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# Retraction of articles by H. Zhong *et al.*

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A series of 41 papers by H. Zhong *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 41 papers by H. Zhong *et al.* are retracted. 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 | DOI | Refcode |
|---|---|---|---|
| *Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thiourea solvate* | Zhong, Zeng, Liu & Luo (2006*a*) | 10.1107/S1600536806041122 | KERQEE |
| *cis-Dichlorobis(1,10-phenanthroline)cobalt(II)* | Zhong, Zeng & Luo (2006) | 10.1107/S1600536806047295 | MEQFOE |
| *Tris(quinolin-8-olato-$\kappa^2N,O$)cobalt(III) glyoxal hemisolvate monohydrate* | Zhong, Zeng, Liu & Luo (2006*b*) | 10.1107/S1600536806050240 | MEQHEW |
| *(8-Quinolinol-$\kappa^2N,O$)bis(8-quinolinolato-$\kappa^2N,O$)nickel(II) glyoxal hemisolvate monohydrate* | Zhong, Zeng, Liu & Luo (2007) | 10.1107/S1600536806053232 | METVUD |
| *Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thioacetamide solvate* | Zhong, Zeng & Luo (2007) | 10.1107/S1600536806053530 | METQIM |
| *(8-Quinolinol-$\kappa^2N,O$)-bis(8-quinolinolato-$\kappa^2N,O$)zinc(II) glyoxal hemisolvate monohydrate* | Zhong, Zeng, Luo, Li & Xiao (2007) | 10.1107/S1600536807001171 | DEXTEG |
| *(Dimethylglyoxime-$\kappa^2N,N'$)bis(1,10-phenanthroline-$\kappa^2N,N'$)nickel(II) dinitrate dihydrate* | Zhong, Zeng, Yang, Luo & Li (2007*a*) | 10.1107/S1600536807004102 | YEYGOZ |
| *(Dimethylglyoxime-$\kappa^2N,N'$)bis(1,10-phenanthroline-$\kappa^2N,N'$)zinc(II) dinitrate dihydrate* | Zhong, Zeng, Yang, Luo & Li (2007*b*) | 10.1107/S1600536807004096 | YEYGUF |
| *Chloridobis(1,10-phenanthroline-$\kappa N,N'$)copper(I) hexahydrate* | Zhong, Zeng, Yang, Luo & Xiao (2007) | 10.1107/S160053680700791X | HEGKOU01 |
| *Tetrakis(pyridine-$\kappa N$)bis(thiocyanato-$\kappa N$)cobalt(II)* | Zhong, Zeng, Yang & Luo (2007*a*) | 10.1107/S1600536807017461 | ITCPCO01 |
| *Tetrakis(pyridine-$\kappa N$)bis(thiocyanato-$\kappa N$)copper(II)* | Zhong, Zeng, Yang & Luo (2007*b*) | 10.1107/S160053680701879X | AVUJEG02 |
| *Tetrakis(nitrato-$\kappa^2O,O'$)bis(4-phenylpyridine-$\kappa N$)cerium(IV)* | Zhong, Zeng, Yang & Luo (2007*c*) | 10.1107/S1600536807018831 | CICDOI |
| *Bis(4,4′-bipyridine-$\kappa^2N,N'$)tetrakis(nitrato-$\kappa^2O,O'$)cerium(IV)* | Zhong, Zeng, Yang & Luo (2007*d*) | 10.1107/S1600536807021502 | YIDNEF |
| *(1,10-Phenanthroline)tris(phenoxyacetato)lanthanum(III)* | Zhong, Zeng, Yang, Luo & Xu (2007) | 10.1107/S1600536807027171 | EDUROL |
| *(1,10-Phenanthroline)tris(phenoxyacetato)cerium(III)* | Zhong, Yang, Luo & Xu (2007*a*) | 10.1107/S1600536807028061 | EDUTUT |
| *(1,10-Phenanthroline)tri(3-phenylpropanoato)lanthanum(III)* | Zhong, Yang, Luo & Xu (2007*b*) | 10.1107/S1600536807028693 | RIGQEE |
| *(1,10-Phenanthroline-$\kappa^2N,N'$)tris(phenoxyacetato)-$\kappa O;\kappa O;\kappa O,O'$-neodymium(III)* | Zhong, Yang, Luo & Xu (2007*c*) | 10.1107/S1600536807030371 | UDUMEM |
| *Bis(2,2′-bipyridyl-$\kappa^2N,N'$)bis(thiocyanato-$\kappa N$)nickel(II)* | Zhong, Yang, Luo & Xu (2007*d*) | 10.1107/S1600536807031613 | YEJGOJ01 |
| *Bis(2,2′-bipyridyl-$\kappa^2N,N'$)bis(isothiocyanato-$\kappa N$)copper(II)* | Zhong, Yang, Luo & Xu (2007*e*) | 10.1107/S1600536807033181 | UFAPOH |
| *Bis(2,2′-bipyridyl-$\kappa^2N,N'$)bis(thiocyanato-$\kappa N$)zinc(II)* | Zhong, Yang, Luo & Xu (2007*f*) | 10.1107/S1600536807035337 | TIGFAR |
| *(1,10-Phenanthroline-$\kappa^2N,N'$)tris(3-phenylpropanoato-$\kappa O$)neodymium(III)* | Zhong, Yang, Luo & Xu (2007*g*) | 10.1107/S1600536807035350 | TIGFEV |
| *2-Fluoro-3,5-dinitrobenzamide monohydrate* | Zhong, Yang, Xie & Luo (2007*j*) | 10.1107/S1600536807038676 | VIKGAY |
| *2-Fluoro-3,5-dinitrobenzoic acid-ammonia (1/1)* | Zhong, Yang, Xie & Luo (2007*k*) | 10.1107/S1600536807039724 | KILKIA |
| *1-Hydroxy-4,6-dinitropyridine-2-carboxamide monohydrate* | Zhong, Yang, Xie & Luo (2007*l*) | 10.1107/S1600536807040779 | AFETAH |
| *N-(2-Hydroxyphenyl)carbamic acid-ammonia (1/1)* | Zhong, Yang, Xie & Luo (2007*m*) | 10.1107/S160053680704086X | AFINAF |
| *catena-Poly[[bis(μ-anilinoacetato-$\kappa^2O:O'$)bis(μ-anilinoacetato-$\kappa^3O,O':O$)bis[(1,10-phenanthroline-$\kappa^2N,N'$)samarium(III)]-μ-anilinoacetato-$\kappa^2O:O'$]* | Zhong, Yang, Xie & Luo (2007*a*) | 10.1107/S1600536807043528 | PILDAQ |
| *2-Hydroxy-5-nitrobenzene-1,3-dicarboxylic acid monohydrate* | Zhong, Yang, Xie & Luo (2007*n*) | 10.1107/S1600536807045199 | XILWIZ |
| *catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dineodymium(III)]-di-μ-anilinoacetato]* | Zhong, Yang, Xie & Luo (2007*b*) | 10.1107/S1600536807048489 | WIMWEV |
| *Hexaaquacopper(II) bis(4-methylbenzenesulfonate)* | Zhong, Yang, Xie & Luo (2007*c*) | 10.1107/S1600536807049525 | TOLSCV01 |

  

**Table 1 (continued)**

| Title | Reference | DOI | Refcode |
|---|---|---|---|
| *catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dilanthanum(III)]-di-μ-anilinoacetato]* | Zhong, Yang, Xie & Luo (2007*d*) | 10.1107/S1600536807051240 | GIMZEI |
| *Hexaaquachromium(II) bis(4-methylbenzenesulfonate)* | Zhong, Yang, Xie & Luo (2007*e*) | 10.1107/S1600536807051227 | GIMZIM |
| *Hexaaquamanganese(II) bis(4-methylbenzenesulfonate)* | Zhong, Yang, Xie & Luo (2007*f*) | 10.1107/S1600536807052051 | QUKQES01 |
| *catena-Poly[[(acetato-κO)(1,10-phenanthroline-$\kappa^2N,N'$)cobalt(II)]-μ-acetato-$\kappa^2O:O'$]* | Zhong, Yang, Xie & Luo (2007*g*) | 10.1107/S1600536807053494 | NIQLAB |
| *Hexaaquanickel(II) bis(4-aminobenzenesulfonate)* | Zhong, Zhong, Xie & Luo (2007*a*) | 10.1107/S1600536807054372 | HIPZOW |
| *catena-Poly[[(acetato-κO)(1,10-phenanthroline-$\kappa^2N,N'$)copper(II)]-μ-acetato-$\kappa^2O:O'$]* | Zhong, Yang, Xie & Luo (2007*h*) | 10.1107/S160053680705622X | XIRGOV |
| *Hexaaquazinc(II) bis(4-aminobenzenesulfonate)* | Zhong, Zhong, Xie & Luo (2007*b*) | 10.1107/S1600536807056498 | XIRJEO |
| *catena-Poly[[(acetato-κO)(1,10-phenanthroline-$\kappa^2N,N'$)nickel(II)]-μ-acetato-$\kappa^2O:O'$]* | Zhong, Yang, Xie & Luo (2007*i*) | 10.1107/S1600536807058540 | HIQJOH |
| *Hexaaquacobalt(II) bis(4-aminobenzenesulfonate)* | Zhong, Xie & Luo (2007) | 10.1107/S1600536807058527 | HIQJUN |
| *catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dieuropium(III)]-di-μ-anilinoacetato]* | Zhong, Yang, Duan & Hong (2007) | 10.1107/S1600536807060643 | YIQMAN |
| *(Dimethylglyoxime-$\kappa^2N,N'$)bis(1,10-phenanthroline-$\kappa^2N,N'$)copper(II) dinitrate dihydrate* | Zhong, Yang, Luo & Li (2007) | 10.1107/S1600536807061193 | YIQNUI |
| *catena-Poly[[(1,10-phenanthroline-$\kappa^2N,N'$)praseodymium(III)]-di-μ-phenoxyacetato-$\kappa^4O:O'$-[(1,10-phenanthroline-$\kappa^2N,N'$)-praseodymium(III)]-di-μ-phenoxyacetato-$\kappa^4O:O'$-di-μ-phenoxyacetato-$\kappa^3O,O':O;\kappa^3O:O,O'$]* | Zhong, Yang, Luo & Xu (2008) | 10.1107/S1600536807068614 | GISJIC |

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# *catena*-Poly[[(1,10-phenanthroline-$\kappa^2N,N'$)praseodymium(III)]-di-$\mu$-phenoxyacetato-$\kappa^4O:O'$-[(1,10-phenanthroline-$\kappa^2N,N'$)praseodymium(III)]-di-$\mu$-phenoxyacetato-$\kappa^4O:O'$-di-$\mu$-phenoxyacetato-$\kappa^3O,O':O;\kappa^3O:O,O'$]

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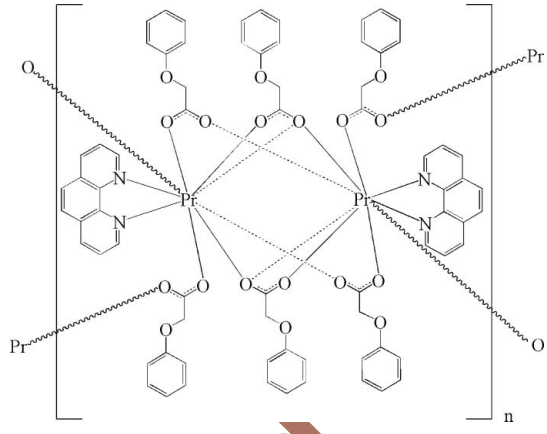
Key indicators: single-crystal X-ray study; $T$ = 273 K; mean $\sigma$(C–C) = 0.008 Å; H-atom completeness 83%; disorder in main residue; $R$ factor = 0.037; $wR$ factor = 0.097; data-to-parameter ratio = 17.1.

The title complex, $[Pr_2(C_8H_7O_3)_6(C_{12}H_8N_2)_2]_n$, which has an inversion centre midway between the two $Pr^{III}$ atoms of the structural unit, forms a one-dimensional polymer bridged alternately by either two bidentate, or two bidentate and two terdentate, phenoxyacetate carboxylate groups. Each $Pr^{III}$ atom is thus nine-coordinated by two N atoms of a 1,10-phenanthroline ligand and seven O atoms from six phenoxyacetate ligands. The coordination geometry at the $Pr^{III}$ atom is distorted tricapped trigonal prismatic. One phenyl ring is disordered over two positions; the site occupancy factors are *ca* 0.6 and 0.4.




## Experimental

### *Crystal data*

$[Pr_2(C_8H_7O_3)_6(C_{12}H_8N_2)_2]$
$M_r$ = 1549.04
Monoclinic, $P2_1/n$
$a$ = 20.204 (4) Å
$b$ = 8.499 (4) Å
$c$ = 20.799 (3) Å
$\beta$ = 107.198 (6)°
$V$ = 3411.8 (17) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.49 mm$^{-1}$
$T$ = 273 (2) K
0.33 × 0.12 × 0.08 mm

### *Data collection*

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.642, $T_{max}$ = 0.890
27763 measured reflections
7712 independent reflections
5037 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.043

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.097
$S$ = 0.90
7712 reflections
452 parameters
144 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.03 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.64 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Pr1—O1 | 2.489 (2) | Pr1—O7 | 2.409 (3) |
| Pr1—O2$^{i}$ | 2.535 (2) | Pr1—O8$^{ii}$ | 2.545 (3) |
| Pr1—O4 | 2.565 (2) | Pr1—N1 | 2.753 (3) |
| Pr1—O5 | 2.817 (3) | Pr1—N2 | 2.720 (3) |
| Pr1—O5$^{i}$ | 2.449 (2) | | |
| O1—Pr1—O4 | 73.62 (8) | O5—Pr1—N1 | 102.34 (9) |
| O1—Pr1—O5 | 65.11 (8) | O7—Pr1—N1 | 77.09 (9) |
| O1—Pr1—O7 | 145.88 (9) | O1—Pr1—N2 | 81.11 (9) |
| O4—Pr1—O5 | 48.17 (8) | O4—Pr1—N2 | 74.08 (9) |
| O4—Pr1—O7 | 138.84 (9) | O5—Pr1—N2 | 118.22 (8) |
| O5—Pr1—O7 | 139.57 (8) | O7—Pr1—N2 | 96.74 (9) |
| O1—Pr1—N1 | 127.55 (9) | N1—Pr1—N2 | 59.78 (10) |
| O4—Pr1—N1 | 63.48 (9) | | |

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

## Related literature

For related literature, see: Allen *et al.* (1987); Daiguebonne *et al.* (2000); Farrugia *et al.* (2000); Kay *et al.* (1972); Ma *et al.* (1999); Mao *et al.* (1998); Starynowicz (1991, 1993); Tsukube & Shinoda (2002); Zhang *et al.* (2005); Zeng *et al.* (2000); Zhong *et al.* (2007).



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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C1—H1···O2$^{i}$ | 0.93 | 2.46 | 3.147 (5) | 130 |
| C10—H10···O4$^{iii}$ | 0.93 | 2.34 | 3.211 (5) | 156 |
| C12—H12···O8$^{ii}$ | 0.93 | 2.47 | 3.063 (5) | 122 |
| C22—H22$B$···O7$^{iv}$ | 0.97 | 2.41 | 3.353 (5) | 166 |

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RT2009).

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# supporting information

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# *catena*-Poly[[(1,10-phenanthroline-$\kappa^2N,N'$)praseodymium(III)]-di-$\mu$-phenoxyacetato-$\kappa^4O:O'$-[(1,10-phenanthroline-$\kappa^2N,N'$)praseodymium(III)]-di-$\mu$-phenoxyacetato-$\kappa^4O:O'$-di-$\mu$-phenoxyacetato-$\kappa^3O,O':O;\kappa^3O:O,O'$]

**H. Zhong, X.-M. Yang, Q.-Y. Luo and Y.-P. Xu**



## S1. Comment

In recent years, there has been great interest in the synthesis of metal organic frameworks (MOFs) with organic ligands and rare earth metals because of their novel structures, fascinating properties and important roles in special materials with potential optical, electronic, magnetic and biological applications (Daiguebonne *et al.*, 2000; Farrugia *et al.*, 2000; Tsukube & Shinoda, 2002; Zhang *et al.*, 2005). These compounds are usually prepared by the reaction of rare-earth metal ions with bi- or multidentate ligands (Starynowicz, 1991, 1993; Kay *et al.*, 1972; Ma *et al.*, 1999; Zeng *et al.*, 2000; Mao *et al.*, 1998). We report herein the crystal structure of the title compound, (I).

In the molecular unit of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The $Pr^{III}$ metal centres are bridged alternatively either by two bidentate, or by two terdentate and two bidentate, phenoxyacetato carboxylate groups with an inversion centre between them. Each Pr atom is nine-coordinated by two N atoms of the 1,10-phenanthroline ligand and seven O atoms from six phenoxyacetate ligands (Table 1), and the coordination geometry at the Pr atom forms a tricapped trigonal prism. The Pr—O bond lengths are in the range 2.409 (3) to 2.817 (3) Å. The Pr—N bond lengths are in the range 2.720 (3) to 2.753 (3) Å. Hydrogen bonds between C—H groups and O atoms of neighbouring phenoxyacetate ligands, with C···O distances of 3.063 (5) to 3.353 (5) Å, generate a layered hydrogen-bonded network (Table 2).

## S2. Experimental

The title compound was synthesized using the hydrothermal method in a 23 ml Teflon-lined Parr bomb, which was then sealed. Praseodymium(III) chloride hexahydrate (71.1 mg, 0.2 mmol), 1,10-phenanthroline (39.6 mg, 0.2 mmol), phenoxyacetic acid (91.3 mg, 0.6 mmol), sodium hydroxide (24 mg, 0.6 mmol) and distilled water (4 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure for 7 d at 413 K and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colorless solution was decanted from small green crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature (yield: 72.7 mg, 36%).

## S3. Refinement

H atoms were positioned geometrically, with C—H = 0.93–0.97 Å, and constrained to ride on their parent atoms, with $U_{iso}$(H) = 1.2$U_{eq}$(C). The phenyl ring defined by C23–C28 shows and in-plane disorder of *ca* 0.4:0.6, and the two phenyl fragments (A and B) were refined as restrained rigid groups, allowing the population to vary. The hydrogen atoms on the disordered phenyl ring were not placed, and as a result of the disorder, slightly larger thermal parameters were observed on the periphery of the molecule.

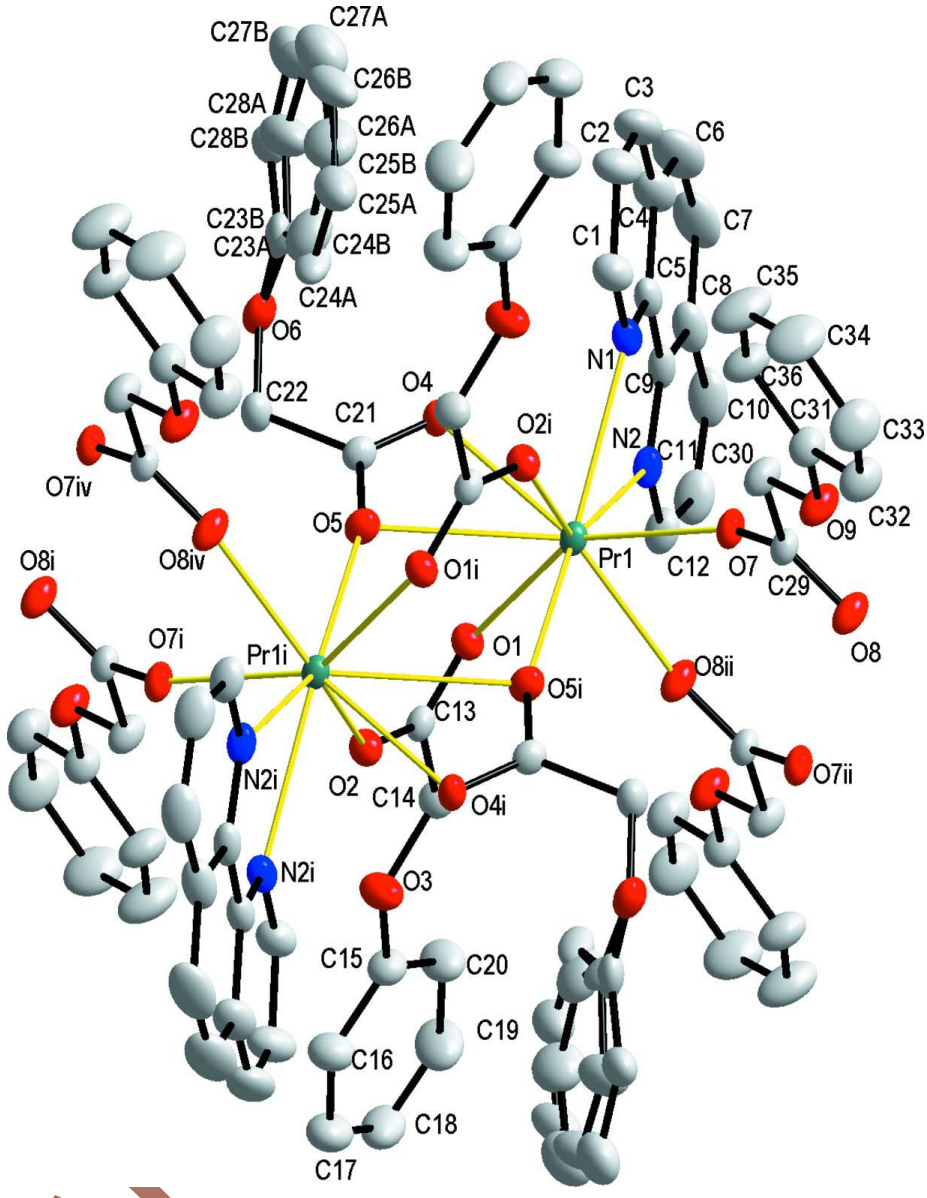


**Figure 1**

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 20% probability level [for symmetry codes, see Tabel 1]. All H atoms have been omitted for clarity.

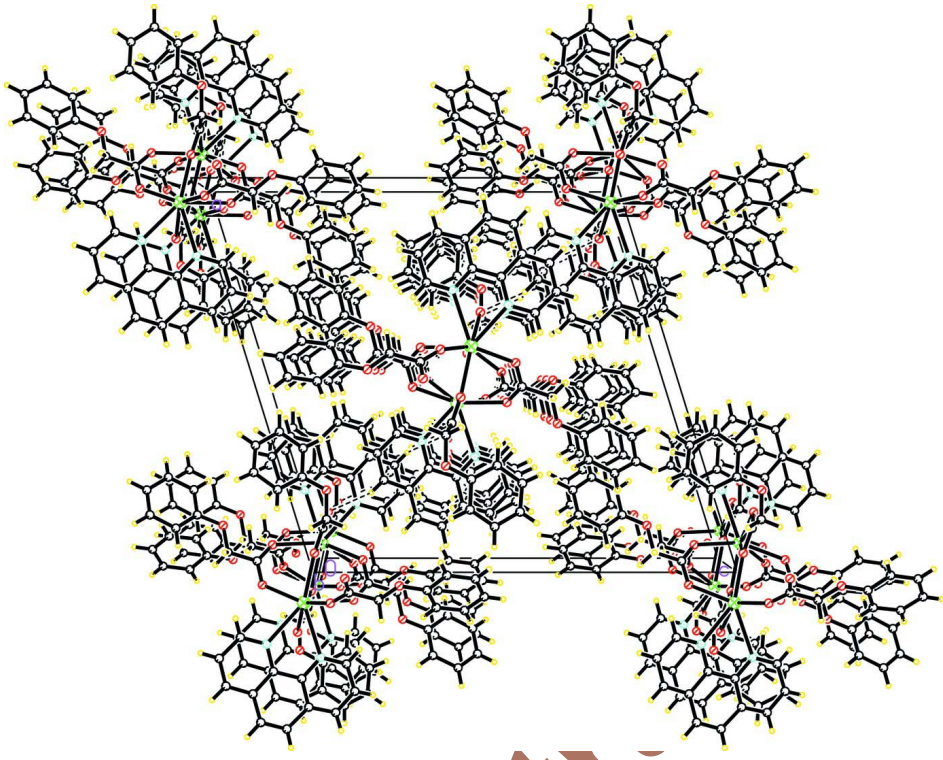

**Figure 2**

View along the *b* axis showing one dimensional polymeric structure, linked by H-bonding.

***catena*-Poly[[(1,10-phenanthroline-$\kappa^2N,N'$)praseodymium(III)]- di-$\mu$-phenoxyacetato-$\kappa^4O:O'$-[(1,10-phenanthroline- $\kappa^2N,N'$)praseodymium(III)]-di-$\mu$-phenoxyacetato-$\kappa^4O:O'$-di-$\mu$- phenoxyacetato-$\kappa^3O,O':O;\kappa^3O:O,O'$]**

*Crystal data*

$[Pr_2(C_8H_7O_3)_6(C_{12}H_8N_2)_2]$
$M_r = 1549.04$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 20.204$ (4) Å
$b = 8.499$ (4) Å
$c = 20.799$ (3) Å
$\beta = 107.198$ (6)°
$V = 3411.8$ (17) Å$^3$
$Z = 2$
$F(000) = 1560$
$D_x = 1.508$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9075 reflections
$\theta = 2.4$–26.9°
$\mu = 1.49$ mm$^{-1}$
$T = 273$ K
Needle, green
0.33 × 0.12 × 0.08 mm

*Data collection*

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.642$, $T_{max} = 0.891$
27763 measured reflections
7712 independent reflections
5037 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.1°$
$h = -26\rightarrow25$
$k = -10\rightarrow11$
$l = -26\rightarrow26$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.097$
$S = 0.90$
7712 reflections
452 parameters
144 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0573P)^2 + 0.9707P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.04$ e Å$^{-3}$
$\Delta\rho_{min} = -0.64$ e Å$^{-3}$

*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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Pr1 | 0.931206 (10) | 0.19065 (2) | 0.964285 (9) | 0.03966 (8) | |
| O1 | 0.97069 (13) | 0.0604 (3) | 0.87489 (11) | 0.0491 (6) | |
| O2 | 1.06691 (13) | −0.0826 (3) | 0.92159 (12) | 0.0516 (6) | |
| O3 | 1.11827 (15) | −0.0166 (4) | 0.82183 (14) | 0.0691 (8) | |
| O4 | 0.84633 (12) | −0.0358 (3) | 0.91883 (12) | 0.0466 (6) | |
| O5 | 0.94657 (13) | −0.1383 (3) | 0.97718 (12) | 0.0518 (7) | |
| O6 | 0.78462 (16) | −0.3257 (3) | 0.89785 (16) | 0.0648 (8) | |
| O7 | 0.94001 (13) | 0.4205 (3) | 1.03407 (12) | 0.0500 (6) | |
| O8 | 1.00785 (15) | 0.6123 (3) | 1.09093 (12) | 0.0590 (7) | |
| O9 | 0.98717 (16) | 0.5273 (3) | 1.20640 (13) | 0.0645 (8) | |
| N1 | 0.79697 (17) | 0.2344 (4) | 0.96683 (16) | 0.0506 (8) | |
| N2 | 0.83406 (18) | 0.3071 (3) | 0.85447 (15) | 0.0498 (8) | |
| C1 | 0.7781 (2) | 0.1926 (5) | 1.0199 (2) | 0.0643 (12) | |
| H1 | 0.8126 | 0.1707 | 1.0598 | 0.077* | |
| C2 | 0.7089 (3) | 0.1797 (6) | 1.0195 (3) | 0.0840 (16) | |
| H2 | 0.6978 | 0.1495 | 1.0580 | 0.101* | |
| C3 | 0.6575 (3) | 0.2127 (7) | 0.9606 (4) | 0.0962 (19) | |
| H3 | 0.6112 | 0.2043 | 0.9591 | 0.115* | |
| C4 | 0.6746 (2) | 0.2581 (7) | 0.9041 (3) | 0.0772 (14) | |
| C5 | 0.7458 (2) | 0.2679 (5) | 0.9084 (2) | 0.0541 (10) | |
| C6 | 0.6231 (3) | 0.2967 (8) | 0.8409 (4) | 0.111 (2) | |
| H6 | 0.5763 | 0.2879 | 0.8372 | 0.133* | |
| C7 | 0.6424 (3) | 0.3448 (8) | 0.7880 (3) | 0.106 (2) | |
| H7 | 0.6085 | 0.3727 | 0.7487 | 0.127* | |
| C8 | 0.7134 (3) | 0.3547 (6) | 0.7899 (2) | 0.0727 (14) | |

| | | | | | |
|---|---|---|---|---|---|
| C9 | 0.7660 (2) | 0.3102 (4) | 0.8506 (2) | 0.0536 (10) | |
| C10 | 0.7358 (3) | 0.4037 (6) | 0.7367 (2) | 0.0878 (17) | |
| H10 | 0.7036 | 0.4392 | 0.6975 | 0.105* | |
| C11 | 0.8031 (3) | 0.4012 (6) | 0.7405 (2) | 0.0819 (15) | |
| H11 | 0.8175 | 0.4331 | 0.7040 | 0.098* | |
| C12 | 0.8524 (3) | 0.3492 (5) | 0.8009 (2) | 0.0644 (12) | |
| H12 | 0.8989 | 0.3448 | 0.8028 | 0.077* | |
| C13 | 1.0286 (2) | 0.0032 (4) | 0.87703 (17) | 0.0442 (9) | |
| C14 | 1.0524 (2) | 0.0512 (5) | 0.81759 (19) | 0.0564 (10) | |
| H14A | 1.0186 | 0.0170 | 0.7763 | 0.068* | |
| H14B | 1.0557 | 0.1649 | 0.8163 | 0.068* | |
| C15 | 1.1460 (2) | 0.0142 (6) | 0.7704 (2) | 0.0646 (12) | |
| C16 | 1.2081 (3) | −0.0565 (7) | 0.7766 (3) | 0.0808 (14) | |
| H16 | 1.2289 | −0.1179 | 0.8141 | 0.097* | |
| C17 | 1.2403 (3) | −0.0368 (7) | 0.7268 (3) | 0.0955 (18) | |
| H17 | 1.2827 | −0.0850 | 0.7309 | 0.115* | |
| C18 | 1.2101 (4) | 0.0526 (7) | 0.6722 (3) | 0.104 (2) | |
| H18 | 1.2318 | 0.0650 | 0.6388 | 0.124* | |
| C19 | 1.1491 (4) | 0.1238 (8) | 0.6659 (3) | 0.109 (2) | |
| H19 | 1.1291 | 0.1856 | 0.6282 | 0.130* | |
| C20 | 1.1148 (3) | 0.1059 (7) | 0.7157 (3) | 0.0847 (16) | |
| H20 | 1.0725 | 0.1548 | 0.7114 | 0.102* | |
| C21 | 0.8840 (2) | −0.1509 (5) | 0.93913 (18) | 0.0457 (9) | |
| C22 | 0.8576 (2) | −0.3140 (5) | 0.9189 (2) | 0.0573 (10) | |
| H22A | 0.8750 | −0.3490 | 0.8825 | 0.069* | |
| H22B | 0.8760 | −0.3842 | 0.9567 | 0.069* | |
| C23A | 0.75531 (19) | −0.3041 (3) | 0.9521 (2) | 0.079 (6) | 0.384 (14) |
| C24A | 0.79664 (17) | −0.2697 (2) | 1.0169 (2) | 0.076 (5) | 0.384 (14) |
| C25A | 0.7671 (2) | −0.2571 (3) | 1.0691 (2) | 0.101 (6) | 0.384 (14) |
| C26A | 0.6962 (3) | −0.2790 (4) | 1.0566 (3) | 0.110 (6) | 0.384 (14) |
| C27A | 0.65490 (19) | −0.3133 (3) | 0.9918 (3) | 0.126 (7) | 0.384 (14) |
| C28A | 0.68444 (18) | −0.3259 (3) | 0.9396 (2) | 0.120 (6) | 0.384 (14) |
| C23B | 0.7508 (2) | −0.3175 (3) | 0.9425 (2) | 0.077 (4) | 0.616 (14) |
| C24B | 0.77565 (17) | −0.2805 (2) | 1.0105 (2) | 0.112 (4) | 0.616 (14) |
| C25B | 0.7302 (2) | −0.2706 (3) | 1.0492 (2) | 0.120 (4) | 0.616 (14) |
| C26B | 0.6599 (2) | −0.2977 (4) | 1.0198 (3) | 0.133 (5) | 0.616 (14) |
| C27B | 0.63499 (18) | −0.3347 (3) | 0.9518 (3) | 0.115 (4) | 0.616 (14) |
| C28B | 0.6804 (2) | −0.3446 (3) | 0.9132 (2) | 0.086 (3) | 0.616 (14) |
| C29 | 0.96861 (15) | 0.4991 (3) | 1.08649 (13) | 0.0453 (9) | |
| C30 | 0.94968 (19) | 0.4431 (3) | 1.14756 (13) | 0.0583 (11) | |
| H30A | 0.9004 | 0.4574 | 1.1402 | 0.070* | |
| H30B | 0.9598 | 0.3316 | 1.1542 | 0.070* | |
| C31 | 0.9746 (2) | 0.4891 (5) | 1.26544 (19) | 0.0558 (10) | |
| C32 | 1.0143 (3) | 0.5695 (6) | 1.3220 (2) | 0.0749 (13) | |
| H32 | 1.0474 | 0.6418 | 1.3181 | 0.090* | |
| C33 | 1.0046 (3) | 0.5419 (7) | 1.3836 (2) | 0.0929 (17) | |
| H33 | 1.0306 | 0.5969 | 1.4212 | 0.111* | |
| C34 | 0.9565 (3) | 0.4332 (9) | 1.3897 (3) | 0.108 (2) | |

| | | | | |
|---|---|---|---|---|
| H34 | 0.9492 | 0.4153 | 1.4312 | 0.130* |
| C35 | 0.9196 (3) | 0.3522 (8) | 1.3342 (3) | 0.108 (2) |
| H35 | 0.8879 | 0.2765 | 1.3386 | 0.129* |
| C36 | 0.9279 (2) | 0.3792 (7) | 1.2721 (2) | 0.0743 (14) |
| H36 | 0.9019 | 0.3230 | 1.2348 | 0.089* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Pr1 | 0.04654 (13) | 0.03356 (12) | 0.03391 (11) | −0.00161 (9) | 0.00420 (8) | 0.00057 (9) |
| O1 | 0.0588 (16) | 0.0479 (16) | 0.0398 (14) | 0.0067 (13) | 0.0132 (12) | 0.0022 (12) |
| O2 | 0.0634 (16) | 0.0494 (16) | 0.0428 (14) | 0.0069 (14) | 0.0167 (12) | 0.0097 (12) |
| O3 | 0.0709 (19) | 0.085 (2) | 0.0591 (18) | 0.0162 (17) | 0.0304 (15) | 0.0209 (16) |
| O4 | 0.0480 (14) | 0.0350 (15) | 0.0484 (14) | 0.0008 (12) | 0.0015 (11) | −0.0027 (11) |
| O5 | 0.0480 (15) | 0.0524 (16) | 0.0462 (15) | −0.0032 (12) | 0.0003 (12) | 0.0071 (12) |
| O6 | 0.0616 (19) | 0.0474 (18) | 0.073 (2) | −0.0128 (14) | 0.0006 (15) | −0.0080 (15) |
| O7 | 0.0718 (17) | 0.0341 (14) | 0.0424 (14) | −0.0063 (13) | 0.0142 (12) | −0.0043 (11) |
| O8 | 0.087 (2) | 0.0515 (18) | 0.0383 (14) | −0.0250 (16) | 0.0177 (13) | −0.0031 (12) |
| O9 | 0.091 (2) | 0.0617 (19) | 0.0416 (15) | −0.0270 (16) | 0.0210 (14) | −0.0058 (13) |
| N1 | 0.0508 (19) | 0.0435 (19) | 0.0498 (19) | 0.0053 (15) | 0.0029 (15) | −0.0074 (15) |
| N2 | 0.065 (2) | 0.0375 (18) | 0.0373 (17) | 0.0016 (16) | −0.0006 (14) | 0.0005 (14) |
| C1 | 0.059 (3) | 0.075 (3) | 0.058 (3) | 0.008 (2) | 0.015 (2) | −0.002 (2) |
| C2 | 0.064 (3) | 0.111 (5) | 0.084 (4) | 0.003 (3) | 0.032 (3) | −0.011 (3) |
| C3 | 0.049 (3) | 0.109 (5) | 0.128 (5) | −0.002 (3) | 0.022 (3) | −0.018 (4) |
| C4 | 0.053 (3) | 0.088 (4) | 0.076 (4) | 0.007 (3) | −0.004 (2) | −0.016 (3) |
| C5 | 0.052 (2) | 0.039 (2) | 0.061 (3) | 0.0057 (18) | 0.0014 (19) | −0.0115 (18) |
| C6 | 0.060 (3) | 0.131 (6) | 0.114 (5) | 0.018 (3) | −0.017 (3) | −0.027 (5) |
| C7 | 0.080 (4) | 0.113 (5) | 0.087 (4) | 0.039 (4) | −0.034 (3) | −0.019 (4) |
| C8 | 0.077 (3) | 0.061 (3) | 0.056 (3) | 0.018 (2) | −0.017 (2) | −0.011 (2) |
| C9 | 0.060 (2) | 0.035 (2) | 0.048 (2) | 0.0049 (19) | −0.0111 (18) | −0.0053 (17) |
| C10 | 0.117 (5) | 0.071 (4) | 0.047 (3) | 0.018 (3) | −0.020 (3) | 0.000 (2) |
| C11 | 0.122 (5) | 0.070 (4) | 0.040 (2) | −0.001 (3) | 0.003 (3) | 0.009 (2) |
| C12 | 0.084 (3) | 0.051 (3) | 0.048 (2) | −0.003 (2) | 0.004 (2) | 0.0067 (19) |
| C13 | 0.058 (2) | 0.035 (2) | 0.038 (2) | −0.0060 (18) | 0.0116 (17) | −0.0025 (15) |
| C14 | 0.066 (3) | 0.056 (3) | 0.049 (2) | 0.006 (2) | 0.0199 (19) | 0.0123 (19) |
| C15 | 0.075 (3) | 0.067 (3) | 0.061 (3) | −0.006 (2) | 0.034 (2) | 0.002 (2) |
| C16 | 0.079 (3) | 0.098 (4) | 0.075 (3) | 0.001 (3) | 0.038 (3) | 0.002 (3) |
| C17 | 0.092 (4) | 0.100 (5) | 0.113 (5) | −0.002 (4) | 0.060 (4) | −0.006 (4) |
| C18 | 0.135 (5) | 0.087 (4) | 0.124 (5) | −0.015 (4) | 0.092 (5) | −0.007 (4) |
| C19 | 0.159 (6) | 0.101 (5) | 0.092 (4) | 0.008 (5) | 0.077 (4) | 0.026 (4) |
| C20 | 0.103 (4) | 0.088 (4) | 0.080 (3) | 0.010 (3) | 0.053 (3) | 0.024 (3) |
| C21 | 0.051 (2) | 0.050 (2) | 0.0325 (18) | −0.0054 (18) | 0.0066 (16) | −0.0032 (16) |
| C22 | 0.062 (3) | 0.045 (2) | 0.058 (3) | 0.002 (2) | 0.008 (2) | −0.0060 (19) |
| C23A | 0.090 (12) | 0.047 (10) | 0.126 (11) | −0.009 (9) | 0.071 (9) | 0.027 (9) |
| C24A | 0.116 (10) | 0.055 (9) | 0.086 (9) | −0.011 (7) | 0.073 (8) | 0.000 (7) |
| C25A | 0.118 (11) | 0.079 (10) | 0.127 (11) | 0.017 (8) | 0.069 (9) | 0.021 (9) |
| C26A | 0.109 (12) | 0.111 (11) | 0.140 (12) | 0.047 (9) | 0.082 (10) | 0.052 (9) |
| C27A | 0.103 (11) | 0.138 (13) | 0.168 (14) | 0.041 (10) | 0.087 (9) | 0.065 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C28A | 0.102 (12) | 0.113 (12) | 0.167 (13) | 0.032 (10) | 0.074 (10) | 0.046 (10) |
| C23B | 0.083 (8) | 0.033 (6) | 0.107 (8) | 0.002 (5) | 0.016 (6) | −0.005 (6) |
| C24B | 0.145 (9) | 0.086 (8) | 0.109 (9) | −0.021 (7) | 0.044 (7) | 0.012 (7) |
| C25B | 0.144 (10) | 0.120 (9) | 0.117 (9) | 0.000 (8) | 0.070 (8) | 0.028 (7) |
| C26B | 0.145 (10) | 0.128 (10) | 0.140 (10) | 0.041 (9) | 0.063 (9) | 0.023 (8) |
| C27B | 0.123 (8) | 0.086 (7) | 0.141 (9) | 0.033 (6) | 0.047 (7) | 0.016 (7) |
| C28B | 0.079 (6) | 0.056 (6) | 0.133 (8) | 0.014 (5) | 0.046 (5) | 0.012 (5) |
| C29 | 0.061 (2) | 0.033 (2) | 0.040 (2) | −0.0035 (18) | 0.0133 (17) | 0.0007 (16) |
| C30 | 0.077 (3) | 0.055 (3) | 0.044 (2) | −0.020 (2) | 0.0193 (19) | −0.0057 (19) |
| C31 | 0.072 (3) | 0.056 (3) | 0.038 (2) | −0.003 (2) | 0.0146 (19) | 0.0016 (18) |
| C32 | 0.092 (3) | 0.077 (3) | 0.054 (3) | −0.019 (3) | 0.017 (2) | −0.009 (2) |
| C33 | 0.122 (5) | 0.108 (5) | 0.042 (3) | −0.021 (4) | 0.014 (3) | −0.009 (3) |
| C34 | 0.133 (5) | 0.146 (6) | 0.055 (3) | −0.031 (5) | 0.043 (3) | 0.009 (4) |
| C35 | 0.124 (5) | 0.141 (6) | 0.066 (4) | −0.059 (4) | 0.041 (3) | −0.003 (4) |
| C36 | 0.081 (3) | 0.091 (4) | 0.053 (3) | −0.033 (3) | 0.023 (2) | −0.003 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Pr1—O1 | 2.489 (2) | C15—C20 | 1.370 (6) |
| Pr1—O2$^{i}$ | 2.535 (2) | C16—C17 | 1.387 (7) |
| Pr1—O4 | 2.565 (2) | C16—H16 | 0.9300 |
| Pr1—O5 | 2.817 (3) | C17—C18 | 1.352 (8) |
| Pr1—O5$^{i}$ | 2.449 (2) | C17—H17 | 0.9300 |
| Pr1—O7 | 2.409 (3) | C18—C19 | 1.345 (8) |
| Pr1—O8$^{ii}$ | 2.545 (3) | C18—H18 | 0.9300 |
| Pr1—N1 | 2.753 (3) | C19—C20 | 1.415 (7) |
| Pr1—N2 | 2.720 (3) | C19—H19 | 0.9300 |
| O1—C13 | 1.255 (4) | C20—H20 | 0.9300 |
| O2—C13 | 1.252 (4) | C21—C22 | 1.500 (5) |
| O2—Pr1$^{i}$ | 2.535 (2) | C22—H22A | 0.9700 |
| O3—C15 | 1.372 (5) | C22—H22B | 0.9700 |
| O3—C14 | 1.429 (5) | C23A—C24B | 1.1792 |
| O4—C21 | 1.235 (4) | C23A—C24A | 1.3900 |
| O5—C21 | 1.282 (4) | C23A—C28A | 1.3900 |
| O5—Pr1$^{i}$ | 2.449 (2) | C23A—C28B | 1.5294 |
| O6—C23B | 1.309 (5) | C24A—C25A | 1.3900 |
| O6—C22 | 1.412 (5) | C24A—C23B | 1.6025 |
| O6—C23A | 1.433 (5) | C24A—C25B | 1.6693 |
| O7—C29 | 1.263 (3) | C25A—C25B | 0.7471 |
| O8—C29 | 1.233 (3) | C25A—C24B | 1.2955 |
| O8—Pr1$^{ii}$ | 2.545 (3) | C25A—C26A | 1.3900 |
| O9—C31 | 1.364 (5) | C26A—C25B | 0.7502 |
| O9—C30 | 1.427 (4) | C26A—C26B | 0.9047 |
| N1—C1 | 1.319 (5) | C26A—C27A | 1.3900 |
| N1—C5 | 1.372 (5) | C27A—C26B | 0.5756 |
| N2—C12 | 1.323 (5) | C27A—C27B | 0.8310 |
| N2—C9 | 1.355 (5) | C27A—C28A | 1.3900 |
| C1—C2 | 1.401 (6) | C27A—C25B | 1.6721 |

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|---|---|---|---|
| C1—H1 | 0.9300 | C28A—C28B | 0.5549 |
| C2—C3 | 1.381 (8) | C28A—C27B | 1.1036 |
| C2—H2 | 0.9300 | C28A—C23B | 1.3252 |
| C3—C4 | 1.373 (8) | C23B—C24B | 1.3900 |
| C3—H3 | 0.9300 | C23B—C28B | 1.3900 |
| C4—C5 | 1.418 (6) | C24B—C25B | 1.3900 |
| C4—C6 | 1.452 (8) | C25B—C26B | 1.3900 |
| C5—C9 | 1.424 (6) | C26B—C27B | 1.3900 |
| C6—C7 | 1.335 (9) | C27B—C28B | 1.3900 |
| C6—H6 | 0.9300 | C29—C30 | 1.5078 |
| C7—C8 | 1.426 (8) | C30—H30A | 0.9700 |
| C7—H7 | 0.9300 | C30—H30B | 0.9700 |
| C8—C10 | 1.377 (7) | C31—C36 | 1.364 (6) |
| C8—C9 | 1.440 (5) | C31—C32 | 1.391 (6) |
| C10—C11 | 1.340 (7) | C32—C33 | 1.372 (6) |
| C10—H10 | 0.9300 | C32—H32 | 0.9300 |
| C11—C12 | 1.423 (6) | C33—C34 | 1.374 (8) |
| C11—H11 | 0.9300 | C33—H33 | 0.9300 |
| C12—H12 | 0.9300 | C34—C35 | 1.361 (8) |
| C13—C14 | 1.509 (5) | C34—H34 | 0.9300 |
| C14—H14A | 0.9700 | C35—C36 | 1.371 (6) |
| C14—H14B | 0.9700 | C35—H35 | 0.9300 |
| C15—C16 | 1.363 (6) | C36—H36 | 0.9300 |

| | | | |
|---|---|---|---|
| O1—Pr1—O4 | 73.62 (8) | C21—C22—H22A | 108.8 |
| O1—Pr1—O5 | 65.11 (8) | O6—C22—H22B | 108.8 |
| O1—Pr1—O7 | 145.88 (9) | C21—C22—H22B | 108.8 |
| O4—Pr1—O5 | 48.17 (8) | H22A—C22—H22B | 107.7 |
| O4—Pr1—O7 | 138.84 (9) | C24B—C23A—C28A | 104.0 |
| O5—Pr1—O7 | 139.57 (8) | C24A—C23A—C28A | 120.0 |
| O1—Pr1—N1 | 127.55 (9) | C24B—C23A—O6 | 137.2 (2) |
| O4—Pr1—N1 | 63.48 (9) | C24A—C23A—O6 | 121.4 (2) |
| O5—Pr1—N1 | 102.34 (9) | C28A—C23A—O6 | 118.6 (2) |
| O7—Pr1—N1 | 77.09 (9) | C24B—C23A—C28B | 125.0 |
| O1—Pr1—N2 | 81.11 (9) | C24A—C23A—C28B | 141.0 |
| O4—Pr1—N2 | 74.08 (9) | O6—C23A—C28B | 97.4 (2) |
| O5—Pr1—N2 | 118.22 (8) | C23A—C24A—C25A | 120.0 |
| O7—Pr1—N2 | 96.74 (9) | C25A—C24A—C23B | 121.0 |
| N1—Pr1—N2 | 59.78 (10) | C23A—C24A—C25B | 93.7 |
| O7—Pr1—O5$^{i}$ | 87.92 (9) | C23B—C24A—C25B | 94.7 |
| O5$^{i}$—Pr1—O1 | 77.99 (9) | C25B—C25A—C24B | 81.0 |
| O7—Pr1—O2$^{i}$ | 75.61 (8) | C24B—C25A—C26A | 102.7 |
| O5$^{i}$—Pr1—O2$^{i}$ | 74.63 (8) | C25B—C25A—C24A | 98.2 |
| O1—Pr1—O2$^{i}$ | 128.25 (9) | C26A—C25A—C24A | 120.0 |
| O7—Pr1—O8$^{ii}$ | 77.23 (9) | C25B—C26A—C26B | 113.9 |
| O5$^{i}$—Pr1—O8$^{ii}$ | 78.03 (9) | C26B—C26A—C25A | 135.7 |
| O1—Pr1—O8$^{ii}$ | 69.56 (9) | C25B—C26A—C27A | 98.3 |
| O2$^{i}$—Pr1—O8$^{ii}$ | 141.78 (8) | C25A—C26A—C27A | 120.0 |

| | | | |
|---|---|---|---|
| O5$^{i}$—Pr1—O4 | 120.85 (9) | C26B—C27A—C27B | 162.1 |
| O2$^{i}$—Pr1—O4 | 84.07 (8) | C26B—C27A—C28A | 145.1 |
| O8$^{ii}$—Pr1—O4 | 133.42 (8) | C27B—C27A—C28A | 52.6 |
| O5$^{i}$—Pr1—N2 | 148.71 (10) | C27B—C27A—C26A | 172.5 |
| O2$^{i}$—Pr1—N2 | 136.51 (10) | C28A—C27A—C26A | 120.0 |
| O8$^{ii}$—Pr1—N2 | 72.96 (10) | C26B—C27A—C25B | 51.6 |
| O5$^{i}$—Pr1—N1 | 150.33 (9) | C27B—C27A—C25B | 146.2 |
| O2$^{i}$—Pr1—N1 | 76.88 (9) | C28A—C27A—C25B | 93.7 |
| O8$^{ii}$—Pr1—N1 | 122.05 (10) | C26B—C27A—C28B | 154.6 |
| O5$^{i}$—Pr1—O5 | 72.90 (10) | C26A—C27A—C28B | 129.4 |
| O2$^{i}$—Pr1—O5 | 65.21 (8) | C25B—C27A—C28B | 103.1 |
| O8$^{ii}$—Pr1—O5 | 129.91 (9) | C28B—C28A—C27B | 109.4 |
| C13—O1—Pr1 | 130.3 (2) | C28B—C28A—C23B | 84.9 |
| C13—O2—Pr1$^{i}$ | 137.7 (2) | C27B—C28A—C23B | 164.8 |
| C15—O3—C14 | 117.6 (3) | C28B—C28A—C27A | 145.7 |
| C21—O4—Pr1 | 101.0 (2) | C23B—C28A—C27A | 128.5 |
| C21—O5—Pr1$^{i}$ | 163.1 (3) | C28B—C28A—C23A | 93.7 |
| C21—O5—Pr1 | 87.9 (2) | C27B—C28A—C23A | 156.7 |
| Pr1$^{i}$—O5—Pr1 | 107.10 (9) | C27A—C28A—C23A | 120.0 |
| C23B—O6—C22 | 119.6 (3) | C28B—C28A—C26B | 155.7 |
| C22—O6—C23A | 112.6 (3) | C27B—C28A—C26B | 46.7 |
| C29—O7—Pr1 | 151.9 (2) | C23B—C28A—C26B | 118.6 |
| C29—O8—Pr1$^{ii}$ | 150.0 (2) | C23A—C28A—C26B | 110.0 |
| C31—O9—C30 | 117.4 (3) | C28B—C28A—C24B | 127.6 |
| C1—N1—C5 | 118.0 (4) | C27B—C28A—C24B | 122.4 |
| C1—N1—Pr1 | 120.6 (3) | C27A—C28A—C24B | 85.7 |
| C5—N1—Pr1 | 119.9 (3) | C26B—C28A—C24B | 75.7 |
| C12—N2—C9 | 118.5 (3) | O6—C23B—C28A | 134.3 (3) |
| C12—N2—Pr1 | 119.6 (3) | O6—C23B—C24B | 128.8 (2) |
| C9—N2—Pr1 | 121.6 (2) | C28A—C23B—C24B | 96.6 |
| N1—C1—C2 | 123.4 (4) | O6—C23B—C28B | 111.1 (3) |
| N1—C1—H1 | 118.3 | C24B—C23B—C28B | 120.0 |
| C2—C1—H1 | 118.3 | O6—C23B—C24A | 115.1 (2) |
| C3—C2—C1 | 118.4 (5) | C28A—C23B—C24A | 110.3 |
| C3—C2—H2 | 120.8 | C28B—C23B—C24A | 133.7 |
| C1—C2—H2 | 120.8 | C23A—C24B—C25A | 153.2 |
| C4—C3—C2 | 120.3 (5) | C25A—C24B—C23B | 152.0 |
| C4—C3—H3 | 119.9 | C23A—C24B—C25B | 121.2 |
| C2—C3—H3 | 119.9 | C23B—C24B—C25B | 120.0 |
| C3—C4—C5 | 118.0 (5) | C25A—C24B—C28A | 111.6 |
| C3—C4—C6 | 123.0 (6) | C25B—C24B—C28A | 79.6 |
| C5—C4—C6 | 119.1 (6) | C25A—C25B—C26A | 136.4 |
| N1—C5—C4 | 121.9 (4) | C25A—C25B—C24B | 67.0 |
| N1—C5—C9 | 118.2 (4) | C26A—C25B—C24B | 156.1 |
| C4—C5—C9 | 120.0 (4) | C25A—C25B—C26B | 172.8 |
| C7—C6—C4 | 120.7 (6) | C24B—C25B—C26B | 120.0 |
| C7—C6—H6 | 119.7 | C25A—C25B—C24A | 55.5 |
| C4—C6—H6 | 119.7 | C26A—C25B—C24A | 167.7 |

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|---|---|---|---|
| C6—C7—C8 | 122.1 (5) | C26B—C25B—C24A | 131.5 |
| C6—C7—H7 | 118.9 | C25A—C25B—C27A | 167.8 |
| C8—C7—H7 | 118.9 | C26A—C25B—C27A | 55.3 |
| C10—C8—C7 | 124.2 (5) | C24B—C25B—C27A | 101.1 |
| C10—C8—C9 | 116.9 (5) | C24A—C25B—C27A | 112.6 |
| C7—C8—C9 | 118.9 (5) | C27A—C26B—C26A | 138.7 |
| N2—C9—C5 | 118.9 (3) | C26A—C26B—C27B | 149.3 |
| N2—C9—C8 | 121.9 (4) | C27A—C26B—C25B | 109.4 |
| C5—C9—C8 | 119.1 (4) | C27B—C26B—C25B | 120.0 |
| C11—C10—C8 | 121.1 (4) | C26A—C26B—C28A | 114.2 |
| C11—C10—H10 | 119.5 | C25B—C26B—C28A | 84.7 |
| C8—C10—H10 | 119.5 | C27A—C27B—C28A | 90.7 |
| C10—C11—C12 | 119.4 (5) | C28A—C27B—C26B | 98.0 |
| C10—C11—H11 | 120.3 | C27A—C27B—C28B | 112.7 |
| C12—C11—H11 | 120.3 | C26B—C27B—C28B | 120.0 |
| N2—C12—C11 | 122.0 (5) | C28A—C28B—C27B | 48.5 |
| N2—C12—H12 | 119.0 | C28A—C28B—C23B | 71.7 |
| C11—C12—H12 | 119.0 | C27B—C28B—C23B | 120.0 |
| O2—C13—O1 | 128.2 (3) | C28A—C28B—C23A | 65.1 |
| O2—C13—C14 | 119.1 (4) | C27B—C28B—C23A | 113.5 |
| O1—C13—C14 | 112.7 (3) | C23B—C28B—C27A | 95.9 |
| O3—C14—C13 | 110.9 (3) | C23A—C28B—C27A | 89.4 |
| O3—C14—H14A | 109.5 | O8—C29—O7 | 126.7 (3) |
| C13—C14—H14A | 109.5 | O8—C29—C30 | 120.06 (18) |
| O3—C14—H14B | 109.5 | O7—C29—C30 | 113.28 (15) |
| C13—C14—H14B | 109.5 | O9—C30—C29 | 111.20 (18) |
| H14A—C14—H14B | 108.0 | O9—C30—H30A | 109.4 |
| C16—C15—C20 | 120.9 (4) | C29—C30—H30A | 109.4 |
| C16—C15—O3 | 114.8 (4) | O9—C30—H30B | 109.4 |
| C20—C15—O3 | 124.3 (4) | C29—C30—H30B | 109.4 |
| C15—C16—C17 | 119.9 (5) | H30A—C30—H30B | 108.0 |
| C15—C16—H16 | 120.0 | C36—C31—O9 | 124.9 (4) |
| C17—C16—H16 | 120.0 | C36—C31—C32 | 119.6 (4) |
| C18—C17—C16 | 120.0 (6) | O9—C31—C32 | 115.5 (4) |
| C18—C17—H17 | 120.0 | C33—C32—C31 | 120.0 (5) |
| C16—C17—H17 | 120.0 | C33—C32—H32 | 120.0 |
| C19—C18—C17 | 120.5 (5) | C31—C32—H32 | 120.0 |
| C19—C18—H18 | 119.7 | C32—C33—C34 | 120.1 (5) |
| C17—C18—H18 | 119.7 | C32—C33—H33 | 119.9 |
| C18—C19—C20 | 120.9 (6) | C34—C33—H33 | 119.9 |
| C18—C19—H19 | 119.5 | C35—C34—C33 | 119.1 (5) |
| C20—C19—H19 | 119.5 | C35—C34—H34 | 120.5 |
| C15—C20—C19 | 117.7 (5) | C33—C34—H34 | 120.5 |
| C15—C20—H20 | 121.2 | C34—C35—C36 | 121.7 (5) |
| C19—C20—H20 | 121.2 | C34—C35—H35 | 119.1 |
| O4—C21—O5 | 122.8 (3) | C36—C35—H35 | 119.1 |
| O4—C21—C22 | 120.2 (3) | C31—C36—C35 | 119.4 (5) |
| O5—C21—C22 | 117.0 (4) | C31—C36—H36 | 120.3 |

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|---|---|---|---|
| O6—C22—C21 | 113.9 (3) | C35—C36—H36 | 120.3 |
| O6—C22—H22A | 108.8 | | |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C1—H1···O2$^{i}$ | 0.93 | 2.46 | 3.147 (5) | 130 |
| C10—H10···O4$^{iii}$ | 0.93 | 2.34 | 3.211 (5) | 156 |
| C12—H12···O8$^{ii}$ | 0.93 | 2.47 | 3.063 (5) | 122 |
| C22—H22*B*···O7$^{iv}$ | 0.97 | 2.41 | 3.353 (5) | 166 |

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