Inorganic Chemistry
including bioinorganic chemistry
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Characterization Data

General Considerations. Melting points were determined in sealed capillary tubes under N_2 and are uncorrected. NMR spectra were recorded at ambient temperatures. Chemical shifts (d) are given relative to residual protium in the deuterated solvent at 7.15 for C_6D_6. IR samples were prepared as mineral oil mulls and taken between KBr plates. Elemental analyses were determined within the College of Chemistry, University of California, Berkeley. Single crystal X-ray structure determinations were performed at CHEXRAY, University of California, Berkeley.

FcC(NCy)NHCy. Mp: 109.5 - 111.0 °C. ^{1}H NMR (C_6D_6, 300 MHz): δ 4.63 (d, J = 6.8 Hz, 1H), 4.28 (t, J = 1.8 Hz, 2H), 4.18 (m, 1H), 3.99 (s, 5H), 3.93 (t, J = 1.8 Hz, 2H), 3.55 (m, 1H), 2.21 (m, 2H), 1.80-1.10 (m, 18H). ^{13}C{^{1}H} NMR (C_6D_6, 75.5 MHz): δ 151.3, 81.4, 69.5, 69.4, 68.2, 58.3, 48.9, 36.5, 33.7, 26.5, 25.3. IR (KBr) 3420 (m), 1619 (vs), 1490 (s), 1301 (w), 1256 (w), 1181 (w), 1156 (w), 1106 (w), 1023 (w), 1003 (w), 888 (w), 830 (m), 722 (w), 568 (w), 488 (w) cm^{-1}. Anal. Calcd for $C_{23}H_{32}N_2Fe$: C, 70.41; H, 8.22; N, 7.14. Found: C, 70.41; H, 8.46; N, 7.05.

[FcC(NCy)$_2$Li(Et$_2$O)]$_2$. Mp: 225 - 230 °C. ^{1}H NMR (C_6D_6, 300 MHz): δ 5.0 - 4.1 (br, 9H), 3.26 (q, 4H), 2.6 - 1.2 (br, 22H), 1.11 (t, 6H). IR (KBr) 1492 (s), 1342 (m), 1305 (w), 1153 (w), 1106 (w), 1064 (w), 1024 (w), 1002 (w), 982 (w), 888 (w), 818 (m), 742 (w), 722 (w), 498 (w), 473 (w) cm^{-1}. Anal. Calcd for $C_{27}H_{41}N_2FeLiO$: C, 68.65; H, 8.75; N, 5.93. Found: C, 68.89; H, 8.62; N, 5.82.

[FcC(NCy)$_2$]$_2$Fe•(Et$_2$O)$_{0.25}$. Mp: 216 - 218 °C. Anal. Calcd for $C_{47}H_{64.5}Fe_3N_4O_{0.25}$: C, 65.86; H, 7.58; N, 6.54. Found: C, 65.69; H, 7.52; N, 6.48. μ_{eff} = 5.02 μ_B.

[FcC(NCy)$_2$]$_2$Co•(Et$_2$O). Mp: 203-207 °C. Anal. Calcd for $C_{50}H_{72}CoFe_2N_4O$: C, 65.58; H, 7.92; N, 6.12. Found: C, 65.42; H, 7.55 N, 6.29. μ_{eff} = 4.62 μ_B.

X-ray Crystallography. Table 1 lists a summary of crystallographic data for all structurally characterized compounds.

General Procedure. A crystal of appropriate size was mounted[1] on a glass capillary using Paratone-N hydrocarbon oil. The crystal was transferred to a Siemens SMART diffractometer/CCD area detector,[2] centered in the beam, and cooled to by nitrogen-flow low-temperature apparatus which had been previously calibrated by a thermocouple placed at the same position as the crystal. Preliminary orientation matrix and cell constants were determined by collection of 60 10-second frames, followed by spot integration and least-squares refinement. A hemisphere of data was collected then the raw data were integrated (XY spot spread = 1.60°; Z spot spread = 0.60°) using SAINT.[3] Cell dimensions reported in Table 1 were calculated from all reflections with I > 10σ. Data analysis and absorption correction were performed using Siemens XPREP.[4] The data were corrected for Lorentz and polarization effects, but no correction for

crystal decay was applied. The reflections measured (θ = 3-45°) were averaged. The structure was solved and refined with the teXsan[5] software package using direct methods[6] and expanded using Fourier techniques.[7] All non-hydrogen atoms were refined anisotropically. Hydrogens were included in structure factor calculations, but were not refined. The disordered Et_2O molecule in the structure of $[FcC(NCy)_2]_2Fe\cdot(Et_2O)_{0.25}$ was located in a diffrence Fourier along the 4-fold axis. The oxygen and two methyl carbons were refined isotropically, with their x and y coordinates constrained at the symmetry site. The two methylene carbons were input at calculated positions and were included in structure factor calculations, but their positions were not refined.The final residuals were refined against the data for which $F^2 > 3\sigma(F^2)$.[8] The quantity minimized by the least squares program was $\Sigma_w(|F_o|-|F_c|)^2$, where w is the weight of a given observation. The p-factor,[8] used to reduce the weight of intense reflections was set to 0.03 throughout the refinement. The analytical forms of the scattering factor tables for the neutral atoms were used[9] and all scattering factors were corrected for both the real and imaginary components of anomalous dispersion.[10] Pertinent details for individual compounds can be found in Table 1.

References

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4. XPREP: Part of the SHELXTL Crystal-Structure Determination Package; Siemens Industrial Automation: Madison, WI, 1994.
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8. $R = [\Sigma||F_o| - |F_c||]/\Sigma|F_o|$, $R_w = \{[\Sigma_w(|F_o| - |F_c|)^2]/\Sigma_w F_o^2\}^{1/2}$, GOF = $\{[\Sigma_w(|F_o| - |F_c|)^2]/(n_o - n_v)\}^{1/2}$, where n_o is the number of observations, n_v the number of variable parameters, and the weights w were given by: $w = 1/\sigma^2(F_o)$, $\sigma(F_o^2) = [\sigma_o^2(F_o^2) +$

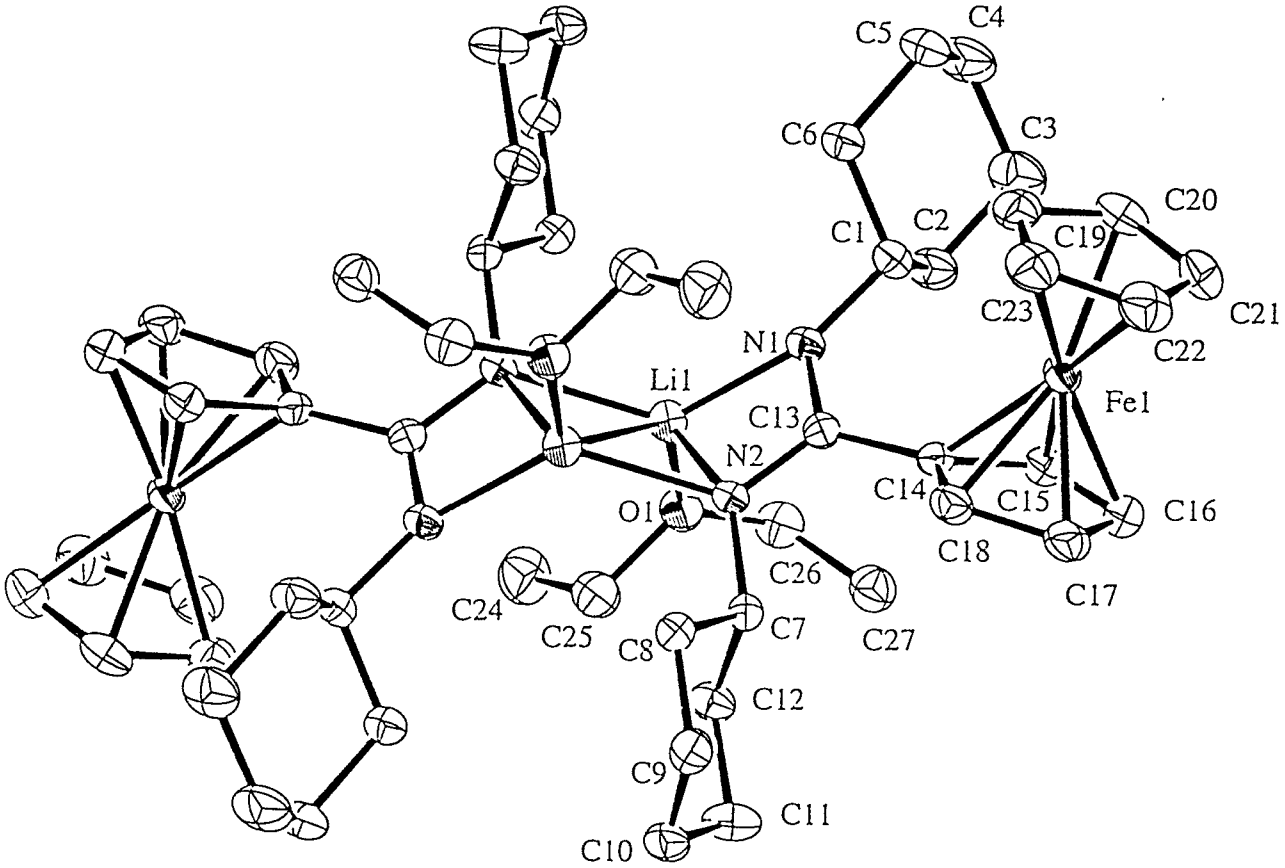
$(pF_o^2)^2]^{1/2}$, where $\sigma^2(F_o)$ is calculated as above from $\sigma(F_o)^2$ and where p is the factor used to lower the weight of intense reflections.

9. Cromer, D. T.; Waber, J. T. *International Tables for X-Ray Crystallography*, The Kynoch Press: Birmingham, England, 1974; Vol. IV; Table 2.2B.
10. Cromer, D. T.; Waber, J. T. *ibid.* ; Table 2.3.1.

Table 1. Crystal Data and Collection Parameters

	$\{[FcC(NCy)_2]Li(Et_2O)\}_2$	$[FcC(NCy)_2]_2Co\cdot(Et_2O)$	$[FcC(NCy)_2]_2Fe\cdot(Et_2O)_{0.25}$
formula	$C_{27}H_{41}FeN2OLi$	$C_{50}H_{72}N_4OFe_2Co$	$C_{47}H_{64.5}N_4OFe_3$
formula wt	472.42	915.77	857.09
space group	P-1 (#2)	$P2_12_12_1$	P4/n (#85)
temp (°C)	-115	-108	-114
a (Å)	10.4093(4)	12.0209(2)	27.2009(3)
b (Å)	10.7630(4)	12.1029(1)	
c (Å)	11.9734(5)	32.8484(7)	11.5815(2)
V ($Å^3$)	1251.1(2)	4779.0(2)	8569.0(4)
α (deg)	92.859(1)	90	90
β (deg)	108.411(1)	90	90
γ (deg)	98.749(1)	90	90
Z	2	4	8
d_{calc} (g/cm^3)	1.254	1.273	1.329
diffractometer	Siemens SMART	Siemens SMART	Siemens SMART
radiation	Mo-Kα	Mo-Kα	Mo-Kα
monochromator	graphite	graphite	graphite

detector	CCD area detector	CCD area detector	CCD area detector
scan type, deg	ω, 0.3	ω, 0.3	ω, 0.3
frame collection time (s)	30	20	30
reflections measured	hemisphere	hemisphere	hemisphere
2θ range (deg)	3-46.5	3-46.5	3-46.5
μ (cm^{-1})	6.23	9.806	10.39
T_{min}, T_{max}	0.912, 0.937	0.653, 0.871	0.744, 0.859
crystal dimensions (mm)	0.14 X 0.15 X 0.07	0.31 X 0.36 X 0.14	0.24 X 0.17 X 0.17
no. of refls measured	5100	20072	35467
no. of uniquie refls	3452	3892	6912
no. of observations ($I > 3\sigma$)	3001	5365	3693
no. of parameters	289	523	486
R_{int} (%)	3.07	6.90	6.60
R (%)	3.78	3.77	3.39
R_w (%)	5.81	4.82	3.92
GOF	2.17	1.27	1.21


C5
C4
C6
C3
C1
C2
C19
C20
C23
C21
C22
N1
Li1
Fe1
C13
N2
C14
C15
C16
O1
C18
C17
C26
C24
C25
C8
C7
C27
C12
C9
C11
C10

Anisotropic Thermal Parameters for $[FeC(NCy)_2Li(Et_2O)]_2$

atom	U11	U22	U33	U12	U13	U23
Fe(1)	0.0241(3)	0.0218(3)	0.0229(3)	0.0038(2)	0.0076(2)	0.0062(2)
O(1)	0.038(1)	0.022(1)	0.027(1)	0.007(1)	0.013(1)	0.001(1)
N(1)	0.019(1)	0.023(1)	0.024(1)	-0.000(1)	0.009(1)	0.005(1)
N(2)	0.021(1)	0.021(1)	0.021(1)	-0.001(1)	0.007(1)	0.004(1)
C(1)	0.021(2)	0.022(2)	0.025(2)	0.004(1)	0.009(1)	0.006(1)
C(2)	0.027(2)	0.030(2)	0.036(2)	0.000(1)	0.016(1)	0.001(1)
C(3)	0.038(2)	0.045(2)	0.048(2)	0.003(2)	0.028(2)	0.003(2)
C(4)	0.030(2)	0.049(2)	0.056(3)	-0.005(2)	0.021(2)	0.011(2)
C(5)	0.036(2)	0.029(2)	0.041(2)	-0.007(2)	0.010(2)	0.009(2)
C(6)	0.025(2)	0.026(2)	0.028(2)	-0.000(1)	0.008(1)	0.005(1)
C(7)	0.020(2)	0.025(2)	0.019(2)	0.001(1)	0.006(1)	0.004(1)
C(8)	0.025(2)	0.028(2)	0.022(2)	-0.001(1)	0.007(1)	0.002(1)
C(9)	0.022(2)	0.041(2)	0.026(2)	0.002(1)	0.011(1)	0.002(1)
C(10)	0.020(2)	0.036(2)	0.034(2)	-0.004(1)	0.007(1)	0.008(2)
C(11)	0.029(2)	0.022(2)	0.052(2)	-0.001(1)	0.014(2)	-0.001(2)
C(12)	0.024(2)	0.027(2)	0.032(2)	0.002(1)	0.014(1)	0.004(1)
C(13)	0.025(2)	0.015(2)	0.020(2)	0.004(1)	0.009(1)	-0.001(1)
C(14)	0.020(2)	0.022(2)	0.020(2)	-0.001(1)	0.007(1)	0.000(1)
C(15)	0.028(2)	0.023(2)	0.025(2)	0.003(1)	0.008(1)	0.003(1)
C(16)	0.038(2)	0.030(2)	0.023(2)	-0.001(2)	0.005(1)	0.003(1)
C(17)	0.029(2)	0.026(2)	0.037(2)	0.002(1)	0.001(2)	0.013(2)
C(18)	0.023(2)	0.030(2)	0.030(2)	0.002(1)	0.011(1)	0.007(1)
C(19)	0.037(2)	0.019(2)	0.034(2)	0.003(1)	0.007(2)	0.002(1)
C(20)	0.038(2)	0.021(2)	0.046(2)	0.003(1)	0.020(2)	0.011(2)
C(21)	0.048(2)	0.031(2)	0.034(2)	0.005(2)	0.013(2)	0.014(2)
C(22)	0.037(2)	0.030(2)	0.049(2)	0.012(2)	0.010(2)	0.014(2)
C(23)	0.045(2)	0.023(2)	0.043(2)	0.010(2)	0.017(2)	0.004(2)
C(24)	0.056(2)	0.035(2)	0.043(2)	0.016(2)	0.011(2)	0.009(2)
C(25)	0.041(2)	0.030(2)	0.033(2)	0.004(2)	0.017(2)	0.001(1)
C(26)	0.033(2)	0.030(2)	0.034(2)	0.007(1)	0.016(2)	-0.000(1)
C(27)	0.040(2)	0.030(2)	0.030(2)	0.005(2)	0.016(2)	0.002(1)
Li(1)	0.027(3)	0.027(3)	0.023(3)	0.003(2)	0.008(2)	0.004(2)

Positional parameters and B(eq) for $[FcC(NCy)_2Li(Et_2O)]_2$.

atom	x	y	z	B(eq)
Fe(1)	0.72438(4)	0.22486(4)	0.89583(4)	1.81(2)
O(1)	0.4002(2)	0.6894(2)	0.6211(2)	2.22(8)
N(1)	0.4550(2)	0.3875(2)	0.6651(2)	1.76(9)
N(2)	0.6391(2)	0.4928(2)	0.6260(2)	1.67(9)
C(1)	0.3847(3)	0.3039(3)	0.7274(3)	1.7(1)
C(2)	0.3037(3)	0.3764(3)	0.7871(3)	2.4(1)
C(3)	0.2190(4)	0.2909(4)	0.8461(3)	3.2(1)
C(4)	0.1198(4)	0.1851(4)	0.7576(4)	3.5(1)
C(5)	0.1971(4)	0.1104(3)	0.6967(3)	2.9(1)
C(6)	0.2833(3)	0.1972(3)	0.6404(3)	2.1(1)
C(7)	0.7789(3)	0.5692(3)	0.6701(3)	1.7(1)
C(8)	0.8624(3)	0.5404(3)	0.5919(3)	2.1(1)
C(9)	1.0084(3)	0.6162(3)	0.6374(3)	2.3(1)
C(10)	1.0100(3)	0.7580(3)	0.6533(3)	2.5(1)
C(11)	0.9202(3)	0.7896(3)	0.7264(3)	2.8(1)
C(12)	0.7746(3)	0.7110(3)	0.6773(3)	2.1(1)
C(13)	0.5906(3)	0.4205(3)	0.6976(3)	1.6(1)
C(14)	0.6902(3)	0.3872(3)	0.8106(3)	1.7(1)
C(15)	0.6801(3)	0.4013(3)	0.9269(3)	2.0(1)
C(16)	0.8061(4)	0.3849(3)	1.0100(3)	2.5(1)
C(17)	0.8961(3)	0.3599(3)	0.9479(3)	2.6(1)
C(18)	0.8237(3)	0.3596(3)	0.8255(3)	2.1(1)
C(19)	0.5937(4)	0.0683(3)	0.7973(3)	2.5(1)
C(20)	0.5757(4)	0.0838(3)	0.9099(3)	2.7(1)
C(21)	0.7041(4)	0.0807(3)	0.9969(3)	3.0(1)
C(22)	0.8000(4)	0.0628(3)	0.9379(3)	3.1(1)
C(23)	0.7309(4)	0.0561(3)	0.8154(3)	2.8(1)
C(24)	0.3199(4)	0.8581(4)	0.5022(3)	3.6(1)
C(25)	0.4397(4)	0.7960(3)	0.5644(3)	2.7(1)
C(26)	0.3831(3)	0.7216(3)	0.7327(3)	2.5(1)
C(27)	0.5109(4)	0.7239(3)	0.8364(3)	2.6(1)
Li(1)	0.4314(5)	0.5289(5)	0.5609(4)	2.0(2)
H(1)	0.859	0.343	0.763	2.4
H(2)	0.602	0.419	0.945	2.4
H(3)	0.525	0.067	0.723	2.9
H(4)	0.988	0.346	0.982	3.2
H(5)	0.827	0.390	1.093	3.0
H(6)	0.894	0.056	0.975	3.8
H(7)	0.771	0.045	0.755	3.5
H(8)	0.493	0.094	0.924	3.2
H(9)	0.723	0.089	1.080	3.5
H(10)	0.824	0.549	0.747	2.0
H(11)	0.450	0.269	0.786	2.2
H(12)	1.056	0.590	0.712	2.9
H(13)	1.054	0.600	0.582	2.9
H(14)	0.223	0.234	0.579	2.6
H(15)	0.334	0.148	0.608	2.6
H(16)	0.914	0.877	0.725	3.4
H(17)	0.961	0.773	0.806	3.4

H(18)	0.367	0.439	0.846	3.0
H(19)	0.243	0.416	0.729	3.0
H(20)	0.867	0.453	0.590	2.6
H(21)	0.818	0.560	0.514	2.6
H(22)	0.731	0.733	0.600	2.8
H(23)	0.724	0.729	0.728	2.8
H(24)	0.280	0.255	0.908	3.9
H(25)	0.168	0.340	0.878	3.9
H(26)	1.102	0.800	0.692	3.1
H(27)	0.977	0.787	0.578	3.1
H(28)	0.132	0.050	0.637	3.7
H(29)	0.256	0.068	0.754	3.7
H(30)	0.074	0.130	0.798	4.1
H(31)	0.054	0.221	0.700	4.1
H(32)	0.537	0.643	0.838	3.0
H(33)	0.583	0.785	0.829	3.0
H(34)	0.494	0.745	0.908	3.0
H(35)	0.280	0.886	0.558	4.2
H(36)	0.351	0.928	0.467	4.2
H(37)	0.253	0.799	0.443	4.2
H(38)	0.358	0.803	0.733	3.2
H(39)	0.311	0.661	0.742	3.2
H(40)	0.506	0.856	0.623	3.3
H(41)	0.479	0.768	0.508	3.3

Intramolecular Distances Involving the Nonhydrogen Atoms for $[Fe(NC_2)_2Li(4l,0)]_2$

atom	atom	distance	ADC(*)	atom	atom	distance	ADC(*)
FE1	C14	2.088(3)	1	C3	C4	1.522(5)	1
FE1	C15	2.065(3)	1	C4	C5	1.528(6)	1
FE1	C16	2.036(3)	1	C5	C6	1.524(4)	1
FE1	C17	2.028(3)	1	C7	C8	1.515(4)	1
FE1	C18	2.024(3)	1	C7	C12	1.533(5)	1
FE1	C19	2.042(3)	1	C8	C9	1.526(4)	1
FE1	C20	2.050(3)	1	C9	C10	1.525(5)	1
FE1	C21	2.041(3)	1	C10	C11	1.529(5)	1
FE1	C22	2.042(3)	1	C11	C12	1.535(5)	1
FE1	C23	2.033(4)	1	C13	C14	1.519(4)	1
O1	C25	1.433(4)	1	C14	C15	1.432(4)	1
O1	C26	1.435(4)	1	C14	C18	1.423(5)	1
O1	LI1	1.951(6)	1	C15	C16	1.416(5)	1
N1	C1	1.455(4)	1	C16	C17	1.413(5)	1
N1	C13	1.325(4)	1	C17	C18	1.420(5)	1
N1	LI1	2.010(6)	1	C19	C20	1.424(5)	1
N2	C7	1.476(4)	1	C19	C23	1.403(5)	1
N2	C13	1.348(4)	1	C20	C21	1.418(5)	1
N2	LI1	2.158(6)	1	C21	C22	1.422(5)	1
N2	LI1	2.111(6)	66602	C22	C23	1.407(5)	1
C1	C2	1.534(5)	1	C24	C25	1.508(5)	1
C1	C6	1.528(4)	1	C26	C27	1.502(5)	1
C2	C3	1.528(5)	1				

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intermolecular Bond Angles Involving the Nonhydrogen Atoms

atom	atom	atom	angle	atom	atom	atom	angle
C18	FE1	C17	41.0(1)	C16	FE1	C19	163.1(1)
C18	FE1	C23	106.3(1)	C16	FE1	C20	124.9(1)
C18	FE1	C16	68.3(1)	C16	FE1	C15	40.4(1)
C18	FE1	C21	156.9(1)	C16	FE1	C14	68.2(1)
C18	FE1	C22	120.6(1)	C21	FE1	C22	40.8(1)
C18	FE1	C19	123.0(1)	C21	FE1	C19	68.2(1)
C18	FE1	C20	160.3(1)	C21	FE1	C20	40.6(1)
C18	FE1	C15	67.8(1)	C21	FE1	C15	123.6(1)
C18	FE1	C14	40.5(1)	C21	FE1	C14	160.5(1)
C17	FE1	C23	118.8(2)	C22	FE1	C19	68.0(1)
C17	FE1	C16	40.7(1)	C22	FE1	C20	68.4(1)
C17	FE1	C21	120.4(1)	C22	FE1	C15	156.7(1)
C17	FE1	C22	103.1(1)	C22	FE1	C14	158.5(1)
C17	FE1	C19	156.1(2)	C19	FE1	C20	40.7(1)
C17	FE1	C20	158.5(1)	C19	FE1	C15	128.2(1)
C17	FE1	C15	68.3(1)	C19	FE1	C14	111.2(1)
C17	FE1	C14	68.7(1)	C20	FE1	C15	111.5(1)
C23	FE1	C16	154.4(2)	C20	FE1	C14	126.0(1)
C23	FE1	C21	68.2(1)	C15	FE1	C14	40.3(1)
C23	FE1	C22	40.4(1)	C25	O1	C26	114.4(2)
C23	FE1	C19	40.3(1)	C25	O1	LI1	114.5(2)
C23	FE1	C20	68.2(1)	C26	O1	LI1	128.2(2)
C23	FE1	C15	162.7(1)	C13	N1	C1	123.6(2)
C23	FE1	C14	124.8(1)	C13	N1	LI1	90.6(2)
C16	FE1	C21	106.4(1)	C1	N1	LI1	142.8(2)
C16	FE1	C22	119.2(1)	C13	N2	C7	120.5(2)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intermolecular Bond Angles Involving the Nonhydrogen Atoms cont

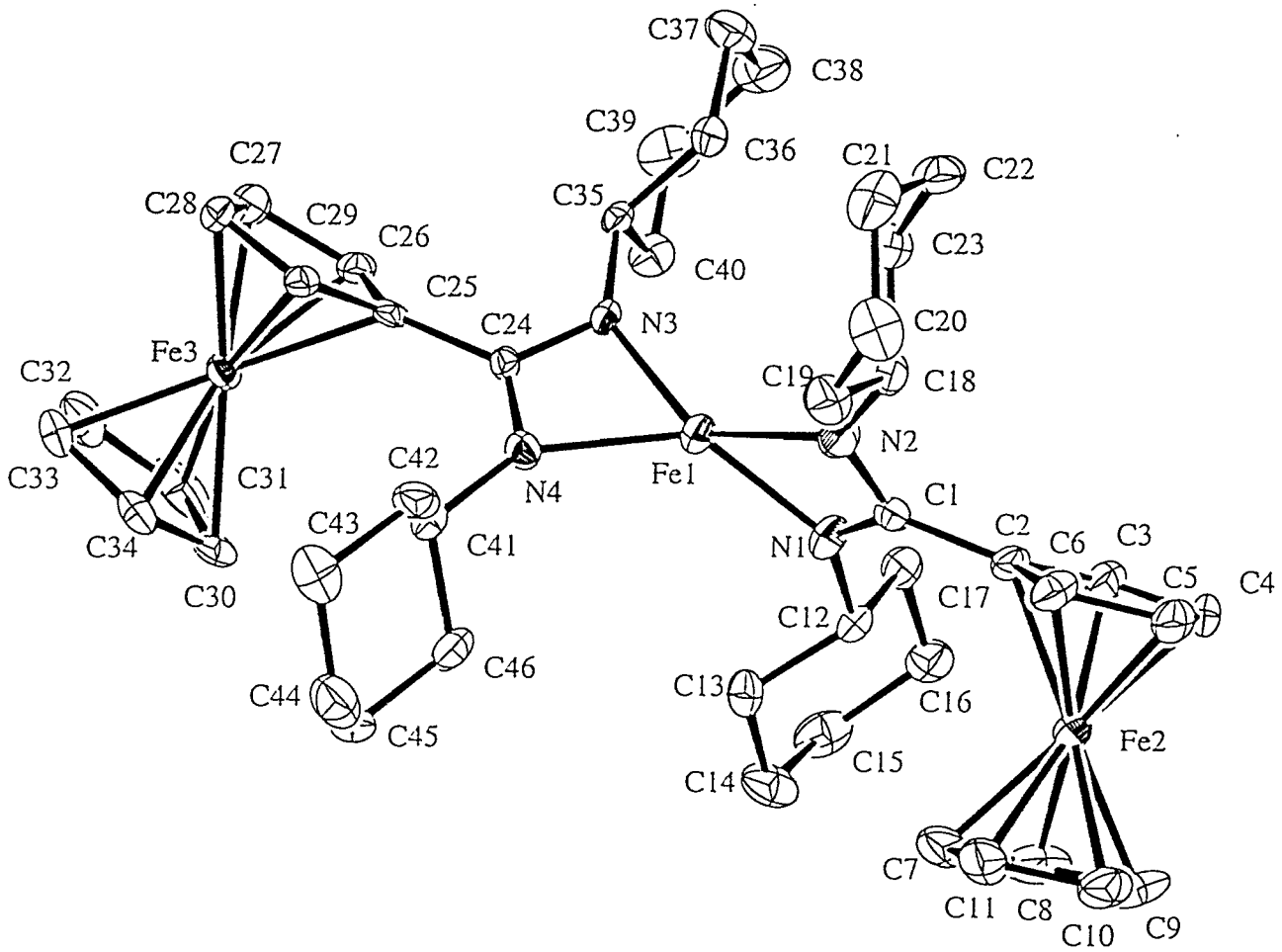
atom	atom	atom	angle	atom	atom	atom	angle
C13	N2	LI1	126.9(2)	C18	C14	FE1	67.3(2)
C13	N2	LI1	83.9(2)	C15	C14	C13	126.5(3)
C7	N2	LI1	109.7(2)	C15	C14	FE1	69.0(2)
C7	N2	LI1	136.6(2)	C13	C14	FE1	137.0(2)
LI1	N2	LI1	70.4(2)	C16	C15	C14	108.7(3)
N1	C1	C6	110.0(2)	C16	C15	FE1	68.7(2)
N1	C1	C2	110.6(3)	C14	C15	FE1	70.7(2)
C6	C1	C2	108.2(3)	C17	C16	C15	108.5(3)
C3	C2	C1	112.8(3)	C17	C16	FE1	69.3(2)
C4	C3	C2	111.2(3)	C15	C16	FE1	70.9(2)
C3	C4	C5	110.6(3)	C16	C17	C18	107.1(3)
C6	C5	C4	111.2(3)	C16	C17	FE1	69.9(2)
C5	C6	C1	113.6(3)	C18	C17	FE1	69.3(2)
N2	C7	C8	111.1(2)	C17	C18	C14	109.6(3)
N2	C7	C12	111.5(2)	C17	C18	FE1	69.6(2)
C8	C7	C12	109.1(2)	C14	C18	FE1	72.2(2)
C7	C8	C9	112.0(3)	C23	C19	C20	108.3(3)
C10	C9	C8	112.1(3)	C23	C19	FE1	69.5(2)
C9	C10	C11	111.9(3)	C20	C19	FE1	69.9(2)
C10	C11	C12	111.6(3)	C21	C20	C19	107.2(3)
C7	C12	C11	111.1(3)	C21	C20	FE1	69.4(2)
N1	C13	N2	115.9(3)	C19	C20	FE1	69.3(2)
N1	C13	C14	124.4(3)	C20	C21	C22	108.1(3)
N2	C13	C14	119.6(3)	C20	C21	FE1	70.1(2)
C18	C14	C15	106.1(3)	C22	C21	FE1	69.7(2)
C18	C14	C13	126.4(3)	C23	C22	C21	107.7(3)

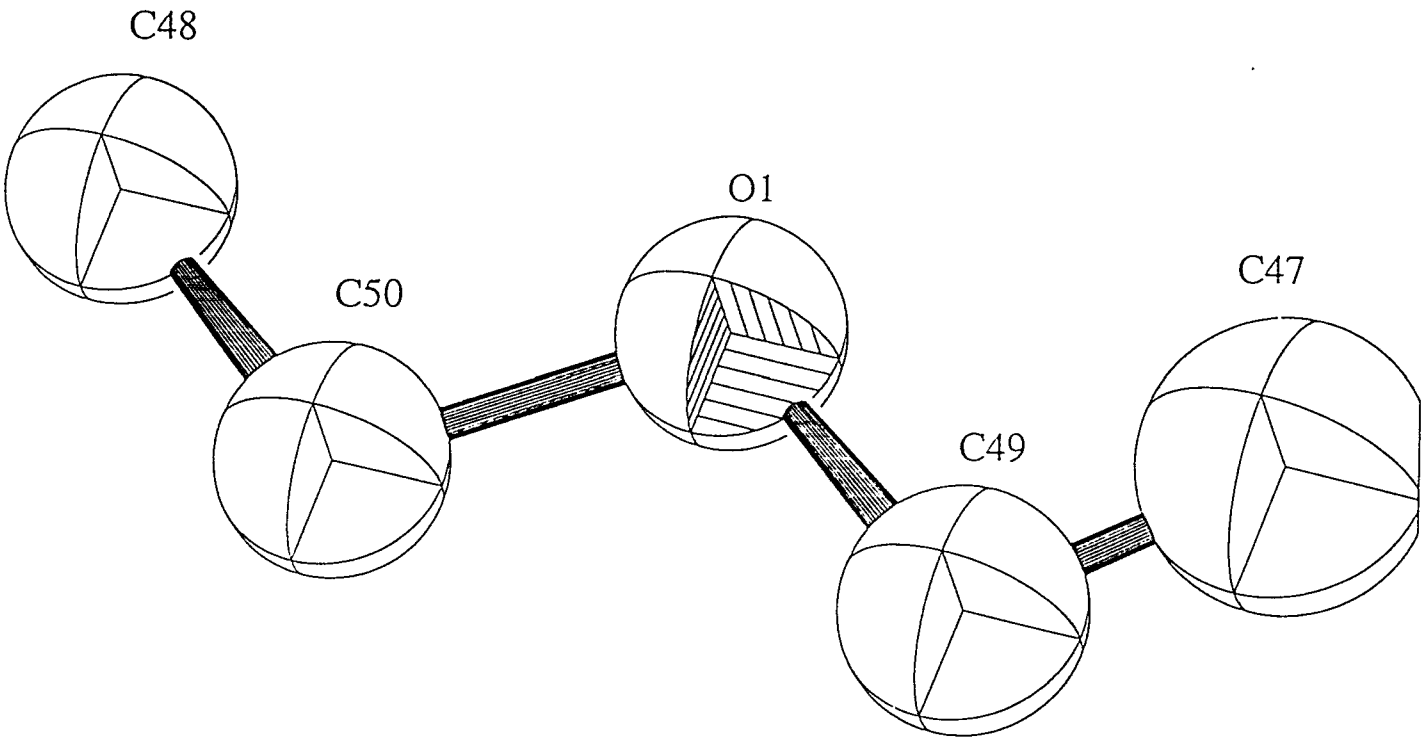
Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

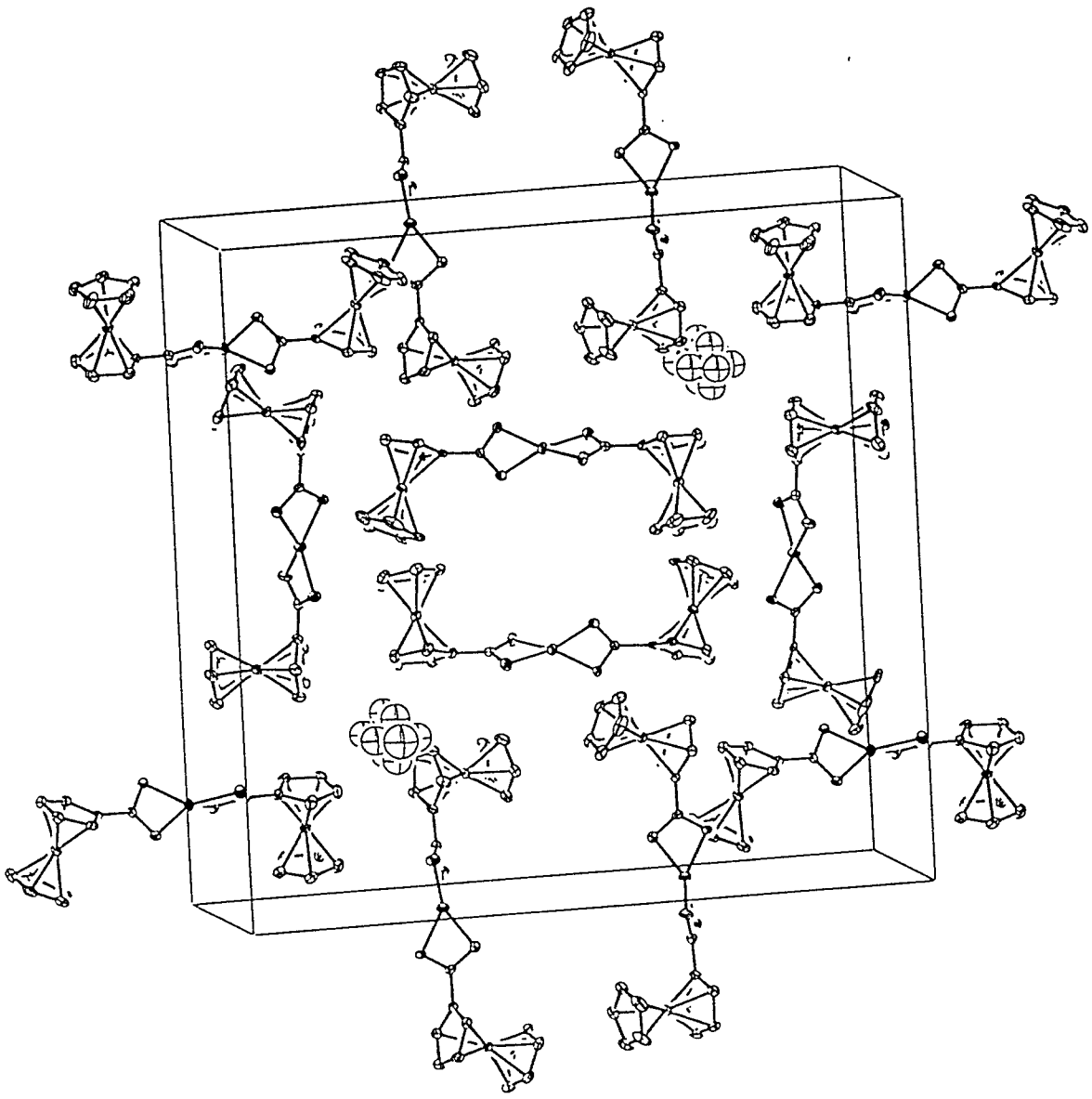
Intermolecular Bond Angles Involving the Nonhydrogen Atoms cont

atom	atom	atom	angle	atom	atom	atom	angle
C23	C22	FE1	69.5(2)				
C21	C22	FE1	69.6(2)				
C19	C23	C22	108.7(3)				
C19	C23	FE1	70.2(2)				
C22	C23	FE1	70.1(2)				
O1	C25	C24	112.6(3)				
O1	C26	C27	113.2(3)				
O1	LI1	N1	119.5(3)				
O1	LI1	N2	110.7(3)				
O1	LI1	N2	116.3(3)				
N1	LI1	N2	125.6(3)				
N1	LI1	N2	65.8(2)				
N2	LI1	N2	109.6(2)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.


C37
C38
C39
C36
C21
C22
C27
C28
C29
C26
C35
C23
C40
C25
C24
N3
C20
Fe3
C19
C18
C32
N2
C42
C33
C31
N4
Fe1
C1
C43
C41
N1
C2
C6
C3
C34
C5
C4
C30
C12
C17
C46
C13
C16
C44
Fe2
C45
C15
C14
C7
C11
C8
C10
C9


C48
O1
C47
C50
C49



Anisotropic Thermal Parameters for $[FcC(NCy)_2]_2Fe\cdot(Et_2O)_{0.25}$.

atom	U11	U22	U33	U12	U13	U23
Fe(1)	0.0243(4)	0.0150(4)	0.0250(5)	0.0005(3)	-0.0018(3)	0.0037(3)
Fe(2)	0.0204(4)	0.0171(4)	0.0288(5)	0.0030(3)	-0.0005(4)	0.0018(3)
Fe(3)	0.0178(4)	0.0178(4)	0.0207(4)	-0.0039(3)	-0.0008(3)	-0.0004(3)
N(1)	0.031(2)	0.016(2)	0.024(3)	0.005(2)	0.002(2)	0.002(2)
N(2)	0.030(2)	0.021(2)	0.025(3)	-0.001(2)	-0.006(2)	0.000(2)
N(3)	0.019(2)	0.015(2)	0.025(3)	0.001(2)	0.002(2)	0.006(2)
N(4)	0.017(2)	0.021(2)	0.025(3)	-0.000(2)	0.003(2)	0.002(2)
C(1)	0.015(2)	0.019(3)	0.024(3)	-0.000(2)	-0.000(2)	0.000(2)
C(2)	0.020(2)	0.015(2)	0.027(3)	0.004(2)	-0.004(2)	-0.000(2)
C(3)	0.023(3)	0.022(3)	0.031(4)	0.005(2)	0.003(2)	0.006(2)
C(4)	0.024(3)	0.019(3)	0.052(4)	-0.004(2)	-0.000(3)	0.016(3)
C(5)	0.033(3)	0.015(3)	0.042(4)	0.000(2)	-0.009(3)	-0.002(3)
C(6)	0.032(3)	0.025(3)	0.026(3)	0.006(2)	-0.009(3)	0.001(2)
C(7)	0.020(3)	0.023(3)	0.078(5)	0.005(2)	-0.002(3)	-0.004(3)
C(8)	0.033(3)	0.042(4)	0.050(5)	0.015(3)	-0.014(3)	-0.013(3)
C(9)	0.043(3)	0.036(3)	0.040(4)	0.022(3)	-0.020(3)	-0.004(3)
C(10)	0.032(3)	0.023(3)	0.054(4)	0.009(2)	-0.011(3)	-0.004(3)
C(11)	0.021(3)	0.026(3)	0.065(5)	0.007(2)	0.011(3)	0.000(3)
C(12)	0.022(3)	0.015(2)	0.019(3)	0.003(2)	-0.001(2)	0.003(2)
C(13)	0.029(3)	0.025(3)	0.024(3)	-0.003(2)	0.006(3)	0.004(2)
C(14)	0.026(3)	0.037(3)	0.043(4)	-0.004(3)	-0.009(3)	-0.014(3)
C(15)	0.044(3)	0.028(3)	0.036(4)	0.012(2)	-0.007(3)	-0.008(3)
C(16)	0.026(3)	0.030(3)	0.029(4)	0.007(2)	0.007(2)	0.002(3)
C(17)	0.026(3)	0.019(3)	0.031(4)	0.002(2)	0.001(3)	-0.002(3)
C(18)	0.030(3)	0.018(2)	0.022(3)	-0.006(2)	-0.006(2)	0.005(2)
C(19)	0.032(3)	0.037(3)	0.036(4)	-0.003(3)	0.004(3)	0.001(3)
C(20)	0.049(4)	0.042(3)	0.027(4)	-0.007(3)	0.009(3)	-0.012(3)
C(21)	0.068(4)	0.036(3)	0.021(3)	-0.008(3)	-0.020(3)	-0.001(3)
C(22)	0.030(3)	0.033(3)	0.042(4)	0.001(3)	-0.016(3)	0.004(3)
C(23)	0.028(3)	0.031(3)	0.028(3)	-0.000(2)	0.001(3)	0.003(3)
C(24)	0.017(2)	0.014(2)	0.018(3)	-0.003(2)	-0.003(2)	0.002(2)
C(25)	0.012(2)	0.015(2)	0.026(3)	-0.002(2)	-0.007(2)	-0.006(2)
C(26)	0.017(2)	0.022(3)	0.020(3)	0.000(2)	-0.004(2)	0.000(2)
C(27)	0.023(3)	0.018(2)	0.032(3)	0.001(2)	-0.000(3)	-0.001(2)
C(28)	0.022(3)	0.019(3)	0.024(3)	-0.001(2)	-0.005(2)	0.008(2)
C(29)	0.015(2)	0.023(3)	0.018(3)	-0.002(2)	-0.003(2)	0.004(2)
C(30)	0.019(3)	0.037(3)	0.034(4)	-0.011(2)	-0.015(3)	0.005(3)
C(31)	0.037(3)	0.066(4)	0.022(4)	-0.030(3)	-0.001(3)	-0.017(3)
C(32)	0.034(3)	0.025(3)	0.054(4)	-0.012(2)	0.001(3)	-0.011(3)
C(33)	0.023(3)	0.028(3)	0.043(4)	-0.011(2)	0.004(3)	0.009(3)
C(34)	0.018(3)	0.029(3)	0.035(4)	-0.009(2)	0.002(2)	0.001(2)
C(35)	0.018(2)	0.016(2)	0.015(3)	0.002(2)	-0.001(2)	0.005(2)
C(36)	0.022(2)	0.017(2)	0.028(3)	-0.001(2)	-0.000(2)	0.001(2)
C(37)	0.021(3)	0.041(3)	0.042(4)	-0.001(2)	0.001(3)	-0.001(3)
C(38)	0.031(3)	0.054(4)	0.036(4)	0.011(3)	0.009(3)	0.008(3)
C(39)	0.043(3)	0.044(4)	0.032(4)	0.013(3)	0.003(3)	-0.011(3)
C(40)	0.030(3)	0.028(3)	0.025(3)	0.002(2)	-0.002(3)	-0.002(3)
C(41)	0.022(3)	0.016(2)	0.029(3)	0.002(2)	-0.000(2)	0.004(2)
C(42)	0.018(3)	0.023(3)	0.044(4)	0.004(2)	-0.002(3)	-0.004(3)
C(43)	0.036(3)	0.033(3)	0.040(4)	-0.005(3)	0.011(3)	-0.011(3)
C(44)	0.027(3)	0.031(3)	0.072(5)	-0.002(2)	0.009(3)	-0.003(3)
C(45)	0.018(3)	0.032(3)	0.061(5)	0.003(2)	-0.005(3)	0.012(3)
C(46)	0.033(3)	0.023(3)	0.033(4)	0.007(2)	-0.001(3)	0.011(3)

Positional parameters and B(eq) for $[FcC(NCy)_2]_2Fe\cdot(Et_2O)_{0.25}$.

atom	x	y	z	B(eq)
Fe(1)	0.84168(2)	0.02089(2)	0.73758(6)	1.69(3)
Fe(2)	0.89681(2)	-0.16176(2)	0.91701(7)	1.74(3)
Fe(3)	0.88751(2)	0.22324(2)	0.65508(6)	1.48(3)
O(1)	1/4	1/4	0.570(1)	9.2(3)
N(1)	0.8541(1)	-0.0269(1)	0.8686(4)	1.9(2)
N(2)	0.8275(1)	-0.0514(1)	0.6991(4)	2.0(2)
N(3)	0.8058(1)	0.0862(1)	0.7389(4)	1.5(2)
N(4)	0.8794(1)	0.0776(1)	0.6634(4)	1.7(2)
C(1)	0.8421(2)	-0.0657(2)	0.8044(4)	1.5(2)
C(2)	0.8427(2)	-0.1180(2)	0.8418(4)	1.6(2)
C(3)	0.8270(2)	-0.1377(2)	0.9505(4)	2.0(2)
C(4)	0.8280(2)	-0.1898(2)	0.9441(5)	2.5(3)
C(5)	0.8452(2)	-0.2032(2)	0.8329(5)	2.4(2)
C(6)	0.8548(2)	-0.1596(2)	0.7711(5)	2.2(2)
C(7)	0.9602(2)	-0.1232(2)	0.9399(6)	3.1(3)
C(8)	0.9446(2)	-0.1428(2)	1.0462(6)	3.3(3)
C(9)	0.9427(2)	-0.1943(2)	1.0343(5)	3.1(3)
C(10)	0.9569(2)	-0.2065(2)	0.9227(6)	2.8(3)
C(11)	0.9680(2)	-0.1622(2)	0.8627(6)	3.0(3)
C(12)	0.8751(2)	-0.0282(2)	0.9847(4)	1.5(2)
C(13)	0.9179(2)	0.0076(2)	0.9919(5)	2.0(2)
C(14)	0.9417(2)	0.0063(2)	1.1114(5)	2.8(3)
C(15)	0.9042(2)	0.0160(2)	1.2063(5)	2.8(3)
C(16)	0.8605(2)	-0.0182(2)	1.1965(5)	2.2(2)
C(17)	0.8370(2)	-0.0154(2)	1.0776(5)	2.0(2)
C(18)	0.8024(2)	-0.0819(2)	0.6147(4)	1.8(2)
C(19)	0.8320(2)	-0.0855(2)	0.5032(5)	2.8(3)
C(20)	0.8049(2)	-0.1147(2)	0.4097(5)	3.1(3)
C(21)	0.7538(2)	-0.0929(2)	0.3862(5)	3.3(3)
C(22)	0.7238(2)	-0.0895(2)	0.4971(5)	2.8(3)
C(23)	0.7513(2)	-0.0607(2)	0.5903(5)	2.3(2)
C(24)	0.8435(2)	0.1090(2)	0.6871(4)	1.3(2)
C(25)	0.8413(2)	0.1618(2)	0.6532(4)	1.4(2)
C(26)	0.8206(2)	0.2016(2)	0.7166(4)	1.5(2)
C(27)	0.8156(2)	0.2430(2)	0.6431(5)	1.9(2)
C(28)	0.8341(2)	0.2295(2)	0.5335(4)	1.7(2)
C(29)	0.8502(2)	0.1805(2)	0.5393(4)	1.5(2)
C(30)	0.9545(2)	0.2098(2)	0.7337(5)	2.4(2)
C(31)	0.9293(2)	0.2495(2)	0.7889(5)	3.3(3)
C(32)	0.9217(2)	0.2863(2)	0.7043(6)	2.9(3)
C(33)	0.9410(2)	0.2701(2)	0.5990(5)	2.5(3)
C(34)	0.9610(2)	0.2230(2)	0.6176(5)	2.2(2)
C(35)	0.7595(2)	0.1093(2)	0.7724(4)	1.3(2)
C(36)	0.7169(2)	0.0763(2)	0.7365(4)	1.8(2)
C(37)	0.6670(2)	0.0981(2)	0.7761(5)	2.7(3)
C(38)	0.6662(2)	0.1074(2)	0.9052(6)	3.2(3)
C(39)	0.7094(2)	0.1400(2)	0.9422(5)	3.1(3)
C(40)	0.7582(2)	0.1175(2)	0.9031(5)	2.2(2)

C(41)	0.9259(2)	0.0923(2)	0.6121(4)	1.7(2)
C(42)	0.9307(2)	0.0730(2)	0.4885(5)	2.2(2)
C(43)	0.9793(2)	0.0885(2)	0.4326(5)	2.9(3)
C(44)	1.0226(2)	0.0719(2)	0.5066(6)	3.4(3)
C(45)	1.0185(2)	0.0888(2)	0.6310(6)	2.9(3)
C(46)	0.9687(2)	0.0730(2)	0.6834(5)	2.4(2)
C(47)	1/4	1/4	0.749(3)	15.0(8)
C(48)	1/4	1/4	0.372(2)	9.0(5)
C(49)	1/4	0.281	0.672	11(1)
C(50)	1/4	0.281	0.467	9(1)
H(1)	0.867	-0.158	0.695	2.0
H(2)	0.849	-0.236	0.805	3.4
H(3)	0.819	-0.212	1.004	3.2
H(4)	0.817	-0.119	1.016	2.5
H(5)	0.965	-0.089	0.923	3.2
H(6)	0.979	-0.159	0.785	3.3
H(7)	0.959	-0.239	0.892	3.4
H(8)	0.933	-0.217	1.093	3.6
H(9)	0.937	-0.125	1.114	4.1
H(10)	0.733	-0.062	0.660	2.9
H(11)	0.755	-0.028	0.565	2.9
H(12)	0.799	-0.114	0.646	2.0
H(13)	0.717	-0.122	0.525	2.9
H(14)	0.694	-0.073	0.481	2.9
H(15)	0.862	-0.101	0.519	3.4
H(16)	0.838	-0.053	0.475	3.4
H(17)	0.758	-0.061	0.355	4.3
H(18)	0.824	-0.114	0.340	3.3
H(19)	0.737	-0.113	0.333	4.3
H(20)	0.801	-0.148	0.435	3.3
H(21)	0.887	-0.060	0.999	1.7
H(22)	0.810	-0.038	1.074	2.2
H(23)	0.825	0.017	1.065	2.2
H(24)	0.871	-0.051	1.210	2.7
H(25)	0.837	-0.009	1.253	2.7
H(26)	0.919	0.011	1.279	3.0
H(27)	0.893	0.049	1.200	3.0
H(28)	0.668	0.077	0.945	4.4
H(29)	0.636	0.123	0.925	4.4
H(30)	0.709	0.143	1.024	3.9
H(31)	0.706	0.172	0.908	3.9
H(32)	0.784	0.139	0.924	2.9
H(33)	0.763	0.087	0.941	2.9
H(34)	0.906	0.040	0.977	2.8
H(35)	0.642	0.076	0.757	3.1
H(36)	0.662	0.128	0.737	3.1
H(37)	0.721	0.045	0.771	2.3
H(38)	0.717	0.073	0.655	2.3
H(39)	0.757	0.140	0.734	1.6
H(40)	0.812	0.201	0.796	1.5
H(41)	0.802	0.274	0.664	2.3
H(42)	0.835	0.250	0.467	2.0
H(43)	0.865	0.163	0.478	1.7
H(44)	0.965	0.180	0.769	2.7

H(45)	0.920	0.251	0.868	3.5
H(46)	0.906	0.317	0.717	3.0
H(47)	0.941	0.288	0.528	2.4
H(48)	0.976	0.203	0.561	2.5
H(49)	0.966	0.086	0.760	2.7
H(50)	0.967	0.038	0.686	2.7
H(51)	0.927	0.127	0.610	2.4
H(52)	1.044	0.075	0.675	3.2
H(53)	1.021	0.124	0.634	3.2
H(54)	0.929	0.038	0.490	2.7
H(55)	0.904	0.086	0.444	2.7
H(56)	1.024	0.037	0.505	3.4
H(57)	1.052	0.085	0.475	3.4
H(58)	0.980	0.123	0.425	3.2
H(59)	0.982	0.074	0.358	3.2
H(60)	0.942	-0.001	0.936	2.8
H(61)	0.956	-0.025	1.123	2.9
H(62)	0.967	0.031	1.115	2.9

Intramolecular Distances Involving the Nonhydrogen Atoms

atom	atom	distance	ADC(*)	atom	atom	distance	ADC(*)
FE1	N1	2.027(4)	1	O1	C49	1.44(1)	2
FE1	N2	2.052(4)	1	O1	C49	1.44(1)	3
FE1	N3	2.027(4)	1	O1	C49	1.44(1)	4
FE1	N4	2.043(4)	1	O1	C50	1.45(1)	1
FE2	C2	2.084(5)	1	O1	C50	1.45(1)	2
FE2	C3	2.047(5)	1	O1	C50	1.45(1)	3
FE2	C4	2.045(5)	1	O1	C50	1.45(1)	4
FE2	C5	2.048(5)	1	N1	C1	1.331(6)	1
FE2	C6	2.041(5)	1	N1	C12	1.462(6)	1
FE2	C7	2.037(5)	1	N2	C1	1.340(6)	1
FE2	C8	2.049(6)	1	N2	C18	1.453(6)	1
FE2	C9	2.046(5)	1	N3	C24	1.340(6)	1
FE2	C10	2.040(5)	1	N3	C35	1.460(5)	1
FE2	C11	2.037(5)	1	N4	C24	1.327(6)	1
FE3	C25	2.092(4)	1	N4	C41	1.453(6)	1
FE3	C26	2.041(5)	1	C1	C2	1.488(6)	1
FE3	C27	2.032(5)	1	C2	C3	1.434(7)	1
FE3	C28	2.031(5)	1	C2	C6	1.434(7)	1
FE3	C29	2.045(5)	1	C3	C4	1.421(6)	1
FE3	C30	2.069(5)	1	C4	C5	1.417(7)	1
FE3	C31	2.052(5)	1	C5	C6	1.411(7)	1
FE3	C32	2.033(5)	1	C7	C8	1.407(8)	1
FE3	C33	2.041(5)	1	C7	C11	1.404(8)	1
FE3	C34	2.046(5)	1	C8	C9	1.411(7)	1
O1	C47	2.08(3)	1	C9	C10	1.389(8)	1
O1	C49	1.44(1)	1	C10	C11	1.425(7)	1

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Distances Involving the Nonhydrogen Atoms cont

atom	atom	distance	ADC(*)	atom	atom	distance	ADC(*)
C12	C13	1.521(6)	1	C37	C38	1.517(8)	1
C12	C17	1.534(7)	1	C38	C39	1.533(8)	1
C13	C14	1.528(7)	1	C39	C40	1.531(7)	1
C14	C15	1.523(8)	1	C41	C42	1.530(7)	1
C15	C16	1.514(7)	1	C41	C46	1.521(7)	1
C16	C17	1.520(7)	1	C42	C43	1.532(7)	1
C18	C19	1.526(7)	1	C43	C44	1.526(8)	1
C18	C23	1.531(7)	1	C44	C45	1.516(9)	1
C19	C20	1.534(8)	1	C45	C46	1.546(7)	1
C20	C21	1.535(8)	1	C47	C49	1.22(2)	1
C21	C22	1.525(8)	1	C47	C49	1 22(2)	2
C22	C23	1.528(7)	1	C47	C49	1.22(2)	3
C24	C25	1.492(6)	1	C47	C49	1.22(2)	4
C25	C26	1.423(6)	1	C48	C50	1.38(2)	1
C25	C29	1.435(7)	1	C48	C50	1.38(2)	2
C26	C27	1.418(7)	1	C48	C50	1.38(2)	3
C27	C28	1.414(7)	1	C48	C50	1.38(2)	4
C28	C29	1.406(6)	1	C49	C49	1.659	2
C30	C31	1.431(8)	1	C49	C49	1.173	3
C30	C34	1.402(8)	1	C49	C49	1.173	4
C31	C32	1.417(8)	1	C50	C50	1.659	2
C32	C33	1.400(8)	1	C50	C50	1.173	3
C33	C34	1.408(7)	1	C50	C50	1.173	4
C35	C36	1.522(6)	1				
C35	C40	1.530(7)	1				
C36	C37	1.551(7)	1				

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms

atom	atom	atom	angle	atom	atom	atom	angle
N1	FE1	N2	65.1(2)	C4	FE2	C8	124.3(3)
N1	FE1	N3	129.5(2)	C4	FE2	C9	107.1(2)
N1	FE1	N4	135.7(2)	C4	FE2	C10	120.4(2)
N2	FE1	N3	138.6(2)	C4	FE2	C11	156.3(2)
N2	FE1	N4	136.6(2)	C5	FE2	C6	40.4(2)
N3	FE1	N4	65.4(1)	C5	FE2	C7	157.9(3)
C2	FE2	C3	40.6(2)	C5	FE2	C8	157.2(2)
C2	FE2	C4	68.4(2)	C5	FE2	C9	119.7(2)
C2	FE2	C5	68.4(2)	C5	FE2	C10	103.7(2)
C2	FE2	C6	40.7(2)	C5	FE2	C11	120.2(2)
C2	FE2	C7	111.0(2)	C6	FE2	C7	124.5(2)
C2	FE2	C8	127.6(2)	C6	FE2	C8	162.3(2)
C2	FE2	C9	162.9(2)	C6	FE2	C9	154.7(2)
C2	FE2	C10	157.0(2)	C6	FE2	C10	119.6(2)
C2	FE2	C11	123.1(2)	C6	FE2	C11	106.1(2)
C3	FE2	C4	40.6(2)	C7	FE2	C8	40.3(2)
C3	FE2	C5	68.3(2)	C7	FE2	C9	67.7(2)
C3	FE2	C6	68.2(2)	C7	FE2	C10	67.9(2)
C3	FE2	C7	126.6(2)	C7	FE2	C11	40.3(2)
C3	FE2	C8	111.7(2)	C8	FE2	C9	40.3(2)
C3	FE2	C9	125.4(2)	C8	FE2	C10	67.5(2)
C3	FE2	C10	158.3(2)	C8	FE2	C11	67.9(3)
C3	FE2	C11	160.6(2)	C9	FE2	C10	39.7(2)
C4	FE2	C5	40.5(2)	C9	FE2	C11	67.8(3)
C4	FE2	C6	68.0(2)	C10	FE2	C11	40.9(2)
C4	FE2	C7	161.3(2)	C25	FE3	C26	40.2(2)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms cont

atom	atom	atom	angle	atom	atom	atom	angle
C25	FE3	C27	68.4(2)	C28	FE3	C32	116.8(2)
C25	FE3	C28	68.2(2)	C28	FE3	C33	103.7(2)
C25	FE3	C29	40.6(2)	C28	FE3	C34	123.6(2)
C25	FE3	C30	113.1(2)	C29	FE3	C30	128.6(2)
C25	FE3	C31	128.3(2)	C29	FE3	C31	165.7(2)
C25	FE3	C32	162.2(2)	C29	FE3	C32	153.0(2)
C25	FE3	C33	157.6(2)	C29	FE3	C33	120.0(2)
C25	FE3	C34	125.7(2)	C29	FE3	C34	110.1(2)
C26	FE3	C27	40.7(2)	C30	FE3	C31	40.6(2)
C26	FE3	C28	68.2(2)	C30	FE3	C32	67.9(2)
C26	FE3	C29	67.8(2)	C30	FE3	C33	67.8(2)
C26	FE3	C30	125.5(2)	C30	FE3	C34	39.8(2)
C26	FE3	C31	109.4(2)	C31	FE3	C32	40.6(2)
C26	FE3	C32	123.6(2)	C31	FE3	C33	68.1(2)
C26	FE3	C33	158.0(2)	C31	FE3	C34	67.6(2)
C26	FE3	C34	160.8(2)	C32	FE3	C33	40.2(2)
C27	FE3	C28	40.7(2)	C32	FE3	C34	67.4(2)
C27	FE3	C29	68.2(2)	C33	FE3	C34	40.3(2)
C27	FE3	C30	157.5(2)	C47	O1	C49	35.1(3)
C27	FE3	C31	119.5(2)	C47	O1	C49	35.1(3)
C27	FE3	C32	103.6(2)	C47	O1	C49	35.1(3)
C27	FE3	C33	120.0(2)	C47	O1	C49	35.1(3)
C27	FE3	C34	157.9(2)	C47	O1	C50	145.2(3)
C28	FE3	C29	40.3(2)	C47	O1	C50	145.2(3)
C28	FE3	C30	161.8(2)	C47	O1	C50	145.2(3)
C28	FE3	C31	153.1(2)	C47	O1	C50	145.2(3)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms cont

atom	atom	atom	angle	atom	atom	atom	angle
C49	O1	C49	70.2(6)	C50	O1	C50	47.6(4)
C49	O1	C49	48.0(4)	C50	O1	C50	69.6(6)
C49	O1	C49	48.0(4)	FE1	N1	C1	92.8(3)
C49	O1	C50	110.102(4)	FE1	N1	C12	140.4(3)
C49	O1	C50	179.7(6)	C1	N1	C12	126.1(4)
C49	O1	C50	132.209(5)	FE1	N2	C1	91.4(3)
C49	O1	C50	132.209(5)	FE1	N2	C18	141.4(3)
C49	O1	C49	48.0(4)	C1	N2	C18	125.9(4)
C49	O1	C49	48.0(4)	FE1	N3	C24	91.9(3)
C49	O1	C50	179.7(6)	FE1	N3	C35	142.7(3)
C49	O1	C50	110.102(4)	C24	N3	C35	125.4(4)
C49	O1	C50	132.209(5)	FE1	N4	C24	91.6(3)
C49	O1	C50	132.209(5)	FE1	N4	C41	144.8(3)
C49	O1	C49	70.2(6)	C24	N4	C41	123.4(4)
C49	O1	C50	132.209(5)	N1	C1	N2	110.6(4)
C49	O1	C50	132.209(5)	N1	C1	C2	126.4(5)
C49	O1	C50	110.102(4)	N2	C1	C2	123.0(4)
C49	O1	C50	179.7(6)	FE2	C2	C1	132.5(3)
C49	O1	C50	132.209(5)	FE2	C2	C3	68.3(3)
C49	O1	C50	132.209(5)	FE2	C2	C6	68.1(3)
C49	O1	C50	179.7(6)	C1	C2	C3	127.5(4)
C49	O1	C50	110.102(4)	C1	C2	C6	126.2(5)
C50	O1	C50	69.6(6)	C3	C2	C6	106.0(4)
C50	O1	C50	47.6(4)	FE2	C3	C2	71.1(3)
C50	O1	C50	47.6(4)	FE2	C3	C4	69.6(3)
C50	O1	C50	47.6(4)	C2	C3	C4	108.7(4)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms cont

atom	atom	atom	angle	atom	atom	atom	angle
FE2	C4	C3	69.8(3)	C13	C12	C17	109.5(4)
FE2	C4	C5	69.9(3)	C12	C13	C14	111.0(4)
C3	C4	C5	108.1(4)	C13	C14	C15	111.5(4)
FE2	C5	C4	69.6(3)	C14	C15	C16	111.4(4)
FE2	C5	C6	69.6(3)	C15	C16	C17	111.6(4)
C4	C5	C6	107.8(4)	C12	C17	C16	109.8(4)
FE2	C6	C2	71.3(3)	N2	C18	C19	110.9(4)
FE2	C6	C5	70.1(3)	N2	C18	C23	109.7(4)
C2	C6	C5	109.3(5)	C19	C18	C23	110.4(4)
FE2	C7	C8	70.3(3)	C18	C19	C20	112.0(4)
FE2	C7	C11	69.8(3)	C19	C20	C21	111.1(4)
C8	C7	C11	108.5(5)	C20	C21	C22	110.9(5)
FE2	C8	C7	69.4(3)	C21	C22	C23	111.4(4)
FE2	C8	C9	69.7(3)	C18	C23	C22	112.4(4)
C7	C8	C9	107.6(5)	N3	C24	N4	111.1(4)
FE2	C9	C8	70.0(3)	N3	C24	C25	122.2(4)
FE2	C9	C10	69.9(3)	N4	C24	C25	126.5(4)
C8	C9	C10	108.5(5)	FE3	C25	C24	138.0(3)
FE2	C10	C9	70.4(3)	FE3	C25	C26	68.0(2)
FE2	C10	C11	69.4(3)	FE3	C25	C29	67.9(2)
C9	C10	C11	108.1(5)	C24	C25	C26	127.8(4)
FE2	C11	C7	69.8(3)	C24	C25	C29	125.2(4)
FE2	C11	C10	69.7(3)	C26	C25	C29	105.8(4)
C7	C11	C10	107.3(6)	FE3	C26	C25	71.8(3)
N1	C12	C13	109.5(4)	FE3	C26	C27	69.3(3)
N1	C12	C17	112.0(4)	C25	C26	C27	109.4(4)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms cont

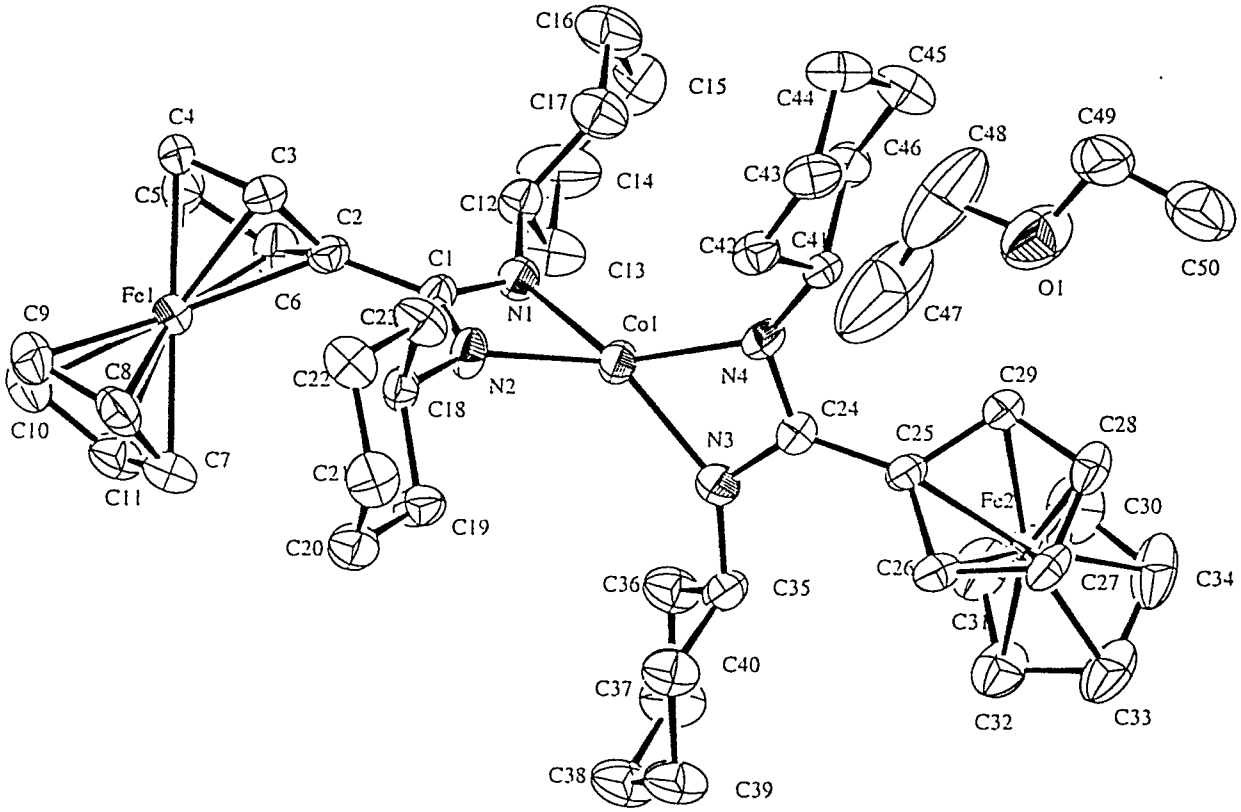
atom	atom	atom	angle	atom	atom	atom	angle
FE3	C27	C26	70.0(3)	C36	C35	C40	109.8(4)
FE3	C27	C28	69.6(3)	C35	C36	C37	111.0(4)
C26	C27	C28	107.4(4)	C36	C37	C38	111.7(4)
FE3	C28	C27	69.7(3)	C37	C38	C39	111.1(5)
FE3	C28	C29	70.4(3)	C38	C39	C40	110.6(4)
C27	C28	C29	108.3(4)	C35	C40	C39	111.7(4)
FE3	C29	C25	71.5(2)	N4	C41	C42	111.2(4)
FE3	C29	C28	69.3(3)	N4	C41	C46	110.4(4)
C25	C29	C28	109.0(4)	C42	C41	C46	109.0(4)
FE3	C30	C31	69.0(3)	C41	C42	C43	111.9(4)
FE3	C30	C34	69.2(3)	C42	C43	C44	110.4(5)
C31	C30	C34	107.2(5)	C43	C44	C45	112.7(5)
FE3	C31	C30	70.3(3)	C44	C45	C46	110.7(4)
FE3	C31	C32	69.0(3)	C41	C46	C45	111.2(4)
C30	C31	C32	107.2(5)	O1	C47	C49	43(1)
FE3	C32	C31	70.4(3)	O1	C47	C49	43(1)
FE3	C32	C33	70.2(3)	O1	C47	C49	43(1)
C31	C32	C33	108.9(5)	O1	C47	C49	43(1)
FE3	C33	C32	69.6(3)	C49	C47	C49	86(2)
FE3	C33	C34	70.0(3)	C49	C47	C49	57(1)
C32	C33	C34	107.4(5)	C49	C47	C49	57(1)
FE3	C34	C30	71.0(3)	C49	C47	C49	57(1)
FE3	C34	C33	69.7(3)	C49	C47	C49	57(1)
C30	C34	C33	109.4(5)	C49	C47	C49	86(2)
N3	C35	C36	109.2(4)	C50	C48	C50	74(1)
N3	C35	C40	110.1(4)	C50	C48	C50	50.5(7)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms cont

atom	atom	atom	angle	atom	atom	atom	angle
C50	C48	C50	50.5(7)				
C50	C48	C50	50.5(7)				
C50	C48	C50	50.5(7)				
C50	C48	C50	74(1)				
O1	C49	C47	102(1)				
O1	C49	C49	54.9(3)				
O1	C49	C49	66.0(2)				
O1	C49	C49	66.0(2)				
C47	C49	C49	47(1)				
C47	C49	C49	61.3(6)				
C47	C49	C49	61.3(6)				
C49	C49	C49	45.0000(3)				
C49	C49	C49	45.0000(3)				
C49	C49	C49	90.0000(6)				
O1	C50	C48	108.1(6)				
O1	C50	C50	55.2(3)				
O1	C50	C50	66.2(2)				
O1	C50	C50	66.2(2)				
C48	C50	C50	52.9(5)				
C48	C50	C50	64.8(3)				
C48	C50	C50	64.8(3)				
C50	C50	C50	45.0000(3)				
C50	C50	C50	45.0000(3)				
C50	C50	C50	90.0000(6)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.


C16
C15
C17
C4
C3
C5
C14
C12
C2
C1
C13
Fe1
C6
C21
N1
Co1
C9
C8
C22
N2
N4
C18
C24
C10
C7
N3
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C29
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C11
C21
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Fe2
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C33
C38
C39
C45
C44
C46
C48
C49
C43
C42
C41
C47
O1
C50

Anisotropic Thermal Parameters for $[FcC(NCy)_2]_2Co \cdot Et_2O$.

atom	U11	U22	U33	U12	U13	U23
Co(1)	0.0301(3)	0.0345(3)	0.0256(3)	0.0031(3)	0.0009(2)	-0.0038(3)
Fe(1)	0.0250(3)	0.0318(3)	0.0310(3)	-0.0016(3)	0.0030(3)	-0.0023(3)
Fe(2)	0.0444(4)	0.0265(3)	0.0299(3)	0.0048(3)	0.0021(3)	-0.0037(3)
O(1)	0.111(4)	0.072(3)	0.050(2)	-0.016(3)	-0.006(3)	-0.002(2)
N(1)	0.024(2)	0.045(2)	0.032(1)	0.006(2)	-0.004(1)	-0.006(2)
N(2)	0.033(2)	0.046(2)	0.021(1)	0.011(2)	0.001(1)	-0.001(2)
N(3)	0.034(2)	0.033(2)	0.034(2)	-0.008(2)	0.004(2)	-0.001(1)
N(4)	0.039(2)	0.027(2)	0.032(2)	-0.002(2)	0.001(1)	-0.010(1)
C(1)	0.029(2)	0.037(3)	0.021(2)	0.004(2)	-0.001(2)	-0.005(2)
C(2)	0.027(2)	0.031(2)	0.027(2)	0.000(2)	-0.004(1)	-0.004(2)
C(3)	0.032(3)	0.030(2)	0.035(2)	-0.005(2)	0.001(2)	-0.007(2)
C(4)	0.024(2)	0.052(2)	0.032(2)	-0.005(2)	0.006(2)	-0.015(2)
C(5)	0.038(2)	0.059(3)	0.027(2)	0.004(3)	0.002(2)	-0.002(2)
C(6)	0.036(2)	0.043(3)	0.034(2)	0.013(2)	0.000(2)	0.006(2)
C(7)	0.033(3)	0.053(3)	0.055(3)	-0.015(2)	0.000(2)	-0.006(2)
C(8)	0.023(2)	0.057(3)	0.043(2)	-0.001(2)	0.005(2)	0.003(2)
C(9)	0.029(2)	0.061(3)	0.049(2)	0.006(2)	0.008(2)	-0.011(2)
C(10)	0.041(3)	0.064(3)	0.044(3)	-0.010(2)	0.014(2)	0.001(2)
C(11)	0.042(3)	0.041(3)	0.060(2)	-0.016(2)	0.009(2)	-0.003(2)
C(12)	0.033(2)	0.036(2)	0.029(2)	0.006(2)	-0.003(2)	-0.001(2)
C(13)	0.047(3)	0.037(2)	0.071(3)	-0.004(3)	-0.020(3)	0.011(3)
C(14)	0.064(4)	0.055(4)	0.083(4)	0.001(3)	-0.042(3)	0.019(3)
C(15)	0.047(3)	0.069(3)	0.055(3)	0.027(3)	-0.017(3)	-0.007(3)
C(16)	0.031(3)	0.069(3)	0.080(4)	0.001(3)	-0.016(3)	0.002(4)
C(17)	0.038(3)	0.046(3)	0.058(3)	-0.000(2)	-0.004(2)	0.005(3)
C(18)	0.026(2)	0.044(2)	0.021(2)	0.006(2)	0.001(2)	-0.002(2)
C(19)	0.034(2)	0.037(3)	0.042(2)	0.002(2)	-0.009(2)	-0.007(2)
C(20)	0.035(3)	0.048(3)	0.041(3)	0.002(2)	-0.006(2)	-0.002(2)
C(21)	0.045(3)	0.050(3)	0.041(2)	0.005(2)	-0.003(2)	0.009(2)
C(22)	0.036(2)	0.034(3)	0.051(3)	0.004(2)	-0.000(2)	0.012(2)
C(23)	0.030(2)	0.046(3)	0.049(3)	-0.002(2)	-0.003(2)	0.011(3)
C(24)	0.032(2)	0.026(2)	0.025(2)	0.001(2)	0.000(2)	-0.001(2)
C(25)	0.032(2)	0.027(2)	0.023(2)	-0.004(2)	-0.002(1)	-0.004(2)
C(26)	0.039(2)	0.028(2)	0.026(2)	-0.005(2)	-0.005(2)	-0.002(2)
C(27)	0.055(2)	0.034(3)	0.022(2)	-0.001(2)	0.001(2)	-0.008(2)
C(28)	0.052(2)	0.026(2)	0.028(2)	0.006(2)	0.008(2)	-0.002(2)
C(29)	0.032(2)	0.033(2)	0.033(2)	-0.002(2)	0.002(2)	-0.010(2)
C(30)	0.064(3)	0.040(3)	0.065(2)	0.025(3)	0.004(3)	0.005(3)
C(31)	0.073(3)	0.029(3)	0.045(3)	0.011(3)	0.001(2)	0.007(2)
C(32)	0.071(4)	0.028(2)	0.049(2)	-0.001(2)	0.005(2)	-0.001(2)
C(33)	0.097(4)	0.032(2)	0.047(3)	0.001(3)	0.012(3)	-0.011(2)
C(34)	0.087(3)	0.034(3)	0.060(2)	0.025(2)	0.027(3)	-0.003(2)
C(35)	0.041(2)	0.032(2)	0.028(2)	-0.005(2)	-0.001(2)	-0.006(2)
C(36)	0.041(3)	0.041(3)	0.044(2)	-0.009(2)	-0.005(2)	0.009(2)
C(37)	0.060(3)	0.039(3)	0.053(3)	-0.009(3)	-0.010(2)	0.018(3)
C(38)	0.052(3)	0.049(3)	0.057(3)	-0.021(3)	-0.006(3)	0.014(2)
C(39)	0.048(3)	0.044(3)	0.056(3)	-0.018(2)	-0.008(3)	0.007(2)
C(40)	0.043(2)	0.042(3)	0.046(3)	-0.004(2)	-0.007(2)	0.007(2)

C(41)	0.027(2)	0.031(2)	0.026(2)	-0.001(2)	-0.002(2)	-0.009(2)
C(42)	0.034(3)	0.029(2)	0.037(2)	0.005(2)	-0.006(2)	-0.004(2)
C(43)	0.048(3)	0.028(2)	0.047(3)	-0.001(2)	-0.009(2)	-0.001(2)
C(44)	0.051(3)	0.045(3)	0.054(3)	-0.016(2)	-0.017(3)	0.002(3)
C(45)	0.032(3)	0.056(3)	0.062(3)	-0.010(2)	-0.004(2)	0.012(3)
C(46)	0.029(2)	0.043(3)	0.036(2)	0.003(2)	-0.005(2)	-0.002(2)
C(47)	0.39(2)	0.12(1)	0.067(5)	-0.11(1)	0.065(9)	-0.012(6)
C(48)	0.21(1)	0.106(7)	0.048(2)	0.064(5)	-0.028(5)	-0.015(4)
C(49)	0.036(3)	0.085(5)	0.114(4)	0.002(3)	0.001(3)	-0.051(4)
C(50)	0.061(4)	0.062(4)	0.109(4)	-0.015(3)	0.012(4)	-0.006(4)

Positional parameters and B(eq) for $[FcC(NCy)_2]_2Co \cdot Et_2O$.

atom	x	y	z	B(eq)
Co(1)	0.95818(5)	0.01437(5)	0.10494(2)	2.38(2)
Fe(1)	1.19929(5)	-0.08574(5)	-0.03768(2)	2.31(2)
Fe(2)	0.81627(6)	0.24954(6)	0.24397(2)	2.65(3)
O(1)	0.5277(4)	0.1820(4)	0.1674(1)	6.1(2)
N(1)	0.9280(3)	0.0171(3)	0.0445(1)	2.7(1)
N(2)	1.0689(3)	-0.0703(3)	0.0716(1)	2.6(2)
N(3)	0.9740(3)	0.1285(3)	0.1490(1)	2.6(2)
N(4)	0.8690(3)	-0.0181(3)	0.1553(1)	2.6(2)
C(1)	1.0175(3)	-0.0446(4)	0.0369(1)	2.3(2)
C(2)	1.0507(4)	-0.0791(4)	-0.0046(1)	2.2(1)
C(3)	1.0742(4)	-0.1894(4)	-0.0185(1)	2.6(2)
C(4)	1.0822(4)	-0.1890(4)	-0.0612(1)	2.9(2)
C(5)	1.0638(4)	-0.0796(5)	-0.0750(1)	3.3(2)
C(6)	1.0452(4)	-0.0108(4)	-0.0402(1)	3.0(2)
C(7)	1.3303(4)	-0.0227(5)	-0.0051(2)	3.7(2)
C(8)	1.3477(4)	-0.1359(5)	-0.0139(1)	3.3(2)
C(9)	1.3478(4)	-0.1485(5)	-0.0566(2)	3.7(2)
C(10)	1.3292(4)	-0.0429(5)	-0.0747(1)	3.9(2)
C(11)	1.3184(4)	0.0341(4)	-0.0422(2)	3.8(2)
C(12)	0.8396(4)	0.0391(4)	0.0155(1)	2.6(2)
C(13)	0.8195(5)	0.1620(4)	0.0119(2)	4.1(2)
C(14)	0.7217(5)	0.1883(5)	-0.0167(2)	5.3(3)
C(15)	0.6168(5)	0.1304(5)	-0.0030(2)	4.5(2)
C(16)	0.6337(4)	0.0083(6)	0.0008(2)	4.7(3)
C(17)	0.7327(4)	-0.0178(5)	0.0293(2)	3.7(2)
C(18)	1.1703(3)	-0.1341(4)	0.0752(1)	2.4(2)
C(19)	1.2523(4)	-0.0772(4)	0.1039(1)	3.0(2)
C(20)	1.3588(4)	-0.1449(4)	0.1102(1)	3.3(2)
C(21)	1.3322(4)	-0.2604(5)	0.1240(1)	3.6(2)
C(22)	1.2531(4)	-0.3173(4)	0.0943(1)	3.2(2)
C(23)	1.1460(4)	-0.2526(5)	0.0898(1)	3.3(2)
C(24)	0.9044(4)	0.0737(4)	0.1735(1)	2.2(2)
C(25)	0.8685(4)	0.1058(4)	0.2151(1)	2.2(2)
C(26)	0.9398(4)	0.1338(4)	0.2493(1)	2.4(2)
C(27)	0.8732(4)	0.1358(4)	0.2849(1)	2.9(2)
C(28)	0.7609(4)	0.1130(4)	0.2738(1)	2.8(2)
C(29)	0.7581(4)	0.0943(4)	0.2309(1)	2.6(2)
C(30)	0.7006(6)	0.3576(5)	0.2219(2)	4.4(2)
C(31)	0.8042(5)	0.3783(4)	0.2035(1)	3.9(2)
C(32)	0.8821(5)	0.4044(5)	0.2348(2)	3.9(2)
C(33)	0.8264(6)	0.4005(5)	0.2727(2)	4.7(2)
C(34)	0.7144(6)	0.3710(5)	0.2647(2)	4.8(2)
C(35)	1.0310(4)	0.2318(4)	0.1594(1)	2.6(2)
C(36)	1.0249(4)	0.3091(4)	0.1221(1)	3.3(2)
C(37)	1.0867(5)	0.4185(5)	0.1303(2)	4.0(2)
C(38)	1.2062(5)	0.3975(5)	0.1439(2)	4.2(2)
C(39)	1.2105(5)	0.3199(5)	0.1802(2)	3.9(2)
C(40)	1.1511(4)	0.2116(4)	0.1709(1)	3.4(2)

C(41)	0.8065(4)	-0.1066(4)	0.1755(1)	2.2(2)
C(42)	0.8737(4)	-0.2132(4)	0.1735(1)	2.7(2)
C(43)	0.8080(5)	-0.3093(4)	0.1922(1)	3.2(2)
C(44)	0.6945(5)	-0.3233(4)	0.1721(2)	4.0(2)
C(45)	0.6290(4)	-0.2171(5)	0.1745(2)	3.9(2)
C(46)	0.6933(4)	-0.1215(4)	0.1549(1)	2.9(2)
C(47)	0.629(1)	0.262(1)	0.1132(2)	15(1)
C(48)	0.538(1)	0.1820(8)	0.1246(2)	9.5(5)
C(49)	0.4470(5)	0.1079(6)	0.1839(2)	6.2(3)
C(50)	0.4371(6)	0.1258(6)	0.2285(2)	6.1(3)
H(1)	1.097	-0.252	-0.078	3.3
H(2)	1.083	-0.253	-0.002	3.2
H(3)	1.031	0.066	-0.041	3.8
H(4)	1.327	0.009	0.021	4.1
H(5)	1.326	-0.027	-0.103	4.5
H(6)	1.064	-0.056	-0.102	3.9
H(7)	1.305	0.111	-0.045	5.0
H(8)	1.358	-0.193	0.005	3.7
H(9)	1.358	-0.216	-0.071	4.2
H(10)	1.017	0.148	0.248	3.0
H(11)	0.694	0.078	0.215	2.9
H(12)	0.699	0.110	0.292	2.9
H(13)	0.820	0.376	0.175	4.1
H(14)	0.899	0.151	0.312	3.4
H(15)	0.634	0.338	0.209	5.5
H(16)	0.858	0.416	0.299	4.7
H(17)	0.658	0.361	0.285	5.2
H(18)	0.958	0.421	0.231	5.0
H(19)	1.204	-0.138	0.049	3.0
H(20)	0.860	0.011	-0.010	2.8
H(21)	0.994	0.266	0.182	3.6
H(22)	0.795	-0.087	0.203	2.8
H(23)	0.798	-0.295	0.220	3.9
H(24)	0.850	-0.375	0.189	3.9
H(25)	1.058	0.273	0.099	3.7
H(26)	0.949	0.325	0.116	3.7
H(27)	1.088	0.462	0.106	4.9
H(28)	1.049	0.458	0.151	4.9
H(29)	1.154	0.166	0.194	4.1
H(30)	1.188	0.176	0.149	4.1
H(31)	0.704	-0.344	0.144	4.7
H(32)	0.655	-0.380	0.186	4.7
H(33)	0.890	-0.230	0.146	3.0
H(34)	0.941	-0.204	0.188	3.0
H(35)	0.651	-0.055	0.158	3.2
H(36)	0.704	-0.137	0.127	3.2
H(37)	0.560	-0.227	0.161	4.6
H(38)	0.615	-0.200	0.202	4.6
H(39)	1.176	0.355	0.203	5.4
H(40)	1.286	0.305	0.187	5.4
H(41)	1.246	0.364	0.122	4.5
H(42)	1.240	0.465	0.151	4.5
H(43)	0.377	0.122	0.172	7.2
H(44)	0.469	0.034	0.179	7.2

H(45)	0.557	0.109	0.116	8.4
H(46)	0.469	0.203	0.113	8.4
H(47)	1.109	-0.249	0.115	4.2
H(48)	1.100	-0.288	0.070	4.2
H(49)	1.272	-0.007	0.093	4.1
H(50)	1.217	-0.067	0.130	4.1
H(51)	1.299	-0.257	0.150	4.1
H(52)	1.399	-0.302	0.126	4.1
H(53)	1.236	-0.390	0.104	3.6
H(54)	1.288	-0.324	0.068	3.6
H(55)	0.804	0.191	0.038	4.1
H(56)	0.885	0.196	0.001	4.1
H(57)	1.399	-0.149	0.085	3.9
H(58)	1.404	-0.110	0.130	3.9
H(59)	0.560	0.144	-0.022	5.0
H(60)	0.595	0.159	0.023	5.0
H(61)	0.568	-0.024	0.011	5.4
H(62)	0.649	-0.021	-0.025	5.4
H(63)	0.709	0.266	-0.017	6.0
H(64)	0.740	0.164	-0.043	6.0
H(65)	0.744	-0.096	0.030	4.5
H(66)	0.715	0.006	0.056	4.5
H(67)	0.507	0.113	0.241	7.6
H(68)	0.414	0.199	0.234	7.6
H(69)	0.384	0.076	0.239	7.6
H(70)	0.696	0.239	0.124	11.6
H(71)	0.633	0.264	0.084	11.6
H(72)	0.608	0.333	0.123	11.6

Intramolecular Distances Involving the Nonhydrogen Atoms

atom	atom	distance	atom	atom	distance
CO1	N1	2.020(4)	N1	N2	2.186(6)
CO1	N2	2.006(4)	N1	C1	1.332(6)
CO1	N3	2.009(4)	N1	C12	1.451(6)
CO1	N4	2.010(4)	N2	C1	1.332(6)
FE1	C2	2.091(5)	N2	C18	1.448(7)
FE1	C3	2.058(5)	N3	N4	2.188(6)
FE1	C4	2.035(5)	N3	C24	1.339(6)
FE1	C5	2.039(6)	N3	C35	1.465(7)
FE1	C6	2.064(5)	N4	C24	1.331(7)
FE1	C7	2.051(6)	N4	C41	1.467(6)
FE1	C8	2.040(6)	C1	C2	1.483(6)
FE1	C9	2.038(6)	C2	C3	1.438(7)
FE1	C10	2.046(6)	C2	C6	1.433(7)
FE1	C11	2.043(6)	C3	C4	1.409(7)
FE2	C25	2.079(5)	C3	C5	2.287(8)
FE2	C26	2.049(5)	C4	C5	1.416(8)
FE2	C27	2.043(6)	C5	C6	1.430(8)
FE2	C28	2.033(5)	C7	C8	1.416(9)
FE2	C29	2.050(6)	C7	C9	2.287(9)
FE2	C30	2.042(6)	C7	C10	2.298(8)
FE2	C31	2.054(6)	C7	C11	1.408(8)
FE2	C32	2.056(7)	C8	C9	1.412(8)
FE2	C33	2.061(6)	C8	C11	2.286(9)
FE2	C34	2.030(6)	C9	C10	1.426(9)
O1	C48	1.412(9)	C9	C11	2.287(9)
O1	C49	1.427(9)	C10	C11	1.421(8)

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Distances Involving the Nonhydrogen Atoms cont

atom	atom	distance	atom	atom	distance
C12	C13	1.512(8)	C35	C36	1.545(7)
C12	C17	1.527(8)	C35	C40	1.513(8)
C13	C14	1.537(8)	C36	C37	1.542(8)
C14	C15	1.51(1)	C37	C38	1.526(9)
C15	C16	1.50(1)	C38	C39	1.519(8)
C16	C17	1.546(8)	C39	C40	1.523(8)
C18	C19	1.529(7)	C41	C42	1.524(7)
C18	C23	1.540(8)	C41	C46	1.530(7)
C19	C20	1.534(8)	C42	C43	1.533(8)
C20	C21	1.504(9)	C43	C44	1.523(8)
C21	C22	1.528(8)	C44	C45	1.509(9)
C22	C23	1.514(8)	C45	C46	1.533(8)
C24	C25	1.484(6)	C47	C48	1.51(2)
C25	C26	1.454(6)	C49	C50	1.49(1)
C25	C29	1.431(7)			
C26	C27	1.417(7)			
C27	C28	1.425(8)			
C28	C29	1.427(7)			
C30	C31	1.41(1)			
C30	C32	2.29(1)			
C30	C34	1.424(9)			
C31	C32	1.428(9)			
C31	C34	2.284(9)			
C32	C33	1.414(8)			
C32	C34	2.28(1)			
C33	C34	1.42(1)			

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms

atom	atom	atom	angle	atom	atom	atom	angle
N1	CO1	N2	65.8(2)	C4	FE1	C8	124.6(3)
N1	CO1	N3	135.5(2)	C4	FE1	C9	105.1(2)
N1	CO1	N4	135.8(2)	C4	FE1	C10	117.3(2)
N2	CO1	N3	133.0(2)	C4	FE1	C11	153.2(2)
N2	CO1	N4	134.7(2)	C5	FE1	C6	40.8(2)
N3	CO1	N4	66.0(2)	C5	FE1	C7	155.9(3)
C2	FE1	C3	40.5(2)	C5	FE1	C8	159.9(2)
C2	FE1	C4	68.3(2)	C5	FE1	C9	122.0(2)
C2	FE1	C5	68.2(2)	C5	FE1	C10	104.1(2)
C2	FE1	C6	40.3(2)	C5	FE1	C11	119.3(3)
C2	FE1	C7	111.7(2)	C6	FE1	C7	123.1(2)
C2	FE1	C8	124.0(2)	C6	FE1	C8	158.6(2)
C2	FE1	C9	157.1(2)	C6	FE1	C9	159.7(2)
C2	FE1	C10	161.9(2)	C6	FE1	C10	123.4(2)
C2	FE1	C11	127.5(2)	C6	FE1	C11	108.3(3)
C3	FE1	C4	40.3(2)	C7	FE1	C8	40.5(2)
C3	FE1	C5	67.8(2)	C7	FE1	C9	68.0(3)
C3	FE1	C6	67.9(2)	C7	FE1	C10	68.2(2)
C3	FE1	C7	128.9(2)	C7	FE1	C11	40.2(2)
C3	FE1	C8	109.9(2)	C8	FE1	C9	40.5(2)
C3	FE1	C9	120.4(3)	C8	FE1	C10	68.6(2)
C3	FE1	C10	153.5(2)	C8	FE1	C11	68.1(3)
C3	FE1	C11	165.3(2)	C9	FE1	C10	40.9(2)
C4	FE1	C5	40.7(2)	C9	FE1	C11	68.2(3)
C4	FE1	C6	68.5(2)	C10	FE1	C11	40.7(2)
C4	FE1	C7	163.3(3)	C25	FE2	C26	41.2(2)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms cont

atom	atom	atom	angle	atom	atom	atom	angle
C25	FE2	C27	68.6(2)	C28	FE2	C32	159.6(2)
C25	FE2	C28	68.8(2)	C28	FE2	C33	121.3(2)
C25	FE2	C29	40.6(2)	C28	FE2	C34	103.2(2)
C25	FE2	C30	125.5(2)	C29	FE2	C30	106.3(3)
C25	FE2	C31	111.2(2)	C29	FE2	C31	122.4(2)
C25	FE2	C32	125.5(2)	C29	FE2	C32	159.4(2)
C25	FE2	C33	159.0(3)	C29	FE2	C33	158.3(2)
C25	FE2	C34	160.2(3)	C29	FE2	C34	121.9(3)
C26	FE2	C27	40.5(2)	C30	FE2	C31	40.2(3)
C26	FE2	C28	68.9(2)	C30	FE2	C32	68.1(3)
C26	FE2	C29	68.8(2)	C30	FE2	C33	68.5(3)
C26	FE2	C30	164.2(2)	C30	FE2	C34	40.9(3)
C26	FE2	C31	128.7(2)	C31	FE2	C32	40.7(2)
C26	FE2	C32	110.9(2)	C31	FE2	C33	68.2(2)
C26	FE2	C33	121.6(3)	C31	FE2	C34	68.0(3)
C26	FE2	C34	154.5(2)	C32	FE2	C33	40.2(2)
C27	FE2	C28	40.9(2)	C32	FE2	C34	67.8(3)
C27	FE2	C29	68.6(2)	C33	FE2	C34	40.5(3)
C27	FE2	C30	153.3(3)	C48	O1	C49	116.0(8)
C27	FE2	C31	164.0(3)	CO1	N1	N2	56.8(1)
C27	FE2	C32	125.5(2)	CO1	N1	C1	91.6(3)
C27	FE2	C33	106.0(2)	CO1	N1	C12	141.2(3)
C27	FE2	C34	118.0(2)	N2	N1	C1	34.8(3)
C28	FE2	C29	40.9(2)	N2	N1	C12	157.4(4)
C28	FE2	C30	117.9(3)	C1	N1	C12	124.9(4)
C28	FE2	C31	154.9(3)	CO1	N2	N1	57.4(2)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms cont

atom	atom	atom	angle	atom	atom	atom	angle
CO1	N2	C1	92.3(3)	FE1	C3	C2	71.0(3)
CO1	N2	C18	141.9(3)	FE1	C3	C4	69.0(3)
N1	N2	C1	34.9(3)	FE1	C3	C5	55.7(2)
N1	N2	C18	160.6(3)	C2	C3	C4	108.9(5)
C1	N2	C18	125.8(4)	C2	C3	C5	72.9(3)
CO1	N3	N4	57.0(2)	C4	C3	C5	36.0(3)
CO1	N3	C24	91.9(3)	FE1	C4	C3	70.8(3)
CO1	N3	C35	143.1(3)	FE1	C4	C5	69.8(3)
N4	N3	C24	34.9(3)	C3	C4	C5	108.1(5)
N4	N3	C35	159.9(3)	FE1	C5	C3	56.5(2)
C24	N3	C35	125.0(4)	FE1	C5	C4	69.5(3)
CO1	N4	N3	57.0(2)	FE1	C5	C6	70.5(3)
CO1	N4	C24	92.1(3)	C3	C5	C4	35.8(3)
CO1	N4	C41	142.0(3)	C3	C5	C6	72.5(3)
N3	N4	C24	35.1(3)	C4	C5	C6	108.3(4)
N3	N4	C41	158.6(3)	FE1	C6	C2	70.8(3)
C24	N4	C41	124.8(4)	FE1	C6	C5	68.7(3)
N1	C1	N2	110.3(4)	C2	C6	C5	107.9(5)
N1	C1	C2	123.1(4)	FE1	C7	C8	69.3(3)
N2	C1	C2	126.6(4)	FE1	C7	C9	55.7(2)
FE1	C2	C1	136.0(3)	FE1	C7	C10	55.8(2)
FE1	C2	C3	68.5(3)	FE1	C7	C11	69.6(3)
FE1	C2	C6	68.8(3)	C8	C7	C9	36.0(3)
C1	C2	C3	127.2(5)	C8	C7	C10	72.2(4)
C1	C2	C6	125.1(5)	C8	C7	C11	108.1(5)
C3	C2	C6	106.7(4)	C9	C7	C10	36.2(2)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms cont

atom	atom	atom	angle	atom	atom	atom	angle
C9	C7	C11	72.1(4)	FE1	C11	C9	55.8(2)
C10	C7	C11	35.9(3)	FE1	C11	C10	69.8(3)
FE1	C8	C7	70.2(4)	C7	C11	C8	36.1(3)
FE1	C8	C9	69.7(3)	C7	C11	C9	72.0(4)
FE1	C8	C11	56.0(2)	C7	C11	C10	108.7(5)
C7	C8	C9	107.9(6)	C8	C11	C9	36.0(2)
C7	C8	C11	35.8(3)	C8	C11	C10	72.6(4)
C9	C8	C11	72.1(4)	C9	C11	C10	36.6(3)
FE1	C9	C7	56.3(2)	N1	C12	C13	110.5(5)
FE1	C9	C8	69.8(3)	N1	C12	C17	109.8(4)
FE1	C9	C10	69.9(3)	C13	C12	C17	109.4(5)
FE1	C9	C11	56.0(2)	C12	C13	C14	112.0(5)
C7	C9	C8	36.1(4)	C13	C14	C15	111.2(6)
C7	C9	C10	72.3(4)	C14	C15	C16	111.7(6)
C7	C9	C11	35.9(2)	C15	C16	C17	110.9(6)
C8	C9	C10	108.4(6)	C12	C17	C16	112.1(5)
C8	C9	C11	72.0(4)	N2	C18	C19	110.7(4)
C10	C9	C11	36.5(3)	N2	C18	C23	111.2(4)
FE1	C10	C7	56.0(2)	C19	C18	C23	110.5(4)
FE1	C10	C9	69.3(3)	C18	C19	C20	112.4(4)
FE1	C10	C11	69.6(3)	C19	C20	C21	111.1(5)
C7	C10	C9	71.4(4)	C20	C21	C22	111.0(4)
C7	C10	C11	35.5(3)	C21	C22	C23	111.0(5)
C9	C10	C11	106.9(5)	C18	C23	C22	110.5(5)
FE1	C11	C7	70.2(3)	N3	C24	N4	110.0(4)
FE1	C11	C8	55.9(2)	N3	C24	C25	127.4(5)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.