

Retraction of articles by T. Liu *et al.*T. Liu,<sup>a\*</sup> Y.-X. Wang,<sup>b</sup> Z.-W. Wang,<sup>a</sup> Z.-P. Xie<sup>a,c</sup> and J. Y. Zhu<sup>d</sup>

<sup>a</sup>College of Engineering, Jingtangshan University, Jian 343009, People's Republic of China, <sup>b</sup>College of Mathematics and Physics, Jingtangshan University, Jian 343009, People's Republic of China, <sup>c</sup>Department of Chemistry, Jiangxi University of Science and Technology, Ganzhou 341000, People's Republic of China, and <sup>d</sup>Department of Information Engineering, Jiangxi University of Science and Technology, Nanchang 330013, People's Republic of China  
Correspondence e-mail: taoliu07@126.com

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A series of 29 papers by Liu *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 29 papers by Liu *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
<i>Tetrakis(pyrazine-κN)bis(thiocyanato-κN)manganese(II)</i>	Liu & Xie (2007a)	10.1107/S1600536807026852	EDUMAS
<i>(Dihydroxyglyoxime-κ<sup>2</sup>N,N')bis(1,10-phenanthroline-κ<sup>2</sup>N,N')copper(II) dinitrate dihydrate</i>	Liu, Wang, Wang & Xie (2007b)	10.1107/S1600536807028255	EDUVAB
<i>Tetrakis(pyrazine-κN)bis(thiocyanato-κN)zinc(II)</i>	Liu & Xie (2007b)	10.1107/S1600536807028735	RIGQAA
<i>Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-lanthanum(III)]</i>	Liu, Wang, Wang & Xie (2007c)	10.1107/S1600536807030917	UDUMIQ
<i>Polymeric KNOF<sub>2</sub></i>	Liu Wang, Wang & Xie (2007a)	10.1107/S1600536807027195	ICSD 240891
<i>(Dihydroxyglyoxime-κ<sup>2</sup>N,N')bis(1,10-phenanthroline-κ<sup>2</sup>N,N')cobalt(II) dinitrate dihydrate</i>	Liu, Wang, Wang & Xie (2007d)	10.1107/S1600536807031224	WIHJED
<i>Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-praseodymium(III)]</i>	Liu, Wang, Wang & Xie (2007e)	10.1107/S1600536807032679	WIHQEK
<i>Tetrakis[μ-(2-pyridyloxy)acetato-κ<sup>2</sup>O:O']bis[(1,10-phenanthroline-κ<sup>2</sup>N,N')-(2-pyridyloxy)acetato-κO]neodymium(III)]</i>	Liu, Wang, Wang & Xie (2007f)	10.1107/S1600536807035349	TIGDAP
<i>(Dihydroxyglyoxime-κ<sup>2</sup>N,N')bis(1,10-phenanthroline-κ<sup>2</sup>N,N')manganese(II) dinitrate dihydrate</i>	Liu, Wang, Wang & Xie (2007g)	10.1107/S1600536807035076	TIGDET
<i>2-Amino-3,5-dinitrobenzoic acid-ammonia (1/1)</i>	Liu & Zhu (2007j)	10.1107/S1600536807040068	KIKQAX
<i>2-Hydroxy-3,5-dinitrobenzamide monohydrate</i>	Liu & Zhu (2007k)	10.1107/S1600536807039712	KIKQEB
<i>2-(1-Hydroxy-2-pyridyl)acetamide monohydrate</i>	Liu & Zhu (2007l)	10.1107/S1600536807040652	CIKQOD
<i>Bis(2,2'-bipyridine-κN,N')bis(thiocyanato-κN)iron(II)</i>	Liu & Zhu (2007a)	10.1107/S1600536807043486	XIFXOA
<i>catena-Poly[hexakis(μ<sub>2</sub>-anilinoacetamide)bis(1,10-phenanthroline)disamarium(III)]</i>	Liu & Zhu (2007b)	10.1107/S1600536807045485	XILNAI
<i>3-Hydroxy-2,4,6-trinitropyridine monohydrate</i>	Liu & Zhu (2007m)	10.1107/S1600536807045230	PILNOO
<i>catena-Poly[hexakis(μ<sub>2</sub>-anilinoacetamide)bis(1,10-phenanthroline)-dipraseodymium(III)]</i>	Liu & Zhu (2007c)	10.1107/S1600536807047733	SILZET
<i>catena-Poly[[tetra-μ-anilinoacetamidato-bis(1,10-phenanthroline)dicerium(III)]-di-μ-anilinoacetamidato]</i>	Liu & Zhu (2007d)	10.1107/S1600536807050969	GIMZOS
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)chromium(II)</i>	Liu & Zhu (2007e)	10.1107/S1600536807051756	WINFAB
<i>2-Ammonio-3-carboxy-5-nitrobenzoate monohydrate</i>	Liu & Zhu (2007n)	10.1107/S1600536807048477	GINFEP
<i>2-(Benzoylhydrazinocarbonyl)benzoic acid</i>	Liu & Zhu (2007o)	10.1107/S160053680705204X	TINZIA
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)vanadium(II)</i>	Liu & Zhu (2007f)	10.1107/S1600536807054529	HIPZIQ
<i>catena-Poly[[nitrate-κO](1,10-phenanthroline-κ<sup>2</sup>N,N')nickel(II)]-μ-acetamido-κ<sup>2</sup>O:N]</i>	Liu & Zhu (2007g)	10.1107/S1600536807056504	XIRGIP
<i>catena-Poly[[nitrate-κO](1,10-phenanthroline-κ<sup>2</sup>N,N')copper(II)]-μ-acetamido-κ<sup>2</sup>O:N]</i>	Liu & Zhu (2007h)	10.1107/S1600536807059077	HIQROP
<i>catena-Poly[[nitrate-κO](1,10-phenanthroline-κ<sup>2</sup>N,N')cobalt(II)]-μ-acetamidato-κ<sup>2</sup>O:N]</i>	Liu & Zhu (2007i)	10.1107/S1600536807060631	YIQMER
<i>N'-Benzoyl-4-nitronicotinohydrazide</i>	Liu & Zhu (2007p)	10.1107/S1600536807053068	CIPVON
<i>N'-(3-Nitro-4-pyridylcarbonyl)pyridine-4-carbohydrazide</i>	Liu & Zhu (2007q)	10.1107/S1600536807054876	RIRWEV

**Table 1 (continued)**

Title	Reference	DOI	Refcode
<i>Ethylenediammonium sulfate</i>	Liu & Zhu (2007r)	10.1107/S1600536807056280	ETDAMS03
<i>Ethylenediammonium perchlorate</i>	Liu & Zhu (2007s)	10.1107/S1600536807059909	HIRYEN
<i>catena-Poly[[[nitrate-κO](1,10-phenanthroline-κ<sup>2</sup>N,N')manganese(II)]-μ-nitrate-κ<sup>2</sup>O:O']</i>	Liu & Zhu (2008)	10.1107/S160053680706254X	MIRROV

## References

Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007a). *Acta Cryst.* **E63**, i170.  
 Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007b). *Acta Cryst.* **E63**, m1887–m1888.  
 Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007c). *Acta Cryst.* **E63**, m2020–m2021.  
 Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007d). *Acta Cryst.* **E63**, m2027–m2028.  
 Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007e). *Acta Cryst.* **E63**, m2080–m2081.  
 Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007f). *Acta Cryst.* **E63**, m2196–m2197.  
 Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007g). *Acta Cryst.* **E63**, m2198–m2199.  
 Liu, T. & Xie, Z.-P. (2007a). *Acta Cryst.* **E63**, m1820.  
 Liu, T. & Xie, Z.-P. (2007b). *Acta Cryst.* **E63**, m1908.  
 Liu, T. & Zhu, J. Y. (2007a). *Acta Cryst.* **E63**, m2506–m2507.

Liu, T. & Zhu, J.-Y. (2007b). *Acta Cryst.* **E63**, m2592–m2593.  
 Liu, T. & Zhu, J. Y. (2007c). *Acta Cryst.* **E63**, m2659–m2660.  
 Liu, T. & Zhu, J. Y. (2007d). *Acta Cryst.* **E63**, m2775–m2776.  
 Liu, T. & Zhu, J. Y. (2007e). *Acta Cryst.* **E63**, m2809.  
 Liu, T. & Zhu, J. Y. (2007f). *Acta Cryst.* **E63**, m2912.  
 Liu, T. & Zhu, J.-Y. (2007g). *Acta Cryst.* **E63**, m2977–m2978.  
 Liu, T. & Zhu, J. Y. (2007h). *Acta Cryst.* **E63**, m3108.  
 Liu, T. & Zhu, J. Y. (2007i). *Acta Cryst.* **E63**, m3144.  
 Liu, T. & Zhu, J.-Y. (2007j). *Acta Cryst.* **E63**, o3829.  
 Liu, T. & Zhu, J. Y. (2007k). *Acta Cryst.* **E63**, o3830.  
 Liu, T. & Zhu, J.-Y. (2007l). *Acta Cryst.* **E63**, o3860.  
 Liu, T. & Zhu, J. Y. (2007m). *Acta Cryst.* **E63**, o4112.  
 Liu, T. & Zhu, J. Y. (2007n). *Acta Cryst.* **E63**, o4267.  
 Liu, T. & Zhu, J. Y. (2007o). *Acta Cryst.* **E63**, o4441.  
 Liu, T. & Zhu, J. Y. (2007p). *Acta Cryst.* **E63**, o4527.  
 Liu, T. & Zhu, J. Y. (2007q). *Acta Cryst.* **E63**, o4574.  
 Liu, T. & Zhu, J.-Y. (2007r). *Acta Cryst.* **E63**, o4660.  
 Liu, T. & Zhu, J. Y. (2007s). *Acta Cryst.* **E63**, o4874.  
 Liu, T. & Zhu, J. Y. (2008). *Acta Cryst.* **E64**, m28.

## catena-Poly[hexakis( $\mu_2$ -anilino-acetamide)bis(1,10-phenanthroline)-diprasedmium(III)]

T. Liu<sup>a\*</sup> and J. Y. Zhu<sup>b</sup>

<sup>a</sup>College of Engineering, Jingtangshan University, Jian 343009, People's Republic of China, and <sup>b</sup>Department of Information Engineering, Jiangxi University of Science and Technology, Nanchang 330013, People's Republic of China  
Correspondence e-mail: taoliu07@126.com

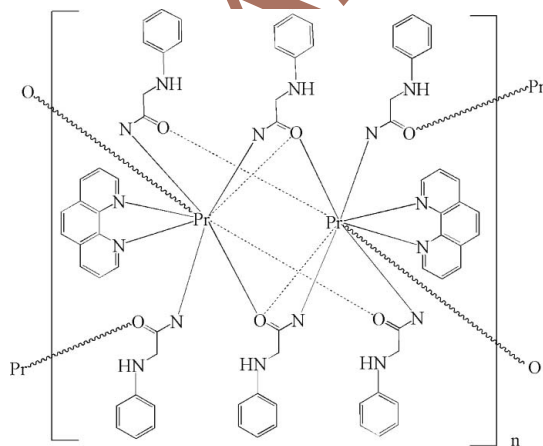
Received 27 September 2007; accepted 28 September 2007

Key indicators: single-crystal X-ray study;  $T = 273$  K; mean  $\sigma(\text{C}-\text{C}) = 0.012$  Å;  $R$  factor = 0.047;  $wR$  factor = 0.138; data-to-parameter ratio = 17.8.

The title compound,  $[\text{Pr}_2(\text{C}_8\text{H}_9\text{N}_2\text{O})_6(\text{C}_{12}\text{H}_8\text{N}_2)_2]_n$ , is a polymeric complex based on a binuclear unit with an inversion centre mid-way between the two  $\text{Pr}^{\text{III}}$  ions, which are bridged by two tridentate, two bidentate and four monodentate (within the binuclear unit) acetamide groups. Each Pr atom is nine-coordinated by two 1,10-phenanthroline N atoms and four O and three N atoms of anilinoacetamide ligands. In the crystal structure,  $\text{C}-\text{H}\cdots\text{O}$ ,  $\text{C}-\text{H}\cdots\text{N}$ ,  $\text{N}-\text{H}\cdots\text{N}$  and  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds result in the formation of a supra-molecular network structure; an  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bond is also present within one ligand.

### Related literature

For a related structure, see: Liu & Zhu (2007). For bond-length data, see: Allen *et al.* (1987).



### Experimental

#### Crystal data

$[\text{Pr}_2(\text{C}_8\text{H}_9\text{N}_2\text{O})_6(\text{C}_{12}\text{H}_8\text{N}_2)_2]$   
 $M_r = 768.63$   
 Monoclinic,  $P2_1/n$   
 $a = 19.9013$  (11) Å  
 $b = 8.6081$  (14) Å  
 $c = 20.581$  (2) Å  
 $\beta = 106.774$  (2)°  
 $V = 3375.8$  (7) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.49$  mm<sup>-1</sup>  
 $T = 273$  (2) K  
 $0.33 \times 0.12 \times 0.08$  mm

#### Data collection

Bruker SMART CCD area-detector diffractometer  
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)  
 $T_{\text{min}} = 0.640$ ,  $T_{\text{max}} = 0.891$   
 26534 measured reflections  
 7311 independent reflections  
 4903 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.042$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$   
 $wR(F^2) = 0.138$   
 $S = 0.96$   
 7311 reflections  
 411 parameters  
 6 restraints  
 H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 1.39$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.72$  e Å<sup>-3</sup>

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

Pr1—O1	2.573 (3)	Pr1—N3	2.458 (3)
Pr1—O2 <sup>i</sup>	2.520 (3)	Pr1—N4	2.863 (4)
Pr1—O3 <sup>ii</sup>	2.543 (3)	Pr1—N4 <sup>i</sup>	2.414 (3)
Pr1—N1	2.715 (4)	Pr1—N5	2.433 (4)
Pr1—N2	2.696 (4)		
O1—Pr1—N1	63.97 (12)	N1—Pr1—N5	77.46 (13)
O1—Pr1—N2	74.94 (11)	N2—Pr1—N3	81.43 (12)
O1—Pr1—N3	72.85 (11)	N2—Pr1—N4	118.48 (11)
O1—Pr1—N4	47.58 (10)	N2—Pr1—N5	95.81 (12)
O1—Pr1—N5	139.78 (12)	N3—Pr1—N4	64.39 (11)
N1—Pr1—N2	59.62 (14)	N3—Pr1—N5	145.60 (12)
N1—Pr1—N3	127.16 (12)	N4—Pr1—N5	140.65 (11)
N1—Pr1—N4	102.53 (12)		

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

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

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C}22-\text{H}22\text{B}\cdots\text{N}5^{\text{iii}}$	0.97	2.39	3.329 (7)	163
$\text{C}12-\text{H}12\cdots\text{N}8^{\text{ii}}$	0.93	2.55	3.395 (8)	151
$\text{C}12-\text{H}12\cdots\text{O}3^{\text{ii}}$	0.93	2.47	3.050 (7)	121
$\text{C}10-\text{H}10\cdots\text{O}1^{\text{iv}}$	0.93	2.33	3.201 (7)	155
$\text{C}1-\text{H}1\cdots\text{O}2^{\text{i}}$	0.93	2.41	3.105 (7)	131
$\text{N}7-\text{H}7\text{A}\cdots\text{O}2$	0.86	2.25	2.605 (5)	105
$\text{N}5-\text{H}5\cdots\text{O}2^{\text{i}}$	0.77 (2)	2.35 (3)	3.083 (5)	159 (6)
$\text{N}4-\text{H}4\cdots\text{N}4^{\text{i}}$	0.86	2.63	3.152 (8)	120
$\text{N}4-\text{H}4\cdots\text{O}2^{\text{i}}$	0.86	2.15	2.905 (5)	146

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); 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: HK2337).

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### References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Liu, T. & Zhu, J.-Y. (2007). *Acta Cryst.* **E63**, m2592–m2593.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Siemens (1996). *SMART*, *SAINT* and *SHELXTL*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Article retracted

**supplementary materials**

**Article retracted**

*Acta Cryst.* (2007). E63, m2659-m2660 [ doi:10.1107/S1600536807047733 ]

***catena*-Poly[hexakis( $\mu_2$ -anilinoacetamide)bis(1,10-phenanthroline)dipraseodymium(III)]**

**T. Liu and J. Y. Zhu**

**Comment**

The crystal structure of *catena*-Poly[hexakis( $\mu_2$ -anilinoacetamide)bis(1,10-phenanthroline)disamarium(III)], (II), has previously been reported (Liu & Zhu, 2007). The crystal structure determination of the title compound, (I), has been carried out in order to elucidate the molecular conformation and to compare it with that of (II). We report herein the crystal structure of (I).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987). It has an inversion centre midway between the two Pr<sup>III</sup> ions, which are bridged by two tridentate, two bidentate and four monodentate acetamide groups. Each Pr atom is nine-coordinated by two N atoms of 1,10-phenanthroline (phen) ligand and four O and three N atoms of anilinoacetamide ligands. The Pr—O and Pr—N bonds are in the range of [2.520 (3)–2.573 (3) Å] and [2.414 (3)–2.863 (4) Å], respectively (Table 1), as in (II).

In the crystal structure, intermolecular C—H $\cdots$ O, C—H $\cdots$ N, N—H $\cdots$ N and N—H $\cdots$ O hydrogen bonds (Table 2, Fig. 2) result in the formation of a supramolecular network structure; intramolecular N—H $\cdots$ O hydrogen bond (Table 2) is also present, as in (II).

The both compounds, (I) and (II), are isostructural.

**Experimental**

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb. Praseodymium (III) nitrate hexahydrate (213.8 mg, 0.5 mmol), phen (198 mg, 1 mmol), anilinoacetamide (290.4 mg, 2 mmol) and distilled water (10 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure up to 453 K over the course of 7 d and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colorless solution was decanted from small colorless crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature.

**Refinement**

H5 and H8 (for NH) were located in difference syntheses and refined isotropically [N—H = 0.77 (2) and 0.81 (5) Å,  $U_{\text{iso}}(\text{H})$  = 0.059 (18) and 0.07 (2) Å<sup>2</sup>]. The remaining H atoms were positioned geometrically, with N—H = 0.86 Å (for NH) and C—H = 0.93 and 0.97 Å, for aromatic and methylene H atoms and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H})$  = 1.2 $U_{\text{eq}}(\text{C}, \text{N})$ .

Figures

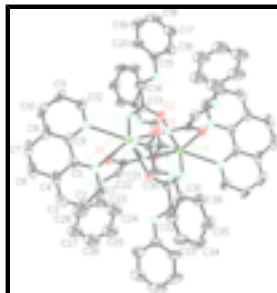


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code (A):  $2 - x, -y, 2 - z$ ]. H atoms have been omitted for clarity.

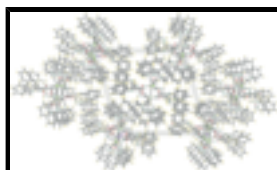


Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

**catena-Poly[hexakis( $\mu_2$ -anilinoacetamide)bis(1,10-phenanthroline)dipraseodymium(III)]**

*Crystal data*

$[\text{Pr}_2(\text{C}_8\text{H}_9\text{N}_2\text{O})_6(\text{C}_{12}\text{H}_8\text{N}_2)_2]$

$M_r = 768.63$

Monoclinic,  $P2_1/n$

Hall symbol:  $-P\ 2_1/n$

$a = 19.9013$  (11) Å

$b = 8.6081$  (14) Å

$c = 20.581$  (2) Å

$\beta = 106.774$  (2)°

$V = 3375.8$  (7) Å<sup>3</sup>

$Z = 4$

$F_{000} = 1560$

$D_x = 1.512$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 8891 reflections

$\theta = 2.6$ – $26.5$ °

$\mu = 1.49$  mm<sup>-1</sup>

$T = 273$  (2) K

Plate, colourless

$0.33 \times 0.12 \times 0.08$  mm

*Data collection*

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 273$ (2) K

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.640$ ,  $T_{\max} = 0.891$

26534 measured reflections

7311 independent reflections

4903 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.042$

$\theta_{\text{max}} = 27.2$ °

$\theta_{\text{min}} = 2.1$ °

$h = -25 \rightarrow 25$

$k = -10 \rightarrow 11$

$l = -26 \rightarrow 26$

Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.138$	$w = 1/[\sigma^2(F_o^2) + (0.0902P)^2 + 0.285P]$
$S = 0.96$	where $P = (F_o^2 + 2F_c^2)/3$
7311 reflections	$(\Delta/\sigma)_{\max} = 0.001$
411 parameters	$\Delta\rho_{\max} = 1.39 \text{ e } \text{\AA}^{-3}$
6 restraints	$\Delta\rho_{\min} = -0.72 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Pr1	0.931196 (13)	0.19067 (3)	0.964285 (12)	0.03954 (11)
O1	0.84617 (16)	-0.0357 (4)	0.91891 (16)	0.0470 (8)
O2	1.06673 (18)	-0.0827 (4)	0.92134 (16)	0.0521 (8)
O3	1.0070 (2)	0.6127 (4)	1.09077 (16)	0.0592 (10)
N1	0.7967 (2)	0.2336 (5)	0.9666 (2)	0.0496 (10)
N2	0.8344 (2)	0.3064 (4)	0.8549 (2)	0.0498 (10)
N3	0.97080 (18)	0.0613 (4)	0.87540 (16)	0.0343 (8)
H3A	0.9396	0.0556	0.8366	0.041*
N4	0.94712 (18)	-0.1394 (5)	0.97706 (17)	0.0364 (8)
H4	0.9440	-0.0483	0.9931	0.044*
N5	0.9401 (2)	0.4226 (4)	1.03380 (17)	0.0347 (8)
H5	0.932 (3)	0.335 (3)	1.035 (3)	0.059 (18)*
N7	1.1181 (2)	-0.0162 (5)	0.8217 (2)	0.0529 (11)
H7A	1.1395	-0.0737	0.8555	0.063*
N8	0.9877 (2)	0.5260 (5)	1.20638 (18)	0.0476 (10)
H8	0.962 (3)	0.600 (4)	1.2049 (19)	0.07 (2)*



## supplementary materials

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N9	0.7855 (2)	-0.3271 (4)	0.8983 (2)	0.0489 (10)
H9	0.7624	-0.3420	0.8565	0.059*
C1	0.7787 (3)	0.1912 (7)	1.0202 (3)	0.0660 (16)
H1	0.8137	0.1683	1.0600	0.079*
C2	0.7092 (4)	0.1793 (9)	1.0196 (4)	0.086 (2)
H2	0.6977	0.1508	1.0587	0.104*
C3	0.6582 (4)	0.2099 (9)	0.9612 (5)	0.092 (2)
H3	0.6113	0.1976	0.9598	0.111*
C4	0.6746 (3)	0.2579 (10)	0.9053 (4)	0.0784 (19)
C5	0.7462 (3)	0.2669 (6)	0.9094 (3)	0.0544 (13)
C6	0.6218 (4)	0.2942 (11)	0.8397 (5)	0.115 (4)
H6	0.5743	0.2828	0.8354	0.138*
C7	0.6417 (4)	0.3421 (11)	0.7878 (4)	0.103 (3)
H7	0.6078	0.3697	0.7479	0.124*
C8	0.7134 (3)	0.3530 (8)	0.7911 (3)	0.0716 (18)
C9	0.7661 (3)	0.3092 (6)	0.8505 (3)	0.0551 (14)
C10	0.7358 (5)	0.4047 (9)	0.7374 (3)	0.090 (2)
H10	0.7033	0.4409	0.6982	0.109*
C11	0.8044 (5)	0.4030 (8)	0.7416 (3)	0.085 (2)
H11	0.8196	0.4369	0.7053	0.102*
C12	0.8526 (3)	0.3500 (7)	0.8007 (3)	0.0665 (16)
H12	0.8997	0.3450	0.8021	0.080*
C13	1.0285 (3)	0.0024 (6)	0.8772 (2)	0.0466 (11)
C14	1.0523 (3)	0.0517 (7)	0.8173 (3)	0.0567 (13)
H14A	1.0181	0.0192	0.7756	0.068*
H14B	1.0561	0.1640	0.8167	0.068*
C15	1.1460 (3)	0.0141 (7)	0.7694 (3)	0.0651 (15)
C16	1.2074 (3)	-0.0556 (9)	0.7760 (3)	0.0800 (19)
H16	1.2279	-0.1170	0.8137	0.096*
C17	1.2398 (4)	-0.0356 (10)	0.7265 (5)	0.096 (2)
H17	1.2831	-0.0820	0.7307	0.115*
C18	1.2086 (5)	0.0530 (10)	0.6708 (5)	0.111 (3)
H18	1.2303	0.0635	0.6367	0.134*
C19	1.1480 (5)	0.1242 (12)	0.6644 (4)	0.112 (3)
H19	1.1276	0.1854	0.6266	0.135*
C20	1.1149 (4)	0.1055 (9)	0.7159 (4)	0.086 (2)
H20	1.0726	0.1550	0.7130	0.103*
C21	0.8838 (3)	-0.1525 (6)	0.9388 (2)	0.0469 (12)
C22	0.8579 (3)	-0.3147 (6)	0.9198 (3)	0.0579 (14)
H22A	0.8764	-0.3512	0.8838	0.069*
H22B	0.8760	-0.3819	0.9587	0.069*
C23	0.7543 (7)	-0.3146 (10)	0.9466 (7)	0.1284 (17)
C24	0.7844 (7)	-0.2801 (10)	1.0107 (7)	0.1284 (17)
H24	0.8325	-0.2621	1.0264	0.154*
C25	0.7416 (6)	-0.2712 (11)	1.0554 (6)	0.1284 (17)
H25	0.7613	-0.2496	1.1012	0.154*
C26	0.6745 (6)	-0.2940 (10)	1.0307 (7)	0.1284 (17)
H26	0.6473	-0.2832	1.0603	0.154*
C27	0.6385 (6)	-0.3346 (10)	0.9613 (6)	0.1284 (17)

H27	0.5906	-0.3550	0.9462	0.154*
C28	0.6799 (6)	-0.3403 (11)	0.9207 (6)	0.1284 (17)
H28	0.6603	-0.3613	0.8748	0.154*
C29	0.9693 (3)	0.4994 (6)	1.0864 (2)	0.0463 (11)
C30	0.9488 (3)	0.4459 (7)	1.1474 (2)	0.0584 (14)
H30A	0.8991	0.4642	1.1402	0.070*
H30B	0.9573	0.3352	1.1536	0.070*
C31	0.9742 (3)	0.4889 (7)	1.2656 (2)	0.0579 (14)
C32	0.9279 (3)	0.3789 (9)	1.2721 (3)	0.0739 (18)
H32	0.9020	0.3237	1.2343	0.089*
C33	0.9195 (5)	0.3498 (12)	1.3343 (4)	0.109 (3)
H33	0.8890	0.2722	1.3395	0.131*
C34	0.9567 (5)	0.4366 (11)	1.3902 (3)	0.105 (3)
H34	0.9487	0.4217	1.4321	0.126*
C35	1.0043 (4)	0.5418 (9)	1.3836 (3)	0.091 (2)
H35	1.0304	0.5962	1.4215	0.109*
C36	1.0145 (3)	0.5696 (8)	1.3221 (3)	0.0743 (17)
H36	1.0478	0.6414	1.3179	0.089*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Pr1	0.04542 (17)	0.03514 (17)	0.03339 (15)	-0.00150 (11)	0.00395 (10)	0.00062 (10)
O1	0.0468 (18)	0.0380 (19)	0.0487 (19)	-0.0002 (15)	0.0018 (14)	-0.0035 (14)
O2	0.063 (2)	0.051 (2)	0.0435 (19)	0.0085 (17)	0.0172 (16)	0.0114 (16)
O3	0.085 (3)	0.055 (2)	0.0387 (19)	-0.026 (2)	0.0200 (18)	-0.0049 (16)
N1	0.047 (2)	0.046 (2)	0.049 (2)	0.0037 (19)	0.0035 (19)	-0.0084 (19)
N2	0.060 (3)	0.045 (3)	0.036 (2)	0.0023 (19)	0.0004 (18)	0.0006 (17)
N3	0.0397 (19)	0.038 (2)	0.0239 (16)	0.0050 (17)	0.0073 (14)	0.0010 (15)
N4	0.0362 (19)	0.0320 (19)	0.0346 (19)	-0.0018 (15)	0.0000 (15)	0.0039 (15)
N5	0.054 (2)	0.0190 (19)	0.0296 (18)	-0.0064 (17)	0.0097 (15)	-0.0053 (14)
N7	0.052 (2)	0.070 (3)	0.043 (2)	0.017 (2)	0.0232 (19)	0.022 (2)
N8	0.068 (3)	0.047 (3)	0.030 (2)	-0.021 (2)	0.0169 (18)	-0.0050 (17)
N9	0.045 (2)	0.037 (2)	0.054 (3)	-0.0137 (18)	-0.0015 (19)	-0.0065 (18)
C1	0.059 (3)	0.080 (5)	0.059 (4)	0.008 (3)	0.018 (3)	0.000 (3)
C2	0.058 (4)	0.121 (7)	0.085 (5)	0.007 (4)	0.028 (4)	-0.010 (4)
C3	0.051 (4)	0.106 (7)	0.118 (7)	-0.004 (4)	0.020 (4)	-0.015 (5)
C4	0.055 (4)	0.094 (5)	0.072 (4)	0.006 (3)	-0.003 (3)	-0.017 (4)
C5	0.054 (3)	0.041 (3)	0.060 (3)	0.007 (2)	0.003 (2)	-0.008 (2)
C6	0.056 (4)	0.157 (10)	0.105 (7)	0.017 (5)	-0.020 (4)	-0.033 (6)
C7	0.079 (5)	0.119 (7)	0.080 (5)	0.038 (5)	-0.028 (4)	-0.018 (5)
C8	0.075 (4)	0.069 (4)	0.048 (3)	0.019 (3)	-0.017 (3)	-0.012 (3)
C9	0.063 (3)	0.037 (3)	0.051 (3)	0.005 (2)	-0.006 (2)	-0.005 (2)
C10	0.120 (6)	0.074 (5)	0.049 (4)	0.017 (4)	-0.021 (4)	0.001 (3)
C11	0.123 (6)	0.082 (5)	0.035 (3)	-0.003 (4)	0.001 (3)	0.013 (3)
C12	0.082 (4)	0.056 (4)	0.052 (3)	0.000 (3)	0.005 (3)	0.009 (3)
C13	0.062 (3)	0.039 (3)	0.037 (2)	-0.012 (2)	0.010 (2)	-0.003 (2)
C14	0.065 (3)	0.058 (3)	0.049 (3)	0.005 (3)	0.019 (2)	0.010 (2)

## supplementary materials

C15	0.070 (4)	0.074 (4)	0.059 (3)	-0.009 (3)	0.031 (3)	0.002 (3)
C16	0.079 (4)	0.099 (5)	0.073 (4)	0.005 (4)	0.040 (4)	-0.002 (4)
C17	0.092 (5)	0.098 (6)	0.115 (6)	-0.003 (5)	0.058 (5)	-0.006 (5)
C18	0.149 (8)	0.086 (6)	0.141 (8)	-0.015 (6)	0.108 (7)	-0.001 (6)
C19	0.153 (8)	0.118 (7)	0.093 (6)	0.022 (7)	0.077 (6)	0.035 (5)
C20	0.100 (5)	0.098 (5)	0.078 (4)	0.003 (4)	0.053 (4)	0.022 (4)
C21	0.048 (3)	0.055 (3)	0.033 (2)	-0.003 (2)	0.004 (2)	-0.005 (2)
C22	0.064 (3)	0.050 (3)	0.055 (3)	0.004 (3)	0.009 (3)	-0.005 (2)
C23	0.139 (4)	0.097 (3)	0.174 (5)	0.017 (3)	0.084 (4)	0.032 (3)
C24	0.139 (4)	0.097 (3)	0.174 (5)	0.017 (3)	0.084 (4)	0.032 (3)
C25	0.139 (4)	0.097 (3)	0.174 (5)	0.017 (3)	0.084 (4)	0.032 (3)
C26	0.139 (4)	0.097 (3)	0.174 (5)	0.017 (3)	0.084 (4)	0.032 (3)
C27	0.139 (4)	0.097 (3)	0.174 (5)	0.017 (3)	0.084 (4)	0.032 (3)
C28	0.139 (4)	0.097 (3)	0.174 (5)	0.017 (3)	0.084 (4)	0.032 (3)
C29	0.058 (3)	0.035 (3)	0.045 (3)	-0.002 (2)	0.014 (2)	0.005 (2)
C30	0.077 (4)	0.057 (3)	0.043 (3)	-0.022 (3)	0.018 (2)	-0.006 (2)
C31	0.076 (4)	0.059 (3)	0.038 (3)	-0.003 (3)	0.015 (2)	0.004 (2)
C32	0.076 (4)	0.096 (5)	0.052 (3)	-0.034 (4)	0.022 (3)	-0.006 (3)
C33	0.124 (7)	0.145 (8)	0.070 (5)	-0.046 (6)	0.046 (5)	0.003 (5)
C34	0.124 (6)	0.148 (8)	0.051 (4)	-0.030 (6)	0.038 (4)	0.007 (5)
C35	0.118 (6)	0.105 (6)	0.045 (3)	-0.018 (5)	0.014 (3)	-0.008 (4)
C36	0.086 (4)	0.082 (5)	0.051 (3)	-0.018 (4)	0.013 (3)	-0.013 (3)

### Geometric parameters (Å, °)

Pr1—O1	2.573 (3)	C8—C9	1.413 (7)
Pr1—O2 <sup>i</sup>	2.520 (3)	C10—C11	1.344 (10)
Pr1—O3 <sup>ii</sup>	2.543 (3)	C10—H10	0.9300
Pr1—N1	2.715 (4)	C11—C12	1.389 (8)
Pr1—N2	2.696 (4)	C11—H11	0.9300
Pr1—N3	2.458 (3)	C12—H12	0.9300
Pr1—N4	2.863 (4)	C13—C14	1.502 (7)
Pr1—N4 <sup>i</sup>	2.414 (3)	C14—H14A	0.9700
Pr1—N5	2.433 (4)	C14—H14B	0.9700
O1—C21	1.250 (6)	C15—C16	1.334 (9)
O2—C13	1.243 (6)	C15—C20	1.350 (9)
O2—Pr1 <sup>i</sup>	2.520 (3)	C16—C17	1.363 (10)
O3—C29	1.217 (6)	C16—H16	0.9300
O3—Pr1 <sup>ii</sup>	2.543 (3)	C17—C18	1.369 (12)
N1—C1	1.306 (7)	C17—H17	0.9300
N1—C5	1.340 (7)	C18—C19	1.325 (11)
N2—C12	1.323 (7)	C18—H18	0.9300
N2—C9	1.336 (7)	C19—C20	1.409 (9)
N3—C13	1.246 (6)	C19—H19	0.9300
N3—H3A	0.8600	C20—H20	0.9300
N4—C21	1.284 (6)	C21—C22	1.500 (7)
N4—Pr1 <sup>i</sup>	2.414 (3)	C22—H22A	0.9700
N4—H4	0.8600	C22—H22B	0.9700

N5—C29	1.258 (6)	C23—C24	1.316 (16)
N5—H5	0.77 (2)	C23—C28	1.438 (16)
N7—C15	1.372 (7)	C24—C25	1.424 (13)
N7—C14	1.413 (6)	C24—H24	0.9300
N7—H7A	0.8600	C25—C26	1.300 (15)
N8—C31	1.360 (6)	C25—H25	0.9300
N8—C30	1.416 (6)	C26—C27	1.444 (16)
N8—H8	0.81 (5)	C26—H26	0.9300
N9—C23	1.319 (12)	C27—C28	1.332 (12)
N9—C22	1.384 (7)	C27—H27	0.9300
N9—H9	0.8600	C28—H28	0.9300
C1—C2	1.384 (9)	C29—C30	1.500 (7)
C1—H1	0.9300	C30—H30A	0.9700
C2—C3	1.357 (11)	C30—H30B	0.9700
C2—H2	0.9300	C31—C32	1.354 (8)
C3—C4	1.348 (11)	C31—C36	1.393 (8)
C3—H3	0.9300	C32—C33	1.363 (9)
C4—C5	1.407 (8)	C32—H32	0.9300
C4—C6	1.486 (11)	C33—C34	1.391 (11)
C5—C9	1.428 (8)	C33—H33	0.9300
C6—C7	1.306 (13)	C34—C35	1.345 (10)
C6—H6	0.9300	C34—H34	0.9300
C7—C8	1.413 (11)	C35—C36	1.359 (9)
C7—H7	0.9300	C35—H35	0.9300
C8—C10	1.379 (10)	C36—H36	0.9300
O1—Pr1—N1	63.97 (12)	N1—C5—C9	118.6 (5)
O1—Pr1—N2	74.94 (11)	C4—C5—C9	119.3 (5)
O1—Pr1—N3	72.85 (11)	C7—C6—C4	120.6 (8)
O1—Pr1—N4	47.58 (10)	C7—C6—H6	119.7
O1—Pr1—N5	139.78 (12)	C4—C6—H6	119.7
N1—Pr1—N2	59.62 (14)	C6—C7—C8	121.4 (7)
N1—Pr1—N3	127.16 (12)	C6—C7—H7	119.3
N1—Pr1—N4	102.53 (12)	C8—C7—H7	119.3
N1—Pr1—N5	77.46 (13)	C10—C8—C9	116.6 (6)
N2—Pr1—N3	81.43 (12)	C10—C8—C7	122.6 (7)
N2—Pr1—N4	118.48 (11)	C9—C8—C7	120.8 (7)
N2—Pr1—N5	95.81 (12)	N2—C9—C8	123.4 (6)
N3—Pr1—N4	64.39 (11)	N2—C9—C5	117.6 (5)
N3—Pr1—N5	145.60 (12)	C8—C9—C5	118.9 (6)
N4—Pr1—N5	140.65 (11)	C11—C10—C8	120.2 (6)
N4 <sup>i</sup> —Pr1—N5	87.92 (13)	C11—C10—H10	119.9
N4 <sup>i</sup> —Pr1—N3	78.38 (12)	C8—C10—H10	119.9
N4 <sup>i</sup> —Pr1—O2 <sup>i</sup>	73.85 (11)	C10—C11—C12	119.5 (6)
N5—Pr1—O2 <sup>i</sup>	76.97 (12)	C10—C11—H11	120.3
N3—Pr1—O2 <sup>i</sup>	127.29 (12)	C12—C11—H11	120.3
N4 <sup>i</sup> —Pr1—O2 <sup>i</sup>	73.85 (11)	N2—C12—C11	122.9 (7)
N5—Pr1—O2 <sup>i</sup>	76.97 (12)	N2—C12—H12	118.5

## supplementary materials

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N3—Pr1—O2 <sup>i</sup>	127.29 (12)	C11—C12—H12	118.5
O2 <sup>i</sup> —Pr1—O2 <sup>i</sup>	0.0 (2)	O2—C13—N3	128.7 (5)
N4 <sup>i</sup> —Pr1—O2 <sup>i</sup>	73.85 (11)	O2—C13—C14	119.7 (5)
N5—Pr1—O2 <sup>i</sup>	76.97 (12)	N3—C13—C14	111.5 (4)
N3—Pr1—O2 <sup>i</sup>	127.29 (12)	N7—C14—C13	109.6 (4)
O2 <sup>i</sup> —Pr1—O2 <sup>i</sup>	0.0 (2)	N7—C14—H14A	109.7
O2 <sup>i</sup> —Pr1—O2 <sup>i</sup>	0.0 (2)	C13—C14—H14A	109.7
N4 <sup>i</sup> —Pr1—O3 <sup>ii</sup>	78.47 (13)	N7—C14—H14B	109.7
N5—Pr1—O3 <sup>ii</sup>	75.71 (12)	C13—C14—H14B	109.7
N3—Pr1—O3 <sup>ii</sup>	70.72 (11)	H14A—C14—H14B	108.2
O2 <sup>i</sup> —Pr1—O3 <sup>ii</sup>	141.45 (11)	C16—C15—C20	122.4 (6)
O2 <sup>i</sup> —Pr1—O3 <sup>ii</sup>	141.45 (11)	C16—C15—N7	113.7 (6)
O2 <sup>i</sup> —Pr1—O3 <sup>ii</sup>	141.45 (11)	C20—C15—N7	123.9 (6)
N4 <sup>i</sup> —Pr1—O1	120.18 (12)	C15—C16—C17	119.0 (7)
O2 <sup>i</sup> —Pr1—O1	83.77 (11)	C15—C16—H16	120.5
O2 <sup>i</sup> —Pr1—O1	83.77 (11)	C17—C16—H16	120.5
O2 <sup>i</sup> —Pr1—O1	83.77 (11)	C16—C17—C18	119.9 (8)
O3 <sup>ii</sup> —Pr1—O1	133.98 (11)	C16—C17—H17	120.1
N4 <sup>i</sup> —Pr1—N2	148.97 (13)	C18—C17—H17	120.1
O2 <sup>i</sup> —Pr1—N2	137.01 (13)	C19—C18—C17	121.4 (7)
O2 <sup>i</sup> —Pr1—N2	137.01 (13)	C19—C18—H18	119.3
O2 <sup>i</sup> —Pr1—N2	137.01 (13)	C17—C18—H18	119.3
O3 <sup>ii</sup> —Pr1—N2	72.71 (13)	C18—C19—C20	118.8 (8)
N4 <sup>i</sup> —Pr1—N1	150.16 (12)	C18—C19—H19	120.6
O2 <sup>i</sup> —Pr1—N1	77.54 (12)	C20—C19—H19	120.6
O2 <sup>i</sup> —Pr1—N1	77.54 (12)	C15—C20—C19	118.4 (7)
O2 <sup>i</sup> —Pr1—N1	77.54 (12)	C15—C20—H20	120.8
O3 <sup>ii</sup> —Pr1—N1	121.54 (14)	C19—C20—H20	120.8
N4 <sup>i</sup> —Pr1—N4	72.79 (13)	O1—C21—N4	121.3 (5)
O2 <sup>i</sup> —Pr1—N4	64.96 (11)	O1—C21—C22	122.4 (4)
O2 <sup>i</sup> —Pr1—N4	64.96 (11)	N4—C21—C22	116.4 (5)
O2 <sup>i</sup> —Pr1—N4	64.96 (11)	N9—C22—C21	113.8 (4)
O3 <sup>ii</sup> —Pr1—N4	130.29 (11)	N9—C22—H22A	108.8
N4 <sup>i</sup> —Pr1—H5	87.3 (18)	C21—C22—H22A	108.8
N3—Pr1—H5	158.2 (15)	N9—C22—H22B	108.8
O2 <sup>i</sup> —Pr1—H5	62.2 (12)	C21—C22—H22B	108.8
O2 <sup>i</sup> —Pr1—H5	62.2 (12)	H22A—C22—H22B	107.7
O2 <sup>i</sup> —Pr1—H5	62.2 (12)	C24—C23—N9	126.5 (12)
O3 <sup>ii</sup> —Pr1—H5	90.5 (12)	C24—C23—C28	122.0 (11)
O1—Pr1—H5	128.9 (14)	N9—C23—C28	111.5 (12)
N2—Pr1—H5	104.0 (17)	C23—C24—C25	118.3 (13)

N1—Pr1—H5	71.8 (17)	C23—C24—H24	120.9
N4—Pr1—H5	126.8 (13)	C25—C24—H24	120.9
C21—O1—Pr1	102.8 (3)	C26—C25—C24	118.6 (13)
C13—O2—Pr1 <sup>i</sup>	138.0 (3)	C26—C25—H25	120.7
C29—O3—Pr1 <sup>ii</sup>	150.1 (3)	C24—C25—H25	120.7
C1—N1—C5	118.9 (5)	C25—C26—C27	125.7 (11)
C1—N1—Pr1	119.2 (4)	C25—C26—H26	117.2
C5—N1—Pr1	120.5 (4)	C27—C26—H26	117.2
C12—N2—C9	117.2 (5)	C28—C27—C26	114.1 (12)
C12—N2—Pr1	120.4 (4)	C28—C27—H27	122.9
C9—N2—Pr1	122.1 (3)	C26—C27—H27	122.9
C13—N3—Pr1	130.8 (3)	C27—C28—C23	121.2 (13)
C13—N3—H3A	114.6	C27—C28—H28	119.4
Pr1—N3—H3A	114.6	C23—C28—H28	119.4
C21—N4—Pr1 <sup>i</sup>	162.9 (4)	O3—C29—N5	127.3 (5)
C21—N4—Pr1	88.2 (3)	O3—C29—C30	119.6 (4)
Pr1 <sup>i</sup> —N4—Pr1	107.21 (13)	N5—C29—C30	112.9 (4)
C21—N4—H4	98.5	N8—C30—C29	110.8 (4)
Pr1 <sup>i</sup> —N4—H4	98.5	N8—C30—H30A	109.5
C29—N5—Pr1	150.9 (3)	C29—C30—H30A	109.5
C29—N5—H5	122 (5)	N8—C30—H30B	109.5
C15—N7—C14	116.7 (4)	C29—C30—H30B	109.5
C15—N7—H7A	121.7	H30A—C30—H30B	108.1
C14—N7—H7A	121.7	C32—C31—N8	124.7 (5)
C31—N8—C30	116.9 (4)	C32—C31—C36	120.7 (5)
C31—N8—H8	86.1 (17)	N8—C31—C36	114.6 (5)
C30—N8—H8	100 (4)	C32—C31—H8	124 (2)
C23—N9—C22	115.2 (8)	C36—C31—H8	107 (2)
C23—N9—H9	122.4	C31—C32—C33	119.5 (6)
C22—N9—H9	122.4	C31—C32—H32	120.3
N1—C1—C2	122.1 (6)	C33—C32—H32	120.3
N1—C1—H1	119.0	C32—C33—C34	119.9 (7)
C2—C1—H1	119.0	C32—C33—H33	120.1
C3—C2—C1	119.0 (7)	C34—C33—H33	120.1
C3—C2—H2	120.5	C35—C34—C33	120.1 (6)
C1—C2—H2	120.5	C35—C34—H34	120.0
C4—C3—C2	120.7 (7)	C33—C34—H34	120.0
C4—C3—H3	119.6	C34—C35—C36	120.7 (7)
C2—C3—H3	119.6	C34—C35—H35	119.7
C3—C4—C5	117.2 (6)	C36—C35—H35	119.7
C3—C4—C6	124.0 (7)	C35—C36—C31	119.0 (6)
C5—C4—C6	118.7 (7)	C35—C36—H36	120.5
N1—C5—C4	122.1 (6)	C31—C36—H36	120.5

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
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## supplementary materials

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C22—H22B…N5 <sup>iii</sup>	0.97	2.39	3.329 (7)	163
C12—H12…N8 <sup>ii</sup>	0.93	2.55	3.395 (8)	151
C12—H12…O3 <sup>ii</sup>	0.93	2.47	3.050 (7)	121
C10—H10…O1 <sup>iv</sup>	0.93	2.33	3.201 (7)	155
C1—H1…O2 <sup>i</sup>	0.93	2.41	3.105 (7)	131
N7—H7A…O2	0.86	2.25	2.605 (5)	105
N5—H5…O2 <sup>i</sup>	0.77 (2)	2.35 (3)	3.083 (5)	159 (6)
N4—H4…N4 <sup>i</sup>	0.86	2.63	3.152 (8)	120
N4—H4…O2 <sup>i</sup>	0.86	2.15	2.905 (5)	146

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

Article retracted

Fig. 1

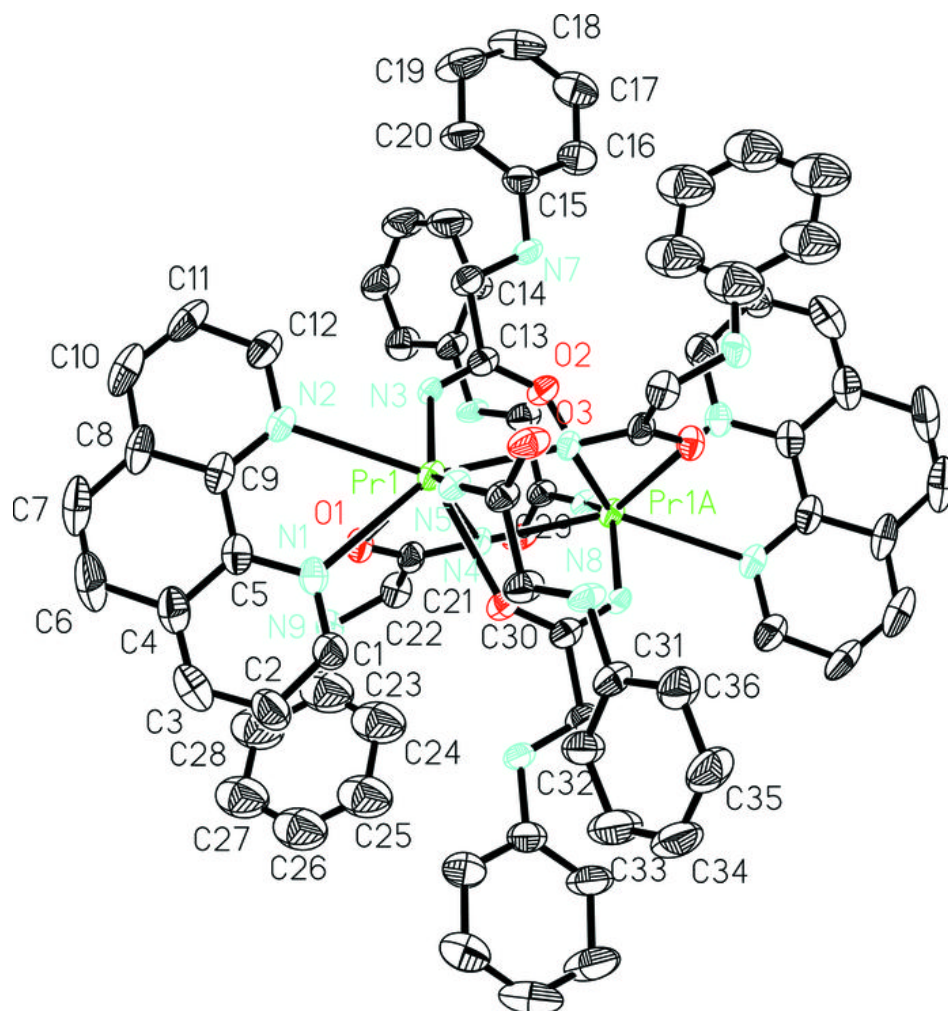
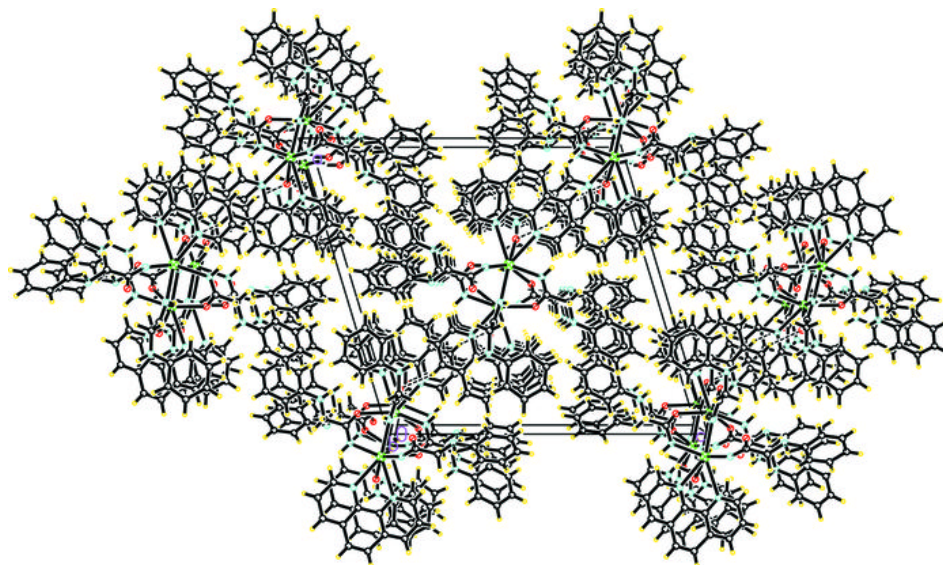




Fig. 2



Article retrac