Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Hexakis(μ-naphthalene-1-acetato)-bis[(1,10-phenanthroline)praseodymium(III)] *N*,*N*-dimethylformamide solvate

Hai-Tao Xia,[a]* Yu-Fen Liu,[a] Da-Qi Wang[b] and Liang Chen[a]

[a]Department of Chemical Engineering, Huaihai Institute of Technology, Lianyungang, Jiangsu 222005, People's Republic of China, and [b]College of Chemistry and Chemical Engineering, Liaocheng University, Shandong 252059, People's Republic of China
Correspondence e-mail: xht161006@hhit.edu.cn

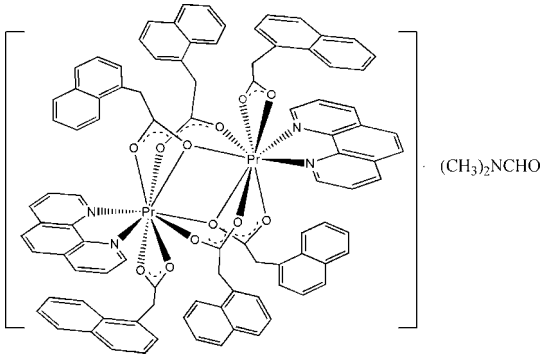
Received 18 September 2007; accepted 24 September 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.011 Å; disorder in main residue; R factor = 0.040; wR factor = 0.100; data-to-parameter ratio = 12.2.

The asymmetric unit of the title compound, $[Pr_2(C_{12}H_9O_2)_6(C_{12}H_8N_2)_2]\cdot C_3H_7NO$, contains two independent half-complex molecules, together with two molecules of solvent; the complex molecules are centrosymmetric. Each Pr^{III} ion is nine-coordinate and the naphthalene acetate (NNA) ligands coordinated to the Pr^{III} ion have three types of coordination mode. One of the NNA ligands is disordered over two sites; the site occupancies refined to 0.565 (17) and 0.435 (17). Molecules are linked into three chains by C—H···O and C—H···π hydrogen bonds and π–π stacking interactions [centroid-to-centroid distance 3.944(3) Å] parallel to the *a*-axis direction and the [011] plane, respectively, and the [011] and *a*-axis chains are linked into sheets parallel to the [011] plane.

Related literature

For related literature, see: Chen & Cai (2005); Liu *et al.* (2007); Zhou *et al.* (2004).



Experimental

Crystal data

$[Pr_2(C_{12}H_9O_2)_6(C_{12}H_8N_2)_2]\cdot C_3H_7NO$
M_r = 1826.48
Triclinic, $P\overline{1}$
a = 13.0204 (12) Å
b = 17.1379 (19) Å
c = 20.417 (3) Å
α = 66.336 (2)°
β = 81.554 (2)°
γ = 85.998 (3)°
V = 4127.2 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.24 mm^{-1}
T = 298 (2) K
0.49 × 0.45 × 0.22 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.583, T_{max} = 0.773
21619 measured reflections
14351 independent reflections
9934 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.100
S = 1.08
14351 reflections
1174 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.75 e Å^{-3}

Table 1
Selected bond lengths (Å).

Pr1—O3^{i}	2.431 (3)	Pr2—O8^{ii}	2.423 (4)
Pr1—O1	2.434 (3)	Pr2—O7	2.443 (4)
Pr1—O5	2.448 (3)	Pr2—O9^{ii}	2.447 (3)
Pr1—O2^{i}	2.474 (3)	Pr2—O12	2.500 (4)
Pr1—O6	2.548 (4)	Pr2—O11	2.552 (4)
Pr1—O4	2.574 (4)	Pr2—O10	2.561 (4)
Pr1—O3	2.619 (4)	Pr2—N4	2.635 (4)
Pr1—N1	2.667 (4)	Pr2—O9	2.644 (4)
Pr1—N2	2.670 (4)	Pr2—N3	2.691 (4)
Pr1—Pr1^{i}	4.0072 (6)		

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

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

Cg is the centroid of the C31–C36 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C26—H26*B*···O13^{iii}	0.97	2.36	3.311 (9)	168
C46—H46···O1	0.93	2.40	3.081 (7)	130
C47—H47···O4^{iv}	0.93	2.59	3.377 (6)	143
C85—H85···O8^{ii}	0.93	2.47	3.149 (7)	130
C92—H92···O10^{v}	0.93	2.55	3.442 (7)	160
C98—H98*A*···O13	0.96	2.37	2.774 (12)	105
C86—H86···*Cg*^{ii}	0.93	2.87	3.706 (12)	151

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

The authors acknowledge the financial support of the Huaihai Institute of Technology Science Foundation.

  doi:10.1107/S160053680704682X

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2404).

References

Chen, Y. & Cai, W.-M. (2005). *Spectrochim. Acta A*, **62**, 863–868.

Liu, Y.-F., Xia, H.-T., Wang, D.-Q. & Yang, S.-P. (2007). *Acta Cryst.* E**63**, m2608–m2609.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen,Germany.

Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.

Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Zhou, Z.-C., Shu, W.-G., Ruan, J.-M., Huang, B.-Y. & Liu, Y.-N. (2004). *Rare Metals*, **23**, 306–310.

supplementary materials

Acta Cryst. (2007). E**63**, m2610-m2611 [**doi:10.1107/S160053680704682X**]

Hexakis(μ-naphthalene-1-acetato)bis[(1,10-phenanthroline)praseodymium(III)] *N*,*N*-dimethylformamide solvate

H.-T. Xia, Y.-F. Liu, D.-Q. Wang and L. Chen

Comment

Rare earth complexes with aromatic carboxylic acids are a kind of luminescent materials with good properties (Zhou *et al.*, 2004). Generally, an organic negative ligand acts as the first ligand to the central ion while a neutral secondary ligand acts as to saturate the coordination number of the rare earth ion and also to improve the fluorescence intensity and stability of the complex. Based on this reason, some rare earth complexes with 1-naphthylacetic acid (NNA) and 1,10-phenanthroline (phen) have been synthesized (Chen & Cai, 2005), however, no report on crystal structures of rare earth complexes with NNA and phen can be found in the literature. Here, we report the synthesis and crystal structure of complex, (I).

In(I), the asymmetric unit consists of two half molecule (*A* and *B*) and one *N*, *N*-dimethylformamide (DMF) solvate. Each half molecule have a symmetric center on the central Pr—Pr bond. Each Pr^{III} ion is nine-coordinated and the stereochemistry each Pr^{III} ion can be described as a distorted monocapped square antiprismatic geometry (Fig. 1). The coordination modes of NNA ligands coordinated to the Pr^{III} ion is consistent with reported Eu complex (Liu *et al.*, 2007). The Pr1—O bond distances are 2.431 (3)–2.619 (4) Å, longer than that 2.423 (4)–2.561 (4) Å of Pr2—O. The dihedral angles between the least square-plane Pr_2O_2 and naphthyl rings are 42.19 (16)–71.32 (11)° for molecule *A* and 49.74 (16)–58.51 (16)° for molecule *B*.

The two molecules of (I) are linked into a chain running parallel to the [011] plane by means of C—H···π hydrogen bond and π···π stacking interaction (Fig. 2 and Table 2). The phen rings (N2C42—C46) in the molecules at (*x*, *y*, *z*) are inclined to one another (N3C85—C89) in the molecules at (1 − *x*, 1 − *y*, 1 − *z*), the separation of the two rings centroids is 3.944 (3) Å, the dihedral angles between the two rings is 2.95°. In the same way, two molecules are linked into two chains parallel to the *a* axis direction by C—H···O hydrogen bonds (Fig. 3 and Table 2), and these two *a* chains are linked into sheets parallel to the [011] plane by [011] chain. The DMF solvate molecules lie in between two sheets. However, there are no direction-specific interactions between adjacent sheets.

Experimental

To a stirred solution of 1-naphthylacetic acid (0.5586 g, 3 mmol) and 1,10-phenanthroline monohydrate (0.198 g, 1 mmol) in 30 ml me thanol, and a solution of $Pr(NO_3)_3·6H_2O$ (0.453 g, 1 mmol) in water (10 ml) was added. The mixed solution was heated to 333 K and stirred for 3 h, and then cooled to room temperature. The precipitate was washed with water and then dissolved in DMF. A colorless crystal suitable for X-ray diffraction was obtained by evaporation of DMF solution [m.p. 548–549 K].

Refinement

The space group was uniquely assigned from the systematic absences. All H atoms were located in difference Fourier maps. H atoms bonded to C atoms were treated as riding atoms, with C—H distances of 0.93 Å (aryl, formyl), 0.97 Å

(methylene) and 0.96 Å (methyl), and with U_{iso}(H) = 1.2U_{eq}(C) (aryl, formyl, methylene) or 1.5U_{eq}(C) (methyl). The NNA ligand bridged to Pr2 were found to be disordered over two sites. The coordinates of these two sites were refined with the occupancies tied to sum to unity, the site occupancies for C50–C60 with attached H atoms and C50'–C60' with attached H atoms refined to 0.565 (17) and 0.435 (17), respectively.

Figures

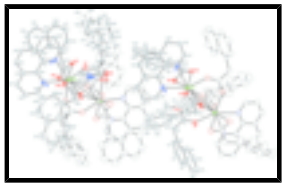


Fig. 1. The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are at the 30% probability level. Unlabelled atoms in the molecular (*a*) are related to labelled atoms by (- *x*, 2 − *y*, − *z*). Unlabelled atoms in the molecule (*b*) are related to labelled atoms by (1 − *x*, 1 − *y*, 1 − *z*). For clarity, the DMF molecular have been omitted.

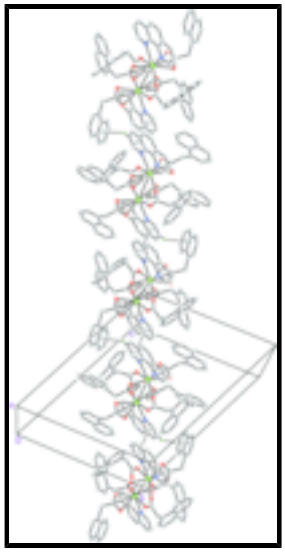


Fig. 2. A larger portion of the crystal structure of (I), showing the formation of a hydrogen-bonded chain built from C—H···π and π···π stacking. For clarity, H atoms not involved in the hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds and π···π stacking.

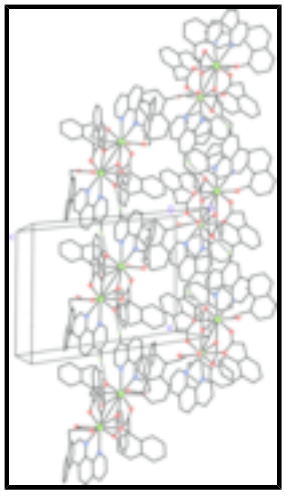


Fig. 3. A larger portion of the crystal structure of (I), showing the formation of a hydrogen-bonded chain built from C—H···O. For clarity, H atoms not involved in the hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds.

Hexakis(μ-naphthalene-1-acetato)bis[(1,10-phenanthroline)praseodymium(III)] *N*,*N*-dimethylformamide solvate

Crystal data

$[Pr_2(C_{12}H_9O_2)_6(C_{12}H_8N_2)_2]\cdot C_3H_7NO$	$Z = 2$
$M_r = 1826.48$	$F_{000} = 1856$
Triclinic, $P\overline{1}$	$D_x = 1.470$ Mg m^{-3}
Hall symbol: -P 1	Melting point: 549 K
$a = 13.0204$ (12) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 17.1379$ (19) Å	Cell parameters from 7370 reflections
$c = 20.417$ (3) Å	$\theta = 2.2$–28.0°
$\alpha = 66.336$ (2)°	$\mu = 1.24$ mm^{-1}
$\beta = 81.554$ (2)°	$T = 298$ (2) K
$\gamma = 85.998$ (3)°	Block, colourless
$V = 4127.2$ (8) Å^3	0.49 × 0.45 × 0.22 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	14351 independent reflections
Radiation source: fine-focus sealed tube	9934 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.023$
$T = 298(2)$ K	$\theta_{max} = 25.0^\circ$
φ and ω scans	$\theta_{min} = 1.3^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -15\rightarrow15$
$T_{min} = 0.583$, $T_{max} = 0.773$	$k = -20\rightarrow20$
21619 measured reflections	$l = -24\rightarrow10$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.040$	H-atom parameters constrained
$wR(F^2) = 0.100$	$w = 1/[\sigma^2(F_o^2) + (0.0262P)^2 + 6.9332P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} = 0.001$
14351 reflections	$\Delta\rho_{max} = 1.56$ e Å^{-3}
1174 parameters	$\Delta\rho_{min} = -0.75$ e Å^{-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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Pr1	0.12209 (2)	0.995948 (16)	0.050714 (15)	0.03165 (9)	
Pr2	0.61837 (2)	0.479311 (17)	0.559170 (16)	0.03783 (9)	
N1	0.3126 (3)	1.0448 (2)	0.0495 (2)	0.0357 (10)	
N2	0.2593 (3)	0.8769 (2)	0.1157 (2)	0.0393 (10)	
N3	0.7446 (3)	0.3471 (3)	0.6218 (2)	0.0468 (12)	
N4	0.8110 (3)	0.5107 (3)	0.5657 (2)	0.0432 (11)	
N5	0.1828 (6)	0.6340 (5)	0.8451 (4)	0.099 (2)	
O1	0.0207 (3)	0.8661 (2)	0.1040 (2)	0.0484 (10)	
O2	−0.1304 (3)	0.8736 (2)	0.06167 (19)	0.0413 (9)	
O3	0.0595 (2)	0.9601 (2)	−0.05013 (19)	0.0415 (9)	
O4	0.2236 (3)	0.9351 (2)	−0.0366 (2)	0.0455 (9)	
O5	0.1096 (3)	1.1156 (2)	0.0882 (2)	0.0443 (9)	
O6	0.1111 (3)	0.9911 (2)	0.17795 (19)	0.0497 (10)	
O7	0.6377 (3)	0.6161 (2)	0.4558 (2)	0.0515 (10)	
O8	0.4972 (3)	0.6407 (2)	0.3992 (2)	0.0556 (11)	
O9	0.5565 (3)	0.4583 (2)	0.44969 (19)	0.0449 (9)	
O10	0.7190 (3)	0.4295 (3)	0.4650 (2)	0.0589 (11)	
O11	0.6152 (3)	0.5839 (2)	0.6199 (2)	0.0491 (10)	
O12	0.5853 (3)	0.4502 (2)	0.6906 (2)	0.0561 (10)	
O13	0.0657 (6)	0.7409 (4)	0.8256 (4)	0.138 (3)	
C1	−0.0614 (4)	0.8342 (3)	0.0990 (3)	0.0403 (13)	
C2	−0.0705 (4)	0.7390 (3)	0.1442 (3)	0.0557 (17)	
H2A	−0.0168	0.7102	0.1235	0.067*	
H2B	−0.0552	0.7286	0.1921	0.067*	
C3	−0.1725 (4)	0.6973 (3)	0.1523 (4)	0.0511 (16)	
C4	−0.2372 (5)	0.6764 (3)	0.2155 (4)	0.0630 (19)	
H4	−0.2177	0.6882	0.2526	0.076*	
C5	−0.3339 (5)	0.6369 (4)	0.2258 (5)	0.080 (2)	
H5	−0.3779	0.6235	0.2690	0.096*	
C6	−0.3611 (6)	0.6190 (4)	0.1723 (5)	0.077 (2)	
H6	−0.4243	0.5929	0.1792	0.093*	
C7	−0.2979 (5)	0.6383 (4)	0.1073 (5)	0.068 (2)	
C8	−0.2007 (5)	0.6772 (3)	0.0963 (4)	0.0567 (17)	

C9	−0.1370 (6)	0.6946 (4)	0.0303 (4)	0.073 (2)
H9	−0.0733	0.7205	0.0221	0.088*
C10	−0.1679 (8)	0.6738 (5)	−0.0228 (5)	0.094 (3)
H10	−0.1245	0.6843	−0.0658	0.112*
C11	−0.2634 (8)	0.6374 (5)	−0.0114 (6)	0.101 (3)
H11	−0.2850	0.6258	−0.0480	0.121*
C12	−0.3264 (7)	0.6181 (4)	0.0513 (6)	0.091 (3)
H12	−0.3891	0.5914	0.0582	0.110*
C13	0.1470 (4)	0.9284 (3)	−0.0640 (3)	0.0352 (12)
C14	0.1551 (4)	0.8837 (4)	−0.1148 (3)	0.0525 (15)
H14A	0.0974	0.8449	−0.1000	0.063*
H14B	0.1470	0.9261	−0.1626	0.063*
C15	0.2532 (5)	0.8346 (4)	−0.1201 (3)	0.0540 (16)
C16	0.3254 (5)	0.8645 (4)	−0.1791 (4)	0.074 (2)
H16	0.3132	0.9159	−0.2168	0.088*
C17	0.4196 (6)	0.8186 (5)	−0.1847 (5)	0.092 (3)
H17	0.4679	0.8396	−0.2259	0.110*
C18	0.4380 (7)	0.7460 (6)	−0.1308 (5)	0.094 (3)
H18	0.5009	0.7179	−0.1346	0.113*
C19	0.3683 (6)	0.7100 (5)	−0.0695 (5)	0.078 (2)
C20	0.2743 (5)	0.7559 (4)	−0.0639 (4)	0.0601 (17)
C21	0.2015 (6)	0.7193 (5)	−0.0014 (4)	0.083 (2)
H21	0.1407	0.7491	0.0042	0.100*
C22	0.2188 (8)	0.6414 (6)	0.0507 (5)	0.115 (3)
H22	0.1688	0.6168	0.0903	0.138*
C23	0.3133 (9)	0.5987 (6)	0.0437 (6)	0.121 (3)
H23	0.3250	0.5459	0.0798	0.145*
C24	0.3866 (8)	0.6307 (6)	−0.0124 (6)	0.105 (3)
H24	0.4492	0.6015	−0.0142	0.126*
C25	0.1147 (4)	1.0706 (3)	0.1537 (3)	0.0412 (13)
C26	0.1283 (5)	1.1189 (4)	0.1990 (3)	0.0603 (17)
H26A	0.1867	1.1566	0.1753	0.072*
H26B	0.0671	1.1546	0.1990	0.072*
C27	0.1455 (5)	1.0692 (4)	0.2756 (3)	0.0552 (16)
C28	0.0668 (6)	1.0653 (5)	0.3276 (4)	0.078 (2)
H28	0.0036	1.0915	0.3147	0.094*
C29	0.0780 (7)	1.0229 (5)	0.4002 (4)	0.100 (3)
H29	0.0219	1.0197	0.4351	0.120*
C30	0.1702 (7)	0.9862 (5)	0.4208 (4)	0.096 (3)
H30	0.1767	0.9584	0.4696	0.115*
C31	0.2567 (6)	0.9898 (4)	0.3686 (4)	0.0705 (19)
C32	0.2429 (5)	1.0310 (3)	0.2948 (3)	0.0527 (15)
C33	0.3289 (5)	1.0341 (4)	0.2432 (4)	0.0626 (17)
H33	0.3220	1.0604	0.1944	0.075*
C34	0.4221 (6)	0.9989 (4)	0.2640 (4)	0.080 (2)
H34	0.4779	1.0013	0.2292	0.095*
C35	0.4345 (6)	0.9597 (5)	0.3363 (5)	0.085 (2)
H35	0.4987	0.9365	0.3497	0.102*
C36	0.3542 (7)	0.9549 (5)	0.3873 (4)	0.085 (2)

H36	0.3634	0.9279	0.4357	0.102*	
C37	0.3381 (4)	1.1259 (3)	0.0189 (3)	0.0455 (14)	
H37	0.2880	1.1657	−0.0026	0.055*	
C38	0.4362 (4)	1.1552 (4)	0.0170 (3)	0.0529 (15)	
H38	0.4508	1.2130	−0.0054	0.063*	
C39	0.5104 (4)	1.0977 (3)	0.0484 (3)	0.0493 (15)	
H39	0.5763	1.1160	0.0477	0.059*	
C40	0.4867 (4)	1.0112 (3)	0.0818 (3)	0.0407 (13)	
C41	0.3850 (4)	0.9869 (3)	0.0815 (3)	0.0351 (12)	
C42	0.3580 (4)	0.8988 (3)	0.1164 (3)	0.0361 (12)	
C43	0.4328 (4)	0.8383 (3)	0.1496 (3)	0.0459 (14)	
C44	0.4026 (5)	0.7529 (4)	0.1819 (3)	0.0629 (18)	
H44	0.4493	0.7108	0.2052	0.075*	
C45	0.3067 (5)	0.7315 (4)	0.1795 (4)	0.068 (2)	
H45	0.2871	0.6746	0.1997	0.082*	
C46	0.2364 (4)	0.7955 (3)	0.1462 (3)	0.0555 (16)	
H46	0.1697	0.7798	0.1456	0.067*	
C47	0.5607 (4)	0.9471 (4)	0.1153 (3)	0.0513 (15)	
H47	0.6278	0.9628	0.1151	0.062*	
C48	0.5351 (4)	0.8657 (4)	0.1467 (3)	0.0540 (16)	
H48	0.5851	0.8253	0.1675	0.065*	
C49	0.5690 (5)	0.6637 (3)	0.4221 (4)	0.0569 (17)	
C50	0.5590 (13)	0.7485 (10)	0.4309 (9)	0.056 (4)	0.565 (17)
H50A	0.5266	0.7895	0.3908	0.067*	0.565 (17)
H50B	0.5118	0.7405	0.4745	0.067*	0.565 (17)
C51	0.6573 (11)	0.7879 (7)	0.4350 (10)	0.066 (5)	0.565 (17)
C52	0.678 (2)	0.786 (2)	0.501 (2)	0.073 (7)	0.565 (17)
H52	0.6326	0.7588	0.5423	0.088*	0.565 (17)
C53	0.767 (4)	0.823 (3)	0.504 (3)	0.086 (9)	0.565 (17)
H53	0.7814	0.8219	0.5477	0.103*	0.565 (17)
C54	0.8356 (18)	0.8634 (11)	0.4415 (13)	0.082 (6)	0.565 (17)
H54	0.8953	0.8887	0.4437	0.098*	0.565 (17)
C55	0.81 (2)	0.87 (3)	0.38 (4)	0.07 (4)	0.565 (17)
C56	0.726 (3)	0.8280 (19)	0.373 (2)	0.070 (9)	0.565 (17)
C57	0.705 (10)	0.830 (7)	0.307 (5)	0.07 (2)	0.565 (17)
H57	0.6450	0.8051	0.3049	0.089*	0.565 (17)
C58	0.773 (6)	0.870 (4)	0.245 (4)	0.082 (11)	0.565 (17)
H58	0.7589	0.8719	0.2009	0.098*	0.565 (17)
C59	0.862 (2)	0.9081 (12)	0.2480 (15)	0.076 (5)	0.565 (17)
H59	0.9077	0.9349	0.2063	0.091*	0.565 (17)
C60	0.883 (6)	0.906 (5)	0.314 (5)	0.079 (15)	0.565 (17)
H60	0.9426	0.9310	0.3158	0.095*	0.565 (17)
C50'	0.5756 (18)	0.7602 (14)	0.3866 (15)	0.076 (7)	0.435 (17)
H50C	0.5431	0.7782	0.3430	0.091*	0.435 (17)
H50D	0.5322	0.7820	0.4186	0.091*	0.435 (17)
C51'	0.678 (2)	0.8062 (15)	0.366 (2)	0.063 (8)	0.435 (17)
C52'	0.701 (12)	0.839 (9)	0.291 (7)	0.071 (17)	0.435 (17)
H52'	0.6569	0.8301	0.2636	0.085*	0.435 (17)
C53'	0.791 (8)	0.887 (5)	0.258 (5)	0.084 (19)	0.435 (17)

H53'	0.8063	0.9090	0.2085	0.101*	0.435 (17)
C54'	0.857 (7)	0.901 (7)	0.300 (7)	0.08 (2)	0.435 (17)
H54'	0.9168	0.9323	0.2780	0.095*	0.435 (17)
C55'	0.83 (3)	0.87 (4)	0.37 (5)	0.07 (4)	0.435 (17)
C56'	0.744 (3)	0.820 (2)	0.4078 (18)	0.065 (10)	0.435 (17)
C57'	0.721 (3)	0.787 (3)	0.482 (2)	0.071 (9)	0.435 (17)
H57'	0.6608	0.7553	0.5045	0.085*	0.435 (17)
C58'	0.787 (5)	0.801 (4)	0.524 (3)	0.082 (11)	0.435 (17)
H58'	0.7713	0.7786	0.5741	0.099*	0.435 (17)
C59'	0.8764 (18)	0.8481 (12)	0.4911 (14)	0.085 (7)	0.435 (17)
H59'	0.9207	0.8575	0.5190	0.102*	0.435 (17)
C60'	0.900 (2)	0.8814 (13)	0.4164 (15)	0.085 (8)	0.435 (17)
H60'	0.9596	0.9131	0.3943	0.102*	0.435 (17)
C61	0.6451 (4)	0.4323 (3)	0.4321 (3)	0.0463 (14)	
C62	0.6600 (5)	0.4080 (4)	0.3675 (3)	0.0651 (18)	
H62A	0.5921	0.4019	0.3561	0.078*	
H62B	0.6943	0.4546	0.3265	0.078*	
C63	0.7217 (6)	0.3276 (4)	0.3764 (4)	0.0670 (18)	
C64	0.8262 (6)	0.3303 (5)	0.3708 (4)	0.087 (2)	
H64	0.8570	0.3815	0.3621	0.104*	
C65	0.8903 (7)	0.2583 (7)	0.3776 (5)	0.107 (3)	
H65	0.9620	0.2621	0.3741	0.129*	
C66	0.8471 (8)	0.1848 (6)	0.3891 (5)	0.104 (3)	
H66	0.8894	0.1370	0.3953	0.125*	
C67	0.7403 (8)	0.1776 (5)	0.3919 (4)	0.086 (2)	
C68	0.6755 (7)	0.2490 (5)	0.3873 (4)	0.076 (2)	
C69	0.5687 (8)	0.2395 (6)	0.3915 (5)	0.103 (3)	
H69	0.5237	0.2850	0.3885	0.124*	
C70	0.5295 (9)	0.1619 (7)	0.4000 (5)	0.123 (3)	
H70	0.4584	0.1565	0.4022	0.148*	
C71	0.5936 (11)	0.0935 (7)	0.4051 (6)	0.131 (4)	
H71	0.5647	0.0420	0.4126	0.157*	
C72	0.6962 (10)	0.0987 (6)	0.3997 (5)	0.115 (3)	
H72	0.7388	0.0524	0.4008	0.138*	
C73	0.5973 (4)	0.5263 (4)	0.6812 (3)	0.0436 (13)	
C74	0.5883 (5)	0.5483 (4)	0.7469 (3)	0.0586 (16)	
H74A	0.5219	0.5765	0.7508	0.070*	
H74B	0.5884	0.4957	0.7895	0.070*	
C75	0.6728 (5)	0.6044 (4)	0.7460 (3)	0.0579 (16)	
C76	0.6530 (6)	0.6847 (4)	0.7422 (4)	0.079 (2)	
H76	0.5858	0.7066	0.7378	0.095*	
C77	0.7314 (7)	0.7362 (5)	0.7448 (5)	0.096 (3)	
H77	0.7165	0.7917	0.7405	0.115*	
C78	0.8276 (7)	0.7036 (5)	0.7533 (4)	0.093 (3)	
H78	0.8781	0.7373	0.7565	0.111*	
C79	0.8557 (6)	0.6214 (4)	0.7578 (4)	0.073 (2)	
C80	0.7764 (5)	0.5717 (4)	0.7524 (3)	0.0566 (16)	
C81	0.8067 (5)	0.4909 (4)	0.7536 (3)	0.0586 (16)	
H81	0.7573	0.4576	0.7487	0.070*	

C82	0.9048 (6)	0.4590 (5)	0.7616 (4)	0.075 (2)
H82	0.9215	0.4055	0.7614	0.090*
C83	0.9794 (6)	0.5064 (6)	0.7700 (4)	0.090 (2)
H83	1.0458	0.4838	0.7774	0.108*
C84	0.9566 (6)	0.5845 (5)	0.7674 (4)	0.086 (2)
H84	1.0083	0.6160	0.7721	0.103*
C85	0.7135 (5)	0.2679 (4)	0.6493 (4)	0.0624 (18)
H85	0.6451	0.2578	0.6472	0.075*
C86	0.7772 (5)	0.1976 (4)	0.6817 (4)	0.073 (2)
H86	0.7514	0.1426	0.7009	0.088*
C87	0.8769 (5)	0.2113 (4)	0.6845 (4)	0.0696 (19)
H87	0.9204	0.1654	0.7058	0.083*
C88	0.9150 (4)	0.2937 (4)	0.6555 (3)	0.0558 (16)
C89	0.8441 (4)	0.3610 (3)	0.6246 (3)	0.0457 (14)
C90	0.8805 (4)	0.4468 (3)	0.5951 (3)	0.0455 (14)
C91	0.9848 (4)	0.4636 (4)	0.5956 (3)	0.0495 (14)
C92	1.0153 (5)	0.5487 (4)	0.5667 (3)	0.0596 (17)
H92	1.0838	0.5619	0.5658	0.072*
C93	0.9452 (5)	0.6123 (4)	0.5399 (3)	0.0590 (17)
H93	0.9643	0.6691	0.5218	0.071*
C94	0.8437 (4)	0.5901 (4)	0.5403 (3)	0.0536 (16)
H94	0.7963	0.6338	0.5215	0.064*
C95	1.0201 (5)	0.3140 (4)	0.6553 (3)	0.0650 (18)
H95	1.0663	0.2699	0.6759	0.078*
C96	1.0533 (5)	0.3934 (4)	0.6267 (3)	0.0609 (17)
H96	1.1225	0.4038	0.6267	0.073*
C97	0.1487 (8)	0.7123 (6)	0.8099 (5)	0.101 (3)
H97	0.1918	0.7480	0.7701	0.121*
C98	0.1213 (9)	0.5751 (7)	0.9091 (6)	0.147 (4)
H98A	0.0559	0.6013	0.9172	0.220*
H98B	0.1579	0.5606	0.9500	0.220*
H98C	0.1096	0.5243	0.9023	0.220*
C99	0.2810 (8)	0.6042 (6)	0.8222 (5)	0.138 (4)
H99A	0.3172	0.6505	0.7831	0.207*
H99B	0.2704	0.5600	0.8064	0.207*
H99C	0.3213	0.5821	0.8617	0.207*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pr1	0.02479 (16)	0.03391 (15)	0.03961 (18)	−0.00079 (11)	−0.01051 (12)	−0.01585 (13)
Pr2	0.02723 (17)	0.03939 (17)	0.0509 (2)	0.00106 (12)	−0.01346 (14)	−0.01950 (15)
N1	0.026 (2)	0.036 (2)	0.044 (3)	−0.0047 (17)	−0.0098 (19)	−0.013 (2)
N2	0.035 (2)	0.036 (2)	0.047 (3)	−0.0018 (18)	−0.012 (2)	−0.015 (2)
N3	0.038 (3)	0.042 (3)	0.062 (3)	0.004 (2)	−0.016 (2)	−0.020 (2)
N4	0.032 (2)	0.047 (3)	0.054 (3)	0.000 (2)	−0.015 (2)	−0.021 (2)
N5	0.124 (6)	0.083 (5)	0.109 (6)	0.023 (5)	−0.051 (5)	−0.049 (5)
O1	0.038 (2)	0.043 (2)	0.059 (3)	−0.0084 (16)	−0.0179 (18)	−0.0106 (18)

O2	0.038 (2)	0.0351 (19)	0.048 (2)	−0.0036 (15)	−0.0131 (18)	−0.0108 (17)
O3	0.026 (2)	0.049 (2)	0.057 (2)	0.0024 (15)	−0.0086 (17)	−0.0282 (19)
O4	0.029 (2)	0.058 (2)	0.061 (3)	0.0034 (16)	−0.0105 (18)	−0.034 (2)
O5	0.047 (2)	0.040 (2)	0.049 (2)	0.0006 (16)	−0.0127 (18)	−0.0182 (18)
O6	0.067 (3)	0.037 (2)	0.049 (2)	−0.0036 (18)	−0.010 (2)	−0.0204 (18)
O7	0.038 (2)	0.046 (2)	0.069 (3)	−0.0053 (17)	−0.017 (2)	−0.018 (2)
O8	0.050 (2)	0.043 (2)	0.073 (3)	−0.0067 (18)	−0.022 (2)	−0.015 (2)
O9	0.032 (2)	0.052 (2)	0.059 (3)	0.0064 (16)	−0.0128 (18)	−0.0296 (19)
O10	0.035 (2)	0.085 (3)	0.069 (3)	0.015 (2)	−0.017 (2)	−0.043 (2)
O11	0.050 (2)	0.046 (2)	0.055 (3)	−0.0044 (18)	−0.007 (2)	−0.023 (2)
O12	0.064 (3)	0.049 (2)	0.057 (3)	−0.0070 (19)	−0.009 (2)	−0.021 (2)
O13	0.129 (6)	0.125 (5)	0.204 (8)	0.056 (4)	−0.078 (5)	−0.101 (5)
C1	0.033 (3)	0.038 (3)	0.048 (3)	−0.005 (2)	−0.005 (3)	−0.015 (3)
C2	0.047 (4)	0.041 (3)	0.068 (4)	−0.007 (3)	−0.020 (3)	−0.005 (3)
C3	0.037 (3)	0.029 (3)	0.075 (5)	−0.002 (2)	−0.016 (3)	−0.005 (3)
C4	0.055 (4)	0.041 (3)	0.077 (5)	−0.001 (3)	−0.011 (4)	−0.006 (3)
C5	0.054 (5)	0.044 (4)	0.109 (7)	0.002 (3)	0.013 (4)	−0.005 (4)
C6	0.054 (5)	0.044 (4)	0.121 (7)	−0.010 (3)	−0.016 (5)	−0.016 (4)
C7	0.062 (5)	0.035 (3)	0.102 (6)	−0.004 (3)	−0.034 (4)	−0.013 (4)
C8	0.053 (4)	0.029 (3)	0.079 (5)	−0.001 (3)	−0.016 (4)	−0.009 (3)
C9	0.080 (5)	0.043 (4)	0.087 (6)	−0.001 (3)	−0.020 (5)	−0.014 (4)
C10	0.120 (8)	0.060 (5)	0.091 (6)	0.006 (5)	−0.027 (6)	−0.016 (4)
C11	0.128 (9)	0.068 (5)	0.111 (8)	0.002 (5)	−0.051 (7)	−0.029 (5)
C12	0.090 (6)	0.054 (4)	0.126 (8)	−0.006 (4)	−0.042 (6)	−0.022 (5)
C13	0.030 (3)	0.038 (3)	0.042 (3)	0.000 (2)	−0.005 (2)	−0.021 (2)
C14	0.048 (4)	0.061 (4)	0.065 (4)	0.008 (3)	−0.016 (3)	−0.040 (3)
C15	0.054 (4)	0.061 (4)	0.063 (4)	0.002 (3)	−0.007 (3)	−0.042 (3)
C16	0.073 (5)	0.067 (4)	0.083 (5)	−0.002 (4)	0.012 (4)	−0.040 (4)
C17	0.077 (6)	0.097 (6)	0.104 (7)	−0.006 (5)	0.024 (5)	−0.055 (6)
C18	0.081 (6)	0.098 (6)	0.116 (8)	0.016 (5)	−0.006 (6)	−0.058 (6)
C19	0.084 (6)	0.080 (5)	0.086 (6)	0.015 (4)	−0.027 (5)	−0.048 (5)
C20	0.060 (4)	0.068 (4)	0.071 (5)	0.008 (3)	−0.020 (4)	−0.044 (4)
C21	0.095 (6)	0.078 (5)	0.074 (5)	0.006 (4)	−0.007 (5)	−0.031 (4)
C22	0.137 (9)	0.113 (7)	0.082 (7)	0.009 (7)	−0.006 (6)	−0.030 (6)
C23	0.141 (10)	0.108 (8)	0.102 (8)	0.020 (7)	−0.034 (7)	−0.027 (6)
C24	0.107 (8)	0.099 (7)	0.115 (8)	0.028 (6)	−0.039 (6)	−0.045 (6)
C25	0.036 (3)	0.043 (3)	0.052 (4)	0.006 (2)	−0.012 (3)	−0.025 (3)
C26	0.084 (5)	0.050 (3)	0.059 (4)	0.009 (3)	−0.025 (4)	−0.030 (3)
C27	0.073 (5)	0.050 (3)	0.052 (4)	0.002 (3)	−0.013 (3)	−0.029 (3)
C28	0.083 (5)	0.089 (5)	0.065 (5)	0.012 (4)	−0.010 (4)	−0.035 (4)
C29	0.099 (7)	0.121 (7)	0.067 (6)	0.006 (5)	0.001 (5)	−0.028 (5)
C30	0.108 (7)	0.108 (6)	0.056 (5)	0.010 (5)	−0.013 (5)	−0.017 (4)
C31	0.081 (5)	0.070 (4)	0.061 (5)	0.004 (4)	−0.017 (4)	−0.024 (4)
C32	0.068 (4)	0.043 (3)	0.055 (4)	0.000 (3)	−0.014 (3)	−0.026 (3)
C33	0.072 (5)	0.061 (4)	0.061 (4)	0.001 (3)	−0.014 (4)	−0.029 (3)
C34	0.079 (6)	0.077 (5)	0.087 (6)	0.004 (4)	−0.005 (5)	−0.040 (5)
C35	0.083 (6)	0.073 (5)	0.103 (7)	0.017 (4)	−0.035 (5)	−0.035 (5)
C36	0.099 (6)	0.082 (5)	0.070 (5)	0.011 (5)	−0.032 (5)	−0.020 (4)
C37	0.040 (3)	0.039 (3)	0.055 (4)	−0.006 (2)	−0.007 (3)	−0.015 (3)

C38	0.048 (4)	0.044 (3)	0.063 (4)	−0.014 (3)	−0.005 (3)	−0.016 (3)
C39	0.034 (3)	0.058 (4)	0.060 (4)	−0.016 (3)	−0.008 (3)	−0.024 (3)
C40	0.031 (3)	0.049 (3)	0.048 (3)	−0.002 (2)	−0.009 (2)	−0.024 (3)
C41	0.030 (3)	0.043 (3)	0.038 (3)	0.000 (2)	−0.008 (2)	−0.021 (2)
C42	0.030 (3)	0.040 (3)	0.043 (3)	0.005 (2)	−0.011 (2)	−0.019 (2)
C43	0.037 (3)	0.046 (3)	0.052 (4)	0.006 (2)	−0.009 (3)	−0.017 (3)
C44	0.049 (4)	0.050 (4)	0.079 (5)	0.016 (3)	−0.023 (3)	−0.011 (3)
C45	0.058 (4)	0.039 (3)	0.095 (5)	0.003 (3)	−0.021 (4)	−0.010 (3)
C46	0.045 (3)	0.038 (3)	0.077 (4)	−0.004 (3)	−0.019 (3)	−0.012 (3)
C47	0.028 (3)	0.067 (4)	0.064 (4)	0.002 (3)	−0.016 (3)	−0.029 (3)
C48	0.032 (3)	0.062 (4)	0.065 (4)	0.014 (3)	−0.018 (3)	−0.020 (3)
C49	0.047 (4)	0.041 (3)	0.081 (5)	−0.006 (3)	−0.011 (3)	−0.019 (3)
C50	0.054 (8)	0.044 (8)	0.078 (11)	−0.001 (6)	−0.014 (9)	−0.031 (9)
C51	0.063 (10)	0.049 (7)	0.091 (14)	0.004 (6)	−0.014 (8)	−0.032 (8)
C52	0.064 (17)	0.058 (9)	0.092 (19)	0.001 (12)	−0.004 (13)	−0.026 (11)
C53	0.09 (2)	0.07 (2)	0.10 (3)	0.008 (16)	−0.020 (16)	−0.026 (17)
C54	0.074 (13)	0.061 (10)	0.104 (18)	0.007 (9)	−0.011 (14)	−0.027 (11)
C55	0.06 (9)	0.05 (3)	0.10 (4)	0.00 (7)	−0.02 (9)	−0.03 (3)
C56	0.062 (19)	0.051 (12)	0.10 (3)	0.009 (11)	−0.012 (17)	−0.029 (16)
C57	0.07 (2)	0.06 (3)	0.09 (4)	0.011 (18)	−0.03 (3)	−0.03 (3)
C58	0.08 (3)	0.06 (2)	0.10 (3)	0.011 (17)	−0.016 (19)	−0.030 (15)
C59	0.067 (14)	0.057 (9)	0.098 (16)	0.014 (8)	−0.020 (12)	−0.025 (11)
C60	0.07 (3)	0.055 (13)	0.11 (4)	0.009 (18)	−0.01 (2)	−0.022 (19)
C50'	0.064 (13)	0.056 (11)	0.101 (19)	0.002 (9)	−0.023 (15)	−0.021 (15)
C51'	0.058 (16)	0.047 (13)	0.09 (3)	0.007 (10)	−0.020 (16)	−0.026 (14)
C52'	0.07 (4)	0.05 (2)	0.09 (5)	0.01 (2)	−0.02 (3)	−0.02 (3)
C53'	0.08 (4)	0.06 (3)	0.10 (4)	0.01 (3)	−0.01 (3)	−0.024 (19)
C54'	0.07 (5)	0.06 (2)	0.10 (5)	0.01 (3)	−0.01 (4)	−0.02 (3)
C55'	0.06 (11)	0.05 (3)	0.09 (5)	0.00 (8)	−0.02 (12)	−0.03 (3)
C56'	0.06 (2)	0.048 (14)	0.09 (3)	0.001 (13)	−0.016 (19)	−0.031 (18)
C57'	0.07 (2)	0.055 (13)	0.09 (3)	0.009 (18)	−0.01 (2)	−0.033 (17)
C58'	0.08 (2)	0.06 (3)	0.10 (3)	0.016 (18)	−0.02 (2)	−0.03 (2)
C59'	0.083 (15)	0.068 (12)	0.104 (19)	0.010 (11)	−0.028 (15)	−0.030 (12)
C60'	0.075 (16)	0.062 (12)	0.11 (2)	0.006 (11)	−0.015 (15)	−0.024 (13)
C61	0.034 (3)	0.053 (3)	0.060 (4)	0.009 (3)	−0.015 (3)	−0.028 (3)
C62	0.060 (4)	0.082 (5)	0.068 (4)	0.023 (3)	−0.021 (3)	−0.044 (4)
C63	0.071 (5)	0.076 (5)	0.069 (5)	0.019 (4)	−0.015 (4)	−0.045 (4)
C64	0.076 (6)	0.102 (6)	0.090 (6)	0.017 (5)	−0.017 (5)	−0.047 (5)
C65	0.089 (7)	0.128 (8)	0.101 (7)	0.033 (6)	−0.020 (5)	−0.043 (7)
C66	0.115 (8)	0.104 (7)	0.086 (6)	0.050 (6)	−0.015 (6)	−0.037 (6)
C67	0.114 (7)	0.084 (6)	0.072 (5)	0.028 (5)	−0.024 (5)	−0.044 (4)
C68	0.091 (6)	0.084 (5)	0.067 (5)	0.020 (4)	−0.018 (4)	−0.044 (4)
C69	0.108 (8)	0.105 (7)	0.098 (7)	−0.001 (6)	−0.022 (6)	−0.038 (6)
C70	0.126 (9)	0.119 (8)	0.125 (9)	−0.016 (7)	−0.022 (7)	−0.043 (7)
C71	0.161 (12)	0.108 (8)	0.123 (9)	−0.007 (9)	−0.028 (9)	−0.041 (7)
C72	0.149 (10)	0.098 (7)	0.095 (7)	0.024 (7)	−0.023 (7)	−0.039 (6)
C73	0.035 (3)	0.050 (3)	0.055 (4)	−0.002 (2)	−0.011 (3)	−0.029 (3)
C74	0.053 (4)	0.072 (4)	0.059 (4)	−0.004 (3)	−0.004 (3)	−0.035 (3)
C75	0.065 (4)	0.061 (4)	0.062 (4)	−0.004 (3)	−0.010 (3)	−0.038 (3)

C76	0.089 (6)	0.075 (5)	0.092 (6)	0.005 (4)	−0.013 (4)	−0.053 (4)
C77	0.116 (8)	0.073 (5)	0.126 (8)	−0.001 (5)	−0.025 (6)	−0.064 (5)
C78	0.100 (7)	0.088 (6)	0.114 (7)	−0.018 (5)	−0.021 (5)	−0.058 (5)
C79	0.080 (5)	0.074 (5)	0.081 (5)	−0.009 (4)	−0.019 (4)	−0.042 (4)
C80	0.064 (4)	0.058 (4)	0.058 (4)	−0.015 (3)	−0.015 (3)	−0.030 (3)
C81	0.060 (4)	0.058 (4)	0.063 (4)	−0.003 (3)	−0.014 (3)	−0.026 (3)
C82	0.074 (5)	0.076 (5)	0.071 (5)	0.004 (4)	−0.020 (4)	−0.023 (4)
C83	0.076 (6)	0.098 (6)	0.093 (6)	0.004 (5)	−0.024 (5)	−0.031 (5)
C84	0.067 (5)	0.103 (6)	0.099 (6)	−0.021 (5)	−0.025 (4)	−0.043 (5)
C85	0.051 (4)	0.049 (4)	0.085 (5)	0.000 (3)	−0.024 (3)	−0.020 (3)
C86	0.072 (5)	0.044 (4)	0.096 (6)	0.010 (3)	−0.021 (4)	−0.017 (4)
C87	0.066 (5)	0.058 (4)	0.077 (5)	0.024 (3)	−0.026 (4)	−0.017 (4)
C88	0.044 (4)	0.061 (4)	0.060 (4)	0.017 (3)	−0.019 (3)	−0.020 (3)
C89	0.038 (3)	0.053 (3)	0.052 (4)	0.006 (3)	−0.015 (3)	−0.025 (3)
C90	0.034 (3)	0.057 (3)	0.051 (4)	0.006 (3)	−0.013 (3)	−0.025 (3)
C91	0.037 (3)	0.064 (4)	0.053 (4)	0.005 (3)	−0.016 (3)	−0.026 (3)
C92	0.039 (4)	0.080 (5)	0.069 (4)	−0.009 (3)	−0.013 (3)	−0.036 (4)
C93	0.048 (4)	0.061 (4)	0.072 (4)	−0.014 (3)	−0.009 (3)	−0.028 (3)
C94	0.040 (3)	0.052 (3)	0.073 (4)	−0.005 (3)	−0.012 (3)	−0.026 (3)
C95	0.049 (4)	0.077 (5)	0.066 (4)	0.022 (3)	−0.028 (3)	−0.022 (4)
C96	0.037 (3)	0.084 (5)	0.064 (4)	0.011 (3)	−0.022 (3)	−0.028 (4)
C97	0.112 (8)	0.087 (6)	0.138 (8)	0.032 (5)	−0.067 (7)	−0.069 (6)
C98	0.169 (11)	0.124 (9)	0.143 (10)	0.008 (8)	−0.041 (9)	−0.043 (8)
C99	0.169 (11)	0.116 (8)	0.147 (10)	0.062 (7)	−0.057 (8)	−0.068 (7)

Geometric parameters (Å, °)

Pr1—O3^{i}	2.431 (3)	C43—C48	1.429 (7)
Pr1—O1	2.434 (3)	C44—C45	1.339 (8)
Pr1—O5	2.448 (3)	C44—H44	0.9300
Pr1—O2^{i}	2.474 (3)	C45—C46	1.395 (8)
Pr1—O6	2.548 (4)	C45—H45	0.9300
Pr1—O4	2.574 (4)	C46—H46	0.9300
Pr1—O3	2.619 (4)	C47—C48	1.324 (7)
Pr1—N1	2.667 (4)	C47—H47	0.9300
Pr1—N2	2.670 (4)	C48—H48	0.9300
Pr1—Pr1^{i}	4.0072 (6)	C49—C50'	1.52 (2)
Pr2—O8^{ii}	2.423 (4)	C49—C50	1.529 (16)
Pr2—O7	2.443 (4)	C50—C51	1.52 (2)
Pr2—O9^{ii}	2.447 (3)	C50—H50A	0.9700
Pr2—O12	2.500 (4)	C50—H50B	0.9700
Pr2—O11	2.552 (4)	C51—C56	1.39 (4)
Pr2—O10	2.561 (4)	C51—C52	1.39 (5)
Pr2—N4	2.635 (4)	C52—C53	1.39 (7)
Pr2—O9	2.644 (4)	C52—H52	0.9300
Pr2—N3	2.691 (4)	C53—C54	1.39 (6)
Pr2—Pr2^{ii}	4.0433 (6)	C53—H53	0.9300
N1—C37	1.319 (6)	C54—C55	1.4 (6)

N1—C41	1.352 (6)	C54—H54	0.9300
N2—C46	1.315 (6)	C55—C56	1.4 (4)
N2—C42	1.367 (6)	C55—C60	1.4 (6)
N3—C85	1.311 (7)	C56—C57	1.39 (10)
N3—C89	1.348 (6)	C57—C58	1.39 (14)
N4—C94	1.322 (6)	C57—H57	0.9300
N4—C90	1.369 (6)	C58—C59	1.39 (7)
N5—C97	1.323 (9)	C58—H58	0.9300
N5—C99	1.427 (10)	C59—C60	1.39 (10)
N5—C98	1.454 (11)	C59—H59	0.9300
O1—C1	1.269 (6)	C60—H60	0.9300
O2—C1	1.244 (6)	C50'—C51'	1.51 (4)
O2—Pr1^{i}	2.474 (3)	C50'—H50C	0.9700
O3—C13	1.272 (5)	C50'—H50D	0.9700
O3—Pr1^{i}	2.431 (3)	C51'—C52'	1.39 (13)
O4—C13	1.246 (6)	C51'—C56'	1.39 (5)
O5—C25	1.256 (6)	C52'—C53'	1.39 (18)
O6—C25	1.252 (6)	C52'—H52'	0.9300
O7—C49	1.252 (7)	C53'—C54'	1.39 (8)
O8—C49	1.256 (7)	C53'—H53'	0.9300
O8—Pr2^{ii}	2.423 (4)	C54'—C55'	1.4 (9)
O9—C61	1.261 (6)	C54'—H54'	0.9300
O9—Pr2^{ii}	2.447 (3)	C55'—C60'	1.4 (7)
O10—C61	1.241 (6)	C55'—C56'	1.4 (5)
O11—C73	1.245 (6)	C56'—C57'	1.39 (6)
O12—C73	1.258 (6)	C57'—C58'	1.39 (9)
O13—C97	1.209 (10)	C57'—H57'	0.9300
C1—C2	1.521 (7)	C58'—C59'	1.39 (8)
C2—C3	1.509 (7)	C58'—H58'	0.9300
C2—H2A	0.9700	C59'—C60'	1.39 (4)
C2—H2B	0.9700	C59'—H59'	0.9300
C3—C4	1.363 (8)	C60'—H60'	0.9300
C3—C8	1.421 (9)	C61—C62	1.519 (8)
C4—C5	1.419 (9)	C62—C63	1.504 (8)
C4—H4	0.9300	C62—H62A	0.9700
C5—C6	1.346 (10)	C62—H62B	0.9700
C5—H5	0.9300	C63—C64	1.351 (9)
C6—C7	1.382 (10)	C63—C68	1.436 (10)
C6—H6	0.9300	C64—C65	1.411 (11)
C7—C8	1.418 (8)	C64—H64	0.9300
C7—C12	1.422 (11)	C65—C66	1.335 (12)
C8—C9	1.405 (9)	C65—H65	0.9300
C9—C10	1.388 (10)	C66—C67	1.395 (12)
C9—H9	0.9300	C66—H66	0.9300
C10—C11	1.377 (11)	C67—C68	1.416 (10)
C10—H10	0.9300	C67—C72	1.447 (12)
C11—C12	1.346 (11)	C68—C69	1.398 (11)
C11—H11	0.9300	C69—C70	1.393 (12)

C12—H12	0.9300	C69—H69	0.9300
C13—C14	1.504 (7)	C70—C71	1.369 (13)
C14—C15	1.494 (7)	C70—H70	0.9300
C14—H14A	0.9700	C71—C72	1.330 (13)
C14—H14B	0.9700	C71—H71	0.9300
C15—C16	1.356 (8)	C72—H72	0.9300
C15—C20	1.418 (8)	C73—C74	1.519 (8)
C16—C17	1.425 (9)	C74—C75	1.505 (8)
C16—H16	0.9300	C74—H74A	0.9700
C17—C18	1.323 (10)	C74—H74B	0.9700
C17—H17	0.9300	C75—C76	1.354 (8)
C18—C19	1.378 (10)	C75—C80	1.428 (8)
C18—H18	0.9300	C76—C77	1.415 (10)
C19—C20	1.423 (9)	C76—H76	0.9300
C19—C24	1.424 (10)	C77—C78	1.341 (10)
C20—C21	1.416 (9)	C77—H77	0.9300
C21—C22	1.361 (10)	C78—C79	1.401 (10)
C21—H21	0.9300	C78—H78	0.9300
C22—C23	1.405 (12)	C79—C84	1.422 (10)
C22—H22	0.9300	C79—C80	1.427 (8)
C23—C24	1.330 (12)	C80—C81	1.404 (8)
C23—H23	0.9300	C81—C82	1.360 (8)
C24—H24	0.9300	C81—H81	0.9300
C25—C26	1.500 (7)	C82—C83	1.380 (10)
C26—C27	1.493 (8)	C82—H82	0.9300
C26—H26A	0.9700	C83—C84	1.333 (10)
C26—H26B	0.9700	C83—H83	0.9300
C27—C28	1.348 (8)	C84—H84	0.9300
C27—C32	1.420 (8)	C85—C86	1.399 (8)
C28—C29	1.389 (10)	C85—H85	0.9300
C28—H28	0.9300	C86—C87	1.348 (9)
C29—C30	1.357 (10)	C86—H86	0.9300
C29—H29	0.9300	C87—C88	1.389 (8)
C30—C31	1.419 (10)	C87—H87	0.9300
C30—H30	0.9300	C88—C89	1.420 (7)
C31—C36	1.403 (10)	C88—C95	1.435 (8)
C31—C32	1.417 (8)	C89—C90	1.432 (7)
C32—C33	1.408 (8)	C90—C91	1.411 (7)
C33—C34	1.364 (9)	C91—C92	1.398 (8)
C33—H33	0.9300	C91—C96	1.432 (8)
C34—C35	1.384 (10)	C92—C93	1.359 (8)
C34—H34	0.9300	C92—H92	0.9300
C35—C36	1.344 (10)	C93—C94	1.399 (7)
C35—H35	0.9300	C93—H93	0.9300
C36—H36	0.9300	C94—H94	0.9300
C37—C38	1.395 (7)	C95—C96	1.323 (8)
C37—H37	0.9300	C95—H95	0.9300
C38—C39	1.362 (7)	C96—H96	0.9300
C38—H38	0.9300	C97—H97	0.9300

C39—C40	1.396 (7)	C98—H98A	0.9600
C39—H39	0.9300	C98—H98B	0.9600
C40—C41	1.417 (6)	C98—H98C	0.9600
C40—C47	1.431 (7)	C99—H99A	0.9600
C41—C42	1.431 (6)	C99—H99B	0.9600
C42—C43	1.404 (7)	C99—H99C	0.9600
C43—C44	1.401 (7)		
$O3^{i}$—Pr1—O1	73.37 (11)	C38—C37—H37	118.3
$O3^{i}$—Pr1—O5	75.11 (11)	C39—C38—C37	119.0 (5)
O1—Pr1—O5	127.67 (12)	C39—C38—H38	120.5
$O3^{i}$—Pr1—$O2^{i}$	78.62 (11)	C37—C38—H38	120.5
O1—Pr1—$O2^{i}$	136.26 (12)	C38—C39—C40	119.5 (5)
O5—Pr1—$O2^{i}$	74.03 (12)	C38—C39—H39	120.2
$O3^{i}$—Pr1—O6	88.75 (12)	C40—C39—H39	120.2
O1—Pr1—O6	86.78 (12)	C39—C40—C41	117.9 (5)
O5—Pr1—O6	51.83 (11)	C39—C40—C47	122.7 (5)
$O2^{i}$—Pr1—O6	125.81 (11)	C41—C40—C47	119.4 (5)
$O3^{i}$—Pr1—O4	124.74 (11)	N1—C41—C40	121.8 (4)
O1—Pr1—O4	87.98 (12)	N1—C41—C42	119.1 (4)
O5—Pr1—O4	144.27 (11)	C40—C41—C42	119.1 (4)
$O2^{i}$—Pr1—O4	81.08 (11)	N2—C42—C43	122.4 (4)
O6—Pr1—O4	142.71 (12)	N2—C42—C41	118.0 (4)
$O3^{i}$—Pr1—O3	75.04 (13)	C43—C42—C41	119.5 (4)
O1—Pr1—O3	69.56 (12)	C44—C43—C42	117.1 (5)
O5—Pr1—O3	137.66 (11)	C44—C43—C48	123.6 (5)
$O2^{i}$—Pr1—O3	71.17 (11)	C42—C43—C48	119.3 (5)
O6—Pr1—O3	154.20 (11)	C45—C44—C43	120.3 (5)
O4—Pr1—O3	49.77 (10)	C45—C44—H44	119.9
$O3^{i}$—Pr1—N1	144.07 (12)	C43—C44—H44	119.9
O1—Pr1—N1	138.19 (12)	C44—C45—C46	119.2 (5)
O5—Pr1—N1	70.72 (12)	C44—C45—H45	120.4
$O2^{i}$—Pr1—N1	81.65 (11)	C46—C45—H45	120.4
O6—Pr1—N1	78.89 (12)	N2—C46—C45	123.6 (5)
O4—Pr1—N1	80.75 (12)	N2—C46—H46	118.2
O3—Pr1—N1	125.68 (12)	C45—C46—H46	118.2
$O3^{i}$—Pr1—N2	146.30 (12)	C48—C47—C40	120.9 (5)
O1—Pr1—N2	76.77 (12)	C48—C47—H47	119.5
O5—Pr1—N2	112.92 (12)	C40—C47—H47	119.5
$O2^{i}$—Pr1—N2	134.88 (12)	C47—C48—C43	121.8 (5)
O6—Pr1—N2	74.21 (13)	C47—C48—H48	119.1
O4—Pr1—N2	68.65 (12)	C43—C48—H48	119.1
O3—Pr1—N2	108.63 (12)	O7—C49—O8	125.7 (5)
N1—Pr1—N2	61.59 (12)	O7—C49—C50'	124.1 (10)
$O3^{i}$—Pr1—$Pr1^{i}$	39.15 (8)	O8—C49—C50'	108.6 (11)
O1—Pr1—$Pr1^{i}$	66.31 (8)	O7—C49—C50	112.4 (8)

O5—Pr1—Pr1^{i}	109.10 (8)	O8—C49—C50	119.4 (8)
O2^{i}—Pr1—Pr1^{i}	70.70 (8)	C51—C50—C49	117.8 (12)
O6—Pr1—Pr1^{i}	125.11 (9)	C51—C50—H50A	107.8
O4—Pr1—Pr1^{i}	85.62 (8)	C49—C50—H50A	107.8
O3—Pr1—Pr1^{i}	35.88 (7)	C51—C50—H50B	107.8
N1—Pr1—Pr1^{i}	150.75 (9)	C49—C50—H50B	107.8
N2—Pr1—Pr1^{i}	135.52 (9)	H50A—C50—H50B	107.2
O8^{ii}—Pr2—O7	135.71 (12)	C56—C51—C52	120 (2)
O8^{ii}—Pr2—O9^{ii}	74.77 (12)	C56—C51—C50	120 (2)
O7—Pr2—O9^{ii}	74.62 (12)	C52—C51—C50	120.2 (17)
O8^{ii}—Pr2—O12	80.13 (13)	C51—C52—C53	120 (3)
O7—Pr2—O12	128.97 (13)	C51—C52—H52	120.0
O9^{ii}—Pr2—O12	87.09 (12)	C53—C52—H52	120.0
O8^{ii}—Pr2—O11	123.85 (13)	C54—C53—C52	120 (4)
O7—Pr2—O11	77.91 (13)	C54—C53—H53	120.0
O9^{ii}—Pr2—O11	76.21 (12)	C52—C53—H53	120.0
O12—Pr2—O11	51.34 (12)	C53—C54—C55	118 (2)
O8^{ii}—Pr2—O10	90.62 (14)	C53—C54—H54	120.0
O7—Pr2—O10	80.59 (13)	C55—C54—H54	120.0
O9^{ii}—Pr2—O10	123.64 (12)	C56—C55—C60	114 (10)
O12—Pr2—O10	144.47 (13)	C56—C55—C54	124 (10)
O11—Pr2—O10	145.05 (13)	C60—C55—C54	120 (10)
O8^{ii}—Pr2—N4	139.13 (13)	C55—C56—C51	117 (10)
O7—Pr2—N4	81.71 (12)	C55—C56—C57	124 (10)
O9^{ii}—Pr2—N4	143.02 (13)	C51—C56—C57	120 (6)
O12—Pr2—N4	86.18 (13)	C58—C57—C56	120 (9)
O11—Pr2—N4	71.27 (13)	C58—C57—H57	120.0
O10—Pr2—N4	78.64 (13)	C56—C57—H57	120.0
O8^{ii}—Pr2—O9	68.76 (12)	C59—C58—C57	120 (7)
O7—Pr2—O9	72.88 (12)	C59—C58—H58	120.0
O9^{ii}—Pr2—O9	74.90 (13)	C57—C58—H58	120.0
O12—Pr2—O9	147.08 (12)	C60—C59—C58	120 (4)
O11—Pr2—O9	143.23 (11)	C60—C59—H59	120.0
O10—Pr2—O9	49.45 (11)	C58—C59—H59	120.0
N4—Pr2—O9	124.51 (12)	C59—C60—C55	120 (10)
O8^{ii}—Pr2—N3	77.85 (13)	C59—C60—H60	120.0
O7—Pr2—N3	135.74 (13)	C55—C60—H60	118.0 (2)
O9^{ii}—Pr2—N3	149.46 (12)	C51'—C50'—C49	122.3 (18)
O12—Pr2—N3	75.05 (14)	C51'—C50'—H50C	106.8
O11—Pr2—N3	109.13 (13)	C49—C50'—H50C	106.8
O10—Pr2—N3	69.46 (13)	C51'—C50'—H50D	106.8
N4—Pr2—N3	61.41 (13)	C49—C50'—H50D	106.8
O9—Pr2—N3	107.33 (12)	H50C—C50'—H50D	106.6
O8^{ii}—Pr2—Pr2^{ii}	66.68 (9)	C52'—C51'—C56'	120 (7)

O7—Pr2—Pr2^{ii}	69.33 (8)	C52'—C51'—C50'	109 (8)
O9^{ii}—Pr2—Pr2^{ii}	39.15 (9)	C56'—C51'—C50'	131 (3)
O12—Pr2—Pr2^{ii}	121.21 (9)	C51'—C52'—C53'	120 (10)
O11—Pr2—Pr2^{ii}	112.31 (8)	C51'—C52'—H52'	120.0
O10—Pr2—Pr2^{ii}	84.84 (9)	C53'—C52'—H52'	120.0
N4—Pr2—Pr2^{ii}	148.64 (9)	C52'—C53'—C54'	120 (10)
O9—Pr2—Pr2^{ii}	35.75 (7)	C52'—C53'—H53'	120.0
N3—Pr2—Pr2^{ii}	135.73 (10)	C54'—C53'—H53'	120.0
C37—N1—C41	118.4 (4)	C53'—C54'—C55'	118 (2)
C37—N1—Pr1	120.9 (3)	C53'—C54'—H54'	120.0
C41—N1—Pr1	120.7 (3)	C55'—C54'—H54'	123.0
C46—N2—C42	117.4 (4)	C60'—C55'—C54'	120 (10)
C46—N2—Pr1	122.0 (3)	C60'—C55'—C56'	114 (10)
C42—N2—Pr1	120.6 (3)	C54'—C55'—C56'	127 (10)
C85—N3—C89	117.6 (5)	C57'—C56'—C51'	120 (4)
C85—N3—Pr2	122.4 (4)	C57'—C56'—C55'	124 (10)
C89—N3—Pr2	120.0 (3)	C51'—C56'—C55'	116 (10)
C94—N4—C90	117.6 (5)	C56'—C57'—C58'	120 (5)
C94—N4—Pr2	120.4 (3)	C56'—C57'—H57'	120.0
C90—N4—Pr2	122.0 (3)	C58'—C57'—H57'	120.0
C97—N5—C99	121.7 (9)	C57'—C58'—C59'	120 (5)
C97—N5—C98	120.9 (9)	C57'—C58'—H58'	120.0
C99—N5—C98	117.5 (8)	C59'—C58'—H58'	120.0
C1—O1—Pr1	142.0 (3)	C60'—C59'—C58'	120 (4)
C1—O2—Pr1^{i}	130.8 (3)	C60'—C59'—H59'	120.0
C13—O3—Pr1^{i}	161.8 (3)	C58'—C59'—H59'	120.0
C13—O3—Pr1	93.1 (3)	C55'—C60'—C59'	122 (2)
Pr1^{i}—O3—Pr1	104.96 (13)	C55'—C60'—H60'	118.0 (2)
C13—O4—Pr1	95.9 (3)	C59'—C60'—H60'	120.0
C25—O5—Pr1	95.4 (3)	O10—C61—O9	121.1 (6)
C25—O6—Pr1	90.8 (3)	O10—C61—C62	120.7 (5)
C49—O7—Pr2	129.0 (3)	O9—C61—C62	118.2 (5)
C49—O8—Pr2^{ii}	137.3 (4)	C63—C62—C61	115.9 (5)
C61—O9—Pr2^{ii}	160.7 (4)	C63—C62—H62A	108.3
C61—O9—Pr2	92.5 (3)	C61—C62—H62A	108.3
Pr2^{ii}—O9—Pr2	105.10 (13)	C63—C62—H62B	108.3
C61—O10—Pr2	97.0 (3)	C61—C62—H62B	108.3
C73—O11—Pr2	92.2 (3)	H62A—C62—H62B	107.4
C73—O12—Pr2	94.3 (3)	C64—C63—C68	118.1 (7)
O2—C1—O1	125.9 (4)	C64—C63—C62	118.5 (7)
O2—C1—C2	120.5 (4)	C68—C63—C62	123.3 (7)
O1—C1—C2	113.6 (5)	C63—C64—C65	122.4 (8)
C3—C2—C1	117.9 (4)	C63—C64—H64	118.8
C3—C2—H2A	107.8	C65—C64—H64	118.8
C1—C2—H2A	107.8	C66—C65—C64	119.3 (9)
C3—C2—H2B	107.8	C66—C65—H65	120.3

C1—C2—H2B	107.8	C64—C65—H65	120.3
H2A—C2—H2B	107.2	C65—C66—C67	122.0 (9)
C4—C3—C8	119.7 (6)	C65—C66—H66	119.0
C4—C3—C2	119.0 (6)	C67—C66—H66	119.0
C8—C3—C2	121.3 (6)	C66—C67—C68	118.7 (9)
C3—C4—C5	121.1 (7)	C66—C67—C72	120.9 (9)
C3—C4—H4	119.5	C68—C67—C72	120.4 (9)
C5—C4—H4	119.5	C69—C68—C67	117.5 (8)
C6—C5—C4	119.1 (7)	C69—C68—C63	123.2 (7)
C6—C5—H5	120.4	C67—C68—C63	119.3 (8)
C4—C5—H5	120.4	C70—C69—C68	120.1 (9)
C5—C6—C7	122.0 (7)	C70—C69—H69	119.9
C5—C6—H6	119.0	C68—C69—H69	119.9
C7—C6—H6	119.0	C71—C70—C69	121.3 (11)
C6—C7—C8	119.7 (8)	C71—C70—H70	119.3
C6—C7—C12	121.8 (7)	C69—C70—H70	119.3
C8—C7—C12	118.5 (8)	C72—C71—C70	121.7 (12)
C9—C8—C7	118.6 (7)	C72—C71—H71	119.1
C9—C8—C3	123.0 (6)	C70—C71—H71	119.1
C7—C8—C3	118.4 (7)	C71—C72—C67	118.9 (10)
C10—C9—C8	120.9 (7)	C71—C72—H72	120.6
C10—C9—H9	119.5	C67—C72—H72	120.6
C8—C9—H9	119.5	O11—C73—O12	122.1 (5)
C11—C10—C9	119.5 (9)	O11—C73—C74	119.3 (5)
C11—C10—H10	120.2	O12—C73—C74	118.6 (5)
C9—C10—H10	120.2	C75—C74—C73	114.9 (5)
C12—C11—C10	121.7 (9)	C75—C74—H74A	108.5
C12—C11—H11	119.1	C73—C74—H74A	108.5
C10—C11—H11	119.1	C75—C74—H74B	108.5
C11—C12—C7	120.7 (8)	C73—C74—H74B	108.5
C11—C12—H12	119.7	H74A—C74—H74B	107.5
C7—C12—H12	119.7	C76—C75—C80	118.4 (6)
O4—C13—O3	120.5 (5)	C76—C75—C74	121.9 (6)
O4—C13—C14	121.4 (5)	C80—C75—C74	119.6 (5)
O3—C13—C14	118.1 (5)	C75—C76—C77	122.1 (7)
C15—C14—C13	116.5 (5)	C75—C76—H76	119.0
C15—C14—H14A	108.2	C77—C76—H76	119.0
C13—C14—H14A	108.2	C78—C77—C76	118.9 (7)
C15—C14—H14B	108.2	C78—C77—H77	120.5
C13—C14—H14B	108.2	C76—C77—H77	120.5
H14A—C14—H14B	107.3	C77—C78—C79	123.2 (8)
C16—C15—C20	117.8 (6)	C77—C78—H78	118.4
C16—C15—C14	120.7 (6)	C79—C78—H78	118.4
C20—C15—C14	121.5 (6)	C78—C79—C84	124.8 (7)
C15—C16—C17	121.3 (7)	C78—C79—C80	116.9 (7)
C15—C16—H16	119.3	C84—C79—C80	118.3 (7)
C17—C16—H16	119.3	C81—C80—C79	116.3 (6)
C18—C17—C16	119.6 (7)	C81—C80—C75	123.3 (6)
C18—C17—H17	120.2	C79—C80—C75	120.4 (6)

C16—C17—H17	120.2	C82—C81—C80	123.1 (6)
C17—C18—C19	123.1 (8)	C82—C81—H81	118.4
C17—C18—H18	118.4	C80—C81—H81	118.4
C19—C18—H18	118.4	C81—C82—C83	119.8 (7)
C18—C19—C20	117.3 (7)	C81—C82—H82	120.1
C18—C19—C24	123.2 (8)	C83—C82—H82	120.1
C20—C19—C24	119.5 (8)	C84—C83—C82	120.1 (8)
C21—C20—C15	121.2 (6)	C84—C83—H83	119.9
C21—C20—C19	117.9 (7)	C82—C83—H83	119.9
C15—C20—C19	120.9 (6)	C83—C84—C79	122.2 (7)
C22—C21—C20	121.3 (8)	C83—C84—H84	118.9
C22—C21—H21	119.4	C79—C84—H84	118.9
C20—C21—H21	119.4	N3—C85—C86	123.9 (6)
C21—C22—C23	119.0 (9)	N3—C85—H85	118.1
C21—C22—H22	120.5	C86—C85—H85	118.1
C23—C22—H22	120.5	C87—C86—C85	118.7 (6)
C24—C23—C22	122.8 (9)	C87—C86—H86	120.7
C24—C23—H23	118.6	C85—C86—H86	120.7
C22—C23—H23	118.6	C86—C87—C88	120.2 (6)
C23—C24—C19	119.4 (9)	C86—C87—H87	119.9
C23—C24—H24	120.3	C88—C87—H87	119.9
C19—C24—H24	120.3	C87—C88—C89	117.1 (6)
O6—C25—O5	121.2 (5)	C87—C88—C95	124.0 (5)
O6—C25—C26	123.4 (5)	C89—C88—C95	119.0 (6)
O5—C25—C26	115.3 (5)	N3—C89—C88	122.5 (5)
C27—C26—C25	118.1 (5)	N3—C89—C90	119.0 (5)
C27—C26—H26A	107.8	C88—C89—C90	118.5 (5)
C25—C26—H26A	107.8	N4—C90—C91	121.9 (5)
C27—C26—H26B	107.8	N4—C90—C89	117.6 (5)
C25—C26—H26B	107.8	C91—C90—C89	120.5 (5)
H26A—C26—H26B	107.1	C92—C91—C90	117.9 (5)
C28—C27—C32	119.7 (6)	C92—C91—C96	123.4 (5)
C28—C27—C26	118.0 (6)	C90—C91—C96	118.8 (5)
C32—C27—C26	122.2 (6)	C93—C92—C91	120.2 (5)
C27—C28—C29	121.4 (7)	C93—C92—H92	119.9
C27—C28—H28	119.3	C91—C92—H92	119.9
C29—C28—H28	119.3	C92—C93—C94	118.4 (6)
C30—C29—C28	120.6 (8)	C92—C93—H93	120.8
C30—C29—H29	119.7	C94—C93—H93	120.8
C28—C29—H29	119.7	N4—C94—C93	124.1 (5)
C29—C30—C31	120.7 (7)	N4—C94—H94	118.0
C29—C30—H30	119.7	C93—C94—H94	118.0
C31—C30—H30	119.7	C96—C95—C88	122.0 (6)
C36—C31—C32	119.4 (7)	C96—C95—H95	119.0
C36—C31—C30	122.7 (7)	C88—C95—H95	119.0
C32—C31—C30	117.9 (7)	C95—C96—C91	121.2 (6)
C33—C32—C31	117.7 (6)	C95—C96—H96	119.4
C33—C32—C27	122.6 (6)	C91—C96—H96	119.4
C31—C32—C27	119.7 (6)	O13—C97—N5	124.9 (11)

C34—C33—C32	120.8 (7)	O13—C97—H97	117.5
C34—C33—H33	119.6	N5—C97—H97	117.5
C32—C33—H33	119.6	N5—C98—H98A	109.5
C33—C34—C35	120.8 (7)	N5—C98—H98B	109.5
C33—C34—H34	119.6	H98A—C98—H98B	109.5
C35—C34—H34	119.6	N5—C98—H98C	109.5
C36—C35—C34	120.3 (8)	H98A—C98—H98C	109.5
C36—C35—H35	119.8	H98B—C98—H98C	109.5
C34—C35—H35	119.8	N5—C99—H99A	109.5
C35—C36—C31	121.0 (7)	N5—C99—H99B	109.5
C35—C36—H36	119.5	H99A—C99—H99B	109.5
C31—C36—H36	119.5	N5—C99—H99C	109.5
N1—C37—C38	123.4 (5)	H99A—C99—H99C	109.5
N1—C37—H37	118.3	H99B—C99—H99C	109.5
$O3^{i}$—Pr1—N1—C37	−28.8 (5)	C15—C20—C21—C22	176.0 (8)
O1—Pr1—N1—C37	−173.0 (4)	C19—C20—C21—C22	−2.4 (11)
O5—Pr1—N1—C37	−47.6 (4)	C20—C21—C22—C23	3.4 (14)
$O2^{i}$—Pr1—N1—C37	28.4 (4)	C21—C22—C23—C24	−1.0 (17)
O6—Pr1—N1—C37	−100.8 (4)	C22—C23—C24—C19	−2.4 (16)
O4—Pr1—N1—C37	110.6 (4)	C18—C19—C24—C23	−177.2 (9)
O3—Pr1—N1—C37	87.9 (4)	C20—C19—C24—C23	3.3 (13)
N2—Pr1—N1—C37	−178.7 (4)	Pr1—O6—C25—O5	8.0 (5)
$Pr1^{i}$—Pr1—N1—C37	47.3 (5)	Pr1—O6—C25—C26	−170.1 (5)
$O3^{i}$—Pr1—N1—C41	150.1 (3)	Pr1—O5—C25—O6	−8.4 (5)
O1—Pr1—N1—C41	5.9 (5)	Pr1—O5—C25—C26	169.9 (4)
O5—Pr1—N1—C41	131.3 (4)	O6—C25—C26—C27	4.2 (9)
$O2^{i}$—Pr1—N1—C41	−152.8 (4)	O5—C25—C26—C27	−174.0 (5)
O6—Pr1—N1—C41	78.1 (4)	C25—C26—C27—C28	−106.8 (7)
O4—Pr1—N1—C41	−70.5 (4)	C25—C26—C27—C32	77.2 (8)
O3—Pr1—N1—C41	−93.2 (4)	C32—C27—C28—C29	−1.4 (11)
N2—Pr1—N1—C41	0.1 (3)	C26—C27—C28—C29	−177.6 (7)
$Pr1^{i}$—Pr1—N1—C41	−133.8 (3)	C27—C28—C29—C30	1.9 (13)
$O3^{i}$—Pr1—N2—C46	33.8 (6)	C28—C29—C30—C31	−0.4 (14)
O1—Pr1—N2—C46	5.7 (4)	C29—C30—C31—C36	178.2 (8)
O5—Pr1—N2—C46	131.3 (4)	C29—C30—C31—C32	−1.5 (12)
$O2^{i}$—Pr1—N2—C46	−138.7 (4)	C36—C31—C32—C33	0.6 (9)
O6—Pr1—N2—C46	96.1 (5)	C30—C31—C32—C33	−179.7 (6)
O4—Pr1—N2—C46	−87.3 (5)	C36—C31—C32—C27	−177.8 (6)
O3—Pr1—N2—C46	−57.1 (5)	C30—C31—C32—C27	1.9 (9)
N1—Pr1—N2—C46	−178.2 (5)	C28—C27—C32—C33	−178.8 (6)
$Pr1^{i}$—Pr1—N2—C46	−28.3 (5)	C26—C27—C32—C33	−2.9 (9)
$O3^{i}$—Pr1—N2—C42	−148.1 (3)	C28—C27—C32—C31	−0.5 (9)
O1—Pr1—N2—C42	−176.2 (4)	C26—C27—C32—C31	175.4 (5)
O5—Pr1—N2—C42	−50.6 (4)	C31—C32—C33—C34	−0.4 (9)
$O2^{i}$—Pr1—N2—C42	39.4 (5)	C27—C32—C33—C34	177.9 (6)
O6—Pr1—N2—C42	−85.8 (4)	C32—C33—C34—C35	−0.3 (10)

O4—Pr1—N2—C42	90.8 (4)	C33—C34—C35—C36	0.7 (12)
O3—Pr1—N2—C42	121.1 (4)	C34—C35—C36—C31	−0.5 (12)
N1—Pr1—N2—C42	−0.1 (4)	C32—C31—C36—C35	−0.2 (11)
Pr1^{i}—Pr1—N2—C42	149.8 (3)	C30—C31—C36—C35	−179.8 (8)
O8^{ii}—Pr2—N3—C85	3.0 (5)	C41—N1—C37—C38	0.7 (8)
O7—Pr2—N3—C85	−142.9 (5)	Pr1—N1—C37—C38	179.6 (4)
O9^{ii}—Pr2—N3—C85	29.7 (6)	N1—C37—C38—C39	−0.2 (9)
O12—Pr2—N3—C85	85.9 (5)	C37—C38—C39—C40	−0.1 (9)
O11—Pr2—N3—C85	124.9 (5)	C38—C39—C40—C41	−0.1 (8)
O10—Pr2—N3—C85	−92.3 (5)	C38—C39—C40—C47	179.4 (6)
N4—Pr2—N3—C85	179.7 (5)	C37—N1—C41—C40	−1.0 (8)
O9—Pr2—N3—C85	−59.9 (5)	Pr1—N1—C41—C40	−179.8 (4)
Pr2^{ii}—Pr2—N3—C85	−33.7 (5)	C37—N1—C41—C42	178.7 (5)
O8^{ii}—Pr2—N3—C89	−178.1 (4)	Pr1—N1—C41—C42	−0.2 (6)
O7—Pr2—N3—C89	36.0 (5)	C39—C40—C41—N1	0.7 (8)
O9^{ii}—Pr2—N3—C89	−151.4 (4)	C47—C40—C41—N1	−178.8 (5)
O12—Pr2—N3—C89	−95.2 (4)	C39—C40—C41—C42	−179.0 (5)
O11—Pr2—N3—C89	−56.2 (4)	C47—C40—C41—C42	1.5 (8)
O10—Pr2—N3—C89	86.6 (4)	C46—N2—C42—C43	−1.5 (8)
N4—Pr2—N3—C89	−1.4 (4)	Pr1—N2—C42—C43	−179.7 (4)
O9—Pr2—N3—C89	119.0 (4)	C46—N2—C42—C41	178.3 (5)
Pr2^{ii}—Pr2—N3—C89	145.2 (4)	Pr1—N2—C42—C41	0.1 (6)
O8^{ii}—Pr2—N4—C94	−173.4 (4)	N1—C41—C42—N2	0.1 (7)
O7—Pr2—N4—C94	27.1 (4)	C40—C41—C42—N2	179.8 (5)
O9^{ii}—Pr2—N4—C94	−23.2 (5)	N1—C41—C42—C43	179.9 (5)
O12—Pr2—N4—C94	−103.2 (4)	C40—C41—C42—C43	−0.5 (8)
O11—Pr2—N4—C94	−52.9 (4)	N2—C42—C43—C44	0.7 (9)
O10—Pr2—N4—C94	109.0 (4)	C41—C42—C43—C44	−179.0 (5)
O9—Pr2—N4—C94	89.6 (4)	N2—C42—C43—C48	178.5 (5)
N3—Pr2—N4—C94	−178.3 (5)	C41—C42—C43—C48	−1.2 (8)
Pr2^{ii}—Pr2—N4—C94	49.4 (5)	C42—C43—C44—C45	1.0 (10)
O8^{ii}—Pr2—N4—C90	6.6 (5)	C48—C43—C44—C45	−176.7 (6)
O7—Pr2—N4—C90	−153.0 (4)	C43—C44—C45—C46	−1.9 (11)
O9^{ii}—Pr2—N4—C90	156.8 (4)	C42—N2—C46—C45	0.6 (9)
O12—Pr2—N4—C90	76.7 (4)	Pr1—N2—C46—C45	178.8 (5)
O11—Pr2—N4—C90	127.1 (4)	C44—C45—C46—N2	1.1 (11)
O10—Pr2—N4—C90	−71.0 (4)	C39—C40—C47—C48	179.7 (6)
O9—Pr2—N4—C90	−90.4 (4)	C41—C40—C47—C48	−0.8 (9)
N3—Pr2—N4—C90	1.7 (4)	C40—C47—C48—C43	−1.0 (10)
Pr2^{ii}—Pr2—N4—C90	−130.6 (4)	C44—C43—C48—C47	179.7 (6)
O3^{i}—Pr1—O1—C1	36.5 (6)	C42—C43—C48—C47	2.0 (9)
O5—Pr1—O1—C1	91.7 (6)	Pr2—O7—C49—O8	−48.1 (9)
O2^{i}—Pr1—O1—C1	−16.0 (7)	Pr2—O7—C49—C50'	148.0 (14)
O6—Pr1—O1—C1	126.1 (6)	Pr2—O7—C49—C50	113.9 (8)
O4—Pr1—O1—C1	−90.8 (6)	Pr2^{ii}—O8—C49—O7	39.4 (11)

O3—Pr1—O1—C1	−43.4 (6)	$Pr2^{ii}$—O8—C49—C50'	−154.7 (12)
N1—Pr1—O1—C1	−164.5 (5)	$Pr2^{ii}$—O8—C49—C50	−121.5 (9)
N2—Pr1—O1—C1	−159.4 (6)	O7—C49—C50—C51	36.0 (16)
$Pr1^{i}$—Pr1—O1—C1	−4.7 (6)	O8—C49—C50—C51	−160.8 (11)
$O3^{i}$—Pr1—O3—C13	−178.1 (3)	C50'—C49—C50—C51	−83 (3)
O1—Pr1—O3—C13	−100.6 (3)	C49—C50—C51—C56	75.7 (19)
O5—Pr1—O3—C13	135.3 (3)	C49—C50—C51—C52	−106 (2)
$O2^{i}$—Pr1—O3—C13	99.0 (3)	C56—C51—C52—C53	0(4)
O6—Pr1—O3—C13	−125.3 (3)	C50—C51—C52—C53	−179 (3)
O4—Pr1—O3—C13	4.8 (3)	C51—C52—C53—C54	0(5)
N1—Pr1—O3—C13	34.7 (3)	C52—C53—C54—C55	4(22)
N2—Pr1—O3—C13	−33.2 (3)	C53—C54—C55—C56	−10 (11)
$Pr1^{i}$—Pr1—O3—C13	−178.1 (3)	C53—C54—C55—C60	−175 (22)
$O3^{i}$—Pr1—O3—$Pr1^{i}$	0.000 (2)	C60—C55—C56—C51	180 (22)
O1—Pr1—O3—$Pr1^{i}$	77.49 (13)	C54—C55—C56—C51	10 (9)
O5—Pr1—O3—$Pr1^{i}$	−46.5 (2)	C60—C55—C56—C57	−9(10)
$O2^{i}$—Pr1—O3—$Pr1^{i}$	−82.84 (13)	C54—C55—C56—C57	−174 (22)
O6—Pr1—O3—$Pr1^{i}$	52.8 (3)	C52—C51—C56—C55	−4(22)
O4—Pr1—O3—$Pr1^{i}$	−177.09 (19)	C50—C51—C56—C55	179 (22)
N1—Pr1—O3—$Pr1^{i}$	−147.14 (12)	C52—C51—C56—C57	180 (6)
N2—Pr1—O3—$Pr1^{i}$	144.95 (12)	C50—C51—C56—C57	−1(6)
$O3^{i}$—Pr1—O4—C13	−8.3 (3)	C55—C56—C57—C58	5(24)
O1—Pr1—O4—C13	59.8 (3)	C51—C56—C57—C58	−180 (6)
O5—Pr1—O4—C13	−123.7 (3)	C56—C57—C58—C59	0(13)
$O2^{i}$—Pr1—O4—C13	−77.7 (3)	C57—C58—C59—C60	0(9)
O6—Pr1—O4—C13	141.8 (3)	C58—C59—C60—C55	−5(23)
O3—Pr1—O4—C13	−4.9 (3)	C56—C55—C60—C59	8(7)
N1—Pr1—O4—C13	−160.6 (3)	C54—C55—C60—C59	175 (22)
N2—Pr1—O4—C13	136.4 (3)	O7—C49—C50'—C51'	22 (3)
$Pr1^{i}$—Pr1—O4—C13	−6.6 (3)	O8—C49—C50'—C51'	−145 (3)
$O3^{i}$—Pr1—O5—C25	104.9 (3)	C50—C49—C50'—C51'	99 (4)
O1—Pr1—O5—C25	50.3 (3)	C49—C50'—C51'—C52'	108 (7)
$O2^{i}$—Pr1—O5—C25	−173.0 (3)	C49—C50'—C51'—C56'	−74 (4)
O6—Pr1—O5—C25	4.5 (3)	C56'—C51'—C52'—C53'	0(15)
O4—Pr1—O5—C25	−125.3 (3)	C50'—C51'—C52'—C53'	179 (9)
O3—Pr1—O5—C25	151.4 (3)	C51'—C52'—C53'—C54'	0(18)
N1—Pr1—O5—C25	−86.4 (3)	C52'—C53'—C54'—C55'	−2(2)
N2—Pr1—O5—C25	−40.5 (3)	C53'—C54'—C55'—C60'	178 (2)
$Pr1^{i}$—Pr1—O5—C25	124.6 (3)	C53'—C54'—C55'—C56'	4(4)
$O3^{i}$—Pr1—O6—C25	−76.4 (3)	C52'—C51'—C56'—C57'	−180 (8)
O1—Pr1—O6—C25	−149.8 (3)	C50'—C51'—C56'—C57'	2(5)
O5—Pr1—O6—C25	−4.5 (3)	C52'—C51'—C56'—C55'	2(2)
$O2^{i}$—Pr1—O6—C25	−1.4 (3)	C50'—C51'—C56'—C55'	−176 (2)
O4—Pr1—O6—C25	127.8 (3)	C60'—C55'—C56'—C57'	3(3)

O3—Pr1—O6—C25	−126.7 (3)	C54'—C55'—C56'—C57'	178 (2)
N1—Pr1—O6—C25	69.7 (3)	C60'—C55'—C56'—C51'	180 (28)
N2—Pr1—O6—C25	133.0 (3)	C54'—C55'—C56'—C51'	−4(4)
Pr1^{i}—Pr1—O6—C25	−91.9 (3)	C51'—C56'—C57'—C58'	180 (4)
O8^{ii}—Pr2—O7—C49	33.4 (6)	C55'—C56'—C57'—C58'	−2(2)
O9^{ii}—Pr2—O7—C49	−14.4 (5)	C56'—C57'—C58'—C59'	0(6)
O12—Pr2—O7—C49	−87.5 (5)	C57'—C58'—C59'—C60'	0(6)
O11—Pr2—O7—C49	−93.2 (5)	C54'—C55'—C60'—C59'	180 (28)
O10—Pr2—O7—C49	114.5 (5)	C56'—C55'—C60'—C59'	−3(3)
N4—Pr2—O7—C49	−165.7 (5)	C58'—C59'—C60'—C55'	2(2)
O9—Pr2—O7—C49	64.2 (5)	Pr2—O10—C61—O9	2.7 (6)
N3—Pr2—O7—C49	161.7 (5)	Pr2—O10—C61—C62	−179.9 (5)
Pr2^{ii}—Pr2—O7—C49	26.5 (5)	Pr2^{ii}—O9—C61—O10	152.9 (8)
O8^{ii}—Pr2—O9—C61	−109.0 (3)	Pr2—O9—C61—O10	−2.6 (6)
O7—Pr2—O9—C61	93.6 (3)	Pr2^{ii}—O9—C61—C62	−24.6 (14)
O9^{ii}—Pr2—O9—C61	171.8 (4)	Pr2—O9—C61—C62	179.9 (5)
O12—Pr2—O9—C61	−129.1 (3)	O10—C61—C62—C63	45.5 (9)
O11—Pr2—O9—C61	132.5 (3)	O9—C61—C62—C63	−137.0 (6)
O10—Pr2—O9—C61	1.4 (3)	C61—C62—C63—C64	−77.8 (8)
N4—Pr2—O9—C61	26.9 (3)	C61—C62—C63—C68	105.0 (8)
N3—Pr2—O9—C61	−39.9 (3)	C68—C63—C64—C65	−2.1 (12)
Pr2^{ii}—Pr2—O9—C61	171.8 (4)	C62—C63—C64—C65	−179.3 (7)
O8^{ii}—Pr2—O9—Pr2^{ii}	79.22 (14)	C63—C64—C65—C66	0.9 (14)
O7—Pr2—O9—Pr2^{ii}	−78.21 (14)	C64—C65—C66—C67	2.4 (15)
O9^{ii}—Pr2—O9—Pr2^{ii}	0.0	C65—C66—C67—C68	−4.3 (14)
O12—Pr2—O9—Pr2^{ii}	59.1 (2)	C65—C66—C67—C72	175.9 (9)
O11—Pr2—O9—Pr2^{ii}	−39.3 (2)	C66—C67—C68—C69	−179.0 (8)
O10—Pr2—O9—Pr2^{ii}	−170.4 (2)	C72—C67—C68—C69	0.7 (11)
N4—Pr2—O9—Pr2^{ii}	−144.95 (13)	C66—C67—C68—C63	3.0 (11)
N3—Pr2—O9—Pr2^{ii}	148.24 (13)	C72—C67—C68—C63	−177.2 (7)
O8^{ii}—Pr2—O10—C61	59.5 (3)	C64—C63—C68—C69	−177.8 (7)
O7—Pr2—O10—C61	−76.9 (3)	C62—C63—C68—C69	−0.6 (11)
O9^{ii}—Pr2—O10—C61	−12.6 (4)	C64—C63—C68—C67	0.1 (11)
O12—Pr2—O10—C61	133.2 (3)	C62—C63—C68—C67	177.2 (6)
O11—Pr2—O10—C61	−129.5 (3)	C67—C68—C69—C70	0.2 (12)
N4—Pr2—O10—C61	−160.3 (4)	C63—C68—C69—C70	178.0 (8)
O9—Pr2—O10—C61	−1.4 (3)	C68—C69—C70—C71	0.6 (15)
N3—Pr2—O10—C61	136.2 (4)	C69—C70—C71—C72	−2.4 (18)
Pr2^{ii}—Pr2—O10—C61	−7.0 (3)	C70—C71—C72—C67	3.3 (17)
O8^{ii}—Pr2—O11—C73	38.0 (3)	C66—C67—C72—C71	177.3 (9)
O7—Pr2—O11—C73	175.6 (3)	C68—C67—C72—C71	−2.5 (14)
O9^{ii}—Pr2—O11—C73	98.7 (3)	Pr2—O11—C73—O12	−2.3 (5)
O12—Pr2—O11—C73	1.2 (3)	Pr2—O11—C73—C74	178.6 (4)
O10—Pr2—O11—C73	−131.2 (3)	Pr2—O12—C73—O11	2.3 (5)
N4—Pr2—O11—C73	−99.2 (3)	Pr2—O12—C73—C74	−178.5 (4)

O9—Pr2—O11—C73	137.7 (3)	O11—C73—C74—C75	−46.9 (8)
N3—Pr2—O11—C73	−49.9 (3)	O12—C73—C74—C75	133.9 (6)
$Pr2^{ii}$—Pr2—O11—C73	114.1 (3)	C73—C74—C75—C76	114.1 (7)
$O8^{ii}$—Pr2—O12—C73	−150.9 (3)	C73—C74—C75—C80	−68.5 (8)
O7—Pr2—O12—C73	−8.4 (4)	C80—C75—C76—C77	−0.4 (11)
$O9^{ii}$—Pr2—O12—C73	−75.9 (3)	C74—C75—C76—C77	177.0 (7)
O11—Pr2—O12—C73	−1.2 (3)	C75—C76—C77—C78	−2.0 (13)
O10—Pr2—O12—C73	132.1 (3)	C76—C77—C78—C79	2.0 (14)
N4—Pr2—O12—C73	67.8 (3)	C77—C78—C79—C84	−179.5 (8)
O9—Pr2—O12—C73	−131.9 (3)	C77—C78—C79—C80	0.3 (12)
N3—Pr2—O12—C73	129.2 (3)	C78—C79—C80—C81	177.1 (6)
$Pr2^{ii}$—Pr2—O12—C73	−96.0 (3)	C84—C79—C80—C81	−3.0 (10)
$Pr1^{i}$—O2—C1—O1	27.5 (8)	C78—C79—C80—C75	−2.7 (10)
$Pr1^{i}$—O2—C1—C2	−152.5 (4)	C84—C79—C80—C75	177.1 (6)
Pr1—O1—C1—O2	−9.6 (10)	C76—C75—C80—C81	−177.1 (6)
Pr1—O1—C1—C2	170.3 (4)	C74—C75—C80—C81	5.4 (9)
O2—C1—C2—C3	−10.1 (9)	C76—C75—C80—C79	2.7 (10)
O1—C1—C2—C3	169.9 (6)	C74—C75—C80—C79	−174.7 (6)
C1—C2—C3—C4	−104.1 (6)	C79—C80—C81—C82	1.9 (10)
C1—C2—C3—C8	78.0 (7)	C75—C80—C81—C82	−178.2 (6)
C8—C3—C4—C5	−1.8 (8)	C80—C81—C82—C83	0.9 (11)
C2—C3—C4—C5	−179.8 (5)	C81—C82—C83—C84	−2.6 (12)
C3—C4—C5—C6	0.8 (9)	C82—C83—C84—C79	1.4 (13)
C4—C5—C6—C7	−0.3 (10)	C78—C79—C84—C83	−178.7 (8)
C5—C6—C7—C8	0.8 (10)	C80—C79—C84—C83	1.5 (12)
C5—C6—C7—C12	179.1 (7)	C89—N3—C85—C86	0.5 (10)
C6—C7—C8—C9	178.8 (6)	Pr2—N3—C85—C86	179.5 (5)
C12—C7—C8—C9	0.5 (8)	N3—C85—C86—C87	−0.7 (11)
C6—C7—C8—C3	−1.8 (8)	C85—C86—C87—C88	−0.1 (11)
C12—C7—C8—C3	179.9 (6)	C86—C87—C88—C89	1.0 (10)
C4—C3—C8—C9	−178.3 (5)	C86—C87—C88—C95	−179.2 (7)
C2—C3—C8—C9	−0.4 (8)	C85—N3—C89—C88	0.4 (9)
C4—C3—C8—C7	2.3 (8)	Pr2—N3—C89—C88	−178.5 (4)
C2—C3—C8—C7	−179.8 (5)	C85—N3—C89—C90	−180.0 (6)
C7—C8—C9—C10	−0.5 (9)	Pr2—N3—C89—C90	1.1 (7)
C3—C8—C9—C10	−179.9 (6)	C87—C88—C89—N3	−1.1 (9)
C8—C9—C10—C11	1.6 (11)	C95—C88—C89—N3	179.0 (6)
C9—C10—C11—C12	−2.8 (12)	C87—C88—C89—C90	179.3 (6)
C10—C11—C12—C7	2.8 (12)	C95—C88—C89—C90	−0.6 (9)
C6—C7—C12—C11	−179.9 (7)	C94—N4—C90—C91	−2.9 (8)
C8—C7—C12—C11	−1.6 (10)	Pr2—N4—C90—C91	177.2 (4)
Pr1—O4—C13—O3	9.0 (5)	C94—N4—C90—C89	178.1 (5)
Pr1—O4—C13—C14	−171.7 (4)	Pr2—N4—C90—C89	−1.9 (7)
$Pr1^{i}$—O3—C13—O4	177.0 (7)	N3—C89—C90—N4	0.5 (8)
Pr1—O3—C13—O4	−8.8 (5)	C88—C89—C90—N4	−179.9 (5)
$Pr1^{i}$—O3—C13—C14	−2.3 (13)	N3—C89—C90—C91	−178.6 (5)
Pr1—O3—C13—C14	171.9 (4)	C88—C89—C90—C91	1.0 (9)

O4—C13—C14—C15	10.8 (8)	N4—C90—C91—C92	1.6 (9)
O3—C13—C14—C15	−169.9 (5)	C89—C90—C91—C92	−179.3 (6)
C13—C14—C15—C16	−106.3 (7)	N4—C90—C91—C96	−179.4 (5)
C13—C14—C15—C20	73.4 (7)	C89—C90—C91—C96	−0.3 (9)
C20—C15—C16—C17	−0.2 (10)	C90—C91—C92—C93	0.8 (9)
C14—C15—C16—C17	179.5 (6)	C96—C91—C92—C93	−178.1 (6)
C15—C16—C17—C18	−0.9 (12)	C91—C92—C93—C94	−1.8 (10)
C16—C17—C18—C19	2.3 (14)	C90—N4—C94—C93	1.8 (9)
C17—C18—C19—C20	−2.3 (13)	Pr2—N4—C94—C93	−178.3 (5)
C17—C18—C19—C24	178.1 (8)	C92—C93—C94—N4	0.6 (10)
C16—C15—C20—C21	−178.2 (6)	C87—C88—C95—C96	179.6 (7)
C14—C15—C20—C21	2.0 (9)	C89—C88—C95—C96	−0.6 (10)
C16—C15—C20—C19	0.1 (9)	C88—C95—C96—C91	1.4 (11)
C14—C15—C20—C19	−179.6 (6)	C92—C91—C96—C95	178.0 (6)
C18—C19—C20—C21	179.5 (7)	C90—C91—C96—C95	−0.9 (10)
C24—C19—C20—C21	−1.0 (10)	C99—N5—C97—O13	178.5 (9)
C18—C19—C20—C15	1.1 (10)	C98—N5—C97—O13	−1.8 (14)
C24—C19—C20—C15	−179.4 (7)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C26—H26B···O13^{iii}	0.97	2.36	3.311 (9)	168
C46—H46···O1	0.93	2.40	3.081 (7)	130
C47—H47···O4^{iv}	0.93	2.59	3.377 (6)	143
C85—H85···O8^{ii}	0.93	2.47	3.149 (7)	130
C92—H92···O10^{v}	0.93	2.55	3.442 (7)	160
C98—H98A···O13	0.96	2.37	2.774 (12)	105
C86—H86···Cg^{ii}	0.93	2.87	3.706 (12)	151

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

Fig. 1

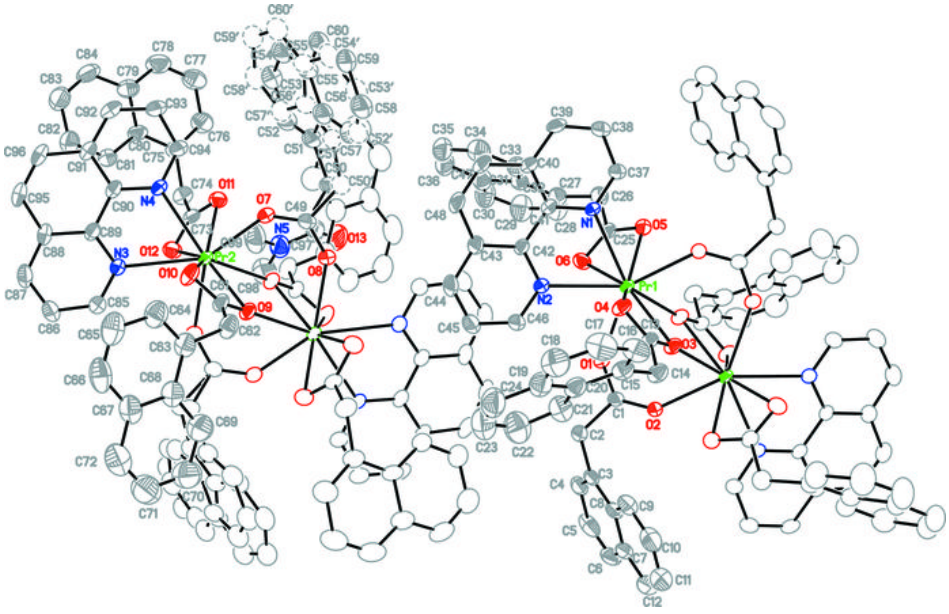


Fig. 2

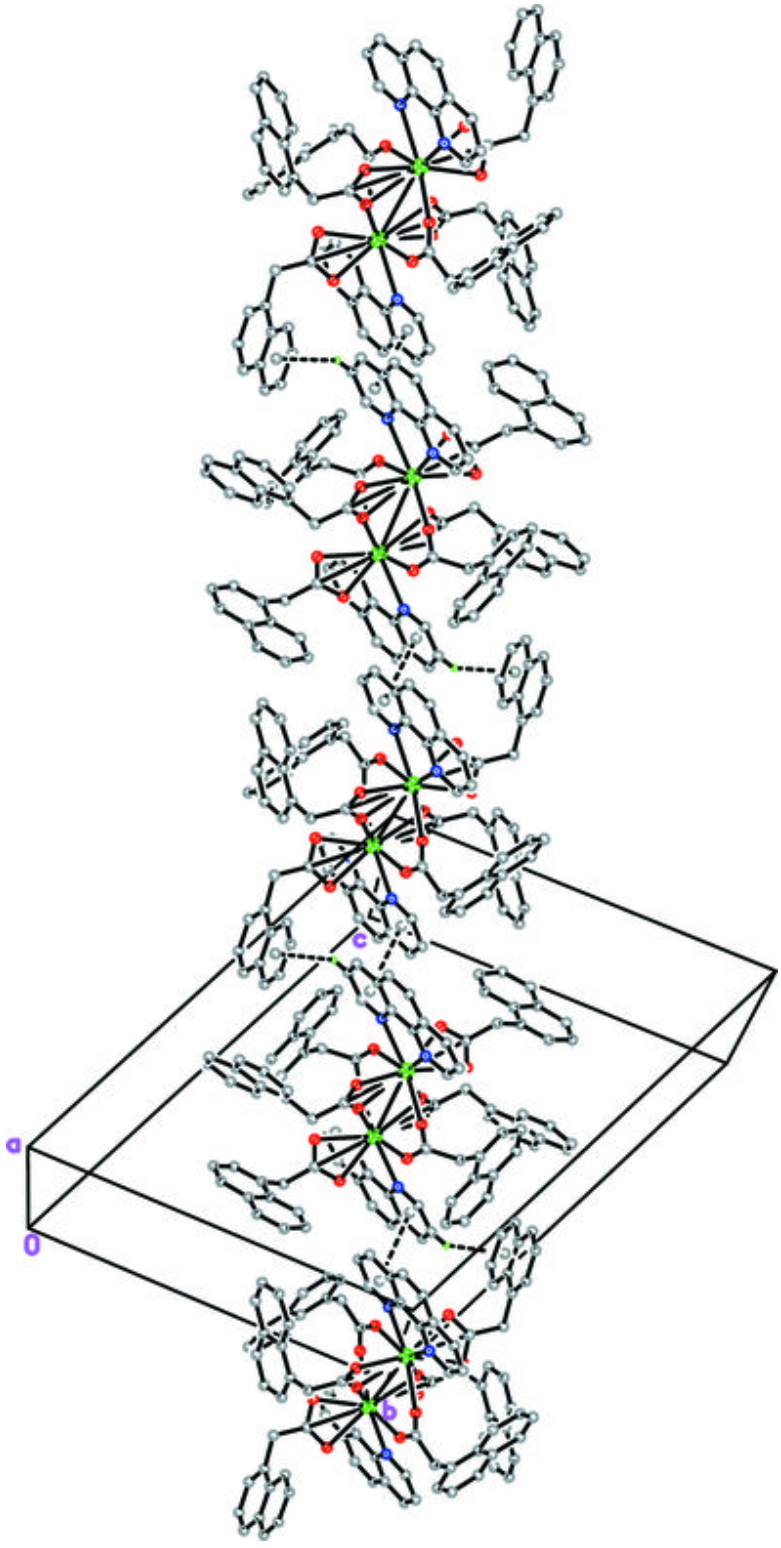


Fig. 3