

Zwitterionic diaqua(1,10-phenanthroline)-
[3-phosphonopropionato(2-)]zinc(II)
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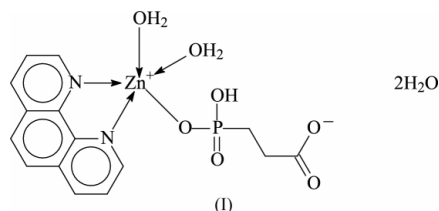
Key indicators

Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.040
 wR factor = 0.120
Data-to-parameter ratio = 16.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

In the crystal structure of the title compound, $[\text{Zn}(\text{C}_{12}\text{H}_8\text{N}_2)(\text{C}_3\text{H}_5\text{O}_5\text{P})(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$, the zinc atom is five-coordinate in a trigonal bipyramidal $\text{N}_2\text{O}_3\text{Zn}$ environment; the apical sites are occupied by the aqua ligand and the N atom of the heterocycle. Hydrogen bonds link the zwitterions and lattice water molecules into a three-dimensional network motif.

Comment

An earlier study described the centrosymmetric dinuclear Cu derivative of 3-phosphonopropionic acid, $[(\text{C}_{12}\text{H}_8\text{N}_2)(\text{C}_3\text{H}_3\text{O}_5\text{P})(\text{H}_2\text{O})\text{Cu}]_2$, in which the dianionic group, $^-\text{OP}(\text{O})(\text{OH})-\text{CH}_2-\text{CH}_2\text{CO}_2^-$, is bonded to two Cu atoms (Zhang *et al.*, 2003). The attempted synthesis of the zinc analog led to the mononuclear compound (I). The phosphato group uses only one end to bond; the negative charge of the anion formally resides at the carboxy $-\text{CO}_2^-$ end, which engages in hydrogen-bonding interactions (Table 2). The Zn atom exhibits a trigonal bipyramidal coordination; the apical sites are occupied by a water ligand and by an N atom of the N-heterocycle. The $\text{Zn}-\text{N}_{\text{apical}}$ distance is marginally longer than the $\text{Zn}-\text{N}_{\text{axial}}$ distance.



Experimental

Zinc diacetate dihydrate (0.22 g, 1.2 mmol), trimethyl 3-phosphonopropionate (0.23 g, 1 mmol), 1,10-phenanthroline (0.20 g, 1 mmol) and water (7 ml) were placed in a 15 ml Teflon-lined stainless-steel bomb, which was then heated at 423 K for 96 h. The bomb was cooled slowly to room temperature and colorless block-like crystals were isolated in about 65% yield. CH&N analysis. Found: C 38.31, H 4.55, N 5.90%; Calc. for $\text{C}_{15}\text{H}_{21}\text{N}_2\text{O}_9\text{PZn}$: C 38.36, H 4.51, N 5.96%.

Crystal data

 $[\text{Zn}(\text{C}_{12}\text{H}_8\text{N}_2)(\text{C}_3\text{H}_5\text{O}_5\text{P})-$
 $(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$
 $M_r = 469.68$
Monoclinic, $C2/c$
 $a = 24.991$ (1) Å
 $b = 7.3516$ (4) Å
 $c = 20.958$ (1) Å
 $\beta = 94.679$ (1)°
 $V = 3837.5$ (4) Å³
 $Z = 8$ $D_x = 1.626$ Mg m⁻³
Mo $K\alpha$ radiation
Cell parameters from 4886
reflections
 $\theta = 2.4-27.0^\circ$
 $\mu = 1.42$ mm⁻¹
 $T = 298$ (2) K
Block, colorless
 $0.22 \times 0.20 \times 0.16$ mm

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Data collection

Bruker SMART APEX area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2002)
 $T_{\min} = 0.619$, $T_{\max} = 0.805$
 10830 measured reflections

4145 independent reflections
 3578 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.020$
 $\theta_{\text{max}} = 27.0^\circ$
 $h = -26 \rightarrow 31$
 $k = -9 \rightarrow 9$
 $l = -26 \rightarrow 19$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.120$
 $S = 1.04$
 4145 reflections
 254 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0743P)^2 + 3.8716P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.66 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.69 \text{ e } \text{\AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

Zn1—O1	1.935 (2)	Zn1—N1	2.091 (2)
Zn1—O1w	2.000 (2)	Zn1—N2	2.137 (2)
Zn1—O2w	2.027 (2)		
O1—Zn1—O1w	93.9 (1)	O1w—Zn1—N1	91.6 (1)
O1—Zn1—O2w	113.2 (1)	O1w—Zn1—N2	163.5 (1)
O1—Zn1—N1	113.9 (1)	O2w—Zn1—N1	132.9 (1)
O1—Zn1—N2	102.2 (1)	O2w—Zn1—N2	90.7 (1)
O1w—Zn1—O2w	86.0 (1)	N1—Zn1—N2	78.8 (1)

Table 2

Hydrogen-bonding geometry (\AA , $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O2—H2o \cdots O3 ⁱ	0.82	1.76	2.553 (3)	161
O1w—H1w1 \cdots O5 ⁱⁱ	0.84	1.66	2.471 (3)	163
O1w—H1w2 \cdots O3w	0.82	2.20	2.718 (4)	121
O2w—H2w1 \cdots O3 ⁱⁱⁱ	0.85	1.81	2.647 (3)	169
O2w—H2w2 \cdots O4 ⁱⁱ	0.85	1.93	2.772 (3)	173
O3w—H3w1 \cdots O4w	0.89	2.04	2.702 (8)	130
O4w—H4w1 \cdots O1w ⁱⁱⁱ	0.86	2.21	2.764 (4)	122

Symmetry codes: (i) $\frac{1}{2} - x, \frac{3}{2} - y, 1 - z$; (ii) $\frac{1}{2} - x, y - \frac{1}{2}, \frac{3}{2} - z$; (iii) $x, y - 1, z$.

The vibration of the lattice water molecules was restrained to be approximately isotropic.

Water H atoms were placed at chemically sensible positions and their $U(H)$ values were set to $1.2U_{\text{eq}}(\text{parent O atom})$. The H atom of the PO_3 group and the carbon-bound H-atoms were placed at

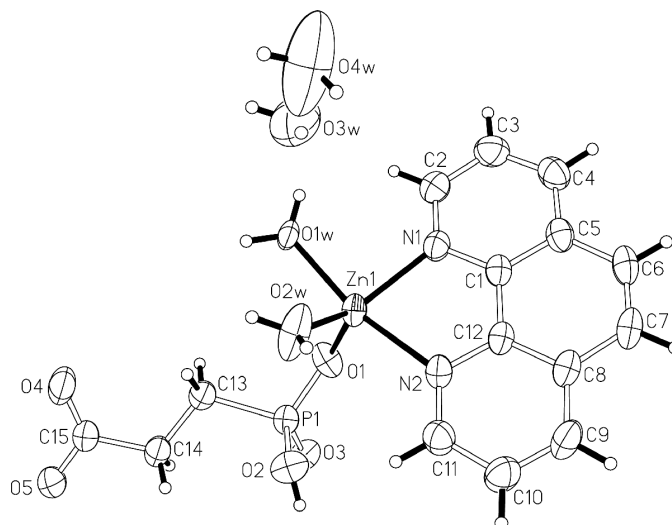


Figure 1

ORTEPII (Johnson, 1976) plot of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii.

calculated positions (O—H 0.82, C—H_{aliphatic} 0.97, C—H_{aromatic} 0.93 \AA) and refined as riding, with $U(H) = 1.2U_{\text{eq}}(C)$. The torsion angle was refined for the hydroxyl group bonded to P.

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: ORTEPII (Johnson, 1976); software used to prepare material for publication: SHELXL97.

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