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Crystallographic report

[(Pyridine)(1,2-bis(2-pyrazinecarboxamido)-4,5-dimethylbenzene)zinc(II)] monohydrate

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The N_4 donor ligand, Me_2bpzb^{2-} and a pyridine molecule are coordinated to the Zinc(II) so that the coordination geometry closely resembles a square-pyramidal environment with a nitrogen atom of the pyridine ligand occupying the apical position. Copyright © 2003 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; zinc(II); N_4 donor ligand

COMMENT

Four nitrogen atoms of the Me_2bpzb^{2-} ligand (H_2Me_2bpzb = 1,2-bis(2-pyrazinecarboxamido)-4,5-dimethylbenzene) and a nitrogen atom of the pyridine ligand are coordinated to the zinc(II) atom (Fig. 1). The two inner Zn–N distances, 2.006(3) and 2.025(3) Å, are somewhat shorter than the outer Zn–N distances, 2.111(3) and 2.125(3) Å. The Zn–N(pyridine) distance is 2.055(4) Å. The angle between the pyridine ring and the N1–N2–N3–N4 plane is 88.12(2)°. The angles between the benzene ring and pyrazine rings of the Me_2bpzb^{2-} ligand are 12.21(3)° and 16.38(2)°. The coordination geometry of the zinc atom closely resembles a square-pyramidal environment with a nitrogen atom of the pyridine ligand in an apical position.

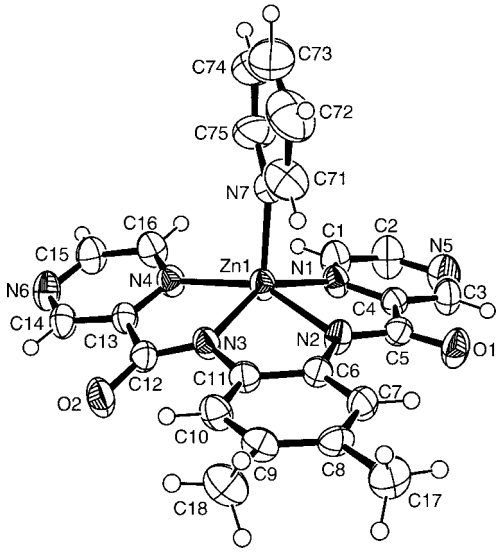

Figure 1. Molecular structure of Zn(Me_2bpzb)(py); the water molecule is not shown. Selected bond distances and angles: Zn(1)–N(1) 2.111(3), Zn(1)–N(2) 2.025(3), Zn(1)–N(3) 2.006(3), Zn(1)–N(4) 2.125(3), Zn(1)–N(7) 2.055(4) Å; N(1)–Zn(1)–N(2) 78.92(13), N(1)–Zn(1)–N(3) 146.95(14), N(1)–Zn(1)–N(4) 107.94(13), N(1)–Zn(1)–N(7) 101.76(14), N(2)–Zn(1)–N(3) 80.22(13), N(2)–Zn(1)–N(4) 151.37(14), N(2)–Zn(1)–N(7) 104.01 (14), N(3)–Zn(1)–N(4) 80.04(13), N(3)–Zn(1)–N(7) 108.00(15), N(4)–Zn(1)–N(7) 101.70(14)°.

EXPERIMENTAL

Bright-orange crystals were isolated from a 1:1 petroleum ether/pyridine solution of a solid that had precipitated from the refluxing (2 h) of 1:1 amounts of $Zn(ClO_4)_2$ and the ligand H_2Me_2bpzb[1] in methanol solution. IR (KBr): ν (C=O) 1614 and ν (C–N) 1577 cm^{-1}. Intensity data were collected at 273 K on an Enraf-Nonius MACH-3 diffractometer for a bright-orange block 0.30 × 0.30 × 0.35 mm^3. $C_{23}H_{21}N_7O_3Zn$, M = 508.84, monoclinic, $P2_1/c$, a = 12.6327(10) Å, b = 9.210(5) Å, c = 19.274(4) Å, β = 102.261(10)°, V = 2191.2(13) $Å^3$, Z = 4, 4284 unique data (R_{int} = 0.029), R = 0.043

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($Rw = 0.101$) with reflections having intensities greater than 2σ. $R = 0.084$ ($Rw = 0.112$) with for all data. Programs used: CAD-4-PC software, XCAD4, SHELXS97, SHELXL97, ORTEP-3 for Windows, CCDC deposition number: 206 512.

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