Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-4,4,4-Trifluoro-2,3-diphenylbut-2-enal

Hoong-Kun Fun,[a]* Shea-Lin Ng,[a] Zhe Li[b] and Jian-Hua Xu[b]

[a]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and [b]Department of Chemistry, Nanjing University, Nanjing 210093, People's Republic of China
Correspondence e-mail: hkfun@usm.my

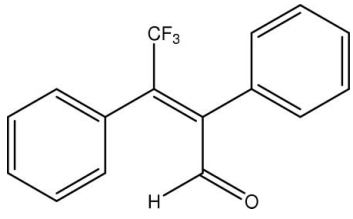
Received 12 June 2007; accepted 13 June 2007

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.074; wR factor = 0.199; data-to-parameter ratio = 16.6.

In the title compound, $C_{16}H_{11}F_3O$, the dihedral angle between the two benzene rings is 4.66 (12)°. In the crystal structure, the molecules are interlinked into columns along the b axis by intermolecular C—H···O interactions and short O···O contacts [2.525 (8) Å]. The crystal structure is further stabilized by weak intermolecular C—H···π interactions. The linkage between the two phenyl rings is disordered over two positions in approximately a 0.6:0.4 ratio.

Related literature

For related literature on values of bond lengths, see: Allen *et al.* (1987). For a related structure, see: van Alem *et al.* (2005);



Experimental

Crystal data

$C_{16}H_{11}F_3O$
M_r = 276.25
Monoclinic, $C2/c$
a = 29.1818 (8) Å
b = 5.8972 (2) Å
c = 17.8356 (6) Å
β = 123.485 (3)°
V = 2559.92 (17) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 100.0 (1) K
0.53 × 0.11 × 0.08 mm

Data collection

Bruker SMART APEX II CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.851, T_{max} = 0.991
24392 measured reflections
3611 independent reflections
2817 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.199
S = 1.07
3611 reflections
217 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the C1–C6 and C11–C16 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5A···O1B^{i}	0.93	2.56	3.491 (4)	175
C13—H13A···O1B^{ii}	0.93	2.50	3.375 (4)	158
C12—H12A···O1A^{i}	0.93	2.58	3.506 (5)	178
C2—H2A···$Cg1^{iii}$	0.93	2.92	3.668 (3)	139
C4—H4A···$Cg2^{iv}$	0.93	2.90	3.662 (2)	141
C15—H15A···$Cg1^{v}$	0.93	2.91	3.618 (2)	134

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

The authors thank the Malaysian Government and Universiti Sains Malaysia for the Scientific Advancement Grant Allocation (SAGA) grant No. 304/PFIZIK/653003/A118.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2389).

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supplementary materials

Acta Cryst. (2007). E**63**, o3255 [**doi:10.1107/S1600536807028966**]

(*E*)-4,4,4-Trifluoro-2,3-diphenylbut-2-enal

H.-K. Fun, S.-L. Ng, Z. Li and J.-H. Xu

Comment

The photochemistry of α,α,α-trifluoroacetophenone is of continuing research interest (van Alem *et al.*, 2005). In continuation of our recent work on photoinduced reactions of ketones with alkynes, the title compound, (I), was obtained by the reaction of photoexcited α,α,α-trifluoroacetophenone with trimethylsilylphenylethyne. A crystallographic analysis of (I) was carried out to elucidate its structure.

Bond lengths and angles in (I) display normal values (Allen *et al.*, 1987). The dihedral angle between the C1—C6 and C11—C16 benzene rings is 4.66 (12)°. The torsion angle of C9—C7A—C8A—C10 and C9—C7B—C8B—C10 are 176.1 (3) and −175.5 (2)°, respectively. The linkage between the two phenyl rings is disordered over two positions.

In the crystal structure, the molecules are interconnected into columns along the *b* axis by intermolecular C13—H13A···O1B and C5—H5A···O1B interactions (Figure 2 and Table 1) together with intermolecular C12—H12A···O1A interactions (Table 1) and short O1A···O1A (−*x*, *y*, 1/2 − *z*) contacts [2.525 (8) Å] (Figure 3). In addition, the crystal structure is further stabilized by C—H···π interactions involving the C1—C6 (centroid *Cg*1) and C11—C16 (centroid *Cg*2) ring (Table 1).

Experimental

The title compound was synthesized by a photo-induced reaction between α,α,α-trifluoroacetophenone (0.05*M*) and an excess amount of 1-phenyl-2-trimethyl-silylacetylene (0.2*M*) in a acetonitrile solution. The title compound was isolated using silica gel column chromatography. Single crystal suitable for X-ray diffraction analysis were obtained by slow evaporation of the solvents from a petroleum ether-ethyl acetate solution (V:V = 2:1).

Refinement

The H atoms on C10 were located in a difference map and refined isotropically. The remaining H atoms were positional geometrically and refined as riding, with C—H = 0.93Å and U_{iso}(H) = 1.2 U_{eq}(C). The ratio of the refined occupancies for the major and minor components of the disordered linkage of C7B/C8B/O1B and C7A/C8A/O1A are 0.614 (4): 0.386 (4).

Figures

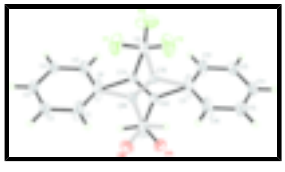


Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. Both disorder components are shown.

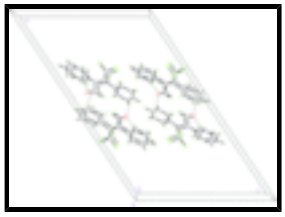


Fig. 2. Packing of the major component of the crystal structure of (I), viewed down the *b* axis. Dashed lines indicate intermolecular C—H···O interactions.

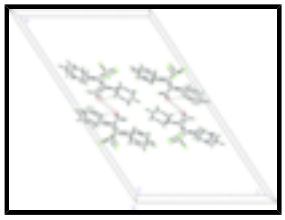


Fig. 3. Packing of the minor component of the crystal structure of (I), viewed down the *b* axis. Dashed lines indicate intermolecular C—H···O interactions and short O···O contact.

(*E*)-4,4,4-Trifluoro-2,3-diphenylbut-2-enal

Crystal data

$C_{16}H_{11}F_3O$	F_{000} = 1136
M_r = 276.25	D_x = 1.434 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 6048 reflections
a = 29.1818 (8) Å	θ = 1.7–29.7º
b = 5.8972 (2) Å	μ = 0.12 mm^{-1}
c = 17.8356 (6) Å	*T* = 100.0 (1) K
β = 123.485 (3)º	Needle, colourless
V = 2559.92 (17) Å^3	0.53 × 0.11 × 0.08 mm
Z = 8	

Data collection

Bruker SMART APEX II CCD area-detector diffractometer	3611 independent reflections
Radiation source: fine-focus sealed tube	2817 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.035
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 29.7º
T = 100.0(1) K	θ_{min} = 1.7º
ω scans	*h* = −40→40
Absorption correction: multi-scan (SADABS; Bruker, 2005)	*k* = −8→8
T_{min} = 0.851, T_{max} = 0.991	*l* = −24→24
24392 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.074$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.199$	$w = 1/[\sigma^2(F_o^2) + (0.077P)^2 + 6.0256P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} < 0.001$
3611 reflections	$\Delta\rho_{max} = 0.53$ e Å^{-3}
217 parameters	$\Delta\rho_{min} = -0.55$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. The data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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 $F^2 > 2$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	0.18069 (11)	0.9487 (5)	0.23530 (19)	0.0464 (7)	
H1A	0.1880	1.0725	0.2726	0.056*	
C2	0.20283 (8)	0.9398 (4)	0.18402 (14)	0.0290 (4)	
H2A	0.2253	1.0566	0.1872	0.035*	
C3	0.19152 (8)	0.7565 (4)	0.12787 (12)	0.0265 (4)	
H3A	0.2062	0.7511	0.0929	0.032*	
C4	0.15853 (8)	0.5809 (4)	0.12336 (13)	0.0267 (4)	
H4A	0.1510	0.4581	0.0855	0.032*	
C5	0.13670 (9)	0.5889 (4)	0.17546 (15)	0.0349 (5)	
H5A	0.1148	0.4709	0.1731	0.042*	
C6	0.14771 (11)	0.7744 (5)	0.23137 (18)	0.0509 (8)	
C7A	0.1405 (2)	0.7075 (8)	0.3129 (3)	0.0206 (11)	0.386 (4)
C8A	0.0984 (2)	0.8206 (8)	0.3060 (3)	0.0211 (11)	0.386 (4)
C7B	0.12592 (13)	0.7038 (5)	0.3454 (2)	0.0219 (7)	0.614 (4)
C8B	0.11472 (13)	0.8185 (5)	0.2723 (2)	0.0211 (7)	0.614 (4)
C9	0.17483 (9)	0.5436 (4)	0.39318 (14)	0.0302 (4)	
F1	0.21769 (8)	0.5581 (4)	0.38942 (15)	0.0710 (6)	
F2	0.15724 (7)	0.3293 (3)	0.37303 (13)	0.0622 (5)	
F3	0.19211 (10)	0.5757 (4)	0.47726 (12)	0.0731 (6)	
C10	0.06815 (8)	0.9881 (4)	0.23205 (13)	0.0256 (4)	
H10A	0.070 (3)	1.000 (13)	0.174 (4)	0.023 (16)*	0.386 (4)
H10B	0.0408 (14)	0.983 (7)	0.252 (2)	0.013 (8)*	0.614 (4)

O1A	0.03311 (17)	1.1142 (8)	0.2254 (3)	0.0326 (11)	0.386 (4)
O1B	0.06237 (11)	1.1301 (5)	0.17911 (18)	0.0350 (7)	0.614 (4)
C11	0.08796 (12)	0.7462 (6)	0.37994 (18)	0.0550 (9)	
C12	0.05262 (9)	0.5710 (4)	0.36590 (15)	0.0345 (5)	
H12A	0.0471	0.4526	0.3273	0.041*	
C13	0.02536 (8)	0.5724 (4)	0.40948 (14)	0.0288 (4)	
H13A	0.0016	0.4546	0.4002	0.035*	
C14	0.03350 (8)	0.7491 (4)	0.46699 (13)	0.0296 (4)	
H14A	0.0153	0.7487	0.4964	0.036*	
C15	0.06837 (9)	0.9249 (4)	0.48076 (14)	0.0320 (5)	
H15A	0.0737	1.0434	0.5192	0.038*	
C16	0.09546 (13)	0.9235 (5)	0.43669 (18)	0.0527 (8)	
H16A	0.1188	1.0425	0.4453	0.063*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0506 (14)	0.0514 (16)	0.0622 (15)	−0.0278 (12)	0.0469 (13)	−0.0355 (13)
C2	0.0296 (9)	0.0292 (11)	0.0369 (10)	−0.0059 (8)	0.0239 (9)	−0.0039 (8)
C3	0.0277 (9)	0.0340 (11)	0.0241 (8)	0.0014 (8)	0.0183 (8)	0.0018 (8)
C4	0.0313 (10)	0.0286 (10)	0.0240 (9)	−0.0014 (8)	0.0177 (8)	−0.0035 (7)
C5	0.0420 (12)	0.0402 (13)	0.0352 (10)	−0.0185 (10)	0.0293 (10)	−0.0141 (9)
C6	0.0582 (15)	0.0696 (19)	0.0547 (14)	−0.0396 (14)	0.0500 (13)	−0.0387 (14)
C7A	0.027 (2)	0.018 (2)	0.021 (2)	0.0024 (19)	0.016 (2)	0.0051 (18)
C8A	0.029 (2)	0.018 (2)	0.020 (2)	−0.005 (2)	0.016 (2)	−0.0026 (18)
C7B	0.0271 (15)	0.0206 (15)	0.0241 (14)	0.0004 (12)	0.0181 (13)	−0.0006 (12)
C8B	0.0265 (15)	0.0179 (15)	0.0251 (14)	−0.0057 (12)	0.0181 (13)	−0.0045 (12)
C9	0.0357 (11)	0.0296 (11)	0.0329 (10)	0.0063 (8)	0.0236 (9)	0.0053 (8)
F1	0.0742 (12)	0.0783 (14)	0.1068 (16)	0.0048 (10)	0.0791 (13)	0.0040 (11)
F2	0.0612 (10)	0.0260 (8)	0.0837 (13)	0.0030 (7)	0.0300 (9)	0.0034 (8)
F3	0.1158 (16)	0.0815 (14)	0.0529 (10)	−0.0030 (12)	0.0660 (12)	−0.0016 (9)
C10	0.0293 (9)	0.0258 (10)	0.0268 (9)	−0.0001 (8)	0.0186 (8)	0.0001 (7)
O1A	0.039 (2)	0.032 (2)	0.032 (2)	0.0098 (17)	0.0223 (18)	0.0025 (17)
O1B	0.0350 (14)	0.0308 (16)	0.0430 (15)	0.0028 (11)	0.0239 (12)	0.0114 (11)
C11	0.0686 (17)	0.077 (2)	0.0508 (14)	−0.0466 (16)	0.0525 (14)	−0.0370 (14)
C12	0.0376 (11)	0.0403 (13)	0.0352 (10)	−0.0130 (9)	0.0260 (9)	−0.0144 (9)
C13	0.0293 (9)	0.0304 (11)	0.0320 (10)	−0.0040 (8)	0.0201 (8)	0.0028 (8)
C14	0.0303 (10)	0.0387 (12)	0.0294 (9)	0.0043 (9)	0.0224 (8)	0.0060 (8)
C15	0.0421 (11)	0.0327 (11)	0.0278 (9)	−0.0030 (9)	0.0235 (9)	−0.0039 (8)
C16	0.0775 (19)	0.0587 (18)	0.0482 (14)	−0.0445 (15)	0.0514 (15)	−0.0287 (13)

Geometric parameters (Å, °)

C1—C2	1.382 (3)	C9—F1	1.292 (2)
C1—C6	1.383 (3)	C9—F3	1.306 (3)
C1—H1A	0.9300	C9—F2	1.337 (3)
C2—C3	1.384 (3)	C10—O1B	1.202 (3)
C2—H2A	0.9300	C10—O1A	1.216 (4)
C3—C4	1.386 (3)	C10—H10A	1.07 (6)

C3—H3A	0.9300	C10—H10B	1.04 (3)
C4—C5	1.387 (3)	O1A—H10B	0.87 (4)
C4—H4A	0.9300	O1B—H10A	0.82 (7)
C5—C6	1.393 (3)	C11—C12	1.382 (3)
C5—H5A	0.9300	C11—C16	1.386 (3)
C6—C8B	1.517 (3)	C12—C13	1.385 (3)
C6—C7A	1.629 (5)	C12—H12A	0.9300
C7A—C8A	1.343 (7)	C13—C14	1.387 (3)
C7A—C9	1.551 (5)	C13—H13A	0.9300
C8A—C10	1.486 (5)	C14—C15	1.376 (3)
C8A—C11	1.571 (5)	C14—H14A	0.9300
C7B—C8B	1.340 (4)	C15—C16	1.389 (3)
C7B—C9	1.521 (4)	C15—H15A	0.9300
C7B—C11	1.556 (4)	C16—H16A	0.9300
C8B—C10	1.512 (4)		
C2—C1—C6	120.3 (2)	F1—C9—C7A	93.6 (2)
C2—C1—H1A	119.9	F3—C9—C7A	127.8 (3)
C6—C1—H1A	119.9	F2—C9—C7A	112.6 (2)
C1—C2—C3	119.80 (19)	O1B—C10—O1A	75.6 (3)
C1—C2—H2A	120.1	O1B—C10—C8A	156.5 (3)
C3—C2—H2A	120.1	O1A—C10—C8A	123.3 (3)
C2—C3—C4	120.40 (17)	O1B—C10—C8B	122.2 (2)
C2—C3—H3A	119.8	O1A—C10—C8B	159.8 (3)
C4—C3—H3A	119.8	O1A—C10—H10A	111 (4)
C3—C4—C5	119.80 (18)	C8A—C10—H10A	126 (4)
C3—C4—H4A	120.1	C8B—C10—H10A	90 (4)
C5—C4—H4A	120.1	O1B—C10—H10B	119 (2)
C4—C5—C6	119.76 (19)	C8A—C10—H10B	83 (2)
C4—C5—H5A	120.1	C8B—C10—H10B	119 (2)
C6—C5—H5A	120.1	H10A—C10—H10B	142 (4)
C1—C6—C5	119.94 (19)	C10—O1A—H10B	57 (2)
C1—C6—C8B	117.2 (2)	C10—O1B—H10A	60 (4)
C5—C6—C8B	121.5 (2)	C12—C11—C16	119.9 (2)
C1—C6—C7A	124.3 (3)	C12—C11—C7B	115.5 (2)
C5—C6—C7A	110.9 (3)	C16—C11—C7B	123.4 (2)
C8A—C7A—C9	119.2 (4)	C12—C11—C8A	121.8 (2)
C8A—C7A—C6	111.1 (4)	C16—C11—C8A	112.1 (3)
C9—C7A—C6	129.7 (3)	C11—C12—C13	119.7 (2)
C7A—C8A—C10	118.5 (4)	C11—C12—H12A	120.1
C7A—C8A—C11	112.0 (4)	C13—C12—H12A	120.1
C10—C8A—C11	129.5 (4)	C12—C13—C14	120.14 (19)
C8B—C7B—C9	120.6 (3)	C12—C13—H13A	119.9
C8B—C7B—C11	117.4 (3)	C14—C13—H13A	119.9
C9—C7B—C11	122.1 (2)	C15—C14—C13	120.37 (17)
C7B—C8B—C10	117.9 (3)	C15—C14—H14A	119.8
C7B—C8B—C6	120.2 (3)	C13—C14—H14A	119.8
C10—C8B—C6	121.9 (3)	C14—C15—C16	119.4 (2)
F1—C9—F3	106.2 (2)	C14—C15—H15A	120.3
F1—C9—F2	106.72 (19)	C16—C15—H15A	120.3

F3—C9—F2	107.1 (2)	C11—C16—C15	120.5 (2)
F1—C9—C7B	124.5 (2)	C11—C16—H16A	119.8
F3—C9—C7B	101.7 (2)	C15—C16—H16A	119.8
F2—C9—C7B	109.5 (2)		
C6—C1—C2—C3	0.6 (4)	C8A—C7A—C9—F3	−42.2 (6)
C1—C2—C3—C4	−0.6 (3)	C6—C7A—C9—F3	136.4 (4)
C2—C3—C4—C5	0.0 (3)	C8A—C7A—C9—F2	94.4 (4)
C3—C4—C5—C6	0.6 (4)	C6—C7A—C9—F2	−87.0 (4)
C2—C1—C6—C5	0.0 (5)	C8A—C7A—C9—C7B	2.8 (3)
C2—C1—C6—C8B	−166.5 (3)	C6—C7A—C9—C7B	−178.6 (7)
C2—C1—C6—C7A	153.0 (3)	C7A—C8A—C10—O1B	−33.0 (10)
C4—C5—C6—C1	−0.5 (4)	C11—C8A—C10—O1B	148.6 (6)
C4—C5—C6—C8B	165.4 (3)	C7A—C8A—C10—O1A	−172.6 (4)
C4—C5—C6—C7A	−157.0 (3)	C11—C8A—C10—O1A	8.9 (6)
C1—C6—C7A—C8A	90.6 (5)	C7A—C8A—C10—C8B	1.0 (3)
C5—C6—C7A—C8A	−114.2 (4)	C11—C8A—C10—C8B	−177.4 (6)
C8B—C6—C7A—C8A	1.1 (3)	C7B—C8B—C10—O1B	164.3 (3)
C1—C6—C7A—C9	−88.1 (5)	C6—C8B—C10—O1B	−16.6 (4)
C5—C6—C7A—C9	67.1 (5)	C7B—C8B—C10—O1A	15.1 (10)
C8B—C6—C7A—C9	−177.6 (7)	C6—C8B—C10—O1A	−165.8 (8)
C9—C7A—C8A—C10	176.1 (3)	C7B—C8B—C10—C8A	−0.5 (3)
C6—C7A—C8A—C10	−2.7 (6)	C6—C8B—C10—C8A	178.6 (5)
C9—C7A—C8A—C11	−5.2 (6)	C8B—C7B—C11—C12	107.9 (3)
C6—C7A—C8A—C11	176.0 (3)	C9—C7B—C11—C12	−73.6 (4)
C9—C7B—C8B—C10	−175.5 (2)	C8B—C7B—C11—C16	−84.8 (4)
C11—C7B—C8B—C10	3.1 (4)	C9—C7B—C11—C16	93.7 (4)
C9—C7B—C8B—C6	5.4 (4)	C8B—C7B—C11—C8A	−1.8 (3)
C11—C7B—C8B—C6	−176.1 (2)	C9—C7B—C11—C8A	176.7 (5)
C1—C6—C8B—C7B	−113.5 (4)	C7A—C8A—C11—C12	−90.1 (5)
C5—C6—C8B—C7B	80.2 (4)	C10—C8A—C11—C12	88.5 (5)
C7A—C6—C8B—C7B	−1.7 (3)	C7A—C8A—C11—C16	117.7 (4)
C1—C6—C8B—C10	67.4 (4)	C10—C8A—C11—C16	−63.8 (5)
C5—C6—C8B—C10	−98.9 (4)	C7A—C8A—C11—C7B	1.1 (3)
C7A—C6—C8B—C10	179.2 (5)	C10—C8A—C11—C7B	179.6 (6)
C8B—C7B—C9—F1	24.0 (4)	C16—C11—C12—C13	−0.7 (5)
C11—C7B—C9—F1	−154.5 (2)	C7B—C11—C12—C13	167.1 (2)
C8B—C7B—C9—F3	143.1 (3)	C8A—C11—C12—C13	−150.9 (3)
C11—C7B—C9—F3	−35.4 (3)	C11—C12—C13—C14	0.0 (4)
C8B—C7B—C9—F2	−103.9 (3)	C12—C13—C14—C15	0.4 (3)
C11—C7B—C9—F2	77.7 (3)	C13—C14—C15—C16	−0.2 (3)
C8B—C7B—C9—C7A	−2.1 (4)	C12—C11—C16—C15	1.0 (5)
C11—C7B—C9—C7A	179.4 (5)	C7B—C11—C16—C15	−165.8 (3)
C8A—C7A—C9—F1	−155.8 (4)	C8A—C11—C16—C15	153.9 (3)
C6—C7A—C9—F1	22.7 (4)	C14—C15—C16—C11	−0.6 (4)

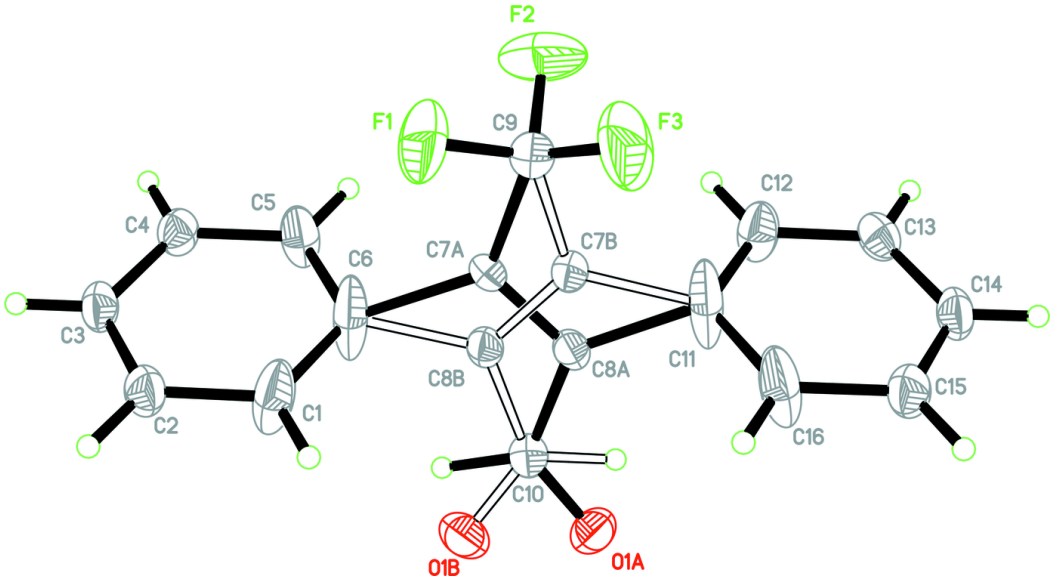
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5A···O1B^{i}	0.93	2.56	3.491 (4)	175

C13—H13A···O1B^{ii}	0.93	2.50	3.375 (4)	158
C12—H12A···O1A^{i}	0.93	2.58	3.506 (5)	178
C2—H2A···Cg1^{iii}	0.93	2.92	3.668 (3)	139
C4—H4A···Cg2^{iv}	0.93	2.90	3.662 (2)	141
C15—H15A···Cg1^{v}	0.93	2.91	3.618 (2)	134

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) −*x*, *y*−1, −*z*+1/2; (iii) −*x*+1/2, *y*+1/2, −*z*+1/2; (iv) *x*, −*y*+1, *z*−1/2; (v) *x*, −*y*+2, *z*+1/2.

Fig. 1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C12
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C4
C13
C7A
C7B
C6
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C8B
C8A
C15
C1
C2
C16
C10
O1B
O1A

Fig. 2

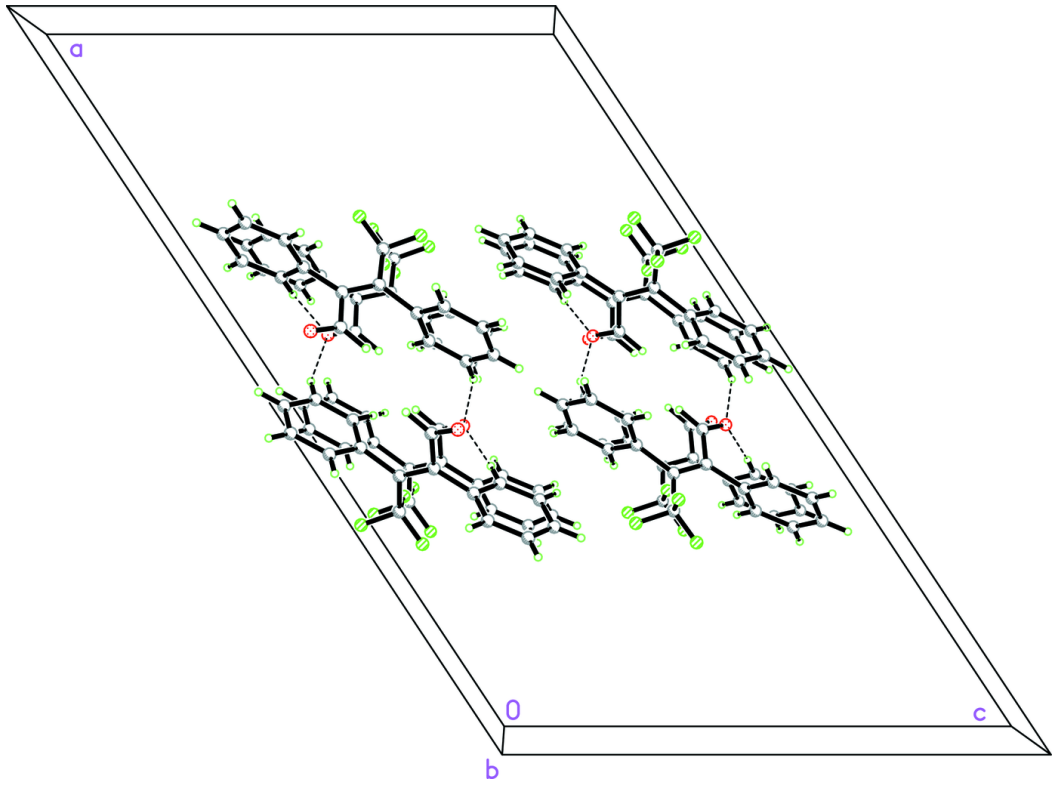

Fig. 3