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

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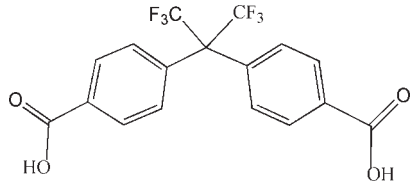
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.040; wR factor = 0.071; data-to-parameter ratio = 11.8.

In the title compound, $C_{17}H_{10}F_6O_4$, 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 O—H···O and C—H···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

$C_{17}H_{10}F_6O_4$
M_r = 392.25
Monoclinic, $P2_1/c$
a = 7.7523 (16) Å
b = 13.381 (3) Å
c = 16.134 (3) Å
β = 102.294 (4)°
V = 1635.2 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.16 mm^{-1}
T = 293 K
0.35 × 0.20 × 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_{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
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···O4^{i}	0.82	1.85	2.661 (2)	169
O3—H3A···O1^{ii}	0.82	1.80	2.603 (2)	165
C15—H15···F1^{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).

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

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supplementary materials

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

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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)°. Strong intermolecular O—H···O and C—H···F hydrogen bonds (Table 1) link the molecules into the 2D wave-like layer structure (Fig. 2).

Experimental

The title compound was prepared by hydrothermal method. A mixture of $Zn(Ac)_2.4H_2O$ (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.

Refinement

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

Figures

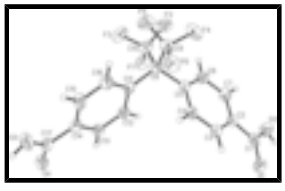

Fig. 1. The molecular structure and labeling of (I). Displacement ellipsoids are drawn at the 30% probability level.

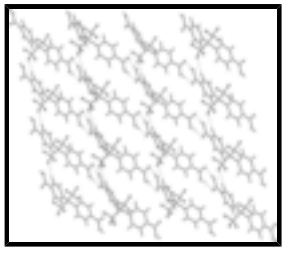

Fig. 2. 2D wave-like layer of (I). Dashed lines denote hydrogen bonds.

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

Crystal data

$C_{17}H_{10}F_6O_4$	$F(000) = 792$
$M_r = 392.25$	$D_x = 1.593$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 775 reflections
$a = 7.7523$ (16) Å	$\theta = 2.7–18.7°$
$b = 13.381$ (3) Å	$\mu = 0.16$ mm^{-1}
$c = 16.134$ (3) Å	$T = 293$ K
$\beta = 102.294$ (4)°	Prism, colorless
$V = 1635.2$ (6) Å^3	0.35 × 0.20 × 0.18 mm
$Z = 4$	

Data collection

Bruker SMART CCD diffractometer	2904 independent reflections
Radiation source: fine-focus sealed tube	1339 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.053$
φ and ω scans	$\theta_{max} = 25.1°$, $\theta_{min} = 2.0°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -9\rightarrow9$
$T_{min} = 0.963$, $T_{max} = 0.972$	$k = -15\rightarrow15$
8113 measured reflections	$l = -13\rightarrow19$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.040$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.071$	H-atom parameters constrained
$S = 1.00$	$w = 1/[\sigma^2(F_o^2) + (0.0135P)^2 + 0.190P]$ where $P = (F_o^2 + 2F_c^2)/3$
2904 reflections	$(\Delta/\sigma)_{max} < 0.001$
246 parameters	$\Delta\rho_{max} = 0.17$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.19$ e Å^{-3}

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^2)

	x	*y*	*z*	U_{iso}*/U_{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^2)

	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, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2A···O4^{i}	0.82	1.85	2.661 (2)	169
O3—H3A···O1^{ii}	0.82	1.80	2.603 (2)	165
C15—H15···F1^{iii}	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*.

Fig. 1

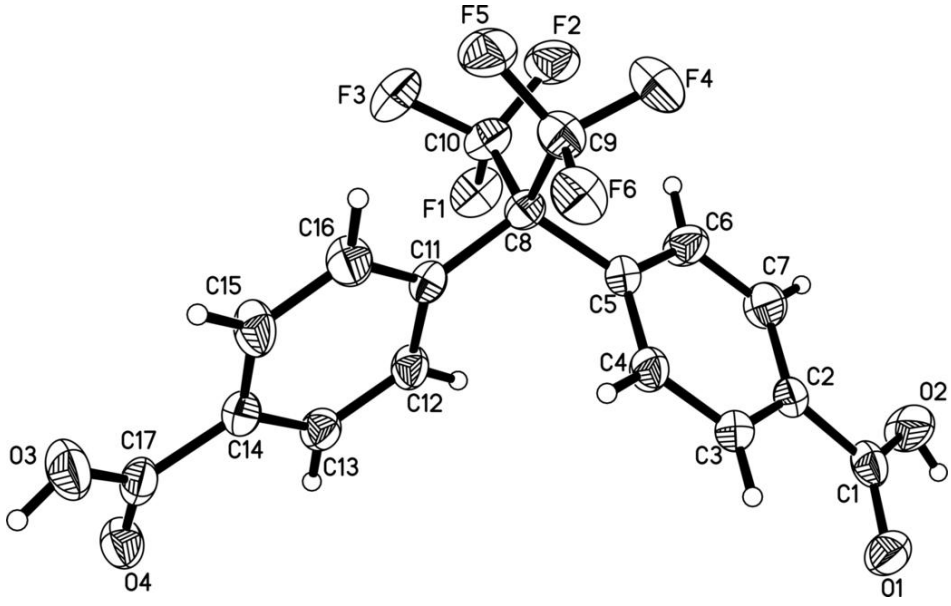
F5
F2
F3
F4
C10
C9
F1
F6
C16
C11
C8
C6
C15
C5
C7
C4
C2
O2
C12
C17
C14
O3
C13
C3
C1
O4
O1

Fig. 2