Supporting Information for

Role of the Metal in the Bonding and Properties of Bimetallic Complexes Involving Manganese, Iron, and Cobalt

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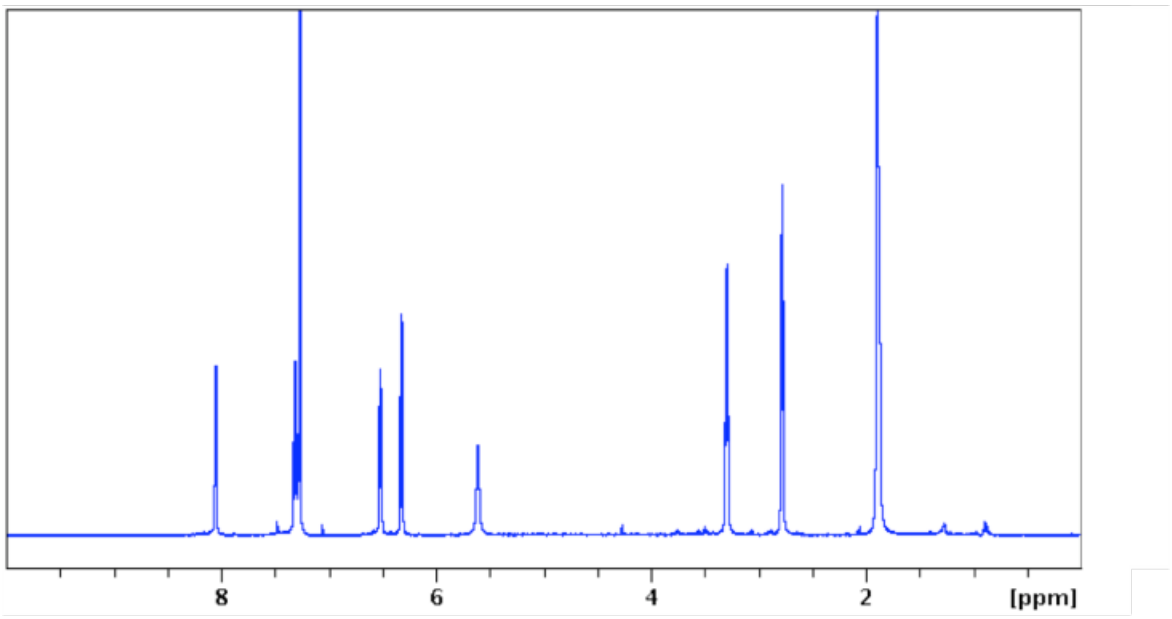
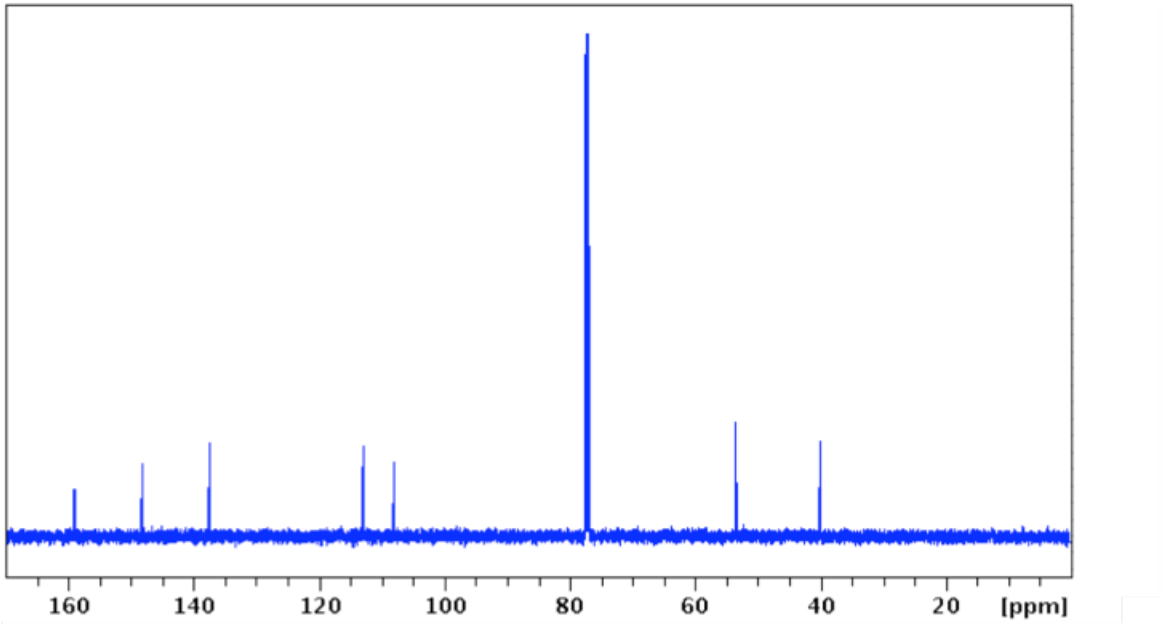
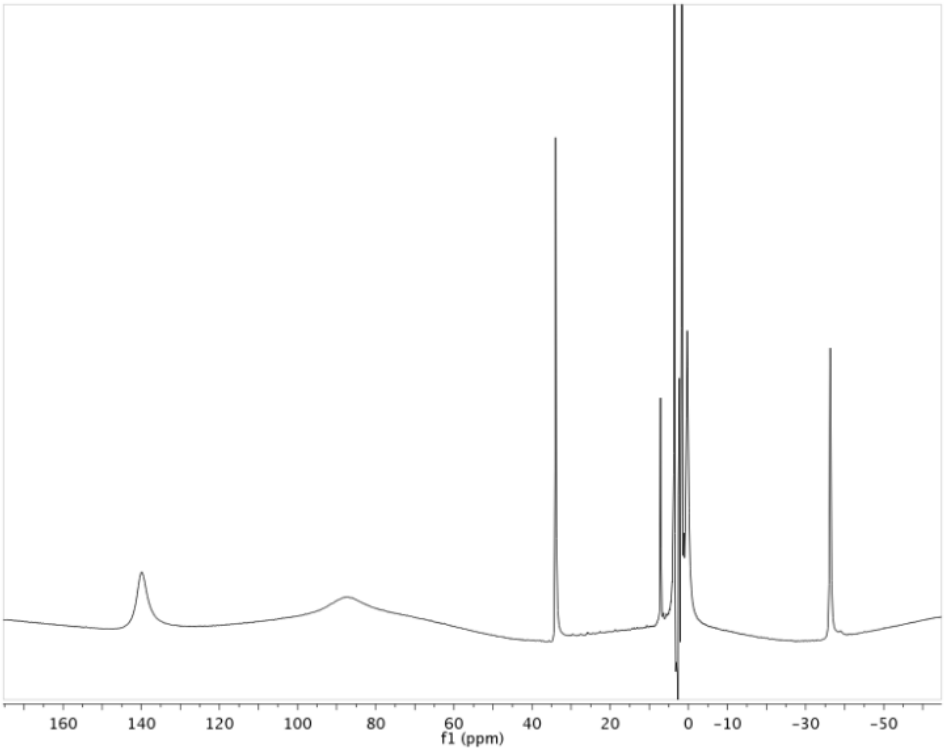


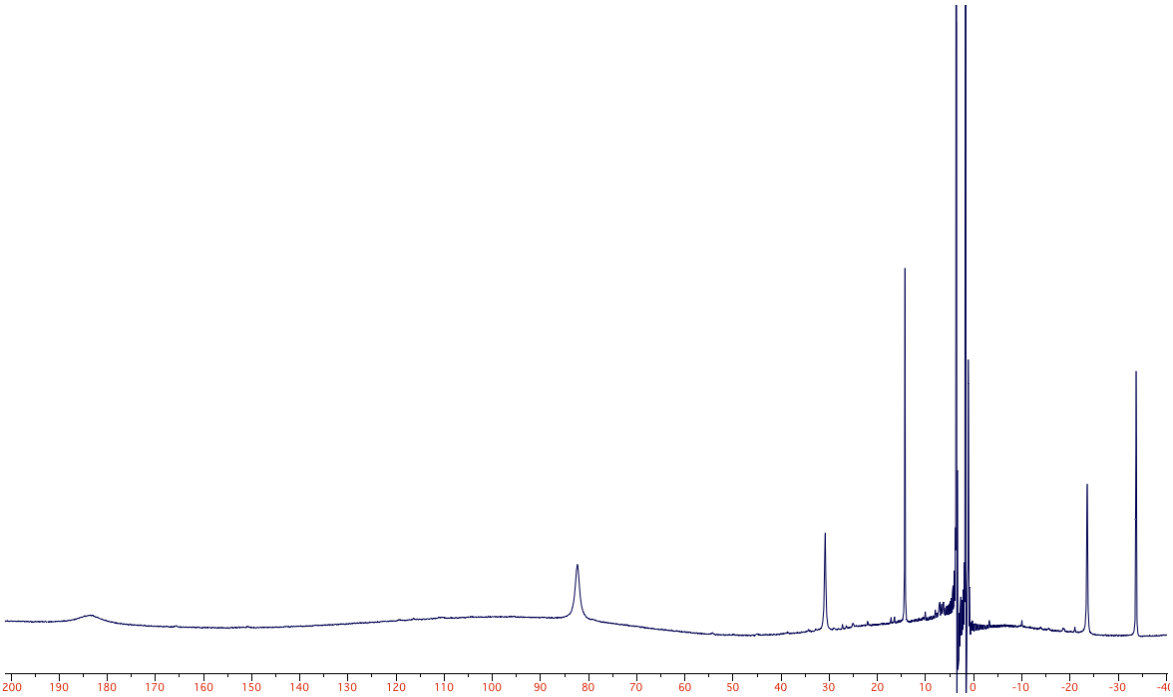
SI Figure 1. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of H_3py_3tren.



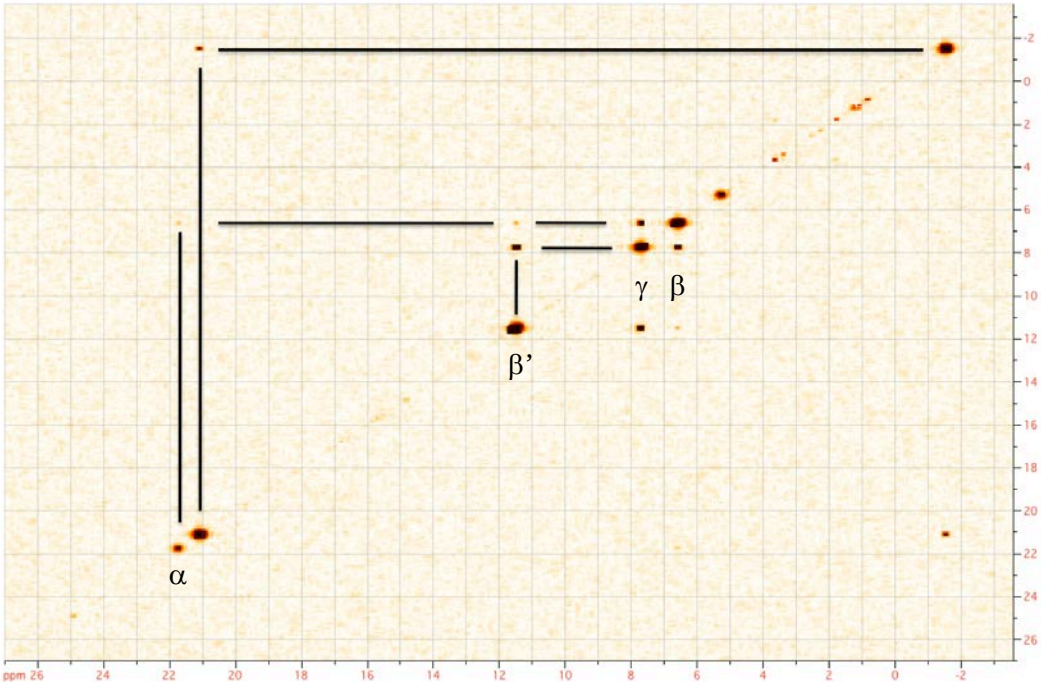
SI Figure 2. ^{13}C NMR spectrum (126 MHz, $CDCl_3$) of H_3py_3tren.



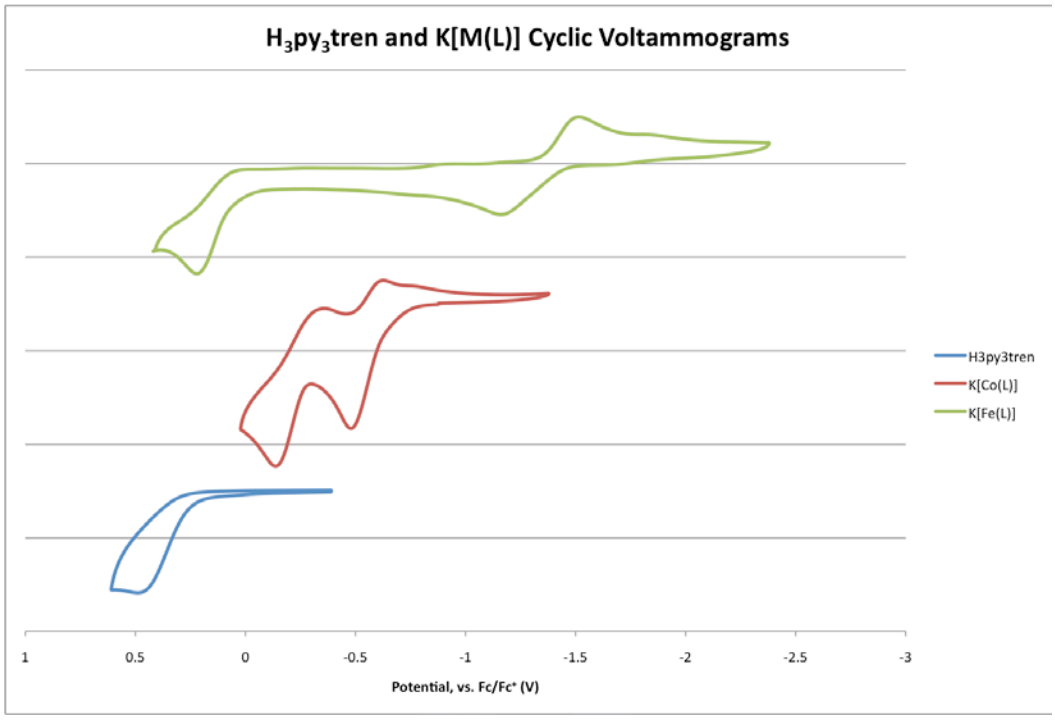
SI Figure 3. ^{1}H NMR spectrum (300 MHz, d_8-THF) of K[Co(py$_3$tren)].



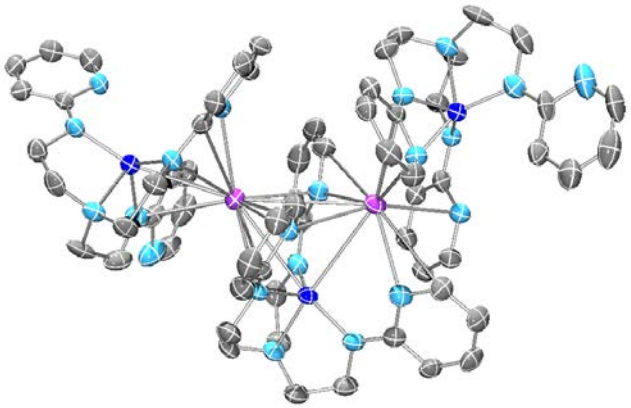
SI Figure 4. ^{1}H NMR spectrum (300 MHz, d_8-THF) of K[Fe(py$_3$tren)].



SI Figure 5. COSY NMR spectrum (300 MHz, CD_2Cl_2) of CoCoCl(py_3tren) **1**.



SI Figure 6. Cyclic voltammograms of H_3(py_3tren), K[Co(py_3tren)], and K[Fe(py_3tren)]. in 0.4 M [nBu_4N]PF_6/THF at 300 mV/s.



SI Figure 7. X-ray structure of K[Co(py$_3$tren)]. The molecule packs as a one-dimensional polymer. The asymmetric unit includes two independent molecules of K[Co(py$_3$tren)]; a third [Co(py$_3$tren)] anion is included to show how the polymer propagates.

SI Table 1. Crystallographic details for K[Co(py$_3$tren)].

	K[Co(py$_3$tren)]
chemical formula	$C_{21}H_{24}N_7CoK$
formula weight	472.50
crystal system	monoclinic
space group	$P2_1/c$
a (Å)	12.955(2)
b (Å)	16.210(3)
c (Å)	21.245(3)
α (deg)	90
β (deg)	106.123(2)
γ (deg)	90
V (Å^3)	4286.0(11)
Z	8
D_{calcd} (g cm^{-3})	1.465
l (Å), μ (mm^{-1})	0.71073, 1.018
T (K)	173(2)
θ range (deg)	1.60 to 26.37
reflns collected	18917
unique reflns	4634
data/restraints/parameters	4634 / 0 / 541
R_1, wR_2 ($I > 2\sigma(I)$)	0.0626, 0.1346

SI Table 1a. Geometrical parameters, including bond lengths (Å) and angles (°) for K[Co(py$_3$tren)].[a]

	Molecule 1	**Molecule 2**
Co−N$_{ap}$ (Å)	2.089(4)	2.089(4)
Co−N$_{eq}$ (Å) [b]	1.955(3)	1.954(3)

[a] Estimated standard deviations (esd) are provided in parentheses. [b] M$_1$−N$_{eq}$ bond lengths are reported as averages.

SI Table 2. Crystallographic details from 30 keV anomalous scattering experiments for the MM'Cl(py_3tren) series, where MM' = CoFe **2**, CoMn **3**, and FeMn **5**.

	2	**3**	**5**
chemical formula	$C_{21}H_{24}N_7Co_{1.04}Fe_{0.96}Cl$	$C_{21}H_{24}N_7Co_{0.998}Mn_{1.002}Cl$	$C_{21}H_{24}N_7Fe_{0.995}Mn_{1.05}Cl$
formula weight	524.82	523.78	520.67
crystal system	monoclinic	monoclinic	monoclinic
space group	$P2_1/n$	$P2_1/n$	$P2_1/n$
a (Å)	9.2450(6)	9.3012(8)	9.3327(9)
b (Å)	12.5597(8)	12.4519(11)	12.4574(12)
c (Å)	18.4751(12)	18.5177(16)	18.4915(19)
α (deg)	90	90	90
β (deg)	98.7240(10)	98.632(2)	98.5268(15)
γ (deg)	90	90	90
V (Å^3)	2120.4(2)	2120.4(3)	2126.1(4)
Z	4	4	4
D_{calcd} (g cm^{-3})	1.644	1.641	1.627
l (Å), μ (mm^{-1})	0.41328, 1.617	0.41328, 0.302	0.41328, 0.279
T (K)	100(2)	100(2)	100(2)
θ range (deg)	1.934 to 24.353	1.902 to 24.670	1.520 to 24.525
reflns collected	17135	17761	17446
unique reflns	14038	14004	12304
data/restraints/parameters	14038 / 0 / 280	14004 / 0 / 280	12304 / 0 / 280
R_1, wR_2 ($I > 2\sigma(I)$)	0.0389, 0.1049	0.0355, 0.1140	0.0379, 0.0880

SI Table 3. Geometrical parameters, including bond lengths (Å) and angle (°) for complexes **2, 3,** and **5**, based on 30 keV data.[a]

	2	**3**	**5**
M_1−M_2 (Å)	2.49693(18)	2.5274(2)	2.5156(2)
r [b]	1.08	1.09	1.08
M_1−N_{ap} (Å)	2.0198(7)	2.0190(8)	2.0536(8)
M_1−N_{eq} (Å) [c]	1.9011±0.0031	1.9051±0.0053	1.9416±0.0067
M_2−Cl (Å)	2.3520(2)	2.3609(3)	2.3587(3)
M_2−N_{py} (Å) [c]	2.1073±0.0069	2.1624±0.0098	2.1768±0.0076
M_1−M_2−Cl (°)	177.407(8)	177.856(9)	177.154(9)

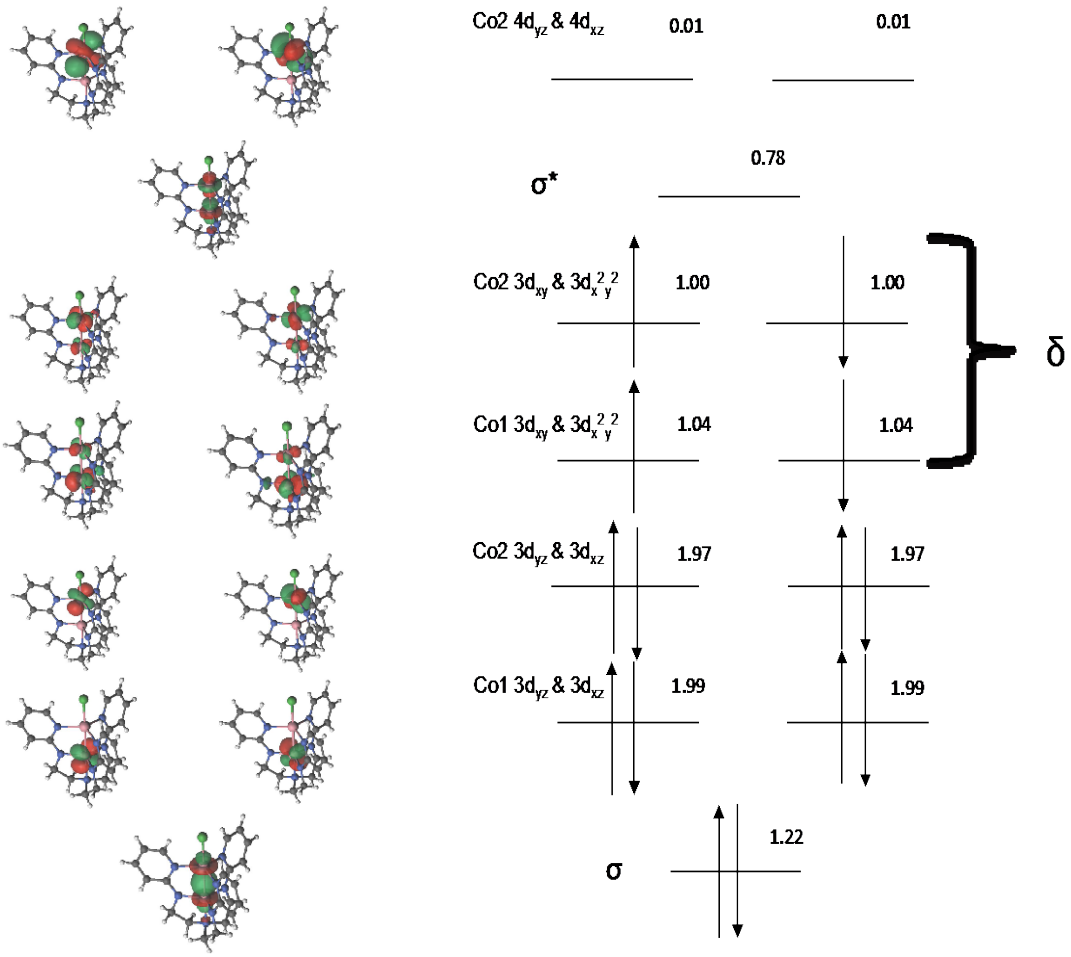
[a] Estimated standard deviations (esd) are provided in parentheses. [b] r = ratio of M_1−M_2 bond distance to the sum of M_1 and M_2 single-bond radii. [c] M_1−N_{eq} and M_2−N_{py} bond lengths are reported as averages.

SI Table 4. CASSCF/CASPT2 Relative Spin State Energies

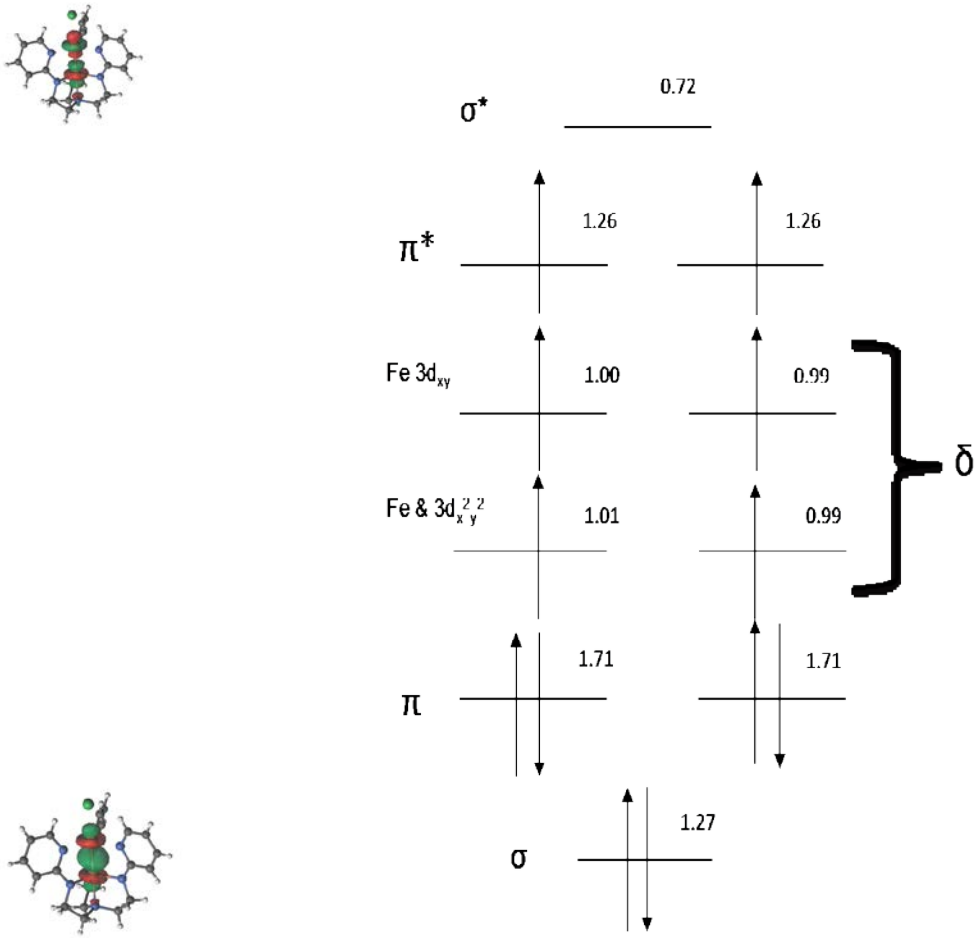
CoCoCl	CASSCF (14/12) Relative Energies (kcal/mol)	CASPT2 Relative Energies (kcal/mol)
singlet	0.00	0.00
triplet	0.81	2.00
quintet	2.43	5.55
septet	4.77	10.74
CoMnCl	CASSCF (12,12) Relative Energies (kcal/mol)	CASPT2 Relative Energies (kcal/mol)
singlet	77.0	72.0
triplet	0.00	0.00
quintet	1.14	2.47
septet	2.84	6.00
nonet	5.04	10.60
CoFeCl	CASSCF (13,12) Relative Energies (kcal/mol)	CASPT2 Relative Energies (kcal/mol)
doublet	0.00	0.00
quartet	0.99	2.26
sextet	2.63	5.80
octet	4.58	9.46
FeMnCl	CASSCF (11,12) Relative Energies (kcal/mol)	CASPT2 Relative Energies (kcal/mol)
doublet	0.00	0.00
quartet	0.71	1.66
sextet	1.94	4.27
octet	3.58	7.94
dectet	5.69	12.58
FeFeCl	CASSCF (12,12) Relative Energies (kcal/mol)	CASPT2 Relative Energies (kcal/mol)
singlet	0.00	0.00
triplet	0.36	4.35
quintet	2.39	4.32
septet	5.14	8.70
nonet	9.34	16.90
FeFeCl	CASSCF (12,15) Relative Energies (kcal/mol)	CASPT2 Relative Energies (kcal/mol)
septet	0.61	3.70
nonet	0.00	0.00
FeFeCl	RASSCF (12/20) Relative Energies (kcal/mol)	RASPT2 Relative Energies (kcal/mol)
singlet	0.00	N/A
septet	2.63 (0.00)	0.02
nonet	3.10 (0.47)	0.00

SI Table 5. Effective Bond Order and Weight of Main Configuration

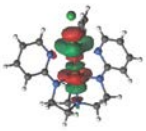
	EBO	Weight of Main Configuration
FeFeCl septet	0.73	28%
CoCoCl singlet	0.22	19%
CoFeCl doublet	0.22	7.0%
CoMnCl triplet	0.22	6.5%
FeMnCl doublet	0.31	2.1%

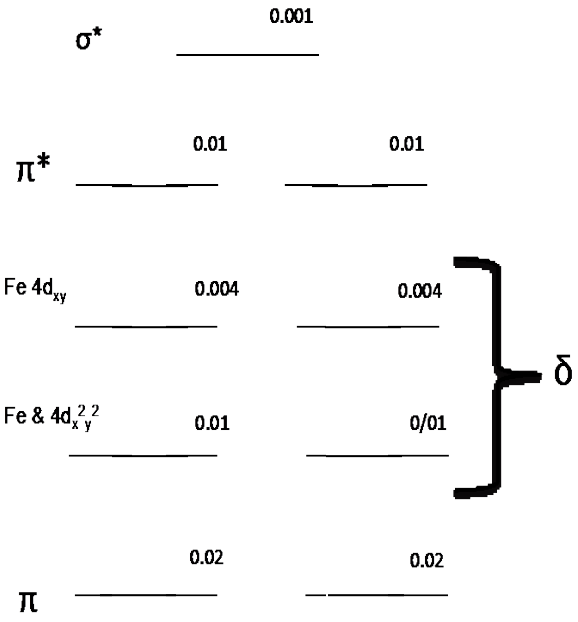


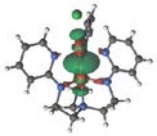
SI Figure 8. MO diagram for CoCoCl(py_3tren), with occupation numbers, showing the full active space.



SI Figure 9. MO diagram for FeFeCl(py_3tren), with occupation numbers, showing the bottom half the active space, comprising 3*d* valence orbitals.







SI Figure 9a. MO diagram for FeFeCl(py$_3$tren), with occupation numbers, showing the top half of the active space, comprising the correlating (and essentially unoccupied) 4*d* orbitals.

SI Table 6. $\langle S^2 \rangle$ Values and Total Energies (in a.u.) of the Considered High-Spin and Spin-Broken-Symmetry Solutions.

	PBE0	HSE	LC− ω PBE
CoCoCl			
HS $(\langle \boldsymbol{S^2} \rangle)$	−4421.10598739646 (12.02)	-4421.28705547 (12.02)	−4421.79456035 (12.01)
BS $(\langle \boldsymbol{S^2} \rangle)$	−4421.1198733571 (2.87)	−4421.30163682 (2.86)	−4421.80998972 (2.86)
CoFeCl			
HS $(\langle \boldsymbol{S^2} \rangle)$	-4302.09152006 (15.79)	-4302.23975166 (15.79)	-4302.74007632 (15.78)
BS $(\langle \boldsymbol{S^2} \rangle)$	-4302.10299312 (3.61)	-4302.25329967 (3.60)	-4302.75692961 (3.61)
CoMnCl			
HS $(\langle \boldsymbol{S^2} \rangle)$	-4189.41541256 (20.02)	-4189.56481805 (20.02)	-4190.0616556 (20.01)
BS $(\langle \boldsymbol{S^2} \rangle)$	-4189.42989109 (4.86)	-4189.57980209 (4.86)	-4190.07762632 (4.87)
FeMnCl			
HS $(\langle \boldsymbol{S^2} \rangle)$	-4070.35204413 (24.78)	-4070.50336987 (24.78)	-4070.99278683 (24.77)
BS $(\langle \boldsymbol{S^2} \rangle)$	-4070.36870057 (4.59)	-4070.52058816 (4.58)	-4071.01094875 (4.60)

.lst file for Complex **2:**

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******************************************************************************
   General Structure Analysis System-II Crystal Structure Refinement
              by Robert B. Von Dreele & Brian H. Toby
                Argonne National Laboratory(C), 2010
 This product includes software developed by the UChicago Argonne, LLC,
           as Operator of Argonne National Laboratory.
                        Please cite:
   B.H. Toby & R.B. Von Dreele, J. Appl. Cryst. 46, 544-549 (2013)
******************************************************************************

 Least squares controls:
 Refinement type:  analytic Hessian
 Maximum number of cycles: 10
 Initial shift factor:  1.000

 Phases:

 Phase name:  FECO
-------------------------------------------------------------------------------------------------------------------------------

 X-ray scattering factors:
   Symbol     fa                                        fb                                        fc
-------------------------------------------------------------------------------------------------------
 C          2.31000   1.02000   1.58860   0.86500  20.84390  10.20750   0.56870  51.65120   0.21560
 Co        12.28410   7.34090   4.00340   2.34880   4.27910   0.27840  13.53590  71.16920   1.01180
 Cl        11.46040   7.19640   6.25560   1.64550   0.01040   1.16620  18.51940  47.77840  -9.55740
 H          0.49300   0.32291   0.14019   0.04081  10.51090  26.12570   3.14236  57.79970   0.00304
 N         12.21260   3.13220   2.01250   1.16630   0.00570   9.89330  28.99750   0.58260 -11.52900
 Fe        11.76950   7.35730   3.52220   2.30450   4.76110   0.30720  15.35350  76.88050   1.03690

 Neutron scattering factors:
   Symbol   isotope       mass       b       resonant terms
-------------------------------------------------------------------------------------------------------
 C       Nat. Abund.     12.011    0.665
 Co      Nat. Abund.     58.933    0.249
 Cl      Nat. Abund.     35.453    0.958
 H       Nat. Abund.      1.008   -0.374
 N       Nat. Abund.     14.007    0.936
 Fe      Nat. Abund.     55.847    0.945

 Space Group: P 21/n
 The lattice is centrosymmetric primitive monoclinic
 Multiplicity of a general site is 4
 The Laue symmetry is 2/m
 The unique monoclinic axis is b
 The inversion center is located at 0,0,0

 The equivalent positions are:
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(1) X , Y , Z (2) 1/2-X ,1/2+Y ,1/2-Z

Atoms:

name	type	refine?	x	y	z	frac	site sym	mult	I/A	Uiso	U11	U22	U33	U12	U13	U23
Co1	Co	F	0.12235	0.14306	0.18227	0.957	1	4	A		0.0101	0.0097	0.0102	0.0108	0.0001	0.0022
Fe1	Fe	F	0.12235	0.14306	0.18227	0.043	1	4	A		0.0000	0.0097	0.0102	0.0108	0.0001	0.0022
Fe2	Fe	F	-0.00706	0.25653	0.08179	0.916	1	4	A		0.0100	0.0088	0.0111	0.0099	-0.0008	0.0010
Co2	Co	F	-0.00706	0.25653	0.08178	0.084	1	4	A		0.0000	0.0088	0.0111	0.0099	-0.0008	0.0010
Cl1	Cl		-0.12737	0.35725	-0.01666	1.000	1	4	A		0.0176	0.0141	0.0223	0.0156	0.0006	-0.0009
N1	N		0.22697	0.05055	0.26316	1.000	1	4	A		0.0145	0.0130	0.0153	0.0158	0.0012	0.0029
C1	C		0.36958	0.10426	0.28728	1.000	1	4	A		0.0174	0.0124	0.0231	0.0168	0.0014	0.0004
H1A	H		0.44070	0.05190	0.31190	1.000	1	4	I	0.0210						
H1B	H		0.35660	0.16090	0.32290	1.000	1	4	I	0.0210						
C2	C		0.42876	0.15256	0.22158	1.000	1	4	A		0.0161	0.0111	0.0190	0.0180	0.0013	0.0013
H2A	H		0.50580	0.20560	0.23850	1.000	1	4	I	0.0190						
H2B	H		0.47220	0.09620	0.19420	1.000	1	4	I	0.0190						
N2	N		0.30734	0.20399	0.17407	1.000	1	4	A		0.0125	0.0100	0.0141	0.0133	-0.0001	0.0011
C3	C		0.33204	0.26317	0.11696	1.000	1	4	A		0.0108	0.0105	0.0103	0.0121	-0.0004	0.0025
C4	C		0.47495	0.28583	0.10009	1.000	1	4	A		0.0138	0.0104	0.0146	0.0169	-0.0016	0.0030
H4A	H		0.55900	0.25900	0.13060	1.000	1	4	I	0.0170						
C5	C		0.48999	0.34625	0.03970	1.000	1	4	A		0.0154	0.0137	0.0150	0.0191	-0.0029	0.0067
H5A	H		0.58460	0.36010	0.02750	1.000	1	4	I	0.0180						
C6	C		0.36512	0.38736	-0.00395	1.000	1	4	A		0.0158	0.0171	0.0151	0.0165	-0.0003	0.0069
H6A	H		0.37350	0.43070	-0.04540	1.000	1	4	I	0.0190						
C7	C		0.22965	0.36376	0.01445	1.000	1	4	A		0.0139	0.0144	0.0139	0.0138	0.0004	0.0039
H7A	H		0.14540	0.39220	-0.01500	1.000	1	4	I	0.0170						
N3	N		0.20973	0.30192	0.07257	1.000	1	4	A		0.0111	0.0109	0.0113	0.0119	-0.0002	0.0027
C8	C		0.24102	-0.05462	0.22764	1.000	1	4	A		0.0188	0.0199	0.0143	0.0237	0.0049	0.0062
H8A	H		0.25790	-0.11060	0.26580	1.000	1	4	I	0.0230						
H8B	H		0.32680	-0.05330	0.20140	1.000	1	4	I	0.0230						
C9	C		0.10262	-0.08115	0.17356	1.000	1	4	A		0.0188	0.0233	0.0116	0.0231	0.0007	0.0069
H9A	H		0.12420	-0.13700	0.13900	1.000	1	4	I	0.0230						
H9B	H		0.02500	-0.10780	0.20040	1.000	1	4	I	0.0230						
N4	N		0.05263	0.01609	0.13328	1.000	1	4	A		0.0149	0.0178	0.0107	0.0171	-0.0009	0.0040
C10	C		-0.06609	0.01432	0.08204	1.000	1	4	A		0.0139	0.0154	0.0128	0.0152	-0.0024	0.0068
C11	C		-0.14788	-0.07979	0.05898	1.000	1	4	A		0.0186	0.0224	0.0149	0.0204	-0.0055	0.0085
H11A	H		-0.11280	-0.14750	0.07710	1.000	1	4	I	0.0220						
C12	C		-0.27596	-0.07286	0.01105	1.000	1	4	A		0.0219	0.0211	0.0223	0.0238	-0.0089	0.0084
H12A	H		-0.33180	-0.13520	-0.00290	1.000	1	4	I	0.0260						
C13	C		-0.32471	0.02662	-0.01766	1.000	1	4	A		0.0221	0.0157	0.0291	0.0213	-0.0056	0.0019
H13A	H		-0.41320	0.03280	-0.05110	1.000	1	4	I	0.0260						
C14	C		-0.24043	0.11488	0.00405	1.000	1	4	A		0.0176	0.0138	0.0222	0.0167	-0.0018	0.0021
H14A	H		-0.27250	0.18210	-0.01600	1.000	1	4	I	0.0210						
N5	N		-0.11373	0.11160	0.05280	1.000	1	4	A		0.0136	0.0125	0.0144	0.0145	-0.0017	0.0034
C15	C		0.12999	0.04970	0.32048	1.000	1	4	A		0.0164	0.0168	0.0189	0.0141	0.0004	0.0038
H15A	H		0.18750	0.03000	0.36820	1.000	1	4	I	0.0200						
H15B	H		0.05190	-0.00410	0.30800	1.000	1	4	I	0.0200						
C16	C		0.06062	0.15999	0.32638	1.000	1	4	A		0.0154	0.0161	0.0195	0.0113	-0.0003	0.0029

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  H16A      H          -0.02380   0.15450   0.35330   1.000    1       4    I  0.0190
  H16B      H           0.13320   0.20920   0.35350   1.000    1       4    I  0.0190
    N6      N           0.01262   0.20059   0.25228   1.000    1       4    A          0.0133  0.0137  0.0154  0.0114  0.0017  0.0025
   C17      C          -0.06772   0.28965   0.24081   1.000    1       4    A          0.0123  0.0101  0.0144  0.0125 -0.0009  0.0029
   C18      C          -0.12586   0.34674   0.29692   1.000    1       4    A          0.0170  0.0170  0.0199  0.0158  0.0003  0.0070
  H18A      H          -0.11080   0.32110   0.34590   1.000    1       4    I  0.0200
   C19      C          -0.20365   0.43921   0.27972   1.000    1       4    A          0.0194  0.0167  0.0200  0.0238  0.0011  0.0089
  H19A      H          -0.24190   0.47750   0.31700   1.000    1       4    I  0.0230
   C20      C          -0.22641   0.47701   0.20764   1.000    1       4    A          0.0182  0.0138  0.0166  0.0253  0.0031  0.0053
  H20A      H          -0.27950   0.54090   0.19500   1.000    1       4    I  0.0220
   C21      C          -0.16924   0.41863   0.15534   1.000    1       4    A          0.0150  0.0120  0.0148  0.0184  0.0016  0.0017
  H21A      H          -0.18510   0.44370   0.10630   1.000    1       4    I  0.0180
    N7      N     XU   -0.09255   0.32738   0.16966   1.000    1       4    A          0.0123  0.0051  0.0138  0.0159 -0.0002 -0.0032

 Unit cell: a = 9.24500  b = 12.55970  c = 18.47510  alpha = 90.000  beta = 98.724  gamma = 90.000  volume = 2120.406  Refine? False

 Spherical harmonics texture: Order:0

 Phase:  FECO  in histogram:  HKLF feco7062.fcf:feco7062
-------------------------------------------------------------------------------------------------------------------------------------------
 Scale factor     :     0.9407  Refine? True

 Phase:  FECO  in histogram:  HKLF feco7659.fcf:feco7659
-------------------------------------------------------------------------------------------------------------------------------------------
 Scale factor     :     0.7638  Refine? True

 Refinement results:
-------------------------------------------------------------------------------------------------------------------------------------------
 Number of function calls: 12  Number of observations:  3638  Number of parameters:  13
 Refinement time =   17.270s,   17.270s/cycle, for 1 cycles
 wR =   29.69%, chi**2 =      68765.7, reduced chi**2 =  18.97
-------------------------------------------------------------------------------------------------------------------------------------------
Variables generated by constraints

 name  :     ::constr:0     ::constr:1
 value :        -0.6459        -0.5883
 sig   :         0.0160         0.0153

 Phases:
 Result for phase:  FECO

 Atoms:
   name      x         y         z      frac   Uiso     U11     U22     U33     U12     U13     U23
-------------------------------------------------------------------------------------------------------------------------------------------
    Co1     Co:
 values:   0.12235   0.14306   0.18227   0.957         0.00966 0.01024 0.01077 0.00007 0.00223 0.00143
 sig   :                               0.011
    Fe1     Fe:
 values:   0.12235   0.14306   0.18227   0.043         0.00966 0.01024 0.01077 0.00007 0.00223 0.00143
 sig   :   0.00000   0.00000   0.00000   0.011         0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
```

```
   Fe2     Fe:
values:  -0.00706   0.25653   0.08179   0.916         0.00883 0.01111 0.00988-0.00080 0.00100 0.00069
sig   :                                 0.011
   Co2     Co:
values:  -0.00706   0.25653   0.08178   0.084         0.00883 0.01111 0.00988-0.00080 0.00100 0.00069
sig   :   0.00000   0.00000   0.00000   0.011         0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
   Cl1     Cl:
values:  -0.12737   0.35725  -0.01666   1.000         0.01408 0.02226 0.01563 0.00058-0.00094 0.00660
sig   :
    N1      N:
values:   0.22697   0.05055   0.26316   1.000         0.01297 0.01525 0.01585 0.00121 0.00289 0.00482
sig   :
    C1      C:
values:   0.36958   0.10426   0.28728   1.000         0.01244 0.02306 0.01681 0.00137 0.00036 0.00724
sig   :
   H1A      H:
values:   0.44070   0.05190   0.31190   1.000 0.02100
sig   :
   H1B      H:
values:   0.35660   0.16090   0.32290   1.000 0.02100
sig   :
    C2      C:
values:   0.42876   0.15256   0.22158   1.000         0.01115 0.01895 0.01801 0.00132 0.00131 0.00479
sig   :
   H2A      H:
values:   0.50580   0.20560   0.23850   1.000 0.01900
sig   :
   H2B      H:
values:   0.47220   0.09620   0.19420   1.000 0.01900
sig   :
    N2      N:
values:   0.30734   0.20399   0.17407   1.000         0.01003 0.01410 0.01325-0.00010 0.00110 0.00305
sig   :
    C3      C:
values:   0.33204   0.26317   0.11696   1.000         0.01053 0.01030 0.01208-0.00039 0.00246-0.00091
sig   :
    C4      C:
values:   0.47495   0.28583   0.10009   1.000         0.01041 0.01461 0.01690-0.00158 0.00305 0.00015
sig   :
   H4A      H:
values:   0.55900   0.25900   0.13060   1.000 0.01700
sig   :
    C5      C:
values:   0.48999   0.34625   0.03970   1.000         0.01369 0.01499 0.01909-0.00293 0.00666-0.00062
sig   :
   H5A      H:
values:   0.58460   0.36010   0.02750   1.000 0.01800
sig   :
    C6      C:
values:   0.36512   0.38736  -0.00395   1.000         0.01710 0.01512 0.01651-0.00029 0.00685 0.00341
```

```
sig   :
   H6A      H:
values:   0.37350   0.43070  -0.04540   1.000 0.01900
sig   :
    C7      C:
values:   0.22965   0.36376   0.01445   1.000         0.01437 0.01391 0.01381 0.00045 0.00387 0.00216
sig   :
   H7A      H:
values:   0.14540   0.39220  -0.01500   1.000 0.01700
sig   :
    N3      N:
values:   0.20973   0.30192   0.07257   1.000         0.01092 0.01127 0.01187-0.00023 0.00267 0.00065
sig   :
    C8      C:
values:   0.24102  -0.05462   0.22764   1.000         0.01991 0.01428 0.02366 0.00493 0.00617 0.00638
sig   :
   H8A      H:
values:   0.25790  -0.11060   0.26580   1.000 0.02300
sig   :
   H8B      H:
values:   0.32680  -0.05330   0.20140   1.000 0.02300
sig   :
    C9      C:
values:   0.10262  -0.08115   0.17356   1.000         0.02332 0.01162 0.02305 0.00070 0.00688 0.00256
sig   :
   H9A      H:
values:   0.12420  -0.13700   0.13900   1.000 0.02300
sig   :
   H9B      H:
values:   0.02500  -0.10780   0.20040   1.000 0.02300
sig   :
    N4      N:
values:   0.05263   0.01609   0.13328   1.000         0.01776 0.01072 0.01712-0.00094 0.00396 0.00047
sig   :
   C10      C:
values:  -0.06609   0.01432   0.08204   1.000         0.01538 0.01283 0.01518-0.00243 0.00678-0.00337
sig   :
   C11      C:
values:  -0.14788  -0.07979   0.05898   1.000         0.02237 0.01487 0.02042-0.00548 0.00855-0.00667
sig   :
  H11A      H:
values:  -0.11280  -0.14750   0.07710   1.000 0.02200
sig   :
   C12      C:
values:  -0.27596  -0.07286   0.01105   1.000         0.02112 0.02231 0.02375-0.00887 0.00838-0.01299
sig   :
  H12A      H:
values:  -0.33180  -0.13520  -0.00290   1.000 0.02600
sig   :
   C13      C:
```

```
values:  -0.32471   0.02662  -0.01766   1.000         0.01575 0.02911 0.02128-0.00560 0.00192-0.01012
sig   :
  H13A      H:
values:  -0.41320   0.03280  -0.05110   1.000 0.02600
sig   :
   C14      C:
values:  -0.24043   0.11488   0.00405   1.000         0.01379 0.02224 0.01671-0.00180 0.00213-0.00420
sig   :
  H14A      H:
values:  -0.27250   0.18210  -0.01600   1.000 0.02100
sig   :
    N5      N:
values:  -0.11373   0.11160   0.05280   1.000         0.01255 0.01437 0.01449-0.00165 0.00336-0.00229
sig   :
   C15      C:
values:   0.12999   0.04970   0.32048   1.000         0.01683 0.01885 0.01411 0.00038 0.00382 0.00603
sig   :
  H15A      H:
values:   0.18750   0.03000   0.36820   1.000 0.02000
sig   :
  H15B      H:
values:   0.05190  -0.00410   0.30800   1.000 0.02000
sig   :
   C16      C:
values:   0.06062   0.15999   0.32638   1.000         0.01607 0.01951 0.01132-0.00027 0.00289 0.00241
sig   :
  H16A      H:
values:  -0.02380   0.15450   0.35330   1.000 0.01900
sig   :
  H16B      H:
values:   0.13320   0.20920   0.35350   1.000 0.01900
sig   :
    N6      N:
values:   0.01262   0.20059   0.25228   1.000         0.01366 0.01538 0.01137 0.00170 0.00249 0.00163
sig   :
   C17      C:
values:  -0.06772   0.28965   0.24081   1.000         0.01011 0.01436 0.01253-0.00089 0.00291-0.00083
sig   :
   C18      C:
values:  -0.12586   0.34674   0.29692   1.000         0.01701 0.01992 0.01576 0.00032 0.00699-0.00249
sig   :
  H18A      H:
values:  -0.11080   0.32110   0.34590   1.000 0.02000
sig   :
   C19      C:
values:  -0.20365   0.43921   0.27972   1.000         0.01673 0.01999 0.02381 0.00112 0.00888-0.00503
sig   :
  H19A      H:
values:  -0.24190   0.47750   0.31700   1.000 0.02300
sig   :
```

```
   C20      C:
values:  -0.22641   0.47701   0.20764   1.000         0.01383 0.01656 0.02535 0.00312 0.00530-0.00219
sig   :
  H20A      H:
values:  -0.27950   0.54090   0.19500   1.000 0.02200
sig   :
   C21      C:
values:  -0.16924   0.41863   0.15534   1.000         0.01203 0.01478 0.01841 0.00162 0.00165-0.00002
sig   :
  H21A      H:
values:  -0.18510   0.44370   0.10630   1.000 0.01800
sig   :
    N7      N:
values:  -0.09255   0.32738   0.16966   1.000         0.00505 0.01378 0.01589-0.00023-0.00325 0.00050
sig   :   0.00052   0.00030   0.00027                 0.00377 0.00200 0.00318 0.00215 0.00287 0.00219

Phase:  FECO  in histogram:  HKLF feco7062.fcf:feco7062
-------------------------------------------------------------------------------------------------------------------------
Final refinement RF, RF^2 = 7.25%, 6.83% on 1504 reflections
HKLF histogram weight factor =  1.000
Scale factor :     0.9407, sig     0.0069

Single crystal extinction: Type:  Lorentzian  Approx:  None


Phase:  FECO  in histogram:  HKLF feco7659.fcf:feco7659
-------------------------------------------------------------------------------------------------------------------------
Final refinement RF, RF^2 = 14.07%, 11.83% on 2134 reflections
HKLF histogram weight factor =  1.000
Scale factor :     0.7638, sig     0.0061

Single crystal extinction: Type:  Lorentzian  Approx:  None
```

.lst file for Complex **3:**

```
******************************************************************************
   General Structure Analysis System-II Crystal Structure Refinement
              by Robert B. Von Dreele & Brian H. Toby
                Argonne National Laboratory(C), 2010
 This product includes software developed by the UChicago Argonne, LLC,
            as Operator of Argonne National Laboratory.
                         Please cite:
   B.H. Toby & R.B. Von Dreele, J. Appl. Cryst. 46, 544-549 (2013)
******************************************************************************

 Least squares controls:
 Refinement type:  analytic Hessian
 Maximum number of cycles: 10
 Initial shift factor:  1.000

 Phases:

 Phase name:  MNCO
-------------------------------------------------------------------------------------------------------------------------------------------

 X-ray scattering factors:
   Symbol     fa                                          fb                                          fc
-------------------------------------------------------------------------------------------------------
 C          2.31000   1.02000   1.58860   0.86500  20.84390  10.20750   0.56870  51.65120   0.21560
 Co        12.28410   7.34090   4.00340   2.34880   4.27910   0.27840  13.53590  71.16920   1.01180
 Cl        11.46040   7.19640   6.25560   1.64550   0.01040   1.16620  18.51940  47.77840  -9.55740
 H          0.49300   0.32291   0.14019   0.04081  10.51090  26.12570   3.14236  57.79970   0.00304
 Mn        11.28190   7.35730   3.01930   2.24410   5.34090   0.34320  17.86740  83.75430   1.08960
 N         12.21260   3.13220   2.01250   1.16630   0.00570   9.89330  28.99750   0.58260 -11.52900

 Neutron scattering factors:
   Symbol   isotope       mass       b       resonant terms
-------------------------------------------------------------------------------------------------
 C       Nat. Abund.     12.011    0.665
 Co      Nat. Abund.     58.933    0.249
 Cl      Nat. Abund.     35.453    0.958
 H       Nat. Abund.      1.008   -0.374
 Mn      Nat. Abund.     54.938   -0.375
 N       Nat. Abund.     14.007    0.936

 Space Group: P 21/n
 The lattice is centrosymmetric primitive monoclinic
 Multiplicity of a general site is 4
 The Laue symmetry is 2/m
 The unique monoclinic axis is b
 The inversion center is located at 0,0,0
```

The equivalent positions are:
(1) X , Y , Z (2) 1/2-X ,1/2+Y ,1/2-Z

Atoms:

name	type	refine?	x	y	z	frac	site sym	mult	I/A	Uiso	U11	U22	U33	U12	U13	U23
Co1	Co	F	0.12032	0.14272	0.17995	0.983	1	4	A		0.0000	0.0092	0.0118	0.0120	0.0000	0.0014
Mn1	Mn	F	0.12032	0.14272	0.17995	0.017	1	4	A		0.0110	0.0092	0.0118	0.0120	0.0000	0.0014
Mn2	Mn	F	-0.00706	0.25869	0.07791	0.985	1	4	A		0.0115	0.0092	0.0129	0.0117	-0.0005	0.0006
Co2	Co	F	-0.00706	0.25869	0.07791	0.015	1	4	A		0.0000	0.0092	0.0129	0.0117	-0.0005	0.0006
Cl1	Cl		-0.12594	0.36149	-0.02046	1.000	1	4	A		0.0182	0.0145	0.0225	0.0167	0.0007	-0.0013
N1	N		0.22191	0.04914	0.26089	1.000	1	4	A		0.0156	0.0131	0.0164	0.0172	0.0011	0.0025
C1	C		0.12591	0.05066	0.31804	1.000	1	4	A		0.0171	0.0161	0.0198	0.0156	-0.0003	0.0021
H1A	H		0.18250	0.03050	0.36560	1.000	1	4	I	0.0210						
H1B	H		0.04690	-0.00250	0.30570	1.000	1	4	I	0.0210						
C2	C		0.05994	0.16264	0.32368	1.000	1	4	A		0.0164	0.0162	0.0206	0.0124	-0.0002	0.0022
H2A	H		-0.02380	0.15850	0.35080	1.000	1	4	I	0.0200						
H2B	H		0.13350	0.21150	0.35040	1.000	1	4	I	0.0200						
N2	N		0.01261	0.20387	0.24985	1.000	1	4	A		0.0140	0.0132	0.0165	0.0124	0.0018	0.0023
C3	C		-0.06701	0.29342	0.23930	1.000	1	4	A		0.0132	0.0104	0.0154	0.0140	-0.0009	0.0027
C4	C		-0.12319	0.35078	0.29579	1.000	1	4	A		0.0180	0.0169	0.0210	0.0170	-0.0001	0.0064
H4A	H		-0.10670	0.32500	0.34460	1.000	1	4	I	0.0220						
C5	C		-0.20149	0.44379	0.27917	1.000	1	4	A		0.0200	0.0167	0.0208	0.0238	0.0008	0.0089
H5A	H		-0.23870	0.48210	0.31680	1.000	1	4	I	0.0240						
C6	C		-0.22612	0.48160	0.20756	1.000	1	4	A		0.0193	0.0140	0.0175	0.0264	0.0031	0.0047
H6A	H		-0.27960	0.54590	0.19530	1.000	1	4	I	0.0230						
C7	C		-0.17042	0.42320	0.15512	1.000	1	4	A		0.0160	0.0117	0.0161	0.0200	0.0014	0.0009
H7A	H		-0.18750	0.44840	0.10620	1.000	1	4	I	0.0190						
N3	N		-0.09274	0.33151	0.16902	1.000	1	4	A		0.0132	0.0102	0.0143	0.0147	0.0008	0.0009
C8	C		0.23331	-0.05725	0.22595	1.000	1	4	A		0.0192	0.0185	0.0156	0.0236	0.0039	0.0041
H8A	H		0.24940	-0.11330	0.26420	1.000	1	4	I	0.0230						
H8B	H		0.31790	-0.05720	0.19930	1.000	1	4	I	0.0230						
C9	C		0.09478	-0.08267	0.17287	1.000	1	4	A		0.0192	0.0212	0.0132	0.0244	0.0010	0.0050
H9A	H		0.11430	-0.14030	0.13890	1.000	1	4	I	0.0230						
H9B	H		0.01740	-0.10770	0.20030	1.000	1	4	I	0.0230						
N4	N		0.04763	0.01468	0.13204	1.000	1	4	A		0.0155	0.0158	0.0121	0.0180	-0.0006	0.0026
C10	C		-0.07065	0.01190	0.08116	1.000	1	4	A		0.0144	0.0142	0.0144	0.0156	-0.0025	0.0057
C11	C		-0.15353	-0.08239	0.06050	1.000	1	4	A		0.0192	0.0204	0.0157	0.0222	-0.0053	0.0077
H11A	H		-0.12030	-0.15020	0.08020	1.000	1	4	I	0.0230						
C12	C		-0.28009	-0.07578	0.01266	1.000	1	4	A		0.0216	0.0191	0.0224	0.0242	-0.0079	0.0078
H12A	H		-0.33750	-0.13830	0.00060	1.000	1	4	I	0.0260						
C13	C		-0.32560	0.02310	-0.01873	1.000	1	4	A		0.0220	0.0149	0.0291	0.0221	-0.0054	0.0017
H13A	H		-0.41270	0.02900	-0.05260	1.000	1	4	I	0.0260						
C14	C		-0.23968	0.11134	0.00094	1.000	1	4	A		0.0181	0.0131	0.0224	0.0181	-0.0020	0.0013
H14A	H		-0.26930	0.17840	-0.02090	1.000	1	4	I	0.0220						
N5	N		-0.11548	0.10862	0.04969	1.000	1	4	A		0.0144	0.0121	0.0158	0.0151	-0.0019	0.0024
C15	C		0.36442	0.10134	0.28440	1.000	1	4	A		0.0184	0.0121	0.0241	0.0185	0.0008	-0.0007
H15A	H		0.43380	0.04780	0.30900	1.000	1	4	I	0.0220						
H15B	H		0.35300	0.15900	0.31980	1.000	1	4	I	0.0220						

```
   C16      C          0.42455   0.14884   0.21872   1.000    1       4    A          0.0170  0.0110  0.0203  0.0187  0.0011  0.0005
  H16A      H          0.50230   0.20150   0.23570   1.000    1       4    I  0.0200
  H16B      H          0.46690   0.09120   0.19170   1.000    1       4    I  0.0200
    N6      N          0.30585   0.20156   0.17125   1.000    1       4    A          0.0134  0.0098  0.0154  0.0148 -0.0003  0.0009
   C17      C          0.33444   0.26187   0.11530   1.000    1       4    A          0.0120  0.0103  0.0114  0.0141 -0.0006  0.0017
   C18      C          0.47713   0.28372   0.09973   1.000    1       4    A          0.0151  0.0104  0.0163  0.0186 -0.0014  0.0026
  H18A      H          0.55960   0.25590   0.13070   1.000    1       4    I  0.0180
   C19      C          0.49537   0.34438   0.04005   1.000    1       4    A          0.0164  0.0132  0.0161  0.0204 -0.0028  0.0058
  H19A      H          0.59030   0.35780   0.02880   1.000    1       4    I  0.0200
   C20      C          0.37343   0.38672  -0.00443   1.000    1       4    A          0.0167  0.0162  0.0159  0.0182 -0.0012  0.0060
  H20A      H          0.38400   0.42980  -0.04570   1.000    1       4    I  0.0200
   C21      C          0.23789   0.36406   0.01310   1.000    1       4    A          0.0145  0.0140  0.0137  0.0158 -0.0000  0.0032
  H21A      H          0.15530   0.39340  -0.01680   1.000    1       4    I  0.0170
    N7      N          0.21561   0.30241   0.07063   1.000    1       4    A          0.0122  0.0108  0.0124  0.0133 -0.0007  0.0018

 Unit cell: a = 9.30120  b = 12.45190  c = 18.51770  alpha = 90.000  beta = 98.632  gamma = 90.000  volume = 2120.382  Refine? False

 Spherical harmonics texture: Order:0

 Phase:  MNCO  in histogram:  HKLF mnco6489.fcf:mnco6489
-------------------------------------------------------------------------------------------------------------------------------------------
 Scale factor     :    27.9960  Refine? True

 Phase:  MNCO  in histogram:  HKLF mnco7659.fcf:mnco7659
-------------------------------------------------------------------------------------------------------------------------------------------
 Scale factor     :    10.2335  Refine? True

 Refinement results:
-------------------------------------------------------------------------------------------------------------------------------------------
 Number of function calls: 12  Number of observations:  3374  Number of parameters:  4
 Refinement time =   15.950s,   15.950s/cycle, for 1 cycles
 wR =   18.60%, chi**2 =      54896.5, reduced chi**2 =  16.29
-------------------------------------------------------------------------------------------------------------------------------------------
Variables generated by constraints

 name  :     ::constr:0     ::constr:1
 value :        -0.6830        -0.6859
 sig   :         0.0166         0.0154

 Phases:
 Result for phase:  MNCO

 Atoms:
   name      x         y         z      frac   Uiso     U11     U22     U33     U12     U13     U23
-------------------------------------------------------------------------------------------------------------------------------------------
    Co1     Co:
 values:   0.12032   0.14272   0.17995   0.983         0.00924 0.01177 0.01197 0.00003 0.00140 0.00116
 sig   :                               0.012
    Mn1     Mn:
 values:   0.12032   0.14272   0.17995   0.017         0.00924 0.01177 0.01197 0.00003 0.00140 0.00116
```

```
sig   :   0.00000   0.00000   0.00000   0.012         0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
   Mn2     Mn:
values:  -0.00706   0.25869   0.07791   0.985         0.00921 0.01293 0.01175-0.00049 0.00063 0.00069
sig   :                                 0.011
   Co2     Co:
values:  -0.00706   0.25869   0.07791   0.015         0.00921 0.01293 0.01175-0.00049 0.00063 0.00069
sig   :   0.00000   0.00000   0.00000   0.011         0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
   Cl1     Cl:
values:  -0.12594   0.36149  -0.02046   1.000         0.01446 0.02247 0.01673 0.00072-0.00127 0.00558
sig   :
    N1      N:
values:   0.22191   0.04914   0.26089   1.000         0.01313 0.01640 0.01722 0.00112 0.00253 0.00361
sig   :
    C1      C:
values:   0.12591   0.05066   0.31804   1.000         0.01613 0.01977 0.01560-0.00025 0.00211 0.00567
sig   :
   H1A      H:
values:   0.18250   0.03050   0.36560   1.000 0.02100
sig   :
   H1B      H:
values:   0.04690  -0.00250   0.30570   1.000 0.02100
sig   :
    C2      C:
values:   0.05994   0.16264   0.32368   1.000         0.01618 0.02064 0.01242-0.00023 0.00218 0.00229
sig   :
   H2A      H:
values:  -0.02380   0.15850   0.35080   1.000 0.02000
sig   :
   H2B      H:
values:   0.13350   0.21150   0.35040   1.000 0.02000
sig   :
    N2      N:
values:   0.01261   0.20387   0.24985   1.000         0.01323 0.01653 0.01236 0.00183 0.00227 0.00131
sig   :
    C3      C:
values:  -0.06701   0.29342   0.23930   1.000         0.01040 0.01540 0.01400-0.00091 0.00272-0.00103
sig   :
    C4      C:
values:  -0.12319   0.35078   0.29579   1.000         0.01689 0.02101 0.01697-0.00006 0.00638-0.00281
sig   :
   H4A      H:
values:  -0.10670   0.32500   0.34460   1.000 0.02200
sig   :
    C5      C:
values:  -0.20149   0.44379   0.27917   1.000         0.01674 0.02078 0.02383 0.00082 0.00893-0.00491
sig   :
   H5A      H:
values:  -0.23870   0.48210   0.31680   1.000 0.02400
sig   :
    C6      C:
```

```
values:  -0.22612   0.48160   0.20756   1.000         0.01397 0.01750 0.02643 0.00314 0.00475-0.00172
sig   :
   H6A      H:
values:  -0.27960   0.54590   0.19530   1.000 0.02300
sig   :
    C7      C:
values:  -0.17042   0.42320   0.15512   1.000         0.01166 0.01611 0.02004 0.00137 0.00092 0.00002
sig   :
   H7A      H:
values:  -0.18750   0.44840   0.10620   1.000 0.01900
sig   :
    N3      N:
values:  -0.09274   0.33151   0.16902   1.000         0.01023 0.01427 0.01468 0.00084 0.00093-0.00025
sig   :
    C8      C:
values:   0.23331  -0.05725   0.22595   1.000         0.01848 0.01560 0.02365 0.00387 0.00408 0.00471
sig   :
   H8A      H:
values:   0.24940  -0.11330   0.26420   1.000 0.02300
sig   :
   H8B      H:
values:   0.31790  -0.05720   0.19930   1.000 0.02300
sig   :
    C9      C:
values:   0.09478  -0.08267   0.17287   1.000         0.02118 0.01322 0.02439 0.00104 0.00504 0.00169
sig   :
   H9A      H:
values:   0.11430  -0.14030   0.13890   1.000 0.02300
sig   :
   H9B      H:
values:   0.01740  -0.10770   0.20030   1.000 0.02300
sig   :
    N4      N:
values:   0.04763   0.01468   0.13204   1.000         0.01584 0.01212 0.01802-0.00060 0.00260 0.00077
sig   :
   C10      C:
values:  -0.07065   0.01190   0.08116   1.000         0.01421 0.01439 0.01562-0.00248 0.00566-0.00346
sig   :
   C11      C:
values:  -0.15353  -0.08239   0.06050   1.000         0.02043 0.01572 0.02222-0.00530 0.00773-0.00672
sig   :
  H11A      H:
values:  -0.12030  -0.15020   0.08020   1.000 0.02300
sig   :
   C12      C:
values:  -0.28009  -0.07578   0.01266   1.000         0.01915 0.02243 0.02423-0.00789 0.00781-0.01130
sig   :
  H12A      H:
values:  -0.33750  -0.13830   0.00060   1.000 0.02600
sig   :
```

```
   C13      C:
values:  -0.32560   0.02310  -0.01873   1.000         0.01491 0.02908 0.02213-0.00543 0.00167-0.00892
sig   :
  H13A      H:
values:  -0.41270   0.02900  -0.05260   1.000 0.02600
sig   :
   C14      C:
values:  -0.23968   0.11134   0.00094   1.000         0.01306 0.02244 0.01811-0.00203 0.00126-0.00368
sig   :
  H14A      H:
values:  -0.26930   0.17840  -0.02090   1.000 0.02200
sig   :
    N5      N:
values:  -0.11548   0.10862   0.04969   1.000         0.01211 0.01580 0.01508-0.00189 0.00245-0.00225
sig   :
   C15      C:
values:   0.36442   0.10134   0.28440   1.000         0.01208 0.02408 0.01848 0.00078-0.00068 0.00627
sig   :
  H15A      H:
values:   0.43380   0.04780   0.30900   1.000 0.02200
sig   :
  H15B      H:
values:   0.35300   0.15900   0.31980   1.000 0.02200
sig   :
   C16      C:
values:   0.42455   0.14884   0.21872   1.000         0.01097 0.02031 0.01869 0.00114 0.00052 0.00436
sig   :
  H16A      H:
values:   0.50230   0.20150   0.23570   1.000 0.02000
sig   :
  H16B      H:
values:   0.46690   0.09120   0.19170   1.000 0.02000
sig   :
    N6      N:
values:   0.30585   0.20156   0.17125   1.000         0.00980 0.01540 0.01480-0.00029 0.00091 0.00277
sig   :
   C17      C:
values:   0.33444   0.26187   0.11530   1.000         0.01031 0.01136 0.01405-0.00062 0.00168-0.00090
sig   :
   C18      C:
values:   0.47713   0.28372   0.09973   1.000         0.01041 0.01626 0.01856-0.00138 0.00264-0.00089
sig   :
  H18A      H:
values:   0.55960   0.25590   0.13070   1.000 0.01800
sig   :
   C19      C:
values:   0.49537   0.34438   0.04005   1.000         0.01319 0.01614 0.02044-0.00283 0.00582-0.00068
sig   :
  H19A      H:
values:   0.59030   0.35780   0.02880   1.000 0.02000
```

```
sig   :
   C20      C:
values:   0.37343   0.38672  -0.00443   1.000         0.01620 0.01588 0.01820-0.00121 0.00595 0.00250
sig   :
  H20A      H:
values:   0.38400   0.42980  -0.04570   1.000 0.02000
sig   :
   C21      C:
values:   0.23789   0.36406   0.01310   1.000         0.01405 0.01374 0.01583-0.00001 0.00324 0.00188
sig   :
  H21A      H:
values:   0.15530   0.39340  -0.01680   1.000 0.01700
sig   :
    N7      N:
values:   0.21561   0.30241   0.07063   1.000         0.01076 0.01237 0.01332-0.00068 0.00179 0.00042
sig   :

Phase:  MNCO  in histogram:  HKLF mnco6489.fcf:mnco6489
-------------------------------------------------------------------------------------------------------------------------
Final refinement RF, RF^2 = 6.39%, 5.08% on 1206 reflections
HKLF histogram weight factor =  1.000
Scale factor :    27.9960, sig     0.1885

Single crystal extinction: Type:  Lorentzian  Approx:  None


Phase:  MNCO  in histogram:  HKLF mnco7659.fcf:mnco7659
-------------------------------------------------------------------------------------------------------------------------
Final refinement RF, RF^2 = 7.71%, 6.43% on 2168 reflections
HKLF histogram weight factor =  1.000
Scale factor :    10.2335, sig     0.0468

Single crystal extinction: Type:  Lorentzian  Approx:  None
```

.lst file for Complex **5:**

```
******************************************************************************
   General Structure Analysis System-II Crystal Structure Refinement
              by Robert B. Von Dreele & Brian H. Toby
                Argonne National Laboratory(C), 2010
 This product includes software developed by the UChicago Argonne, LLC,
           as Operator of Argonne National Laboratory.
                         Please cite:
   B.H. Toby & R.B. Von Dreele, J. Appl. Cryst. 46, 544-549 (2013)
******************************************************************************

 Least squares controls:
 Refinement type:  analytic Hessian
 Maximum number of cycles: 10
 Initial shift factor:  1.000

 Phases:

 Phase name:  MNFE
-------------------------------------------------------------------------------------------------------------------------------------------

 X-ray scattering factors:
   Symbol     fa                                          fb                                          fc
-------------------------------------------------------------------------------------------------------
 C          2.31000   1.02000   1.58860   0.86500  20.84390  10.20750   0.56870  51.65120   0.21560
 Cl        11.46040   7.19640   6.25560   1.64550   0.01040   1.16620  18.51940  47.77840  -9.55740
 H          0.49300   0.32291   0.14019   0.04081  10.51090  26.12570   3.14236  57.79970   0.00304
 Mn        11.28190   7.35730   3.01930   2.24410   5.34090   0.34320  17.86740  83.75430   1.08960
 N         12.21260   3.13220   2.01250   1.16630   0.00570   9.89330  28.99750   0.58260 -11.52900
 Fe        11.76950   7.35730   3.52220   2.30450   4.76110   0.30720  15.35350  76.88050   1.03690

 Neutron scattering factors:
   Symbol   isotope       mass       b       resonant terms
-----------------------------------------------------------------------------------------------
 C       Nat. Abund.     12.011    0.665
 Cl      Nat. Abund.     35.453    0.958
 H       Nat. Abund.      1.008   -0.374
 Mn      Nat. Abund.     54.938   -0.375
 N       Nat. Abund.     14.007    0.936
 Fe      Nat. Abund.     55.847    0.945

 Space Group: P 21/n
 The lattice is centrosymmetric primitive monoclinic
 Multiplicity of a general site is 4
 The Laue symmetry is 2/m
 The unique monoclinic axis is b
 The inversion center is located at 0,0,0
```

The equivalent positions are:
(1) X , Y , Z (2) 1/2-X ,1/2+Y ,1/2-Z

Atoms:

name	type	refine?	x	y	z	frac	site sym	mult	I/A	Uiso	U11	U22	U33	U12	U13	U23
Fe1	Fe	F	0.12023	0.14192	0.17699	0.952	1	4	A		0.0101	0.0098	0.0100	0.0106	-0.0000	0.0015
Mn1	Mn	F	0.12023	0.14192	0.17699	0.048	1	4	A		0.0101	0.0098	0.0100	0.0106	-0.0000	0.0015
Mn2	Mn	F	-0.00631	0.25883	0.07634	0.993	1	4	A		0.0107	0.0096	0.0117	0.0109	-0.0008	0.0013
Fe2	Fe	F	-0.00631	0.25883	0.07634	0.007	1	4	A		0.0107	0.0096	0.0117	0.0109	-0.0008	0.0013
Cl1	Cl		-0.12383	0.36148	-0.02217	1.000	1	4	A		0.0171	0.0150	0.0204	0.0152	0.0006	-0.0007
N1	N		0.22166	0.04633	0.25957	1.000	1	4	A		0.0138	0.0124	0.0146	0.0145	0.0008	0.0024
C1	C		0.23161	-0.05998	0.22441	1.000	1	4	A		0.0178	0.0183	0.0134	0.0221	0.0034	0.0043
H1A	H		0.24750	-0.11620	0.26260	1.000	1	4	I	0.0210						
H1B	H		0.31570	-0.06040	0.19750	1.000	1	4	I	0.0210						
C2	C		0.09306	-0.08579	0.17127	1.000	1	4	A		0.0179	0.0217	0.0110	0.0216	0.0008	0.0054
H2A	H		0.11210	-0.14450	0.13790	1.000	1	4	I	0.0210						
H2B	H		0.01560	-0.10940	0.19890	1.000	1	4	I	0.0210						
N2	N		0.04723	0.01058	0.12920	1.000	1	4	A		0.0142	0.0162	0.0106	0.0160	-0.0010	0.0026
C3	C		-0.07226	0.00969	0.07943	1.000	1	4	A		0.0134	0.0144	0.0127	0.0142	-0.0022	0.0051
C4	C		-0.15725	-0.08336	0.05910	1.000	1	4	A		0.0176	0.0202	0.0140	0.0201	-0.0056	0.0079
H4A	H		-0.12570	-0.15150	0.07840	1.000	1	4	I	0.0210						
C5	C		-0.28407	-0.07491	0.01192	1.000	1	4	A		0.0202	0.0189	0.0209	0.0222	-0.0083	0.0079
H5A	H		-0.34260	-0.13660	-0.00010	1.000	1	4	I	0.0240						
C6	C		-0.32768	0.02475	-0.01871	1.000	1	4	A		0.0200	0.0139	0.0254	0.0207	-0.0049	0.0023
H6A	H		-0.41510	0.03190	-0.05200	1.000	1	4	I	0.0240						
C7	C		-0.24024	0.11201	0.00077	1.000	1	4	A		0.0164	0.0124	0.0200	0.0167	-0.0019	0.0020
H7A	H		-0.26880	0.17950	-0.02060	1.000	1	4	I	0.0200						
N3	N		-0.11510	0.10725	0.04895	1.000	1	4	A		0.0129	0.0118	0.0138	0.0134	-0.0020	0.0028
C8	C		0.36419	0.09772	0.28282	1.000	1	4	A		0.0170	0.0128	0.0216	0.0160	0.0013	-0.0002
H8A	H		0.43290	0.04370	0.30700	1.000	1	4	I	0.0200						
H8B	H		0.35360	0.15490	0.31880	1.000	1	4	I	0.0200						
C9	C		0.42565	0.14638	0.21752	1.000	1	4	A		0.0160	0.0112	0.0193	0.0173	0.0010	0.0011
H9A	H		0.50480	0.19720	0.23510	1.000	1	4	I	0.0190						
H9B	H		0.46560	0.08890	0.18940	1.000	1	4	I	0.0190						
N4	N		0.30988	0.20232	0.17098	1.000	1	4	A		0.0126	0.0103	0.0141	0.0132	0.0000	0.0015
C10	C		0.33737	0.26247	0.11500	1.000	1	4	A		0.0110	0.0109	0.0100	0.0124	-0.0006	0.0024
C11	C		0.47893	0.28458	0.09883	1.000	1	4	A		0.0141	0.0107	0.0146	0.0172	-0.0014	0.0027
H11A	H		0.56150	0.25730	0.12960	1.000	1	4	I	0.0170						
C12	C		0.49613	0.34531	0.03886	1.000	1	4	A		0.0150	0.0131	0.0145	0.0187	-0.0029	0.0062
H12A	H		0.59040	0.35870	0.02730	1.000	1	4	I	0.0180						
C13	C		0.37413	0.38748	-0.00533	1.000	1	4	A		0.0157	0.0168	0.0144	0.0172	-0.0015	0.0067
H13A	H		0.38390	0.43070	-0.04670	1.000	1	4	I	0.0190						
C14	C		0.23973	0.36447	0.01290	1.000	1	4	A		0.0135	0.0140	0.0127	0.0144	0.0002	0.0038
H14A	H		0.15710	0.39370	-0.01680	1.000	1	4	I	0.0160						
N5	N		0.21802	0.30268	0.07051	1.000	1	4	A		0.0109	0.0111	0.0102	0.0116	-0.0007	0.0027
C15	C		0.12544	0.04908	0.31681	1.000	1	4	A		0.0156	0.0160	0.0177	0.0133	-0.0003	0.0027
H15A	H		0.18160	0.02860	0.36450	1.000	1	4	I	0.0190						
H15B	H		0.04630	-0.00380	0.30470	1.000	1	4	I	0.0190						

```
   C16      C          0.06048   0.16131   0.32281   1.000    1       4    A          0.0150  0.0162  0.0182  0.0109 -0.0001  0.0026
  H16A      H         -0.02210   0.15750   0.35070   1.000    1       4    I  0.0180
  H16B      H          0.13440   0.21000   0.34900   1.000    1       4    I  0.0180
    N6      N          0.01108   0.20279   0.24915   1.000    1       4    A          0.0132  0.0139  0.0153  0.0107  0.0018  0.0027
   C17      C         -0.06749   0.29232   0.23885   1.000    1       4    A          0.0121  0.0100  0.0144  0.0122 -0.0008  0.0029
   C18      C         -0.12388   0.34990   0.29532   1.000    1       4    A          0.0165  0.0175  0.0189  0.0145  0.0007  0.0067
  H18A      H         -0.10770   0.32400   0.34420   1.000    1       4    I  0.0200
   C19      C         -0.20162   0.44298   0.27885   1.000    1       4    A          0.0185  0.0163  0.0194  0.0214  0.0008  0.0081
  H19A      H         -0.23860   0.48160   0.31640   1.000    1       4    I  0.0220
   C20      C         -0.22608   0.48063   0.20679   1.000    1       4    A          0.0176  0.0138  0.0157  0.0237  0.0033  0.0040
  H20A      H         -0.27950   0.54460   0.19450   1.000    1       4    I  0.0210
   C21      C         -0.17043   0.42218   0.15435   1.000    1       4    A          0.0146  0.0113  0.0145  0.0177  0.0015  0.0008
  H21A      H         -0.18740   0.44750   0.10540   1.000    1       4    I  0.0180
    N7      N         -0.09288   0.33072   0.16832   1.000    1       4    A          0.0119  0.0103  0.0126  0.0129  0.0009  0.0016

 Unit cell: a = 9.33270  b = 12.45740  c = 18.49150  alpha = 90.000  beta = 98.527  gamma = 90.000  volume = 2126.081  Refine? False

 Spherical harmonics texture: Order:0

 Phase:  MNFE  in histogram:  HKLF mnfe_6489.fcf:mnfe_6489
-------------------------------------------------------------------------------------------------------------------------------------------
 Scale factor     :     0.9760  Refine? True

 Phase:  MNFE  in histogram:  HKLF mnfe_7062.fcf:mnfe_7062
-------------------------------------------------------------------------------------------------------------------------------------------
 Scale factor     :     0.8610  Refine? True

 Refinement results:
-------------------------------------------------------------------------------------------------------------------------------------------
 Number of function calls: 8  Number of observations:  2748  Number of parameters:  4
 Refinement time =   10.580s,   10.580s/cycle, for 1 cycles
 wR =   20.56%, chi**2 =      24958.8, reduced chi**2 =   9.10
-------------------------------------------------------------------------------------------------------------------------------------------
Variables generated by constraints

 name  :     ::constr:0     ::constr:1
 value :        -0.6395        -0.6994
 sig   :         0.0228         0.0209

 Phases:
 Result for phase:  MNFE

 Atoms:
   name      x         y         z      frac   Uiso     U11     U22     U33     U12     U13     U23
-------------------------------------------------------------------------------------------------------------------------------------------
    Fe1     Fe:
 values:   0.12023   0.14192   0.17699   0.952         0.00982 0.01001 0.01058-0.00003 0.00152 0.00139
 sig   :                               0.016
    Mn1     Mn:
 values:   0.12023   0.14192   0.17699   0.048         0.00982 0.01001 0.01058-0.00003 0.00152 0.00139
```

```
sig   :   0.00000   0.00000   0.00000   0.016         0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
   Mn2     Mn:
values:  -0.00631   0.25883   0.07634   0.995         0.00959 0.01168 0.01086-0.00078 0.00133 0.00001
sig   :                                 0.015
   Fe2     Fe:
values:  -0.00631   0.25883   0.07634   0.005         0.00959 0.01168 0.01086-0.00078 0.00133 0.00001
sig   :   0.00000   0.00000   0.00000   0.015         0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
   Cl1     Cl:
values:  -0.12383   0.36148  -0.02217   1.000         0.01501 0.02036 0.01515 0.00056-0.00074 0.00471
sig   :
    N1      N:
values:   0.22166   0.04633   0.25957   1.000         0.01240 0.01460 0.01450 0.00080 0.00240 0.00370
sig   :
    C1      C:
values:   0.23161  -0.05998   0.22441   1.000         0.01830 0.01340 0.02210 0.00340 0.00430 0.00480
sig   :
   H1A      H:
values:   0.24750  -0.11620   0.26260   1.000 0.02100
sig   :
   H1B      H:
values:   0.31570  -0.06040   0.19750   1.000 0.02100
sig   :
    C2      C:
values:   0.09306  -0.08579   0.17127   1.000         0.02170 0.01100 0.02160 0.00080 0.00540 0.00160
sig   :
   H2A      H:
values:   0.11210  -0.14450   0.13790   1.000 0.02100
sig   :
   H2B      H:
values:   0.01560  -0.10940   0.19890   1.000 0.02100
sig   :
    N2      N:
values:   0.04723   0.01058   0.12920   1.000         0.01620 0.01060 0.01600-0.00100 0.00260 0.00030
sig   :
    C3      C:
values:  -0.07226   0.00969   0.07943   1.000         0.01440 0.01270 0.01420-0.00220 0.00510-0.00300
sig   :
    C4      C:
values:  -0.15725  -0.08336   0.05910   1.000         0.02020 0.01400 0.02010-0.00560 0.00790-0.00620
sig   :
   H4A      H:
values:  -0.12570  -0.15150   0.07840   1.000 0.02100
sig   :
    C5      C:
values:  -0.28407  -0.07491   0.01192   1.000         0.01890 0.02090 0.02220-0.00830 0.00790-0.01130
sig   :
   H5A      H:
values:  -0.34260  -0.13660  -0.00010   1.000 0.02400
sig   :
    C6      C:
```

```
values:  -0.32768   0.02475  -0.01871   1.000         0.01390 0.02540 0.02070-0.00490 0.00230-0.00820
sig   :
   H6A      H:
values:  -0.41510   0.03190  -0.05200   1.000 0.02400
sig   :
    C7      C:
values:  -0.24024   0.11201   0.00077   1.000         0.01240 0.02000 0.01670-0.00190 0.00200-0.00400
sig   :
   H7A      H:
values:  -0.26880   0.17950  -0.02060   1.000 0.02000
sig   :
    N3      N:
values:  -0.11510   0.10725   0.04895   1.000         0.01180 0.01380 0.01340-0.00200 0.00280-0.00250
sig   :
    C8      C:
values:   0.36419   0.09772   0.28282   1.000         0.01280 0.02160 0.01600 0.00130-0.00020 0.00560
sig   :
   H8A      H:
values:   0.43290   0.04370   0.30700   1.000 0.02000
sig   :
   H8B      H:
values:   0.35360   0.15490   0.31880   1.000 0.02000
sig   :
    C9      C:
values:   0.42565   0.14638   0.21752   1.000         0.01120 0.01930 0.01730 0.00100 0.00110 0.00470
sig   :
   H9A      H:
values:   0.50480   0.19720   0.23510   1.000 0.01900
sig   :
   H9B      H:
values:   0.46560   0.08890   0.18940   1.000 0.01900
sig   :
    N4      N:
values:   0.30988   0.20232   0.17098   1.000         0.01030 0.01410 0.01320 0.00000 0.00150 0.00270
sig   :
   C10      C:
values:   0.33737   0.26247   0.11500   1.000         0.01090 0.01000 0.01240-0.00060 0.00240-0.00070
sig   :
   C11      C:
values:   0.47893   0.28458   0.09883   1.000         0.01070 0.01460 0.01720-0.00140 0.00270-0.00020
sig   :
  H11A      H:
values:   0.56150   0.25730   0.12960   1.000 0.01700
sig   :
   C12      C:
values:   0.49613   0.34531   0.03886   1.000         0.01310 0.01450 0.01870-0.00290 0.00620-0.00030
sig   :
  H12A      H:
values:   0.59040   0.35870   0.02730   1.000 0.01800
sig   :
```

```
   C13      C:
values:   0.37413   0.38748  -0.00533   1.000         0.01680 0.01440 0.01720-0.00150 0.00670 0.00260
sig   :
  H13A      H:
values:   0.38390   0.43070  -0.04670   1.000 0.01900
sig   :
   C14      C:
values:   0.23973   0.36447   0.01290   1.000         0.01400 0.01270 0.01440 0.00020 0.00380 0.00170
sig   :
  H14A      H:
values:   0.15710   0.39370  -0.01680   1.000 0.01600
sig   :
    N5      N:
values:   0.21802   0.30268   0.07051   1.000         0.01110 0.01020 0.01160-0.00070 0.00270 0.00060
sig   :
   C15      C:
values:   0.12544   0.04908   0.31681   1.000         0.01600 0.01770 0.01330-0.00030 0.00270 0.00520
sig   :
  H15A      H:
values:   0.18160   0.02860   0.36450   1.000 0.01900
sig   :
  H15B      H:
values:   0.04630  -0.00380   0.30470   1.000 0.01900
sig   :
   C16      C:
values:   0.06048   0.16131   0.32281   1.000         0.01620 0.01820 0.01090-0.00010 0.00260 0.00220
sig   :
  H16A      H:
values:  -0.02210   0.15750   0.35070   1.000 0.01800
sig   :
  H16B      H:
values:   0.13440   0.21000   0.34900   1.000 0.01800
sig   :
    N6      N:
values:   0.01108   0.20279   0.24915   1.000         0.01390 0.01530 0.01070 0.00180 0.00270 0.00100
sig   :
   C17      C:
values:  -0.06749   0.29232   0.23885   1.000         0.01000 0.01440 0.01220-0.00080 0.00290-0.00050
sig   :
   C18      C:
values:  -0.12388   0.34990   0.29532   1.000         0.01750 0.01890 0.01450 0.00070 0.00670-0.00230
sig   :
  H18A      H:
values:  -0.10770   0.32400   0.34420   1.000 0.02000
sig   :
   C19      C:
values:  -0.20162   0.44298   0.27885   1.000         0.01630 0.01940 0.02140 0.00080 0.00810-0.00440
sig   :
  H19A      H:
values:  -0.23860   0.48160   0.31640   1.000 0.02200
```

```
sig   :
   C20      C:
values:  -0.22608   0.48063   0.20679   1.000         0.01380 0.01570 0.02370 0.00330 0.00400-0.00180
sig   :
  H20A      H:
values:  -0.27950   0.54460   0.19450   1.000 0.02100
sig   :
   C21      C:
values:  -0.17043   0.42218   0.15435   1.000         0.01130 0.01450 0.01770 0.00150 0.00080 0.00000
sig   :
  H21A      H:
values:  -0.18740   0.44750   0.10540   1.000 0.01800
sig   :
    N7      N:
values:  -0.09288   0.33072   0.16832   1.000         0.01030 0.01260 0.01290 0.00090 0.00160-0.00020
sig   :

Phase:  MNFE  in histogram:  HKLF mnfe_6489.fcf:mnfe_6489
-------------------------------------------------------------------------------------------------------------------------
Final refinement RF, RF^2 = 7.28%, 6.11% on 1174 reflections
HKLF histogram weight factor =  1.000
Scale factor :     0.9758, sig     0.0065

Single crystal extinction: Type:  Lorentzian  Approx:  None


Phase:  MNFE  in histogram:  HKLF mnfe_7062.fcf:mnfe_7062
-------------------------------------------------------------------------------------------------------------------------
Final refinement RF, RF^2 = 9.49%, 7.60% on 1574 reflections
HKLF histogram weight factor =  1.000
Scale factor :     0.8611, sig     0.0055

Single crystal extinction: Type:  Lorentzian  Approx:  None
```