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# Tetrakis(2,5-pyridinedicarboxylato)tetrazinc(II) octahydrate

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**Key indicators**

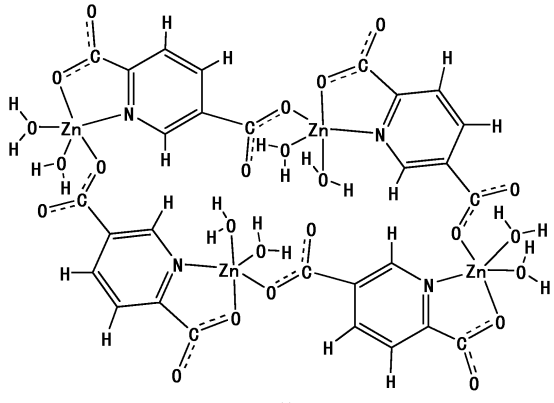
Single-crystal X-ray study
$T$ = 293 K
Mean $\sigma$(C–C) = 0.006 Å
$R$ factor = 0.041
$wR$ factor = 0.121
Data-to-parameter ratio = 10.0

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

A zinc(II) coordination discrete complex, $[Zn_4(pydc)_4(H_2O)_8]$ (pydc = 2,5-pyridinedicarboxylate, $C_7H_3NO_4$), has been prepared from the hydrothermal reaction of $[Zn(CH_3COO)_2]\cdot 2H_2O$ and $H_2$pydc in $H_2O$. The complex exhibits a rectangular structure formed from four zinc(II) and four pydc bridging ligands. The rectangular structure is interconnected by hydrogen bonds to form a three-dimensional network.

## Comment

In the last few years, much effort has been devoted to the use of transition metal ions with exo-bidentate ligands, such as polypyridyl or pyrazines and 1,4-benzenedicarboxylate, to generate polymeric metal–organic coordination polymers with two- or three-dimensional networks. Very recently, Goodgame *et al.* (1999) reported a new type of metal–organic large-pore zeotype, *i.e.* $[Zn(dimto)_2]_n\cdot n$DMF [dimto = 2,4,6-tri(1-imidazolyl)-1,3,5-triazin-2-one], which was generated from zinc bromide and 2,4,6-tri(1-imidazolyl)-1,3,5-triazine (timt). Li *et al.* (1999) reported a porous polymer, $[\{Zn_4O(bdc)_3\}(dmf)_8(C_6H_5Cl)]_n$ (bdc = 1,4-benzenedicarboxylate), which could absorb and desorb nitrogen gas. Several infinite two- and three-dimensional coordination polymers with 1,4-benzenedicarboxylate as a bridging ligand have been prepared (Hagrman *et al.*, 1999; Li *et al.*, 1998; Groenman *et al.*, 1999). However, reports on coordination polymers based on a metal cluster framework have not received much attention in this respect, although several three-dimensional polymers consisting of a metal oxide interconnected by organic molecules have been reported (Liang *et al.*, 2000). Herein we report a coordination complex, $[Zn_4(pydc)_4(H_2O)_8]$ (pydc = pyridine-2,5-dicarboxylate), (I), prepared from hydrothermal reaction of $[Zn(CH_3COO)_2]\cdot 2H_2O$ and $H_2$pydc in $H_2O$.



(I)

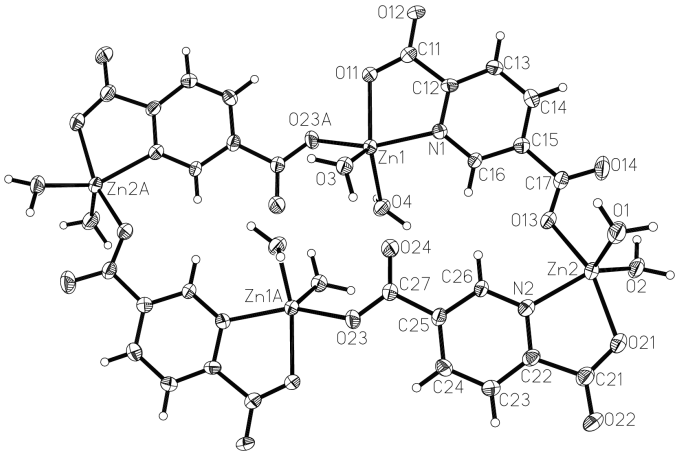



**Figure 1**
The structure of $[Zn_4(pydc)_4(H_2O)_8]$. Displacement ellipsoids are plotted at the 50% probability level.

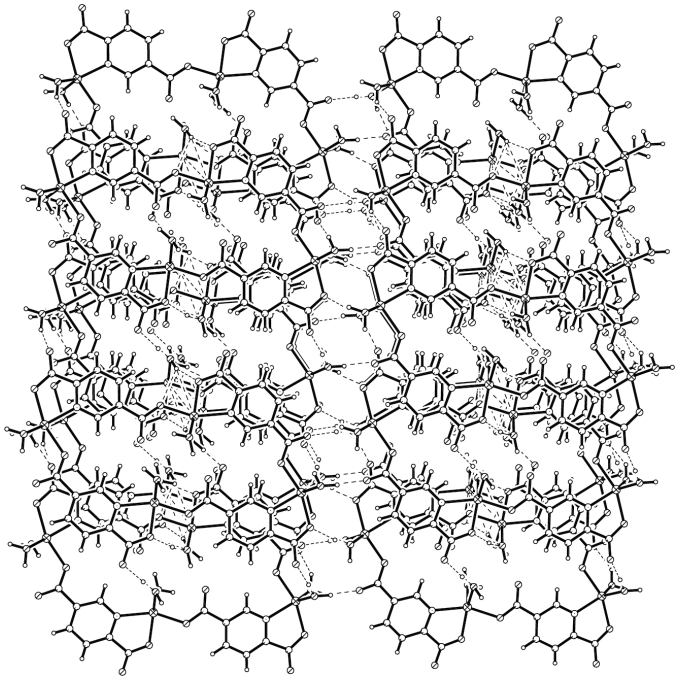


**Figure 2**
Packing diagram of $[Zn_4(pydc)_4(H_2O)_8]$.

Crystallographic analysis reveals that the compound is a discrete $[Zn_4(pydc)_4(H_2O)_8]$ molecule, in which the four Zn atoms are connected by four pydc ligands through bridges forming a rectangular structure, as shown in Fig. 1. The molecules are connected by hydrogen-bonding interactions involving the carboxylate groups and $H_2O$, with an average O···O distance of 2.708 Å, to form a three-dimensional network, as shown in Fig. 2. The coordination environment of the zinc centre in the complex is distorted bipyramidal $\{ZnO_4N\}$, of which one N atom and two O atoms are from the pydc ligand and the other two O atoms are from water molecules. Zn—O bond lengths are in the range 1.985 (4)–2.107 (3) Å and the Zn—N distances range from 2.070 (4) to 2.113 (3) Å.

## Experimental

A mixture of $[Zn(CH_3COO)_2].2H_2O$ (0.220 g, 1.0 mmol), $H_2$pydc (0.167 g, 1.0 mmol), and $H_2O$ (16 ml) in a molar ratio of *ca* 1:1:890 was sealed in a 25 ml stainless-steel reactor with a Teflon liner. The reaction system was heated at 443 K for 72 h. Slow cooling to room temperature yielded prismatic colourless crystals of the complex, which were collected by filtration.

*Crystal data*

$[Zn_4(C_7H_3NO_4)_4(H_2O)_8]$
$M_r$ = 1066.02
Triclinic, $P\overline{1}$
$a$ = 7.0512 (6) Å
$b$ = 7.3853 (6) Å
$c$ = 18.4652 (14) Å
$\alpha$ = 90.022 (1)°
$\beta$ = 96.985 (1)°
$\gamma$ = 115.630 (1)°
$V$ = 859.02 (12) Å$^3$
$Z$ = 1
$D_x$ = 2.061 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 423 reflections
$\theta$ = 8.1–19.6°
$\mu$ = 2.87 mm$^{-1}$
$T$ = 293 (2) K
Prism, colourless
0.36 × 0.18 × 0.12 mm

*Data collection*

SMART CCD diffractometer
$\omega$ scans
Absorption correction: empirical (*SHELXTL*; Sheldrick, 1997)
$T_{min}$ = 0.350, $T_{max}$ = 0.709
4717 measured reflections
3021 independent reflections
2472 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028
$\theta_{max}$ = 25.0°
$h = -8 \rightarrow 8$
$k = -8 \rightarrow 8$
$l = -21 \rightarrow 15$
Intensity decay: none

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.121
$S$ = 1.07
3021 reflections
303 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0701P)^2 + 0.0949P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.56 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.22 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Zn1—O3 | 2.009 (3) | Zn2—O1 | 1.985 (4) |
| Zn1—O23$^{i}$ | 2.020 (3) | Zn2—O2 | 2.010 (4) |
| Zn1—O4 | 2.039 (3) | Zn2—O13 | 2.040 (3) |
| Zn1—O11 | 2.107 (3) | Zn2—N2 | 2.070 (4) |
| Zn1—N1 | 2.113 (3) | Zn2—O21 | 2.103 (3) |
| | | | |
| O3—Zn1—O23$^{i}$ | 99.90 (14) | O1—Zn2—O2 | 113.39 (16) |
| O3—Zn1—O4 | 102.40 (13) | O1—Zn2—O13 | 99.80 (15) |
| O23$^{i}$—Zn1—O4 | 91.22 (13) | O2—Zn2—O13 | 89.91 (14) |
| O3—Zn1—O11 | 106.09 (13) | O1—Zn2—N2 | 110.78 (16) |
| O23$^{i}$—Zn1—O11 | 83.20 (12) | O2—Zn2—N2 | 135.66 (16) |
| O4—Zn1—O11 | 151.49 (14) | O13—Zn2—N2 | 86.40 (13) |
| O3—Zn1—N1 | 99.89 (13) | O1—Zn2—O21 | 102.65 (15) |
| O23$^{i}$—Zn1—N1 | 156.01 (14) | O2—Zn2—O21 | 88.50 (14) |
| O4—Zn1—N1 | 97.65 (13) | O13—Zn2—O21 | 156.16 (14) |
| O11—Zn1—N1 | 78.38 (12) | N2—Zn2—O21 | 78.25 (13) |

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

Data collection: *SMART* (Siemens, 1994); cell refinement: *SMART*; data reduction: *SMART*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXTL* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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