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Crystallographic report

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

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The molecular structure of $[Zn(O_2CC_6H_4NO_2-m)_2(pyridine)_2]$ exhibits a distorted N_2O_2 tetrahedral geometry; the molecule has two fold symmetry. Copyright © 2004 John Wiley & Sons, Ltd.

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

COMMENT

The zinc atom in $[Zn(O_2CC_6H_4NO_2-m)_2(pyridine)_2]$, Fig. 1, lies on a two fold axis and is in a distorted tetrahedral N_2O_2 coordination environment defined by two nitrogen atoms of the pyridine molecules and two oxygen atoms derived from the monodentate m-nitrobenzoate ligands. The structure is similar, for example, to those reported for $[zinc(2-pyrrolecarboxylato)_2(1-methylimidazole)_2^1$ and $[Zn(O_2CCH_3)_2(pyridine)_2.^2$

EXPERIMENTAL

An aqueous solution of ZnO (1.0 mmol) was added to a 50% ethanol solution of *m*-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 ethanol solution to give colorless crystals, m.p. 178–179 °C. Intensity data were collected at 298 K on a Bruker Smart 1000 CCD for a block $0.27 \times 0.39 \times 0.45$ mm³. C₂₄H₁₈N₄O₈Zn, M = 555.79, monoclinic, C2/c, a = 14.982(6), b = 6.372(3), c = 24.808(10) Å, $\beta = 90.852(6)$ °, V = 2367.9(17) ų, Z = 4,2093 unique data ($\theta_{\rm max} = 25.0$ °), R = 0.030 (1753 data with $I > 2\sigma(I)$), wR = 0.072 (all data). Programs used: SHELXL and ORTEP. CCDC deposition number: 247032.

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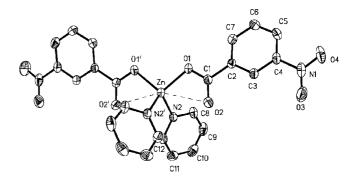


Figure 1. The molecular structure of $[Zn(O_2CC_6H_4NO_2-m)_2 (pyridine)_2]$. Key geometric parameters: Zn-O1 1.9611(16), Zn1-N2 2.0411(18), $Zn\cdots O2$ 2.7782(18) Å; O1-Zn-N2 105.98(7), $O1-Zn-O1^i$, 101.77(9), $O1-Zn-N2^i$ 118.54(7), $N2-Zn-N2^i$ 106.72(11)°. Symmetry code i: 1-x, y, 3/2-z.

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