

Acetone[μ -*N,N'*-bis(3-methoxy-2-oxido-benzylidene)-1,2-propanediamine]-trinitratocopper(II)praseodymium(III)

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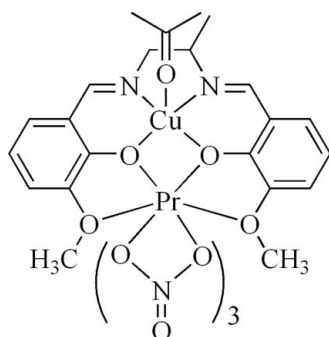
Received 9 July 2007; accepted 14 July 2007

Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; disorder in main residue; R factor = 0.036; wR factor = 0.110; data-to-parameter ratio = 15.8.

In the title complex (systematic name: (acetone-2 κ O){6,6'-dimethoxy-2,2'-[propane-1,2-diylbis(nitrilomethylidene)]-diphenolato-1 κ^4 O¹,O^{1'},O⁶,O^{6'}:2 κ^4 O¹,N,N',O^{1'}}trinitrato-1 κ^6 O,O'-copper(II)praseodymium(III)), [CuPr(C₁₉H₂₀N₂O₄)(NO₃)₃(C₃H₆O)], the Cu^{II} ion is five-coordinated by two O atoms and two N atoms of the deprotonated Schiff base and by the acetone, giving rise to a square-pyramidal geometry, whereas the Pr^{III} ion is ten-coordinated by six nitrate O atoms and four O atoms of the deprotonated Schiff base. The C atoms, with attached H atoms, of the diaminopropane link are disordered over two positions with site occupancy factors of *ca* 0.7 and 0.3.

Related literature

See Kara *et al.* (2000) for a similar copper–lanthanum complex of the same Schiff base.



Experimental

Crystal data

[CuPr(C₁₉H₂₀N₂O₄)(NO₃)₃·(C₃H₆O)]
 $M_r = 784.64$
 Monoclinic, $P2_1/c$
 $a = 9.879$ (3) Å
 $b = 18.887$ (7) Å
 $c = 15.676$ (5) Å

$\beta = 95.376$ (14)°
 $V = 2912.2$ (16) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 2.46$ mm⁻¹
 $T = 295$ (2) K
 $0.39 \times 0.25 \times 0.24$ mm

Data collection

Rigaku RAXIS-RAPID diffractometer
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.447$, $T_{\max} = 0.567$

25560 measured reflections
 6654 independent reflections
 5376 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.110$
 $S = 1.11$
 6654 reflections
 421 parameters

56 restraints
 H-atom parameters constrained
 $\Delta\rho_{\max} = 1.00$ e Å⁻³
 $\Delta\rho_{\min} = -0.75$ e Å⁻³

Table 1

Selected bond lengths (Å).

Cu1—O3	1.897 (3)	Pr1—O7	2.528 (4)
Cu1—O1	1.905 (3)	Pr1—O11	2.538 (4)
Cu1—N1	1.907 (5)	Pr1—O5	2.559 (4)
Cu1—N2	1.915 (4)	Pr1—O10	2.571 (4)
Cu1—O14	2.594 (4)	Pr1—O8	2.588 (4)
Pr1—O1	2.427 (3)	Pr1—O2	2.658 (3)
Pr1—O3	2.436 (3)	Pr1—O4	2.661 (3)
Pr1—O13	2.518 (5)		

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXL97*.

The authors gratefully acknowledge financial support from the National Natural Science Foundation of China (grant Nos. 20572018 and 20672032), Heilongjiang Province (grant Nos. 1055HZ001, ZJG0504 and JC200605) and Heilongjiang University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2296).

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supplementary materials

Acta Cryst. (2007). E63, m2192 [doi:10.1107/S1600536807034460]

Acetone[μ -*N,N'*-bis(3-methoxy-2-oxidobenzylidene)-1,2-propanediamine]trinitratocopper(II)praseodymium(III)

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Comment

As shown in Fig. 1, the octodentate Schiff base ligand links Cu and Pr atoms into a dinuclear complex through two phenolate O atoms, which is similar with the bonding reported for another copper-lanthanum complex of the same ligand (Kara *et al.*, 2000). The Pr^{III} centre in (I) is ten-coordinated by four oxygen atoms from the ligand and six oxygen atoms from three nitrate ions. The Cu^{II} center is five-coordinate by two nitrogen atoms and two oxygen atoms from the ligand and one oxygen atom from acetone in a square-pyramidal geometry.

Experimental

The title complex was obtained by the treatment of copper(II) acetate monohydrate with the Schiff base in methanol/acetone (4:1). The first two reactants were refluxed for 6 h, and the mixture was refluxed for another 3 h after the addition of praseodymium (III) nitrate hexahydrate. The reaction mixture was cooled and filtered; diethyl ether was allowed to diffuse slowly into the solution of the filtrate. Single crystals were obtained after several days. Analysis calculated for C₂₂H₂₆CuN₅O₁₄Pr: C, 33.49; H, 3.32; Cu, 8.05; N, 8.88; Pr, 17.86; found: C, 33.10; H, 3.05; Cu, 7.85; N, 8.25; Pr, 17.23%.

Refinement

H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic C), C—H = 0.97 Å (methylene C), C—H = 0.98 Å (methine C), and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or C—H = 0.96 Å (methyl C) and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$. In complex (I), the diaminopropane is disordered and was refined with a split model over two positions, and with an occupancy of 0.289 (11) for C8, C9, C10, and 0.711 (11) for C8', C9', C10'.

Figures

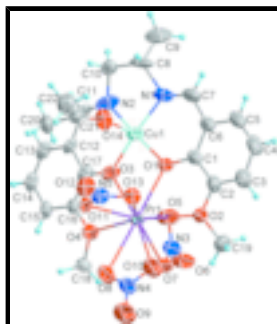


Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids. The disordered C8', C9', C10' and all H atoms have been omitted.

supplementary materials

(acetone-2κO){6,6'-dimethoxy-2,2'-[propane-1,2- diylbis(nitrilomethylidyne)]diphenolato-1κ⁴O¹,O^{1'},O⁶,O^{6'}:2κ⁴O¹,N,N',O^{1'}}trinitrato- 1κ⁶O,O'-copper(II)neodymium(III)

Crystal data

[CuPr(C ₁₉ H ₂₀ N ₂ O ₄)(NO ₃) ₃ (C ₃ H ₆ O)]	$F_{000} = 1555$
$M_r = 784.64$	$D_x = 1.790 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
Hall symbol: -P 2ybc	$\lambda = 0.71073 \text{ \AA}$
$a = 9.879 (3) \text{ \AA}$	Cell parameters from 20972 reflections
$b = 18.887 (7) \text{ \AA}$	$\theta = 3.0\text{--}27.5^\circ$
$c = 15.676 (5) \text{ \AA}$	$\mu = 2.46 \text{ mm}^{-1}$
$\beta = 95.376 (14)^\circ$	$T = 295 (2) \text{ K}$
$V = 2912.2 (16) \text{ \AA}^3$	Block, colourless
$Z = 4$	$0.39 \times 0.25 \times 0.24 \text{ mm}$

Data collection

Rigaku RAXIS-RAPID diffractometer	6654 independent reflections
Radiation source: fine-focus sealed tube	5376 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.033$
$T = 295(2) \text{ K}$	$\theta_{\text{max}} = 27.5^\circ$
ω scans	$\theta_{\text{min}} = 3.0^\circ$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -12 \rightarrow 12$
$T_{\text{min}} = 0.447$, $T_{\text{max}} = 0.567$	$k = -24 \rightarrow 24$
25560 measured reflections	$l = -20 \rightarrow 20$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.110$	$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2 + 1.9949P]$
$S = 1.11$	where $P = (F_o^2 + 2F_c^2)/3$
6654 reflections	$(\Delta/\sigma)_{\text{max}} = 0.004$
421 parameters	$\Delta\rho_{\text{max}} = 1.01 \text{ e \AA}^{-3}$
56 restraints	$\Delta\rho_{\text{min}} = -0.75 \text{ e \AA}^{-3}$
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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C1	0.8680 (4)	0.2350 (2)	0.3353 (3)	0.0444 (9)	
C2	0.9441 (5)	0.1951 (2)	0.3985 (3)	0.0480 (10)	
C3	1.0029 (6)	0.2261 (3)	0.4713 (4)	0.0676 (15)	
H1	1.0514	0.1989	0.5131	0.081*	
C4	0.9895 (6)	0.2994 (3)	0.4825 (4)	0.0748 (17)	
H2	1.0267	0.3207	0.5328	0.090*	
C5	0.9234 (5)	0.3387 (3)	0.4211 (4)	0.0684 (16)	
H3	0.9178	0.3874	0.4291	0.082*	
C6	0.8622 (5)	0.3091 (2)	0.3451 (3)	0.0520 (11)	
C7	0.7993 (6)	0.3557 (3)	0.2800 (5)	0.0760 (18)	
H4	0.8057	0.4041	0.2907	0.091*	
C11	0.5822 (7)	0.2497 (4)	0.0017 (4)	0.0783 (19)	
H11	0.5442	0.2763	-0.0444	0.094*	
C12	0.5947 (5)	0.1744 (3)	-0.0112 (3)	0.0594 (13)	
C13	0.5531 (6)	0.1477 (4)	-0.0920 (3)	0.0750 (18)	
H12	0.5149	0.1782	-0.1342	0.090*	
C14	0.5669 (7)	0.0777 (4)	-0.1105 (3)	0.0761 (19)	
H13	0.5369	0.0608	-0.1647	0.091*	
C15	0.6248 (5)	0.0325 (3)	-0.0499 (3)	0.0606 (13)	
H14	0.6348	-0.0151	-0.0630	0.073*	
C16	0.6688 (5)	0.0572 (3)	0.0312 (3)	0.0492 (11)	
C17	0.6527 (5)	0.1276 (3)	0.0526 (3)	0.0493 (11)	
C18	0.7768 (6)	-0.0526 (3)	0.0730 (4)	0.0636 (14)	
H15	0.6997	-0.0816	0.0546	0.095*	
H17	0.8273	-0.0742	0.1214	0.095*	
H16	0.8340	-0.0480	0.0270	0.095*	
C19	1.0568 (7)	0.0843 (3)	0.4255 (4)	0.0703 (16)	
H18	1.1406	0.1102	0.4268	0.106*	
H19	1.0667	0.0397	0.3976	0.106*	
H20	1.0345	0.0764	0.4830	0.106*	
C20	0.3179 (7)	0.1927 (4)	0.1389 (4)	0.0841 (19)	
H21	0.2896	0.2285	0.0975	0.126*	
H22	0.2443	0.1604	0.1444	0.126*	

supplementary materials

H23	0.3942	0.1674	0.1204	0.126*	
C21	0.3576 (6)	0.2265 (3)	0.2231 (4)	0.0620 (13)	
C22	0.2484 (8)	0.2423 (5)	0.2793 (5)	0.102 (2)	
H24	0.2131	0.1987	0.2997	0.154*	
H25	0.1767	0.2680	0.2474	0.154*	
H26	0.2849	0.2703	0.3272	0.154*	
Cu1	0.70339 (7)	0.24136 (3)	0.17375 (4)	0.05314 (16)	
Pr1	0.78327 (2)	0.072680 (11)	0.251884 (13)	0.03820 (9)	
N1	0.7363 (6)	0.3368 (2)	0.2097 (4)	0.0833 (17)	
N2	0.6188 (6)	0.2829 (3)	0.0708 (3)	0.0736 (14)	
N3	1.0501 (4)	0.0451 (2)	0.1849 (3)	0.0553 (10)	
N4	0.7742 (5)	-0.0693 (2)	0.3381 (3)	0.0607 (11)	
N5	0.5171 (6)	0.0863 (3)	0.3227 (4)	0.0774 (15)	
O1	0.8088 (3)	0.19986 (16)	0.2688 (2)	0.0501 (7)	
O2	0.9507 (3)	0.12417 (17)	0.3795 (2)	0.0516 (8)	
O3	0.6936 (4)	0.14686 (17)	0.13258 (18)	0.0510 (8)	
O4	0.7309 (3)	0.01636 (17)	0.09667 (19)	0.0496 (7)	
O5	0.9915 (4)	0.1033 (2)	0.1734 (3)	0.0686 (10)	
O6	1.1512 (6)	0.0298 (3)	0.1524 (4)	0.1089 (19)	
O7	0.9956 (4)	0.00182 (18)	0.2334 (3)	0.0631 (9)	
O8	0.7247 (5)	-0.0603 (2)	0.2635 (2)	0.0707 (11)	
O9	0.7751 (6)	-0.1266 (2)	0.3731 (3)	0.1046 (17)	
O10	0.8210 (5)	-0.0157 (2)	0.3766 (2)	0.0715 (10)	
O11	0.5273 (5)	0.0602 (3)	0.2508 (3)	0.0887 (14)	
O12	0.4092 (6)	0.0918 (4)	0.3531 (5)	0.133 (2)	
O13	0.6254 (5)	0.1080 (3)	0.3616 (3)	0.0890 (13)	
O14	0.4757 (4)	0.2408 (2)	0.2439 (3)	0.0718 (11)	
C8	0.622 (2)	0.3855 (8)	0.1689 (15)	0.067 (6)	0.289 (11)
H5	0.5540	0.3932	0.2097	0.080*	0.289 (11)
C9	0.674 (4)	0.4528 (12)	0.143 (2)	0.139 (15)	0.289 (11)
H6	0.7042	0.4485	0.0868	0.209*	0.289 (11)
H7	0.7491	0.4668	0.1829	0.209*	0.289 (11)
H8	0.6036	0.4879	0.1423	0.209*	0.289 (11)
C10	0.5539 (19)	0.3537 (8)	0.0867 (10)	0.044 (4)	0.289 (11)
H9	0.4575	0.3474	0.0917	0.053*	0.289 (11)
H10	0.5643	0.3853	0.0390	0.053*	0.289 (11)
C8'	0.7006 (12)	0.3867 (5)	0.1348 (6)	0.083 (3)	0.711 (11)
C9'	0.7917 (14)	0.3991 (6)	0.0717 (10)	0.128 (6)	0.711 (11)
C10'	0.6150 (14)	0.3613 (5)	0.0732 (7)	0.088 (3)	0.711 (11)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.042 (2)	0.037 (2)	0.054 (2)	-0.0015 (18)	0.0044 (19)	-0.0046 (18)
C2	0.048 (2)	0.046 (2)	0.049 (2)	-0.006 (2)	-0.004 (2)	-0.0070 (19)
C3	0.069 (3)	0.064 (3)	0.066 (3)	0.001 (3)	-0.014 (3)	-0.013 (3)
C4	0.071 (4)	0.064 (4)	0.086 (4)	-0.003 (3)	-0.013 (3)	-0.036 (3)
C5	0.055 (3)	0.043 (3)	0.106 (5)	-0.002 (2)	-0.003 (3)	-0.024 (3)

C6	0.040 (2)	0.038 (2)	0.077 (3)	-0.0029 (19)	0.000 (2)	-0.007 (2)
C7	0.065 (3)	0.029 (2)	0.131 (6)	-0.001 (2)	-0.009 (4)	0.003 (3)
C11	0.081 (4)	0.098 (5)	0.055 (3)	0.029 (4)	0.003 (3)	0.038 (3)
C12	0.053 (3)	0.086 (4)	0.038 (2)	0.012 (3)	0.000 (2)	0.017 (2)
C13	0.066 (3)	0.115 (6)	0.042 (3)	0.005 (4)	-0.004 (2)	0.019 (3)
C14	0.066 (3)	0.122 (6)	0.038 (2)	-0.010 (4)	-0.009 (2)	0.003 (3)
C15	0.055 (3)	0.086 (4)	0.040 (2)	-0.014 (3)	0.003 (2)	-0.008 (2)
C16	0.045 (2)	0.065 (3)	0.038 (2)	-0.006 (2)	0.0057 (19)	-0.001 (2)
C17	0.046 (2)	0.069 (3)	0.0327 (19)	0.001 (2)	0.0031 (18)	0.007 (2)
C18	0.077 (4)	0.054 (3)	0.060 (3)	0.006 (3)	0.008 (3)	-0.014 (2)
C19	0.076 (4)	0.054 (3)	0.074 (4)	0.009 (3)	-0.027 (3)	0.001 (3)
C20	0.067 (4)	0.092 (5)	0.090 (4)	-0.020 (3)	-0.006 (3)	-0.011 (4)
C21	0.055 (3)	0.057 (3)	0.074 (3)	-0.003 (2)	0.005 (3)	0.004 (3)
C22	0.073 (4)	0.131 (7)	0.107 (5)	0.001 (5)	0.026 (4)	-0.014 (5)
Cu1	0.0654 (4)	0.0380 (3)	0.0542 (3)	0.0070 (3)	-0.0038 (3)	0.0120 (2)
Pr1	0.04735 (15)	0.03195 (13)	0.03429 (13)	0.00098 (9)	-0.00148 (9)	0.00179 (8)
N1	0.096 (4)	0.031 (2)	0.116 (4)	-0.002 (2)	-0.026 (3)	0.014 (3)
N2	0.094 (4)	0.065 (3)	0.062 (3)	0.027 (3)	0.003 (3)	0.029 (2)
N3	0.055 (2)	0.043 (2)	0.069 (3)	-0.0001 (19)	0.014 (2)	-0.0002 (19)
N4	0.080 (3)	0.041 (2)	0.057 (2)	-0.011 (2)	-0.014 (2)	0.0130 (18)
N5	0.072 (3)	0.081 (4)	0.084 (4)	0.004 (3)	0.030 (3)	0.008 (3)
O1	0.0594 (19)	0.0348 (16)	0.0529 (17)	0.0021 (14)	-0.0111 (15)	0.0018 (13)
O2	0.0605 (19)	0.0394 (16)	0.0507 (17)	0.0038 (14)	-0.0174 (15)	0.0000 (14)
O3	0.068 (2)	0.0476 (18)	0.0362 (15)	0.0119 (15)	-0.0032 (14)	0.0074 (13)
O4	0.0578 (18)	0.0493 (18)	0.0407 (15)	0.0011 (15)	-0.0005 (14)	-0.0058 (13)
O5	0.068 (2)	0.052 (2)	0.089 (3)	0.0092 (18)	0.024 (2)	0.021 (2)
O6	0.098 (3)	0.073 (3)	0.169 (5)	0.016 (3)	0.080 (4)	0.014 (3)
O7	0.062 (2)	0.0446 (19)	0.084 (2)	0.0074 (16)	0.0117 (19)	0.0159 (17)
O8	0.098 (3)	0.052 (2)	0.056 (2)	-0.020 (2)	-0.023 (2)	0.0102 (16)
O9	0.147 (4)	0.064 (3)	0.094 (3)	-0.021 (3)	-0.035 (3)	0.031 (2)
O10	0.095 (2)	0.0604 (19)	0.0561 (17)	-0.0169 (17)	-0.0104 (17)	0.0087 (15)
O11	0.058 (2)	0.114 (4)	0.094 (3)	-0.008 (2)	0.009 (2)	-0.020 (3)
O12	0.081 (4)	0.170 (6)	0.159 (6)	0.005 (4)	0.070 (4)	0.004 (5)
O13	0.0882 (15)	0.0920 (16)	0.0874 (15)	0.0007 (10)	0.0117 (10)	-0.0043 (10)
O14	0.060 (2)	0.080 (3)	0.075 (2)	-0.012 (2)	0.004 (2)	-0.017 (2)
C8	0.076 (12)	0.023 (7)	0.106 (15)	0.018 (8)	0.029 (11)	0.014 (8)
C9	0.17 (4)	0.10 (2)	0.15 (3)	0.07 (2)	0.04 (3)	0.00 (2)
C10	0.042 (5)	0.043 (5)	0.047 (5)	-0.001 (3)	0.002 (3)	0.009 (3)
C8'	0.090 (4)	0.069 (4)	0.088 (4)	0.001 (3)	0.006 (3)	0.013 (3)
C9'	0.128 (10)	0.070 (7)	0.197 (15)	-0.013 (7)	0.073 (10)	0.023 (8)
C10'	0.089 (3)	0.088 (3)	0.088 (3)	0.0016 (11)	0.0086 (11)	0.0014 (11)

Geometric parameters (Å, °)

C1—O1	1.325 (5)	C21—C22	1.485 (9)
C1—C2	1.406 (7)	C22—H24	0.9600
C1—C6	1.410 (6)	C22—H25	0.9600
C2—C3	1.363 (7)	C22—H26	0.9600
C2—O2	1.375 (5)	Cu1—O3	1.897 (3)

supplementary materials

C3—C4	1.404 (8)	Cu1—O1	1.905 (3)
C3—H1	0.9300	Cu1—N1	1.907 (5)
C4—C5	1.336 (9)	Cu1—N2	1.915 (4)
C4—H2	0.9300	Cu1—O14	2.594 (4)
C5—C6	1.401 (7)	Cu1—Pr1	3.4774 (12)
C5—H3	0.9300	Pr1—O1	2.427 (3)
C6—C7	1.443 (8)	Pr1—O3	2.436 (3)
C7—N1	1.266 (9)	Pr1—O13	2.518 (5)
C7—H4	0.9300	Pr1—O7	2.528 (4)
C11—N2	1.273 (9)	Pr1—O11	2.538 (4)
C11—C12	1.444 (9)	Pr1—O5	2.559 (4)
C11—H11	0.9300	Pr1—O10	2.571 (4)
C12—C13	1.388 (8)	Pr1—O8	2.588 (4)
C12—C17	1.416 (7)	Pr1—O2	2.658 (3)
C13—C14	1.363 (9)	Pr1—O4	2.661 (3)
C13—H12	0.9300	N1—C8	1.549 (19)
C14—C15	1.363 (8)	N2—C10	1.514 (17)
C14—H13	0.9300	N3—O6	1.199 (6)
C15—C16	1.384 (6)	N3—O5	1.247 (6)
C15—H14	0.9300	N3—O7	1.270 (5)
C16—O4	1.381 (6)	N4—O9	1.214 (5)
C16—C17	1.384 (7)	N4—O8	1.236 (5)
C17—O3	1.331 (5)	N4—O10	1.244 (5)
C18—O4	1.440 (6)	N5—O12	1.212 (7)
C18—H15	0.9600	N5—O11	1.244 (7)
C18—H17	0.9600	N5—O13	1.250 (7)
C18—H16	0.9600	C8—C9	1.444 (19)
C19—O2	1.430 (6)	C8—C10	1.52 (3)
C19—H18	0.9600	C8—H5	0.9800
C19—H19	0.9600	C9—H6	0.9600
C19—H20	0.9600	C9—H7	0.9600
C20—C21	1.486 (8)	C9—H8	0.9600
C20—H21	0.9600	C10—H9	0.9700
C20—H22	0.9600	C10—H10	0.9700
C20—H23	0.9600	C8'—C10'	1.313 (12)
C21—O14	1.213 (6)	C8'—C9'	1.417 (13)
O1—C1—C2	116.9 (4)	O1—Pr1—O8	167.01 (13)
O1—C1—C6	124.3 (4)	O3—Pr1—O8	123.00 (12)
C2—C1—C6	118.7 (4)	O13—Pr1—O8	93.01 (16)
C3—C2—O2	125.1 (5)	O7—Pr1—O8	71.80 (14)
C3—C2—C1	121.1 (5)	O11—Pr1—O8	71.42 (16)
O2—C2—C1	113.8 (4)	O5—Pr1—O8	116.62 (14)
C2—C3—C4	119.4 (6)	O10—Pr1—O8	48.21 (12)
C2—C3—H1	120.3	O1—Pr1—O2	60.30 (10)
C4—C3—H1	120.3	O3—Pr1—O2	121.56 (11)
C5—C4—C3	120.2 (5)	O13—Pr1—O2	76.72 (15)
C5—C4—H2	119.9	O7—Pr1—O2	79.38 (12)
C3—C4—H2	119.9	O11—Pr1—O2	126.05 (14)
C4—C5—C6	122.2 (5)	O5—Pr1—O2	78.91 (13)

C4—C5—H3	118.9	O10—Pr1—O2	68.27 (11)
C6—C5—H3	118.9	O8—Pr1—O2	115.44 (11)
C5—C6—C1	118.1 (5)	O1—Pr1—O4	120.33 (10)
C5—C6—C7	118.7 (5)	O3—Pr1—O4	60.17 (11)
C1—C6—C7	123.2 (5)	O13—Pr1—O4	130.59 (15)
N1—C7—C6	126.0 (5)	O7—Pr1—O4	77.04 (12)
N1—C7—H4	117.0	O11—Pr1—O4	81.28 (14)
C6—C7—H4	117.0	O5—Pr1—O4	75.36 (13)
N2—C11—C12	125.7 (5)	O10—Pr1—O4	115.93 (11)
N2—C11—H11	117.2	O8—Pr1—O4	69.57 (11)
C12—C11—H11	117.2	O2—Pr1—O4	152.68 (11)
C13—C12—C17	118.9 (6)	O1—Pr1—Cu1	31.75 (8)
C13—C12—C11	117.7 (5)	O3—Pr1—Cu1	31.62 (8)
C17—C12—C11	123.4 (5)	O13—Pr1—Cu1	82.12 (12)
C14—C13—C12	121.3 (6)	O7—Pr1—Cu1	127.44 (8)
C14—C13—H12	119.3	O11—Pr1—Cu1	83.65 (13)
C12—C13—H12	119.3	O5—Pr1—Cu1	77.87 (8)
C13—C14—C15	120.1 (5)	O10—Pr1—Cu1	151.01 (9)
C13—C14—H13	119.9	O8—Pr1—Cu1	150.37 (9)
C15—C14—H13	119.9	O2—Pr1—Cu1	91.98 (7)
C14—C15—C16	120.3 (6)	O4—Pr1—Cu1	91.49 (7)
C14—C15—H14	119.9	C7—N1—C8	118.2 (9)
C16—C15—H14	119.9	C7—N1—Cu1	125.5 (4)
O4—C16—C17	114.1 (4)	C8—N1—Cu1	110.0 (8)
O4—C16—C15	125.0 (5)	C11—N2—C10	119.0 (7)
C17—C16—C15	120.9 (5)	C11—N2—Cu1	125.6 (4)
O3—C17—C16	117.4 (4)	C10—N2—Cu1	112.4 (7)
O3—C17—C12	124.2 (5)	O6—N3—O5	123.1 (4)
C16—C17—C12	118.4 (4)	O6—N3—O7	121.0 (5)
O14—C21—C22	122.0 (6)	O5—N3—O7	115.9 (4)
O14—C21—C20	120.1 (5)	O9—N4—O8	122.3 (5)
C22—C21—C20	117.9 (6)	O9—N4—O10	121.3 (5)
O3—Cu1—O1	83.45 (13)	O8—N4—O10	116.3 (4)
O3—Cu1—N1	172.5 (2)	O12—N5—O11	122.6 (7)
O1—Cu1—N1	95.29 (19)	O12—N5—O13	121.7 (7)
O3—Cu1—N2	95.40 (19)	O11—N5—O13	115.7 (5)
O1—Cu1—N2	172.52 (19)	C1—O1—Cu1	125.3 (3)
N1—Cu1—N2	84.9 (2)	C1—O1—Pr1	128.0 (3)
O3—Cu1—O14	96.98 (14)	Cu1—O1—Pr1	106.14 (14)
O1—Cu1—O14	95.65 (14)	C2—O2—C19	116.8 (4)
N1—Cu1—O14	90.5 (2)	C2—O2—Pr1	118.7 (3)
N2—Cu1—O14	91.82 (19)	C19—O2—Pr1	124.2 (3)
O3—Cu1—Pr1	42.32 (9)	C17—O3—Cu1	125.4 (3)
O1—Cu1—Pr1	42.11 (9)	C17—O3—Pr1	128.5 (3)
N1—Cu1—Pr1	137.31 (17)	Cu1—O3—Pr1	106.06 (13)
N2—Cu1—Pr1	137.64 (17)	C16—O4—C18	116.3 (4)
O14—Cu1—Pr1	91.37 (10)	C16—O4—Pr1	119.4 (3)
O1—Pr1—O3	62.71 (11)	C18—O4—Pr1	124.0 (3)
O1—Pr1—O13	74.17 (15)	N3—O5—Pr1	96.6 (3)

supplementary materials

O3—Pr1—O13	99.66 (15)	N3—O7—Pr1	97.5 (3)
O1—Pr1—O7	117.25 (12)	N4—O8—Pr1	97.3 (3)
O3—Pr1—O7	117.54 (11)	N4—O10—Pr1	98.0 (3)
O13—Pr1—O7	142.44 (15)	N5—O11—Pr1	97.0 (4)
O1—Pr1—O11	100.69 (14)	N5—O13—Pr1	97.9 (4)
O3—Pr1—O11	75.97 (15)	C21—O14—Cu1	137.6 (4)
O13—Pr1—O11	49.37 (16)	C9—C8—C10	105 (2)
O7—Pr1—O11	141.92 (14)	C9—C8—N1	112 (2)
O1—Pr1—O5	75.49 (12)	C10—C8—N1	111.2 (12)
O3—Pr1—O5	75.65 (12)	C9—C8—H5	109.7
O13—Pr1—O5	147.72 (16)	C10—C8—H5	109.7
O7—Pr1—O5	49.57 (11)	N1—C8—H5	109.7
O11—Pr1—O5	149.61 (16)	N2—C10—C8	109.2 (12)
O1—Pr1—O10	123.59 (12)	N2—C10—H9	109.8
O3—Pr1—O10	166.77 (13)	C8—C10—H9	109.8
O13—Pr1—O10	73.02 (16)	N2—C10—H10	109.8
O7—Pr1—O10	71.38 (13)	C8—C10—H10	109.8
O11—Pr1—O10	91.06 (16)	H9—C10—H10	108.3
O5—Pr1—O10	116.49 (13)	C10 ['] —C8 ['] —C9 [']	87.5 (10)
O1—C1—C2—C3	-176.6 (5)	O11—Pr1—O2—C19	117.3 (4)
C6—C1—C2—C3	5.0 (7)	O5—Pr1—O2—C19	-81.8 (4)
O1—C1—C2—O2	2.8 (6)	O10—Pr1—O2—C19	42.7 (4)
C6—C1—C2—O2	-175.6 (4)	O8—Pr1—O2—C19	32.5 (5)
O2—C2—C3—C4	179.4 (5)	O4—Pr1—O2—C19	-62.0 (5)
C1—C2—C3—C4	-1.3 (8)	Cu1—Pr1—O2—C19	-159.1 (4)
C2—C3—C4—C5	-2.1 (10)	C16—C17—O3—Cu1	171.8 (3)
C3—C4—C5—C6	1.8 (10)	C12—C17—O3—Cu1	-8.0 (6)
C4—C5—C6—C1	2.0 (8)	C16—C17—O3—Pr1	-3.9 (6)
C4—C5—C6—C7	-176.6 (6)	C12—C17—O3—Pr1	176.3 (3)
O1—C1—C6—C5	176.5 (4)	O1—Cu1—O3—C17	-165.9 (4)
C2—C1—C6—C5	-5.2 (7)	N2—Cu1—O3—C17	6.7 (4)
O1—C1—C6—C7	-5.1 (8)	O14—Cu1—O3—C17	99.2 (4)
C2—C1—C6—C7	173.3 (5)	Pr1—Cu1—O3—C17	-176.5 (4)
C5—C6—C7—N1	-177.4 (6)	O1—Cu1—O3—Pr1	10.57 (15)
C1—C6—C7—N1	4.1 (10)	N2—Cu1—O3—Pr1	-176.85 (19)
N2—C11—C12—C13	-178.1 (6)	O14—Cu1—O3—Pr1	-84.35 (15)
N2—C11—C12—C17	-1.1 (10)	O1—Pr1—O3—C17	167.1 (4)
C17—C12—C13—C14	0.0 (9)	O13—Pr1—O3—C17	-126.4 (4)
C11—C12—C13—C14	177.1 (6)	O7—Pr1—O3—C17	58.9 (4)
C12—C13—C14—C15	-1.1 (10)	O11—Pr1—O3—C17	-82.8 (4)
C13—C14—C15—C16	0.6 (9)	O5—Pr1—O3—C17	86.2 (4)
C14—C15—C16—O4	-178.7 (5)	O10—Pr1—O3—C17	-71.2 (7)
C14—C15—C16—C17	1.2 (7)	O8—Pr1—O3—C17	-26.4 (4)
O4—C16—C17—O3	-2.2 (6)	O2—Pr1—O3—C17	153.3 (3)
C15—C16—C17—O3	177.9 (4)	O4—Pr1—O3—C17	5.1 (3)
O4—C16—C17—C12	177.6 (4)	Cu1—Pr1—O3—C17	176.3 (5)
C15—C16—C17—C12	-2.3 (7)	O1—Pr1—O3—Cu1	-9.26 (13)
C13—C12—C17—O3	-178.5 (5)	O13—Pr1—O3—Cu1	57.21 (19)
C11—C12—C17—O3	4.5 (8)	O7—Pr1—O3—Cu1	-117.44 (15)

C13—C12—C17—C16	1.7 (7)	O11—Pr1—O3—Cu1	100.87 (18)
C11—C12—C17—C16	-175.3 (5)	O5—Pr1—O3—Cu1	-90.11 (17)
O3—Cu1—Pr1—O1	164.2 (2)	O10—Pr1—O3—Cu1	112.4 (5)
N1—Cu1—Pr1—O1	-4.6 (3)	O8—Pr1—O3—Cu1	157.23 (16)
N2—Cu1—Pr1—O1	168.9 (3)	O2—Pr1—O3—Cu1	-23.1 (2)
O14—Cu1—Pr1—O1	-96.91 (18)	O4—Pr1—O3—Cu1	-171.2 (2)
O1—Cu1—Pr1—O3	-164.2 (2)	C17—C16—O4—C18	-166.9 (4)
N1—Cu1—Pr1—O3	-168.8 (3)	C15—C16—O4—C18	13.0 (6)
N2—Cu1—Pr1—O3	4.6 (3)	C17—C16—O4—Pr1	6.4 (5)
O14—Cu1—Pr1—O3	98.87 (18)	C15—C16—O4—Pr1	-173.7 (4)
O3—Cu1—Pr1—O13	-123.2 (2)	O1—Pr1—O4—C16	-24.4 (3)
O1—Cu1—Pr1—O13	72.6 (2)	O3—Pr1—O4—C16	-5.8 (3)
N1—Cu1—Pr1—O13	68.0 (3)	O13—Pr1—O4—C16	70.5 (3)
N2—Cu1—Pr1—O13	-118.6 (3)	O7—Pr1—O4—C16	-138.5 (3)
O14—Cu1—Pr1—O13	-24.35 (15)	O11—Pr1—O4—C16	73.0 (3)
O3—Cu1—Pr1—O7	82.4 (2)	O5—Pr1—O4—C16	-87.4 (3)
O1—Cu1—Pr1—O7	-81.86 (19)	O10—Pr1—O4—C16	159.9 (3)
N1—Cu1—Pr1—O7	-86.5 (3)	O8—Pr1—O4—C16	146.3 (3)
N2—Cu1—Pr1—O7	87.0 (3)	O2—Pr1—O4—C16	-107.6 (3)
O14—Cu1—Pr1—O7	-178.77 (15)	Cu1—Pr1—O4—C16	-10.4 (3)
O3—Cu1—Pr1—O11	-73.46 (19)	O1—Pr1—O4—C18	148.4 (4)
O1—Cu1—Pr1—O11	122.31 (19)	O3—Pr1—O4—C18	167.0 (4)
N1—Cu1—Pr1—O11	117.7 (3)	O13—Pr1—O4—C18	-116.7 (4)
N2—Cu1—Pr1—O11	-68.8 (3)	O7—Pr1—O4—C18	34.2 (4)
O14—Cu1—Pr1—O11	25.40 (14)	O11—Pr1—O4—C18	-114.3 (4)
O3—Cu1—Pr1—O5	82.27 (19)	O5—Pr1—O4—C18	85.3 (4)
O1—Cu1—Pr1—O5	-81.96 (19)	O10—Pr1—O4—C18	-27.3 (4)
N1—Cu1—Pr1—O5	-86.6 (3)	O8—Pr1—O4—C18	-40.9 (4)
N2—Cu1—Pr1—O5	86.9 (3)	O2—Pr1—O4—C18	65.2 (4)
O14—Cu1—Pr1—O5	-178.87 (13)	Cu1—Pr1—O4—C18	162.4 (4)
O3—Cu1—Pr1—O10	-154.1 (3)	O6—N3—O5—Pr1	173.0 (6)
O1—Cu1—Pr1—O10	41.7 (3)	O7—N3—O5—Pr1	-6.6 (5)
N1—Cu1—Pr1—O10	37.0 (3)	O1—Pr1—O5—N3	151.2 (3)
N2—Cu1—Pr1—O10	-149.5 (3)	O3—Pr1—O5—N3	-143.8 (3)
O14—Cu1—Pr1—O10	-55.3 (2)	O13—Pr1—O5—N3	130.8 (4)
O3—Cu1—Pr1—O8	-41.0 (3)	O7—Pr1—O5—N3	3.9 (3)
O1—Cu1—Pr1—O8	154.7 (3)	O11—Pr1—O5—N3	-122.4 (4)
N1—Cu1—Pr1—O8	150.1 (3)	O10—Pr1—O5—N3	30.6 (4)
N2—Cu1—Pr1—O8	-36.4 (3)	O8—Pr1—O5—N3	-23.7 (4)
O14—Cu1—Pr1—O8	57.8 (2)	O2—Pr1—O5—N3	89.3 (3)
O3—Cu1—Pr1—O2	160.48 (17)	O4—Pr1—O5—N3	-81.4 (3)
O1—Cu1—Pr1—O2	-3.74 (17)	Cu1—Pr1—O5—N3	-176.2 (3)
N1—Cu1—Pr1—O2	-8.4 (3)	O6—N3—O7—Pr1	-172.9 (5)
N2—Cu1—Pr1—O2	165.1 (3)	O5—N3—O7—Pr1	6.6 (5)
O14—Cu1—Pr1—O2	-100.65 (12)	O1—Pr1—O7—N3	-39.8 (3)
O3—Cu1—Pr1—O4	7.59 (17)	O3—Pr1—O7—N3	31.9 (3)
O1—Cu1—Pr1—O4	-156.63 (17)	O13—Pr1—O7—N3	-139.4 (3)
N1—Cu1—Pr1—O4	-161.2 (3)	O11—Pr1—O7—N3	134.8 (3)
N2—Cu1—Pr1—O4	12.2 (3)	O5—Pr1—O7—N3	-3.8 (3)

supplementary materials

O14—Cu1—Pr1—O4	106.45 (11)	O10—Pr1—O7—N3	-158.7 (3)
C6—C7—N1—C8	151.3 (10)	O8—Pr1—O7—N3	150.3 (3)
C6—C7—N1—Cu1	2.2 (10)	O2—Pr1—O7—N3	-88.2 (3)
O1—Cu1—N1—C7	-5.6 (6)	O4—Pr1—O7—N3	77.9 (3)
N2—Cu1—N1—C7	-178.1 (7)	Cu1—Pr1—O7—N3	-3.9 (3)
O14—Cu1—N1—C7	90.1 (6)	O9—N4—O8—Pr1	-177.8 (6)
Pr1—Cu1—N1—C7	-2.5 (8)	O10—N4—O8—Pr1	3.7 (6)
O1—Cu1—N1—C8	-156.8 (9)	O1—Pr1—O8—N4	-57.1 (7)
N2—Cu1—N1—C8	30.7 (9)	O3—Pr1—O8—N4	-169.7 (3)
O14—Cu1—N1—C8	-61.1 (9)	O13—Pr1—O8—N4	-66.1 (4)
Pr1—Cu1—N1—C8	-153.7 (9)	O7—Pr1—O8—N4	78.8 (4)
C12—C11—N2—C10	-157.0 (9)	O11—Pr1—O8—N4	-111.2 (4)
C12—C11—N2—Cu1	1.6 (10)	O5—Pr1—O8—N4	100.6 (4)
O3—Cu1—N2—C11	-3.6 (6)	O10—Pr1—O8—N4	-2.2 (3)
N1—Cu1—N2—C11	168.9 (6)	O2—Pr1—O8—N4	10.6 (4)
O14—Cu1—N2—C11	-100.7 (6)	O4—Pr1—O8—N4	161.4 (4)
Pr1—Cu1—N2—C11	-6.7 (7)	Cu1—Pr1—O8—N4	-145.4 (3)
O3—Cu1—N2—C10	156.2 (8)	O9—N4—O10—Pr1	177.7 (6)
N1—Cu1—N2—C10	-31.4 (8)	O8—N4—O10—Pr1	-3.7 (6)
O14—Cu1—N2—C10	59.0 (8)	O1—Pr1—O10—N4	169.4 (3)
Pr1—Cu1—N2—C10	153.1 (8)	O3—Pr1—O10—N4	54.6 (7)
C2—C1—O1—Cu1	-178.7 (3)	O13—Pr1—O10—N4	112.4 (4)
C6—C1—O1—Cu1	-0.4 (6)	O7—Pr1—O10—N4	-79.7 (4)
C2—C1—O1—Pr1	10.9 (6)	O11—Pr1—O10—N4	65.8 (4)
C6—C1—O1—Pr1	-170.8 (3)	O5—Pr1—O10—N4	-100.9 (4)
O3—Cu1—O1—C1	177.2 (4)	O8—Pr1—O10—N4	2.2 (3)
N1—Cu1—O1—C1	4.7 (4)	O2—Pr1—O10—N4	-165.4 (4)
O14—Cu1—O1—C1	-86.4 (4)	O4—Pr1—O10—N4	-15.0 (4)
Pr1—Cu1—O1—C1	-172.2 (4)	Cu1—Pr1—O10—N4	144.6 (3)
O3—Cu1—O1—Pr1	-10.62 (15)	O12—N5—O11—Pr1	-179.4 (6)
N1—Cu1—O1—Pr1	176.9 (2)	O13—N5—O11—Pr1	2.0 (6)
O14—Cu1—O1—Pr1	85.78 (15)	O1—Pr1—O11—N5	-59.3 (4)
O3—Pr1—O1—C1	-178.9 (4)	O3—Pr1—O11—N5	-117.5 (4)
O13—Pr1—O1—C1	71.1 (4)	O13—Pr1—O11—N5	-1.2 (4)
O7—Pr1—O1—C1	-70.3 (4)	O7—Pr1—O11—N5	125.6 (4)
O11—Pr1—O1—C1	113.1 (4)	O5—Pr1—O11—N5	-138.8 (4)
O5—Pr1—O1—C1	-97.8 (4)	O10—Pr1—O11—N5	65.2 (4)
O10—Pr1—O1—C1	14.6 (4)	O8—Pr1—O11—N5	110.0 (4)
O8—Pr1—O1—C1	61.8 (7)	O2—Pr1—O11—N5	1.6 (5)
O2—Pr1—O1—C1	-12.4 (3)	O4—Pr1—O11—N5	-178.7 (4)
O4—Pr1—O1—C1	-160.8 (3)	Cu1—Pr1—O11—N5	-86.2 (4)
Cu1—Pr1—O1—C1	171.9 (4)	O12—N5—O13—Pr1	179.4 (6)
O3—Pr1—O1—Cu1	9.23 (13)	O11—N5—O13—Pr1	-2.0 (6)
O13—Pr1—O1—Cu1	-100.80 (19)	O1—Pr1—O13—N5	121.0 (4)
O7—Pr1—O1—Cu1	117.86 (15)	O3—Pr1—O13—N5	63.1 (4)
O11—Pr1—O1—Cu1	-58.74 (19)	O7—Pr1—O13—N5	-124.6 (4)
O5—Pr1—O1—Cu1	90.34 (17)	O11—Pr1—O13—N5	1.2 (4)
O10—Pr1—O1—Cu1	-157.25 (15)	O5—Pr1—O13—N5	141.5 (4)
O8—Pr1—O1—Cu1	-110.1 (5)	O10—Pr1—O13—N5	-105.5 (4)

O2—Pr1—O1—Cu1	175.69 (19)	O8—Pr1—O13—N5	-61.1 (4)
O4—Pr1—O1—Cu1	27.34 (19)	O2—Pr1—O13—N5	-176.5 (4)
C3—C2—O2—C19	-19.1 (7)	O4—Pr1—O13—N5	4.4 (5)
C1—C2—O2—C19	161.5 (5)	Cu1—Pr1—O13—N5	89.6 (4)
C3—C2—O2—Pr1	166.4 (4)	C22—C21—O14—Cu1	-171.4 (5)
C1—C2—O2—Pr1	-13.0 (5)	C20—C21—O14—Cu1	8.2 (10)
O1—Pr1—O2—C2	12.7 (3)	O3—Cu1—O14—C21	-52.6 (6)
O3—Pr1—O2—C2	26.8 (3)	O1—Cu1—O14—C21	-136.6 (6)
O13—Pr1—O2—C2	-66.4 (3)	N1—Cu1—O14—C21	128.0 (6)
O7—Pr1—O2—C2	142.7 (3)	N2—Cu1—O14—C21	43.1 (6)
O11—Pr1—O2—C2	-68.6 (4)	Pr1—Cu1—O14—C21	-94.7 (6)
O5—Pr1—O2—C2	92.2 (3)	C7—N1—C8—C9	65 (2)
O10—Pr1—O2—C2	-143.2 (3)	Cu1—N1—C8—C9	-140.9 (18)
O8—Pr1—O2—C2	-153.4 (3)	C7—N1—C8—C10	-178.0 (11)
O4—Pr1—O2—C2	112.1 (3)	Cu1—N1—C8—C10	-24.4 (16)
Cu1—Pr1—O2—C2	15.0 (3)	C11—N2—C10—C8	-175.3 (11)
O1—Pr1—O2—C19	-161.3 (5)	Cu1—N2—C10—C8	23.4 (15)
O3—Pr1—O2—C19	-147.2 (4)	C9—C8—C10—N2	121.7 (18)
O13—Pr1—O2—C19	119.5 (4)	N1—C8—C10—N2	0.8 (18)
O7—Pr1—O2—C19	-31.3 (4)		

Fig. 1

