Acta Crystallographica Section E
**Structure Reports**
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# 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 |
|---|---|---|---|---|
| *trans-Bis{1-[3-(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/S160053680500187X | FEYSUY |
| *Bis(salicylaldehydo)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 |
| *Tetraaqua(1,10-phenanthroline-κ$^2$N,N′)copper(II) naphthalene-1,5-disulfonate dihydrate* | Liu *et al.* (2006) | Author | 10.1107/S1600536806030637 | GENYOO |
| *Tetraaqua(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 *et al.* (2006) | Journal | 10.1107/S160053680604565X | HESPEP |
| *Bis(2-formylphenolato-κ$^2$O,O′)iron(II)* | Yang *et al.* (2007) | Author | 10.1107/S1600536807021721 | PIFCAJ |
| *2,6-Dimethoxybenzohydrazide* | Qadeer *et al.* (2007*a*) | Journal | 10.1107/S1600536807022593 | PIFHES |
| *2-(2,4-Dichlorophenylsulfanyl)acetohydrazide* | Qadeer *et al.* (2007*b*) | Journal | 10.1107/S1600536807022891 | YIFSOW |
| *{6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoeuropium(III)zinc(II)* | Hu *et al.* (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}-trinitratopraseodymium(III)zinc(II)* | Chen *et al.* (2007) | Author | 10.1107/S1600536807032540 | WIHRIP |
| *{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)nickel(II)* | Sui, Li *et al.* (2007) | Author | 10.1107/S1600536807032618 | UFACUA |
| *{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1κ$^4$O$^1$,O$^{1'}$,O$^6$,O$^{6'}$:2κ$^4$O$^1$,N,N′,O$^{1'}$}(methanol-1κO)-μ-nitrato-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-nitrato-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-nitrato-dinitratopraseodymium(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-nitrato-dinitratolutetium(III)zinc(II)* | Sui, Sui *et al.* (2007) | Author | 10.1107/S1600536807037737 | AFEFOH |
| *catena-Poly[[chloridonickel(II)]-di-μ-chlorido-[chloridonickel(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 *et al.* (2007*a*) | Author | 10.1107/S1600536807040640 | DIKYUS |
| *trans-Bis(ethylenediamine-κ$^2$N,N′)bis(nitrato-κO)zinc(II)* | Liu, Zeng & Chen (2007) | Author | 10.1107/S1600536807042390 | XIKYEW |
| *[N,N′-(o-Phenylene)bis(picolinamido)-κ$^4$N,N′,N″,N‴]cobalt(II)* | Liu & Zeng (2007*a*) | Author | 10.1107/S1600536807044571 | XILFII |
| *[N,N′-(o-Phenylene)dipicolinamide-κ$^4$N]nickel(II)* | Liu & Zeng (2007*b*) | Author | 10.1107/S1600536807048386 | WINWEW |
| *{2,2′-[o-Phenylenebis(nitrilomethylidyne)]diphenolato}manganese(II)* | Liu *et al.* (2007*b*) | Author | 10.1107/S1600536807052993 | VIQPIV |
| *N-(2-Amino-3-pyridyl)urea monohydrate* | Li *et al.* (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$^1$,O$^2$)-copper(II)* | Liu & Wen (2007) | Author | 10.1107/S1600536807054244 | HIQCAM |
| *μ-Acetato-tri-μ-ferrocenecarboxylatobis[(N,N-dimethylformamide)-copper(II)]* | Liu, Lin *et al.* (2007) | Journal | 10.1107/S1600536807059041 | HIQQEE |

**Table 1 (continued)**

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

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# {6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-$\mu$-nitrato-dinitrato-praseodymium(III)zinc(II)

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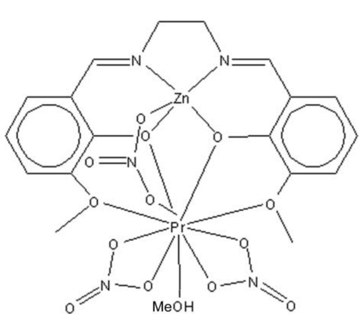
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.025; $wR$ factor = 0.076; data-to-parameter ratio = 17.4.

In the title heteronuclear $Zn^{II}$–$Pr^{III}$ complex (systematic name: {6,6′-dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^1,O^{1'},O^6,O^{6'}$:2$\kappa^4O^1,N,N',O^{1'}$}-(methanol-1$\kappa O$)-$\mu$-nitrato-1:2$\kappa^2O$:$O'$-dinitrato-1$\kappa^4O,O'$-praseodymium(III)zinc(II)), [PrZn($C_{18}H_{18}N_2O_4$)($NO_3$)$_3$($CH_4O$)], with the hexadentate Schiff base compartmental ligand $N,N'$-bis(3-methoxysalicylidene)ethylenediamine ($H_2L$), the Pr and Zn atoms are triply bridged by two phenolate O atoms provided by the Schiff base ligand and one nitrate. The five-coordinate Zn atom is in a square-pyramidal geometry, with the donor centers of two imine N atoms, two phenolate O atoms and one of the bridging nitrate O atoms. The $Pr^{III}$ center has a tenfold coordination environment of O atoms, involving the phenolate O atoms, two methoxy O atoms, one methanol O atom, and two O atoms from two nitrates and one from the bridging nitrate. Strong intermolecular O—H···O and some weak C—H···O interactions generate a two-dimensional layer structure.

## Related literature

For related literature, see: Baggio *et al.* (2000); Caravan *et al.* (1999); Edder *et al.* (2000); Knoer *et al.* (2005); Sui *et al.* (2006, 2007).




## Experimental

*Crystal data*

[PrZn($C_{18}H_{18}N_2O_4$)($NO_3$)$_3$($CH_4O$)]
$M_r$ = 750.70
Monoclinic, $P2_1/n$
$a$ = 9.6011 (4) Å
$b$ = 13.8046 (5) Å
$c$ = 20.0375 (7) Å
$\beta$ = 91.629 (1)°
$V$ = 2654.68 (17) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 2.79 mm$^{-1}$
$T$ = 293 (2) K
0.30 × 0.22 × 0.15 mm

*Data collection*

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min}$ = 0.488, $T_{max}$ = 0.679
19675 measured reflections
6372 independent reflections
5465 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.076
$S$ = 1.00
6372 reflections
367 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.74 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.70 e Å$^{-3}$



**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Pr1—O1 | 2.4634 (19) | Pr1—O11 | 2.459 (2) |
| Pr1—O2 | 2.4517 (17) | Pr1—O14 | 2.5302 (19) |
| Pr1—O3 | 2.568 (2) | Zn1—O1 | 2.0212 (18) |
| Pr1—O4 | 2.584 (2) | Zn1—O2 | 2.0155 (19) |
| Pr1—O6 | 2.8027 (19) | Zn1—O13 | 2.005 (2) |
| Pr1—O7 | 2.7945 (19) | Zn1—N1 | 2.027 (3) |
| Pr1—O8 | 2.648 (2) | Zn1—N2 | 2.070 (2) |
| Pr1—O9 | 2.638 (2) | | |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C18—H18$B$···O9 | 0.96 | 2.38 | 3.015 (4) | 124 |
| C17—H17$B$···O3 | 0.96 | 2.45 | 3.178 (4) | 133 |
| C5—H5···O3$^{i}$ | 0.93 | 2.57 | 3.429 (4) | 154 |
| C7—H7···O8$^{i}$ | 0.93 | 2.49 | 3.391 (4) | 165 |
| O14—H14$A$···O13$^{ii}$ | 0.875 (18) | 1.84 (2) | 2.689 (3) | 162 (3) |

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *APEX2*; software used to prepare material for publication: *APEX2* and *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2355).

  

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**supplementary materials**

*Acta Cryst.* (2007). E**63**, m2275-m2276 [ **doi:10.1107/S1600536807037488** ]

# {6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}methanol-$\mu$-nitrato-dinitratopraseodymium(III)zinc(II)

**Y. Sui, X.-N. Fang and M.-W. Yuan**



## Comment

The potential applications of trivalent lanthanide complexes as contrast agent for magnetic resonance imaging and stains for fluorescence imaging have prompted considerable interest in the preparation, magnetic and optical properties of 3 d–4f hetorometallic dinuclear complexes (Baggio *et al.*, 2000; Caravan *et al.*, 1999; Edder *et al.*, 2000; Knoer *et al.*, 2005). As part of our investigations into the structure and applications of 3 d–4f hetorometallic Schiff base complexes (Sui *et al.*, 2006; Sui *et al.*, 2007), we report here the synthesis and X-ray crystal structure analysis of the title complex, (I), a new $Zn^{II}$–$Pr^{III}$ complex with salen-type Schiff base *N*,*N*'-bis(3-methoxysalicylidene) ethylenediamine ($H_2L$).

Complex (I) crystallizes in the space group $P2_1/n$, with zinc and praseodymium triply bridged by two phenolate O atoms provided by a salen-type Schiff base ligand and one nitrate. The inner salen-type cavity is occupied by zinc(II), while praseodymium(III) is present in the open and larger portion of the dinucleating compartmental Schiff base ligand.

The $Pr^{III}$ center has a decacoordination environment of O atoms, involving the phenolate O atoms, two methoxy O atoms, one methanol O atom, two O atoms from two nitrates and one from the bridging nitrate. The five kinds of Pr—O bond distances are significantly different, the longest being the Pr—*O*(methoxy) separations and the shortest being the Pr—O(phenolate) and Pr—O11(bridging nitrate).

The $Zn^{II}$ is in a square-pyramidal geometry and is five-coordinated by two imine N atoms, two phenolate O atoms and one of the bridging nitrate O atoms. The Zn atom is 0.5835 (3)Å above the mean $N_2O_2$ plane with an average deviation from the plane of 0.0959 (4) Å, which construct the bottom of square-pyramid. The Zn—O13(bridging nitrate) separation is 2.005 (2)Å and the angles of this Zn—O vector with the Zn—N or Zn—O bonds lie between 103.2 (3)° and 115.6 (3)°, which suggesting that the $Zn^{II}$ is in a slightly distorted square-pyramidal conformation.

Adjacent molecules are held together by strong interactions [O14—H14A··· $O13^{i}$ = 2.689 (3); symmetry codes: (i) 3/2 − *x*, *y* − 1/2, 1/2 − *z*] and weak interactions [C7—H7···$O8^{ii}$ = 3.391 (4) and C5—H5···$O3^{ii}$ = 3.429 (4); symmetry codes:(ii) 1/2 + *x*, 1/2 − *y*, 1/2 + *z*]. These link the molecules into a two-dimensional layer structure (Fig. 2).

## Experimental

$H_2L$ was prepared by the 2:1 condensation of 3-methoxysalicylaldehyde and ethylenediamine in methanol. Complex (I) was obtained by the treatment of zinc(II) acetate dihydrate (0.188 g, 1 mmol) with $H_2L$ (0.328 g, 1 mmol) in methanol solution (80 ml) under reflux for 3 h and then for another 3 h after the addition of praseodymium(III) nitrate hexahydrate (0.435 g, 1 mmol). The reaction mixture was cooled and the resulting precipitate was filtered off, washed with diethyl ether and dried *in vacuo*. Single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation at room temperature of a methanol solution. Analysis calculated for $C_{19}H_{22}N_5O_{14}PrZn$: C 30.40, H 2.95, N 9.33, Pr 18.77, Zn 8.71%; found: C 30.15, H 2.92, N 9.38, Pr 18.59, Zn 8.66%. IR (KBr, $cm^{-1}$): 1640(C═N), 1386,1490(nitrate).

## Refinement

The H bound O atom was found from a difference Fourier map and refined freely. The H atoms were positioned geometrically and treated as riding on their parent atoms, with C—H distances of 0.93 (aromatic), 0.97 (methylene) and 0.96 Å (methyl), and with $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms and $1.2U_{eq}(C)$ for other H atoms. The methyl group of methanol was constrainted as idealized no-rotating $CH_3$ group.

## Figures

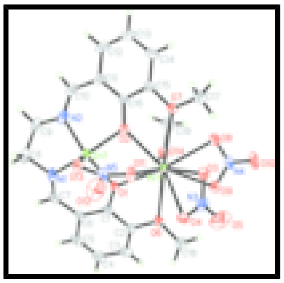

Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids.

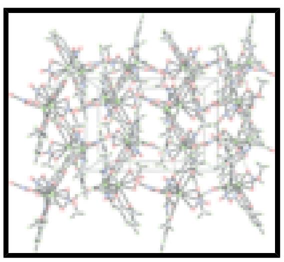

Fig. 2. The packing diagram of (I), viewed along the *c* axis; hydrogen bonds are shown as dashed lines.



## {6,6'-dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-\ 1κ$^4$*O*$^1$,*O*$^{1'}$,*O*$^6$,*O*$^{6'}$:2κ$^4$*O*$^1$,*N*,\ *N*',*O*$^{1'}$)(methanol-1κ*O*)-μ-nitrato-1:2κ$^2$*O*:*O*'-\ dinitrato-1κ$^4$*O*,*O*'-praseodymium(III)zinc(II)

### *Crystal data*

| | |
|---|---|
| $[PrZn(C_{18}H_{18}N_2O_4)(NO_3)_3(CH_4O)]$ | $F_{000} = 1488$ |
| $M_r = 750.70$ | $D_x = 1.878$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2yn | Cell parameters from 6083 reflections |
| *a* = 9.6011 (4) Å | θ = 1.8–28.3º |
| *b* = 13.8046 (5) Å | μ = 2.79 mm$^{-1}$ |
| *c* = 20.0375 (7) Å | *T* = 293 (2) K |
| β = 91.629 (1)º | Block, yellow |
| *V* = 2654.68 (17) Å$^3$ | 0.30 × 0.22 × 0.15 mm |
| *Z* = 4 | |

*Data collection*

| | |
|---|---|
| Bruker APEXII area-detector diffractometer | 6372 independent reflections |
| Radiation source: fine-focus sealed tube | 5465 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.020$ |
| $T = 293(2)$ K | $\theta_{max} = 28.3°$ |
| φ and ω scans | $\theta_{min} = 1.8°$ |
| Absorption correction: multi-scan (SADABS; Bruker, 2004) | $h = -12 \rightarrow 12$ |
| $T_{min} = 0.488$, $T_{max} = 0.679$ | $k = -18 \rightarrow 18$ |
| 19675 measured reflections | $l = -26 \rightarrow 26$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.025$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.076$ | $w = 1/[\sigma^2(F_o^2) + (0.0512P)^2 + 0.717P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.00$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 6372 reflections | $\Delta\rho_{max} = 0.74$ e Å$^{-3}$ |
| 367 parameters | $\Delta\rho_{min} = -0.70$ e Å$^{-3}$ |
| 5 restraints | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | |

*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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| Pr1 | 0.721733 (14) | 0.278496 (10) | 0.113900 (6) | 0.02796 (6) |
| Zn1 | 0.68898 (3) | 0.37172 (2) | 0.273215 (15) | 0.03249 (8) |
| O1 | 0.82378 (19) | 0.28226 (13) | 0.22807 (9) | 0.0329 (4) |

| | | | | |
|---|---|---|---|---|
| O2 | 0.55769 (18) | 0.32507 (14) | 0.19980 (9) | 0.0352 (4) |
| O3 | 0.7364 (2) | 0.36395 (17) | 0.00049 (10) | 0.0464 (5) |
| O7 | 0.4591 (2) | 0.35441 (16) | 0.08039 (10) | 0.0438 (5) |
| O6 | 0.9691 (2) | 0.18028 (15) | 0.14816 (10) | 0.0385 (4) |
| C1 | 0.9349 (3) | 0.23950 (19) | 0.25573 (13) | 0.0302 (5) |
| O4 | 0.9351 (2) | 0.33213 (17) | 0.04734 (11) | 0.0463 (5) |
| N1 | 0.7947 (3) | 0.35333 (18) | 0.36133 (12) | 0.0419 (6) |
| C11 | 0.3434 (3) | 0.3729 (2) | 0.25103 (16) | 0.0411 (7) |
| N2 | 0.5233 (3) | 0.36915 (18) | 0.33710 (12) | 0.0443 (6) |
| C16 | 0.4263 (3) | 0.35504 (18) | 0.19526 (15) | 0.0332 (6) |
| C6 | 0.9764 (3) | 0.2473 (2) | 0.32366 (14) | 0.0387 (6) |
| C12 | 0.2019 (3) | 0.3977 (2) | 0.2390 (2) | 0.0540 (9) |
| H12 | 0.1453 | 0.4076 | 0.2753 | 0.065* |
| N3 | 0.8672 (3) | 0.3668 (2) | −0.00158 (14) | 0.0494 (6) |
| C2 | 1.0167 (3) | 0.1826 (2) | 0.21401 (14) | 0.0354 (6) |
| C15 | 0.3670 (3) | 0.3692 (2) | 0.13133 (16) | 0.0385 (6) |
| C14 | 0.2281 (3) | 0.3947 (2) | 0.12128 (19) | 0.0496 (8) |
| H14 | 0.1906 | 0.4031 | 0.0784 | 0.060* |
| C5 | 1.0960 (3) | 0.1962 (3) | 0.34674 (17) | 0.0506 (8) |
| H5 | 1.1232 | 0.2003 | 0.3916 | 0.061* |
| C3 | 1.1330 (3) | 0.1341 (2) | 0.23812 (18) | 0.0473 (7) |
| H3 | 1.1853 | 0.0965 | 0.2096 | 0.057* |
| C7 | 0.9014 (3) | 0.3013 (2) | 0.37299 (14) | 0.0426 (7) |
| H7 | 0.9343 | 0.2975 | 0.4170 | 0.051* |
| C9 | 0.5654 (4) | 0.3618 (3) | 0.40742 (15) | 0.0550 (9) |
| H9A | 0.5585 | 0.2951 | 0.4221 | 0.066* |
| H9B | 0.5043 | 0.4009 | 0.4342 | 0.066* |
| C10 | 0.3950 (3) | 0.3688 (2) | 0.31916 (17) | 0.0469 (8) |
| H10 | 0.3298 | 0.3656 | 0.3525 | 0.056* |
| O5 | 0.9252 (4) | 0.4006 (3) | −0.04924 (16) | 0.1051 (13) |
| C8 | 0.7151 (4) | 0.3971 (3) | 0.41655 (15) | 0.0543 (9) |
| H8A | 0.7188 | 0.4672 | 0.4143 | 0.065* |
| H8B | 0.7537 | 0.3766 | 0.4595 | 0.065* |
| C13 | 0.1462 (3) | 0.4075 (2) | 0.1768 (2) | 0.0565 (9) |
| H13 | 0.0523 | 0.4229 | 0.1709 | 0.068* |
| O14 | 0.6428 (2) | 0.11820 (14) | 0.16097 (11) | 0.0407 (5) |
| O8 | 0.5706 (2) | 0.18210 (16) | 0.02343 (10) | 0.0444 (5) |
| O11 | 0.7639 (2) | 0.45080 (15) | 0.13810 (10) | 0.0462 (5) |
| O9 | 0.7876 (2) | 0.14450 (16) | 0.02637 (11) | 0.0469 (5) |
| N4 | 0.6692 (3) | 0.13211 (18) | 0.00000 (12) | 0.0433 (6) |
| C18 | 1.0643 (4) | 0.1419 (3) | 0.10131 (17) | 0.0534 (8) |
| H18A | 1.1529 | 0.1736 | 0.1070 | 0.080* |
| H18B | 1.0284 | 0.1527 | 0.0567 | 0.080* |
| H18C | 1.0756 | 0.0736 | 0.1088 | 0.080* |
| C17 | 0.4082 (4) | 0.3800 (3) | 0.01438 (18) | 0.0603 (9) |
| H17A | 0.3363 | 0.3355 | 0.0004 | 0.090* |
| H17B | 0.4833 | 0.3770 | −0.0162 | 0.090* |
| H17C | 0.3711 | 0.4446 | 0.0149 | 0.090* |
| C4 | 1.1719 (4) | 0.1414 (3) | 0.30528 (19) | 0.0563 (9) |

| | | | | |
|---|---|---|---|---|
| H4 | 1.2502 | 0.1086 | 0.3217 | 0.068* |
| O13 | 0.7476 (2) | 0.50348 (14) | 0.24262 (10) | 0.0397 (4) |
| N5 | 0.7784 (3) | 0.51487 (19) | 0.18159 (13) | 0.0450 (6) |
| O10 | 0.6494 (3) | 0.0758 (2) | −0.04565 (13) | 0.0748 (8) |
| O12 | 0.8398 (4) | 0.6104 (2) | 0.16159 (19) | 0.0994 (11) |
| C19 | 0.5002 (4) | 0.0896 (3) | 0.1617 (2) | 0.0641 (10) |
| H19A | 0.4715 | 0.0842 | 0.2071 | 0.096* |
| H19B | 0.4891 | 0.0281 | 0.1398 | 0.096* |
| H19C | 0.4438 | 0.1372 | 0.1388 | 0.096* |
| H14A | 0.695 (3) | 0.085 (2) | 0.1890 (14) | 0.049 (10)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Pr1 | 0.03016 (9) | 0.03434 (9) | 0.01918 (8) | 0.00085 (5) | −0.00257 (6) | −0.00135 (5) |
| Zn1 | 0.03917 (17) | 0.03690 (16) | 0.02147 (15) | −0.00117 (12) | 0.00195 (13) | −0.00117 (12) |
| O1 | 0.0310 (9) | 0.0455 (10) | 0.0218 (9) | 0.0064 (7) | −0.0045 (8) | −0.0012 (7) |
| O2 | 0.0279 (9) | 0.0467 (11) | 0.0309 (10) | 0.0051 (8) | 0.0010 (8) | −0.0056 (8) |
| O3 | 0.0436 (12) | 0.0658 (14) | 0.0295 (10) | 0.0013 (10) | −0.0048 (9) | 0.0085 (10) |
| O7 | 0.0347 (10) | 0.0606 (13) | 0.0355 (11) | 0.0099 (9) | −0.0079 (9) | −0.0066 (10) |
| O6 | 0.0360 (10) | 0.0503 (11) | 0.0289 (10) | 0.0089 (9) | −0.0044 (8) | −0.0049 (8) |
| C1 | 0.0300 (12) | 0.0358 (13) | 0.0243 (12) | −0.0039 (10) | −0.0071 (10) | 0.0061 (10) |
| O4 | 0.0344 (10) | 0.0598 (13) | 0.0446 (12) | −0.0017 (9) | 0.0003 (9) | 0.0093 (11) |
| N1 | 0.0589 (16) | 0.0453 (13) | 0.0214 (11) | −0.0059 (11) | −0.0011 (11) | −0.0020 (10) |
| C11 | 0.0375 (15) | 0.0331 (13) | 0.0535 (18) | −0.0023 (11) | 0.0161 (14) | −0.0038 (12) |
| N2 | 0.0562 (16) | 0.0452 (13) | 0.0324 (12) | 0.0001 (11) | 0.0155 (12) | 0.0006 (10) |
| C16 | 0.0261 (12) | 0.0308 (12) | 0.0430 (15) | −0.0012 (9) | 0.0031 (11) | −0.0057 (11) |
| C6 | 0.0377 (15) | 0.0491 (15) | 0.0288 (14) | −0.0065 (12) | −0.0105 (12) | 0.0100 (12) |
| C12 | 0.0365 (16) | 0.0433 (16) | 0.083 (3) | −0.0003 (13) | 0.0257 (18) | −0.0069 (17) |
| N3 | 0.0529 (16) | 0.0583 (16) | 0.0375 (14) | −0.0004 (13) | 0.0097 (13) | 0.0086 (12) |
| C2 | 0.0329 (13) | 0.0372 (13) | 0.0356 (14) | −0.0009 (11) | −0.0058 (11) | 0.0040 (11) |
| C15 | 0.0280 (13) | 0.0370 (14) | 0.0502 (18) | 0.0007 (10) | −0.0025 (12) | −0.0085 (12) |
| C14 | 0.0306 (15) | 0.0485 (17) | 0.069 (2) | 0.0031 (12) | −0.0097 (15) | −0.0067 (15) |
| C5 | 0.0479 (18) | 0.065 (2) | 0.0376 (17) | −0.0001 (16) | −0.0171 (15) | 0.0134 (16) |
| C3 | 0.0382 (15) | 0.0488 (17) | 0.054 (2) | 0.0104 (13) | −0.0084 (14) | 0.0078 (15) |
| C7 | 0.0538 (18) | 0.0525 (16) | 0.0208 (13) | −0.0126 (14) | −0.0123 (13) | 0.0044 (12) |
| C9 | 0.078 (2) | 0.0580 (19) | 0.0297 (15) | 0.0055 (17) | 0.0211 (16) | 0.0010 (14) |
| C10 | 0.0505 (18) | 0.0418 (15) | 0.0497 (18) | −0.0006 (13) | 0.0237 (15) | −0.0034 (13) |
| O5 | 0.088 (2) | 0.159 (3) | 0.070 (2) | 0.005 (2) | 0.0345 (18) | 0.060 (2) |
| C8 | 0.089 (3) | 0.0498 (17) | 0.0248 (14) | 0.0031 (17) | 0.0052 (16) | −0.0079 (13) |
| C13 | 0.0278 (14) | 0.0485 (18) | 0.093 (3) | 0.0055 (12) | 0.0044 (17) | −0.0041 (18) |
| O14 | 0.0426 (11) | 0.0401 (10) | 0.0391 (11) | −0.0037 (9) | −0.0017 (9) | 0.0098 (9) |
| O8 | 0.0465 (12) | 0.0521 (12) | 0.0339 (11) | 0.0026 (10) | −0.0125 (9) | −0.0035 (10) |
| O11 | 0.0671 (14) | 0.0404 (10) | 0.0311 (9) | −0.0039 (10) | 0.0038 (10) | −0.0018 (7) |
| O9 | 0.0455 (12) | 0.0539 (12) | 0.0410 (12) | 0.0031 (9) | −0.0027 (10) | −0.0154 (9) |
| N4 | 0.0611 (16) | 0.0402 (13) | 0.0282 (12) | −0.0015 (11) | −0.0069 (12) | −0.0022 (10) |
| C18 | 0.0475 (18) | 0.069 (2) | 0.0438 (18) | 0.0174 (16) | 0.0048 (15) | −0.0088 (16) |
| C17 | 0.057 (2) | 0.080 (3) | 0.0426 (18) | 0.0153 (18) | −0.0166 (16) | −0.0036 (18) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C4 | 0.0482 (18) | 0.067 (2) | 0.052 (2) | 0.0128 (16) | −0.0194 (16) | 0.0164 (17) |
| O13 | 0.0536 (12) | 0.0339 (9) | 0.0319 (8) | −0.0046 (8) | 0.0031 (9) | −0.0028 (7) |
| N5 | 0.0571 (15) | 0.0421 (12) | 0.0360 (10) | 0.0030 (11) | 0.0036 (12) | −0.0023 (9) |
| O10 | 0.100 (2) | 0.0690 (17) | 0.0543 (16) | 0.0012 (15) | −0.0202 (15) | −0.0343 (14) |
| O12 | 0.135 (3) | 0.0654 (18) | 0.099 (3) | −0.0109 (19) | 0.030 (2) | 0.0017 (18) |
| C19 | 0.051 (2) | 0.073 (2) | 0.069 (2) | −0.0208 (18) | −0.0020 (18) | 0.015 (2) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Pr1—O1 | 2.4634 (19) | C12—H12 | 0.9300 |
| Pr1—O2 | 2.4517 (17) | N3—O5 | 1.212 (4) |
| Pr1—O3 | 2.568 (2) | C2—C3 | 1.378 (4) |
| Pr1—O4 | 2.584 (2) | C15—C14 | 1.389 (4) |
| Pr1—O6 | 2.8027 (19) | C14—C13 | 1.391 (5) |
| Pr1—O7 | 2.7945 (19) | C14—H14 | 0.9300 |
| Pr1—O8 | 2.648 (2) | C5—C4 | 1.351 (5) |
| Pr1—O9 | 2.638 (2) | C5—H5 | 0.9300 |
| Pr1—O11 | 2.459 (2) | C3—C4 | 1.390 (5) |
| Pr1—O14 | 2.5302 (19) | C3—H3 | 0.9300 |
| Zn1—O1 | 2.0212 (18) | C7—H7 | 0.9300 |
| Zn1—O2 | 2.0155 (19) | C9—C8 | 1.523 (5) |
| Zn1—O13 | 2.005 (2) | C9—H9A | 0.9700 |
| Zn1—N1 | 2.027 (3) | C9—H9B | 0.9700 |
| Zn1—N2 | 2.070 (2) | C10—H10 | 0.9300 |
| O1—C1 | 1.327 (3) | C8—H8A | 0.9700 |
| O2—C16 | 1.328 (3) | C8—H8B | 0.9700 |
| O3—N3 | 1.259 (3) | C13—H13 | 0.9300 |
| O7—C15 | 1.385 (3) | O14—C19 | 1.425 (4) |
| O7—C17 | 1.441 (4) | O14—H14A | 0.875 (18) |
| O6—C2 | 1.384 (3) | O8—N4 | 1.272 (3) |
| O6—C18 | 1.431 (4) | O11—N5 | 1.247 (3) |
| C1—C2 | 1.404 (4) | O9—N4 | 1.252 (3) |
| C1—C6 | 1.411 (4) | N4—O10 | 1.211 (3) |
| O4—N3 | 1.256 (3) | C18—H18A | 0.9600 |
| N1—C7 | 1.268 (4) | C18—H18B | 0.9600 |
| N1—C8 | 1.490 (4) | C18—H18C | 0.9600 |
| C11—C16 | 1.412 (4) | C17—H17A | 0.9600 |
| C11—C12 | 1.416 (4) | C17—H17B | 0.9600 |
| C11—C10 | 1.440 (5) | C17—H17C | 0.9600 |
| N2—C10 | 1.273 (4) | C4—H4 | 0.9300 |
| N2—C9 | 1.458 (4) | O13—N5 | 1.276 (3) |
| C16—C15 | 1.401 (4) | N5—O12 | 1.503 (4) |
| C6—C5 | 1.415 (4) | C19—H19A | 0.9600 |
| C6—C7 | 1.446 (5) | C19—H19B | 0.9600 |
| C12—C13 | 1.350 (5) | C19—H19C | 0.9600 |
| O2—Pr1—O11 | 73.34 (7) | O2—C16—C11 | 123.8 (3) |
| O2—Pr1—O1 | 65.73 (6) | C15—C16—C11 | 118.4 (3) |
| O11—Pr1—O1 | 74.79 (7) | C1—C6—C5 | 118.8 (3) |
| O2—Pr1—O14 | 76.25 (7) | C1—C6—C7 | 124.5 (3) |

| | | | |
|---|---|---|---|
| O11—Pr1—O14 | 145.28 (7) | C5—C6—C7 | 116.7 (3) |
| O1—Pr1—O14 | 77.75 (7) | C13—C12—C11 | 122.3 (3) |
| O2—Pr1—O3 | 123.59 (7) | C13—C12—H12 | 118.9 |
| O11—Pr1—O3 | 73.58 (7) | C11—C12—H12 | 118.9 |
| O1—Pr1—O3 | 141.43 (7) | O5—N3—O4 | 121.5 (3) |
| O14—Pr1—O3 | 139.13 (7) | O5—N3—O3 | 121.3 (3) |
| O2—Pr1—O4 | 145.25 (7) | O4—N3—O3 | 117.3 (2) |
| O11—Pr1—O4 | 72.31 (7) | C3—C2—O6 | 124.4 (3) |
| O1—Pr1—O4 | 99.97 (7) | C3—C2—C1 | 121.6 (3) |
| O14—Pr1—O4 | 133.89 (7) | O6—C2—C1 | 113.9 (2) |
| O3—Pr1—O4 | 49.27 (7) | O7—C15—C14 | 124.2 (3) |
| O2—Pr1—O9 | 145.23 (7) | O7—C15—C16 | 113.7 (2) |
| O11—Pr1—O9 | 140.19 (7) | C14—C15—C16 | 122.1 (3) |
| O1—Pr1—O9 | 122.39 (6) | C15—C14—C13 | 118.6 (3) |
| O14—Pr1—O9 | 73.42 (7) | C15—C14—H14 | 120.7 |
| O3—Pr1—O9 | 73.35 (7) | C13—C14—H14 | 120.7 |
| O4—Pr1—O9 | 69.47 (7) | C4—C5—C6 | 121.6 (3) |
| O2—Pr1—O8 | 105.18 (6) | C4—C5—H5 | 119.2 |
| O11—Pr1—O8 | 134.83 (7) | C6—C5—H5 | 119.2 |
| O1—Pr1—O8 | 147.35 (7) | C2—C3—C4 | 119.8 (3) |
| O14—Pr1—O8 | 69.60 (7) | C2—C3—H3 | 120.1 |
| O3—Pr1—O8 | 70.59 (7) | C4—C3—H3 | 120.1 |
| O4—Pr1—O8 | 102.57 (7) | N1—C7—C6 | 125.6 (3) |
| O9—Pr1—O8 | 47.90 (7) | N1—C7—H7 | 117.2 |
| O2—Pr1—O7 | 58.48 (6) | C6—C7—H7 | 117.2 |
| O11—Pr1—O7 | 80.04 (7) | N2—C9—C8 | 109.2 (2) |
| O1—Pr1—O7 | 123.20 (6) | N2—C9—H9A | 109.8 |
| O14—Pr1—O7 | 98.03 (7) | C8—C9—H9A | 109.8 |
| O3—Pr1—O7 | 71.74 (7) | N2—C9—H9B | 109.8 |
| O4—Pr1—O7 | 119.44 (7) | C8—C9—H9B | 109.8 |
| O9—Pr1—O7 | 109.56 (6) | H9A—C9—H9B | 108.3 |
| O8—Pr1—O7 | 63.31 (6) | N2—C10—C11 | 124.8 (3) |
| O2—Pr1—O6 | 120.77 (6) | N2—C10—H10 | 117.6 |
| O11—Pr1—O6 | 106.62 (7) | C11—C10—H10 | 117.6 |
| O1—Pr1—O6 | 58.06 (6) | N1—C8—C9 | 106.4 (3) |
| O14—Pr1—O6 | 75.31 (6) | N1—C8—H8A | 110.4 |
| O3—Pr1—O6 | 111.82 (6) | C9—C8—H8A | 110.4 |
| O4—Pr1—O6 | 65.58 (6) | N1—C8—H8B | 110.4 |
| O9—Pr1—O6 | 66.82 (6) | C9—C8—H8B | 110.4 |
| O8—Pr1—O6 | 111.63 (6) | H8A—C8—H8B | 108.6 |
| O7—Pr1—O6 | 173.01 (6) | C12—C13—C14 | 120.5 (3) |
| O13—Zn1—O2 | 104.00 (8) | C12—C13—H13 | 119.7 |
| O13—Zn1—O1 | 103.21 (8) | C14—C13—H13 | 119.7 |
| O2—Zn1—O1 | 82.72 (7) | C19—O14—Pr1 | 123.0 (2) |
| O13—Zn1—N1 | 104.00 (9) | C19—O14—H14A | 113 (2) |
| O2—Zn1—N1 | 151.99 (9) | Pr1—O14—H14A | 122 (2) |
| O1—Zn1—N1 | 90.13 (9) | N4—O8—Pr1 | 97.25 (16) |
| O13—Zn1—N2 | 115.59 (9) | N5—O11—Pr1 | 147.00 (18) |
| O2—Zn1—N2 | 88.29 (9) | N4—O9—Pr1 | 98.31 (16) |

| | | | |
|---|---|---|---|
| O1—Zn1—N2 | 141.20 (9) | O10—N4—O9 | 121.8 (3) |
| N1—Zn1—N2 | 80.43 (11) | O10—N4—O8 | 121.7 (3) |
| C1—O1—Zn1 | 127.04 (17) | O9—N4—O8 | 116.5 (2) |
| C1—O1—Pr1 | 132.26 (16) | O6—C18—H18A | 109.5 |
| Zn1—O1—Pr1 | 100.70 (7) | O6—C18—H18B | 109.5 |
| C16—O2—Zn1 | 121.57 (16) | H18A—C18—H18B | 109.5 |
| C16—O2—Pr1 | 131.41 (17) | O6—C18—H18C | 109.5 |
| Zn1—O2—Pr1 | 101.26 (7) | H18A—C18—H18C | 109.5 |
| N3—O3—Pr1 | 97.09 (17) | H18B—C18—H18C | 109.5 |
| C15—O7—C17 | 115.7 (2) | O7—C17—H17A | 109.5 |
| C15—O7—Pr1 | 117.96 (17) | O7—C17—H17B | 109.5 |
| C17—O7—Pr1 | 126.35 (18) | H17A—C17—H17B | 109.5 |
| C2—O6—C18 | 115.7 (2) | O7—C17—H17C | 109.5 |
| C2—O6—Pr1 | 118.49 (15) | H17A—C17—H17C | 109.5 |
| C18—O6—Pr1 | 124.85 (18) | H17B—C17—H17C | 109.5 |
| O1—C1—C2 | 117.2 (2) | C5—C4—C3 | 120.1 (3) |
| O1—C1—C6 | 124.8 (3) | C5—C4—H4 | 120.0 |
| C2—C1—C6 | 118.0 (2) | C3—C4—H4 | 120.0 |
| N3—O4—Pr1 | 96.37 (16) | N5—O13—Zn1 | 118.65 (17) |
| C7—N1—C8 | 121.5 (3) | O11—N5—O13 | 123.9 (2) |
| C7—N1—Zn1 | 127.8 (2) | O11—N5—O12 | 118.2 (2) |
| C8—N1—Zn1 | 110.0 (2) | O13—N5—O12 | 117.8 (3) |
| C16—C11—C12 | 117.9 (3) | O14—C19—H19A | 109.5 |
| C16—C11—C10 | 123.9 (3) | O14—C19—H19B | 109.5 |
| C12—C11—C10 | 118.2 (3) | H19A—C19—H19B | 109.5 |
| C10—N2—C9 | 120.8 (3) | O14—C19—H19C | 109.5 |
| C10—N2—Zn1 | 125.4 (2) | H19A—C19—H19C | 109.5 |
| C9—N2—Zn1 | 113.7 (2) | H19B—C19—H19C | 109.5 |
| O2—C16—C15 | 117.8 (2) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C18—H18B···O9 | 0.96 | 2.38 | 3.015 (4) | 124 |
| C17—H17B···O3 | 0.96 | 2.45 | 3.178 (4) | 133 |
| C5—H5···O3$^{i}$ | 0.93 | 2.57 | 3.429 (4) | 154 |
| C7—H7···O8$^{i}$ | 0.93 | 2.49 | 3.391 (4) | 165 |
| O14—H14A···O13$^{ii}$ | 0.875 (18) | 1.84 (2) | 2.689 (3) | 162 (3) |

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

**Fig. 1**

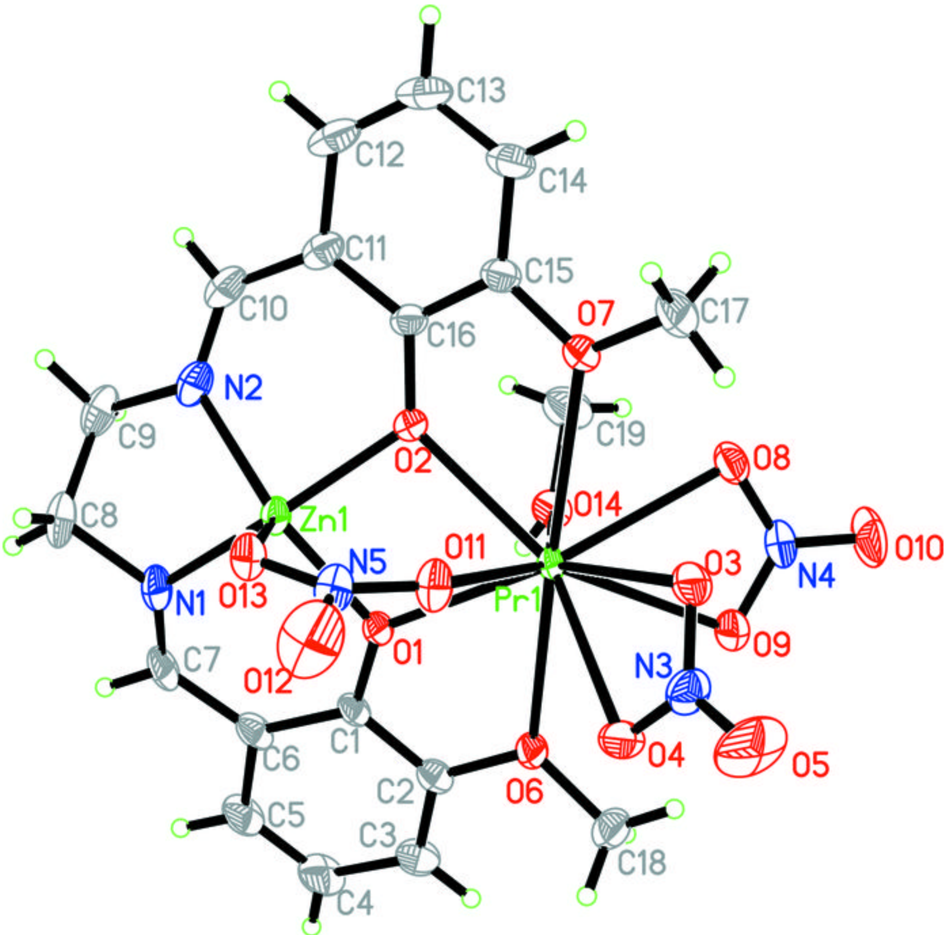
C13
C12
C14
C11
C15
C10
C16
O7
C17
N2
C19
C9
O2
O8
C8
Zn1
O14
N5
O11
O3
N4
O10
N1
O13
Pr1
O1
O9
C7
O12
N3
C1
C6
O4
O5
C2
O6
C5
C3
C4
C18

Fig. 2