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Crystallographic report

Cis-[Zn(3,5-dinitrobenzoato)$_2$(1,10-phenanthroline)$_2$]·CH_3CH_2OH

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***Cis*-[Zn(3,5-dinitrobenzoato)$_2$(1,10-phenanthroline)$_2$]·CH_3CH_2OH features unidentate and *cis*-disposed 3,5-dinitrobenzoate ligands and chelating 1,10-phenanthroline ligands so that a distorted octahedral N_4O_2 coordination geometry results. Copyright © 2004 John Wiley & Sons, Ltd.**

KEYWORDS: crystal structure; zinc; 3,5-dinitrobenzoic acid; 1,10-phenanthroline

COMMENT

The title complex, Fig. 1, features unidentate 3,5-dinitrobenzoate and chelating 1,10-phenanthroline ligands. The zinc center is in a distorted octahedral N_4O_2 coordination environment with *cis*-carboxylate ligands. The ethanol molecule of crystallization forms an H-bond with the non-coordinating O8 atom.

EXPERIMENTAL

An aqueous solution of $Zn(OAc)_2$ (1.0 mmol) was added to an ethanol solution of 3,5-dinitrobenzoic acid (2.0 mmol) and 1,10-phenanthroline (2.0 mmol) and stirred for 5 h at 30 °C. The white solid was obtained by filtration. The product was recrystallized from acetonitrile solution to give colorless crystals, m.p. 254–256 °C. IR (KBr) v: 3457, 3042, 2960, 2880, 1700, 1413, 850, 735 cm^{-1}. Intensity data were collected at 298 K on a Bruker Smart 1000 CCD for a block 0.16 × 0.36 × 0.45 mm^3. $C_{40}H_{28}N_8O_{13}Zn$, $M = 894.07$, $P2_1/c$, $a = 19.141(2)$, $b = 19.6815(17)$, $c = 10.0521(10)$ Å, $\beta = 95.668(2)°$, $V = 3768.3(7)$ $Å^3$, $Z = 4$, 6641 unique data ($\theta_{max} = 25.0°$), $R_1 = 0.048$ [3750 data with $I > 2\sigma(I)$], $wR_2 = 0.104$ (all data). Programs used: SHELXL and ORTEP. CCDC deposition no. 236304.

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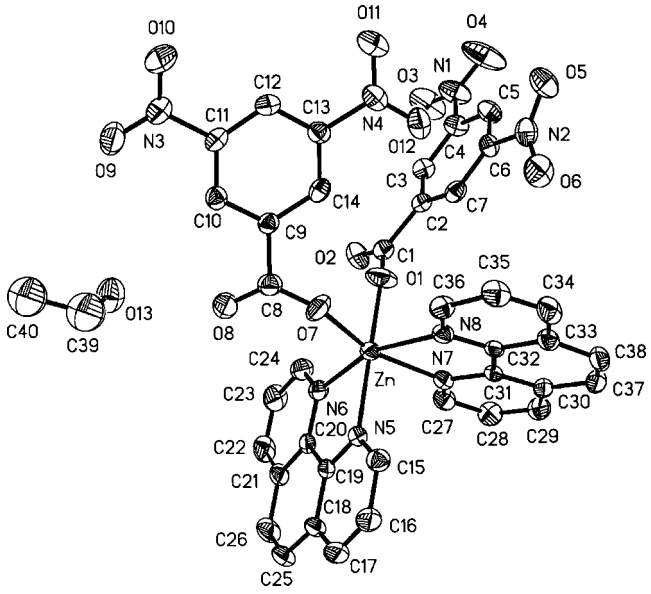

Figure 1. Molecular structure of *cis*-[Zn($O_2CC_6H_3(NO_2)_2$-3,5)(1,10-phenanthroline)$_2$·CH_3OH; H atoms are omitted. Key geometric parameters: Zn-O1 2.046(3), Zn-O7 2.009(3), Zn-N5 2.186(3), Zn-N6 2.130(3), Zn-N7 2.240(3), Zn-N8 2.165(3) Å; O1-Zn-O7 86.62(13), O1-Zn-N5 175.32(12), O7-Zn-N7 162.72(11), N6-Zn-N8, 160.82(12)°.