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Crystallographic report

[(1,3-Bis(4-pyridyl)propane)(diaqua)zinc(II)] diperchlorate dihydrate

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Four ligands of 1,3-bis(4-pyridyl)propane and two water molecules are coordinated to the zinc(II) atom so that the coordination geometry closely resembles a *trans*-N_4O_2 octahedral environment.

KEYWORDS: crystal structure; zinc(II); 1,3-bis(4-pyridyl)propane

COMMENT

Four nitrogen atoms derived from four ligands of 1,3-bis(4-pyridyl)propane (bpp)[1] and two water molecules are coordinated to the zinc(II) atom in the title complex. The Zn–N distances range from 2.151(3) to 2.177(4) Å, and the Zn–O distances are 2.135(3) and 2.138(3) Å. Two water molecules are also coordinated to the zinc(II) atom that define an O–Zn–O angle of 173.81(11)°. The coordination geometry of the zinc atom closely resembles an octahedral environment, with two oxygen atoms occupying mutually trans positions.

EXPERIMENTAL

Colorless crystals were isolated under the conditions such that an aqueous solution of $Zn(ClO_4)_2$ was carefully layered by a methanol solution of the ligand 1,3-bis(4-pyridyl)propane. IR (KBr): ν(O–H) 3423 and $\nu(ClO_4^-)$ 1130–1080 cm^{-1}. Anal. Found: C, 55.70; H, 5.42; N, 10.00%. Calc. for $C_{52}H_{64}Cl_2N_8O_{12}Zn$: C, 55.30; H, 5.72; N, 9.92%. Intensity data were collected at 150 K on a Nonius Kappa-CCD diffractometer using Mo Kα ($\lambda = 0.710\,73$ Å) radiation for a colorless crystal $0.04 \times 0.08 \times 0.10$ mm^3. $C_{52}H_{64}Cl_2N_8O_{12}Zn$, $M = 1129.38$, orthorhombic, *Pbca*, $a = 18.9895(7)$ Å, $b = 15.8278(8)$ Å, $c = 36.9050(13)$ Å, $V = 11092.2(8)$ $Å^3$, $Z = 8$, 9715 unique data ($\theta_{max} = 25.0°$), $R = 0.058$ (4501 reflections with $I \geq 2\sigma(I)$), $wR = 0.137$ (all data). Programs used: DENZO-SMN software package, SHEXTL V5.0, ORTEP-3. CCDC deposition number: 230886.

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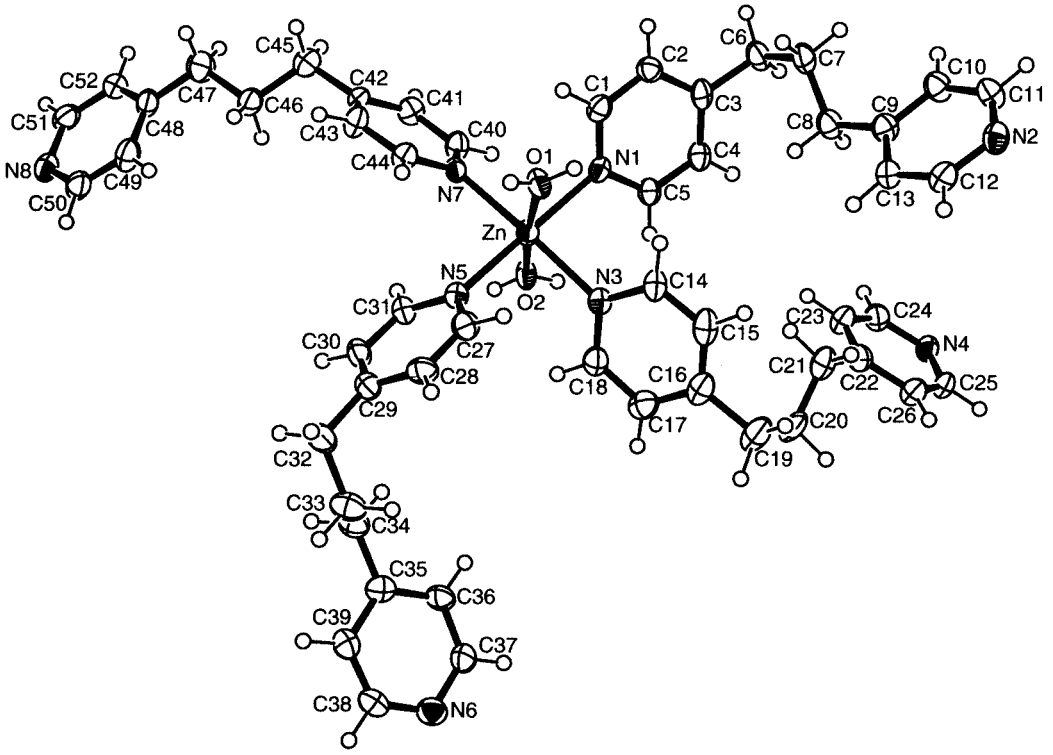

Figure 1. Molecular structure of the cation in $[Zn(bpp)_4(H_2O)_2](ClO_4)_2 \cdot 2H_2O$; the perchlorate anions and water molecules are not shown. Selected bond distances and angles: Zn–O1 2.138(3), Zn–O2 2.135(3), Zn–N1 2.173(3), Zn–N3 2.177(4), Zn–N5 2.171(3), Zn–N7 2.151(3) Å; O1–Zn–O2 173.81(11), O1–Zn–N1 85.19(12), O1–Zn–N3 90.56(13), O1–Zn–N5 91.18(12), O1–Zn–N7 92.57(13), O2–Zn–N1 88.82(12), O2–Zn–N3 87.09(13), O2–Zn–N5 94.77(12), O2–Zn–N7 89.11(13), N1–Zn–N3 90.31(13), N1–Zn–N5 176.17(13), N1–Zn–N7 91.13(13), N3–Zn–N5 88.49(13), N3–Zn–N7 176.66(13), N5–Zn–N7 90.26(13)°.