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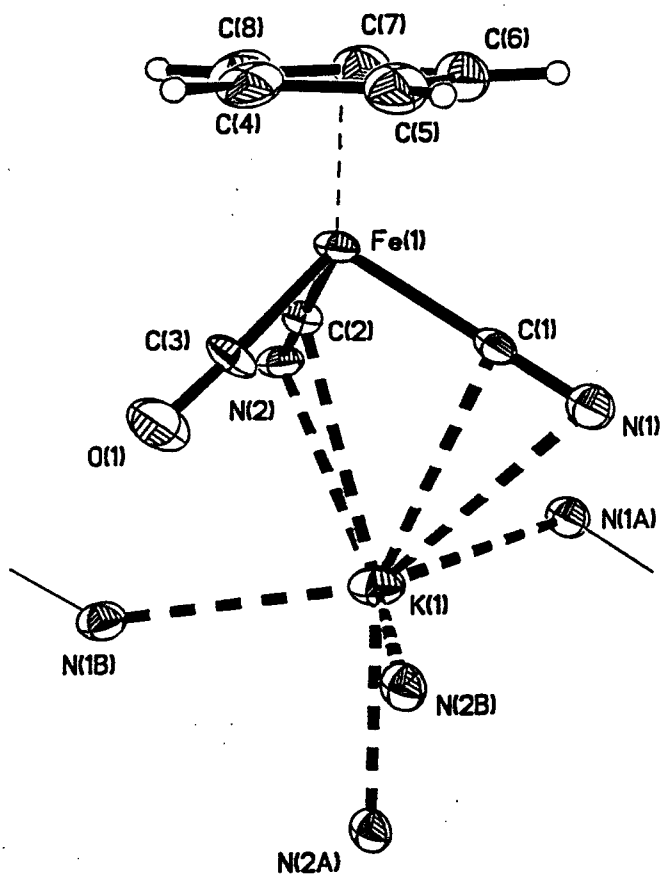
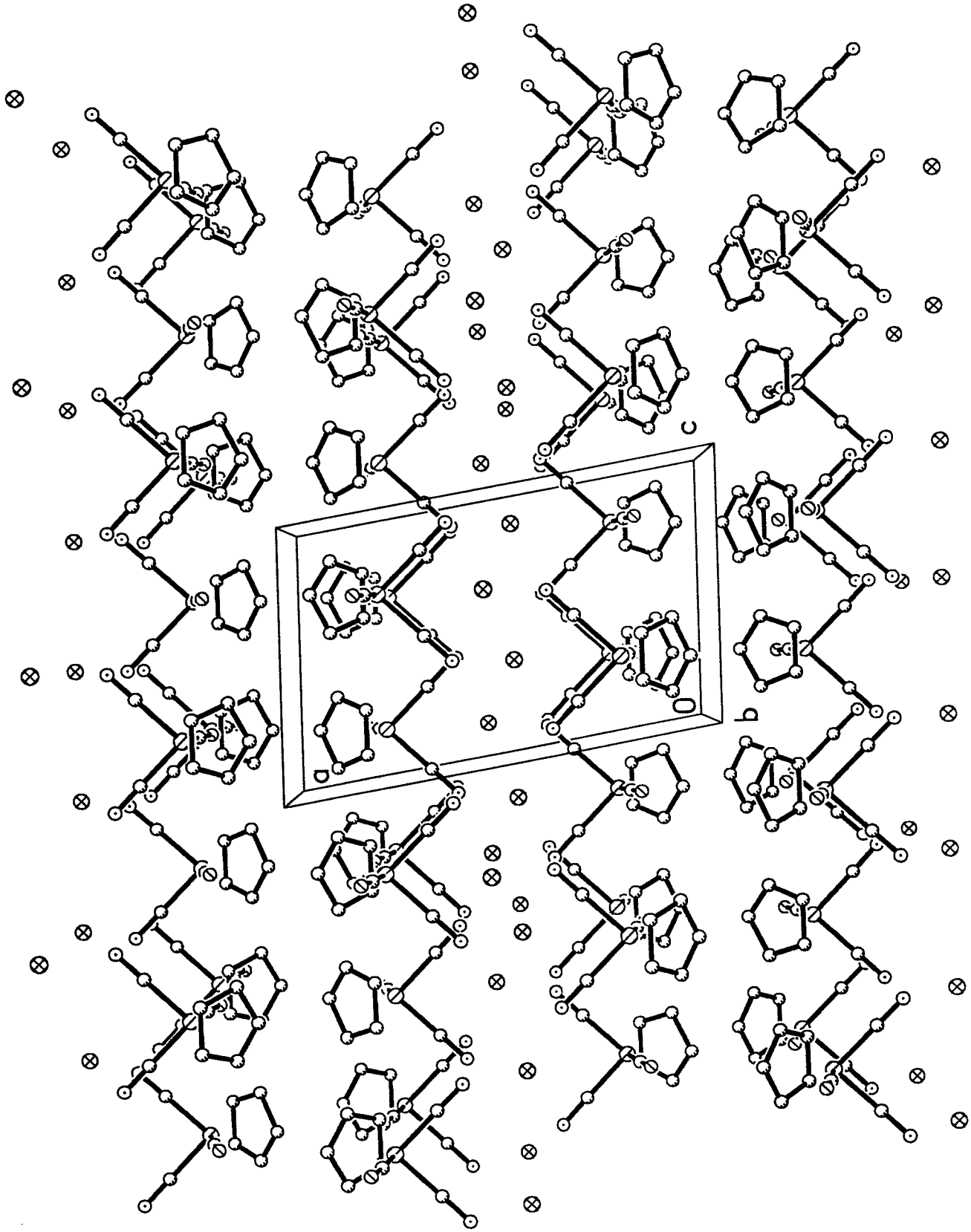
Supplementary Materials for $FeCp(CN)_2(CO)K$



Contents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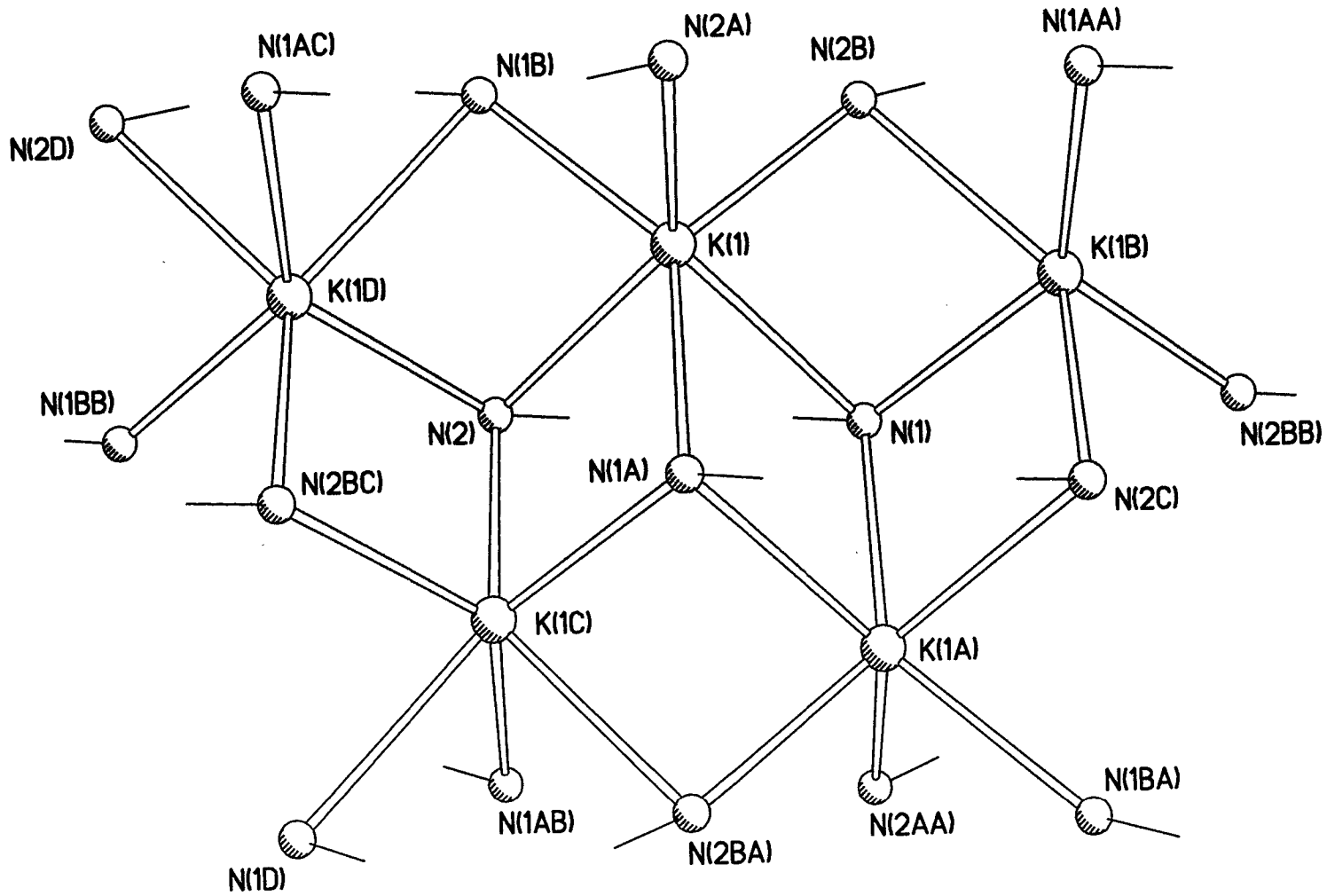

The crystals of $FeCp(CO)(CN)_2K$ were grown from ethanol. All of the crystals examined were small needles (widths ~0.02mm) and were extremely sensitive to moisture. Initially a crystal was selected and a cell determined at -80°C on a Siemens P4 sealed-tube diffractometer. The cell parameters were a=8.7254, b=7.8478, c=26.8272, α=90.000, β=99.115, γ=90.000, which is an *F* -superlattice of the cell a=8.7254, b=7.8478, c=13.4319, α=90.000, β=99.115, γ=90.000. A data set was collected and the structure solved in the supercell, however the structure failed to refine properly. The subcell was then chosen and the structure was solved and refined (disordered model) to R(F) ~ 8%. It was decided to recollect the data on a rotating anode, due to the small size and poor scattering power of the crystals.

A yellow needle (0.02 x 0.02 x 0.30mm) was mounted on a glass fiber at room temperature. Preliminary examination and data collection was performed on a Rigaku AFC5 rotating anode diffractometer (oriented graphite monochrometer; CuKa radiation) at 193(2) degK. Cell parameters were calculated from the least-squares fit for 25 high-angle reflections (2θ>45°).Omega scans for several intense reflections indicated acceptable crystal quality.

Data was collected for 6.66 to 120° 2θ at 193(2) K. Scan width for data collection was 1.42 +0.3tanθ° in ω with a fixed scan rate of 8 deg/min. Weak reflections were rescanned (maximum of two rescans and the counts for each scan were accumulated. The three standards, collected every 150 reflections, showed no significant trends. Background measurement by stationary crystal and stationary counter technique at the beginning and the end of each scan for 1/2 the total scan time. Lorentz and polarization corrections were applied to all reflections. A semi-empirical absorption correction was applied. A total of 866 unique reflections wit $I \geq 2\sigma(I)$ (Rint = 0.0445) were observed. The structure was solved by Direct Methods (Sheldrick, 1986). The final model was refined as a disordered structure with the CO and the Cp moieties disordered (50/50) between two positions related by a pseudo mirror plane. The Fe atom and the two CN ligands site on the pseudo mirror plane. Similarity restraints were applied to the Cp and CO moieties (Sheldick, 1993) as well as thermal parameter equality constraints placed on the equivalent atoms of the disordered Cp and CO moieties. Full-matrix least-squares anisotropic refinement for all non-Hydrogen atoms yielded $wR(F^2)[I \geq 2\sigma(I)] = 0.162$ and $R(F)[I \geq 2\sigma] = 0.066$ at convergence.(Sheldrick, 1993) Hydrogen atoms were placed in idealized positions with isotropic thermal parameters fixed at 1.5 times the attached atom. Neutral atom scattering factors and anomalous scattering factors were taken from the International Table for X-ray Crystallography Vol C.

Footnotes

Sheldrick, G. (1986) SHELXS-86 Program for Crystal Structure Solution, Institut fur Anorganische Chemie der Universitat, Tammanstrasse 4, D-3400 Gottingen, Germany.
Sheldrick, G. (1993) SHELXL-93 Program for Crystal Structure Refinement, Institut fur Anorganische Chemie der Universitat, Tammanstrasse 4, D-3400 Gottingen, Germany.

Table 1. Crystal data and structure refinement for 1.

Identification code	dd312
Empirical formula	$C_{16}H_{10}Fe_2K_2N_4O_2$
Formula weight	480.18
Temperature	193(2) K
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 13.442(3) Å alpha = 90° b = 7.852(2) Å beta = 99.60(3)° c = 8.731(2) Å gamma = 90°
Volume, Z	908.5(3) $Å^3$, 2
Density (calculated)	1.755 Mg/m^3
Absorption coefficient	17.070 mm^{-1}
F(000)	480
Crystal size	0.30 x 0.02 x 0.02 mm
θ range for data collection	3.33 to 60.07°
Limiting indices	$-15 \le h \le 14$, $-8 \le k \le 0$, $0 \le l \le 9$
Reflections collected	1460
Independent reflections	1354 (R_{int} = 0.0445)
Absorption correction	Psi-scan
Max. and min. transmission	0.9793 and 0.6410
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1323 / 48 / 179
Goodness-of-fit on F^2	1.022
Final R indices [$I>2\sigma(I)$]	R1 = 0.0655, wR2 = 0.1615
R indices (all data)	R1 = 0.1266, wR2 = 0.2401
Largest diff. peak and hole	1.909 and -0.528 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	2253(1)	25(2)	3075(2)	16(1)
K(1)	5327(1)	2779(3)	6358(2)	27(1)
N(1)	3913(6)	-95(9)	5942(9)	25(2)
N(2)	3843(5)	-327(9)	968(9)	22(2)
C(1)	3289(6)	-43(10)	4865(10)	18(2)
C(2)	3244(7)	-142(11)	1767(10)	21(2)
C(3)	2018(16)	-2136(26)	3051(26)	25(3)
O(1)	1817(11)	-3505(19)	3028(18)	38(2)
C(4)	701(21)	559(31)	2621(38)	34(3)
C(5)	1119(14)	1251(28)	4109(27)	36(3)
C(6)	1856(14)	2501(27)	3784(26)	32(3)
C(7)	1847(14)	2497(27)	2149(26)	30(2)
C(8)	1154(14)	1305(28)	1522(26)	35(3)
O(1′)	2175(11)	3597(18)	3018(18)	38(2)
C(3′)	2261(16)	2204(25)	3015(25)	25(3)
C(4′)	683(21)	-124(28)	2764(37)	34(3)
C(5′)	1098(14)	-941(28)	4155(27)	36(3)
C(6′)	1672(15)	-2360(29)	3727(27)	32(3)
C(7′)	1631(14)	-2357(27)	2112(27)	30(2)
C(8′)	1025(14)	-955(29)	1457(26)	35(3)

Table 3. Bond lengths [Å] and angles [°] for 1.

Fe(1)-C(3')	1.71(2)	Fe(1)-C(3)	1.73(2)
Fe(1)-C(2)	1.898(9)	Fe(1)-C(1)	1.913(9)
Fe(1)-C(4')	2.09(3)	Fe(1)-C(5')	2.09(2)
Fe(1)-C(8)	2.09(2)	Fe(1)-C(4)	2.10(3)
Fe(1)-C(5)	2.13(2)	Fe(1)-C(8')	2.13(2)
Fe(1)-C(6)	2.13(2)	Fe(1)-C(7)	2.14(2)
Fe(1)-C(6')	2.14(2)	Fe(1)-C(7')	2.16(2)
K(1)-N(2)#1	2.805(8)	K(1)-N(2)#2	2.887(8)
K(1)-N(1)#3	2.930(8)	K(1)-N(1)	2.934(8)
K(1)-N(2)#4	3.088(8)	K(1)-C(2)#4	3.099(9)
K(1)-C(1)#4	3.143(8)	K(1)-N(1)#4	3.194(8)
K(1)-C(2)#1	3.427(9)	K(1)-C(3)#4	3.56(2)
K(1)-C(1)	3.595(9)	K(1)-O(1)#4	3.83(2)
N(1)-C(1)	1.151(12)	N(1)-K(1)#5	2.930(8)
N(1)-K(1)#4	3.194(8)	N(2)-C(2)	1.159(11)
N(2)-K(1)#6	2.805(8)	N(2)-K(1)#7	2.887(8)
N(2)-K(1)#4	3.088(8)	C(1)-K(1)#4	3.143(8)
C(1)-K(1)#5	3.900(9)	C(2)-K(1)#4	3.099(9)
C(2)-K(1)#6	3.427(9)	C(2)-K(1)#7	3.942(9)
C(3)-O(1)	1.11(3)	C(3)-K(1)#4	3.56(2)
O(1)-K(1)#4	3.83(2)	C(4)-C(8)	1.35(4)
C(4)-C(5)	1.43(4)	C(5)-C(6)	1.46(3)
C(6)-C(7)	1.43(3)	C(6)-Fe(1)#1	4.17(2)
C(7)-C(8)	1.37(3)	C(7)-Fe(1)#6	4.17(2)
O(1')-C(3')	1.10(2)	C(4')-C(5')	1.40(4)
C(4')-C(8')	1.45(4)	C(5')-C(6')	1.44(3)
C(6')-C(7')	1.40(3)	C(6')-K(1)#4	4.06(2)
C(7')-C(8')	1.43(3)	C(7')-K(1)#4	4.10(2)

C(3')-Fe(1)-C(2)	92.4(7)	C(3)-Fe(1)-C(2)	94.1(8)
C(3')-Fe(1)-C(1)	92.6(8)	C(3)-Fe(1)-C(1)	95.1(8)
C(2)-Fe(1)-C(1)	90.1(4)	C(3')-Fe(1)-C(4')	93.6(9)
C(2)-Fe(1)-C(4')	135.6(9)	C(1)-Fe(1)-C(4')	133.4(9)
C(3')-Fe(1)-C(5')	112.7(9)	C(2)-Fe(1)-C(5')	153.6(7)
C(1)-Fe(1)-C(5')	96.6(7)	C(4')-Fe(1)-C(5')	39.3(9)
C(3)-Fe(1)-C(8)	110.9(10)	C(2)-Fe(1)-C(8)	97.7(6)
C(1)-Fe(1)-C(8)	152.1(7)	C(3)-Fe(1)-C(4)	91.1(10)
C(2)-Fe(1)-C(4)	132.5(9)	C(1)-Fe(1)-C(4)	136.4(9)
C(8)-Fe(1)-C(4)	37.7(10)	C(3)-Fe(1)-C(5)	107.9(9)
C(2)-Fe(1)-C(5)	155.7(7)	C(1)-Fe(1)-C(5)	98.1(7)
C(8)-Fe(1)-C(5)	65.1(8)	C(4)-Fe(1)-C(5)	39.6(10)
C(3')-Fe(1)-C(8')	110.4(10)	C(2)-Fe(1)-C(8')	96.9(6)
C(1)-Fe(1)-C(8')	155.5(7)	C(4')-Fe(1)-C(8')	40.3(10)
C(5')-Fe(1)-C(8')	67.4(8)	C(3)-Fe(1)-C(6)	147.6(9)
C(2)-Fe(1)-C(6)	118.2(6)	C(1)-Fe(1)-C(6)	88.4(6)
C(8)-Fe(1)-C(6)	64.3(8)	C(4)-Fe(1)-C(6)	65.4(9)
C(5)-Fe(1)-C(6)	39.9(8)	C(3)-Fe(1)-C(7)	148.6(10)
C(2)-Fe(1)-C(7)	89.8(6)	C(1)-Fe(1)-C(7)	116.1(6)
C(8)-Fe(1)-C(7)	37.8(8)	C(4)-Fe(1)-C(7)	64.2(8)
C(5)-Fe(1)-C(7)	66.0(8)	C(6)-Fe(1)-C(7)	39.0(8)
C(3')-Fe(1)-C(6')	152.4(9)	C(2)-Fe(1)-C(6')	115.0(7)
C(1)-Fe(1)-C(6')	90.4(6)	C(4')-Fe(1)-C(6')	65.1(8)
C(5')-Fe(1)-C(6')	39.7(8)	C(8')-Fe(1)-C(6')	65.4(8)
C(3')-Fe(1)-C(7')	149.0(9)	C(2)-Fe(1)-C(7')	88.4(6)
C(1)-Fe(1)-C(7')	118.4(6)	C(4')-Fe(1)-C(7')	65.4(9)

C(5')-Fe(1)-C(7')	66.0(8)
C(6')-Fe(1)-C(7')	38.0(8)
N(2)#1-K(1)-N(1)#3	80.6(2)
N(2)#1-K(1)-N(1)	95.8(2)
N(1)#3-K(1)-N(1)	132.02(13)
N(2)#2-K(1)-N(2)#4	136.0(3)
N(1)-K(1)-N(2)#4	76.0(2)
N(2)#2-K(1)-C(2)#4	116.0(2)
N(1)-K(1)-C(2)#4	83.3(2)
N(2)#1-K(1)-C(1)#4	153.5(2)
N(1)#3-K(1)-C(1)#4	121.1(2)
N(2)#4-K(1)-C(1)#4	70.8(2)
N(2)#1-K(1)-N(1)#4	133.6(2)
N(1)#3-K(1)-N(1)#4	141.0(3)
N(2)#4-K(1)-N(1)#4	87.2(2)
C(1)#4-K(1)-N(1)#4	20.9(2)
N(2)#2-K(1)-C(2)#1	102.3(2)
N(1)-K(1)-C(2)#1	84.6(2)
C(2)#4-K(1)-C(2)#1	138.73(12)
N(1)#4-K(1)-C(2)#1	140.8(2)
N(2)#2-K(1)-C(3)#4	71.3(4)
N(1)-K(1)-C(3)#4	121.5(4)
C(2)#4-K(1)-C(3)#4	46.4(4)
N(1)#4-K(1)-C(3)#4	65.1(4)
N(2)#1-K(1)-C(1)	85.0(2)
N(1)#3-K(1)-C(1)	141.7(2)
N(2)#4-K(1)-C(1)	92.7(2)
C(1)#4-K(1)-C(1)	85.0(2)
C(2)#1-K(1)-C(1)	77.6(2)
N(2)#1-K(1)-O(1)#4	125.9(3)
N(1)#3-K(1)-O(1)#4	66.2(3)
N(2)#4-K(1)-O(1)#4	76.1(3)
C(1)#4-K(1)-O(1)#4	60.9(3)
C(2)#1-K(1)-O(1)#4	136.2(3)
C(1)-K(1)-O(1)#4	145.9(3)
C(1)-N(1)-K(1)	116.2(6)
C(1)-N(1)-Fe(1)	0.3(5)
K(1)-N(1)-Fe(1)	116.5(3)
K(1)#5-N(1)-K(1)#4	91.4(2)
Fe(1)-N(1)-K(1)#4	76.8(2)
C(2)-N(2)-K(1)#7	151.2(7)
C(2)-N(2)-Fe(1)	2.0(5)
K(1)#7-N(2)-Fe(1)	149.4(3)
K(1)#6-N(2)-K(1)#4	101.1(2)
Fe(1)-N(2)-K(1)#4	78.6(2)
N(1)-C(1)-K(1)#4	82.0(6)
N(1)-C(1)-K(1)	47.1(5)
K(1)#4-C(1)-K(1)	95.0(2)
Fe(1)-C(1)-K(1)#5	151.9(4)
K(1)-C(1)-K(1)#5	74.7(2)
N(2)-C(2)-K(1)#4	78.7(6)
N(2)-C(2)-K(1)#6	49.0(5)
K(1)#4-C(2)-K(1)#6	88.4(2)
Fe(1)-C(2)-K(1)#7	156.4(4)
K(1)#6-C(2)-K(1)#7	69.6(2)
O(1)-C(3)-K(1)#4	95.8(14)
C(3)-O(1)-Fe(1)	2.1(12)
Fe(1)-O(1)-K(1)#4	69.6(3)
C(8)-C(4)-Fe(1)	70.8(14)
C(8')-Fe(1)-C(7')	39.0(8)
N(2)#1-K(1)-N(2)#2	84.1(2)
N(2)#2-K(1)-N(1)#3	98.6(2)
N(2)#2-K(1)-N(1)	128.9(2)
N(2)#1-K(1)-N(2)#4	134.13(11)
N(1)#3-K(1)-N(2)#4	73.3(2)
N(2)#1-K(1)-C(2)#4	154.9(2)
N(1)#3-K(1)-C(2)#4	81.6(2)
N(2)#4-K(1)-C(2)#4	21.6(2)
N(2)#2-K(1)-C(1)#4	78.1(2)
N(1)-K(1)-C(1)#4	80.8(2)
C(2)#4-K(1)-C(1)#4	51.2(2)
N(2)#2-K(1)-N(1)#4	72.3(2)
N(1)-K(1)-N(1)#4	71.5(2)
C(2)#4-K(1)-N(1)#4	69.9(2)
N(2)#1-K(1)-C(2)#1	18.2(2)
N(1)#3-K(1)-C(2)#1	77.8(2)
N(2)#4-K(1)-C(2)#1	117.2(2)
C(1)#4-K(1)-C(2)#1	161.0(2)
N(2)#1-K(1)-C(3)#4	142.7(4)
N(1)#3-K(1)-C(3)#4	76.0(4)
N(2)#4-K(1)-C(3)#4	64.8(4)
C(1)#4-K(1)-C(3)#4	46.8(4)
C(2)#1-K(1)-C(3)#4	151.6(4)
N(2)#2-K(1)-C(1)	115.0(2)
N(1)-K(1)-C(1)	16.7(2)
C(2)#4-K(1)-C(1)	98.5(2)
N(1)#4-K(1)-C(1)	70.7(2)
C(3)#4-K(1)-C(1)	130.6(4)
N(2)#2-K(1)-O(1)#4	61.7(3)
N(1)-K(1)-O(1)#4	138.2(3)
C(2)#4-K(1)-O(1)#4	60.5(3)
N(1)#4-K(1)-O(1)#4	76.6(3)
C(3)#4-K(1)-O(1)#4	16.7(4)
C(1)-N(1)-K(1)#5	141.8(7)
K(1)#5-N(1)-K(1)	101.9(2)
K(1)#5-N(1)-Fe(1)	141.6(3)
C(1)-N(1)-K(1)#4	77.1(6)
K(1)-N(1)-K(1)#4	108.5(2)
C(2)-N(2)-K(1)#6	112.9(6)
K(1)#6-N(2)-K(1)#7	95.9(2)
K(1)#6-N(2)-Fe(1)	114.7(3)
C(2)-N(2)-K(1)#4	79.8(6)
K(1)#7-N(2)-K(1)#4	94.4(2)
N(1)-C(1)-Fe(1)	179.5(8)
Fe(1)-C(1)-K(1)#4	97.6(3)
Fe(1)-C(1)-K(1)	133.3(4)
N(1)-C(1)-K(1)#5	27.7(5)
K(1)#4-C(1)-K(1)#5	76.2(2)
N(2)-C(2)-Fe(1)	176.8(8)
Fe(1)-C(2)-K(1)#4	99.4(3)
Fe(1)-C(2)-K(1)#6	133.9(4)
N(2)-C(2)-K(1)#7	20.6(5)
K(1)#4-C(2)-K(1)#7	76.0(2)
O(1)-C(3)-Fe(1)	177(2)
Fe(1)-C(3)-K(1)#4	87.7(8)
C(3)-O(1)-K(1)#4	67.5(13)
C(8)-C(4)-C(5)	109(2)
C(5)-C(4)-Fe(1)	71.2(14)

C(4)-C(5)-C(6)	105(2)	C(4)-C(5)-Fe(1)	69.1(14)
C(6)-C(5)-Fe(1)	70.3(12)	C(7)-C(6)-C(5)	108(2)
C(7)-C(6)-Fe(1)	70.6(13)	C(5)-C(6)-Fe(1)	69.8(12)
C(7)-C(6)-Fe(1)#1	151.4(14)	C(5)-C(6)-Fe(1)#1	97.3(13)
Fe(1)-C(6)-Fe(1)#1	133.1(8)	C(8)-C(7)-C(6)	107(2)
C(8)-C(7)-Fe(1)	69.2(12)	C(6)-C(7)-Fe(1)	70.4(13)
C(8)-C(7)-Fe(1)#6	98.9(14)	C(6)-C(7)-Fe(1)#6	150.8(14)
Fe(1)-C(7)-Fe(1)#6	133.2(8)	C(4)-C(8)-C(7)	112(2)
C(4)-C(8)-Fe(1)	72(2)	C(7)-C(8)-Fe(1)	73.1(13)
C(3')-O(1')-Fe(1)	4.2(12)	O(1')-C(3')-Fe(1)	173(2)
C(5')-C(4')-C(8')	110(2)	C(5')-C(4')-Fe(1)	70.5(14)
C(8')-C(4')-Fe(1)	71.5(14)	C(4')-C(5')-C(6')	106(2)
C(4')-C(5')-Fe(1)	70.2(14)	C(6')-C(5')-Fe(1)	72.1(12)
C(7')-C(6')-C(5')	109(2)	C(7')-C(6')-Fe(1)	71.7(13)
C(5')-C(6')-Fe(1)	68.1(12)	C(7')-C(6')-K(1)#4	81.6(12)
C(5')-C(6')-K(1)#4	130.1(13)	Fe(1)-C(6')-K(1)#4	70.0(5)
C(6')-C(7')-C(8')	109(2)	C(6')-C(7')-Fe(1)	70.3(13)
C(8')-C(7')-Fe(1)	69.4(12)	C(6')-C(7')-K(1)#4	78.6(12)
C(8')-C(7')-K(1)#4	131.6(13)	Fe(1)-C(7')-K(1)#4	69.1(5)
C(7')-C(8')-C(4')	105(2)	C(7')-C(8')-Fe(1)	71.7(12)
C(4')-C(8')-Fe(1)	68.2(14)		

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1/2,z+1/2 #2 -x+1,y+1/2,-z+1/2 #3 -x+1,y+1/2,-z+3/2

#4 -x+1,-y,-z+1 #5 -x+1,y-1/2,-z+3/2 #6 x,-y+1/2,z-1/2

#7 -x+1,y-1/2,-z+1/2

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 1.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
Fe(1)	11(1)	11(1)	28(1)	0(1)	5(1)	1(1)
K(1)	20(1)	25(1)	37(1)	4(1)	6(1)	5(1)
N(1)	18(4)	22(4)	35(4)	-4(4)	2(3)	-1(3)
N(2)	17(3)	19(4)	29(4)	3(3)	2(3)	5(3)
C(1)	14(4)	12(4)	28(4)	-5(4)	5(3)	1(4)
C(2)	20(4)	18(4)	23(4)	-4(4)	0(3)	4(4)
C(3)	33(7)	16(6)	27(6)	-7(7)	9(6)	6(6)
O(1)	43(6)	22(5)	49(6)	-5(5)	7(5)	4(5)
C(4)	15(4)	38(8)	50(6)	0(7)	7(4)	7(7)
C(5)	25(5)	37(6)	48(6)	-1(6)	9(5)	5(5)
C(6)	25(5)	25(5)	45(6)	-1(6)	2(5)	-1(5)
C(7)	21(5)	24(5)	45(6)	-2(6)	7(5)	-2(5)
C(8)	19(5)	38(6)	46(6)	0(6)	2(5)	6(5)
O(1')	43(6)	22(5)	49(6)	-5(5)	7(5)	4(5)
C(3')	33(7)	16(6)	27(6)	-7(7)	9(6)	6(6)
C(4')	15(4)	38(8)	50(6)	0(7)	7(4)	7(7)
C(5')	25(5)	37(6)	48(6)	-1(6)	9(5)	5(5)
C(6')	25(5)	25(5)	45(6)	-1(6)	2(5)	-1(5)
C(7')	21(5)	24(5)	45(6)	-2(6)	7(5)	-2(5)
C(8')	19(5)	38(6)	46(6)	0(6)	2(5)	6(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(4A)	186(21)	-297(31)	2436(38)	51
H(5A)	950(14)	955(28)	5101(27)	54
H(6A)	2273(14)	3202(27)	4533(26)	48
H(7A)	2251(14)	3196(27)	1591(26)	45
H(8A)	1004(14)	1034(28)	435(26)	52
H(4'A)	239(21)	840(28)	2686(37)	51
H(5'B)	1017(14)	-617(28)	5187(27)	54
H(6'A)	2026(15)	-3177(29)	4434(27)	48
H(7'A)	1957(14)	-3167(27)	1538(27)	45
H(8'A)	876(14)	-632(29)	383(26)	52

S12

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wR and all goodnesses of fit S are based on F^2^, conventional R-factors R
are based on F, with F set to zero for negative F^2^. The observed criterion
of F^2^ > 2sigma(F^2^) is used only for calculating _R_factor_obs etc. and is
not relevant to the choice of reflections for refinement.  R-factors based
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C3' Fe1 C7' 149.0(9) . . ?
C2 Fe1 C7' 88.4(6) . . ?
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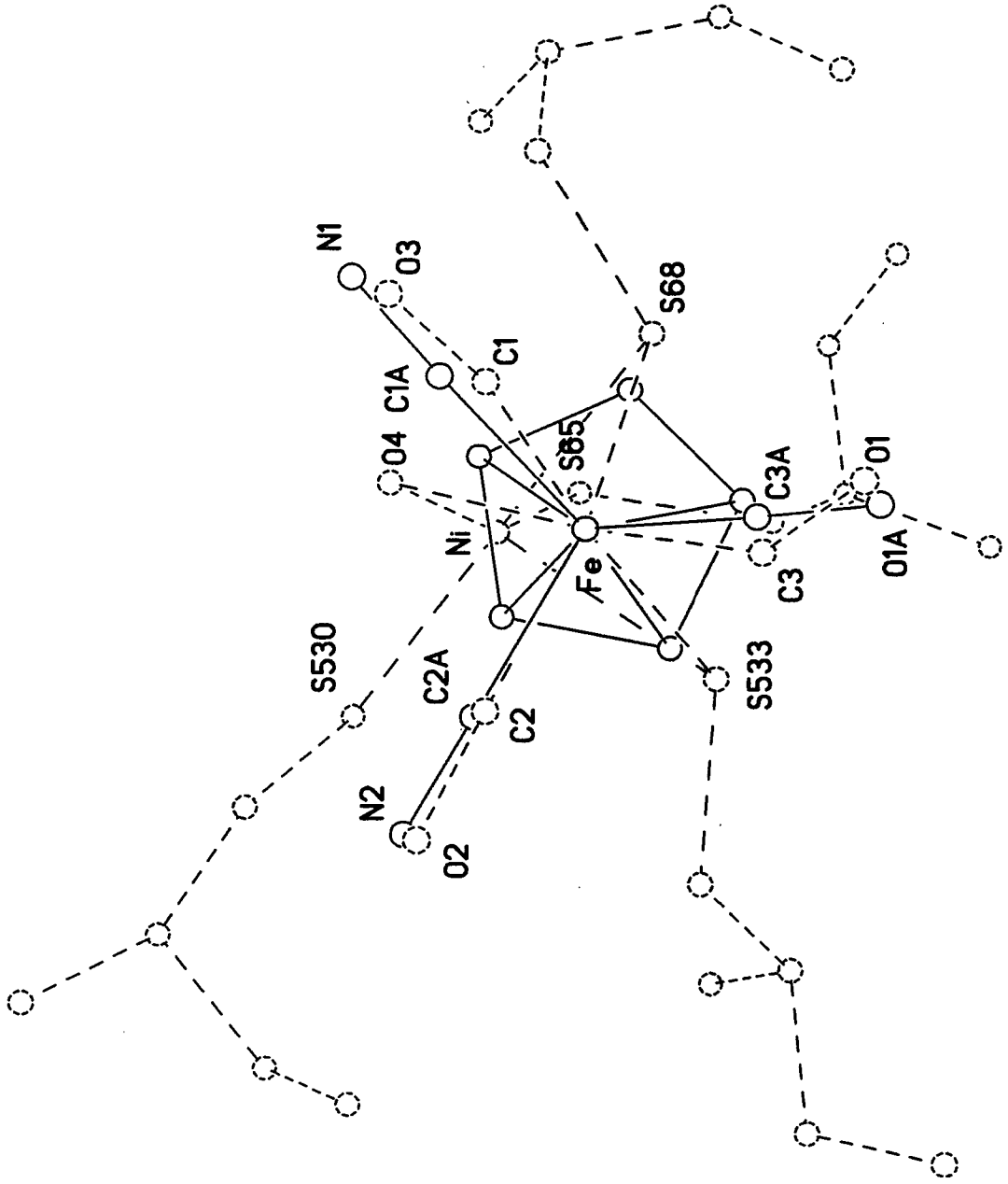
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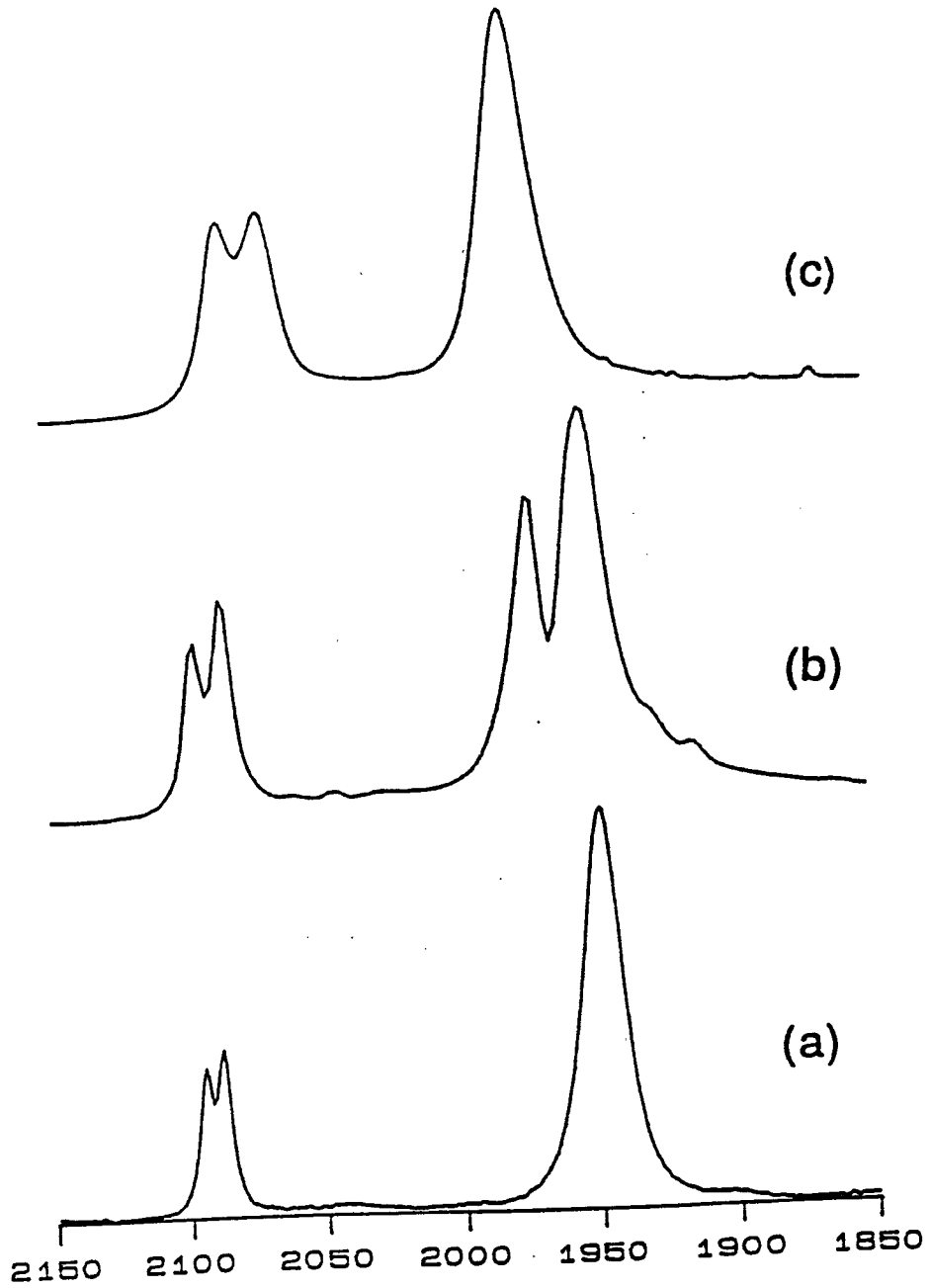

Figure 1S. Infrared spectra of $K[(\eta^5\text{-}C_5H_5)Fe(CN)_2(CO)]$ in the ν_{CN} and ν_{CO} region: (a) CH_3CN, (b) KBr, and (c) H_2O.