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catena-Poly[[tris(acetonitrile-κN)-praseodymium(III)]tris(μ-trifluoromethanesulfonato-$\kappa^2 O$:O')]

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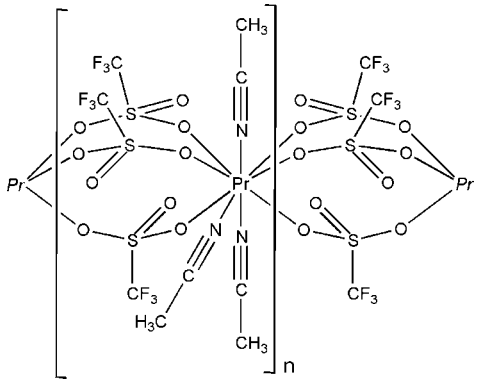
Key indicators: single-crystal X-ray study; T = 103 K; mean σ(C–C) = 0.008 Å; R factor = 0.036; wR factor = 0.076; data-to-parameter ratio = 16.9.

In the colourless title compound, $[Pr(CF_3O_3S)_3(CH_3CN)_3]_n$, the three trifluoromethanesulfonate anions form three bridges *via* O:O'-coordination between two Pr^{III} atoms. The structure contains $[Pr(NCMe)_3$-$\mu_2(OTf)_3-Pr(NCMe)_3$-$\mu_2(OTf)_3]_n$ (NCMe is acetonitrile; OTf is trifluoromethanesulfonate) chains parallel to the a axis. The Pr^{III} atom is nine-coordinate in a distorted tricapped trigonal-prismatic environment.

Related literature

For the isostructural Eu^{III} and U^{III} compounds, see: Tang *et al.* (2011) and Natrajan *et al.* (2005), respectively.



Experimental

Crystal data

$[Pr(CF_3O_3S)_3(C_2H_3N)_3]$
M_r = 711.28
Triclinic, $P\overline{1}$
a = 5.8044 (6) Å
b = 10.5062 (10) Å
c = 18.9887 (19) Å
α = 97.307 (1)°
β = 94.163 (1)°
γ = 91.695 (1)°
V = 1144.7 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.52 mm^{-1}
T = 103 K
0.24 × 0.02 × 0.01 mm

Data collection

Bruker APEXII Quazar diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.578, T_{max} = 0.978
20544 measured reflections
5251 independent reflections
4674 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.076
S = 1.16
5251 reflections
311 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.04 e Å^{-3}
$\Delta\rho_{min}$ = −1.15 e Å^{-3}

Table 1
Selected bond lengths (Å).

Pr1—O1^{i}	2.435 (3)	Pr1—O8^{i}	2.473 (3)
Pr1—O2	2.464 (3)	Pr1—N1	2.621 (4)
Pr1—O4^{i}	2.455 (3)	Pr1—N2	2.648 (4)
Pr1—O5	2.464 (3)	Pr1—N3	2.651 (4)
Pr1—O7	2.459 (3)		

Symmetry code: (i) $x+1, y, z$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XPMA* (Zsolnai, 1996) and *ORTEP-3* (Farrugia, 2012); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: VN2063).

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supporting information

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catena-Poly[[tris(acetonitrile-κN)praseodymium(III)]tris(μ-trifluoromethanesulfonato-$\kappa^2 O$:O')]

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S1. Comment

The coordination environment of the Pr^{III} atom ion in the title compound can be described as a distorted trigonal tricapped prism. 6 O atoms are forming the trigonal prismatic environment around the Pr^{III} atom and the three N atoms of the coordinated MeCN solvent molecules are forming the cappings over the rectangular sides of the prism. The metal-O distances in the title compound are with an average of 2.458 (13) Å about 0.05 Å longer than in the corresponding Eu complex (Tang *et al.*, 2011) and 0.04 Å shorter than in its U analogue (Natrajan *et al.*, 2005) reflecting the effects of the lanthanide contraction and also the change from a lanthanide to an actinide ion. The metal-N distances with 2.588 (17) Å for the Eu complex are about 0.05 Å shorter than for the here presented Pr compound with 2.640 (17) Å, whereas the latter are found to be in very good agreement with those in the U complex with 2.651 (14) Å. The ion size increase while changing the metal ion in the complex from Pr to U seems to influence more the shorter metal-O distances than the longer metal-N distances for the solvent molecules forming the cappings of the trigonal prism.

S2. Experimental

Crystals from the title compound precipitated after a ligand exchange reaction from 103.1 mg (0.13 mmol) $[Pr(H_2O)_9](OTf)_3$ in 2 ml of MeCN. Crystals in the form of needles suitable for x-ray analysis were obtained by re-crystallization from hot MeCN.

S3. Refinement

All H atoms were placed on geometrical positions according to the hybridization of the atoms they are bound to. One common isotropic *U* value was used and refined for all hydrogen atoms.

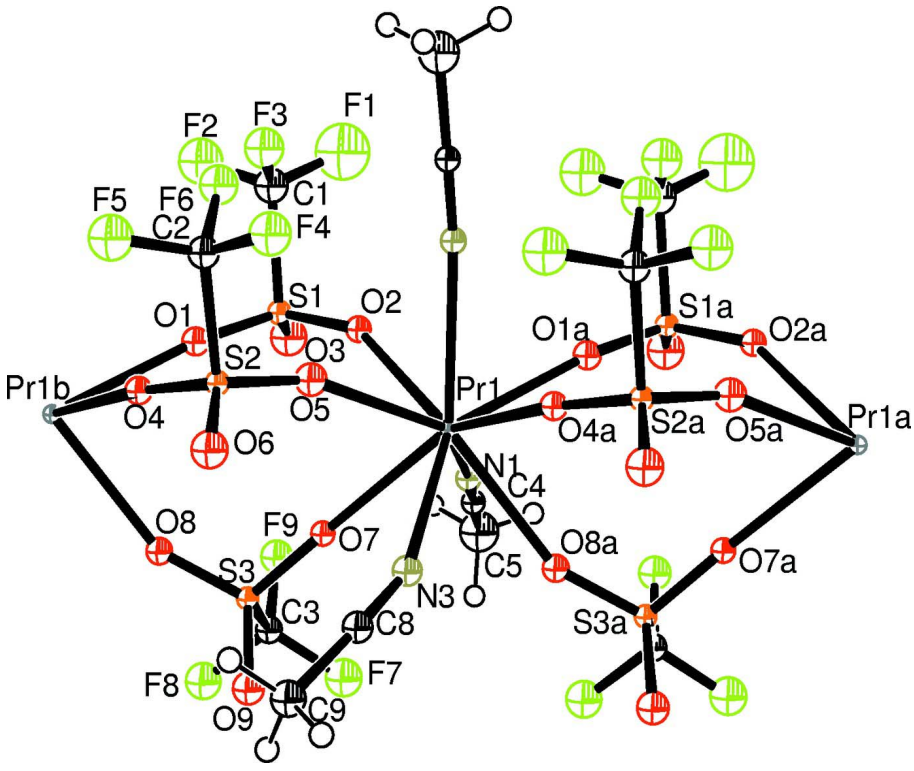

Figure 1

Molecular structure of the title compound; ellipsoids at the 50% probability level (symmetry codes: a = x + 1, y, z; b = x - 1, y, z).

***catena*-Poly[[tris(acetonitrile-κN)praseodymium(III)]tris(μ- trifluoromethanesulfonato-κ^2O:O')]**

Crystal data

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Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 5.8044 (6) Å
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α = 97.307 (1)°
β = 94.163 (1)°
γ = 91.695 (1)°
V = 1144.7 (2) Å^3
Z = 2
F(000) = 688
D_x = 2.064 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9222 reflections
θ = 2.2–28.1°
μ = 2.52 mm^{-1}
T = 103 K
Needle, colourless
0.24 × 0.02 × 0.01 mm

Data collection

Bruker APEXII Quazar diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 66 pixels mm^{-1}
combined ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.578, T_{max} = 0.978
20544 measured reflections
5251 independent reflections
4674 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 28.2°, θ_{min} = 1.1°
h = −7→7
k = −13→13
l = −25→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.076$
$S = 1.16$
5251 reflections
311 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0169P)^2 + 4.422P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.04$ e Å^{-3}
$\Delta\rho_{min} = -1.15$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Pr1	1.07535 (4)	0.07978 (2)	0.262548 (13)	0.01276 (7)
S1	0.56250 (16)	0.18346 (10)	0.15067 (6)	0.0158 (2)
S2	0.61165 (16)	0.18294 (10)	0.39162 (6)	0.0158 (2)
S3	0.55261 (16)	−0.16488 (10)	0.24609 (6)	0.0147 (2)
F1	0.6947 (6)	0.3922 (3)	0.10237 (19)	0.0467 (9)
F2	0.3309 (6)	0.3778 (3)	0.11712 (19)	0.0450 (9)
F3	0.5755 (5)	0.4245 (3)	0.20746 (15)	0.0299 (6)
F4	0.7997 (5)	0.3949 (3)	0.46088 (18)	0.0440 (8)
F5	0.4258 (5)	0.3828 (3)	0.45649 (18)	0.0422 (8)
F6	0.5975 (5)	0.4226 (3)	0.36502 (17)	0.0344 (7)
F7	0.7193 (5)	−0.3223 (3)	0.14700 (16)	0.0320 (7)
F8	0.3474 (5)	−0.3357 (3)	0.14802 (16)	0.0338 (7)
F9	0.5120 (4)	−0.1770 (3)	0.10682 (14)	0.0258 (6)
O1	0.3838 (5)	0.1578 (3)	0.19688 (18)	0.0240 (7)
O2	0.7937 (5)	0.1773 (3)	0.18415 (17)	0.0216 (7)
O3	0.5278 (6)	0.1225 (3)	0.07935 (17)	0.0276 (7)
O4	0.3864 (5)	0.1540 (3)	0.35450 (17)	0.0223 (7)
O5	0.7984 (5)	0.1725 (3)	0.34527 (17)	0.0230 (7)
O6	0.6489 (5)	0.1277 (3)	0.45609 (17)	0.0270 (7)
O7	0.7431 (5)	−0.0746 (3)	0.24309 (17)	0.0208 (7)
O8	0.3323 (5)	−0.1040 (3)	0.25044 (16)	0.0186 (6)
O9	0.5924 (5)	−0.2595 (3)	0.29293 (17)	0.0233 (7)
N1	1.0406 (6)	−0.0433 (4)	0.1330 (2)	0.0225 (8)
N2	1.1033 (6)	0.3339 (4)	0.2835 (2)	0.0216 (8)
N3	1.0456 (6)	−0.0546 (4)	0.3708 (2)	0.0214 (8)

C1	0.5396 (8)	0.3551 (4)	0.1440 (3)	0.0238 (10)
C2	0.6081 (8)	0.3553 (5)	0.4193 (3)	0.0270 (11)
C3	0.5309 (7)	−0.2545 (4)	0.1566 (2)	0.0207 (9)
C4	1.0185 (7)	−0.1019 (5)	0.0786 (3)	0.0219 (10)
C5	0.9892 (9)	−0.1778 (6)	0.0081 (3)	0.0377 (13)
H5A	0.9788	−0.2693	0.0134	0.083 (9)*
H5B	1.1219	−0.1607	−0.0189	0.083 (9)*
H5C	0.8472	−0.1540	−0.0174	0.083 (9)*
C6	1.0979 (7)	0.4424 (5)	0.2948 (3)	0.0261 (11)
C7	1.0879 (10)	0.5816 (5)	0.3096 (5)	0.057 (2)
H7A	0.9471	0.6098	0.2854	0.083 (9)*
H7B	1.2236	0.6219	0.2923	0.083 (9)*
H7C	1.0864	0.6067	0.3611	0.083 (9)*
C8	0.9551 (7)	−0.1080 (4)	0.4105 (2)	0.0212 (9)
C9	0.8291 (8)	−0.1738 (5)	0.4598 (3)	0.0283 (11)
H9A	0.7095	−0.1184	0.4790	0.083 (9)*
H9B	0.9365	−0.1933	0.4989	0.083 (9)*
H9C	0.7567	−0.2538	0.4346	0.083 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pr1	0.00653 (9)	0.01308 (12)	0.01839 (12)	−0.00110 (7)	0.00174 (7)	0.00089 (8)
S1	0.0118 (4)	0.0162 (5)	0.0198 (5)	−0.0006 (4)	0.0023 (4)	0.0039 (4)
S2	0.0104 (4)	0.0182 (5)	0.0177 (5)	−0.0012 (4)	0.0018 (4)	−0.0015 (4)
S3	0.0101 (4)	0.0124 (5)	0.0215 (5)	−0.0011 (3)	0.0013 (4)	0.0017 (4)
F1	0.069 (2)	0.0256 (17)	0.051 (2)	−0.0047 (15)	0.0294 (18)	0.0160 (16)
F2	0.0451 (19)	0.0280 (17)	0.059 (2)	0.0138 (14)	−0.0205 (16)	0.0072 (16)
F3	0.0326 (15)	0.0204 (15)	0.0351 (17)	0.0005 (11)	0.0012 (12)	−0.0014 (12)
F4	0.0312 (16)	0.0360 (18)	0.055 (2)	−0.0067 (13)	−0.0136 (14)	−0.0178 (16)
F5	0.0357 (16)	0.0319 (18)	0.056 (2)	0.0040 (13)	0.0219 (15)	−0.0165 (15)
F6	0.0276 (15)	0.0199 (15)	0.056 (2)	−0.0004 (11)	0.0017 (13)	0.0051 (14)
F7	0.0307 (15)	0.0266 (16)	0.0381 (17)	0.0115 (12)	0.0087 (12)	−0.0034 (13)
F8	0.0293 (15)	0.0263 (16)	0.0419 (18)	−0.0140 (12)	0.0013 (12)	−0.0068 (13)
F9	0.0236 (13)	0.0315 (16)	0.0222 (14)	0.0012 (11)	0.0006 (10)	0.0031 (12)
O1	0.0164 (14)	0.0217 (17)	0.0349 (19)	−0.0018 (12)	0.0103 (13)	0.0036 (14)
O2	0.0137 (14)	0.0215 (17)	0.0292 (18)	−0.0002 (12)	−0.0021 (12)	0.0045 (14)
O3	0.0307 (17)	0.0279 (19)	0.0228 (18)	−0.0002 (14)	0.0009 (13)	−0.0010 (14)
O4	0.0141 (14)	0.0206 (17)	0.0297 (18)	−0.0033 (12)	−0.0037 (12)	−0.0019 (14)
O5	0.0198 (15)	0.0198 (17)	0.0299 (18)	0.0023 (12)	0.0111 (13)	−0.0002 (14)
O6	0.0243 (16)	0.034 (2)	0.0228 (18)	0.0030 (14)	0.0035 (13)	0.0051 (15)
O7	0.0120 (13)	0.0223 (17)	0.0275 (18)	−0.0090 (11)	0.0001 (12)	0.0034 (14)
O8	0.0146 (14)	0.0171 (16)	0.0242 (17)	0.0023 (11)	0.0031 (11)	0.0010 (13)
O9	0.0208 (15)	0.0204 (17)	0.0304 (19)	−0.0004 (12)	0.0013 (13)	0.0110 (14)
N1	0.0139 (17)	0.029 (2)	0.024 (2)	0.0009 (15)	0.0015 (14)	0.0008 (18)
N2	0.0129 (16)	0.020 (2)	0.032 (2)	−0.0025 (14)	0.0031 (14)	0.0038 (17)
N3	0.0165 (17)	0.022 (2)	0.026 (2)	0.0023 (14)	0.0029 (15)	0.0017 (17)
C1	0.025 (2)	0.018 (2)	0.029 (3)	0.0009 (17)	0.0011 (18)	0.008 (2)

C2	0.018 (2)	0.025 (3)	0.034 (3)	−0.0017 (18)	0.0005 (18)	−0.010 (2)
C3	0.0157 (19)	0.017 (2)	0.027 (3)	−0.0003 (16)	0.0022 (17)	−0.0055 (19)
C4	0.0127 (19)	0.029 (3)	0.024 (3)	0.0004 (17)	0.0024 (16)	0.005 (2)
C5	0.038 (3)	0.051 (4)	0.021 (3)	0.000 (2)	0.002 (2)	−0.006 (2)
C6	0.0120 (19)	0.023 (3)	0.044 (3)	−0.0016 (16)	0.0060 (18)	0.004 (2)
C7	0.032 (3)	0.016 (3)	0.123 (7)	−0.001 (2)	0.022 (3)	0.002 (3)
C8	0.017 (2)	0.022 (2)	0.025 (2)	0.0014 (17)	0.0001 (17)	0.002 (2)
C9	0.022 (2)	0.041 (3)	0.023 (2)	−0.005 (2)	0.0025 (18)	0.010 (2)

Geometric parameters (Å, º)

Pr1—O1^{i}	2.435 (3)	F4—C2	1.340 (5)
Pr1—O2	2.464 (3)	F5—C2	1.333 (5)
Pr1—O4^{i}	2.455 (3)	F6—C2	1.320 (6)
Pr1—O5	2.464 (3)	F7—C3	1.333 (5)
Pr1—O7	2.459 (3)	F8—C3	1.332 (5)
Pr1—O8^{i}	2.473 (3)	F9—C3	1.324 (5)
Pr1—N1	2.621 (4)	O1—Pr1^{ii}	2.435 (3)
Pr1—N2	2.648 (4)	O4—Pr1^{ii}	2.455 (3)
Pr1—N3	2.651 (4)	O8—Pr1^{ii}	2.473 (3)
S1—O3	1.420 (3)	N1—C4	1.130 (6)
S1—O1	1.447 (3)	N2—C6	1.134 (6)
S1—O2	1.450 (3)	N3—C8	1.142 (6)
S1—C1	1.832 (5)	C4—C5	1.464 (7)
S2—O6	1.426 (3)	C5—H5A	0.9800
S2—O5	1.443 (3)	C5—H5B	0.9800
S2—O4	1.445 (3)	C5—H5C	0.9800
S2—C2	1.822 (5)	C6—C7	1.457 (7)
S3—O9	1.429 (3)	C7—H7A	0.9800
S3—O7	1.444 (3)	C7—H7B	0.9800
S3—O8	1.449 (3)	C7—H7C	0.9800
S3—C3	1.829 (5)	C8—C9	1.457 (6)
F1—C1	1.322 (5)	C9—H9A	0.9800
F2—C1	1.320 (5)	C9—H9B	0.9800
F3—C1	1.326 (5)	C9—H9C	0.9800
O1^{i}—Pr1—O4^{i}	75.59 (11)	O9—S3—C3	105.0 (2)
O1^{i}—Pr1—O7	139.23 (11)	O7—S3—C3	102.39 (19)
O4^{i}—Pr1—O7	139.22 (11)	O8—S3—C3	103.59 (19)
O1^{i}—Pr1—O2	88.88 (10)	S1—O1—Pr1^{ii}	170.4 (2)
O4^{i}—Pr1—O2	137.29 (10)	S1—O2—Pr1	151.05 (19)
O7—Pr1—O2	75.57 (10)	S2—O4—Pr1^{ii}	162.7 (2)
O1^{i}—Pr1—O5	137.30 (11)	S2—O5—Pr1	161.1 (2)
O4^{i}—Pr1—O5	88.00 (10)	S3—O7—Pr1	169.2 (2)
O7—Pr1—O5	76.01 (10)	S3—O8—Pr1^{ii}	155.19 (18)
O2—Pr1—O5	76.90 (11)	C4—N1—Pr1	175.9 (4)
O1^{i}—Pr1—O8^{i}	77.31 (10)	C6—N2—Pr1	174.3 (3)
O4^{i}—Pr1—O8^{i}	79.12 (10)	C8—N3—Pr1	156.4 (3)

O7—Pr1—O8^{i}	88.37 (10)	F2—C1—F1	109.2 (4)
O2—Pr1—O8^{i}	136.43 (10)	F2—C1—F3	108.1 (4)
O5—Pr1—O8^{i}	138.43 (10)	F1—C1—F3	108.5 (4)
O1^{i}—Pr1—N1	71.04 (11)	F2—C1—S1	110.0 (3)
O4^{i}—Pr1—N1	137.12 (11)	F1—C1—S1	109.9 (3)
O7—Pr1—N1	68.20 (11)	F3—C1—S1	111.1 (3)
O2—Pr1—N1	68.43 (11)	F6—C2—F5	107.8 (4)
O5—Pr1—N1	134.88 (11)	F6—C2—F4	107.8 (4)
O8^{i}—Pr1—N1	68.00 (11)	F5—C2—F4	108.2 (4)
O1^{i}—Pr1—N2	70.21 (11)	F6—C2—S2	112.9 (3)
O4^{i}—Pr1—N2	70.03 (11)	F5—C2—S2	110.0 (3)
O7—Pr1—N2	132.10 (10)	F4—C2—S2	110.0 (3)
O2—Pr1—N2	67.28 (11)	F9—C3—F8	108.5 (4)
O5—Pr1—N2	67.15 (11)	F9—C3—F7	108.1 (4)
O8^{i}—Pr1—N2	139.51 (10)	F8—C3—F7	108.3 (4)
N1—Pr1—N2	120.35 (12)	F9—C3—S3	111.7 (3)
O1^{i}—Pr1—N3	136.38 (11)	F8—C3—S3	110.3 (3)
O4^{i}—Pr1—N3	71.01 (11)	F7—C3—S3	109.8 (3)
O7—Pr1—N3	68.24 (11)	N1—C4—C5	179.8 (6)
O2—Pr1—N3	134.74 (10)	C4—C5—H5A	109.5
O5—Pr1—N3	68.85 (11)	C4—C5—H5B	109.5
O8^{i}—Pr1—N3	69.59 (11)	H5A—C5—H5B	109.5
N1—Pr1—N3	118.54 (12)	C4—C5—H5C	109.5
N2—Pr1—N3	120.91 (12)	H5A—C5—H5C	109.5
O3—S1—O1	115.7 (2)	H5B—C5—H5C	109.5
O3—S1—O2	115.4 (2)	N2—C6—C7	179.2 (5)
O1—S1—O2	112.91 (19)	C6—C7—H7A	109.5
O3—S1—C1	104.8 (2)	C6—C7—H7B	109.5
O1—S1—C1	103.3 (2)	H7A—C7—H7B	109.5
O2—S1—C1	102.54 (19)	C6—C7—H7C	109.5
O6—S2—O5	115.65 (19)	H7A—C7—H7C	109.5
O6—S2—O4	114.9 (2)	H7B—C7—H7C	109.5
O5—S2—O4	113.45 (19)	N3—C8—C9	177.2 (5)
O6—S2—C2	105.1 (2)	C8—C9—H9A	109.5
O5—S2—C2	102.6 (2)	C8—C9—H9B	109.5
O4—S2—C2	102.99 (19)	H9A—C9—H9B	109.5
O9—S3—O7	115.75 (18)	C8—C9—H9C	109.5
O9—S3—O8	115.15 (19)	H9A—C9—H9C	109.5
O7—S3—O8	112.91 (18)	H9B—C9—H9C	109.5

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