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catena-Poly[[(acetato-κO)[4-(1*H*-pyrazol-3-yl)pyridine-κN^1]zinc]-μ-acetato-$\kappa^2 O:O'$]

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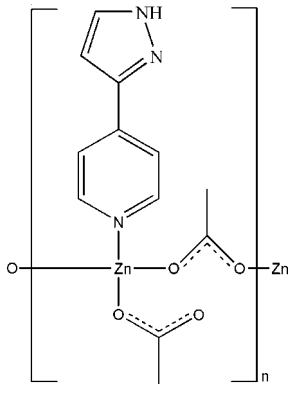
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.056; wR factor = 0.131; data-to-parameter ratio = 13.7.

In the title compound, $[Zn(CH_3CO_2)_2(C_8H_7N_3)]_n$, the Zn^{II} atom is coordinated by one N atom from a 4-(1*H*-pyrazol-3-yl)pyridine ligand and three O atoms from two bridging and one terminal acetate ligands, forming a distorted tetrahedral geometry. The bridging acetate ligands link the Zn atoms into a chain along [001]. N—H···O hydrogen bonds and π–π interactions between the pyridine and pyrazole rings [centroid–centroid distance = 3.927 (3) Å] connect the chains into a layer parallel to (011).

Related literature

For background to complexes of 4-(1*H*-pyrazol-3-yl)pyridine, see: Davies *et al.* (2005). For the synthesis of the ligand, see: Davies *et al.* (2003).



Experimental

Crystal data

$[Zn(C_2H_3O_2)_2(C_8H_7N_3)]$ M_r = 322.58
Monoclinic, $P2_1/c$
a = 16.371 (3) Å
b = 8.8526 (18) Å
c = 9.5041 (19) Å
β = 94.18 (3)°
V = 1373.7 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.80 mm^{-1}
T = 293 K
0.28 × 0.23 × 0.19 mm

Data collection

Rigaku SCXmini CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.632, T_{max} = 0.726
11822 measured reflections
2479 independent reflections
1957 reflections with $I > 2\sigma(I)$
R_{int} = 0.068

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.131
S = 1.06
2479 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—N1	2.026 (4)	Zn1—O3	1.958 (3)
Zn1—O1	1.942 (4)	Zn1—O4^{i}	1.984 (3)

Symmetry code: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O2^{ii}	0.86	1.93	2.769 (6)	163

Symmetry code: (ii) $-x, -y+1, -z+2$.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2465).

References

Brandenburg, K. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Davies, G. M., Adams, H. & Ward, M. D. (2005). *Acta Cryst.* C**61**, m485–m487.
Davies, G. M., Jeffery, J. C. & Ward, M. D. (2003). *New J. Chem.* **27**, 1550–1553.
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2011). E**67**, m1512 [**doi:10.1107/S1600536811040190**]

catena-Poly[[(acetato-κO)[4-(1*H*-pyrazol-3-yl)pyridine-κN^1]zinc]-μ-acetato-$\kappa^2 O:O'$]

Z.-D. Tan, F.-J. Tan, B. Tan and Z.-W. Yi

Comment

Pyridine derivatives are an important class of ligands for constructing metal–organic frameworks. 4-(1*H*-Pyrazol-3-yl)pyridine can be used as pyridine ligand in building coordination compounds (Davies *et al.*, 2005). In the present paper, we report the synthesis and structure of the title compound.

As shown in Fig. 1, the Zn^{II} atom exhibits a distorted tetrahedral coordination geometry, defined by one N atom from a 4-(1*H*-pyrazol-3-yl)pyridine ligand and three O atoms from two types of acetate ligands (Table 1). One acetate anion coordinates the Zn atom as a monodentate terminal ligand. The other acetate anion links the Zn atoms *via* two O atoms, forming a one-dimensional chain along [0 0 1] (Fig. 2). N—H···O hydrogen bonds (Table 2) and π–π interactions between the pyridine and pyrazole rings [centroid–centroid distance = 3.927 (3) Å] connect the chains into a layer parallel to (0 1 1) (Fig. 3).

Experimental

4-(1*H*-Pyrazol-3-yl)pyridine was prepared according to the published method of Davies *et al.* (2003). An aqueous solution (20 ml) containing zinc acetate (0.1 mmol, 22 mg) and 4-(1*H*-pyrazol-3-yl)pyridine (0.2 mmol, 29 mg) was stirred for a few minutes in air. Colorless crystals were obtained by allowing the solution to stand at room temperature for a few weeks.

Refinement

H atoms were placed at calculated positions and refined as riding atoms, with C—H = 0.93 and N—H = 0.86 Å and with $U_{iso}(H) = 1.2U_{eq}(C, N)$.

Figures

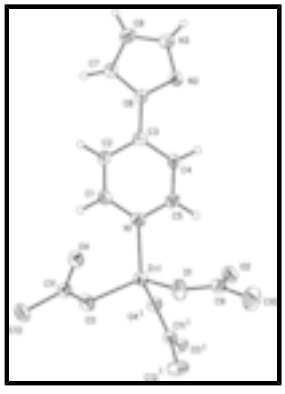

Fig. 1. The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) *x*, 3/2-*y*, 1/2+*z*.]

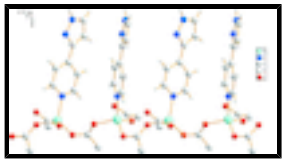

Fig. 2. A view of the one-dimensional structure of the title compound along [0 0 1].

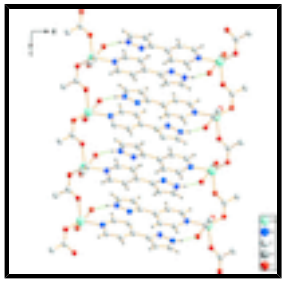

Fig. 3. A view of the layer network. Hydrogen bonds are shown as dashed lines.

catena-Poly[[(acetato-κ*O*)[4-(1*H*-pyrazol-3- yl)pyridine-κN^1]zinc]-μ-acetato-κ^2*O*:*O*']

Crystal data

$[Zn(C_2H_3O_2)_2(C_8H_7N_3)]$	$F(000) = 648$
$M_r = 322.58$	$D_x = 1.560$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 11614 reflections
$a = 16.371$ (3) Å	$\theta = 3.2$–$27.6°$
$b = 8.8526$ (18) Å	$\mu = 1.80$ mm^{-1}
$c = 9.5041$ (19) Å	$T = 293$ K
$\beta = 94.18$ (3)°	Block, colourless
$V = 1373.7$ (5) Å^3	0.28 × 0.23 × 0.19 mm
$Z = 4$	

Data collection

Rigaku SCXmini CCD diffractometer	2479 independent reflections
Radiation source: fine-focus sealed tube	1957 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.068$
ω scans	$\theta_{max} = 25.2°$, $\theta_{min} = 3.2°$
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)	$h = -19 \rightarrow 19$
$T_{min} = 0.632$, $T_{max} = 0.726$	$k = -10 \rightarrow 10$
11822 measured reflections	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.056$	Hydrogen site location: inferred from neighbouring sites

$wR(F^2) = 0.131$	H-atom parameters constrained
$S = 1.06$	$w = 1/[\sigma^2(F_o^2) + (0.063P)^2 + 1.9274P]$ where $P = (F_o^2 + 2F_c^2)/3$
2479 reflections	$(\Delta/\sigma)_{max} < 0.001$
181 parameters	$\Delta\rho_{max} = 0.51$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.54$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.34131 (3)	0.68665 (6)	1.02084 (6)	0.0343 (2)
N1	0.2233 (2)	0.7526 (5)	0.9820 (4)	0.0348 (9)
C3	0.0573 (3)	0.8142 (5)	0.9123 (5)	0.0325 (11)
C4	0.0820 (3)	0.6924 (5)	0.9969 (5)	0.0362 (11)
H4	0.0430	0.6294	1.0325	0.043*
C5	0.1635 (3)	0.6647 (6)	1.0280 (5)	0.0372 (12)
H5	0.1784	0.5813	1.0836	0.045*
C1	0.1992 (3)	0.8734 (6)	0.9045 (5)	0.0403 (12)
H1	0.2393	0.9371	0.8736	0.048*
C2	0.1192 (3)	0.9082 (5)	0.8682 (5)	0.0365 (12)
H2	0.1059	0.9938	0.8146	0.044*
N3	−0.1561 (3)	0.7919 (5)	0.8372 (5)	0.0491 (12)
H3	−0.2025	0.7466	0.8393	0.059*
C6	−0.0297 (3)	0.8401 (5)	0.8676 (5)	0.0331 (11)
N2	−0.0849 (3)	0.7342 (5)	0.8937 (5)	0.0454 (11)
C7	−0.0660 (3)	0.9619 (6)	0.7937 (5)	0.0438 (13)
H7	−0.0402	1.0480	0.7624	0.053*
C8	−0.1469 (3)	0.9277 (7)	0.7774 (6)	0.0495 (14)
H8	−0.1880	0.9870	0.7333	0.059*
O3	0.4195 (2)	0.8246 (4)	0.9418 (3)	0.0453 (9)
O1	0.3590 (2)	0.4837 (4)	0.9518 (4)	0.0500 (10)
O2	0.2878 (2)	0.3956 (4)	1.1226 (4)	0.0501 (10)
C9	0.3292 (3)	0.3761 (6)	1.0208 (6)	0.0405 (12)
C10	0.3494 (5)	0.2163 (7)	0.9709 (8)	0.072 (2)
C11	0.4183 (3)	0.8446 (5)	0.8100 (5)	0.0334 (11)
C12	0.4840 (3)	0.9438 (7)	0.7551 (6)	0.0578 (17)
O4	0.3643 (2)	0.7841 (4)	0.7269 (3)	0.0373 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0330 (3)	0.0415 (4)	0.0283 (3)	−0.0030 (3)	0.0026 (2)	−0.0012 (3)
N1	0.035 (2)	0.039 (2)	0.030 (2)	−0.004 (2)	0.0011 (18)	−0.0030 (19)
C3	0.034 (3)	0.034 (3)	0.030 (3)	0.003 (2)	0.005 (2)	−0.005 (2)
C4	0.039 (3)	0.034 (3)	0.036 (3)	−0.004 (2)	0.007 (2)	0.008 (2)
C5	0.040 (3)	0.041 (3)	0.030 (3)	0.003 (2)	0.003 (2)	0.006 (2)
C1	0.040 (3)	0.041 (3)	0.040 (3)	−0.010 (2)	0.004 (2)	0.003 (2)

C2	0.042 (3)	0.032 (3)	0.036 (3)	0.001 (2)	0.005 (2)	0.007 (2)
N3	0.032 (2)	0.053 (3)	0.061 (3)	−0.001 (2)	−0.002 (2)	0.007 (2)
C6	0.037 (3)	0.031 (3)	0.031 (3)	0.000 (2)	0.004 (2)	0.000 (2)
N2	0.034 (3)	0.039 (3)	0.063 (3)	−0.004 (2)	0.003 (2)	0.008 (2)
C7	0.045 (3)	0.043 (3)	0.043 (3)	−0.002 (3)	0.000 (2)	0.010 (3)
C8	0.042 (3)	0.054 (4)	0.052 (3)	0.009 (3)	−0.001 (3)	0.010 (3)
O3	0.048 (2)	0.061 (2)	0.0267 (19)	−0.0171 (18)	0.0011 (15)	0.0038 (17)
O1	0.068 (3)	0.038 (2)	0.046 (2)	−0.0065 (19)	0.0162 (19)	−0.0039 (17)
O2	0.044 (2)	0.046 (2)	0.062 (3)	−0.0055 (18)	0.0122 (19)	0.0023 (19)
C9	0.036 (3)	0.042 (3)	0.042 (3)	−0.004 (2)	−0.008 (2)	−0.001 (3)
C10	0.094 (5)	0.037 (4)	0.086 (5)	0.005 (3)	0.006 (4)	−0.013 (3)
C11	0.036 (3)	0.035 (3)	0.030 (3)	0.002 (2)	0.004 (2)	0.001 (2)
C12	0.047 (3)	0.075 (4)	0.052 (4)	−0.023 (3)	0.005 (3)	0.015 (3)
O4	0.042 (2)	0.044 (2)	0.0258 (17)	−0.0044 (16)	0.0040 (15)	−0.0009 (15)

Geometric parameters (Å, °)

Zn1—N1	2.026 (4)	N3—C8	1.344 (7)
Zn1—O1	1.942 (4)	N3—N2	1.348 (6)
Zn1—O3	1.958 (3)	N3—H3	0.8600
Zn1—O4^{i}	1.984 (3)	C6—N2	1.338 (6)
N1—C1	1.341 (6)	C6—C7	1.395 (7)
N1—C5	1.348 (6)	C7—C8	1.356 (7)
C3—C4	1.387 (6)	C7—H7	0.9300
C3—C2	1.398 (7)	C8—H8	0.9300
C3—C6	1.475 (7)	O3—C11	1.264 (6)
C4—C5	1.368 (7)	O1—C9	1.274 (6)
C4—H4	0.9300	O2—C9	1.233 (6)
C5—H5	0.9300	C9—C10	1.536 (8)
C1—C2	1.365 (7)	C11—O4	1.261 (5)
C1—H1	0.9300	C11—C12	1.510 (7)
C2—H2	0.9300		
O1—Zn1—O3	109.25 (16)	C3—C2—H2	120.2
O1—Zn1—O4^{i}	115.59 (15)	C8—N3—N2	112.7 (4)
O3—Zn1—O4^{i}	102.40 (14)	C8—N3—H3	123.6
O1—Zn1—N1	111.65 (17)	N2—N3—H3	123.6
O3—Zn1—N1	113.05 (16)	N2—C6—C7	111.5 (4)
O4^{i}—Zn1—N1	104.60 (15)	N2—C6—C3	119.3 (4)
C1—N1—C5	116.5 (4)	C7—C6—C3	129.2 (4)
C1—N1—Zn1	124.6 (3)	C6—N2—N3	103.7 (4)
C5—N1—Zn1	118.7 (3)	C8—C7—C6	105.1 (5)
C4—C3—C2	116.7 (4)	C8—C7—H7	127.4
C4—C3—C6	121.4 (4)	C6—C7—H7	127.4
C2—C3—C6	121.8 (4)	N3—C8—C7	106.9 (5)
C5—C4—C3	120.2 (4)	N3—C8—H8	126.5
C5—C4—H4	119.9	C7—C8—H8	126.5
C3—C4—H4	119.9	C11—O3—Zn1	120.3 (3)
N1—C5—C4	123.1 (5)	C9—O1—Zn1	116.5 (3)

N1—C5—H5	118.4	O2—C9—O1	123.5 (5)
C4—C5—H5	118.4	O2—C9—C10	121.0 (5)
N1—C1—C2	123.9 (5)	O1—C9—C10	115.5 (5)
N1—C1—H1	118.1	O4—C11—O3	121.4 (4)
C2—C1—H1	118.1	O4—C11—C12	121.0 (4)
C1—C2—C3	119.5 (5)	O3—C11—C12	117.6 (4)
C1—C2—H2	120.2	C11—O4—Zn1^{ii}	129.6 (3)

Symmetry codes: (i) *x*, −*y*+3/2, *z*+1/2; (ii) *x*, −*y*+3/2, *z*−1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O2^{iii}	0.86	1.93	2.769 (6)	163

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

Fig. 1

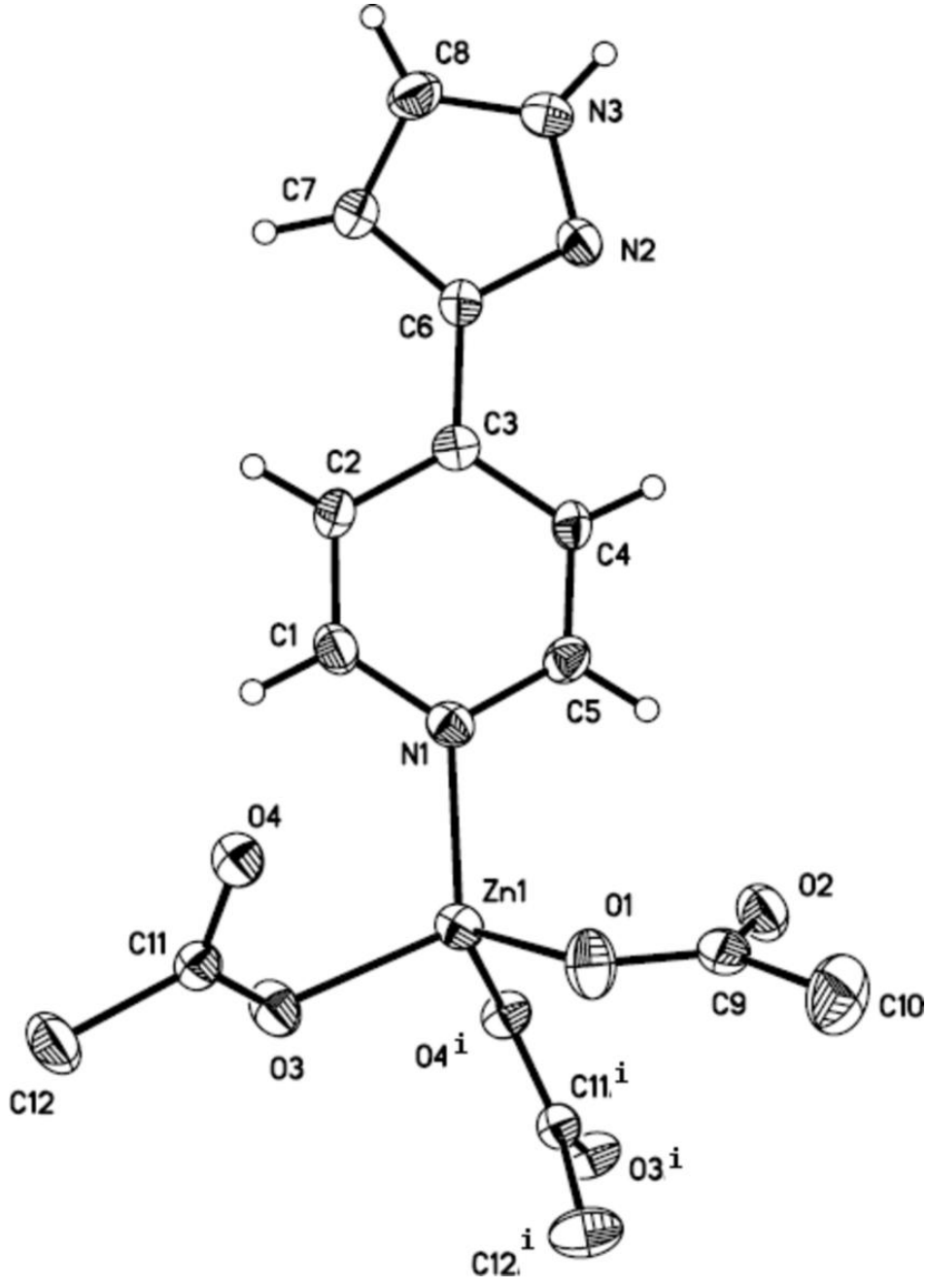
C8
N3
C7
N2
C6
C3
C2
C4
C1
C5
N1
O4
Zn1
O1
O2
C11
C9
C10
O3
C12
O4 i
C11 i
O3 i
C12 i

Fig. 2

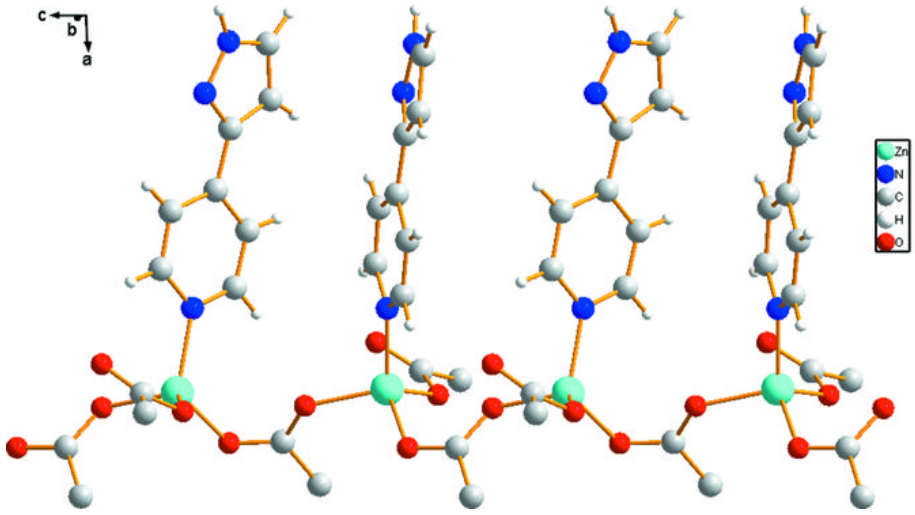

Fig. 3