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## Structure Reports

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 (Croconato- $\kappa^2O,O'$ )bis(1,10-phenanthroline- $\kappa^2N,N'$ )zinc(II)

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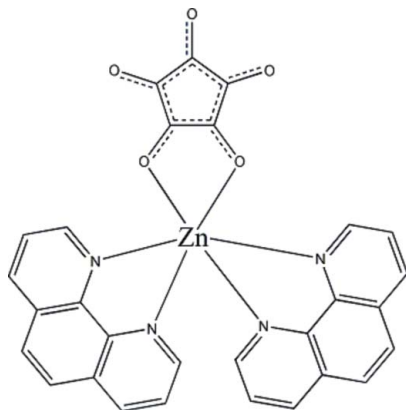
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 Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(C-C) = 0.003$  Å;  $R$  factor = 0.029;  $wR$  factor = 0.096; data-to-parameter ratio = 14.7.

In the title compound,  $[Zn(C_5O_5)(C_{12}H_8N_2)_2]$ , the Zn atom is in a slightly distorted octahedral environment. The molecule lies across a twofold rotation axis, around which two 1,10-phenanthroline ligands are arranged. There are short contacts between the 1,10-phenanthroline groups and the O atoms of the croconate ligand, which probably stabilize the crystal structure *via* weak C—H...O interactions.

## Related literature

For related literature, see: Braga *et al.* (2002); Carranza *et al.* (2004); Castro *et al.* (1992, 2002); Chen *et al.* (2005, 2007, 2008); Faus *et al.* (1994); Maji *et al.* (2003); Seitz & Imming (1992); Sletten *et al.* (1998); Wang *et al.* (2002).



## Experimental

## Crystal data

$[Zn(C_5O_5)(C_{12}H_8N_2)_2]$   
 $M_r = 565.83$   
 Orthorhombic, *Pbcn*  
 $a = 12.2605$  (4) Å  
 $b = 11.0133$  (3) Å  
 $c = 17.2745$  (5) Å  
 $V = 2332.55$  (12) Å<sup>3</sup>  
 $Z = 4$

 Mo  $K\alpha$  radiation  
 $\mu = 1.11$  mm<sup>-1</sup>
 $T = 293$  (2) K  
 $0.28 \times 0.23 \times 0.15$  mm

## Data collection

Bruker APEX2 CCD area-detector diffractometer  
 Absorption correction: multi-scan (*APEX2*; Bruker, 2005)  
 $T_{\min} = 0.743$ ,  $T_{\max} = 0.782$   
 (expected range = 0.805–0.847)

9769 measured reflections  
 2627 independent reflections  
 2164 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.019$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$   
 $wR(F^2) = 0.096$   
 $S = 1.28$   
 2627 reflections

179 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.29$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.32$  e Å<sup>-3</sup>

Table 1

Selected bond lengths (Å).

N1—Zn1	2.1493 (15)	O1—Zn1	2.1325 (14)
N2—Zn1	2.1664 (17)		

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C6—H6...O1 <sup>i</sup>	0.93	2.47	3.295 (2)	149
C11—H11...O3 <sup>ii</sup>	0.93	2.55	3.147 (2)	122

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2254).

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**supplementary materials**

*Acta Cryst.* (2008). E64, m1507-m1508 [ doi:10.1107/S1600536808033709 ]

## (Croconato- $\kappa^2O,O'$ )bis(1,10-phenanthroline- $\kappa^2N,N'$ )zinc(II)

H. Chen, P. Li, L. Dong, X. Zhu and Q. Fang

### Comment

The dianion of croconic acid(4,5-dihydroxycyclopent-4-ene-1,2,3-trione),  $(C_5O_5)^{2-}$ , is one of the cyclic aromatic oxocarbons  $(CO)_n^{2-}$  characterized by extensive delocalization of the  $\pi$  electrons all over the ring (Seitz & Imming, 1992). Previous reports reveal that croconate is a polydent ligand(Chen *et al.*, 2005, Maji *et al.*, 2003, Wang *et al.*, 2002, Sletten *et al.*, 1998). According to the concept of 'molecular self-organization' and 'molecular engineering', transition metal croconates associated with another ligand such as terpyridine (Castro *et al.* 2002), bis((bis(2-pyridylcarbonyl) amido (Maji *et al.*, 2003), 2,2'-bipyridine (Castro *et al.*, 1992) or the tetrakis(2-pyridyl)pyrazine (Carranza *et al.* 2004) show interesting properties in magnetism, biochemistry, catalyst *et al.*

1,10-Phenanthroline(phen) is a well known neutral bidentate ligand. There have been considerable interests in the synthesis of open-framework phen-based metal complexes because of their interesting structure chemistry and potential applications(Faus *et al.* 1994). Recently, many research activities have focused on the synthesis of hybrid framework by incorporate organic ligand in the structure of phen-based complexes. Among the family of cyclic oxocarbons of the formula  $(CO)_n^{2-}$  [ $n=2-6$  for oxalate, delatate, squarate, croconate and rhodizonate anions, respectively], the croconate moiety,  $(C_5O_5)^{2-}$ , was found to be a good candidate and has been successfully incorporated into phen-based frameworks in our previous work,  $[M(\text{phen})_2(C_5O_5)]$  ( $M=$  Cu, Ni, Co, Mn) (Chen *et al.*, 2005, 2007, 2008). Here, we report a new member of this family:  $[Zn(\text{phen})_2(C_5O_5)]$ .

In the title structure, asymmetry unit contains a phen moiety and half a croconate group coordinated with a zinc ion. The title compound lies across twofold rotation axes which passes through the Zn atom and bisects the croconate ligand, around which two phen ligand are arranged in a chiral propeller manner. A unit cell contains four  $[Zn(\text{phen})_2(C_5O_5)]$  molecules.

As a good  $\pi$ -conjugation system, the croconate dianion('free' ligand) in its simple salt has a planar  $D_{5h}$  conformation with five almost identical C?O bonds and five almost identical C?C bonds, such as in  $Rb_2C_5O_5$  and  $Cs_2C_5O_5$  crystals (Braga *et al.*, 2002). However, the coordinated ligand in title complex obviously deviates from  $D_{5h}$  symmetry. The C?O bond involving coordinated O atoms is longer than that involving the uncoordinated O atoms. In the title complex, the C?O bond lengths are 1.229 (3) Å and 1.228 (4) Å for the uncoordinated O atoms and 1.277 (2) Å for the coordinated O atoms.

The molecular conformation of  $[Zn(\text{phen})_2(C_5O_5)]$  is close to  $[Co(\text{phen})_2(C_5O_5)]$  and  $[Ni(\text{phen})_2(C_5O_5)]$  while different from  $[Cu(\text{phen})_2(C_5O_5)]$  and  $[Mn(\text{phen})_2(C_5O_5)]$ . The dihedral angle between the two phen planes for the title compound is 85.3 (1)° and the croconate and phen planes are also effectively perpendicular, with a dihedral angle of 87.7 (1)°. Compared with our previous reported result(Chen *et al.* 2005, 2007, 2008), the crystal growth method not only influence crystal packing motif, but also have effect on the molecular configuration. The crystal of  $[Zn(\text{phen})_2(C_5O_5)]$ ,  $[Co(\text{phen})_2(C_5O_5)]$  and  $[Ni(\text{phen})_2(C_5O_5)]$  are grown by hydrothermal method while the crystal of  $[Cu(\text{phen})_2(C_5O_5)]$  and  $[Mn(\text{phen})_2(C_5O_5)]$  are obtained by solvent evaporation under room temperature. Correspondingly, the crystal packing motif for crystal of Ni,

## supplementary materials

Co, and Zn complexes are  $P_{bcn}$ , while it is  $C2/c$  for Cu and Mn complexes. As for the molecular configuration, the dihedral angles between the two phen planes for the complexes of Zn, Co, Ni are  $87.7 (1)^\circ$ ,  $85.7 (1)^\circ$ ,  $86.0 (1)^\circ$  which are almost perpendicular to each other, but they are  $46.5 (1)^\circ$  and  $40.7 (1)^\circ$  for Cu and Mn complexes.

According to the Jahn-teller effect theory (if a d-orbital of a transition metal ion is empty or full-filled and the other equivalent orbital is half full-filled, the coordinate environment of the transition metal ion will be distorted to form a more stable configuration),  $Cu^{2+}$  and  $Mn^{2+}$  have a strong tendency to Jahn-teller distortion while  $Zn^{2+}$  and  $Ni^{2+}$  are not. So, the local polyhedral  $MN_4O_2$  ( $M=Zn, Co, Ni$ ) in their complexes are close to the octahedral while  $MN_4O_2$  ( $M=Mn, Cu$ ) in their complexes are severely distorted from the octahedral. In the title compound, the values of the angles subtended by the bidentate at zinc atom [ $77.37 (6)^\circ$ ] deviate significantly from the ideal value of  $90^\circ$  due to the small bite size of the five-membered planar chelate rings.

As shown in Fig.2, the dipole moments of  $[Zn(phen)_2(C_5O_5)]$  are arranged alternatively along +b and -b directions. There are short contacts between the phen groups and the O atoms of the croconate [e.g.  $C(6)-H(6)\cdots O(1)$  ( $x, -y, -1/2 + z$ ) and  $C(11)-H(11)\cdots O(3)$  ( $-1/2 + x, -1/2 + y, 3/2 - z$ ), which probably stabilize the crystal structure.

### Experimental

$[K_2(C_5O_5)]$  (0.10 g) and  $Zn(CH_3COO)_2 \cdot 2H_2O$  (0.10 g) were dissolved in solvent of water 15 ml. The mixture was heated to 340–350 K under continuous stirring for 20 min. To the resulting yellow solution, an ethanol solution (10 ml) of 1,10-phenanthroline (0.1 mol/L) was added to cause an immediate precipitation of yellow microcrystal. After the solutions were left to stand at room temperature for 30 minutes, they were collected by filter suction, washed with water. Then the obtained precipitation and 15 ml water was placed in the teflon liner of an autoclave, which was sealed and heated to 433 K for 48 h, cooled at speed of 10 K/min, whereupon yellow block of  $[Zn(phen)_2(C_5O_5)]$  were obtained.

### Refinement

All H atoms were geometrically fixed and allowed to ride on their attached atoms, which  $C-H = 0.93 \text{ \AA}$  and  $U_{iso}(H) = 1.2 U_{eq}(C)$ .

### Figures

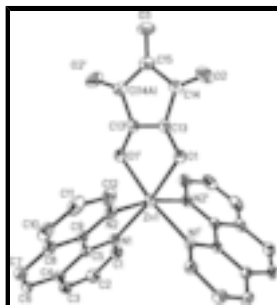


Fig. 1. Molecular structure with thermal ellipsoids at 30% probability levels. [symmetry code:  $-x + 1/2, y, -z + 3/2$ ]

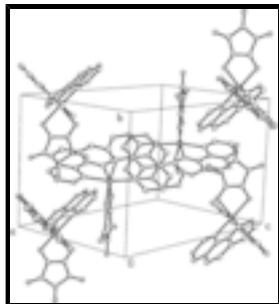


Fig. 2. A packing diagram of the title compound.

**(Croconato- $\kappa^2O,O'$ )bis(1,10-phenanthroline- $\kappa^2N,N'$ )zinc(II)**
*Crystal data*
 $[Zn(C_5O_5)(C_{12}H_8N_2)_2]$ 
 $M_r = 565.83$ 

 Orthorhombic, *Pbcn*

Hall symbol: -P 2n 2ab

 $a = 12.2605 (4) \text{ \AA}$ 
 $b = 11.0133 (3) \text{ \AA}$ 
 $c = 17.2745 (5) \text{ \AA}$ 
 $V = 2332.55 (12) \text{ \AA}^3$ 
 $Z = 4$ 
 $F_{000} = 1152$ 
 $D_x = 1.611 \text{ Mg m}^{-3}$ 

 Mo  $K\alpha$  radiation

 $\lambda = 0.71073 \text{ \AA}$ 

Cell parameters from 3967 reflections

 $\theta = 2.8\text{--}27.5^\circ$ 
 $\mu = 1.11 \text{ mm}^{-1}$ 
 $T = 293 (2) \text{ K}$ 

Prism, yellow

 $0.28 \times 0.23 \times 0.15 \text{ mm}$ 
*Data collection*

 Bruker APEXII CCD area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

 Detector resolution:  $10.0 \text{ pixels mm}^{-1}$ 
 $T = 295(2) \text{ K}$ 
 $\varphi$  and  $\omega$  scans

 Absorption correction: multi-scan  
(APEX2; Bruker, 2005)

 $T_{\min} = 0.743$ ,  $T_{\max} = 0.782$ 

9769 measured reflections

2627 independent reflections

 2164 reflections with  $I > 2\sigma(I)$ 
 $R_{\text{int}} = 0.019$ 
 $\theta_{\max} = 27.6^\circ$ 
 $\theta_{\min} = 2.4^\circ$ 
 $h = -15 \rightarrow 14$ 
 $k = -14 \rightarrow 13$ 
 $l = -21 \rightarrow 21$ 
*Refinement*

 Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.029$ 
 $wR(F^2) = 0.096$ 

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0414P)^2 + 0.6435P]$$

 where  $P = (F_o^2 + 2F_c^2)/3$ 
 $(\Delta/\sigma)_{\max} < 0.001$

## supplementary materials

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$S = 1.28$	$\Delta\rho_{\max} = 0.29 \text{ e } \text{\AA}^{-3}$
2627 reflections	$\Delta\rho_{\min} = -0.32 \text{ e } \text{\AA}^{-3}$
179 parameters	Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0037 (5)
Secondary atom site location: difference Fourier map	

### 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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	1.14583 (16)	-0.08987 (18)	0.66696 (12)	0.0370 (4)
H1	1.1977	-0.0725	0.7047	0.044*
C2	1.17077 (19)	-0.1768 (2)	0.61125 (13)	0.0442 (5)
H2	1.2374	-0.2171	0.6123	0.053*
C3	1.09642 (18)	-0.20164 (18)	0.55543 (12)	0.0411 (5)
H3	1.1121	-0.2598	0.5180	0.049*
C4	0.99594 (16)	-0.14043 (18)	0.55356 (12)	0.0346 (4)
C5	0.97663 (15)	-0.05585 (16)	0.61341 (10)	0.0284 (4)
C6	0.91524 (18)	-0.15647 (19)	0.49514 (12)	0.0406 (5)
H6	0.9282	-0.2110	0.4551	0.049*
C7	0.82034 (19)	-0.09419 (19)	0.49667 (13)	0.0434 (5)
H7	0.7700	-0.1051	0.4570	0.052*
C8	0.79598 (16)	-0.01181 (19)	0.55831 (11)	0.0371 (4)
C9	0.87469 (15)	0.00774 (16)	0.61615 (11)	0.0305 (4)
C10	0.69824 (18)	0.0534 (2)	0.56380 (14)	0.0503 (6)
H10	0.6443	0.0438	0.5264	0.060*
C11	0.68264 (19)	0.1309 (2)	0.62399 (15)	0.0535 (6)
H11	0.6177	0.1740	0.6281	0.064*
C12	0.76426 (18)	0.1457 (2)	0.67964 (13)	0.0460 (5)
H12	0.7522	0.1985	0.7208	0.055*
C13	0.96697 (16)	0.35065 (18)	0.78378 (11)	0.0334 (4)
C14	0.94811 (17)	0.47521 (18)	0.80990 (13)	0.0409 (5)
C15	1.0000	0.5549 (3)	0.7500	0.0419 (7)
N1	1.05186 (12)	-0.03074 (13)	0.66885 (9)	0.0290 (3)
N2	0.85892 (13)	0.08653 (15)	0.67547 (9)	0.0352 (4)

O1	0.93325 (12)	0.25245 (13)	0.81491 (8)	0.0415 (3)
O2	0.89952 (16)	0.50881 (16)	0.86832 (11)	0.0659 (5)
O3	1.0000	0.6664 (2)	0.7500	0.0560 (7)
Zn1	1.0000	0.10546 (3)	0.7500	0.03197 (13)

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0350 (10)	0.0405 (11)	0.0355 (11)	0.0036 (8)	-0.0035 (8)	0.0000 (8)
C2	0.0441 (11)	0.0421 (11)	0.0465 (13)	0.0118 (9)	0.0055 (10)	-0.0014 (9)
C3	0.0551 (13)	0.0326 (10)	0.0356 (11)	0.0030 (9)	0.0093 (9)	-0.0061 (9)
C4	0.0457 (11)	0.0278 (8)	0.0302 (10)	-0.0086 (8)	0.0057 (8)	-0.0008 (8)
C5	0.0348 (9)	0.0270 (9)	0.0235 (9)	-0.0044 (7)	-0.0003 (7)	0.0029 (7)
C6	0.0579 (13)	0.0387 (11)	0.0253 (10)	-0.0166 (10)	-0.0015 (9)	-0.0029 (8)
C7	0.0504 (12)	0.0458 (12)	0.0340 (12)	-0.0204 (10)	-0.0078 (9)	0.0041 (9)
C8	0.0347 (9)	0.0427 (11)	0.0340 (11)	-0.0090 (8)	-0.0040 (8)	0.0107 (8)
C9	0.0325 (9)	0.0317 (9)	0.0275 (10)	-0.0034 (7)	0.0032 (7)	0.0062 (7)
C10	0.0369 (11)	0.0632 (15)	0.0507 (14)	-0.0041 (10)	-0.0093 (10)	0.0208 (12)
C11	0.0378 (11)	0.0656 (15)	0.0572 (15)	0.0163 (11)	0.0031 (10)	0.0239 (13)
C12	0.0486 (12)	0.0514 (13)	0.0380 (12)	0.0166 (10)	0.0035 (9)	0.0067 (10)
C13	0.0377 (9)	0.0342 (10)	0.0283 (10)	-0.0010 (8)	0.0009 (8)	-0.0019 (8)
C14	0.0403 (11)	0.0357 (10)	0.0468 (13)	0.0004 (9)	0.0011 (9)	-0.0078 (9)
C15	0.0364 (14)	0.0334 (15)	0.056 (2)	0.000	-0.0102 (13)	0.000
N1	0.0323 (8)	0.0298 (8)	0.0250 (8)	0.0014 (6)	0.0021 (6)	0.0004 (6)
N2	0.0361 (8)	0.0388 (9)	0.0307 (9)	0.0075 (7)	0.0039 (7)	0.0040 (7)
O1	0.0567 (9)	0.0360 (7)	0.0320 (8)	-0.0025 (6)	0.0138 (6)	0.0001 (6)
O2	0.0795 (12)	0.0528 (10)	0.0653 (12)	-0.0019 (9)	0.0307 (10)	-0.0207 (9)
O3	0.0662 (16)	0.0286 (11)	0.0731 (18)	0.000	-0.0109 (12)	0.000
Zn1	0.0409 (2)	0.03008 (19)	0.0249 (2)	0.000	0.00062 (12)	0.000

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

C1—N1	1.324 (2)	C10—H10	0.9300
C1—C2	1.391 (3)	C11—C12	1.397 (3)
C1—H1	0.9300	C11—H11	0.9300
C2—C3	1.355 (3)	C12—N2	1.333 (3)
C2—H2	0.9300	C12—H12	0.9300
C3—C4	1.405 (3)	C13—O1	1.277 (2)
C3—H3	0.9300	C13—C13 <sup>i</sup>	1.420 (4)
C4—C5	1.412 (3)	C13—C14	1.462 (3)
C4—C6	1.424 (3)	C14—O2	1.229 (3)
C5—N1	1.358 (2)	C14—C15	1.498 (3)
C5—C9	1.433 (3)	C15—O3	1.229 (4)
C6—C7	1.351 (3)	C15—C14 <sup>i</sup>	1.498 (3)
C6—H6	0.9300	N1—Zn1	2.1493 (15)
C7—C8	1.430 (3)	N2—Zn1	2.1664 (17)
C7—H7	0.9300	O1—Zn1	2.1325 (14)
C8—C10	1.400 (3)	Zn1—O1 <sup>i</sup>	2.1325 (14)

## supplementary materials

C8—C9	1.406 (3)	Zn1—N1 <sup>i</sup>	2.1493 (15)
C9—N2	1.357 (2)	Zn1—N2 <sup>i</sup>	2.1664 (17)
C10—C11	1.359 (4)		
N1—C1—C2	123.14 (19)	N2—C12—H12	119.0
N1—C1—H1	118.4	C11—C12—H12	119.0
C2—C1—H1	118.4	O1—C13—C13 <sup>i</sup>	122.05 (11)
C3—C2—C1	118.91 (19)	O1—C13—C14	127.84 (18)
C3—C2—H2	120.5	C13 <sup>i</sup> —C13—C14	110.10 (12)
C1—C2—H2	120.5	O2—C14—C13	127.8 (2)
C2—C3—C4	120.63 (19)	O2—C14—C15	126.6 (2)
C2—C3—H3	119.7	C13—C14—C15	105.61 (19)
C4—C3—H3	119.7	O3—C15—C14 <sup>i</sup>	125.84 (13)
C3—C4—C5	116.54 (18)	O3—C15—C14	125.84 (13)
C3—C4—C6	124.48 (19)	C14 <sup>i</sup> —C15—C14	108.3 (3)
C5—C4—C6	118.96 (18)	C1—N1—C5	118.26 (17)
N1—C5—C4	122.48 (17)	C1—N1—Zn1	128.09 (13)
N1—C5—C9	118.00 (17)	C5—N1—Zn1	113.65 (12)
C4—C5—C9	119.52 (17)	C12—N2—C9	118.54 (18)
C7—C6—C4	121.43 (19)	C12—N2—Zn1	128.01 (15)
C7—C6—H6	119.3	C9—N2—Zn1	113.37 (12)
C4—C6—H6	119.3	C13—O1—Zn1	107.30 (12)
C6—C7—C8	121.09 (19)	O1—Zn1—O1 <sup>i</sup>	81.23 (7)
C6—C7—H7	119.5	O1—Zn1—N1	170.49 (6)
C8—C7—H7	119.5	O1 <sup>i</sup> —Zn1—N1	94.20 (5)
C10—C8—C9	117.4 (2)	O1—Zn1—N1 <sup>i</sup>	94.20 (5)
C10—C8—C7	123.7 (2)	O1 <sup>i</sup> —Zn1—N1 <sup>i</sup>	170.49 (6)
C9—C8—C7	118.88 (19)	N1—Zn1—N1 <sup>i</sup>	91.48 (8)
N2—C9—C8	122.48 (18)	O1—Zn1—N2	94.54 (6)
N2—C9—C5	117.50 (17)	O1 <sup>i</sup> —Zn1—N2	93.84 (6)
C8—C9—C5	120.02 (18)	N1—Zn1—N2	77.37 (6)
C11—C10—C8	119.6 (2)	N1 <sup>i</sup> —Zn1—N2	94.83 (6)
C11—C10—H10	120.2	O1—Zn1—N2 <sup>i</sup>	93.84 (6)
C8—C10—H10	120.2	O1 <sup>i</sup> —Zn1—N2 <sup>i</sup>	94.54 (6)
C10—C11—C12	119.9 (2)	N1—Zn1—N2 <sup>i</sup>	94.83 (6)
C10—C11—H11	120.0	N1 <sup>i</sup> —Zn1—N2 <sup>i</sup>	77.37 (6)
C12—C11—H11	120.0	N2—Zn1—N2 <sup>i</sup>	168.95 (9)
N2—C12—C11	121.9 (2)		

Symmetry codes: (i)  $-x+2, y, -z+3/2$ .

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C6—H6 $\cdots$ O1 <sup>ii</sup>	0.93	2.47	3.295 (2)	149
C11—H11 $\cdots$ O3 <sup>iii</sup>	0.93	2.55	3.147 (2)	122

Symmetry codes: (ii)  $x, -y, z-1/2$ ; (iii)  $x-1/2, y-1/2, -z+3/2$ .

Fig. 1

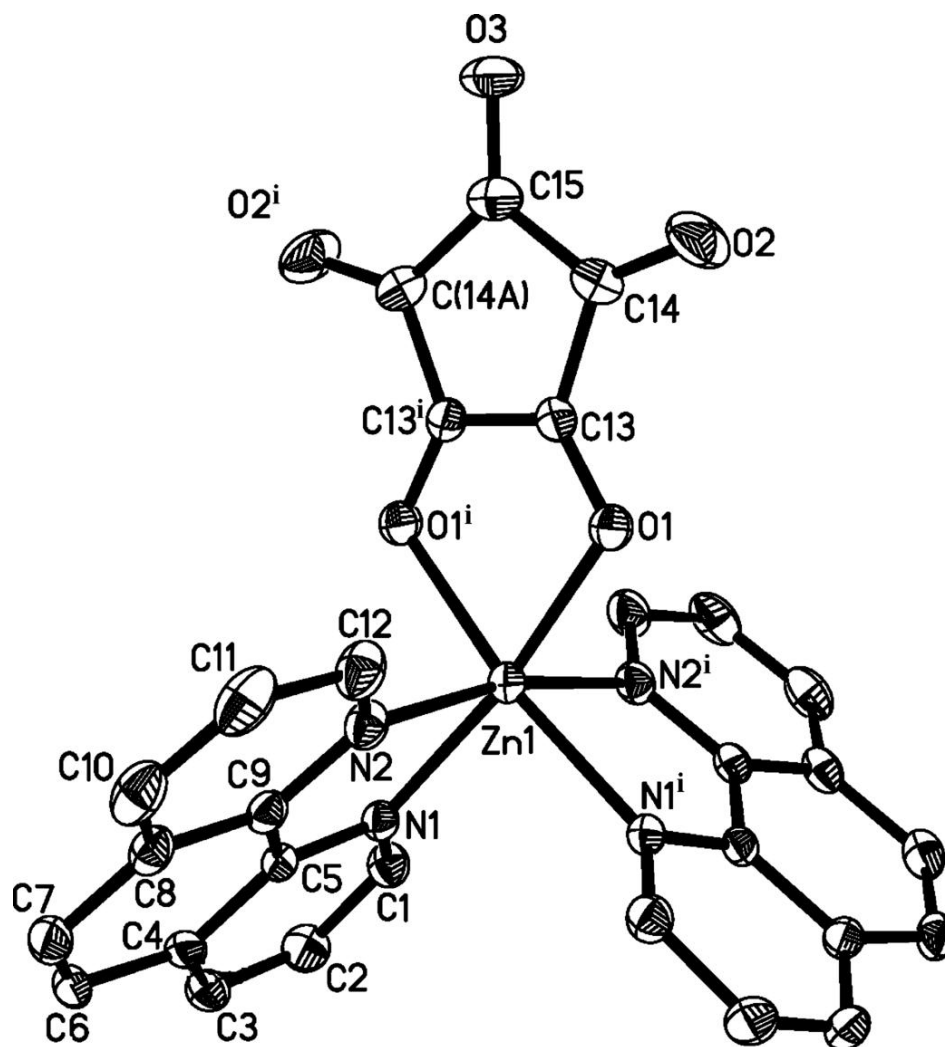


Fig. 2

