

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

## 4,4'-(1,1,1,3,3,3-Hexafluoropropane-2,2-diyl)dibenzoic acid

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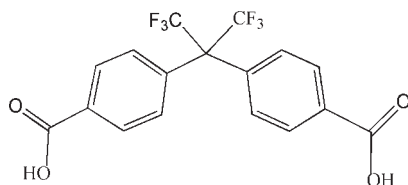
Received 19 March 2010; accepted 14 May 2010

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.040;  $wR$  factor = 0.071; data-to-parameter ratio = 11.8.

In the title compound,  $\text{C}_{17}\text{H}_{10}\text{F}_6\text{O}_4$ , the two benzene rings are twisted with respect to each other, making a dihedral angle of  $67.43$  ( $12$ )°. In the crystal, adjacent molecules are linked by  $\text{O}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\text{F}$  hydrogen bonding, forming a wave-like layered supramolecular structure.

## Related literature

For the use of bibenzoic acids as bridging ligands for the synthesis of novel solid-state architectures, see: Zou *et al.* (2007). For the structures of related dibenzoic acid compounds, see: Potts *et al.* (2007); Lian *et al.* (2007).



## Experimental

## Crystal data

$\text{C}_{17}\text{H}_{10}\text{F}_6\text{O}_4$   
 $M_r = 392.25$   
 Monoclinic,  $P2_1/c$   
 $a = 7.7523$  (16) Å  
 $b = 13.381$  (3) Å  
 $c = 16.134$  (3) Å  
 $\beta = 102.294$  (4)°

$V = 1635.2$  (6) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.16$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.35 \times 0.20 \times 0.18$  mm

## Data collection

Bruker SMART CCD  
 diffractometer  
 Absorption correction: multi-scan  
 (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.963$ ,  $T_{\max} = 0.972$

8113 measured reflections  
 2904 independent reflections  
 1339 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.053$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$   
 $wR(F^2) = 0.071$   
 $S = 1.00$   
 2904 reflections

246 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.17$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.19$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O}2-\text{H}2\text{A}\cdots\text{O}4^{\text{i}}$	0.82	1.85	2.661 (2)	169
$\text{O}3-\text{H}3\text{A}\cdots\text{O}1^{\text{ii}}$	0.82	1.80	2.603 (2)	165
$\text{C}15-\text{H}15\cdots\text{F}1^{\text{iii}}$	0.93	2.48	3.382 (3)	163

Symmetry codes: (i)  $x - 1, -y + \frac{1}{2}, z + \frac{1}{2}$ ; (ii)  $x + 1, -y + \frac{1}{2}, z - \frac{1}{2}$ ; (iii)  $x + 1, y, z$ .

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999).

This project was supported by the Natural Scientific Foundation of Shaanxi Province, China (grant No. SJ08B11), the Key Laboratory Foundation of Shaanxi Provincial Education Office, China (Nos. 08JZ82, 07 J K435, 08 J K490, 09 J K816, 09 J K826 and 09 J K815) and the Special Scientific Research Foundation of Yan'an University (No. D2009-139).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2737).

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## supporting information

*Acta Cryst.* (2010). E66, o1390 [https://doi.org/10.1107/S1600536810017745]

**4,4'-(1,1,1,3,3,3-Hexafluoropropane-2,2-diyl)dibenzoic acid****Long Tang, Ya-Pan Wu, Feng Fu, Zhu-Lian Zhang and Dan Zheng****S1. Comment**

The rational design and synthesis of novel solid-state architectures are of current interest in the field of supramolecular chemistry and crystal engineering, due to intriguing structural motifs that can be created by various intermolecular interactions. Supramolecular chemistry uses molecular recognition processes that rely heavily on the understanding of the recognition properties of the functional groups involved in these interactions (Zou *et al.*, 2007). Herein, we reported the organic crystal structure of  $C_{17}H_{10}F_6O_4$ , which is similar to that of the reported compounds (Potts *et al.* 2007; Lian *et al.*, 2007).

The molecular structure is shown in Fig. 1. The dihedral angle between the two benzene rings of the flexible  $H_2hfipbb$  molecule is  $67.43(12)^\circ$ . Strong intermolecular  $O—H\cdots O$  and  $C—H\cdots F$  hydrogen bonds (Table 1) link the molecules into the 2D wave-like layer structure (Fig. 2).

**S2. Experimental**

The title compound was prepared by hydrothermal method. A mixture of  $Zn(Ac)_2 \cdot 4H_2O$  (0.20 mmol), 2,2'-bipyridine (bipy 0.20 mmol), 4,4'-(hexafluoroisopropylidene)bis(benzoic acid) ( $H_2hfipbb$  0.20 mmol) and water (10 ml) was stirred for 20 min. The mixture was then transferred to a 23 ml Teflon-lined autoclave and kept at 433 K for 72 h under autogenous pressure. Then the mixture was cooled to room temperature slowly, the targeted Zn complex was not obtained. Colorless single crystals of the title compound suitable for X-ray analysis were obtained from the reaction mixture.

**S3. Refinement**

H atoms were included in the riding approximation with  $C—H = 0.93$  and  $O—H = 0.82 \text{ \AA}$ ,  $U_{iso}(H) = 1.2U_{eq}(C,O)$ .

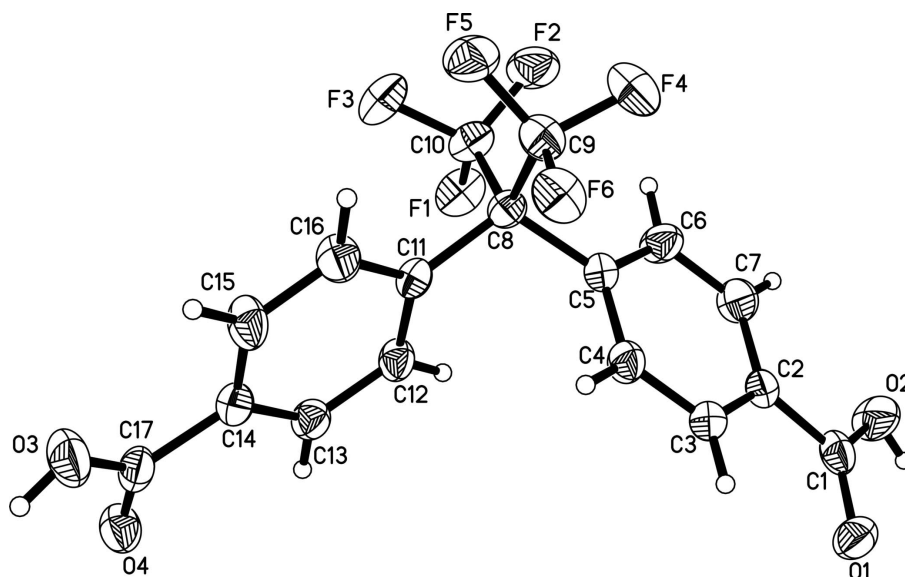


Figure 1

The molecular structure and labeling of (I). Displacement ellipsoids are drawn at the 30% probability level.

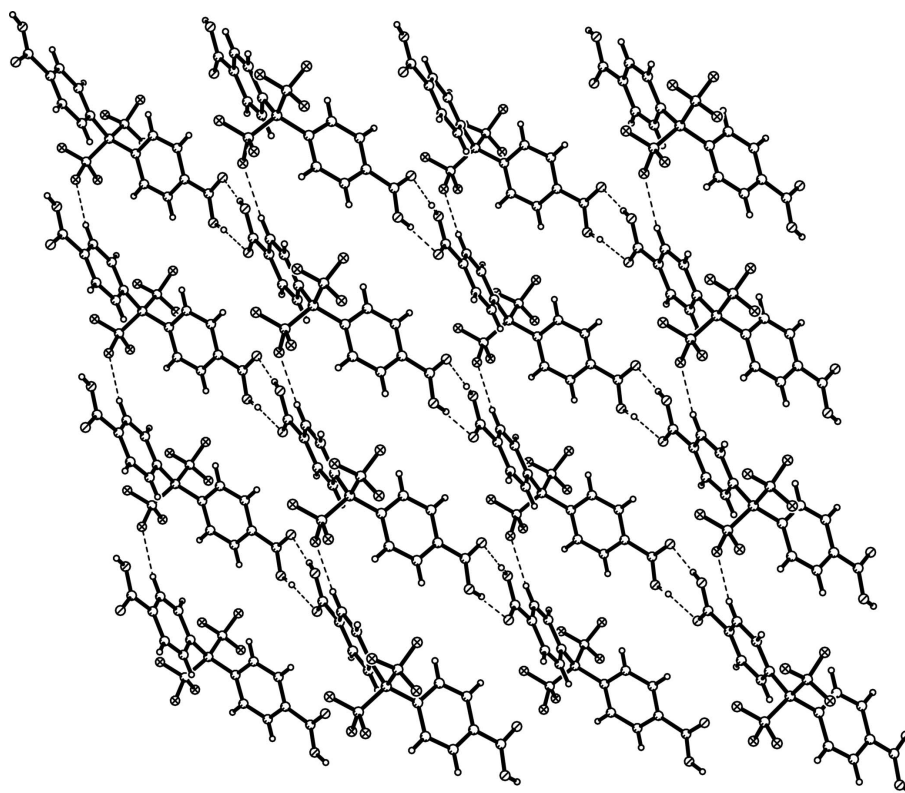


Figure 2

2D wave-like layer of (I). Dashed lines denote hydrogen bonds.

## 4,4'-(1,1,1,3,3,3-Hexafluoropropane-2,2-diyl)dibenzoic acid

## Crystal data

C<sub>17</sub>H<sub>10</sub>F<sub>6</sub>O<sub>4</sub> $M_r = 392.25$ Monoclinic,  $P2_1/c$ 

Hall symbol: -P 2ybc

 $a = 7.7523$  (16) Å $b = 13.381$  (3) Å $c = 16.134$  (3) Å $\beta = 102.294$  (4)° $V = 1635.2$  (6) Å<sup>3</sup> $Z = 4$  $F(000) = 792$  $D_x = 1.593$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 775 reflections

 $\theta = 2.7$ – $18.7$ ° $\mu = 0.16$  mm<sup>-1</sup> $T = 293$  K

Prism, colorless

 $0.35 \times 0.20 \times 0.18$  mm

## Data collection

Bruker SMART CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 $\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

 $T_{\min} = 0.963$ ,  $T_{\max} = 0.972$ 

8113 measured reflections

2904 independent reflections

1339 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.053$  $\theta_{\max} = 25.1$ °,  $\theta_{\min} = 2.0$ ° $h = -9 \rightarrow 9$  $k = -15 \rightarrow 15$  $l = -13 \rightarrow 19$ 

## Refinement

Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.040$  $wR(F^2) = 0.071$  $S = 1.00$ 

2904 reflections

246 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

 $w = 1/[\sigma^2(F_o^2) + (0.0135P)^2 + 0.190P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} < 0.001$  $\Delta\rho_{\max} = 0.17$  e Å<sup>-3</sup> $\Delta\rho_{\min} = -0.19$  e Å<sup>-3</sup>

## Special details

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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<sup>2</sup>)

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	-0.2346 (4)	0.0955 (2)	0.4514 (2)	0.0540 (8)
C2	-0.1474 (3)	0.04538 (17)	0.38975 (18)	0.0467 (7)
C3	0.0256 (3)	0.06770 (16)	0.38831 (17)	0.0482 (7)
H3	0.0908	0.1094	0.4295	0.058*

C4	0.1019 (3)	0.02807 (17)	0.32574 (17)	0.0491 (7)
H4	0.2188	0.0435	0.3254	0.059*
C5	0.0090 (3)	-0.03396 (17)	0.26363 (17)	0.0438 (7)
C6	-0.1618 (3)	-0.05959 (18)	0.26780 (19)	0.0599 (8)
H6	-0.2251	-0.1042	0.2286	0.072*
C7	-0.2381 (3)	-0.01936 (19)	0.32963 (19)	0.0612 (8)
H7	-0.3539	-0.0363	0.3309	0.073*
C8	0.1010 (3)	-0.07485 (17)	0.19469 (18)	0.0430 (7)
C9	0.2103 (4)	-0.1652 (2)	0.2347 (2)	0.0584 (8)
C10	-0.0290 (4)	-0.1105 (2)	0.1152 (2)	0.0586 (8)
C11	0.2132 (3)	0.00552 (17)	0.16376 (15)	0.0412 (7)
C12	0.1452 (3)	0.10175 (17)	0.14883 (16)	0.0489 (7)
H12	0.0372	0.1171	0.1621	0.059*
C13	0.2346 (3)	0.17475 (18)	0.11477 (16)	0.0500 (7)
H13	0.1856	0.2382	0.1045	0.060*
C14	0.3958 (3)	0.15424 (18)	0.09593 (16)	0.0460 (7)
C15	0.4658 (3)	0.05969 (19)	0.11157 (18)	0.0609 (8)
H15	0.5758	0.0454	0.1002	0.073*
C16	0.3744 (3)	-0.01372 (19)	0.14386 (17)	0.0575 (8)
H16	0.4223	-0.0776	0.1524	0.069*
C17	0.4938 (4)	0.2307 (2)	0.05836 (17)	0.0513 (8)
O1	-0.1535 (2)	0.15916 (13)	0.50126 (12)	0.0654 (6)
O2	-0.3969 (3)	0.07246 (13)	0.44691 (15)	0.0814 (7)
H2A	-0.4415	0.1127	0.4745	0.098*
O3	0.6508 (3)	0.20695 (12)	0.05373 (14)	0.0748 (6)
H3A	0.7020	0.2563	0.0408	0.090*
O4	0.4229 (2)	0.31255 (13)	0.03316 (12)	0.0628 (6)
F1	-0.14945 (18)	-0.04108 (11)	0.08519 (10)	0.0701 (5)
F2	-0.11835 (19)	-0.19326 (11)	0.12709 (10)	0.0760 (5)
F3	0.05259 (19)	-0.13151 (11)	0.05246 (11)	0.0747 (5)
F4	0.1158 (2)	-0.22673 (10)	0.27230 (11)	0.0775 (5)
F5	0.2745 (2)	-0.22093 (10)	0.17918 (11)	0.0736 (5)
F6	0.3482 (2)	-0.13628 (10)	0.29418 (11)	0.0664 (5)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.054 (2)	0.0537 (18)	0.062 (3)	0.0027 (15)	0.0283 (19)	0.0126 (16)
C2	0.0535 (19)	0.0446 (15)	0.046 (2)	-0.0039 (14)	0.0196 (17)	0.0041 (14)
C3	0.0538 (18)	0.0478 (15)	0.044 (2)	-0.0051 (13)	0.0139 (17)	-0.0007 (14)
C4	0.0454 (17)	0.0559 (16)	0.049 (2)	-0.0061 (14)	0.0176 (17)	-0.0013 (15)
C5	0.0483 (18)	0.0442 (15)	0.041 (2)	-0.0032 (13)	0.0150 (16)	0.0021 (14)
C6	0.0547 (19)	0.0644 (17)	0.064 (3)	-0.0151 (14)	0.0211 (18)	-0.0206 (16)
C7	0.0477 (19)	0.0698 (19)	0.073 (3)	-0.0114 (15)	0.0275 (19)	-0.0068 (18)
C8	0.0423 (15)	0.0464 (15)	0.039 (2)	0.0000 (12)	0.0060 (15)	-0.0044 (14)
C9	0.055 (2)	0.0553 (19)	0.065 (3)	-0.0058 (16)	0.014 (2)	0.0039 (18)
C10	0.057 (2)	0.0604 (19)	0.059 (3)	0.0039 (16)	0.014 (2)	-0.0142 (18)
C11	0.0412 (16)	0.0499 (16)	0.0327 (19)	0.0042 (13)	0.0078 (14)	-0.0010 (13)

C12	0.0463 (17)	0.0543 (16)	0.051 (2)	0.0059 (13)	0.0216 (16)	0.0019 (15)
C13	0.0556 (18)	0.0479 (15)	0.049 (2)	0.0062 (14)	0.0162 (16)	0.0005 (14)
C14	0.0464 (17)	0.0536 (17)	0.039 (2)	0.0017 (14)	0.0107 (15)	0.0016 (14)
C15	0.0453 (17)	0.0694 (19)	0.076 (3)	0.0081 (15)	0.0307 (17)	0.0128 (17)
C16	0.0542 (19)	0.0532 (17)	0.070 (2)	0.0142 (14)	0.0240 (18)	0.0094 (16)
C17	0.0479 (19)	0.0664 (19)	0.044 (2)	-0.0031 (16)	0.0188 (17)	-0.0045 (16)
O1	0.0729 (14)	0.0669 (13)	0.0592 (16)	-0.0006 (10)	0.0205 (12)	-0.0136 (11)
O2	0.0789 (15)	0.0848 (15)	0.096 (2)	-0.0088 (12)	0.0523 (14)	-0.0270 (13)
O3	0.0644 (14)	0.0759 (14)	0.0945 (18)	-0.0037 (11)	0.0400 (13)	0.0129 (13)
O4	0.0660 (13)	0.0586 (11)	0.0685 (15)	0.0055 (10)	0.0252 (11)	0.0127 (11)
F1	0.0562 (10)	0.0868 (11)	0.0613 (13)	0.0170 (8)	-0.0013 (9)	-0.0071 (9)
F2	0.0732 (11)	0.0693 (10)	0.0835 (14)	-0.0196 (8)	0.0125 (10)	-0.0244 (10)
F3	0.0710 (11)	0.0992 (12)	0.0547 (12)	0.0075 (9)	0.0151 (10)	-0.0247 (9)
F4	0.0733 (11)	0.0613 (10)	0.1000 (16)	-0.0059 (8)	0.0231 (11)	0.0212 (9)
F5	0.0774 (12)	0.0578 (9)	0.0885 (15)	0.0155 (8)	0.0242 (11)	-0.0058 (9)
F6	0.0562 (10)	0.0689 (10)	0.0677 (13)	0.0017 (8)	-0.0013 (9)	0.0144 (9)

*Geometric parameters (Å, °)*

C1—O1	1.246 (3)	C9—F5	1.340 (3)
C1—O2	1.283 (3)	C10—F1	1.333 (3)
C1—C2	1.477 (3)	C10—F3	1.332 (3)
C2—C7	1.377 (3)	C10—F2	1.341 (3)
C2—C3	1.379 (3)	C11—C16	1.379 (3)
C3—C4	1.380 (3)	C11—C12	1.393 (3)
C3—H3	0.9300	C12—C13	1.378 (3)
C4—C5	1.380 (3)	C12—H12	0.9300
C4—H4	0.9300	C13—C14	1.375 (3)
C5—C6	1.383 (3)	C13—H13	0.9300
C5—C8	1.544 (3)	C14—C15	1.379 (3)
C6—C7	1.374 (3)	C14—C17	1.479 (3)
C6—H6	0.9300	C15—C16	1.377 (3)
C7—H7	0.9300	C15—H15	0.9300
C8—C10	1.530 (3)	C16—H16	0.9300
C8—C11	1.532 (3)	C17—O4	1.254 (3)
C8—C9	1.538 (3)	C17—O3	1.276 (3)
C9—F4	1.331 (3)	O2—H2A	0.8200
C9—F6	1.333 (3)	O3—H3A	0.8200
O1—C1—O2	123.7 (3)	F6—C9—C8	111.0 (2)
O1—C1—C2	120.3 (3)	F5—C9—C8	114.0 (3)
O2—C1—C2	115.9 (3)	F1—C10—F3	106.3 (3)
C7—C2—C3	118.5 (3)	F1—C10—F2	106.5 (2)
C7—C2—C1	121.4 (3)	F3—C10—F2	106.1 (2)
C3—C2—C1	119.9 (3)	F1—C10—C8	111.9 (2)
C2—C3—C4	119.9 (2)	F3—C10—C8	111.6 (2)
C2—C3—H3	120.0	F2—C10—C8	113.9 (2)
C4—C3—H3	120.0	C16—C11—C12	117.4 (2)

C5—C4—C3	121.5 (2)	C16—C11—C8	123.4 (2)
C5—C4—H4	119.2	C12—C11—C8	119.0 (2)
C3—C4—H4	119.2	C13—C12—C11	121.4 (2)
C4—C5—C6	118.1 (2)	C13—C12—H12	119.3
C4—C5—C8	119.1 (2)	C11—C12—H12	119.3
C6—C5—C8	122.8 (2)	C14—C13—C12	120.3 (2)
C7—C6—C5	120.2 (3)	C14—C13—H13	119.9
C7—C6—H6	119.9	C12—C13—H13	119.9
C5—C6—H6	119.9	C13—C14—C15	118.9 (2)
C6—C7—C2	121.6 (2)	C13—C14—C17	121.5 (2)
C6—C7—H7	119.2	C15—C14—C17	119.5 (2)
C2—C7—H7	119.2	C14—C15—C16	120.6 (2)
C10—C8—C11	105.3 (2)	C14—C15—H15	119.7
C10—C8—C9	108.2 (2)	C16—C15—H15	119.7
C11—C8—C9	112.9 (2)	C11—C16—C15	121.3 (2)
C10—C8—C5	113.1 (2)	C11—C16—H16	119.3
C11—C8—C5	111.55 (19)	C15—C16—H16	119.3
C9—C8—C5	105.9 (2)	O4—C17—O3	123.8 (3)
F4—C9—F6	106.7 (3)	O4—C17—C14	120.6 (3)
F4—C9—F5	106.3 (2)	O3—C17—C14	115.6 (3)
F6—C9—F5	106.7 (2)	C1—O2—H2A	109.5
F4—C9—C8	111.7 (2)	C17—O3—H3A	109.5
O1—C1—C2—C7	-174.9 (2)	C11—C8—C10—F1	-70.1 (3)
O2—C1—C2—C7	2.1 (4)	C9—C8—C10—F1	168.9 (2)
O1—C1—C2—C3	1.2 (4)	C5—C8—C10—F1	51.9 (3)
O2—C1—C2—C3	178.2 (2)	C11—C8—C10—F3	48.8 (3)
C7—C2—C3—C4	2.2 (4)	C9—C8—C10—F3	-72.2 (3)
C1—C2—C3—C4	-173.9 (2)	C5—C8—C10—F3	170.8 (2)
C2—C3—C4—C5	0.1 (4)	C11—C8—C10—F2	169.0 (2)
C3—C4—C5—C6	-3.0 (4)	C9—C8—C10—F2	48.0 (3)
C3—C4—C5—C8	179.2 (2)	C5—C8—C10—F2	-69.0 (3)
C4—C5—C6—C7	3.6 (4)	C10—C8—C11—C16	-94.9 (3)
C8—C5—C6—C7	-178.7 (2)	C9—C8—C11—C16	22.9 (4)
C5—C6—C7—C2	-1.3 (4)	C5—C8—C11—C16	142.0 (2)
C3—C2—C7—C6	-1.6 (4)	C10—C8—C11—C12	80.3 (3)
C1—C2—C7—C6	174.5 (3)	C9—C8—C11—C12	-161.9 (2)
C4—C5—C8—C10	-159.9 (2)	C5—C8—C11—C12	-42.7 (3)
C6—C5—C8—C10	22.4 (3)	C16—C11—C12—C13	0.6 (4)
C4—C5—C8—C11	-41.5 (3)	C8—C11—C12—C13	-174.9 (2)
C6—C5—C8—C11	140.9 (2)	C11—C12—C13—C14	-1.1 (4)
C4—C5—C8—C9	81.7 (3)	C12—C13—C14—C15	0.1 (4)
C6—C5—C8—C9	-95.9 (3)	C12—C13—C14—C17	179.3 (2)
C10—C8—C9—F4	-73.2 (3)	C13—C14—C15—C16	1.3 (4)
C11—C8—C9—F4	170.6 (2)	C17—C14—C15—C16	-177.8 (3)
C5—C8—C9—F4	48.3 (3)	C12—C11—C16—C15	0.9 (4)
C10—C8—C9—F6	167.9 (2)	C8—C11—C16—C15	176.1 (3)
C11—C8—C9—F6	51.7 (3)	C14—C15—C16—C11	-1.9 (4)

C5—C8—C9—F6	-70.7 (3)	C13—C14—C17—O4	-8.7 (4)
C10—C8—C9—F5	47.3 (3)	C15—C14—C17—O4	170.4 (3)
C11—C8—C9—F5	-68.9 (3)	C13—C14—C17—O3	171.5 (3)
C5—C8—C9—F5	168.8 (2)	C15—C14—C17—O3	-9.4 (4)

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O2—H2 <i>A</i> ...O4 <sup>i</sup>	0.82	1.85	2.661 (2)	169
O3—H3 <i>A</i> ...O1 <sup>ii</sup>	0.82	1.80	2.603 (2)	165
C15—H15...F1 <sup>iii</sup>	0.93	2.48	3.382 (3)	163

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