

Retraction of articles

This article reports the retraction of 39 articles published in *Acta Crystallographica Section E* between 2004 and 2009.

After thorough investigation (see Harrison *et al.*, 2010), 39 additional articles are retracted as a result of problems with the data sets or incorrect atom assignments. Full details of all the articles are given in Table 1.

Table 1

Details of articles to be retracted, in order of publication.

| Title | Reference | Retracted by | DOI | Refcode |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------|--------------|---------------------------|---------|
| <i>trans</i> -Bis[1-β-(cyclohexylamino)propyliminomethyl]-2-naphtholato]copper(II) dichloride dihydrate | Zhang (2004) | Journal | 10.1107/S1600536804028296 | BIPDUA |
| Bis(4-bromo-2-formylphenolato-κ ² O,O')copper(II) | Sun & Gao (2005) | Author | 10.1107/S16005368050187X | FEYSUY |
| Bis(salicylaldehyde)zinc(II) | Xiong & Liu (2005) | Journal | 10.1107/S1600536805010913 | GAMDUU |
| Bis(4-bromo-2-formylphenolato-κ ² O,O')zinc(II) | Chen (2006) | Journal | 10.1107/S1600536805040432 | SAZCUS |
| Bis(2-formylphenolato-κ ² O,O')nickel(II) | Li & Chen (2006) | Journal | 10.1107/S1600536806012931 | IDAZAP |
| Bis(2-formylphenolato)cobalt(II) | Qiu (2006) | Journal | 10.1107/S1600536806015704 | GEJDUV |
| Bis(2-formylphenolato-κ ² O,O')manganese(II) | Wang & Fang (2006) | Journal | 10.1107/S1600536806021039 | IDOVED |
| Tetraqua(1,10-phenanthroline-κ ² N,N')copper(II) naphthalene-1,5-disulfonate dihydrate | Liu <i>et al.</i> (2006) | Author | 10.1107/S1600536806030637 | GENYOO |
| Tetraqua(1,10-phenanthroline-κ ² N,N')nickel(II) naphthalene-1,5-disulfonate dihydrate | Liu & Fan (2006) | Author | 10.1107/S1600536806035410 | KERBEP |
| {6,6'-Diethoxy-2,2'-ethane-1,2-diylbis(nitrilomethylidyne)}diphenolato]-trinitratolutetium(III)copper(II) | Sui <i>et al.</i> (2006) | Journal | 10.1107/S160053680604565X | HESPEP |
| Bis(2-formylphenolato-κ ² O,O')iron(II) | Yang <i>et al.</i> (2007) | Author | 10.1107/S1600536807021721 | PIFCAJ |
| 2,6-Dimethoxybenzohydrazide | Qadeer <i>et al.</i> (2007a) | Journal | 10.1107/S1600536807022593 | PIFHES |
| 2-(2,4-Dichlorophenylsulfanylmethylidyne)acetohydrazide | Qadeer <i>et al.</i> (2007b) | Journal | 10.1107/S1600536807022891 | YIFSOW |
| {6,6'-Diethoxy-2,2'-ethane-1,2-diylbis(nitrilomethylidyne)}diphenolato]-trinitratoeuropium(III)zinc(II) | Hu <i>et al.</i> (2007) | Author | 10.1107/S1600536807031121 | WIHKEE |
| {μ-6,6'-Diethoxy-2,2'-ethane-1,2-diylbis(nitrilomethylidyne)}diphenolato]-trinitratocerium(III)zinc(II) | Sui, Zhang, Hu & Yin (2007) | Author | 10.1107/S1600536807032564 | WIHREL |
| {μ-6,6'-Diethoxy-2,2'-ethane-1,2-diylbis(nitrilomethylidyne)}diphenolato]-trinitratorpaseodymium(III)zinc(II) | Chen <i>et al.</i> (2007) | Author | 10.1107/S1600536807032540 | WIHRIP |
| {μ-6,6'-Diethoxy-2,2'-ethane-1,2-diylbis(nitrilomethylidyne)}diphenolato]-trinitratorpaseodymium(III)nickel(II) | Sui, Li <i>et al.</i> (2007) | Author | 10.1107/S1600536807032618 | UFACUA |
| {6,6'-Dimethoxy-2,2'-ethane-1,2-diylbis(nitrilomethylidyne)}diphenolato-1κ ⁴ O ^I ,O ^V ,O ⁶ :2κ ⁴ O ^I ,N,N',O ^V](methanol-1κO)-μ-nitrito-1:2κ ² O:O'-dinitrato-1κ ⁴ O,O'-cerium(III)zinc(II) | Sui, Fang, Hu & Lin (2007) | Author | 10.1107/S1600536807033314 | UDUYIC |
| {6,6'-Dimethoxy-2,2'-ethane-1,2-diylbis(nitrilomethylidyne)}diphenolato]-methanol-μ-nitrito-dinitratosamarium(III)nickel(II) | Sui, Zhang, Hu & Jiang (2007) | Author | 10.1107/S1600536807037130 | AFECEU |
| {6,6'-Dimethoxy-2,2'-ethane-1,2-diylbis(nitrilomethylidyne)}diphenolato]-methanol-μ-nitrito-dinitratorpaseodymium(III)zinc(II) | Sui, Fang & Yuan (2007) | Author | 10.1107/S1600536807037488 | AFICEY |
| {6,6'-Dimethoxy-2,2'-ethane-1,2-diylbis(nitrilomethylidyne)}diphenolato]-methanol-μ-nitrito-dinitratolutetium(III)zinc(II) | Sui, Sui <i>et al.</i> (2007) | Author | 10.1107/S1600536807037737 | AFEFOH |
| catena-Poly[chloridonickel(II)-di-μ-chlorido-schloridonickel(II)]-μ-4,4'-methylenebis(3,5-dimethylpyrazole)-κ ² N ² :N ^{2'}] | Huang & Chen (2007) | Author | 10.1107/S1600536807039384 | VIJYOD |
| {2,2'-{o-Phenylenebis(nitrilomethylidyne)}}diphenolato]zinc(II) | Liu <i>et al.</i> (2007a) | Author | 10.1107/S1600536807040640 | DIKYUS |
| trans-Bis(ethylenediamine-2 ^N ,N')bis(nitrato-κO)zinc(II) | Liu, Zeng & Chen (2007) | Author | 10.1107/S1600536807042390 | XIKYEW |
| [N,N'-{o-Phenylenebis(picolinamido)}-κ ² N,N',N'',N''']cobalt(II) | Liu & Zeng (2007a) | Author | 10.1107/S1600536807044571 | XILFII |
| [N,N'-{o-Phenylenebis(picolinamide)}-κ ⁴ N]nickel(II) | Liu & Zeng (2007b) | Author | 10.1107/S1600536807048386 | WINWEW |
| {2,2'-{o-Phenylenebis(nitrilomethylidyne)}}diphenolato)manganese(II) | Liu <i>et al.</i> (2007b) | Author | 10.1107/S1600536807052993 | VIQPIV |
| N-(2-Amino-3-pyridyl)urea monohydrate | Li <i>et al.</i> (2007) | Author | 10.1107/S1600536807047526 | SIMFEA |
| N-(2-Fluorophenyl)carbamic acid monohydrate | Yang (2007) | Author | 10.1107/S1600536807052464 | WINMOW |
| Aqua(dimethylglyoxime-κ ² N,N')(3,5-dinitro-2-oxidobenzoato-κ ² O ^I ,O ²)-copper(II) | Liu & Wen (2007) | Author | 10.1107/S1600536807054244 | HIQCAM |
| μ-Acetoato-tri-μ-ferrocenecarboxylatobis[(N,N-dimethylformamide)-copper(II)] | Liu, Lin <i>et al.</i> (2007) | Journal | 10.1107/S1600536807059041 | HIQQEE |

addenda and errata

Table 1 (continued)

| Title | Reference | Retracted by | DOI | Refcode |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------|--------------|---------------------------|---------|
| { μ -6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato- μ -nitro-dinitratoeuropium(III)zinc(II)} | Hu <i>et al.</i> (2008) | Author | 10.1107/S160053680706151X | MIRPAF |
| Bis(4-chloro-2-formylphenolato)nickel(II) | Li <i>et al.</i> (2008) | Author | 10.1107/S1600536807056309 | RISTET |
| { μ -6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato- μ -nitro-dinitratoterbium(III)zinc(II)} | Chen <i>et al.</i> (2008) | Author | 10.1107/S1600536808006958 | QIXHIP |
| Bis(2-ethoxy-6-formylphenolato- κ^2O^1,O^6)nickel(II) | Han (2008) | Journal | 10.1107/S160053680800809X | QIXLIT |
| { μ -6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato- μ -nitro-dinitratoholmium(III)zinc(II)} | Xiao, Sui <i>et al.</i> (2008) | Author | 10.1107/S1600536808013743 | BIZTUA |
| { μ -6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato- μ -trinitratoholmium(III)nickel(II)} | Xiao, Fu <i>et al.</i> (2008) | Author | 10.1107/S1600536808013755 | BIZVAI |
| Hydrogen-bonding patterns in the cocrystal terephthalic acid-4,4'-bipyridine (2/1) | Wang <i>et al.</i> (2009) | Journal | 10.1107/S160053680903236X | DUCZEH |
| { μ -6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato- μ -1 $k^4O^1,O^r,O^6,O^{r'}:2k^4O^1,N,N',O^{r'}$ (ethanol-1 k O)- μ -nitro-1:2 $k^2O:O'$ -dinitrato-1 k^2O,O' -samarium(III)zinc(II)} | Huang <i>et al.</i> (2009) | Journal | 10.1107/S1600536809033558 | YUCWAV |

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trans-Bis(ethylenediamine- $\kappa^2 N,N'$)-bis(nitrato- κO)zinc(II)

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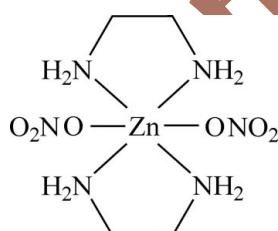
Received 14 August 2007; accepted 29 August 2007

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(C-C) = 0.007$ Å;
 R factor = 0.048; wR factor = 0.148; data-to-parameter ratio = 14.1.

In the title compound, $[Zn(NO_3)_2(C_2H_8N_2)_2]$, the Zn^{II} atom lies on a centre of inversion and is coordinated by four N atoms belonging to two ethylenediamine molecules and two O atoms belonging to two nitrate anions arranged in a *trans* manner. The Zn^{II} ion displays a distorted octahedral coordination geometry. Adjacent complexes are connected by $N-H\cdots O$ hydrogen bonds formed between the H atoms of the amino groups and the uncoordinated O atoms of the nitrate anions.

Related literature

For the structure of the analogous Cu^{II} compound, see: Komiyama & Lingafelter (1964); Fronczek *et al.* (1995); Manriquez *et al.* (1996).



Experimental

Crystal data

$[Zn(NO_3)_2(C_2H_8N_2)_2]$
 $M_r = 309.62$
Monoclinic, $P2_1/c$
 $a = 8.2127$ (7) Å
 $b = 9.9673$ (8) Å
 $c = 7.9733$ (7) Å
 $\beta = 111.171$ (1)°

Data collection

Bruker APEXII CCD diffractometer

Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
 $T_{min} = 0.668$, $T_{max} = 0.823$

3715 measured reflections
1116 independent reflections

811 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.026$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.148$
 $S = 1.07$
1116 reflections

79 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.71$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.84$ e Å⁻³

Table 1
Selected geometric parameters (Å, °).

| | | | |
|-------------------------|-------------|-------------------------|------------|
| O2—Zn1 | 2.568 (3) | Zn1—N1 | 2.002 (4) |
| Zn1—N2 | 1.989 (4) | | |
| N2 ⁱ —Zn1—N2 | 180.0 | N2 ⁱ —Zn1—O2 | 92.14 (15) |
| N2 ⁱ —Zn1—N1 | 95.11 (16) | N2—Zn1—O2 | 87.86 (15) |
| N2—Zn1—N1 | 84.89 (16) | N1—Zn1—O2 | 91.40 (15) |
| N1—Zn1—N1 ⁱ | 180.00 (14) | N1 ⁱ —Zn1—O2 | 88.60 (15) |

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

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

| D—H···A | D—H | H···A | D···A | D—H···A |
|----------------------------|------|-------|-----------|---------|
| N1—H3B···O3 ⁱⁱ | 0.90 | 2.29 | 3.023 (6) | 138 |
| N1—H3A···O3 | 0.90 | 2.22 | 3.015 (6) | 147 |
| N2—H4A···O1 ⁱⁱⁱ | 0.90 | 2.13 | 3.025 (5) | 176 |
| N2—H4A···O2 ⁱⁱⁱ | 0.90 | 2.58 | 3.235 (5) | 130 |
| N2—H4B···O1 ^{iv} | 0.90 | 2.16 | 3.027 (6) | 161 |

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

The authors are grateful to the Natural Science Foundation of Jiangxi Province (grant Nos. 0520036 and 0620029) for support of this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2235).

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supplementary materials

Article retracted

Acta Cryst. (2007). E63, m2462 [doi:10.1107/S1600536807042390]

trans-Bis(ethylenediamine- κ^2N,N')bis(nitrato- κO)zinc(II)

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Comment

The title compound (Fig. 1) is a mononuclear Zn^{II} complex. The Zn^{II} atom lies on a centre of inversion and is coordinated to four N atoms belonging to two ethylenediamine molecules and two O atoms belonging to two nitrate anions arranged in a *trans* manner. In the crystal, adjacent molecules are connected by N—H \cdots O hydrogen bonds involving the H atoms of the amino groups and the non-bonded O atoms of the nitrate ions (Fig. 2).

Experimental

Ethylenediamine (0.120 g, 0.002 mol) and $Zn(NO_3)_2$ (0.189 g, 0.001 mol) were added to 25 ml methanol. The mixture was heated for 5 h under reflux with stirring and the resulting solution was filtered. Single crystals suitable for X-ray diffraction were formed after a week by slow evaporation of the filtrate.

Refinement

H atoms were placed at calculated positions and refined as riding on their parent C or N atoms, with C—H = 0.97 Å or N—H = 0.90 Å, and with $U_{iso}(H) = 1.2U_{eq}(C/N)$.

Figures

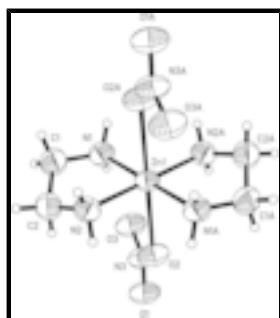


Fig. 1. The molecular structure of the title compound with displacement ellipsoids drawn at 50% probability for non-H atoms.

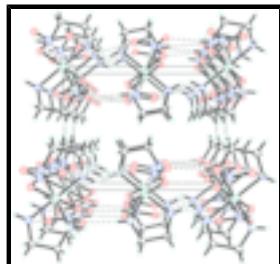


Fig. 2. Unit-cell contents viewed along the c axis. H bonds are shown as dashed lines.

supplementary materials

trans-Bis(ethylenediamine- κ^2N,N')bis(nitrato- κO) zinc(II)

Crystal data

| | |
|---------------------------------------------------------------------------------------------------|-------------------------------------------|
| [Zn(NO ₃) ₂ (C ₂ H ₈ N ₂) ₂] | $F_{000} = 320$ |
| $M_r = 309.62$ | $D_x = 1.689 \text{ Mg m}^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| Hall symbol: -P 2ybc | $\lambda = 0.71073 \text{ \AA}$ |
| $a = 8.2127 (7) \text{ \AA}$ | Cell parameters from 2202 reflections |
| $b = 9.9673 (8) \text{ \AA}$ | $\theta = 2.7\text{--}27.8^\circ$ |
| $c = 7.9733 (7) \text{ \AA}$ | $\mu = 2.05 \text{ mm}^{-1}$ |
| $\beta = 111.171 (1)^\circ$ | $T = 293 (2) \text{ K}$ |
| $V = 608.63 (9) \text{ \AA}^3$ | Block, colourless |
| $Z = 2$ | $0.24 \times 0.17 \times 0.09 \text{ mm}$ |

Data collection

| | |
|----------------------------------------------------------|---------------------------------------|
| Bruker APEXII CCD diffractometer | 1116 independent reflections |
| Radiation source: fine-focus sealed tube | 811 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{\text{int}} = 0.026$ |
| $T = 293(2) \text{ K}$ | $\theta_{\text{max}} = 25.5^\circ$ |
| φ and ω scans | $\theta_{\text{min}} = 2.7^\circ$ |
| Absorption correction: multi-scan (SADABS; Bruker, 1997) | $h = -9 \rightarrow 9$ |
| $T_{\text{min}} = 0.668$, $T_{\text{max}} = 0.823$ | $k = -12 \rightarrow 11$ |
| 3715 measured reflections | $l = -9 \rightarrow 9$ |

Refinement

| | |
|----------------------------------------------------------------|----------------------------------------------------------|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.048$ | H-atom parameters constrained |
| $wR(F^2) = 0.148$ | $w = 1/[\sigma^2(F_o^2) + (0.0901P)^2 + 0.4042P]$ |
| $S = 1.07$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 1116 reflections | $(\Delta/\sigma)_{\text{max}} < 0.001$ |
| 79 parameters | $\Delta\rho_{\text{max}} = 0.71 \text{ e \AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{\text{min}} = -0.84 \text{ e \AA}^{-3}$ |
| | 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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|------------|------------|------------|----------------------------------|
| Zn1 | 1.0000 | 0.5000 | 0.5000 | 0.0411 (3) |
| N3 | 0.8252 (6) | 0.5573 (4) | 0.8297 (6) | 0.0547 (11) |
| O1 | 0.7756 (5) | 0.6261 (4) | 0.9285 (5) | 0.0637 (10) |
| O2 | 0.9006 (5) | 0.6110 (3) | 0.7375 (5) | 0.0600 (10) |
| O3 | 0.7984 (5) | 0.4342 (4) | 0.8202 (6) | 0.0675 (11) |
| C2 | 0.6379 (8) | 0.5160 (5) | 0.3000 (9) | 0.0620 (15) |
| H2A | 0.5473 | 0.5332 | 0.1840 | 0.074* |
| H2B | 0.5968 | 0.5474 | 0.3929 | 0.074* |
| N1 | 0.8360 (5) | 0.3461 (4) | 0.4743 (6) | 0.0544 (11) |
| H3B | 0.8856 | 0.2696 | 0.4563 | 0.065* |
| H3A | 0.8125 | 0.3370 | 0.5755 | 0.065* |
| N2 | 0.7978 (5) | 0.5876 (4) | 0.3128 (6) | 0.0515 (11) |
| H4A | 0.7904 | 0.6739 | 0.3423 | 0.062* |
| H4B | 0.8120 | 0.5853 | 0.2061 | 0.062* |
| C1 | 0.6745 (7) | 0.3712 (5) | 0.3217 (8) | 0.0649 (15) |
| H1A | 0.5784 | 0.3256 | 0.3408 | 0.078* |
| H1B | 0.6851 | 0.3356 | 0.2128 | 0.078* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|------------|------------|------------|--------------|-------------|--------------|
| O2 | 0.090 (3) | 0.044 (2) | 0.062 (2) | -0.0035 (18) | 0.045 (2) | -0.0026 (16) |
| O3 | 0.095 (3) | 0.039 (2) | 0.075 (3) | -0.0047 (19) | 0.039 (2) | 0.0023 (19) |
| Zn1 | 0.0495 (5) | 0.0314 (5) | 0.0439 (5) | 0.0007 (3) | 0.0187 (3) | 0.0030 (3) |
| N3 | 0.082 (3) | 0.037 (2) | 0.056 (3) | -0.001 (2) | 0.039 (2) | 0.000 (2) |
| O1 | 0.093 (3) | 0.052 (2) | 0.060 (2) | 0.0047 (19) | 0.044 (2) | -0.0022 (17) |
| C2 | 0.058 (3) | 0.052 (3) | 0.069 (4) | -0.001 (2) | 0.014 (3) | 0.002 (2) |
| N1 | 0.057 (2) | 0.037 (2) | 0.069 (3) | -0.0039 (18) | 0.021 (2) | -0.0027 (19) |
| N2 | 0.054 (2) | 0.044 (2) | 0.054 (3) | 0.0043 (18) | 0.0172 (19) | 0.0036 (18) |
| C1 | 0.061 (3) | 0.049 (3) | 0.076 (4) | -0.004 (2) | 0.014 (3) | -0.003 (3) |

supplementary materials

Geometric parameters (\AA , $^\circ$)

| | | | |
|--------------------------------------|-------------|------------|-----------|
| O2—N3 | 1.241 (5) | C2—H2A | 0.970 |
| O2—Zn1 | 2.568 (3) | C2—H2B | 0.970 |
| O3—N3 | 1.243 (6) | N1—C1 | 1.462 (6) |
| Zn1—N2 ⁱ | 1.989 (4) | N1—H3B | 0.900 |
| Zn1—N2 | 1.989 (4) | N1—H3A | 0.900 |
| Zn1—N1 | 2.002 (4) | N2—H4A | 0.900 |
| Zn1—N1 ⁱ | 2.002 (4) | N2—H4B | 0.900 |
| N3—O1 | 1.221 (5) | C1—H1A | 0.970 |
| C2—N2 | 1.466 (7) | C1—H1B | 0.970 |
| C2—C1 | 1.472 (7) | | |
| N3—O2—Zn1 | 127.6 (3) | H2A—C2—H2B | 108.3 |
| N2 ⁱ —Zn1—N2 | 180.0 | C1—N1—Zn1 | 109.2 (3) |
| N2 ⁱ —Zn1—N1 | 95.11 (16) | C1—N1—H3B | 109.8 |
| N2—Zn1—N1 | 84.89 (16) | Zn1—N1—H3B | 109.8 |
| N2 ⁱ —Zn1—N1 ⁱ | 84.89 (16) | C1—N1—H3A | 109.8 |
| N2—Zn1—N1 ⁱ | 95.11 (16) | Zn1—N1—H3A | 109.8 |
| N1—Zn1—N1 ⁱ | 180.00 (14) | H3B—N1—H3A | 108.3 |
| N2 ⁱ —Zn1—O2 | 92.14 (15) | C2—N2—Zn1 | 108.9 (3) |
| N2—Zn1—O2 | 87.86 (15) | C2—N2—H4A | 109.9 |
| N1—Zn1—O2 | 91.40 (15) | Zn1—N2—H4A | 109.9 |
| N1 ⁱ —Zn1—O2 | 88.60 (15) | C2—N2—H4B | 109.9 |
| O1—N3—O2 | 119.6 (4) | Zn1—N2—H4B | 109.9 |
| O1—N3—O3 | 120.0 (4) | H4A—N2—H4B | 108.3 |
| O2—N3—O3 | 120.3 (4) | N1—C1—C2 | 110.6 (4) |
| N2—C2—C1 | 109.2 (5) | N1—C1—H1A | 109.5 |
| N2—C2—H2A | 109.8 | C2—C1—H1A | 109.5 |
| C1—C2—H2A | 109.8 | N1—C1—H1B | 109.5 |
| N2—C2—H2B | 109.8 | C2—C1—H1B | 109.5 |
| C1—C2—H2B | 109.8 | H1A—C1—H1B | 108.1 |

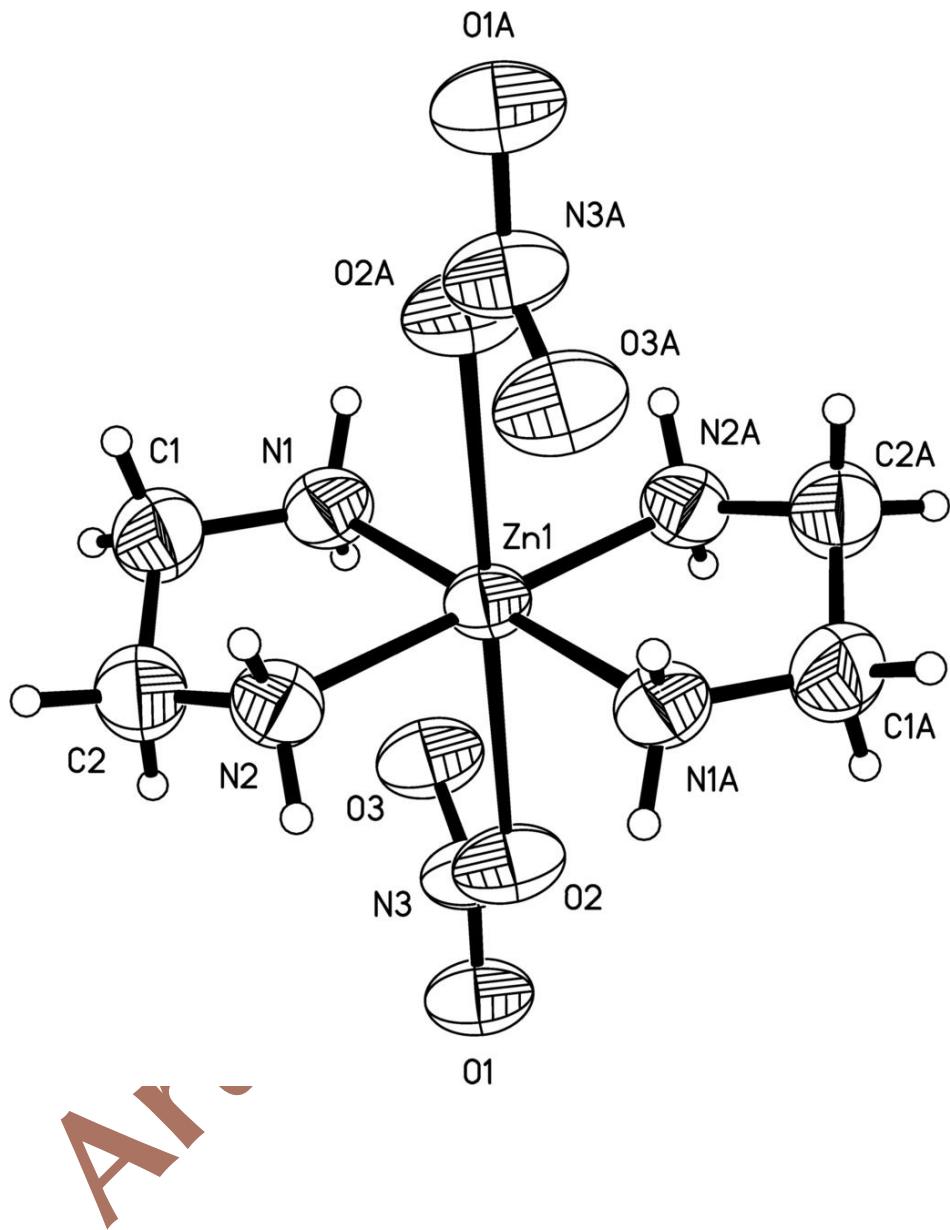
Symmetry codes: (i) $-x+2, -y+1, -z+1$.

Hydrogen-bond geometry (\AA , $^\circ$)

| $D—\text{H}\cdots A$ | $D—\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D—\text{H}\cdots A$ |
|------------------------------------------|--------------|--------------------|-------------|----------------------|
| N1—H3B ⁱⁱ —O3 ⁱⁱ | 0.90 | 2.29 | 3.023 (6) | 138 |
| N1—H3A ⁱⁱⁱ —O3 | 0.90 | 2.22 | 3.015 (6) | 147 |
| N2—H4A ⁱⁱⁱ —O1 ⁱⁱⁱ | 0.90 | 2.13 | 3.025 (5) | 176 |
| N2—H4A ⁱⁱⁱ —O2 ⁱⁱⁱ | 0.90 | 2.58 | 3.235 (5) | 130 |
| N2—H4B ^{iv} —O1 ^{iv} | 0.90 | 2.16 | 3.027 (6) | 161 |

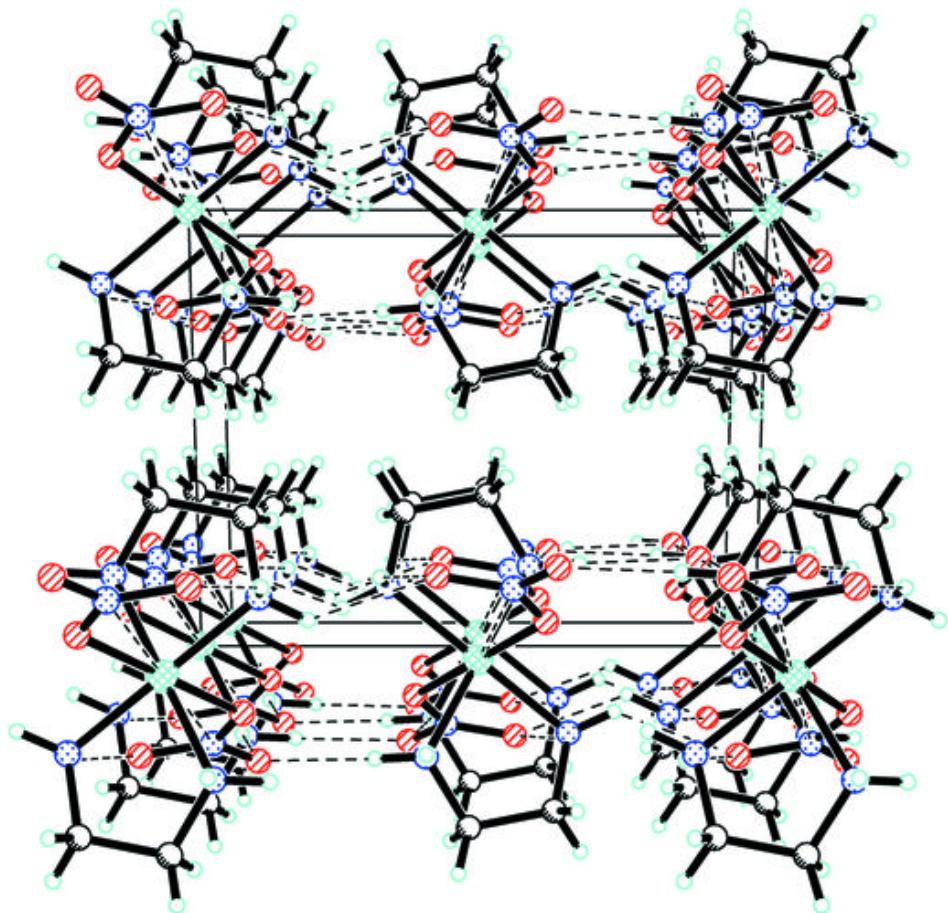
Symmetry codes: (ii) $x, -y+1/2, z-1/2$; (iii) $x, -y+3/2, z-1/2$; (iv) $x, y, z-1$.

Fig. 1



supplementary materials

Fig. 2



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