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Crystallographic report

{[Zn($O_2CC_6H_4NO_2$-*m*)(1,10-phenanthroline)$_2$] $O_2CC_6H_4NO_2$-*m*}·$2H_2O$·$HO_2CC_6H_4NO_2$-*m*

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The structure of {[Zn($O_2CC_6H_4NO_2$-*m*)(1,10-phenanthroline)$_2$]$O_2CC_6H_4NO_2$-*m*}·$2H_2O$·$HO_2CC_6H_4NO_2$-*m* features chelating *m*-nitrobenzoate and 1,10-phenanthroline ligands so that a distorted octahedron N_4O_2 coordination geometry results. Copyright © 2005 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; zinc, *m*-nitrobenzoate; 1,10-phenanthroline

COMMENT

The structure of {[Zn($O_2CC_6H_4NO_2$-*m*)(1,10-phenanthroline)$_2$]$O_2CC_6H_4NO_2$-*m*} · $2H_2O$ · $HO_2CC_6H_4NO_2$-*m* (Fig. 1) features a chelating *m*-nitrobenzoate ligand that forms unsymmetric Zn–O bonds. The zinc center is in a distorted octahedral N_4O_2 coordination environment that is defined by four nitrogen atoms derived from two 1,10-phenanthroline ligands and two carboxyl oxygen atoms of the *m*-nitrobenzoate ligand. The coordination complex is similar, for example, to those reported for [Zn($O_2CCH_2C_6H_5$)(1, 10-phen)$_2$]NO_3[1] and [Zn(O_2CCH_3)(1, 10-phen)$_2$]ClO_4.[2]

EXPERIMENTAL

An aqueous solution of $Zn(O_2CCH_3)_2$ (1.0 mmol) was added to an ethanol solution of *m*-nitrobenzoic acid (2.0 mmol) and 1,10-phenanthroline (2.0 mmol) and stirred for 8 h at 30 °C. The white solid was obtained by filtration. The product was recrystallized from an acetonitrile solution of the complex to give colorless crystals, m.p. 287–289 °C. IR (KBr) ν(cm^{-1}): 3088, 3041, 2965, 2871, 1702, 1573, 1532, 1438, 1413, 852, 731. Intensity data were collected at 293 K on a Bruker Smart 1000 CCD for a block 0.08 × 0.17 × 0.22 mm^3. $C_{45}H_{33}N_7O_{14}Zn$, $M = 961.15$, $P\bar{1}$, $a = 12.107(6)$, $b = 14.173(7)$, $c = 15.726(8)$ Å, $\alpha = 116.420(9)$, $\beta = 90.528(9)$, $\gamma = 114.337(8)°$, $V = 2139.7(19)$Å^3, $Z = 2$, 7494 unique data ($\theta_{max} = 25.0°$), $R = 0.056$ (3140 data with $I > 2\sigma(I)$), $wR = 0.122$ (all data). Programs used: SHELXL and ORTEP. CCDC deposition number: 227567.

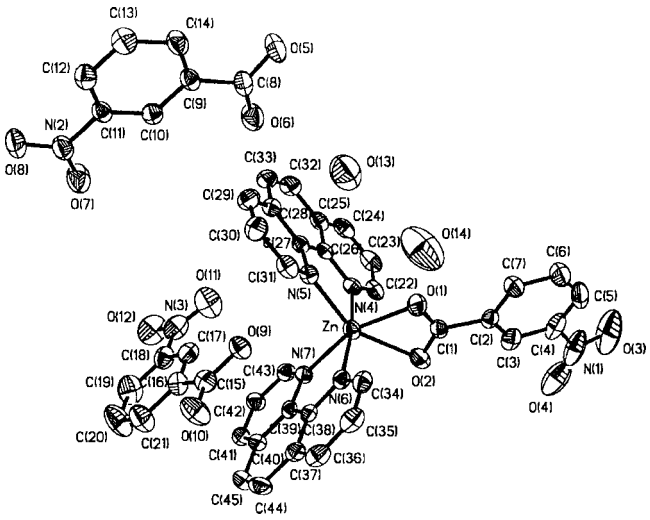

Figure 1. The molecular structure of {[Zn($O_2CC_6H_4NO_2$-*m*)(1, 10-phenanthroline)$_2$]$O_2CC_6H_4NO_2$-*m*} · $2H_2O$ · $HO_2CC_6H_4NO_2$-*m*; H atoms are omitted for clarity. Key geometric parameters: Zn–O1 2.131(4), Zn–O2 2.295(5), Zn–N4 2.170(5), Zn–N5 2.107(5), Zn–N6 2.149(5), Zn–N7 2.118(5) Å; O1–Zn–O2 59.55(18), O1–Zn–N4 95.56(18), O1–Zn–N5 98.43(19), O1–Zn–N6 93.04(19), O1–Zn–N7 159.43(18), O2–Zn–N4 87.59(19), O2–Zn–N5 152.26(17), O2–Zn–N6 97.13(17), O2–Zn–N7 102.47(19), N4–Zn–N5 77.4(2), N4–Zn–N6 171.39(19), N4–Zn–N7 93.38(19), N5–Zn–N6 100.98(19), N5–Zn–N7, 101.59(19), N6–Zn–N7 78.6(2)°.

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