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Crystal structure of bis(acetonitrile)-diaqua-dichloridoiron(II), $C_4H_{10}Cl_2N_2O_2Fe$

Table 1: Data collection and handling.

Crystal:	Green block
Size:	$0.50 \times 0.47 \times 0.18$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	1.98 mm^{-1}
Diffractometer, scan mode:	CCD Area Detector, φ and ω
θ_{max} , completeness:	25.0° , >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	2290, 883, 0.104
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 702
$N(\text{param})_{\text{refined}}$:	54
Programs:	Bruker [1], SHELX [2, 3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Fe1	0.0000	0.5000	0.0000	0.0281(4)
Cl1	−0.18298(11)	0.75902(11)	−0.01789(11)	0.0341(4)
O1	0.0246(5)	0.5157(3)	−0.2459(4)	0.0438(8)
H1A	−0.0621	0.5618	−0.3017	0.053*
H1B	0.0459	0.4196	−0.2865	0.053*
N1	0.2287(4)	0.6664(4)	0.0660(5)	0.0476(9)
C1	0.3235(5)	0.7615(5)	0.1265(5)	0.0370(10)
C2	0.4467(5)	0.8846(5)	0.2044(6)	0.0484(11)
H2A	0.4459	0.8815	0.3200	0.073*
H2B	0.4161	0.9970	0.1643	0.073*
H2C	0.5596	0.8564	0.1805	0.073*

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Abstract

$C_4H_{10}Cl_2N_2O_2Fe$, monoclinic, $P2_1/c$ (no. 14), $a = 7.8501(10)$ Å, $b = 7.8289(10)$ Å, $c = 8.2974(17)$ Å, $\beta = 97.840(2)^\circ$, $V = 505.17(14)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0447$, $wR_{\text{ref}}(F^2) = 0.1237$, $T = 298(2)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

Iron(II) chloride tetrahydrate (1.447 g, 10 mmol) was added to acetonitrile (30 mL). The reaction was stirred at 343 K for 24 h. After cooling, the resulting green solution was allowed to evaporate slowly at room temperature for a week, yielding green block crystals.

Experimental details

All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were assigned with common isotropic displacement factors $U_{\text{iso}}(\text{H}) = 1.5$ times $U_{\text{eq}}(\text{O, water})$, (C, methyl) and refined as riding on their parent atom.

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Comment

The solvent ligands which contain N atom have a high binding affinity to a range of metal ions, and are ligands ubiquitous in coordination chemistry [4, 5]. It has been shown that these complexes have been used in the fields of magnetism, catalysis, enzymatic reactions and biological activities [6, 7].

In this paper, we report the synthesis and crystal structure of a iron complex with acetonitrile ligand. The title structure contains one iron ion, two chloride ions, two acetonitrile ligands and two coordinated water molecules located at a center of inversion. The iron atom is six-coordinated by two chlorido ligands, two N atoms from two acetonitrile ligands and two coordinated water O atoms. Among them, the Fe–O bond lengths are 2.079(3) Å, Fe–N bond lengths are 2.225(4) Å and the Fe–Cl ones are 2.4777(9) Å, respectively. Bond lengths are in the expected ranges [8–10]. Adjacent complexes are connected by OH⋯Cl hydrogen bonds (*cf.* the figure).

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