CRYSTALLOGRAPHIC COMMUNICATIONS
ISSN 2056-9890

N,*N*,2,4,6-Pentamethylanilinium hexafluorophosphate–1,4,7,10,13,16-hexaoxacyclooctadecane (2/1). Corrigendum

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In the paper by Chang *et al.* [*Acta Cryst.* (2014), E**70**, o72], there is an error in the order of the authors.

The order of the authors in the paper by Chang *et al.* (2014) is incorrect and should be as given above.

References

Chang, Y. Q., Zhang, Y. & Lian, H. L. (2014). *Acta Cryst.* E**70**, o72.

Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N,*N*,2,4,6-Pentamethylanilinium hexafluorophosphate–1,4,7,10,13,16-hexaoxacyclooctadecane (2/1)

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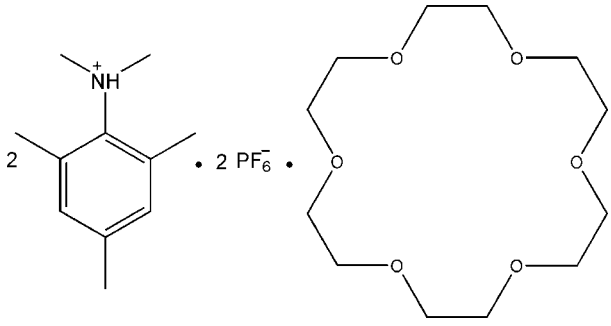
Received 26 November 2013; accepted 13 December 2013

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.083; wR factor = 0.195; data-to-parameter ratio = 15.2.

In the title compound, $2C_{11}H_{18}N^+\cdot 2PF_6^-\cdot C_{12}H_{24}O_6$, the 18-crown-6 molecule has crystallographically imposed inversion symmetry. In the crystal, it interacts with the cation through weak C—H···O hydrogen bonds. The cations and anions are further linked *via* N—H···F and C—H···F hydrogen bonds, leading to a sandwich structure .

Related literature

For background to the development of ferroelectric pure organic or inorganic compounds, see: Haertling (1999); Homes *et al.* (2001). For the structure of a related compound, see: Zhang (2013).



Experimental

Crystal data

$2C_{11}H_{18}N^+\cdot 2PF_6^-\cdot C_{12}H_{24}O_6$
M_r = 882.78
Monoclinic, $P2_1/c$
a = 8.9122 (18) Å
b = 16.775 (3) Å
c = 15.136 (3) Å
β = 103.71 (3)°
V = 2198.4 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 293 K
0.40 × 0.30 × 0.20 mm

Data collection

Rigaku Mercury2 (2x2 bin mode) diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.832, T_{max} = 1.000
18170 measured reflections
3858 independent reflections
2524 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.083
$wR(F^2)$ = 0.195
S = 1.20
3858 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*C*···F4	0.91	2.38	3.077 (5)	134
C16—H16*A*···O3^{i}	0.96	2.52	3.334 (5)	143
C16—H16*B*···O2^{ii}	0.96	2.51	3.443 (5)	164
C16—H16*C*···O1^{i}	0.96	2.57	3.381 (5)	143
C17—H17*B*···F4	0.96	2.54	3.122 (6)	119

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ5098).

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Haertling, G. H. (1999). *J. Am. Ceram. Soc.* **82**, 797–810.
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Zhang, Y. (2013). *Acta Cryst.* E**69**, o31.

supporting information

Acta Cryst. (2014). E**70**, o72 [https://doi.org/10.1107/S1600536813033734]

N,*N*,2,4,6-Pentamethylanilinium hexafluorophosphate–1,4,7,10,13,16-hexaoxacyclooctadecane (2/1)

Yi Qi Chang, Yuan Zhang and Huo Lin Lian

S1. Comment

As a continuation of our studies on the development of novel ferroelectric pure organic or inorganic compounds (Haertling *et al.*, 1999; Homes *et al.*, 2001), we investigated the physical properties of the title compound. Recently the crystal structure of the strictly related compound *N*,*N*,2,4,6-pentamethylanilinium hexafluorophosphate was reported by our group (Zhang, 2013). The dielectric constant of the title compound as a function of the temperature indicates that the permittivity is basically temperature-independent (dielectric constant equaling to 4.1 to 6.1), suggesting that this compound should be not a real ferroelectrics or there may be no distinct phase transition occurring within the measured temperature range. Similarly, below the melting point (180°C) of the compound, the dielectric constant as a function of temperature also goes smoothly, and there is no dielectric anomaly observed (dielectric constant equaling to 4.1 to 6.1). Herein, we report the synthesis and crystal structure of the title compound.

The asymmetric unit of the title compound (Fig. 1) consists of one *N*,*N*,2,4,6-pentamethylanilinium cation, one hexafluorophosphate anion and one half of a 1,4,7,10,13,16-hexaoxacyclooctadecane molecule. Bond distances and bond angles are not unusual. In the crystal structure (Fig. 2), the 18-crown-6 molecule interacts with the cation through weak C—H···O hydrogen bonds (Table 1). Cation and anion are further linked *via* N—H···F and C—H···F hydrogen bonds. Dipole–dipole and van der Waals interactions are effective in stabilizing the molecular packing.

S2. Experimental

A mixture of *N*,*N*,2,4,6-pentamethylbenzenamine (1.36 g, 10 mmol), hexafluorophosphoric acid(1.90 g, 10 mmol) and 1,4,7,10,13,16-hexaoxacyclooctadecane (2.64, 10 mmol) in methanol(30 ml) was stirred until clear. After several days, the title compound was formed and recrystallized from a methanol solution to afford colourless prismatic crystals suitable for X-ray analysis.

S3. Refinement

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.97 Å, N—H = 0.91 Å, and U_{iso}(H) = 1.2 U_{eq}(C, N) or 1.5 U_{eq}(C) for methyl H atoms

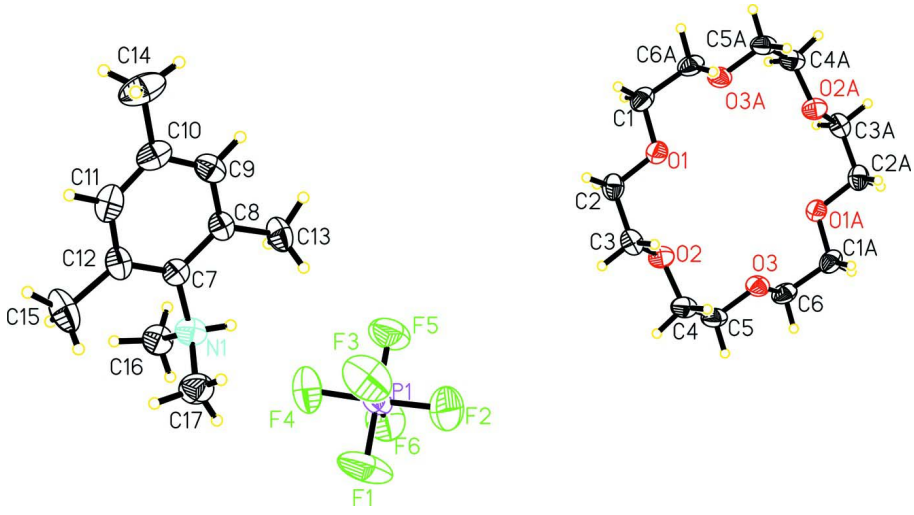

Figure 1

Perspective view of the title compound, showing the displacement ellipsoids drawn at the 30% probability level. Atoms with the suffix A are generated by symmetry code -x, 2-y, 1-z.

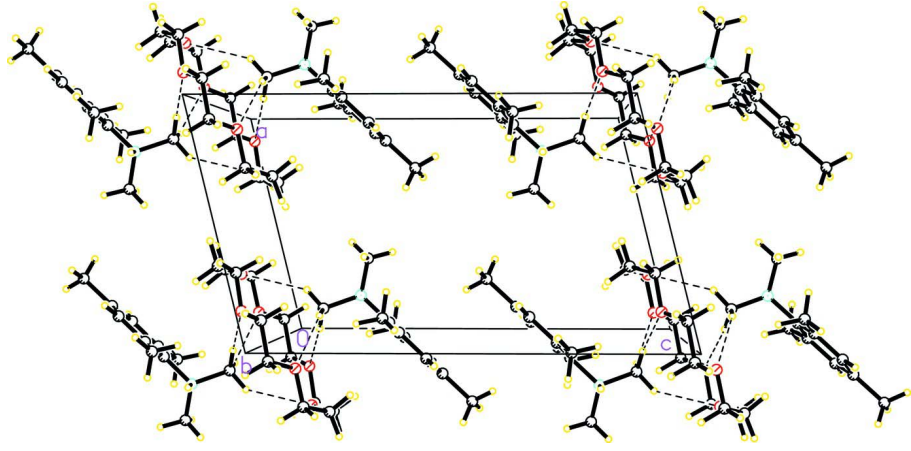

Figure 2

Crystal packing of the title compound viewed along the *b* axis, showing the hydrogen bonding network (dashed lines).

N,*N*,2,4,6-Pentamethylanilinium hexafluorophosphate–1,4,7,10,13,16-hexaoxacyclooctadecane (2/1)

Crystal data

$2C_{11}H_{18}N^{+}\cdot 2PF_6^{-}\cdot C_{12}H_{24}O_6$
$M_r = 882.78$
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Hall symbol: -P 2ybc
$a = 8.9122\ (18)$ Å
$b = 16.775\ (3)$ Å
$c = 15.136\ (3)$ Å
$\beta = 103.71\ (3)°$
$V = 2198.4\ (8)$ Å^3
$Z = 2$

$F(000) = 928$
$D_x = 1.334$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3858 reflections
$\theta = 2.6–25.0°$
$\mu = 0.19$ mm^{-1}
$T = 293$ K
Prism, colourless
0.40 × 0.30 × 0.20 mm

Data collection

Rigaku Mercury2 (2x2 bin mode) diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
CCD_Profile_fitting scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.832, T_{max} = 1.000
18170 measured reflections
3858 independent reflections
2524 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 25.0°, θ_{min} = 3.0°
h = −10→10
k = −19→19
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.083
$wR(F^2)$ = 0.195
S = 1.20
3858 reflections
253 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
$w = 1/[\sigma^2(F_o^2) + (0.0528P)^2 + 2.P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
P1	0.47256 (14)	0.24011 (8)	0.74636 (8)	0.0722 (4)
F6	0.4805 (5)	0.2762 (2)	0.6529 (2)	0.1280 (12)
F5	0.3159 (4)	0.2840 (2)	0.7412 (3)	0.1289 (12)
F4	0.3770 (4)	0.16651 (18)	0.6942 (2)	0.1268 (12)
F3	0.4597 (5)	0.2030 (2)	0.8388 (2)	0.1461 (15)
F2	0.5602 (5)	0.3133 (2)	0.7981 (3)	0.1507 (15)
F1	0.6268 (5)	0.1971 (3)	0.7510 (3)	0.1725 (19)
O3	0.2823 (3)	1.00490 (16)	0.45178 (17)	0.0589 (7)
O2	0.1340 (3)	0.85340 (16)	0.45499 (17)	0.0612 (7)
O1	−0.1059 (3)	0.85014 (16)	0.55077 (17)	0.0609 (7)
C6	0.2987 (5)	1.0742 (3)	0.4023 (3)	0.0651 (11)
H6A	0.2276	1.0722	0.3429	0.078*
H6B	0.4029	1.0771	0.3936	0.078*
C4	0.2945 (5)	0.8633 (3)	0.4624 (3)	0.0673 (11)
H4A	0.3358	0.8166	0.4386	0.081*
H4B	0.3480	0.8696	0.5257	0.081*

C5	0.3191 (5)	0.9355 (3)	0.4095 (3)	0.0647 (11)
H5A	0.4261	0.9378	0.4056	0.078*
H5B	0.2548	0.9321	0.3482	0.078*
C2	−0.0682 (5)	0.7856 (2)	0.5001 (3)	0.0616 (11)
H2A	−0.1249	0.7899	0.4371	0.074*
H2B	−0.0961	0.7357	0.5243	0.074*
C3	0.1010 (5)	0.7875 (2)	0.5061 (3)	0.0630 (11)
H3A	0.1573	0.7927	0.5691	0.076*
H3B	0.1329	0.7384	0.4821	0.076*
C1	−0.2661 (5)	0.8535 (3)	0.5475 (3)	0.0664 (11)
H1A	−0.2971	0.8060	0.5751	0.080*
H1B	−0.3247	0.8560	0.4848	0.080*
C7	0.0742 (4)	0.0080 (2)	0.7882 (2)	0.0501 (9)
N1	0.1899 (4)	0.0220 (2)	0.7330 (2)	0.0679 (10)
H1C	0.1970	0.0761	0.7327	0.081*
C9	−0.1049 (5)	0.0657 (3)	0.8628 (3)	0.0647 (11)
H9A	−0.1532	0.1104	0.8797	0.078*
C12	0.0381 (5)	−0.0678 (2)	0.8125 (3)	0.0616 (11)
C11	−0.0714 (6)	−0.0732 (3)	0.8639 (3)	0.0726 (13)
H11A	−0.0971	−0.1235	0.8816	0.087*
C8	0.0030 (4)	0.0760 (2)	0.8112 (2)	0.0537 (10)
C10	−0.1433 (5)	−0.0085 (3)	0.8899 (3)	0.0675 (12)
C13	0.0349 (6)	0.1585 (2)	0.7817 (3)	0.0774 (13)
H13A	−0.0270	0.1963	0.8049	0.116*
H13B	0.0099	0.1611	0.7164	0.116*
H13C	0.1422	0.1709	0.8048	0.116*
C16	0.1342 (6)	0.0025 (3)	0.6344 (3)	0.0709 (12)
H16A	0.2140	0.0142	0.6035	0.106*
H16B	0.0443	0.0338	0.6087	0.106*
H16C	0.1085	−0.0531	0.6277	0.106*
C17	0.3506 (5)	−0.0026 (3)	0.7753 (4)	0.0873 (15)
H17A	0.3774	0.0142	0.8377	0.131*
H17B	0.4196	0.0217	0.7433	0.131*
H17C	0.3588	−0.0595	0.7724	0.131*
C15	0.1046 (7)	−0.1451 (3)	0.7880 (4)	0.1037 (18)
H15A	0.0592	−0.1889	0.8131	0.156*
H15B	0.2144	−0.1452	0.8123	0.156*
H15C	0.0827	−0.1503	0.7230	0.156*
C14	−0.2611 (6)	−0.0173 (4)	0.9466 (3)	0.109 (2)
H14A	−0.2989	0.0344	0.9579	0.164*
H14B	−0.2137	−0.0423	1.0034	0.164*
H14C	−0.3455	−0.0496	0.9144	0.164*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0737 (8)	0.0786 (9)	0.0619 (7)	0.0147 (7)	0.0115 (6)	−0.0153 (6)
F6	0.166 (3)	0.134 (3)	0.090 (2)	−0.004 (2)	0.044 (2)	0.010 (2)

F5	0.105 (2)	0.129 (3)	0.155 (3)	0.044 (2)	0.035 (2)	−0.003 (2)
F4	0.177 (3)	0.088 (2)	0.106 (2)	−0.022 (2)	0.017 (2)	−0.0247 (18)
F3	0.202 (4)	0.166 (4)	0.074 (2)	0.046 (3)	0.041 (2)	0.022 (2)
F2	0.155 (3)	0.151 (3)	0.140 (3)	−0.030 (3)	0.023 (2)	−0.065 (3)
F1	0.126 (3)	0.232 (5)	0.158 (3)	0.101 (3)	0.031 (3)	−0.019 (3)
O3	0.0604 (17)	0.0714 (18)	0.0509 (15)	−0.0010 (14)	0.0253 (13)	−0.0022 (14)
O2	0.0529 (16)	0.0711 (18)	0.0599 (16)	0.0049 (14)	0.0138 (12)	0.0084 (14)
O1	0.0557 (17)	0.0676 (18)	0.0605 (16)	−0.0109 (14)	0.0164 (13)	−0.0133 (14)
C6	0.053 (2)	0.090 (3)	0.057 (2)	−0.012 (2)	0.0249 (19)	0.003 (2)
C4	0.054 (3)	0.079 (3)	0.070 (3)	0.011 (2)	0.019 (2)	−0.001 (2)
C5	0.050 (2)	0.092 (3)	0.058 (2)	0.004 (2)	0.0234 (19)	−0.004 (2)
C2	0.076 (3)	0.054 (2)	0.054 (2)	−0.009 (2)	0.013 (2)	0.0014 (19)
C3	0.075 (3)	0.055 (2)	0.056 (2)	0.007 (2)	0.011 (2)	−0.003 (2)
C1	0.061 (3)	0.074 (3)	0.066 (3)	−0.019 (2)	0.018 (2)	0.000 (2)
C7	0.054 (2)	0.059 (2)	0.0350 (18)	−0.0008 (19)	0.0063 (16)	0.0018 (17)
N1	0.065 (2)	0.083 (3)	0.055 (2)	0.0083 (18)	0.0140 (17)	0.0001 (18)
C9	0.067 (3)	0.078 (3)	0.046 (2)	0.014 (2)	0.006 (2)	−0.008 (2)
C12	0.081 (3)	0.053 (2)	0.046 (2)	0.001 (2)	0.005 (2)	−0.0007 (19)
C11	0.089 (3)	0.069 (3)	0.052 (2)	−0.019 (3)	0.002 (2)	0.008 (2)
C8	0.061 (2)	0.055 (2)	0.040 (2)	0.0030 (19)	0.0023 (18)	−0.0010 (17)
C10	0.052 (2)	0.105 (4)	0.040 (2)	−0.010 (3)	0.0013 (18)	0.006 (2)
C13	0.110 (4)	0.049 (3)	0.075 (3)	0.005 (2)	0.026 (3)	0.001 (2)
C16	0.087 (3)	0.085 (3)	0.045 (2)	−0.004 (2)	0.023 (2)	−0.006 (2)
C17	0.067 (3)	0.090 (4)	0.100 (4)	0.011 (3)	0.010 (3)	0.010 (3)
C15	0.164 (6)	0.057 (3)	0.091 (4)	0.021 (3)	0.032 (4)	0.001 (3)
C14	0.073 (3)	0.187 (6)	0.070 (3)	−0.025 (4)	0.024 (3)	0.011 (3)

Geometric parameters (Å, º)

P1—F1	1.539 (3)	C7—C8	1.390 (5)
P1—F6	1.556 (3)	C7—N1	1.492 (5)
P1—F3	1.560 (3)	N1—C17	1.482 (5)
P1—F2	1.562 (4)	N1—C16	1.493 (5)
P1—F5	1.564 (3)	N1—H1C	0.9100
P1—F4	1.598 (3)	C9—C10	1.380 (6)
O3—C5	1.404 (5)	C9—C8	1.385 (6)
O3—C6	1.409 (5)	C9—H9A	0.9300
O2—C4	1.418 (4)	C12—C11	1.389 (6)
O2—C3	1.419 (4)	C12—C15	1.507 (6)
O1—C2	1.412 (4)	C11—C10	1.364 (6)
O1—C1	1.418 (4)	C11—H11A	0.9300
C6—C1^{i}	1.495 (6)	C8—C13	1.503 (5)
C6—H6A	0.9700	C10—C14	1.512 (6)
C6—H6B	0.9700	C13—H13A	0.9600
C4—C5	1.497 (6)	C13—H13B	0.9600
C4—H4A	0.9700	C13—H13C	0.9600
C4—H4B	0.9700	C16—H16A	0.9600
C5—H5A	0.9700	C16—H16B	0.9600

C5—H5B	0.9700	C16—H16C	0.9600
C2—C3	1.490 (6)	C17—H17A	0.9600
C2—H2A	0.9700	C17—H17B	0.9600
C2—H2B	0.9700	C17—H17C	0.9600
C3—H3A	0.9700	C15—H15A	0.9600
C3—H3B	0.9700	C15—H15B	0.9600
C1—C6^{i}	1.495 (6)	C15—H15C	0.9600
C1—H1A	0.9700	C14—H14A	0.9600
C1—H1B	0.9700	C14—H14B	0.9600
C7—C12	1.382 (5)	C14—H14C	0.9600

F1—P1—F6	89.5 (2)	C12—C7—C8	122.7 (4)
F1—P1—F3	91.6 (2)	C12—C7—N1	122.0 (4)
F6—P1—F3	178.3 (2)	C8—C7—N1	115.4 (3)
F1—P1—F2	90.6 (3)	C17—N1—C7	116.1 (3)
F6—P1—F2	91.4 (2)	C17—N1—C16	115.4 (4)
F3—P1—F2	89.9 (2)	C7—N1—C16	114.5 (3)
F1—P1—F5	179.7 (2)	C17—N1—H1C	102.6
F6—P1—F5	90.2 (2)	C7—N1—H1C	102.6
F3—P1—F5	88.7 (2)	C16—N1—H1C	102.6
F2—P1—F5	89.4 (2)	C10—C9—C8	122.3 (4)
F1—P1—F4	91.5 (2)	C10—C9—H9A	118.9
F6—P1—F4	89.15 (19)	C8—C9—H9A	118.9
F3—P1—F4	89.5 (2)	C7—C12—C11	116.6 (4)
F2—P1—F4	177.8 (2)	C7—C12—C15	126.6 (4)
F5—P1—F4	88.5 (2)	C11—C12—C15	116.9 (4)
C5—O3—C6	112.2 (3)	C10—C11—C12	123.4 (4)
C4—O2—C3	112.6 (3)	C10—C11—H11A	118.3
C2—O1—C1	112.3 (3)	C12—C11—H11A	118.3
O3—C6—C1^{i}	110.0 (3)	C9—C8—C7	117.3 (4)
O3—C6—H6A	109.7	C9—C8—C13	119.2 (4)
C1^{i}—C6—H6A	109.7	C7—C8—C13	123.5 (4)
O3—C6—H6B	109.7	C11—C10—C9	117.7 (4)
C1^{i}—C6—H6B	109.7	C11—C10—C14	121.5 (5)
H6A—C6—H6B	108.2	C9—C10—C14	120.7 (5)
O2—C4—C5	109.0 (3)	C8—C13—H13A	109.5
O2—C4—H4A	109.9	C8—C13—H13B	109.5
C5—C4—H4A	109.9	H13A—C13—H13B	109.5
O2—C4—H4B	109.9	C8—C13—H13C	109.5
C5—C4—H4B	109.9	H13A—C13—H13C	109.5
H4A—C4—H4B	108.3	H13B—C13—H13C	109.5
O3—C5—C4	110.4 (3)	N1—C16—H16A	109.5
O3—C5—H5A	109.6	N1—C16—H16B	109.5
C4—C5—H5A	109.6	H16A—C16—H16B	109.5
O3—C5—H5B	109.6	N1—C16—H16C	109.5
C4—C5—H5B	109.6	H16A—C16—H16C	109.5
H5A—C5—H5B	108.1	H16B—C16—H16C	109.5
O1—C2—C3	108.6 (3)	N1—C17—H17A	109.5

O1—C2—H2A	110.0	N1—C17—H17B	109.5
C3—C2—H2A	110.0	H17A—C17—H17B	109.5
O1—C2—H2B	110.0	N1—C17—H17C	109.5
C3—C2—H2B	110.0	H17A—C17—H17C	109.5
H2A—C2—H2B	108.4	H17B—C17—H17C	109.5
O2—C3—C2	108.7 (3)	C12—C15—H15A	109.5
O2—C3—H3A	109.9	C12—C15—H15B	109.5
C2—C3—H3A	109.9	H15A—C15—H15B	109.5
O2—C3—H3B	109.9	C12—C15—H15C	109.5
C2—C3—H3B	109.9	H15A—C15—H15C	109.5
H3A—C3—H3B	108.3	H15B—C15—H15C	109.5
O1—C1—C6^{i}	109.3 (3)	C10—C14—H14A	109.5
O1—C1—H1A	109.8	C10—C14—H14B	109.5
C6^{i}—C1—H1A	109.8	H14A—C14—H14B	109.5
O1—C1—H1B	109.8	C10—C14—H14C	109.5
C6^{i}—C1—H1B	109.8	H14A—C14—H14C	109.5
H1A—C1—H1B	108.3	H14B—C14—H14C	109.5

Symmetry code: (i) $-x$, $-y+2$, $-z+1$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*C*···F4	0.91	2.38	3.077 (5)	134
C16—H16*A*···O3^{ii}	0.96	2.52	3.334 (5)	143
C16—H16*B*···O2^{iii}	0.96	2.51	3.443 (5)	164
C16—H16*C*···O1^{ii}	0.96	2.57	3.381 (5)	143
C17—H17*B*···F4	0.96	2.54	3.122 (6)	119

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