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Crystallographic report

Tris{2-[2-(1-methyl)imidazolyl]methyliminoethyl}-aminezinc(II) dihexafluorophosphate

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The cation in the title compound has crystallographic threefold symmetry. The zinc atom is in a distorted octahedral geometry, being coordinated by three nitrogen atoms of the imine and three nitrogen atoms of imidazole. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; complex; imidazole; zinc

COMMENT

Metal complexes of imidazole and its derivatives are of current interest in the investigation of model complexes relevant to metalloenzymes, as imidazole, a residue of histidine, is frequently found to coordinate metal ions in the active centers of metalloenzymes.[1] We have recently reported a series of metal complexes with imidazole-containing ligands for mimicking the active sites of some metalloenzymes.[2,3] As a sequel to this work, we report herein the synthesis and crystal structure of a mononuclear zinc(II) complex with a polydentate ligand, tris{2-[2-(1-methyl)imidazolyl]methyliminoethyl}amine [$(mim)_3$tren], namely [Zn$(mim)_3$tren]$(PF_6)_2$ (Fig 1).

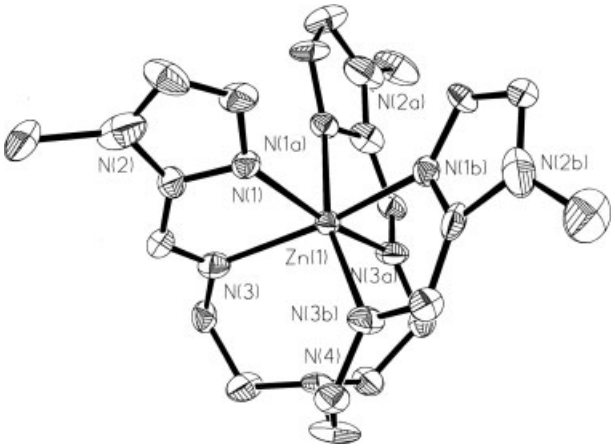

Figure 1. An ORTEP view of the cation $[Zn(mim)_3tren]^{2+}$ in $[Zn(mim)_3tren](PF_6)_2$. Key geometric parameters: Zn(1)–N(3) 2.23(2), Zn(1)–N(1) 2.17(2) Zn(1)···N(4) 3.079 Å; N(1)–Zn(1)–N(3)^i 164.9(8); N(1)^i–Zn(1)–N(1) 88.4(7), N(3)–Zn(1)–N(3)^{ii} 99.4(6), N(1)^i–Zn(1)–N(3) 95.6(8) N(1)–Zn(1)–N(3) 77.2(8)°. Symmetry operation $i: -y+1, x-y, -z$; $ii: -x+y+1, -x+1, z$.

EXPERIMENTAL

Methyl-imidazole-2-carbaldehyde (3.0 mmol, 0.330 g) was added to a solution of tri(2-aminoethyl)amine (tren, 1.0 mmol, 0.146 g) in dried methanol. The mixture was refluxed for 2 h. Then a solution of $ZnCl_2$ (1 mmol 0.136 g) and an aqueous methanol (10 ml, 1:1 v/v) solution of $NaPF_6$ (2 mmol, 0.340 g) were added. The reaction mixture turned pale yellow. After filtration, the solution was allowed to stand at room temperature for 4 days, and pale yellow crystals of [Zn$(mim)_3$tren]$(PF_6)_2$ were collected. IR (KBr, cm^{-1}): ν(C=N) 1637. Intensity data was collected at 293 K on a Siemens R3m diffractometer for a block $0.30 \times 0.35 \times 0.50$ mm^3. $C_{21}H_{30}F_{l2}N_{10}P_2Zn$, $M = 777.86$, trigonal, $P31c$, $a = 11.005(4)$, $b = 11.005(4)$, $c = 14.967(9)$ Å, $\beta = 120.0(7)°$, $V = 1569.8(10)$ Å^3, $Z = 2$, 1070 unique data ($\theta_{max} = 25.0°$), $R = 0.079$, $wR = 0.133$, $\rho_{max} = 0.72$ e$^-$ Å^{-3}. Programs used: R3m Software, SHELXS and SHELXL. CCDC deposition number: 213502.

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