Crystal structure of 1,3-bis(2 -pyridylimino)isoindolinato-(dichloro)iron(III), $Fe(C_{18}H_{12}N_5)Cl_2$

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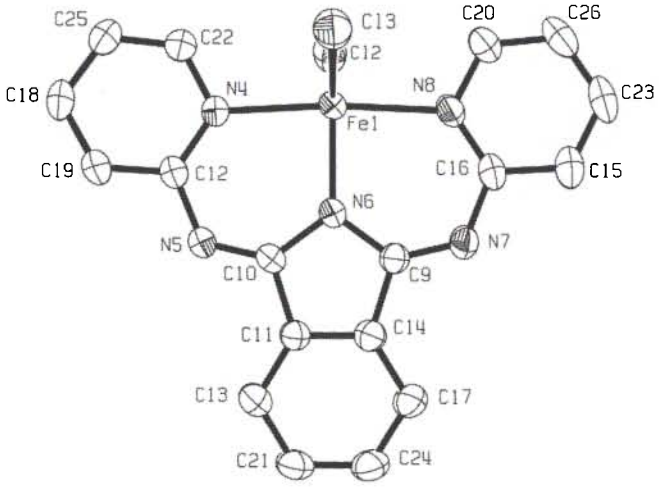
Received May 18, 1999, CCDC-No. 1267/191



Abstract

$C_{18}H_{12}Cl_2FeN_5$, triclinic, $P\bar{1}$ (No. 2), a = 8.8039(5) Å, b = 9.6444(4) Å, c = 11.3739(6) Å, α = 78.470(3)°, β = 77.976(2)°, γ = 76.058(2)°, V = 905.2 Å^3, Z = 2, ρ_m = 1.250 g·cm^{-3}, $R_{gt}(F)$ = 0.032, $wR(F)$ = 0.049, T = 298 K.

Source of material

The compound was prepared by adding 1,3-bis(2′-pyridylimino)isoindoline to a solution of $FeCl_2$ in refluxing MeOH under O_2. The brown precipitate was crystallized by diffusion of Et_2O into a CH_2Cl_2 solution.

Discussion

In the complex the Fe(III) environment is trigonal bipyramidal with two chlorine atoms and one N of the tridentate 1,3-bis-(2′-pyridylimino) isoindolinato ligand in basal positions while further two N atoms of the ligand occupy the apical positions. The Fe–N distances of 2.149(1) Å, 1.963(1) Å and 2.147(1) Å are comparable to those of the Mo(II) [1] and Ni(II) [2] complexes of the 1,3-bis(2′-pyridylimino) isoindoline ligand.

Table 1. Data collection and handling.

Crystal:	dark brown prism, size 0.2 × 0.3 × 0.3 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	185.8 cm^{-1}
Diffractometer, scan mode:	Nonius Kappa-CCD, 90 exposures, $\Delta\varphi$ = 2°
$2\theta_{max}$:	50.9°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	3360, 3360
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 3\ \sigma(I_{obs})$, 2936
$N(param)_{refined}$:	235
Program:	maXus [3]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(13)	2*i*	0.1902	0.0502	0.4085	0.05
H(15)	2*i*	0.8466	0.4282	0.5333	0.05
H(17)	2*i*	0.6795	0.2083	0.3121	0.05
H(18)	2*i*	–0.2633	0.0809	0.9453	0.05
H(19)	2*i*	–0.1151	0.0566	0.7497	0.05
H(20)	2*i*	0.4789	0.4944	0.8841	0.05
H(21)	2*i*	0.3619	0.0149	0.2285	0.05
H(22)	2*i*	0.0430	0.3124	0.9870	0.05
H(23)	2*i*	0.9010	0.5435	0.6774	0.05
H(24)	2*i*	0.6052	0.0887	0.1820	0.05
H(25)	2*i*	–0.1854	0.2200	1.0630	0.05
H(26)	2*i*	0.7157	0.5784	0.8544	0.05

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe(1)	2*i*	0.30290(2)	0.33540(2)	0.78700(1)	0.03420(9)	0.0383(1)	0.03070(9)	–0.01490(7)	–0.00390(6)	–0.00950(7)
Cl(2)	2*i*	0.15590(4)	0.55540(3)	0.80330(3)	0.0485(2)	0.0450(2)	0.0816(2)	–0.0145(1)	0.0024(2)	–0.0266(2)
Cl(3)	2*i*	0.38660(4)	0.20350(4)	0.95540(3)	0.0572(2)	0.0701(2)	0.0389(2)	–0.0256(2)	–0.0155(1)	0.0051(1)
N(4)	2*i*	0.0947(1)	0.2437(1)	0.82860(8)	0.0336(5)	0.0420(5)	0.0358(5)	–0.0158(4)	–0.0003(4)	–0.0108(4)
N(5)	2*i*	0.1245(1)	0.1505(1)	0.64250(8)	0.0339(5)	0.0487(5)	0.0380(5)	–0.0176(4)	–0.0029(4)	–0.0141(4)
N(6)	2*i*	0.3498(1)	0.26150(9)	0.63180(7)	0.0316(4)	0.0346(5)	0.0322(4)	–0.0128(4)	–0.0041(3)	–0.0077(4)

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Table 3. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(7)	2*i*	0.6063(1)	0.32440(9)	0.53940(8)	0.0352(5)	0.0405(5)	0.0365(5)	–0.0153(4)	–0.0034(4)	–0.0031(4)
N(8)	2*i*	0.5213(1)	0.4109(1)	0.73190(8)	0.0378(5)	0.0424(5)	0.0371(5)	–0.0184(4)	–0.0094(4)	–0.0059(4)
C(9)	2*i*	0.4854(1)	0.2697(1)	0.54230(9)	0.0344(5)	0.0307(5)	0.0314(5)	–0.0092(4)	–0.0044(4)	–0.0035(4)
C(10)	2*i*	0.2555(1)	0.1892(1)	0.59050(9)	0.0349(5)	0.0343(5)	0.0331(5)	–0.0102(4)	–0.0077(4)	–0.0088(5)
C(11)	2*i*	0.3328(1)	0.1549(1)	0.46920(9)	0.0389(6)	0.0366(5)	0.0308(5)	–0.0131(5)	–0.0038(4)	–0.0062(5)
C(12)	2*i*	0.0479(1)	0.1703(1)	0.7587(1)	0.0320(5)	0.0394(6)	0.0386(6)	–0.0130(5)	–0.0057(4)	–0.0085(5)
C(13)	2*i*	0.2876(1)	0.0838(1)	0.3920(1)	0.0497(7)	0.0545(7)	0.0410(6)	–0.0229(6)	–0.0066(5)	–0.0132(6)
C(14)	2*i*	0.4745(1)	0.2006(1)	0.44090(9)	0.0409(6)	0.0322(5)	0.0314(5)	–0.0104(4)	–0.0059(4)	–0.0025(5)
C(15)	2*i*	0.7702(1)	0.4412(1)	0.6066(1)	0.0368(6)	0.0508(7)	0.0556(7)	–0.0193(5)	–0.0093(5)	–0.0005(6)
C(16)	2*i*	0.6274(1)	0.3918(1)	0.6290(1)	0.0330(5)	0.0333(5)	0.0415(6)	–0.0128(4)	–0.0121(5)	0.0017(5)
C(17)	2*i*	0.5794(1)	0.1776(1)	0.3340(1)	0.0490(7)	0.0440(6)	0.0353(6)	–0.0179(5)	0.0022(5)	–0.0056(5)
C(18)	2*i*	–0.1733(2)	0.1244(2)	0.9140(1)	0.0444(7)	0.0707(9)	0.0599(8)	–0.0339(7)	0.0081(6)	–0.0167(7)
C(19)	2*i*	–0.0859(1)	0.1097(2)	0.8012(1)	0.0437(7)	0.0720(9)	0.0522(7)	–0.0331(6)	0.0007(6)	–0.0233(7)
C(20)	2*i*	0.5557(2)	0.4802(1)	0.8124(1)	0.0510(7)	0.0555(7)	0.0486(7)	–0.0241(6)	–0.0109(6)	–0.0134(6)
C(21)	2*i*	0.3915(2)	0.0625(1)	0.2841(1)	0.0663(8)	0.0576(7)	0.0344(6)	–0.0239(7)	–0.0042(6)	–0.0171(6)
C(22)	2*i*	0.0065(1)	0.2589(1)	0.9391(1)	0.0487(7)	0.0589(7)	0.0433(6)	–0.0255(6)	0.0056(5)	–0.0216(6)
C(23)	2*i*	0.8023(2)	0.5101(1)	0.6907(1)	0.0419(7)	0.0544(7)	0.0727(9)	–0.0249(6)	–0.0223(6)	0.0001(7)
C(24)	2*i*	0.5343(2)	0.1071(1)	0.2564(1)	0.0595(8)	0.0522(7)	0.0320(6)	–0.0175(6)	0.0033(5)	–0.0116(5)
C(25)	2*i*	–0.1263(2)	0.2029(1)	0.9846(1)	0.0467(7)	0.0649(8)	0.0463(7)	–0.0248(6)	0.0107(6)	–0.0180(6)
C(26)	2*i*	0.6932(2)	0.5302(1)	0.7952(1)	0.0598(8)	0.0523(7)	0.0608(8)	–0.0250(6)	–0.0282(7)	–0.0070(6)

Acknowledgments. We thank the Hungarian Research Fund (OTKA T-016285 and T-030400) and French-Hungarian Bilateral Grant (Balaton Project, F-23/96) for financial support.

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