0.6950	3.8660	-2.2670
H	-0.2060	2.1680	-2.2020
H	-1.8020	2.6610	-1.5970
Complex 5			
Fe	-0.2430	4.2580	5.1220
Cl	-1.8490	2.6300	4.9500
Cl	-1.0360	6.2020	4.2010
N	1.2610	3.5880	3.5480
N	-0.5180	4.7810	7.3160
N	1.6470	4.0190	6.0440
C	-0.2750	2.0740	0.6060
H	-0.6610	1.1750	0.3080
C	0.8140	4.5390	1.4240
C	3.6080	2.9400	3.0380
H	3.2860	2.7970	2.0070
H	4.0130	1.9890	3.3900
H	4.4030	3.6880	3.0340
C	0.2710	2.2040	1.8980
C	-1.7880	5.4670	9.1930
H	-2.6840	5.7560	9.5920
C	2.5050	3.3830	3.9420
C	0.7940	3.4480	2.3250
C	3.9730	3.4700	5.9710
H	4.8100	3.1720	5.4670
C	2.9760	4.4350	9.4680
H	3.8470	4.3470	9.9970
C	4.0800	3.7360	7.3500
H	4.9860	3.6250	7.8140
C	1.8010	4.8450	10.1360
H	1.8380	5.0470	11.1380
C	2.9500	4.1490	8.0820
C	-0.6370	5.3750	10.0040
H	-0.6980	5.5980	11.0010
C	2.7240	3.6190	5.3130
C	-1.6810	5.1540	7.8210
H	-2.4990	5.2130	7.2130
C	0.5870	4.9730	9.4260
C	1.7320	4.2790	7.3730
C	0.5750	4.6840	8.0390

C	-0.2860	3.1720	-0.2740
C	0.2660	4.4000	0.1350
H	0.2760	5.1960	-0.5080
Br	0.3140	0.6930	2.9910
Br	1.5890	6.1730	1.8790
Cl	-0.9490	3.0120	-1.8240
Complex 6			
Fe	-0.2410	4.2640	5.1240
Cl	-1.8520	2.6440	4.9460
Cl	-1.0240	6.2140	4.2060
N	1.2630	3.5920	3.5520
N	-0.5160	4.7850	7.3190
N	1.6480	4.0160	6.0490
C	-0.2730	2.0890	0.6050
H	-0.6620	1.1950	0.2990
C	0.8240	4.5480	1.4280
C	3.6090	2.9350	3.0440
H	3.2890	2.7960	2.0120
H	4.0100	1.9830	3.3950
H	4.4070	3.6800	3.0430
C	0.2710	2.2140	1.8970
C	-1.7870	5.4720	9.1950
H	-2.6830	5.7630	9.5930
C	2.5060	3.3810	3.9470
C	0.7980	3.4550	2.3280
C	3.9710	3.4590	5.9790
H	4.8080	3.1580	5.4760
C	2.9720	4.4190	9.4760
H	3.8420	4.3260	10.0070
C	4.0770	3.7200	7.3590
H	4.9820	3.6050	7.8230
C	1.7980	4.8320	10.1430
H	1.8340	5.0320	11.1460
C	2.9470	4.1370	8.0900
C	-0.6380	5.3730	10.0080
H	-0.7000	5.5940	11.0050
C	2.7240	3.6130	5.3190
C	-1.6790	5.1600	7.8230
H	-2.4960	5.2240	7.2130
C	0.5850	4.9670	9.4310
C	1.7310	4.2730	7.3790
C	0.5750	4.6810	8.0430
C	-0.2780	3.1880	-0.2720

C	0.2780	4.4130	0.1380
H	0.2880	5.2050	-0.5070
Br	0.3060	0.7010	2.9870
Br	1.6040	6.1800	1.8870
Br	-1.0040	3.0170	-1.9770
Complex 7			
Fe	-0.2800	4.1810	5.1580
Cl	-1.8510	2.5140	5.0660
Cl	-1.1630	6.0810	4.2270
N	1.2240	3.5430	3.5670
N	-0.5290	4.7550	7.3420
N	1.6260	3.9870	6.0600
C	-0.4110	2.2370	0.5720
H	-0.8750	1.3940	0.2230
C	0.8970	4.5840	1.4580
C	3.5520	2.8180	3.0650
H	3.2180	2.6450	2.0420
H	3.9420	1.8720	3.4450
H	4.3600	3.5500	3.0300
C	0.1470	2.2640	1.8710
C	-1.7820	5.4740	9.2190
H	-2.6760	5.7650	9.6230
C	2.4630	3.3090	3.9620
C	0.7680	3.4620	2.3310
C	3.9500	3.4350	5.9750
H	4.7820	3.1240	5.4700
C	2.9920	4.4820	9.4580
H	3.8690	4.4090	9.9800
C	4.0730	3.7340	7.3460
H	4.9840	3.6350	7.8020
C	1.8230	4.9010	10.1310
H	1.8710	5.1260	11.1280
C	2.9510	4.1640	8.0800
C	-0.6210	5.4100	10.0180
H	-0.6710	5.6560	11.0090
C	2.6950	3.5700	5.3270
C	-1.6890	5.1290	7.8530
H	-2.5160	5.1660	7.2550
C	0.6000	5.0050	9.4330
C	1.7250	4.2750	7.3820
C	0.5730	4.6850	8.0530
C	-0.3370	3.3580	-0.2680
H	-0.7510	3.3250	-1.2020

C	0.3200	4.5170	0.1680
H	0.3800	5.3120	-0.4730
C	0.0720	1.0080	2.6650
H	0.5120	1.1020	3.6580
H	-0.9690	0.7040	2.7830
H	0.6080	0.2140	2.1410
C	1.6520	5.8080	1.8490
H	1.5920	6.5960	1.0960
H	1.2720	6.2140	2.7830
H	2.7050	5.5580	1.9840
Complex 8			
Fe	-0.3450	3.9850	5.2030
Cl	-1.7400	2.1710	5.2960
Cl	-1.4520	5.7280	4.2040
N	1.1680	3.4230	3.5880
N	-0.5750	4.6830	7.3530
N	1.5940	3.9920	6.0530
C	-0.2100	2.1650	0.4430
H	-0.5480	1.3080	0.0000
C	0.8060	4.5710	1.5480
C	-1.1360	0.1160	2.5270
H	-1.1260	-0.6780	3.2760
H	-1.3290	-0.3420	1.5550
H	-1.9540	0.8010	2.7540
C	3.5210	2.7900	3.0730
H	3.1780	2.5480	2.0670
H	3.9760	1.8890	3.4870
H	4.2820	3.5680	2.9840
C	0.2370	2.1600	1.7850
C	0.2260	0.8570	2.5260
H	0.9710	0.2000	2.0700
H	0.5250	0.9890	3.5670
C	-1.8260	5.4320	9.2200
H	-2.7270	5.6850	9.6310
C	2.4220	3.2570	3.9720
C	0.7320	3.3800	2.3410
C	3.9450	3.5740	5.9370
H	4.7810	3.2830	5.4280
C	3.0100	4.7790	9.3750
H	3.9030	4.7960	9.8740
C	4.0830	3.9650	7.2830
H	5.0090	3.9490	7.7180
C	1.8330	5.1630	10.0550

H	1.8910	5.4540	11.0340
C	2.9550	4.3730	8.0210
C	-0.6420	5.4990	9.9840
H	-0.6830	5.8030	10.9600
C	2.6680	3.5970	5.3160
C	-1.7450	5.0070	7.8760
H	-2.5880	4.9480	7.3020
C	0.5880	5.1420	9.3890
C	1.7070	4.3640	7.3530
C	0.5480	4.7350	8.0320
C	1.4610	5.8160	2.0830
H	1.1170	5.9940	3.1020
H	2.5360	5.6260	2.1400
C	1.2660	7.1530	1.3260
H	1.7240	7.9670	1.8930
H	0.2030	7.3720	1.2070
H	1.7430	7.1150	0.3450
C	-0.1980	3.3360	-0.3220
H	-0.5450	3.3220	-1.2840
C	0.3050	4.5230	0.2240
H	0.3150	5.3470	-0.3780
Complex 9			
Fe	-0.1980	4.5960	4.8890
Cl	-1.9130	3.2500	4.1750
Cl	-0.6840	6.7480	4.2670
N	1.4960	3.8610	3.5390
N	-0.8500	4.7180	7.0640
N	1.5200	4.2260	6.0640
C	0.6780	1.5170	0.8460
H	0.5490	0.5220	0.6420
C	1.0090	4.2940	1.2550
C	3.9740	3.8630	3.2580
H	3.7920	3.7150	2.1950
H	4.6070	3.0430	3.5970
H	4.5230	4.7980	3.3770
C	1.0570	1.9590	2.1410
C	-2.4400	5.0260	8.7930
H	-3.4040	5.2080	9.0800
C	2.7110	3.9340	4.0550
C	1.1910	3.3790	2.3460
C	3.8810	3.9280	6.2740
H	4.8100	3.8030	5.8680
C	2.2910	4.2010	9.6750

H	3.0790	4.0880	10.3180
C	3.7610	3.9680	7.6770
H	4.5990	3.8700	8.2550
C	0.9980	4.4200	10.1990
H	0.8670	4.4560	11.2130
C	2.4970	4.1450	8.2760
C	-1.4250	4.8450	9.7570
H	-1.6540	4.8970	10.7520
C	2.7240	4.0390	5.4590
C	-2.0990	4.9570	7.4250
H	-2.8150	5.0920	6.7090
C	-0.1010	4.5980	9.3300
C	1.3880	4.2920	7.4110
C	0.1180	4.5360	7.9320
C	0.4790	2.4040	-0.2140
H	0.2130	2.0510	-1.1370
C	0.6580	3.7730	-0.0130
H	0.5280	4.3880	-0.8190
C	0.4520	0.8980	4.4430
C	1.3210	0.8580	3.1600
C	2.8240	0.6500	3.4960
H	-0.6000	0.7900	4.1790
H	0.5950	1.8220	4.9990
H	0.7080	0.0650	5.1030
H	1.0370	-0.1030	2.7160
H	3.0030	-0.3830	3.8060
H	3.1390	1.2850	4.3210
H	3.4510	0.8480	2.6240
C	-0.0790	6.5800	0.9390
C	1.1950	5.7880	1.3600
C	2.4360	6.2810	0.5640
H	-0.9670	6.1640	1.4180
H	-0.2310	6.5500	-0.1410
H	0.0120	7.6270	1.2350
H	1.3930	6.0630	2.3970
H	2.6030	7.3450	0.7470
H	2.3040	6.1360	-0.5100
H	3.3320	5.7430	0.8770
Complex 10			
Fe	-0.2460	4.4550	4.9540
Cl	-2.0150	3.0770	4.4780
Cl	-0.6660	6.5460	4.1140
N	1.3400	3.6900	3.5080

N	-0.7170	4.8650	7.1400
N	1.4720	3.9060	6.0660
C	0.0960	2.5310	0.2740
H	-0.3450	1.7160	-0.1620
C	1.3170	4.8140	1.4110
C	0.4190	2.5230	1.6500
C	-2.1130	5.5900	8.9110
H	-3.0080	5.9690	9.2270
C	2.4890	3.3030	4.0340
C	1.0310	3.6770	2.2240
C	3.7050	3.0570	6.2090
H	4.5520	2.6840	5.7740
C	2.4150	3.9130	9.6380
H	3.1970	3.6750	10.2540
C	3.6760	3.2140	7.6090
H	4.4980	2.9540	8.1600
C	1.2280	4.4310	10.2000
H	1.1670	4.5600	11.2130
C	2.5240	3.7250	8.2400
C	-1.0910	5.2910	9.8370
H	-1.2450	5.4540	10.8350
C	2.5720	3.4150	5.4330
C	-1.8770	5.3560	7.5380
H	-2.6010	5.5640	6.8480
C	0.1350	4.7670	9.3700
C	1.4270	4.0630	7.4120
C	0.2570	4.5750	7.9720
C	0.3710	3.6490	-0.5260
C	0.9780	4.7790	0.0390
H	1.1730	5.5820	-0.5660
H	0.1310	3.6390	-1.5200
C	4.5590	3.6950	2.7790
H	4.5160	4.6950	2.9930
C	5.6240	3.2090	1.9990
H	6.3380	3.8530	1.6500
C	5.7110	1.8370	1.7020
H	6.4850	1.4840	1.1350
C	4.7330	0.9490	2.1870
H	4.7990	-0.0490	1.9750
C	3.6670	1.4340	2.9670
H	2.9700	0.7730	3.3200
C	3.5650	2.8130	3.2610
C	1.9710	6.0550	1.9090
H	1.3260	6.9150	1.7200

H	2.1860	6.0280	2.9770
H	2.9160	6.2080	1.3820
C	0.1010	1.2810	2.4060
H	0.3590	1.3450	3.4630
H	-0.9680	1.0690	2.3360
H	0.6500	0.4400	1.9780
Complex 11			
Fe	-0.1690	4.5330	5.0310
Cl	-2.0950	3.4460	4.4150
Cl	-0.4010	6.7470	4.4920
N	1.3320	3.7710	3.4880
N	-0.6180	4.6490	7.2570
N	1.5420	3.7980	6.0410
C	-0.1780	2.4500	0.4350
H	-0.6970	1.6420	0.0760
C	1.2090	4.7450	1.3250
C	0.2380	2.4980	1.7900
C	-1.9890	5.1470	9.1240
H	-2.8740	5.4960	9.4980
C	2.5450	3.4810	3.9320
C	0.9260	3.6760	2.2360
C	3.7870	2.9730	6.0480
H	4.6320	2.6680	5.5610
C	2.5180	3.3220	9.5720
H	3.3020	2.9980	10.1430
C	3.7660	2.9260	7.4560
H	4.5930	2.5960	7.9590
C	1.3380	3.7650	10.2110
H	1.2850	3.7520	11.2320
C	2.6150	3.3310	8.1610
C	-0.9680	4.7010	9.9900
H	-1.1130	4.7260	11.0030
C	2.6440	3.4210	5.3360
C	-1.7650	5.1040	7.7300
H	-2.4880	5.4230	7.0830
C	0.2450	4.2260	9.4450
C	1.5110	3.7760	7.3960
C	0.3530	4.2250	8.0320
C	0.1150	3.4790	-0.4650
C	0.8180	4.6050	-0.0270
H	1.0380	5.3280	-0.7150
H	-0.1790	3.4070	-1.4430
C	4.7380	4.1670	3.0950

H	4.7200	4.9850	3.7100
C	5.8500	3.9780	2.2540
H	6.6230	4.6480	2.2680
C	5.8990	2.8690	1.3910
H	6.7060	2.7320	0.7790
C	4.8360	1.9490	1.3720
H	4.8720	1.1420	0.7450
C	3.7250	2.1370	2.2140
H	2.9690	1.4530	2.1820
C	3.6590	3.2500	3.0870
C	0.4310	0.9850	4.0020
C	-0.1040	1.2550	2.5740
H	0.0190	0.0430	4.3680
H	0.1340	1.7650	4.6980
H	1.5160	0.8900	4.0030
H	-1.1940	1.1920	2.6250
H	0.2350	0.3940	1.9890
C	1.1870	7.3150	1.3520
C	1.9340	6.0030	1.7040
H	1.6670	8.1600	1.8510
H	0.1450	7.2670	1.6720
H	1.2120	7.5010	0.2770
H	2.1450	6.0370	2.7730
H	2.9010	6.0100	1.1930
Complex 12			
Fe	-0.3440	4.4330	4.6470
Cl	-1.9930	3.2450	3.5790
Cl	-0.5830	6.6430	4.0970
N	1.5260	3.7630	3.5150
N	-1.3350	4.4790	6.6920
N	1.1170	3.8180	6.0480
C	0.5230	2.2740	0.3360
H	0.0480	1.4620	-0.0640
C	1.7130	4.6390	1.3090
C	0.8420	2.3290	1.7190
C	-3.1570	4.8410	8.1620
H	-4.1320	5.1140	8.3060
C	2.6230	3.6080	4.2430
C	1.3830	3.5720	2.2140
C	3.3460	3.1710	6.6090
H	4.3040	2.9320	6.3480
C	1.2320	3.3700	9.7140
H	1.8770	3.1010	10.4610

C	2.9860	3.1020	7.9690
H	3.6890	2.8300	8.6610
C	-0.0990	3.7090	10.0410
H	-0.4000	3.6780	11.0180
C	1.6700	3.4060	8.3690
C	-2.3490	4.4640	9.2550
H	-2.7390	4.4640	10.2010
C	2.3830	3.5420	5.6330
C	-2.5960	4.8360	6.8670
H	-3.1600	5.1080	6.0600
C	-1.0050	4.0940	9.0270
C	0.7560	3.7730	7.3540
C	-0.5540	4.1200	7.6840
C	0.8380	3.3060	-0.5500
C	1.4520	4.4620	-0.0700
H	1.6900	5.1870	-0.7500
H	0.6210	3.2150	-1.5460
C	4.9220	4.4370	4.0750
H	4.6950	5.2110	4.7050
C	6.2340	4.3390	3.5740
H	6.9380	5.0280	3.8460
C	6.5750	3.2950	2.6960
H	7.5270	3.2250	2.3300
C	5.6040	2.3500	2.3220
H	5.8500	1.5910	1.6830
C	4.2950	2.4470	2.8290
H	3.6140	1.7450	2.5520
C	3.9320	3.4890	3.7120
C	1.4600	7.1870	1.2950
C	2.3220	5.9590	1.7200
C	3.7740	6.1150	1.1810
H	0.4040	7.0100	1.4940
H	1.5640	7.4000	0.2290
H	1.7720	8.0760	1.8480
H	2.3920	6.0110	2.8080
H	4.2640	6.9670	1.6580
H	3.7820	6.2760	0.1010
H	4.3630	5.2230	1.3870
C	0.7100	0.9820	4.0290
C	0.5290	1.0420	2.4830
C	1.2700	-0.2100	1.8980
H	0.2940	0.0520	4.4250
H	0.1830	1.7890	4.5250
H	1.7650	1.0110	4.3010

H	-0.5400	0.8600	2.3280
H	0.9590	-1.1210	2.4150
H	2.3500	-0.1120	2.0060
H	1.0490	-0.3660	0.8430
Complex 13			
Fe	-0.2020	4.4140	5.1020
Cl	-1.8760	2.8630	4.9230
Cl	-0.7190	6.4780	4.2540
N	1.2200	3.6320	3.5190
N	-0.4570	4.8880	7.3000
N	1.6610	4.0230	6.0130
C	-0.2600	2.0710	0.5480
H	-0.5450	1.1630	0.1710
C	0.5030	4.5940	1.5130
C	3.5570	2.9880	2.9550
H	3.2260	2.9170	1.9200
H	3.9430	2.0100	3.2500
H	4.3690	3.7160	2.9890
C	0.3230	2.1670	1.8350
C	-1.6880	5.5940	9.1960
H	-2.5650	5.9270	9.6020
C	2.4690	3.4050	3.8890
C	0.7020	3.4520	2.3210
C	3.9520	3.3600	5.9140
H	4.7710	3.0360	5.3970
C	3.0040	4.2600	9.4440
H	3.8670	4.1060	9.9710
C	4.0730	3.5720	7.3020
H	4.9720	3.3990	7.7590
C	1.8540	4.7180	10.1240
H	1.9000	4.8860	11.1320
C	2.9660	4.0200	8.0500
C	-0.5480	5.4030	10.0050
H	-0.5980	5.5990	11.0080
C	2.7110	3.5910	5.2640
C	-1.5960	5.3180	7.8140
H	-2.4060	5.4490	7.2070
C	0.6510	4.9420	9.4170
C	1.7570	4.2400	7.3480
C	0.6240	4.6970	8.0210
C	-0.4580	3.2160	-0.2440
C	-0.0750	4.4770	0.2380
H	-0.2160	5.3100	-0.3390

H	0.7830	5.5200	1.8450
H	-0.8800	3.1300	-1.1710
C	0.5270	0.9340	2.6430
H	0.0400	1.0350	3.6130
H	0.1190	0.0450	2.1570
H	1.5920	0.7670	2.8020
Complex 14			
Fe	-0.2290	4.5160	5.1800
Cl	-1.8950	2.9590	4.9770
Cl	-0.6910	6.5470	4.2290
N	1.2560	3.6910	3.6810
N	-0.5690	5.0700	7.3470
N	1.5890	4.1340	6.1820
C	-0.1980	2.1990	0.6640
H	-0.5740	1.3210	0.2990
C	0.7990	4.6480	1.6030
C	3.5890	2.9420	3.2490
H	3.2990	2.8330	2.2040
H	3.9300	1.9680	3.6030
H	4.4210	3.6460	3.2860
C	0.3000	2.2720	1.9890
C	-1.8680	5.8580	9.1640
H	-2.7560	6.2170	9.5210
C	2.4770	3.4320	4.1160
C	0.7990	3.5230	2.4570
C	3.8680	3.4250	6.2050
H	4.7030	3.0680	5.7360
C	2.7870	4.4660	9.6580
H	3.6240	4.3150	10.2270
C	3.9340	3.6850	7.5890
H	4.8080	3.5110	8.0910
C	1.6170	4.9640	10.2710
H	1.6230	5.1660	11.2740
C	2.8040	4.1780	8.2720
C	-0.7660	5.6800	10.0270
H	-0.8550	5.9110	11.0200
C	2.6620	3.6580	5.4940
C	-1.7220	5.5330	7.7980
H	-2.5040	5.6540	7.1520
C	0.4490	5.1820	9.5060
C	1.6320	4.3940	7.5110
C	0.4780	4.8900	8.1200
C	-0.1930	3.3250	-0.1780

C	0.3060	4.5490	0.2910
H	0.3120	5.3680	-0.3210
H	1.1610	5.5480	1.9280
H	-0.5550	3.2530	-1.1320
C	1.2270	-0.0680	2.3390
C	0.2640	1.0370	2.8320
H	1.1850	-0.9210	3.0190
H	2.2530	0.3020	2.3110
H	0.9480	-0.4120	1.3410
H	0.5200	1.2550	3.8710
H	-0.7550	0.6420	2.8380
Complex 15			
Fe	-0.1790	4.5710	5.0870
Cl	-1.9890	3.1830	4.8700
Cl	-0.5330	6.6760	4.2590
N	1.2120	3.6650	3.5390
N	-0.4460	5.0260	7.2880
N	1.6510	4.0870	6.0210
C	-0.3360	2.1270	0.5740
H	-0.6540	1.2420	0.1700
C	0.4680	4.6030	1.5780
C	3.5590	3.0740	2.9620
H	3.2250	3.0130	1.9260
H	3.9590	2.0990	3.2440
H	4.3620	3.8120	3.0030
C	0.2940	2.1540	1.8510
C	-1.6760	5.7560	9.1760
H	-2.5450	6.1180	9.5750
C	2.4680	3.4700	3.9000
C	0.6780	3.4400	2.3560
C	3.9310	3.3800	5.9370
H	4.7490	3.0460	5.4240
C	2.9600	4.2460	9.4690
H	3.8110	4.0580	10.0050
C	4.0390	3.5670	7.3290
H	4.9280	3.3670	7.7950
C	1.8150	4.7290	10.1410
H	1.8520	4.8800	11.1520
C	2.9330	4.0280	8.0720
C	-0.5560	5.5080	9.9990
H	-0.6130	5.6920	11.0040
C	2.7010	3.6430	5.2780
C	-1.5740	5.4960	7.7920

H	-2.3700	5.6680	7.1750
C	0.6320	5.0080	9.4210
C	1.7390	4.2890	7.3580
C	0.6150	4.7810	8.0220
C	-0.5520	3.2900	-0.1830
C	-0.1430	4.5310	0.3180
H	-0.2900	5.3800	-0.2330
H	0.7660	5.5210	1.9170
H	-1.0040	3.2310	-1.0980
C	0.7610	0.7240	4.0460
C	0.4720	0.8040	2.5180
C	1.5280	-0.0580	1.7610
H	0.1410	1.4190	4.6040
H	1.8080	0.9180	4.2690
H	0.5360	-0.2800	4.4150
H	-0.4900	0.2870	2.4140
H	1.5980	-1.0550	2.2010
H	2.5120	0.4110	1.8100
H	1.2600	-0.1840	0.7110
Complex 16			
Fe	-0.1410	4.4220	5.0720
Cl	-1.7750	2.8390	4.8110
Cl	-0.6520	6.4860	4.2220
N	1.3350	3.6820	3.5210
N	-0.4630	4.8720	7.2660
N	1.6960	4.0260	6.0330
C	-0.0650	2.1650	0.5060
H	-0.3510	1.2440	0.1620
C	0.7270	4.6780	1.4770
C	3.6670	2.9690	3.0300
H	3.3660	2.9040	1.9840
H	4.0120	1.9800	3.3380
H	4.4990	3.6720	3.0870
C	0.4580	2.2780	1.8090
C	-1.7500	5.5560	9.1320
H	-2.6400	5.8810	9.5160
C	2.5640	3.4200	3.9290
C	0.8580	3.5420	2.3020
C	3.9850	3.3510	5.9970
H	4.8180	3.0260	5.5030
C	2.9350	4.2290	9.5040
H	3.7820	4.0690	10.0550
C	4.0650	3.5540	7.3900

H	4.9490	3.3740	7.8730
C	1.7650	4.6800	10.1540
H	1.7810	4.8400	11.1640
C	2.9380	4.0010	8.1080
C	-0.6330	5.3610	9.9720
H	-0.7130	5.5470	10.9750
C	2.7660	3.5940	5.3130
C	-1.6180	5.2930	7.7510
H	-2.4110	5.4270	7.1210
C	0.5830	4.9100	9.4140
C	1.7520	4.2300	7.3720
C	0.5980	4.6780	8.0160
C	-0.2010	3.3010	-0.3230
C	0.2020	4.5590	0.1780
H	0.1180	5.4000	-0.4000
Br	0.6040	0.7340	2.8450
H	1.0180	5.5990	1.8150
C	-0.7570	3.1520	-1.6890
H	-0.8060	4.1050	-2.2190
H	-0.1300	2.4720	-2.2690
H	-1.7670	2.7410	-1.6330
Complex 17			
Fe	-0.1880	4.4020	5.1110
Cl	-1.8120	2.8020	4.9000
Cl	-0.7390	6.4550	4.2590
N	1.2580	3.6660	3.5320
N	-0.4640	4.8650	7.3080
N	1.6740	4.0310	6.0320
C	-0.1970	2.1090	0.5620
H	-0.4840	1.1890	0.2210
C	0.5930	4.6420	1.4950
C	3.5850	2.9710	2.9910
H	3.2600	2.8970	1.9530
H	3.9460	1.9880	3.2970
H	4.4120	3.6820	3.0250
C	0.3560	2.2390	1.8520
C	-1.7140	5.5510	9.1980
H	-2.5980	5.8720	9.5990
C	2.4990	3.4180	3.9130
C	0.7550	3.5120	2.3260
C	3.9680	3.3770	5.9480
H	4.7920	3.0560	5.4370
C	2.9900	4.2680	9.4730

H	3.8510	4.1190	10.0060
C	4.0780	3.5900	7.3370
H	4.9750	3.4210	7.8010
C	1.8310	4.7130	10.1460
H	1.8690	4.8790	11.1540
C	2.9630	4.0310	8.0780
C	-0.5770	5.3720	10.0140
H	-0.6360	5.5640	11.0170
C	2.7310	3.6040	5.2900
C	-1.6110	5.2800	7.8160
H	-2.4190	5.4030	7.2040
C	0.6310	4.9270	9.4310
C	1.7590	4.2440	7.3670
C	0.6160	4.6860	8.0350
C	-0.3560	3.2410	-0.2590
C	0.0400	4.5080	0.2090
H	-0.0730	5.3340	-0.3840
Br	0.5420	0.7050	2.8950
H	0.8830	5.5690	1.8190
F	-0.8700	3.1170	-1.4520
Complex 18			
Fe	-0.1810	4.4090	5.1190
Cl	-1.8090	2.8140	4.9020
Cl	-0.7210	6.4640	4.2660
N	1.2680	3.6680	3.5440
N	-0.4610	4.8720	7.3160
N	1.6770	4.0310	6.0460
C	-0.1840	2.1160	0.5710
H	-0.4730	1.1980	0.2280
C	0.6110	4.6460	1.5060
C	3.5940	2.9650	3.0100
H	3.2720	2.8930	1.9710
H	3.9510	1.9810	3.3170
H	4.4230	3.6740	3.0470
C	0.3660	2.2430	1.8610
C	-1.7160	5.5610	9.2030
H	-2.5990	5.8850	9.6020
C	2.5070	3.4160	3.9290
C	0.7670	3.5150	2.3370
C	3.9690	3.3690	5.9690
H	4.7940	3.0460	5.4600
C	2.9840	4.2620	9.4910
H	3.8430	4.1110	10.0260

C	4.0760	3.5810	7.3580
H	4.9710	3.4090	7.8250
C	1.8240	4.7100	10.1600
H	1.8600	4.8760	11.1690
C	2.9610	4.0260	8.0960
C	-0.5810	5.3770	10.0220
H	-0.6420	5.5690	11.0250
C	2.7350	3.6000	5.3070
C	-1.6090	5.2900	7.8210
H	-2.4150	5.4150	7.2060
C	0.6270	4.9290	9.4430
C	1.7590	4.2430	7.3820
C	0.6160	4.6880	8.0460
C	-0.3380	3.2480	-0.2510
C	0.0610	4.5130	0.2180
H	-0.0480	5.3380	-0.3750
Br	0.5440	0.7080	2.9050
H	0.9020	5.5720	1.8300
Br	-1.0680	3.0720	-1.9530
Complex Fe19			
Fe	-1.1730	-3.1620	3.0440
N	0.0310	-1.5060	1.8980
Cl	0.4730	-3.7770	4.5200
C	1.1770	-1.7080	1.2580
N	-2.2590	-1.3690	3.2810
Cl	-1.6760	-4.5200	1.2650
C	1.8110	-0.6240	0.6020
H	2.6950	-0.7500	0.1010
N	-3.0340	-3.5820	4.4100
C	1.2100	0.6480	0.6440
H	1.6590	1.4370	0.1720
C	-0.0050	0.8150	1.3390
C	-0.6810	2.0490	1.4370
H	-0.2990	2.8880	0.9930
C	-1.8920	2.1370	2.1510
H	-2.3710	3.0390	2.2110
C	-2.4370	0.9920	2.7760
C	-3.6460	1.0280	3.4960
H	-4.1720	1.9010	3.5870
C	-4.1430	-0.1400	4.0990
H	-5.0220	-0.0770	4.6140
C	-3.4290	-1.3610	3.9900
C	-1.7600	-0.2510	2.6840

C	-0.5590	-0.3320	1.9650
C	1.7790	-2.9740	1.2210
C	1.4270	-3.9060	0.2190
H	0.7230	-3.6710	-0.4860
C	2.0430	-5.1710	0.1770
H	1.7770	-5.8450	-0.5450
C	3.0250	-5.5090	1.1250
H	3.4710	-6.4280	1.0950
C	3.3970	-4.5790	2.1120
H	4.1160	-4.8220	2.7980
C	2.7820	-3.3140	2.1570
H	3.0690	-2.6460	2.8780
C	-3.8600	-2.5680	4.5820
C	-5.1410	-2.6640	5.3440
H	-5.3420	-3.6670	5.7200
H	-5.9750	-2.3860	4.6970
H	-5.1130	-1.9890	6.2010
C	-3.1290	-4.7860	4.9450
C	-2.6170	-5.0170	6.2570
C	-2.6190	-6.3340	6.7710
H	-2.2390	-6.5340	7.7000
C	-3.1550	-7.3960	6.0290
H	-3.1460	-8.3440	6.4120
C	-3.7190	-7.1530	4.7690
H	-4.1290	-7.9400	4.2570
C	-3.7330	-5.8520	4.2170
C	-2.1180	-3.9080	7.1190
H	-1.6820	-4.2680	8.0540
H	-1.3570	-3.3260	6.6040
H	-2.9450	-3.2460	7.3740
C	-4.4200	-5.6820	2.9080
H	-5.4660	-5.9820	3.0050
H	-4.4070	-4.6530	2.5490
H	-3.9460	-6.3140	2.1550
Complex Fe20			
Fe	-1.1470	-3.0900	3.0280
N	-0.0670	-1.2180	2.1130
Cl	0.4860	-3.6980	4.5220
C	1.1160	-1.2460	1.5100
N	-2.4110	-1.4400	3.3920
Cl	-1.4460	-4.2830	1.0900
C	1.6660	-0.0450	0.9970
H	2.5750	-0.0360	0.5260

N	-3.0220	-3.8260	4.2320
C	0.9440	1.1540	1.1390
H	1.3310	2.0270	0.7710
C	-0.3060	1.1340	1.7910
C	-1.1010	2.2840	1.9830
H	-0.7850	3.1970	1.6430
C	-2.3390	2.1850	2.6460
H	-2.9040	3.0280	2.7760
C	-2.7950	0.9350	3.1250
C	-4.0250	0.7850	3.7910
H	-4.6340	1.5920	3.9480
C	-4.4290	-0.4800	4.2480
H	-5.3280	-0.5520	4.7280
C	-3.6000	-1.6140	4.0450
C	-1.9990	-0.2240	2.9370
C	-0.7700	-0.1170	2.2710
C	1.8390	-2.4390	1.3740
C	1.6310	-3.2800	0.2580
H	0.9440	-3.0320	-0.4600
C	2.3680	-4.4710	0.1170
H	2.2070	-5.0800	-0.6890
C	3.3300	-4.8230	1.0810
H	3.8640	-5.6880	0.9790
C	3.5590	-3.9800	2.1840
H	4.2620	-4.2330	2.8810
C	2.8220	-2.7900	2.3270
H	3.0060	-2.1840	3.1320
C	-3.9370	-2.9110	4.4880
C	-5.2220	-3.2000	5.1930
H	-5.3350	-4.2500	5.4630
H	-6.0620	-2.9360	4.5480
H	-5.2790	-2.6160	6.1120
C	-3.0340	-5.0950	4.5960
C	-2.5260	-5.4660	5.8810
C	-2.4250	-6.8470	6.1820
H	-2.0520	-7.1700	7.0750
C	-2.8450	-7.8250	5.2710
H	-2.7540	-8.8170	5.5060
C	-3.4070	-7.4450	4.0460
H	-3.7250	-8.1800	3.4090
C	-3.5370	-6.0820	3.6960
C	-4.2200	-5.7600	2.4030
H	-4.1360	-4.7010	2.1530
H	-3.7400	-6.3160	1.5940

C	-5.7300	-6.0960	2.4180
H	-6.1810	-5.8060	1.4670
H	-6.2340	-5.5530	3.2190
H	-5.8910	-7.1670	2.5590
C	-2.1650	-4.4170	6.8960
H	-1.5760	-3.6370	6.4150
H	-3.0930	-3.9520	7.2350
C	-1.3720	-4.8360	8.1590
H	-1.1200	-3.9510	8.7460
H	-0.4440	-5.3380	7.8770
H	-1.9680	-5.5000	8.7870
Complex Fe21			
Fe	-1.0640	-3.1120	3.1150
N	0.2780	-1.5780	1.9500
Cl	0.4210	-3.5270	4.8100
C	1.4740	-1.8480	1.4380
N	-2.1340	-1.2970	3.0750
Cl	-1.3090	-4.6090	1.3970
C	2.1870	-0.8340	0.7520
H	3.1100	-1.0140	0.3470
N	-3.1010	-3.4330	4.2540
C	1.6120	0.4430	0.6270
H	2.1180	1.1830	0.1330
C	0.3410	0.6850	1.1880
C	-0.3150	1.9310	1.1150
H	0.1250	2.7230	0.6370
C	-1.5840	2.0960	1.7010
H	-2.0470	3.0070	1.6390
C	-2.2090	1.0170	2.3650
C	-3.4750	1.1330	2.9660
H	-3.9870	2.0190	2.9370
C	-4.0510	0.0270	3.6140
H	-4.9710	0.1520	4.0380
C	-3.3630	-1.2140	3.6680
C	-1.5550	-0.2390	2.4420
C	-0.2920	-0.3960	1.8550
C	2.0580	-3.1180	1.5560
C	1.8470	-4.0980	0.5600
H	1.2560	-3.8970	-0.2510
C	2.4490	-5.3660	0.6710
H	2.2850	-6.0740	-0.0480
C	3.2780	-5.6590	1.7690
H	3.7130	-6.5810	1.8500

C	3.5130	-4.6810	2.7530
H	4.1220	-4.8920	3.5470
C	2.9120	-3.4130	2.6440
H	3.1010	-2.7100	3.3620
C	-3.8820	-2.3660	4.3010
C	-5.2220	-2.3370	4.9670
H	-5.5040	-3.2870	5.4190
H	-5.9910	-2.0810	4.2370
H	-5.2250	-1.5860	5.7580
C	-3.3840	-4.6140	4.7840
C	-3.0430	-4.8820	6.1520
C	-3.4450	-6.1160	6.7180
H	-3.2330	-6.3420	7.6920
C	-4.1540	-7.0650	5.9770
H	-4.4330	-7.9500	6.4080
C	-4.4920	-6.7950	4.6480
H	-5.0280	-7.5050	4.1440
C	-4.1220	-5.5800	4.0200
C	-1.0580	-4.5170	7.7330
C	-2.3200	-3.9060	7.0490
C	-3.2700	-3.2970	8.1200
H	-0.4750	-5.1040	7.0220
H	-1.3300	-5.1710	8.5630
H	-0.4210	-3.7220	8.1260
H	-1.9610	-3.0610	6.4590
H	-2.7420	-2.5450	8.7090
H	-3.6440	-4.0640	8.7990
H	-4.1220	-2.8120	7.6460
C	-6.1090	-5.1400	2.5080
C	-4.5730	-5.3650	2.5960
C	-4.1390	-6.5120	1.6330
H	-6.4140	-4.3100	3.1450
H	-6.6590	-6.0310	2.8180
H	-6.3970	-4.8980	1.4820
H	-4.1190	-4.4540	2.2010
H	-4.2300	-6.1860	0.5950
H	-4.7620	-7.4000	1.7620
H	-3.1030	-6.8010	1.8130
Complex Fe22			
Fe	1.6840	1.4250	6.1540
Cl	1.0140	-0.7630	6.3130
Cl	3.8390	2.0130	6.6750
N	0.3230	2.8990	5.4980

C	-0.2530	3.1920	7.7940
N	1.8210	1.5790	3.8180
C	-0.4190	3.5370	6.4450
C	0.8680	1.8350	9.3130
C	2.6660	0.7830	3.1890
C	1.8080	0.8270	9.5680
C	0.2070	3.1850	4.1670
C	-1.3550	4.5420	6.0890
C	4.0110	1.2040	2.9610
C	1.0160	2.4650	3.2650
C	-1.0090	3.8330	8.8090
C	-2.1100	5.1850	7.0970
H	-2.7880	5.9110	6.8530
C	3.1580	1.1540	9.8260
H	3.4670	2.1300	9.8190
C	0.9580	2.6760	1.8690
C	-0.7830	3.4230	10.1390
H	-1.2970	3.8480	10.9150
C	-1.9380	4.8320	8.4500
H	-2.4930	5.3070	9.1660
C	0.0150	1.9780	1.0800
H	-0.6430	1.3250	1.5110
C	-0.7160	4.1840	3.7640
H	-0.8360	4.4340	2.7800
C	-1.4910	4.8570	4.7240
H	-2.1530	5.5750	4.4190
C	2.3450	-1.5390	9.8890
H	2.0500	-2.5170	9.9160
C	0.1650	2.4140	10.3970
H	0.3320	2.1120	11.3610
C	3.6920	-1.2060	10.1240
H	4.3740	-1.9420	10.3180
C	1.8370	3.5900	1.2440
H	2.5140	4.1220	1.7950
C	4.0970	0.1410	10.0960
H	5.0740	0.3830	10.2730
C	1.4050	-0.5270	9.6190
H	0.4280	-0.7860	9.4580
C	-0.0320	2.1750	-0.3130
H	-0.7140	1.6630	-0.8780
C	0.8570	3.0750	-0.9280
H	0.8230	3.2160	-1.9400
C	1.7890	3.7840	-0.1490
H	2.4310	4.4430	-0.5960

N	0.6250	2.2530	8.0760
C	2.2340	-0.4970	2.7290
C	4.9030	0.3300	2.3000
H	5.8730	0.6080	2.1280
C	3.1580	-1.3400	2.0710
H	2.8730	-2.2640	1.7350
C	4.4830	-0.9330	1.8610
H	5.1400	-1.5550	1.3850
C	4.5510	2.5320	3.3610
H	5.4010	2.3980	4.0330
H	4.8920	3.0710	2.4740
H	3.8180	3.1580	3.8680
C	0.8470	-1.0170	2.8810
H	0.4160	-1.2020	1.8950
H	0.8630	-1.9570	3.4350
H	0.1870	-0.3300	3.4090
Complex Fe23			
Fe	1.4790	1.4480	6.2270
Cl	0.5850	-0.6470	6.4980
Cl	3.5760	1.9240	7.0230
N	0.3670	2.9430	5.2380
C	-0.5050	3.5210	7.3810
N	1.9790	1.3440	3.9360
C	-0.4440	3.7310	5.9970
C	0.2640	2.2560	9.1740
C	2.8560	0.4270	3.5580
C	1.0670	1.2180	9.6670
C	0.4730	3.0930	3.8850
C	-1.2240	4.7590	5.4100
C	4.2540	0.7330	3.5610
C	1.3430	2.2270	3.1880
C	-1.3370	4.3220	8.2050
C	-2.0540	5.5610	6.2260
H	-2.6220	6.3070	5.8150
C	2.3880	1.4800	10.0970
H	2.7750	2.4260	10.0430
C	1.5070	2.3220	1.7890
C	-1.3400	4.0420	9.5870
H	-1.9190	4.5850	10.2320
C	-2.1100	5.3440	7.6170
H	-2.7160	5.9340	8.1930
C	0.6710	1.5880	0.9180
H	-0.0690	0.9900	1.2910

C	-0.2930	4.1080	3.2550
H	-0.2500	4.2620	2.2450
C	-1.1350	4.9350	4.0170
H	-1.6800	5.6640	3.5480
C	1.3530	-1.1300	10.2930
H	0.9760	-2.0780	10.3690
C	-0.5330	2.9990	10.0800
H	-0.5320	2.7910	11.0830
C	2.6740	-0.8660	10.6990
H	3.2570	-1.6210	11.0660
C	2.4670	3.1990	1.2380
H	3.0460	3.7830	1.8450
C	3.1900	0.4400	10.6040
H	4.1480	0.6340	10.9050
C	0.5500	-0.0920	9.7850
H	-0.4120	-0.3000	9.5030
C	0.8360	1.6800	-0.4770
H	0.2360	1.1340	-1.1000
C	1.8220	2.5270	-1.0140
H	1.9440	2.5910	-2.0270
C	2.6320	3.2920	-0.1570
H	3.3390	3.9200	-0.5470
N	0.2360	2.5550	7.8810
C	2.4140	-0.8970	3.2390
C	5.1800	-0.3110	3.3250
H	6.1870	-0.1350	3.3550
C	3.3840	-1.9020	3.0110
H	3.1040	-2.8660	2.8140
C	4.7520	-1.6150	3.0550
H	5.4380	-2.3570	2.8900
C	5.6990	2.6540	2.6810
C	4.8210	2.0940	3.8290
H	5.8890	3.7160	2.8450
H	5.2080	2.5310	1.7160
H	6.6620	2.1410	2.6450
H	4.0340	2.8230	4.0280
H	5.4370	2.0450	4.7300
C	0.5620	-1.8960	1.7810
C	0.9760	-1.3100	3.1550
H	-0.5260	-1.9670	1.7220
H	0.9730	-2.8980	1.6460
H	0.9140	-1.2660	0.9640
H	0.7870	-2.0720	3.9150
H	0.3080	-0.4760	3.3730

Complex Fe24			
Fe	1.7990	1.5180	6.1700
Cl	1.3090	-0.6990	6.4930
Cl	3.8890	2.3100	6.6850
N	0.4450	2.9470	5.4200
C	-0.9610	-0.1450	2.1200
H	-0.8220	0.9170	1.9170
H	-2.0000	-0.2800	2.4280
H	-0.7980	-0.7070	1.1980
C	-0.3110	3.2140	7.6640
N	1.8980	1.5210	3.8230
C	-0.3830	3.5610	6.3080
C	0.7430	1.9000	9.2670
C	2.3740	0.4670	3.1850
C	1.7060	0.9360	9.6000
C	0.4840	3.2880	4.0970
C	-1.2960	4.5600	5.8850
C	3.7540	0.4010	2.8120
C	1.3900	2.6020	3.2590
C	-1.1690	3.8220	8.6160
C	-2.1550	5.1660	6.8290
H	-2.8260	5.8820	6.5370
C	3.0610	1.3040	9.7600
H	3.3540	2.2770	9.6360
C	4.7740	1.4390	3.2040
H	4.2930	2.2330	3.7780
C	1.7290	3.0680	1.9590
C	-1.0380	3.4100	9.9580
H	-1.6310	3.8090	10.6900
C	-2.0960	4.7960	8.1870
H	-2.7260	5.2440	8.8580
C	0.0070	-0.6170	3.2400
H	-0.1440	0.0780	4.0690
C	1.5670	2.3000	0.7790
H	1.1820	1.3600	0.8120
C	-0.4040	4.2920	3.6320
H	-0.4290	4.5670	2.6480
C	-1.2940	4.9160	4.5230
H	-1.9350	5.6320	4.1710
C	2.2920	-1.3720	10.1690
H	2.0120	-2.3440	10.3220
C	-0.0760	2.4380	10.2900
H	0.0230	2.1360	11.2630

C	3.6420	-1.0010	10.3030
H	4.3440	-1.7020	10.5500
C	2.2880	4.3660	1.8310
H	2.4410	4.9500	2.6580
C	4.0260	0.3380	10.1020
H	5.0060	0.6090	10.2070
C	1.3260	-0.4080	9.8250
H	0.3470	-0.6950	9.7340
C	1.9330	2.8140	-0.4790
H	1.8060	2.2460	-1.3200
C	2.4740	4.1060	-0.5820
H	2.7390	4.4790	-1.4960
C	2.6530	4.8820	0.5750
H	3.0500	5.8220	0.5030
C	5.8700	0.8450	4.1340
H	5.4140	0.3210	4.9760
H	6.5010	1.6440	4.5320
H	6.5090	0.1420	3.5970
C	5.4080	2.1510	1.9750
H	4.6330	2.5320	1.3100
H	6.0450	1.4720	1.4050
H	6.0190	2.9960	2.3020
N	0.5830	2.3140	8.0150
C	1.4600	-0.5770	2.8140
C	4.1820	-0.6940	2.0240
H	5.1600	-0.7830	1.7370
C	1.9440	-1.6170	1.9840
H	1.3200	-2.3530	1.6480
C	3.2870	-1.6820	1.5990
H	3.6140	-2.4520	1.0110
C	-0.4460	-2.0070	3.7890
H	0.3100	-2.4350	4.4480
H	-0.6270	-2.7140	2.9770
H	-1.3740	-1.9040	4.3560
Complex Co19			
Co	-1.2280	-3.1200	3.0520
N	0.1370	-1.6390	1.9430
Cl	0.3220	-3.8690	4.5220
C	1.2630	-1.9500	1.3080
N	-2.1270	-1.2970	3.2890
Cl	-1.8280	-4.3790	1.2700
C	2.0100	-0.9290	0.6700
H	2.8810	-1.1390	0.1740

N	-3.0840	-3.4300	4.3760
C	1.5410	0.3980	0.7180
H	2.0710	1.1420	0.2570
C	0.3410	0.6800	1.4010
C	-0.2170	1.9730	1.5030
H	0.2490	2.7740	1.0710
C	-1.4250	2.1690	2.2010
H	-1.8180	3.1120	2.2630
C	-2.0860	1.0760	2.8070
C	-3.2990	1.2130	3.5080
H	-3.7460	2.1290	3.6000
C	-3.9090	0.0880	4.0890
H	-4.7890	0.2210	4.5910
C	-3.3020	-1.1900	3.9780
C	-1.5240	-0.2220	2.7140
C	-0.3290	-0.4110	2.0110
C	1.7350	-3.2700	1.2530
C	1.3120	-4.1390	0.2220
H	0.6490	-3.8190	-0.4900
C	1.7980	-5.4580	0.1580
H	1.4810	-6.0850	-0.5850
C	2.7240	-5.9140	1.1140
H	3.0760	-6.8730	1.0690
C	3.1690	-5.0490	2.1300
H	3.8480	-5.3790	2.8200
C	2.6830	-3.7300	2.1960
H	3.0230	-3.1100	2.9360
C	-3.8380	-2.3630	4.5490
C	-5.1340	-2.3660	5.2930
H	-5.4150	-3.3550	5.6550
H	-5.9340	-2.0170	4.6370
H	-5.0650	-1.7050	6.1580
C	-3.2670	-4.6250	4.9080
C	-2.7880	-4.8910	6.2270
C	-2.8740	-6.2080	6.7340
H	-2.5160	-6.4350	7.6660
C	-3.4630	-7.2330	5.9810
H	-3.5130	-8.1820	6.3580
C	-4.0020	-6.9510	4.7180
H	-4.4540	-7.7100	4.2000
C	-3.9340	-5.6480	4.1730
C	-2.2420	-3.8170	7.1050
H	-1.8360	-4.2060	8.0410
H	-1.4480	-3.2670	6.6040

H	-3.0390	-3.1170	7.3560
C	-4.6100	-5.4290	2.8660
H	-5.6700	-5.6720	2.9590
H	-4.5410	-4.3990	2.5170
H	-4.1710	-6.0800	2.1080
Complex Co20			
Co	-1.1010	-3.0240	3.1270
N	0.1380	-1.5790	1.8320
Cl	0.3680	-3.1070	4.8430
C	1.3550	-1.8170	1.3520
N	-2.2810	-1.3700	2.9050
Cl	-1.1950	-4.6780	1.5890
C	2.0010	-0.8300	0.5650
H	2.9380	-0.9840	0.1820
N	-3.0660	-3.4420	4.2660
C	1.3390	0.3850	0.3060
H	1.7960	1.1030	-0.2600
C	0.0490	0.5920	0.8350
C	-0.6980	1.7720	0.6340
H	-0.3140	2.5420	0.0780
C	-1.9830	1.9000	1.1980
H	-2.5120	2.7630	1.0430
C	-2.5320	0.8500	1.9680
C	-3.8090	0.9240	2.5540
H	-4.3880	1.7600	2.4370
C	-4.3010	-0.1540	3.3100
H	-5.2310	-0.0640	3.7210
C	-3.5160	-1.3250	3.4850
C	-1.7850	-0.3370	2.1710
C	-0.5100	-0.4570	1.6090
C	2.0300	-3.0220	1.5970
C	1.9170	-4.1020	0.6920
H	1.3310	-4.0210	-0.1440
C	2.6100	-5.3040	0.9270
H	2.5150	-6.0840	0.2730
C	3.4340	-5.4320	2.0590
H	3.9350	-6.3060	2.2310
C	3.5730	-4.3540	2.9520
H	4.1790	-4.4430	3.7700
C	2.8820	-3.1510	2.7180
H	3.0040	-2.3710	3.3700
C	-3.9390	-2.4490	4.2250
C	-5.2780	-2.4730	4.8920

H	-5.4800	-3.4000	5.4270
H	-6.0640	-2.3460	4.1470
H	-5.3440	-1.6570	5.6140
C	-3.2510	-4.5980	4.8880
C	-2.9010	-4.7280	6.2740
C	-3.1850	-5.9510	6.9310
H	-2.9570	-6.0830	7.9190
C	-3.7960	-7.0160	6.2630
H	-3.9890	-7.8900	6.7590
C	-4.1570	-6.8760	4.9210
H	-4.6240	-7.6670	4.4740
C	-3.9010	-5.6810	4.2040
C	-0.9790	-4.0470	7.8280
C	-2.2920	-3.6220	7.1020
C	-3.3090	-3.0420	8.1250
H	-0.3320	-4.6200	7.1620
H	-1.1890	-4.6650	8.7030
H	-0.4320	-3.1640	8.1630
H	-2.0210	-2.7860	6.4540
H	-2.8740	-2.1870	8.6470
H	-3.5930	-3.7900	8.8690
H	-4.2130	-2.7020	7.6200
C	-5.9340	-5.5310	2.6940
C	-4.3820	-5.6130	2.7750
C	-3.8590	-6.7860	1.8900
H	-6.3060	-4.6890	3.2760
H	-6.3980	-6.4430	3.0750
H	-6.2510	-5.3900	1.6590
H	-4.0160	-4.6970	2.3080
H	-3.9800	-6.5420	0.8320
H	-4.4070	-7.7100	2.0850
H	-2.8030	-6.9780	2.0790
Complex Co21			
Co	-1.1010	-3.0240	3.1270
N	0.1380	-1.5790	1.8320
Cl	0.3680	-3.1070	4.8430
C	1.3550	-1.8170	1.3520
N	-2.2810	-1.3700	2.9050
Cl	-1.1950	-4.6780	1.5890
C	2.0010	-0.8300	0.5650
H	2.9380	-0.9840	0.1820
N	-3.0660	-3.4420	4.2660
C	1.3390	0.3850	0.3060

H	1.7960	1.1030	-0.2600
C	0.0490	0.5920	0.8350
C	-0.6980	1.7720	0.6340
H	-0.3140	2.5420	0.0780
C	-1.9830	1.9000	1.1980
H	-2.5120	2.7630	1.0430
C	-2.5320	0.8500	1.9680
C	-3.8090	0.9240	2.5540
H	-4.3880	1.7600	2.4370
C	-4.3010	-0.1540	3.3100
H	-5.2310	-0.0640	3.7210
C	-3.5160	-1.3250	3.4850
C	-1.7850	-0.3370	2.1710
C	-0.5100	-0.4570	1.6090
C	2.0300	-3.0220	1.5970
C	1.9170	-4.1020	0.6920
H	1.3310	-4.0210	-0.1440
C	2.6100	-5.3040	0.9270
H	2.5150	-6.0840	0.2730
C	3.4340	-5.4320	2.0590
H	3.9350	-6.3060	2.2310
C	3.5730	-4.3540	2.9520
H	4.1790	-4.4430	3.7700
C	2.8820	-3.1510	2.7180
H	3.0040	-2.3710	3.3700
C	-3.9390	-2.4490	4.2250
C	-5.2780	-2.4730	4.8920
H	-5.4800	-3.4000	5.4270
H	-6.0640	-2.3460	4.1470
H	-5.3440	-1.6570	5.6140
C	-3.2510	-4.5980	4.8880
C	-2.9010	-4.7280	6.2740
C	-3.1850	-5.9510	6.9310
H	-2.9570	-6.0830	7.9190
C	-3.7960	-7.0160	6.2630
H	-3.9890	-7.8900	6.7590
C	-4.1570	-6.8760	4.9210
H	-4.6240	-7.6670	4.4740
C	-3.9010	-5.6810	4.2040
C	-0.9790	-4.0470	7.8280
C	-2.2920	-3.6220	7.1020
C	-3.3090	-3.0420	8.1250
H	-0.3320	-4.6200	7.1620
H	-1.1890	-4.6650	8.7030

H	-0.4320	-3.1640	8.1630
H	-2.0210	-2.7860	6.4540
H	-2.8740	-2.1870	8.6470
H	-3.5930	-3.7900	8.8690
H	-4.2130	-2.7020	7.6200
C	-5.9340	-5.5310	2.6940
C	-4.3820	-5.6130	2.7750
C	-3.8590	-6.7860	1.8900
H	-6.3060	-4.6890	3.2760
H	-6.3980	-6.4430	3.0750
H	-6.2510	-5.3900	1.6590
H	-4.0160	-4.6970	2.3080
H	-3.9800	-6.5420	0.8320
H	-4.4070	-7.7100	2.0850
H	-2.8030	-6.9780	2.0790
Complex Co22			
Co	1.4870	1.3430	6.0990
Cl	0.7940	-0.8050	5.9320
Cl	3.5250	1.8470	6.9440
N	0.2580	2.8530	5.4670
C	-0.5970	2.8910	7.6830
N	1.9540	1.7170	3.8790
C	-0.5980	3.3910	6.3760
C	0.3430	1.3540	9.1480
C	2.8920	0.9920	3.2960
C	1.2500	0.3140	9.4000
C	0.3120	3.2920	4.1740
C	-1.4840	4.4410	6.0250
C	4.2450	1.4470	3.2910
C	1.2380	2.6700	3.3160
C	-1.4710	3.4170	8.6670
C	-2.3570	4.9720	7.0020
H	-3.0020	5.7300	6.7640
C	2.5550	0.5980	9.8630
H	2.8570	1.5660	10.0070
C	1.3880	3.0500	1.9630
C	-1.4030	2.8500	9.9560
H	-2.0060	3.1850	10.7110
C	-2.3500	4.4640	8.3160
H	-2.9880	4.8600	9.0110
C	0.6590	2.3910	0.9470
H	0.0030	1.6420	1.1780
C	-0.5560	4.3390	3.7720

H	-0.5510	4.6980	2.8140
C	-1.4490	4.9090	4.6970
H	-2.0690	5.6640	4.3950
C	1.7570	-2.0770	9.5100
H	1.4650	-3.0500	9.3870
C	-0.4880	1.8080	10.2020
H	-0.4360	1.3930	11.1370
C	3.0610	-1.7850	9.9500
H	3.7180	-2.5440	10.1420
C	2.2630	4.1030	1.6110
H	2.7870	4.6080	2.3300
C	3.4580	-0.4480	10.1310
H	4.4030	-0.2350	10.4580
C	0.8520	-1.0330	9.2440
H	-0.0970	-1.2630	8.9360
C	0.8230	2.7620	-0.4010
H	0.2970	2.2770	-1.1320
C	1.7060	3.8020	-0.7430
H	1.8250	4.0700	-1.7230
C	2.4230	4.4740	0.2630
H	3.0600	5.2340	0.0140
N	0.2460	1.9170	7.9490
C	2.5540	-0.2390	2.6570
C	5.2390	0.6450	2.6840
H	6.2170	0.9470	2.6730
C	3.5790	-1.0090	2.0620
H	3.3620	-1.9000	1.6040
C	4.9110	-0.5750	2.0790
H	5.6410	-1.1450	1.6450
C	4.6980	2.7410	3.8730
H	5.1370	3.3620	3.0890
H	3.8910	3.3100	4.3340
H	5.4560	2.5580	4.6360
C	1.1700	-0.7780	2.5530
H	1.1200	-1.7640	3.0190
H	0.4260	-0.1420	3.0310
H	0.8950	-0.8790	1.5010
Complex Co23			
Co	1.3730	1.1090	5.9870
Cl	0.3030	-0.8660	5.7270
Cl	3.4960	1.2040	6.7650
N	0.3170	2.8000	5.5340
C	-0.3780	2.8020	7.8060

N	1.8340	1.6220	3.7890
C	-0.4110	3.3740	6.5290
C	0.4710	1.0850	9.1180
C	2.7890	0.9560	3.1560
C	1.2560	-0.0700	9.2530
C	0.3290	3.2980	4.2630
C	-1.2010	4.5270	6.2960
C	4.1390	1.4370	3.2130
C	1.1480	2.6480	3.3160
C	-1.1080	3.3720	8.8800
C	-1.9330	5.1000	7.3610
H	-2.5050	5.9350	7.2080
C	2.5880	0.0210	9.7160
H	3.0000	0.9300	9.9440
C	1.2560	3.1140	1.9850
C	-1.0100	2.7340	10.1330
H	-1.5100	3.0970	10.9480
C	-1.8840	4.5270	8.6480
H	-2.4190	4.9550	9.4080
C	0.6200	2.4310	0.9240
H	0.0500	1.6040	1.1050
C	-0.4680	4.4370	3.9730
H	-0.5090	4.8360	3.0330
C	-1.2220	5.0490	4.9890
H	-1.7840	5.8750	4.7670
C	1.4910	-2.5030	9.1300
H	1.0910	-3.4210	8.9210
C	-0.2140	1.5800	10.2570
H	-0.1400	1.1120	11.1650
C	2.8230	-2.4010	9.5690
H	3.3920	-3.2440	9.6760
C	1.9830	4.2930	1.6980
H	2.4260	4.8260	2.4510
C	3.3700	-1.1400	9.8660
H	4.3360	-1.0670	10.1930
C	0.7070	-1.3440	8.9810
H	-0.2650	-1.4370	8.6750
C	0.7440	2.8910	-0.4000
H	0.2880	2.3850	-1.1630
C	1.4910	4.0500	-0.6760
H	1.5830	4.3830	-1.6380
C	2.1050	4.7540	0.3740
H	2.6400	5.6030	0.1760
N	0.3530	1.7200	7.9570

C	2.4860	-0.2280	2.4090
C	5.1560	0.6950	2.5670
H	6.1350	0.9860	2.6260
C	3.5340	-0.8890	1.7250
H	3.3470	-1.7130	1.1490
C	4.8570	-0.4470	1.8170
H	5.6030	-0.9540	1.3360
C	5.2770	3.7280	3.0280
C	4.5640	2.6860	3.9270
H	5.3440	4.6840	3.5500
H	4.7340	3.8780	2.0950
H	6.2900	3.4030	2.7880
H	3.7180	3.1880	4.3990
H	5.2530	2.4110	4.7290
C	0.9970	-2.2960	2.6980
C	1.1130	-0.8090	2.2710
H	-0.0550	-2.5690	2.8050
H	1.5030	-2.4710	3.6480
H	1.4390	-2.9510	1.9450
H	0.3830	-0.2390	2.8470
H	0.8120	-0.7380	1.2230
Complex Co24			
Co	1.7130	1.5120	6.1410
Cl	1.4420	-0.7240	6.3410
Cl	3.6580	2.4910	6.7570
N	0.2910	2.7930	5.4270
C	-0.7050	-0.2080	1.9230
H	-0.6370	0.8660	1.7610
H	-1.7460	-0.4300	2.1690
H	-0.4520	-0.7250	0.9950
C	-0.5600	2.8610	7.6420
N	1.9200	1.6040	3.8500
C	-0.6290	3.2710	6.3060
C	0.5980	1.5900	9.2050
C	2.5090	0.6200	3.1940
C	1.6560	0.7260	9.5250
C	0.3440	3.2130	4.1290
C	-1.6270	4.1920	5.9010
C	3.9040	0.6820	2.8830
C	1.3450	2.6590	3.3040
C	-1.5040	3.3200	8.5940
C	-2.5770	4.6480	6.8430
H	-3.3120	5.3030	6.5630

C	2.9530	1.2380	9.7570
H	3.1340	2.2430	9.6950
C	4.8140	1.7890	3.3470
H	4.2430	2.5230	3.9180
C	1.6940	3.2150	2.0420
C	-1.3620	2.8520	9.9170
H	-2.0150	3.1420	10.6490
C	-2.5200	4.2100	8.1820
H	-3.2160	4.5490	8.8520
C	0.2340	-0.6460	3.0810
H	-0.0160	0.0030	3.9220
C	1.6720	2.4880	0.8260
H	1.3880	1.5110	0.8010
C	-0.6220	4.1490	3.6780
H	-0.6350	4.4770	2.7100
C	-1.6080	4.6250	4.5610
H	-2.3060	5.2910	4.2210
C	2.4880	-1.5280	9.9970
H	2.3180	-2.5330	10.0880
C	-0.3020	1.9790	10.2280
H	-0.1940	1.6390	11.1890
C	3.7800	-1.0120	10.2030
H	4.5500	-1.6410	10.4410
C	2.1190	4.5680	1.9960
H	2.1690	5.1270	2.8520
C	4.0110	0.3700	10.0860
H	4.9490	0.7460	10.2430
C	1.4280	-0.6620	9.6660
H	0.4930	-1.0530	9.5240
C	2.0440	3.0910	-0.3890
H	2.0200	2.5510	-1.2570
C	2.4510	4.4360	-0.4130
H	2.7190	4.8750	-1.2960
C	2.4890	5.1750	0.7820
H	2.7890	6.1520	0.7690
C	5.9150	1.2620	4.3120
H	5.4680	0.6780	5.1190
H	6.4580	2.0980	4.7570
H	6.6330	0.6300	3.7870
C	5.4370	2.5900	2.1680
H	4.6600	2.9330	1.4850
H	6.1470	1.9820	1.6050
H	5.9660	3.4680	2.5460
N	0.4210	2.0480	7.9690

C	1.7010	-0.4770	2.7390
C	4.4580	-0.3470	2.0830
H	5.4510	-0.3450	1.8400
C	2.3080	-1.4460	1.9030
H	1.7620	-2.2160	1.5120
C	3.6690	-1.3890	1.5850
H	4.0870	-2.1100	0.9910
C	-0.1380	-2.0860	3.5550
H	0.6130	-2.4820	4.2400
H	-0.2220	-2.7730	2.7110
H	-1.0990	-2.0750	4.0740
Complex Ni19			
Ni	-1.2760	-3.0690	3.0360
N	0.1920	-1.7940	1.8710
Cl	0.2470	-3.5930	4.6000
C	1.2760	-2.2230	1.2370
N	-2.0040	-1.2490	3.2370
Cl	-2.1590	-4.0050	1.1960
C	2.0980	-1.2880	0.5610
H	2.9420	-1.5860	0.0640
N	-3.0880	-3.2780	4.3920
C	1.7420	0.0760	0.5730
H	2.3270	0.7590	0.0850
C	0.5780	0.4810	1.2610
C	0.1240	1.8160	1.3380
H	0.6460	2.5670	0.8790
C	-1.0560	2.1240	2.0470
H	-1.3730	3.0960	2.0880
C	-1.7920	1.1030	2.6930
C	-2.9820	1.3440	3.4050
H	-3.3580	2.2930	3.4810
C	-3.6680	0.2810	4.0210
H	-4.5290	0.4900	4.5290
C	-3.1610	-1.0420	3.9350
C	-1.3320	-0.2350	2.6260
C	-0.1680	-0.5320	1.9090
C	1.6170	-3.5840	1.2300
C	1.0680	-4.4560	0.2640
H	0.4160	-4.1050	-0.4440
C	1.4130	-5.8200	0.2570
H	1.0060	-6.4480	-0.4400
C	2.3220	-6.3210	1.2070
H	2.5720	-7.3120	1.2030

C	2.8900	-5.4560	2.1600
H	3.5550	-5.8190	2.8470
C	2.5440	-4.0920	2.1690
H	2.9700	-3.4750	2.8660
C	-3.7720	-2.1610	4.5390
C	-5.0610	-2.0620	5.2830
H	-5.4050	-3.0230	5.6650
H	-5.8390	-1.6770	4.6210
H	-4.9480	-1.3850	6.1320
C	-3.3150	-4.4420	4.9740
C	-2.8530	-4.6690	6.3070
C	-2.9560	-5.9690	6.8560
H	-2.6070	-6.1690	7.7970
C	-3.5500	-7.0120	6.1330
H	-3.6090	-7.9480	6.5390
C	-4.0860	-6.7630	4.8620
H	-4.5480	-7.5310	4.3670
C	-4.0060	-5.4770	4.2790
C	-2.3090	-3.5760	7.1620
H	-1.8970	-3.9450	8.1040
H	-1.5220	-3.0280	6.6500
H	-3.1090	-2.8760	7.4050
C	-4.6980	-5.2880	2.9770
H	-5.7500	-5.5650	3.0780
H	-4.6690	-4.2570	2.6270
H	-4.2420	-5.9270	2.2180
Complex Ni20			
Ni	-1.0770	-3.0300	3.4090
N	0.4310	-1.7110	2.3500
Cl	0.0090	-2.9550	5.3710
C	1.6520	-2.0640	1.9700
N	-2.0420	-1.3260	3.1960
Cl	-1.2670	-4.4010	1.6410
C	2.4690	-1.1170	1.3010
H	3.4150	-1.3580	0.9930
N	-3.1660	-3.4060	4.2210
C	1.9660	0.1780	1.0620
H	2.5490	0.8690	0.5840
C	0.6610	0.5030	1.4890
C	0.0550	1.7660	1.3080
H	0.5640	2.5210	0.8420
C	-1.2570	1.9970	1.7720
H	-1.6790	2.9190	1.6360

C	-1.9810	0.9680	2.4200
C	-3.2860	1.1400	2.9200
H	-3.7630	2.0410	2.8260
C	-3.9480	0.0740	3.5560
H	-4.8930	0.2340	3.9100
C	-3.3090	-1.1870	3.6880
C	-1.3800	-0.3030	2.5900
C	-0.0740	-0.5180	2.1390
C	2.1410	-3.3550	2.2160
C	2.0850	-4.3430	1.2060
H	1.6840	-4.1290	0.2890
C	2.5770	-5.6390	1.4520
H	2.5260	-6.3510	0.7200
C	3.1380	-5.9550	2.7020
H	3.4920	-6.8970	2.8810
C	3.2160	-4.9720	3.7060
H	3.6310	-5.2000	4.6120
C	2.7260	-3.6750	3.4620
H	2.8040	-2.9680	4.1980
C	-3.9110	-2.3180	4.2800
C	-5.2800	-2.2690	4.8740
H	-5.5950	-3.2230	5.2960
H	-6.0050	-1.9860	4.1090
H	-5.3030	-1.5310	5.6780
C	-3.5530	-4.6400	4.4970
C	-3.3710	-5.1910	5.8040
C	-3.7940	-6.5200	6.0470
H	-3.6940	-6.9400	6.9740
C	-4.3670	-7.2980	5.0340
H	-4.6460	-8.2630	5.2240
C	-4.5720	-6.7450	3.7650
H	-5.0060	-7.3320	3.0470
C	-4.2070	-5.4090	3.4810
C	-4.5590	-4.8820	2.1230
H	-4.1230	-3.8990	1.9410
H	-4.1500	-5.5520	1.3610
C	-6.0830	-4.7440	1.8970
H	-6.2700	-4.2980	0.9180
H	-6.5270	-4.1020	2.6600
H	-6.5730	-5.7180	1.9280
C	-2.8100	-4.4270	6.9620
H	-2.5570	-3.4050	6.6800
H	-3.5830	-4.3490	7.7300
C	-1.5530	-5.0710	7.6000

H	-1.0900	-4.3670	8.2940
H	-0.8220	-5.3400	6.8360
H	-1.8180	-5.9690	8.1600
Complex Ni21			
Ni	-1.0410	-3.0730	3.2240
N	0.6860	-1.8730	2.3720
Cl	0.0420	-3.3660	5.1660
C	1.8860	-2.3400	2.0500
N	-1.7730	-1.2480	3.1070
Cl	-1.3320	-4.1530	1.2810
C	2.8580	-1.4500	1.5260
H	3.7930	-1.7780	1.2680
N	-3.1730	-3.2350	4.0160
C	2.5270	-0.0900	1.3600
H	3.2200	0.5600	0.9830
C	1.2370	0.3560	1.7190
C	0.7970	1.6920	1.5960
H	1.4230	2.4120	1.2280
C	-0.5140	2.0440	1.9820
H	-0.8170	3.0170	1.8870
C	-1.3970	1.0660	2.4940
C	-2.7150	1.3550	2.8950
H	-3.0820	2.3080	2.8250
C	-3.5420	0.3330	3.3960
H	-4.4930	0.5790	3.6770
C	-3.0560	-0.9970	3.5030
C	-0.9580	-0.2750	2.6190
C	0.3430	-0.6140	2.2320
C	2.2110	-3.6940	2.2190
C	1.9900	-4.6190	1.1740
H	1.5890	-4.3130	0.2830
C	2.3190	-5.9770	1.3440
H	2.1490	-6.6430	0.5870
C	2.8860	-6.4190	2.5530
H	3.1240	-7.4050	2.6770
C	3.1310	-5.5010	3.5910
H	3.5490	-5.8200	4.4670
C	2.8010	-4.1430	3.4230
H	2.9950	-3.4860	4.1840
C	-3.8170	-2.0800	3.9960
C	-5.2300	-1.8920	4.4470
H	-5.6940	-2.8110	4.8040
H	-5.8340	-1.5190	3.6190

H	-5.2630	-1.1690	5.2630
C	-3.6670	-4.3890	4.4420
C	-3.5740	-4.7400	5.8320
C	-4.1350	-5.9680	6.2600
H	-4.0870	-6.2560	7.2400
C	-4.7880	-6.8240	5.3700
H	-5.1820	-7.7080	5.7020
C	-4.9200	-6.4570	4.0290
H	-5.4320	-7.0940	3.4150
C	-4.3830	-5.2420	3.5350
C	-1.8480	-4.5670	7.7180
C	-2.9610	-3.8560	6.8910
C	-4.0430	-3.2600	7.8370
H	-1.1800	-5.1340	7.0670
H	-2.2720	-5.2600	8.4480
H	-1.2540	-3.8290	8.2620
H	-2.4870	-2.9930	6.4210
H	-3.5880	-2.5500	8.5310
H	-4.5330	-4.0420	8.4210
H	-4.8050	-2.7300	7.2660
C	-6.1560	-4.5790	1.8470
C	-4.6540	-4.9050	2.0890
C	-4.1700	-6.0100	1.1010
H	-6.4880	-3.7820	2.5110
H	-6.7850	-5.4550	2.0190
H	-6.3080	-4.2450	0.8180
H	-4.1170	-3.9960	1.8170
H	-4.1340	-5.6140	0.0840
H	-4.8410	-6.8710	1.1030
H	-3.1720	-6.3610	1.3680
Complex Ni22			
Ni	1.4140	1.3980	6.0920
Cl	0.3600	-0.5780	5.9260
Cl	3.3700	2.1840	6.8610
N	0.2540	2.8650	5.4640
C	-0.5560	2.9790	7.6940
N	1.9010	1.6540	3.8870
C	-0.5740	3.4440	6.3750
C	0.4010	1.4550	9.1630
C	2.8390	0.9060	3.3310
C	1.3020	0.4040	9.3890
C	0.2970	3.2690	4.1600
C	-1.4460	4.5000	6.0150

C	4.1890	1.3710	3.2830
C	1.2020	2.6090	3.3050
C	-1.3920	3.5440	8.6870
C	-2.2870	5.0720	6.9990
H	-2.9230	5.8360	6.7560
C	2.6290	0.6750	9.7930
H	2.9480	1.6390	9.9220
C	1.3620	2.9670	1.9470
C	-1.2950	3.0020	9.9870
H	-1.8710	3.3650	10.7500
C	-2.2600	4.5980	8.3280
H	-2.8740	5.0240	9.0260
C	0.7310	2.2230	0.9240
H	0.1340	1.4260	1.1520
C	-0.5620	4.3200	3.7470
H	-0.5700	4.6510	2.7800
C	-1.4270	4.9300	4.6740
H	-2.0390	5.6890	4.3640
C	1.7880	-1.9920	9.4810
H	1.4810	-2.9620	9.3720
C	-0.3910	1.9480	10.2310
H	-0.3170	1.5520	11.1720
C	3.1120	-1.7140	9.8640
H	3.7680	-2.4800	10.0300
C	2.1550	4.0850	1.5950
H	2.6080	4.6500	2.3180
C	3.5310	-0.3800	10.0230
H	4.4920	-0.1780	10.3080
C	0.8840	-0.9380	9.2500
H	-0.0790	-1.1590	8.9810
C	0.9100	2.5750	-0.4270
H	0.4550	2.0290	-1.1630
C	1.7120	3.6800	-0.7670
H	1.8420	3.9350	-1.7490
C	2.3310	4.4360	0.2440
H	2.9090	5.2430	-0.0040
N	0.2750	1.9970	7.9590
C	2.5080	-0.3630	2.7670
C	5.1870	0.5350	2.7310
H	6.1640	0.8410	2.6950
C	3.5380	-1.1700	2.2300
H	3.3280	-2.0900	1.8350
C	4.8680	-0.7290	2.2180
H	5.6020	-1.3240	1.8270

C	4.6380	2.7070	3.7610
H	5.0730	3.2660	2.9300
H	3.8320	3.3080	4.1770
H	5.3990	2.5860	4.5350
C	1.1270	-0.9080	2.6730
H	1.0590	-1.8430	3.2330
H	0.3720	-0.2240	3.0570
H	0.8820	-1.1110	1.6290
Complex Ni23			
Ni	1.3320	1.1410	5.9680
Cl	-0.1610	-0.5070	5.6680
Cl	3.4500	1.3960	6.6670
N	0.4050	2.8470	5.6360
C	-0.1700	2.8120	7.9420
N	1.7560	1.6400	3.7880
C	-0.2340	3.4280	6.6880
C	0.6530	0.9930	9.1300
C	2.6600	0.9440	3.1130
C	1.3820	-0.2060	9.1460
C	0.3780	3.3800	4.3790
C	-0.9640	4.6320	6.5360
C	4.0230	1.3900	3.0880
C	1.1090	2.7150	3.3710
C	-0.7980	3.3790	9.0770
C	-1.5980	5.2080	7.6610
H	-2.1260	6.0800	7.5680
C	2.7380	-0.2130	9.5490
H	3.2040	0.6550	9.8280
C	1.1860	3.2070	2.0460
C	-0.6630	2.6830	10.2960
H	-1.0910	3.0410	11.1540
C	-1.5130	4.5880	8.9260
H	-1.9750	5.0190	9.7300
C	0.5600	2.5220	0.9790
H	0.0210	1.6730	1.1500
C	-0.3700	4.5690	4.1700
H	-0.4460	4.9950	3.2440
C	-1.0280	5.1930	5.2460
H	-1.5520	6.0560	5.0800
C	1.4930	-2.6270	8.8100
H	1.0400	-3.5050	8.5450
C	0.0700	1.4790	10.3280
H	0.1710	0.9690	11.2100

C	2.8470	-2.6230	9.1920
H	3.3790	-3.4960	9.2010
C	1.8790	4.4090	1.7670
H	2.3260	4.9380	2.5200
C	3.4680	-1.4170	9.5650
H	4.4500	-1.4150	9.8490
C	0.7620	-1.4250	8.7940
H	-0.2270	-1.4490	8.5290
C	0.6510	3.0090	-0.3390
H	0.2000	2.5010	-1.1030
C	1.3570	4.1950	-0.6040
H	1.4230	4.5490	-1.5610
C	1.9670	4.8980	0.4500
H	2.4750	5.7650	0.2590
N	0.5000	1.6850	8.0080
C	2.2930	-0.2470	2.4080
C	4.9890	0.6030	2.4170
H	5.9770	0.8700	2.4200
C	3.2900	-0.9610	1.7010
H	3.0550	-1.7970	1.1610
C	4.6270	-0.5530	1.7190
H	5.3370	-1.0960	1.2210
C	5.2010	3.6450	2.7700
C	4.5190	2.6470	3.7400
H	5.3300	4.6110	3.2620
H	4.6010	3.7880	1.8720
H	6.1870	3.2840	2.4720
H	3.7140	3.1840	4.2430
H	5.2460	2.3780	4.5110
C	0.7500	-2.2300	2.8820
C	0.9000	-0.7880	2.3320
H	-0.3090	-2.4790	2.9840
H	1.2300	-2.3250	3.8580
H	1.2020	-2.9560	2.2030
H	0.1960	-0.1480	2.8630
H	0.5840	-0.7910	1.2850
Complex Ni24			
Ni	1.6270	1.5240	6.1220
Cl	1.0080	-0.6250	6.2970
Cl	3.4090	2.7850	6.6470
N	0.2460	2.7550	5.4500
C	-0.6470	-0.3190	1.7190
H	-0.6120	0.7540	1.5360

H	-1.6940	-0.5790	1.8980
H	-0.3110	-0.8450	0.8240
C	-0.5470	2.8550	7.6840
N	1.8590	1.5690	3.8570
C	-0.6540	3.2420	6.3450
C	0.6730	1.6050	9.2160
C	2.4810	0.6000	3.2080
C	1.7480	0.7440	9.4870
C	0.2760	3.1650	4.1480
C	-1.6640	4.1540	5.9540
C	3.8860	0.6870	2.9500
C	1.2770	2.6220	3.3130
C	-1.4610	3.3210	8.6600
C	-2.5890	4.6190	6.9190
H	-3.3330	5.2680	6.6510
C	3.0550	1.2580	9.6470
H	3.2310	2.2630	9.5750
C	4.7550	1.8240	3.4230
H	4.1430	2.5670	3.9330
C	1.6350	3.1990	2.0620
C	-1.2680	2.8680	9.9820
H	-1.8960	3.1630	10.7340
C	-2.4910	4.2010	8.2630
H	-3.1690	4.5470	8.9470
C	0.2260	-0.6920	2.9500
H	-0.0970	-0.0170	3.7440
C	1.6840	2.4820	0.8400
H	1.4480	1.4950	0.7990
C	-0.7090	4.0870	3.7080
H	-0.7440	4.4030	2.7370
C	-1.6790	4.5680	4.6080
H	-2.3890	5.2260	4.2740
C	2.6100	-1.5080	9.9100
H	2.4490	-2.5130	10.0090
C	-0.1930	2.0010	10.2660
H	-0.0490	1.6710	11.2250
C	3.9110	-0.9900	10.0450
H	4.6950	-1.6180	10.2400
C	2.0090	4.5680	2.0340
H	2.0140	5.1240	2.8950
C	4.1320	0.3930	9.9170
H	5.0760	0.7710	10.0230
C	1.5320	-0.6450	9.6380
H	0.5910	-1.0380	9.5460

C	2.0660	3.1090	-0.3600
H	2.0910	2.5730	-1.2310
C	2.4170	4.4690	-0.3640
H	2.6950	4.9250	-1.2360
C	2.3910	5.1990	0.8360
H	2.6530	6.1870	0.8370
C	5.8110	1.3480	4.4600
H	5.3270	0.7950	5.2690
H	6.3270	2.2060	4.8960
H	6.5570	0.6980	3.9980
C	5.4210	2.6020	2.2520
H	4.6710	2.9090	1.5220
H	6.1720	1.9950	1.7440
H	5.9130	3.5010	2.6300
N	0.4470	2.0510	7.9860
C	1.7090	-0.5030	2.7030
C	4.4950	-0.3420	2.1900
H	5.4990	-0.3270	1.9970
C	2.3720	-1.4680	1.9050
H	1.8570	-2.2470	1.4880
C	3.7470	-1.3990	1.6620
H	4.2050	-2.1180	1.0980
C	-0.1410	-2.1270	3.4470
H	0.5770	-2.4850	4.1850
H	-0.1610	-2.8400	2.6200
H	-1.1300	-2.1230	3.9110