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Crystallographic report

Bis(4-nitrobenzoato)bis(pyridine)zinc(II)

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The molecular structure of $[Zn(O_2CC_6H_4NO_2\text{-}p)_2(pyridine)_2]$ exhibits a distorted N_2O_2 tetrahedral geometry around the zinc atom owing to the presence of monodentate *p*-nitrobenzoate ligands; the molecule has twofold symmetry. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; zinc; *p*-nitrobenzoate; pyridine

COMMENT

The zinc center in $[Zn(O_2CC_6H_4NO_2\text{-}p)_2(pyridine)_2]$, Fig. 1, lies on a twofold axis of symmetry and is in a distorted tetrahedral N_2O_2 coordination environment defined by two nitrogen atoms from the pyridine molecules and two carboxyl oxygen atoms derived from monodentate *p*-nitrobenzoate ligands. The structure is similar, for example, to those reported for $[Zn(2\text{-pyrrolecarboxylato})_2(1\text{-methylimidazole})_2]$[1] and $[Zn(O_2CCH_3)_2(pyridine)_2]$.[2]

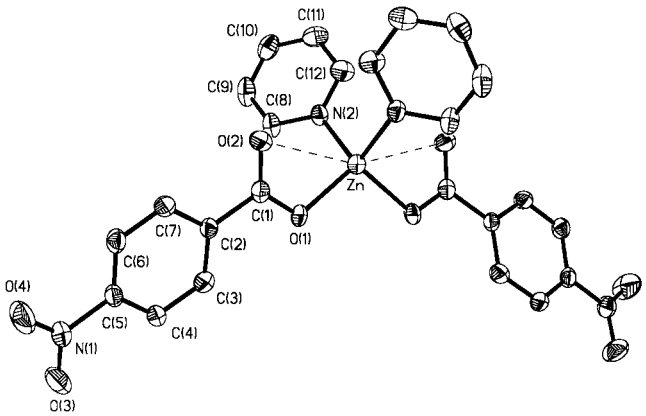

Figure 1. The molecular structure of $[Zn(O_2CC_6H_4NO_2\text{-}p)_2(pyridine)_2]$; hydrogen atoms have been omitted for clarity. Key geometric parameters: Zn–O1 1.934(4), Zn1–N2 2.033(5), Zn···O2 2.751(5), N1–O4 1.183(7), N1–O3 1.197(7), N1–C5 1.450(7) Å; O1–Zn–O1^i, 101.2(3), O1–Zn–N2 104.82(18), O1–Zn–N2^i 121.20(19), N2–Zn–N2^i 104.9(3), O4–N1–O3 123.1(6)°. Symmetry operation *i*: $1-x, y, -z+3/2$.

EXPERIMENTAL

An aqueous solution of ZnO (1.0 mmol) was added to a 50% ethanol solution of sodium *p*-nitrobenzoic acid (2.0 mmol) and pyridine (2.0 mmol) and stirred for 8.0 h at 30 °C. The white solid was obtained by filtration. The product was recrystallized from an acetonitrile solution of the compound to give colorless crystals, m.p. 166–168 °C. Intensity data were collected at 293 K on a Bruker Smart 1000 CCD for a block $0.08 \times 0.15 \times 0.25$ mm^3. $C_{24}H_{18}N_4O_8Zn$, $M = 555.79$, monoclinic, $C2/c$, $a = 14.84(3)$, $b = 6.245(12)$, $c = 24.55(5)$ Å, $\beta = 92.14(3)°$, $V = 2273(8)$ Å^3, $Z = 4$, 1820 unique data ($\theta_{max} = 25.0°$), $R = 0.053$ (1331 data with $I > 2\sigma(I)$), $wR = 0.168$ (all data). Programs used: SHELXL and ORTEP. CCDC deposition number: 227568.

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