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2-[3-(Trifluoromethyl)phenoxy]ethyl 1-oxo-2,6,7-trioxa-1λ^5-phosphabicyclo-[2.2.2]octane-4-carboxylate

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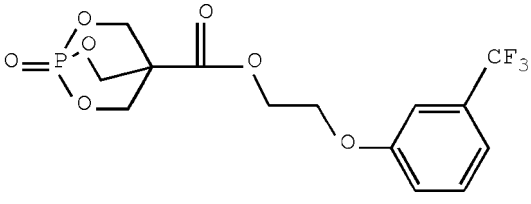
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.052; wR factor = 0.137; data-to-parameter ratio = 14.0.

In the crystal structure of the title compound, $C_{14}H_{14}F_3O_7P$, the central chain, which connects the phosphate bicyclic system and the benzene ring, is made up of an approximately planar C—C(O)—O—C(H_2) fragment and a C(H_2)—O—C(Ph) link; the mean planes make a dihedral angle of 75.9 (2)°. The F atoms are disordered over two positions; the site occupancy factors are *ca* 0.6 and 0.4.

Related literature

For industrial and biological applications of heterocyclic compounds involving bicyclic phosphate, see: Ratz (1966); Li *et al.*, (2002). Many related derivatives have been prepared by Verkade & Reynolds (1960) and Sheng & He (2006). For the synthesis of the starting material, see: Chen & Jin (2000). For related literature, see: Nimrod *et al.* (1968).



Experimental

Crystal data

$C_{14}H_{14}F_3O_7P$
M_r = 382.22
Monoclinic, $P2_1/n$
a = 5.7824 (3) Å
b = 27.5060 (16) Å
c = 10.2878 (6) Å
β = 96.738 (1)°
V = 1624.98 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 295 (2) K
0.30 × 0.20 × 0.06 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: none
18233 measured reflections
3547 independent reflections
2332 reflections with $I > 2\sigma(I)$
R_{int} = 0.091

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.137
S = 0.98
3547 reflections
254 parameters
30 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: YA2064).

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supporting information

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2-[3-(Trifluoromethyl)phenoxy]ethyl 1-oxo-2,6,7-trioxa-1λ^5-phosphabicyclo-[2.2.2]octane-4-carboxylate

Wei Wang, Wei-Dong Wang, Shao-Bin Wang, Yun-Li Shen and Hong-Wu He

S1. Comment

Heterocyclic derivatives containing bicyclic phosphate system are important compounds with versatile industrial and biological applications (Ratz, 1966; Li *et al.*, 2002). In continuation of our work on new biologically active heterocyclic derivatives, we report here the crystal structure of the title compound,(I) (Fig.1).Bond lengths and angles of the phosphorus-containing bicyclic cage of (I) are close to those observed previously in similar compounds (Nimrod *et al.*, 1968; Sheng & He, 2006). The central chain of the molecule, which connects phosphate bicyclic system and benzene ring, is made up of approximately planar C4—C5—O6—C6 fragment and C7—O7—C8 link; their mean planes form dihedral angle of 75.9 (2)°.

S2. Experimental

The solution of anhydrous 1-oxo-2,6,7-trioxa-1λ^5-phospha-bicyclo[2.2.2] octane-4-carbonyl chloride (Chen & Jin, 2000) (1.14 g, 0.0055 mol) in 5 ml of acetonitrile was added dropwise under stirring to the solution of 2-(3-trifluoromethyl-phenoxy)ethanol (1.03 g, 0.005 mol) and triethylamine (0.61 g, 0.006 mol) in 25 ml of acetonitrile. The stirring was continued for about 3 h. Then, the solvent was removed under reduced pressure and the residue was washed with water (20 ml). The raw product was recrystallized from acetonitrile, yielding the title compound as a white solid with 81% yield. Colourless crystals of (I) suitable for X-ray structure analysis were grown from the mixture of dichloromethane and n-hexane (*v*/*v*, 1:8).

S3. Refinement

It was apparent at an early stage, that the CF_3 group showed rotational disorder, and two alternative positions were revealed for each of the F atoms. Refinement of the s.o.f.'s for the F atoms indicated noticeable differences in occupancies of each of the two orientations of the CF_3 group [0.59 (2) *versus*. 0.41 (2)]. The C—F bond distances were restrained during the refinement using the SADI command (*SHELXL97*; Sheldrick, 2008). H atoms were included in the refinement in riding model approximation with C—H = 0.93 Å for aromatic and 0.97 Å for all other H atoms; U_{iso}(H) = 1.2U_{eq} of the carrier C atom.

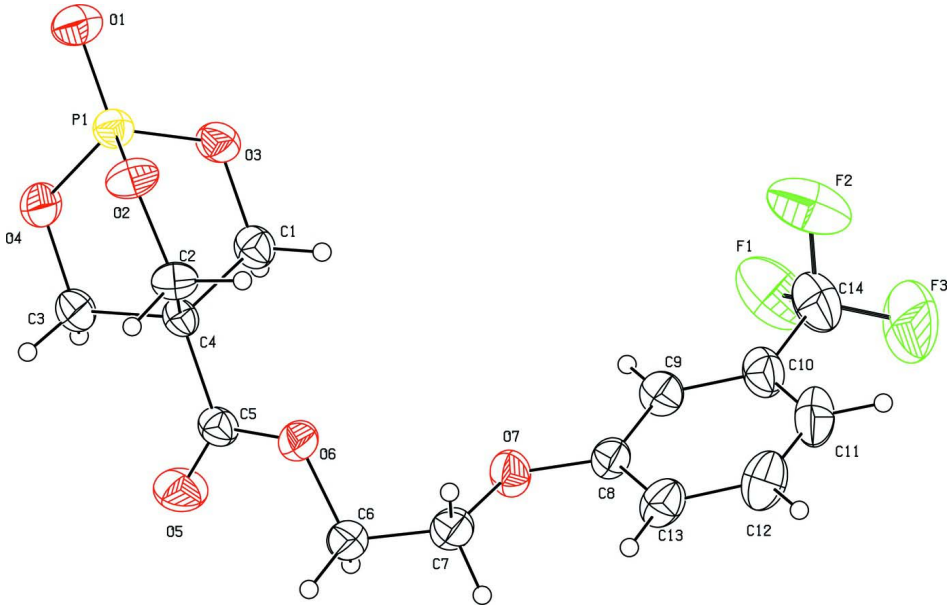

Figure 1

The structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme; the minor component of the CF_3 group disorder is omitted. H atoms are shown as small spheres of arbitrary radius.

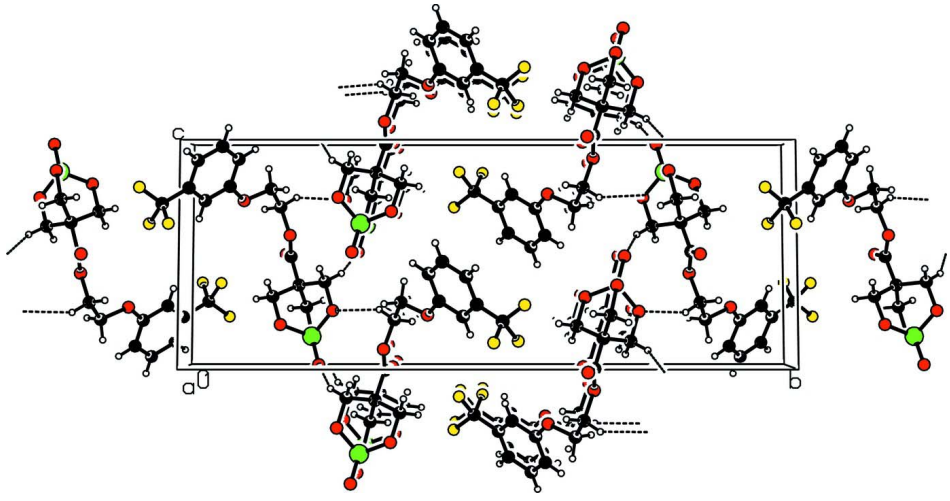

Figure 2

Packing diagram for (I).

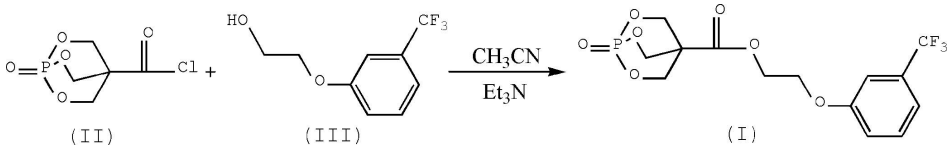

Figure 3

The formation of the title compound, (I).

2-[3-(Trifluoromethyl)phenoxy]ethyl 1-oxo-2,6,7-trioxa-1λ^5-phosphabicyclo[2.2.2]octane-4-carboxylate

Crystal data

$C_{14}H_{14}F_3O_7P$
$M_r = 382.22$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 5.7824$ (3) Å
$b = 27.5060$ (16) Å
$c = 10.2878$ (6) Å
$\beta = 96.738$ (1)°
$V = 1624.98$ (16) Å^3
$Z = 4$
$F(000) = 784$
$D_x = 1.562$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4355 reflections
$\theta = 2.4$–19.3°
$\mu = 0.24$ mm^{-1}
$T = 295$ K
Plate, colourless
0.30 × 0.20 × 0.06 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
18233 measured reflections
3547 independent reflections
2332 reflections with $I > 2\sigma(I)$
$R_{int} = 0.091$
$\theta_{max} = 27.0°$, $\theta_{min} = 1.5°$
$h = -7 \rightarrow 7$
$k = -35 \rightarrow 35$
$l = -13 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.137$
$S = 0.98$
3547 reflections
254 parameters
30 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
$w = 1/[\sigma^2(F_o^2) + (0.0771P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ 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}	Occ. (<1)
C1	0.3969 (4)	0.14250 (8)	0.3106 (2)	0.0518 (6)	
H1A	0.5300	0.1356	0.3744	0.062*	
H1B	0.3031	0.1133	0.2985	0.062*	
C2	0.4076 (4)	0.22884 (9)	0.3762 (2)	0.0502 (6)	
H2A	0.3254	0.2552	0.4134	0.060*	

H2B	0.5473	0.2218	0.4350	0.060*	
C3	0.0422 (4)	0.19358 (11)	0.2599 (2)	0.0579 (7)	
H3A	−0.0585	0.1653	0.2523	0.069*	
H3B	−0.0459	0.2207	0.2886	0.069*	
C4	0.2525 (3)	0.18376 (8)	0.3603 (2)	0.0405 (5)	
C5	0.1682 (4)	0.16870 (8)	0.4885 (2)	0.0479 (6)	
C6	0.2903 (5)	0.15256 (10)	0.7125 (2)	0.0630 (7)	
H6A	0.1908	0.1241	0.7030	0.076*	
H6B	0.2108	0.1778	0.7559	0.076*	
C7	0.5158 (5)	0.14044 (9)	0.7905 (2)	0.0602 (7)	
H7A	0.6266	0.1666	0.7853	0.072*	
H7B	0.4938	0.1356	0.8817	0.072*	
C8	0.8002 (4)	0.07776 (9)	0.7983 (2)	0.0497 (6)	
C9	0.8907 (5)	0.03932 (9)	0.7345 (2)	0.0567 (7)	
H9	0.8138	0.0281	0.6557	0.068*	
C10	1.0948 (5)	0.01744 (10)	0.7873 (3)	0.0665 (8)	
C11	1.2075 (6)	0.03407 (13)	0.9055 (3)	0.0844 (9)	
H11	1.3452	0.0195	0.9418	0.101*	
C12	1.1166 (6)	0.07149 (13)	0.9678 (3)	0.0832 (9)	
H12	1.1933	0.0824	1.0469	0.100*	
C13	0.9127 (5)	0.09386 (10)	0.9166 (2)	0.0657 (7)	
H13	0.8516	0.1194	0.9610	0.079*	
C14	1.1925 (6)	−0.02293 (13)	0.7178 (4)	0.0947 (11)	
F1	1.0315 (9)	−0.0476 (3)	0.6324 (13)	0.136 (3)	0.591 (16)
F2	1.3280 (17)	−0.0092 (4)	0.6315 (8)	0.136 (4)	0.591 (16)
F3	1.295 (3)	−0.0570 (4)	0.7881 (7)	0.202 (7)	0.591 (16)
F1′	1.0849 (18)	−0.0629 (3)	0.7297 (14)	0.115 (5)	0.409 (16)
F2′	1.4149 (10)	−0.0324 (4)	0.7722 (12)	0.113 (4)	0.409 (16)
F3′	1.218 (3)	−0.0137 (5)	0.5991 (8)	0.135 (6)	0.409 (16)
O1	0.4623 (3)	0.22048 (7)	0.00883 (16)	0.0676 (5)	
O2	0.4701 (3)	0.24307 (6)	0.24834 (15)	0.0583 (5)	
O3	0.4763 (3)	0.15669 (6)	0.18650 (16)	0.0570 (5)	
O4	0.1178 (3)	0.20463 (7)	0.13298 (16)	0.0661 (5)	
O5	−0.0280 (3)	0.15716 (8)	0.49924 (19)	0.0766 (6)	
O6	0.3411 (3)	0.16937 (6)	0.58442 (16)	0.0580 (5)	
O7	0.5992 (3)	0.09700 (6)	0.73729 (15)	0.0592 (5)	
P1	0.38795 (10)	0.20768 (2)	0.13331 (6)	0.0473 (2)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0521 (14)	0.0443 (13)	0.0594 (15)	0.0020 (10)	0.0080 (11)	−0.0002 (11)
C2	0.0553 (15)	0.0499 (13)	0.0472 (14)	−0.0098 (11)	0.0134 (11)	−0.0049 (11)
C3	0.0347 (13)	0.0757 (17)	0.0628 (16)	0.0004 (11)	0.0039 (11)	0.0092 (13)
C4	0.0319 (11)	0.0415 (12)	0.0478 (13)	−0.0008 (9)	0.0041 (9)	−0.0008 (9)
C5	0.0428 (13)	0.0444 (13)	0.0577 (15)	−0.0006 (10)	0.0116 (12)	0.0022 (11)
C6	0.0696 (18)	0.0645 (16)	0.0583 (16)	0.0197 (13)	0.0215 (13)	0.0145 (13)
C7	0.0821 (19)	0.0515 (14)	0.0485 (14)	0.0154 (13)	0.0141 (13)	−0.0017 (11)

C8	0.0545 (14)	0.0476 (13)	0.0467 (13)	0.0021 (11)	0.0042 (11)	0.0045 (11)
C9	0.0610 (16)	0.0507 (14)	0.0583 (16)	−0.0001 (12)	0.0065 (13)	−0.0031 (12)
C10	0.0608 (17)	0.0529 (15)	0.086 (2)	0.0086 (13)	0.0088 (16)	0.0105 (14)
C11	0.070 (2)	0.086 (2)	0.092 (2)	0.0152 (17)	−0.0144 (18)	0.018 (2)
C12	0.085 (2)	0.089 (2)	0.0686 (19)	−0.0008 (18)	−0.0211 (17)	0.0045 (17)
C13	0.083 (2)	0.0616 (16)	0.0499 (15)	0.0021 (14)	−0.0007 (14)	−0.0002 (12)
C14	0.085 (3)	0.079 (3)	0.120 (3)	0.024 (2)	0.012 (3)	−0.001 (2)
F1	0.126 (4)	0.084 (4)	0.202 (9)	0.010 (3)	0.037 (5)	−0.061 (5)
F2	0.108 (5)	0.159 (6)	0.151 (8)	−0.032 (5)	0.055 (5)	−0.069 (6)
F3	0.268 (16)	0.152 (9)	0.190 (7)	0.147 (11)	0.042 (9)	0.040 (6)
F1′	0.123 (6)	0.066 (5)	0.163 (11)	−0.031 (4)	0.044 (7)	−0.051 (6)
F2′	0.062 (4)	0.092 (5)	0.178 (10)	0.033 (3)	−0.018 (4)	−0.038 (5)
F3′	0.165 (12)	0.141 (11)	0.099 (5)	0.060 (10)	0.018 (7)	−0.018 (6)
O1	0.0735 (13)	0.0802 (13)	0.0510 (11)	−0.0054 (10)	0.0153 (9)	0.0008 (9)
O2	0.0748 (12)	0.0507 (9)	0.0518 (10)	−0.0220 (8)	0.0168 (8)	−0.0027 (8)
O3	0.0627 (11)	0.0535 (10)	0.0572 (11)	0.0088 (8)	0.0178 (8)	−0.0041 (8)
O4	0.0411 (10)	0.1008 (14)	0.0544 (11)	0.0014 (9)	−0.0035 (8)	0.0136 (9)
O5	0.0527 (11)	0.0998 (15)	0.0798 (14)	−0.0187 (10)	0.0189 (10)	0.0094 (11)
O6	0.0479 (10)	0.0716 (11)	0.0551 (10)	0.0023 (8)	0.0082 (8)	0.0188 (9)
O7	0.0657 (11)	0.0579 (10)	0.0524 (10)	0.0154 (8)	−0.0006 (8)	−0.0095 (8)
P1	0.0443 (4)	0.0516 (4)	0.0460 (4)	−0.0027 (3)	0.0054 (3)	−0.0017 (3)

Geometric parameters (Å, º)

C1—O3	1.460 (3)	C8—O7	1.361 (3)
C1—C4	1.532 (3)	C8—C9	1.380 (3)
C1—H1A	0.9700	C8—C13	1.384 (3)
C1—H1B	0.9700	C9—C10	1.378 (4)
C2—O2	1.458 (2)	C9—H9	0.9300
C2—C4	1.528 (3)	C10—C11	1.388 (4)
C2—H2A	0.9700	C10—C14	1.469 (5)
C2—H2B	0.9700	C11—C12	1.351 (5)
C3—O4	1.457 (3)	C11—H11	0.9300
C3—C4	1.525 (3)	C12—C13	1.378 (4)
C3—H3A	0.9700	C12—H12	0.9300
C3—H3B	0.9700	C13—H13	0.9300
C4—C5	1.516 (3)	C14—F3′	1.274 (7)
C5—O5	1.196 (3)	C14—F1′	1.277 (6)
C5—O6	1.320 (3)	C14—F3	1.284 (5)
C6—O6	1.459 (3)	C14—F2	1.307 (6)
C6—C7	1.487 (3)	C14—F2′	1.366 (6)
C6—H6A	0.9700	C14—F1	1.382 (6)
C6—H6B	0.9700	O1—P1	1.4416 (18)
C7—O7	1.422 (3)	O2—P1	1.5625 (16)
C7—H7A	0.9700	O3—P1	1.5689 (17)
C7—H7B	0.9700	O4—P1	1.5642 (18)
O3—C1—C4	109.50 (18)	C9—C10—C11	119.6 (3)

O3—C1—H1A	109.8	C9—C10—C14	119.9 (3)
C4—C1—H1A	109.8	C11—C10—C14	120.5 (3)
O3—C1—H1B	109.8	C12—C11—C10	119.9 (3)
C4—C1—H1B	109.8	C12—C11—H11	120.1
H1A—C1—H1B	108.2	C10—C11—H11	120.1
O2—C2—C4	109.03 (16)	C11—C12—C13	121.5 (3)
O2—C2—H2A	109.9	C11—C12—H12	119.3
C4—C2—H2A	109.9	C13—C12—H12	119.3
O2—C2—H2B	109.9	C12—C13—C8	119.1 (3)
C4—C2—H2B	109.9	C12—C13—H13	120.5
H2A—C2—H2B	108.3	C8—C13—H13	120.5
O4—C3—C4	110.18 (18)	F3′—C14—F1′	112.2 (6)
O4—C3—H3A	109.6	F3′—C14—F3	125.9 (8)
C4—C3—H3A	109.6	F1′—C14—F3	61.0 (5)
O4—C3—H3B	109.6	F3′—C14—F2	31.0 (6)
C4—C3—H3B	109.6	F1′—C14—F2	130.6 (7)
H3A—C3—H3B	108.1	F3—C14—F2	108.7 (5)
C5—C4—C3	108.98 (18)	F3′—C14—F2′	102.7 (6)
C5—C4—C2	111.94 (18)	F1′—C14—F2′	104.0 (5)
C3—C4—C2	109.88 (19)	F3—C14—F2′	44.0 (5)
C5—C4—C1	109.37 (18)	F2—C14—F2′	73.9 (5)
C3—C4—C1	109.12 (19)	F3′—C14—F1	68.6 (6)
C2—C4—C1	107.51 (18)	F1′—C14—F1	48.5 (4)
O5—C5—O6	125.3 (2)	F3—C14—F1	103.3 (5)
O5—C5—C4	124.0 (2)	F2—C14—F1	97.1 (5)
O6—C5—C4	110.72 (18)	F2′—C14—F1	134.3 (5)
O6—C6—C7	107.6 (2)	F3′—C14—C10	114.3 (6)
O6—C6—H6A	110.2	F1′—C14—C10	112.7 (4)
C7—C6—H6A	110.2	F3—C14—C10	117.1 (5)
O6—C6—H6B	110.2	F2—C14—C10	114.0 (5)
C7—C6—H6B	110.2	F2′—C14—C10	110.0 (5)
H6A—C6—H6B	108.5	F1—C14—C10	114.4 (3)
O7—C7—C6	107.2 (2)	C2—O2—P1	115.51 (13)
O7—C7—H7A	110.3	C1—O3—P1	114.91 (13)
C6—C7—H7A	110.3	C3—O4—P1	114.44 (13)
O7—C7—H7B	110.3	C5—O6—C6	117.12 (18)
C6—C7—H7B	110.3	C8—O7—C7	117.31 (18)
H7A—C7—H7B	108.5	O1—P1—O2	115.14 (10)
O7—C8—C9	115.4 (2)	O1—P1—O4	114.40 (10)
O7—C8—C13	124.7 (2)	O2—P1—O4	104.46 (10)
C9—C8—C13	119.9 (2)	O1—P1—O3	114.17 (10)
C10—C9—C8	120.1 (2)	O2—P1—O3	103.61 (9)
C10—C9—H9	119.9	O4—P1—O3	103.71 (10)
C8—C9—H9	119.9		

O4—C3—C4—C5	−175.80 (19)	C9—C10—C14—F1′	−76.8 (9)
O4—C3—C4—C2	61.2 (3)	C11—C10—C14—F1′	103.7 (9)
O4—C3—C4—C1	−56.4 (3)	C9—C10—C14—F3	−144.7 (10)

O2—C2—C4—C5	−176.43 (17)	C11—C10—C14—F3	35.8 (11)
O2—C2—C4—C3	−55.2 (2)	C9—C10—C14—F2	86.9 (7)
O2—C2—C4—C1	63.4 (2)	C11—C10—C14—F2	−92.6 (7)
O3—C1—C4—C5	179.40 (17)	C9—C10—C14—F2′	167.6 (7)
O3—C1—C4—C3	60.3 (2)	C11—C10—C14—F2′	−11.9 (8)
O3—C1—C4—C2	−58.9 (2)	C9—C10—C14—F1	−23.6 (8)
C3—C4—C5—O5	13.7 (3)	C11—C10—C14—F1	156.9 (7)
C2—C4—C5—O5	135.5 (2)	C4—C2—O2—P1	−5.5 (2)
C1—C4—C5—O5	−105.5 (3)	C4—C1—O3—P1	−2.6 (2)
C3—C4—C5—O6	−167.4 (2)	C4—C3—O4—P1	−4.5 (3)
C2—C4—C5—O6	−45.6 (3)	O5—C5—O6—C6	2.9 (4)
C1—C4—C5—O6	73.4 (2)	C4—C5—O6—C6	−175.99 (19)
O6—C6—C7—O7	−71.8 (3)	C7—C6—O6—C5	161.0 (2)
O7—C8—C9—C10	179.5 (2)	C9—C8—O7—C7	−172.2 (2)
C13—C8—C9—C10	−1.0 (4)	C13—C8—O7—C7	8.4 (4)
C8—C9—C10—C11	0.5 (4)	C6—C7—O7—C8	−176.9 (2)
C8—C9—C10—C14	−179.0 (3)	C2—O2—P1—O1	−176.46 (15)
C9—C10—C11—C12	0.0 (5)	C2—O2—P1—O4	57.23 (18)
C14—C10—C11—C12	179.5 (3)	C2—O2—P1—O3	−51.09 (18)
C10—C11—C12—C13	0.0 (5)	C3—O4—P1—O1	−177.70 (18)
C11—C12—C13—C8	−0.5 (5)	C3—O4—P1—O2	−50.93 (19)
O7—C8—C13—C12	−179.5 (3)	C3—O4—P1—O3	57.31 (19)
C9—C8—C13—C12	1.0 (4)	C1—O3—P1—O1	−178.26 (15)
C9—C10—C14—F3′	52.8 (10)	C1—O3—P1—O2	55.75 (17)
C11—C10—C14—F3′	−126.7 (10)	C1—O3—P1—O4	−53.13 (17)