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Tetrakis(μ-2-nitrobenzoato-κ²O:O′)bis[(pyridine-κN)zinc(II)]

Guo-Liang Zhao* and Yi-Hang Wen

Zhejiang Key Laboratory for Reactive Chemistry on Solid Surfaces, Institute of Physical Chemistry, Zhejiang Normal University, Jinhua, Zhejiang 321004, People's Republic of China

Correspondence e-mail: sky53@zjnu.cn

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.045
wR factor = 0.103
Data-to-parameter ratio = 12.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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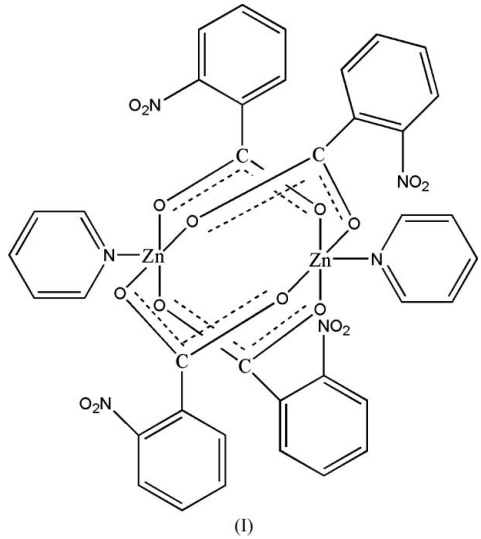
In the centrosymmetric title compound, $[Zn_2(C_7H_4NO_4)_4(C_5H_5N)_2]$, the Zn atom has a distorted square-pyramidal coordination, formed by four carboxylate O atoms and one pyridine N atom. Two Zn atoms are linked by four bridging bidentate 2-nitrobenzoate ligands to form a paddle-wheel cage structure.

Comment

One strategy in the synthesis of coordination compounds is the building-block approach (Ikeda *et al.*, 2004; Wen *et al.*, 2005), *i.e.* appropriate ligands are combined together. The combination of 2-nitrobenzoic acid and zinc hydroxide in the presence of pyridine furnishes the centrosymmetric dinuclear title compound, (I) (Fig. 1).



(I)

The Zn atom is five-coordinated by four O atoms of the carboxylate groups from four different 2-nitrobenzoates and the N atom of pyridine in a square-pyramidal geometry. The Zn lies 0.403 (2) Å out of the basal plane in the direction of the apical N atom. The dinuclear molecule features a paddle-wheel $[Zn_2O_8]$ unit with a $Zn\cdots Zn^{i}$ (symmetry code as in Table 1) separation of 3.0299 (8) Å. Another such paddle-wheel dizinc structure has recently been reported (Yang *et al.*, 2005).

Experimental

A mixture of $Zn(OH)_2$ (0.099 g, 1 mmol), 2-nitrobenzoic acid (0.335 g, 2 mmol) and water (20 ml) was sealed in a 30 ml Teflon-lined stainless steel reactor and heated to 413 K for 48 h. A colourless solution was obtained after cooling the reaction to room temperature.

Pyridine (0.16 g, 2 mmol) was added dropwise to the above solution with constant stirring for 2 h. Colourless single crystals were obtained after 5 d.

Crystal data

$[Zn_2(C_7H_4NO_4)_4(C_5H_5N)_2]$	$Z = 1$
$M_r = 953.39$	$D_x = 1.668$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 7.9627$ (9) Å	Cell parameters from 2612 reflections
$b = 10.4988$ (12) Å	$\theta = 1.7$–$25.2°$
$c = 12.3751$ (14) Å	$\mu = 1.35$ mm^{-1}
$\alpha = 76.616$ (2)°	$T = 293$ (2) K
$\beta = 87.507$ (2)°	Prism, colourless
$\gamma = 70.685$ (2)°	0.25 × 0.13 × 0.11 mm
$V = 949.18$ (19) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3360 independent reflections
ω scans	2987 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.020$
$T_{min} = 0.810$, $T_{max} = 0.862$	$\theta_{max} = 25.2°$
5090 measured reflections	$h = -9 \rightarrow 8$
	$k = -12 \rightarrow 7$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0445P)^2 + 0.6749P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.045$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.103$	$\Delta\rho_{max} = 0.52$ e Å^{-3}
$S = 1.04$	$\Delta\rho_{min} = -0.28$ e Å^{-3}
3360 reflections	
280 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Zn1—N3	2.026 (3)	Zn1—O5^{i}	2.060 (2)
Zn1—O1^{i}	2.030 (2)	Zn1—O6	2.065 (2)
Zn1—O2	2.040 (2)	Zn1—Zn1^{i}	3.0299 (8)
N3—Zn1—O1^{i}	102.34 (11)	O2—Zn1—O5^{i}	88.69 (11)
N3—Zn1—O2	100.62 (11)	N3—Zn1—O6	96.67 (10)
O1^{i}—Zn1—O2	157.04 (10)	O1^{i}—Zn1—O6	89.49 (10)
N3—Zn1—O5^{i}	105.89 (10)	O2—Zn1—O6	87.56 (10)
O1^{i}—Zn1—O5^{i}	85.36 (11)	O5^{i}—Zn1—O6	157.44 (10)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

The H atoms were positioned geometrically and refined using a riding model [C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$].

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXTL*.

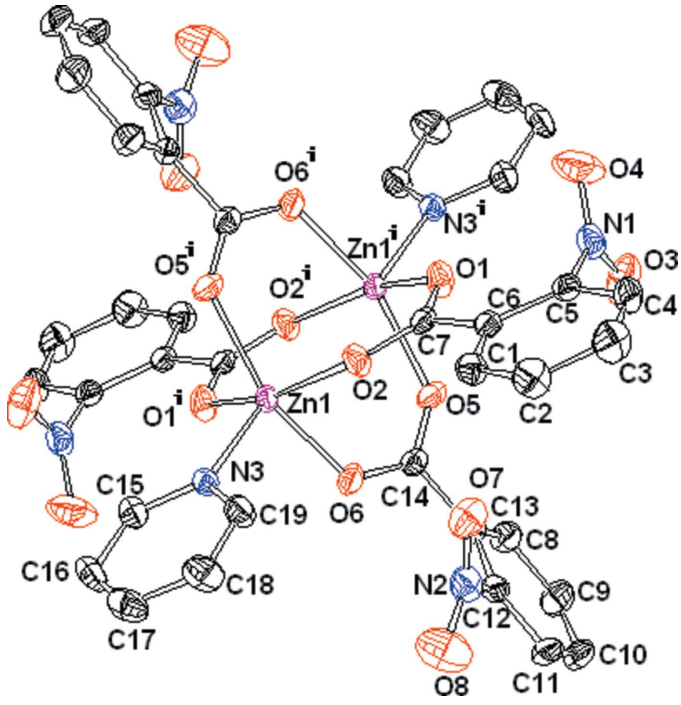


Figure 1
A view of the molecule of (I), showing the atom-labelling scheme, with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted for clarity [symmetry code: (i) $1-x, 1-y, 1-z$].

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