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catena-Poly[[diaquazinc(II)]-μ-2,2′-bipyridine-3,3′-dicarboxyato-$\kappa^4N,N':O,O'$]

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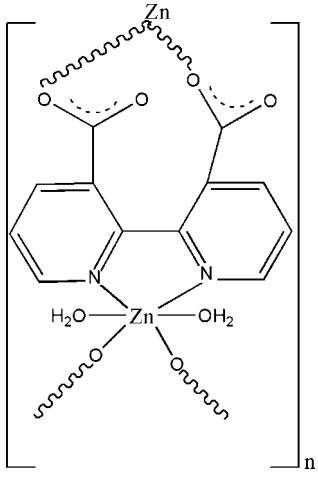
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.042; wR factor = 0.128; data-to-parameter ratio = 10.9.

In the title complex, $[Zn(C_{12}H_6N_2O_4)(H_2O)_2]_n$, the Zn atom, located on a twofold axis, is six-coordinated in a distorted octahedral arrangement, with two N atoms and two O atoms of two symmetry-related 2,2′-bipyridine-3,3′-dicarboxyate (dcbp) ligands located in the equatorial plane, while the two O atoms of the water molecules occupy the axial positions. The dcbp ligand acts as a bridging ligand, linking adjacent Zn ions and forming a one-dimensional infinite chain parallel to the b axis. O—H···O hydrogen bonds involving the coordinated water molecules connect adjacent chains to form layers parallel to the (001) plane.

Related literature

For related literature, see: Gokel *et al.* (2004); Shan *et al.* (2001); Starova *et al.* (2007).



Experimental

Crystal data

$[Zn(C_{12}H_6N_2O_4)(H_2O)_2]$
M_r = 343.59
Monoclinic, $C2/c$
a = 11.3254 (15) Å
b = 7.8829 (10) Å
c = 13.1264 (17) Å
β = 100.519 (2)°
V = 1152.2 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.17 mm^{-1}
T = 298 (2) K
0.28 × 0.22 × 0.19 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.572, T_{max} = 0.666
2925 measured reflections
1044 independent reflections
1007 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.128
S = 1.17
1044 reflections
96 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H11···O3^{i}	0.84	1.92	2.744 (4)	167
O1—H12···O3^{ii}	0.84	1.88	2.648 (4)	151

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* (Bruker, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2251).

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supplementary materials

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catena-Poly[[diaquazinc(II)]-μ-2,2'-bipyridine-3,3'-dicarboxyato-$\kappa^4N,N':O,O'$]

L. Lu, J. Wang, B.-Z. Zhao and F.-C. Zeng

Comment

Transition metal complexes with 2,2'-bipyridine derivatives are suitable models for the study of excited state dynamics. In addition, they are of interest for the development of light-energy conversion devices and optical sensors (Gokel *et al.*, 2004; Shan *et al.*, 2001). One of the simplest carbonyl-containing derivatives of 2,2'-bipyridine is the 3,3'-dicarboxy-2,2'-bipyridine molecule (dcbp). Indeed, the molecule of dcbp has two available centres for complexation: nitrogen atoms of bipyridine fragment and oxygen atoms of the carboxylic groups. The carbonyl groups are capable to form chelates when pyridine rings turn from *trans*-conformation to *cis*-conformation (Starova *et al.*, 2007).

The Zn atom, located on a twofold axis, is six-coordinated in a distorted octahedral arrangement, with two N atoms and two O atoms of two symmetry related dcbp ligands are located in the basal plane whereas two O atoms of water molecule occupy the apical positions. The dcbp ligand acts then as a bridging ligand linking adjacent Zn ions and forming a one-dimensional infinite chain parallel to the *b* axis. O—H···O hydrogen bongs involving the coordinated water molecules connect adjacent chains to form layers parallel to the (0 0 1) plane (Table 1).

Experimental

ZnSO4(0.016 g, 0.01 mmol), dcbp (0.018 g, 0.012 mmol) and NaOH(0.048 mmol,0.12 mmol), were added in a mixed solvent of ethanol and acetonitrile, the mixture was heated for five hours under reflux. during the process stirring and influx were required. The resultant was then filtered to give a pure solution which was infiltrated by diethyl ether freely in a closed vessel, a weeks later some single crystals of the size suitable for X-Ray diffraction analysis.

Refinement

All H atoms attached to C were fixed geometrically and treated as riding with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). H atoms of the coordinated water molecules were located in difference Fourier maps and included in the subsequent refinement as riding on their parent O atoms using restraints (O—H= 0.84 (1)Å and H···H= 1.39 (2) Å) with U_{iso}(H) = 1.5U_{eq}(O).

Figures

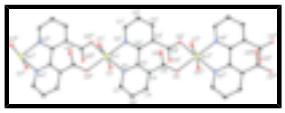


Fig. 1. Partial view of the polymeric chain in (I) with the atom-labelling scheme. Displacement ellipsoids are drawn at the 60% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i) 1 − *x*, *y*, 1/2 − *z*; (ii) *x*, *y* − 1, *z*; (iii) 1 − *x*, *y* − 1, 1/2 − *z*; (iv) *x*, 1 + *y*, *z*; (v) 1 − *x*, 1 + *y*, 1/2 − *z*]

catena-Poly[[diaquazinc(II)]-μ-2,2'-bipyridine-3,3'-dicarboxyato- $\kappa^4N,N':O,O'$]

Crystal data

$[Zn(C_{12}H_6N_2O_4)(H_2O)_2]$	F_{000} = 696
M_r = 343.59	D_x = 1.981 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 1044 reflections
a = 11.3254 (15) Å	θ = 3.2–25.2º
b = 7.8829 (10) Å	μ = 2.17 mm^{-1}
c = 13.1264 (17) Å	*T* = 298 (2) K
β = 100.519 (2)º	Block, colourless
V = 1152.2 (3) Å^3	0.28 × 0.22 × 0.19 mm
Z = 4	

Data collection

Bruker APEXII area-detector diffractometer	1044 independent reflections
Radiation source: fine-focus sealed tube	1007 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.039
Detector resolution: 0 pixels mm^{-1}	θ_{max} = 25.2º
T = 298(2) K	θ_{min} = 3.2º
φ and ω scans	*h* = −13→11
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	*k* = −9→9
T_{min} = 0.572, T_{max} = 0.666	*l* = −15→15
2925 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.042	H-atom parameters constrained
$wR(F^2)$ = 0.128	$w = 1/[\sigma^2(F_o^2) + (0.0557P)^2 + 12.6528P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.17	$(\Delta/\sigma)_{max} < 0.001$
1044 reflections	$\Delta\rho_{max}$ = 0.69 e Å^{-3}
96 parameters	$\Delta\rho_{min}$ = −0.60 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.5000	0.20313 (9)	0.2500	0.0168 (3)
N1	0.4346 (3)	0.4119 (4)	0.1576 (2)	0.0076 (7)
O1	0.3250 (2)	0.1908 (3)	0.2842 (2)	0.0107 (6)
H11	0.2660	0.2311	0.2436	0.016*
H12	0.3135	0.0913	0.3028	0.016*
O2	0.4605 (2)	1.0082 (3)	0.1389 (2)	0.0089 (6)
O3	0.6348 (2)	0.8655 (4)	0.1726 (2)	0.0116 (6)
C1	0.3727 (3)	0.3937 (5)	0.0605 (3)	0.0102 (8)
H1	0.3487	0.2856	0.0370	0.012*
C2	0.3435 (4)	0.5300 (5)	−0.0057 (3)	0.0114 (8)
H2	0.2948	0.5163	−0.0703	0.014*
C3	0.3891 (3)	0.6873 (5)	0.0275 (3)	0.0093 (8)
H3	0.3746	0.7803	−0.0166	0.011*
C4	0.4571 (3)	0.7073 (5)	0.1272 (3)	0.0065 (8)
C5	0.4707 (3)	0.5671 (5)	0.1932 (3)	0.0066 (8)
C6	0.5228 (4)	0.8741 (5)	0.1492 (3)	0.0079 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0171 (4)	0.0127 (4)	0.0197 (4)	0.000	0.0011 (3)	0.000
N1	0.0071 (15)	0.0062 (16)	0.0086 (16)	0.0004 (12)	−0.0008 (13)	−0.0006 (13)
O1	0.0061 (13)	0.0083 (14)	0.0173 (15)	0.0012 (10)	0.0011 (11)	0.0034 (11)
O2	0.0103 (13)	0.0038 (13)	0.0109 (13)	0.0012 (10)	−0.0027 (10)	−0.0008 (10)
O3	0.0079 (14)	0.0081 (14)	0.0177 (15)	0.0002 (11)	−0.0009 (11)	0.0002 (11)
C1	0.0078 (18)	0.0088 (19)	0.0131 (19)	−0.0015 (15)	−0.0004 (15)	−0.0030 (16)
C2	0.0103 (19)	0.013 (2)	0.0096 (19)	0.0012 (16)	−0.0013 (15)	−0.0029 (16)
C3	0.0076 (19)	0.0108 (19)	0.0085 (19)	0.0029 (15)	−0.0010 (15)	0.0000 (15)
C4	0.0056 (18)	0.0046 (19)	0.0093 (19)	0.0019 (14)	0.0016 (15)	−0.0021 (14)
C5	0.0060 (17)	0.0063 (18)	0.007 (2)	0.0000 (14)	0.0009 (14)	−0.0020 (15)
C6	0.0134 (19)	0.0063 (19)	0.0039 (17)	−0.0016 (15)	0.0009 (14)	0.0000 (14)

Geometric parameters (Å, °)

Zn1—N1^{i}	2.098 (3)	O2—Zn1^{iv}	2.110 (3)
Zn1—N1	2.098 (3)	O3—C6	1.252 (5)
Zn1—O2^{ii}	2.110 (3)	C1—C2	1.383 (6)
Zn1—O2^{iii}	2.110 (3)	C1—H1	0.9300
Zn1—O1	2.113 (3)	C2—C3	1.383 (6)
Zn1—O1^{i}	2.113 (3)	C2—H2	0.9300
N1—C1	1.345 (5)	C3—C4	1.401 (6)
N1—C5	1.346 (5)	C3—H3	0.9300
O1—H11	0.8379	C4—C5	1.395 (5)
O1—H12	0.8388	C4—C6	1.513 (5)
O2—C6	1.264 (5)	C5—C5^{i}	1.519 (7)
N1^{i}—Zn1—N1	76.67 (18)	H11—O1—H12	113.1
N1^{i}—Zn1—O2^{ii}	168.29 (12)	C6—O2—Zn1^{iv}	119.4 (2)
N1—Zn1—O2^{ii}	99.41 (12)	N1—C1—C2	122.4 (4)
N1^{i}—Zn1—O2^{iii}	99.41 (12)	N1—C1—H1	118.8
N1—Zn1—O2^{iii}	168.29 (12)	C2—C1—H1	118.8
O2^{ii}—Zn1—O2^{iii}	86.50 (15)	C3—C2—C1	117.8 (4)
N1^{i}—Zn1—O1	99.16 (12)	C3—C2—H2	121.1
N1—Zn1—O1	85.01 (12)	C1—C2—H2	121.1
O2^{ii}—Zn1—O1	91.41 (11)	C2—C3—C4	120.3 (4)
O2^{iii}—Zn1—O1	84.74 (11)	C2—C3—H3	119.8
N1^{i}—Zn1—O1^{i}	85.01 (12)	C4—C3—H3	119.8
N1—Zn1—O1^{i}	99.16 (12)	C5—C4—C3	118.1 (3)
O2^{ii}—Zn1—O1^{i}	84.74 (11)	C5—C4—C6	125.1 (3)
O2^{iii}—Zn1—O1^{i}	91.41 (11)	C3—C4—C6	116.3 (3)
O1—Zn1—O1^{i}	174.72 (15)	N1—C5—C4	120.8 (3)
C1—N1—C5	119.9 (3)	N1—C5—C5^{i}	113.1 (2)
C1—N1—Zn1	122.2 (3)	C4—C5—C5^{i}	126.1 (2)
C5—N1—Zn1	117.3 (2)	O3—C6—O2	126.3 (4)
Zn1—O1—H11	121.2	O3—C6—C4	116.1 (3)
Zn1—O1—H12	107.9	O2—C6—C4	117.5 (3)

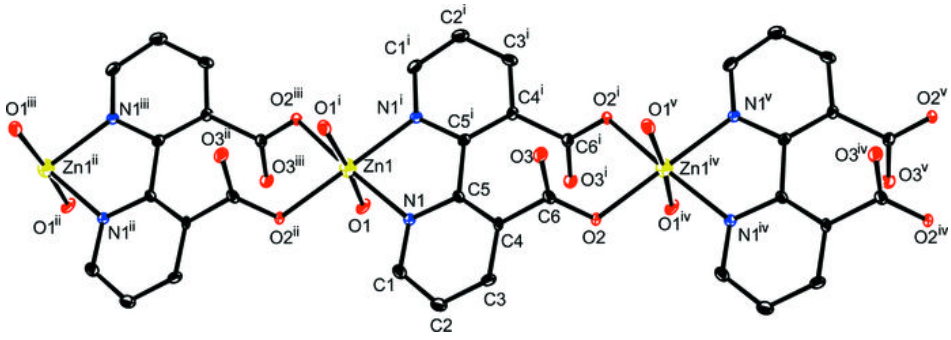
Symmetry codes: (i) −*x*+1, *y*, −*z*+1/2; (ii) *x*, *y*−1, *z*; (iii) −*x*+1, *y*−1, −*z*+1/2; (iv) *x*, *y*+1, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H11···O3^{v}	0.84	1.92	2.744 (4)	167
O1—H12···O3^{iii}	0.84	1.88	2.648 (4)	151

Symmetry codes: (v) *x*−1/2, *y*−1/2, *z*; (iii) −*x*+1, *y*−1, −*z*+1/2.

Fig. 1


O1iii
N1iii
O2iii
O1i
C2i
C1i
C3i
N1i
C4i
O2i
O1v
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Zn1ii
O3ii
O3iii
Zn1
C5i
C6i
O3
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O3iv
O3v
O1ii
N1ii
O2ii
O1
N1
C5
C6
O2
O1iv
N1iv
O2iv
C4
C1
C3
C2