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1,5-Bis(4-fluorophenyl)penta-1,4-dien-3-one

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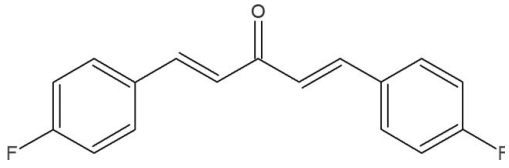
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.094; wR factor = 0.275; data-to-parameter ratio = 18.6.

The title compound, $C_{17}H_{12}FO$, a derivative of the anti-oxidant, antibacterial and anti-inflammatory compound curcumin, crystallizes with three independent molecules (*A*, *B* and *C*) in the asymmetric unit. Molecule *C* is found to have whole-molecule disorder with an approximate 2:1 ratio of occupancies. The mean planes of the two 4-fluorophenyl groups in *A*, *B* and *C* form dihedral angles of 54.8 (2), 54.3 (1) and 52.4 (8)°, respectively. The angles between the mean plane of the penta-1,4-dien-3-one group and those of the two 4-fluorophenyl rings are 26.9 (3) and 33.7 (7)° in molecule *A*, 25.3 (1) and 34.2 (6)° in *B*, and 28.0 (9) and 30.8 (1)° in *C*. The crystal structure is stabilized by intermolecular hydrogen bonds.

Related literature

For the synthesis of the title compound, see: Furniss *et al.* (1989). For biological activity of the title compound and curcumin, see: Reksohadiprodjo *et al.* (2004) and Filler & Kabayashi (1992), respectively. For related structures, see: Harrison *et al.* (2006); Butcher *et al.* (2006).



Experimental

Crystal data

$C_{17}H_{12}F_2O$
M_r = 270.27
Monoclinic, *Cc*
a = 90.019 (14) Å
b = 5.8228 (9) Å
c = 7.5301 (12) Å
β = 90.868 (4)°
V = 3946.5 (11) Å^3
Z = 12
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 173 K
0.50 × 0.25 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
5194 measured reflections
5194 independent reflections
3837 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.094
$wR(F^2)$ = 0.275
S = 1.06
5194 reflections
541 parameters
50 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7*CA*—H7*CA*···O1*CB*^{i}	0.95	2.38	3.260 (8)	153
C11*D*—H11*D*···O1*CA*^{i}	0.95	2.50	3.379 (9)	154

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2006); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* (Bruker, 2000).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2156).

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supplementary materials

Acta Cryst. (2007). E**63**, o3213-o3214 [**doi:10.1107/S1600536807026116**]

1,5-Bis(4-fluorophenyl)penta-1,4-dien-3-one

R. J. Butcher, J. P. Jasinski, B. K. Sarojini, H. S. Yathirajan, S. Bindya and B. Narayana

Comment

The title compound, (I), is a biologically active compound. Derivatives of dibenzylidene acetone, cyclopentanone and cyclohexanone derivatives exhibit potent anti-inflammatory, anti-bacterial and anti-oxidant activity. Certain derivatives inhibit glutathione S-transferace (GST) but do not irritate the gastrointestinal tract. Curcumin, 1,5-di(4-hydroxy-3-methoxyphenyl)penta-1,4-dien-3-one, is a major constituent of turmeric, the commonly used spice. It has been widely used as an anti-inflammatory, anti-bacterial, anti-oxidant, anti-hepatotoxic, hypocholesterolanemia, anti-cyclooxygenase, anti-cancer and radical scavenger agent. It is reported that curcumin is non-toxic at high doses and substitution on the aromatic rings with electron-donating and -withdrawing groups increases anti-inflammatory activity (Reksohadiprodjo *et al.*, 2004). Recently, fluorinated organic compounds have attracted attention due to the ability of fluorine to act as a polar-hydrogen or hydroxyl mimic. Therefore, substitution of hydrogen by fluorine has been a strategy in designing molecules for biological activity studies (Filler & Kabayashi, 1992). Most recently, a redetermination of 1,5-bis(4-methoxyphenyl)penta-1,4-dien-3-one at 120 (2) K (Harrison *et al.*, 2006) and the crystal structure of 1,5-bis(4-chlorophenyl)penta-1,4-dien-3-one have been reported (Butcher *et al.*, 2006).

Experimental

The title compound was synthesized according to the method reported in the literature (Furniss *et al.*, 1989). A solution of of NaOH (25 g) in water (250 ml) and ethanol (200 ml) was placed in a 500 ml bolt head flask fitted with a mechanical stirrer. The flask was immersed in a water bath and the temperature of the solution was maintained at 393–398 K. The solution was stirred vigorously and to it was added one half of a previously prepared mixture of 4-fluorobenzaldehyde (31 g, 0.25 mol) and acetone (7.3 g, 0.125 mol). A flocculent precipitate formed within 2–3 minutes. After 15 minutes, the remainder of the aldehyde-acetone mixture was added and the stirring was continued for a further 30 min. The crude product obtained was filtered and washed with cold water to eliminate the alkali as completely as possible. The compound was purified from ethanol (yield:80%). The crystal growth was done in acetone:toluene (1:1) solvent by the slow evaporation technique; m.p. 383–387 K. Analysis for $C_{17}H_{12}FO$: Found (Calculated): C: 75.44 (75.55); H: 4.42 (4.48).

Refinement

The H atoms were included in the riding model approximation with C—H = 0.95 Å, and with $U_{iso}(H) = 1.17–1.21U_{eq}(C)$.

Figures

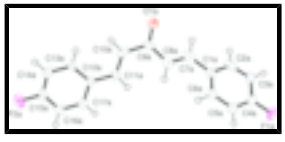

Fig. 1. Molecular structure of molecule A for $C_{17}H_{12}FO$, (I), showing atom labeling and 50% probability displacement ellipsoids.

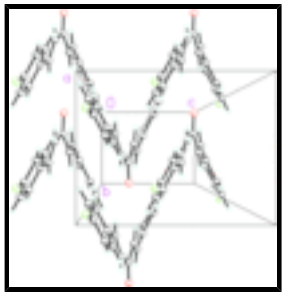

Fig. 2. Packing diagram of $C_{17}H_{12}FO$ viewed down the *a* axis.

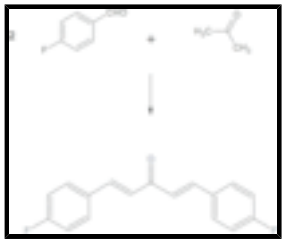

Fig. 3. The formation of the title compound.

1,5-Bis(4-fluorophenyl)penta-1,4-dien-3-one

Crystal data

$C_{17}H_{12}F_2O$	F_{000} = 1680
M_r = 270.27	D_x = 1.365 Mg m^{-3}
Monoclinic, *Cc*	Mo *K*α radiation λ = 0.71073 Å
a = 90.019 (14) Å	Cell parameters from 4065 reflections
b = 5.8228 (9) Å	θ = 2.7–28.1°
c = 7.5301 (12) Å	μ = 0.10 mm^{-1}
β = 90.868 (4)°	*T* = 173 K
V = 3946.5 (11) Å^3	Chunk, colorless
Z = 12	0.50 × 0.25 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer	R_{int} = 0.035
φ and ω scans	θ_{max} = 29.1°
Absorption correction: none	θ_{min} = 0.9°
5194 measured reflections	*h* = −122→122
5194 independent reflections	*k* = 0→7
3837 reflections with $I > 2\sigma(I)$	*l* = 0→10

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.144P)^2 + 6.6257P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.094	$(\Delta/\sigma)_{max}$ = 0.035

$wR(F^2) = 0.275$	$\Delta\rho_{max} = 0.58$ e Å^{-3}
$S = 1.06$	$\Delta\rho_{min} = -0.33$ e Å^{-3}
5194 reflections	Extinction correction: none
541 parameters	Absolute structure: Flack (1983), 4789 Friedel pairs
50 restraints	Flack parameter: 0.0 (13)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
F1A	0.27702 (2)	1.0336 (4)	−0.16569 (16)	0.0621 (6)	
F2A	0.12761 (2)	0.8795 (4)	0.39939 (18)	0.0603 (6)	
O1A	0.20685 (3)	0.1533 (4)	0.0811 (3)	0.0507 (6)	
C1A	0.24120 (3)	0.6308 (5)	−0.0358 (3)	0.0296 (6)	
C2A	0.25580 (3)	0.5584 (5)	−0.0047 (4)	0.0400 (7)	
H2AA	0.2574	0.4113	0.0469	0.048*	
C3A	0.26790 (3)	0.6875 (6)	−0.0444 (4)	0.0417 (8)	
H3AA	0.2777	0.6350	−0.0192	0.050*	
C4A	0.26526 (3)	0.9004 (6)	−0.1237 (3)	0.0372 (7)	
C5A	0.25130 (3)	0.9750 (5)	−0.1640 (3)	0.0315 (6)	
H5AA	0.2499	1.1163	−0.2249	0.038*	
C6A	0.23928 (3)	0.8451 (5)	−0.1163 (3)	0.0310 (6)	
H6AA	0.2295	0.9017	−0.1384	0.037*	
C7A	0.22878 (3)	0.4774 (5)	0.0134 (4)	0.0391 (7)	
H7AA	0.2310	0.3192	0.0286	0.047*	
C8A	0.21516 (3)	0.5388 (5)	0.0376 (3)	0.0342 (7)	
H8AA	0.2123	0.6951	0.0255	0.041*	
C9A	0.20407 (3)	0.3606 (5)	0.0845 (3)	0.0353 (7)	
C10A	0.18896 (3)	0.4326 (5)	0.1406 (4)	0.0385 (7)	
H10A	0.1816	0.3160	0.1452	0.046*	
C11A	0.18483 (3)	0.6404 (5)	0.1841 (3)	0.0311 (6)	
H11A	0.1920	0.7596	0.1791	0.037*	
C12A	0.16973 (3)	0.7010 (5)	0.2404 (3)	0.0283 (6)	
C13A	0.15755 (3)	0.5540 (5)	0.2024 (3)	0.0300 (6)	
H13A	0.1590	0.4146	0.1395	0.036*	
C14A	0.14334 (3)	0.6158 (5)	0.2582 (4)	0.0348 (7)	
H14A	0.1350	0.5184	0.2361	0.042*	
C15A	0.14170 (3)	0.8213 (5)	0.3459 (4)	0.0389 (7)	
C16A	0.15295 (3)	0.9684 (5)	0.3852 (4)	0.0364 (7)	
H16A	0.1512	1.1078	0.4473	0.044*	
C17A	0.16707 (3)	0.9064 (4)	0.3308 (3)	0.0299 (6)	
H17A	0.1752	1.0067	0.3557	0.036*	

F1B	0.11450 (2)	0.3744 (4)	0.4610 (2)	0.0547 (6)	
F2B	−0.03545 (2)	0.5312 (4)	1.0134 (2)	0.0534 (6)	
O1B	0.03519 (3)	−0.3460 (4)	0.7792 (3)	0.0456 (6)	
C1B	0.07269 (3)	0.1959 (5)	0.6194 (3)	0.0272 (6)	
C2B	0.08485 (3)	0.0555 (4)	0.6522 (3)	0.0291 (6)	
H2BA	0.0834	−0.0860	0.7123	0.035*	
C3B	0.09880 (3)	0.1140 (5)	0.6010 (4)	0.0348 (7)	
H3BA	0.1070	0.0153	0.6256	0.042*	
C4B	0.10081 (3)	0.3173 (6)	0.5135 (4)	0.0356 (7)	
C5B	0.08905 (3)	0.4645 (5)	0.4777 (4)	0.0357 (7)	
H5BA	0.0906	0.6053	0.4171	0.043*	
C6B	0.07488 (3)	0.4028 (5)	0.5320 (3)	0.0338 (7)	
H6BA	0.0667	0.5024	0.5092	0.041*	
C7B	0.05745 (3)	0.1417 (5)	0.6736 (3)	0.0283 (6)	
H7BA	0.0505	0.2639	0.6776	0.034*	
C8B	0.05280 (3)	−0.0686 (5)	0.7175 (3)	0.0293 (6)	
H8BA	0.0601	−0.1860	0.7145	0.035*	
C9B	0.03801 (3)	−0.1415 (4)	0.7694 (3)	0.0260 (6)	
C10B	0.02679 (3)	0.0351 (5)	0.8148 (4)	0.0327 (7)	
H10B	0.0297	0.1914	0.8253	0.039*	
C11B	0.01251 (3)	−0.0249 (4)	0.8412 (3)	0.0250 (6)	
H11B	0.0102	−0.1832	0.8281	0.030*	
C12B	0.00010 (3)	0.1266 (5)	0.8881 (3)	0.0287 (6)	
C13B	−0.01418 (3)	0.0495 (5)	0.8496 (3)	0.0271 (6)	
H13B	−0.0157	−0.0957	0.7947	0.032*	
C14B	−0.02632 (3)	0.1887 (5)	0.8927 (4)	0.0353 (7)	
H14B	−0.0362	0.1401	0.8666	0.042*	
C15B	−0.02373 (3)	0.3929 (5)	0.9720 (4)	0.0359 (7)	
C16B	−0.00952 (3)	0.4799 (5)	1.0111 (4)	0.0346 (7)	
H16B	−0.0082	0.6266	1.0642	0.041*	
C17B	0.00251 (3)	0.3412 (5)	0.9686 (4)	0.0312 (6)	
H17B	0.0123	0.3917	0.9940	0.037*	
F1CA	0.44648 (3)	0.4141 (6)	−0.3573 (4)	0.0623 (9)	0.6844 (16)
F2CA	0.29806 (3)	0.5303 (6)	0.2078 (4)	0.0578 (8)	0.6844 (16)
O1CA	0.36780 (3)	−0.3478 (5)	−0.0692 (6)	0.0507 (8)	0.6844 (16)
F1CB	0.44252 (7)	0.5412 (14)	−0.3731 (10)	0.0623 (9)	0.32
F2CB	0.29393 (7)	0.3939 (13)	0.1870 (10)	0.0578 (8)	0.32
O1CB	0.37554 (8)	−0.3589 (12)	−0.0905 (12)	0.0507 (8)	0.32
C1C	0.405100 (18)	0.1904 (3)	−0.2208 (2)	0.0276 (8)	0.6844 (16)
C2C	0.41751 (2)	0.0561 (3)	−0.1830 (3)	0.0289 (9)	0.6844 (16)
H2CA	0.4164	−0.0873	−0.1245	0.035*	0.6844 (16)
C3C	0.431549 (19)	0.1317 (4)	−0.2306 (4)	0.0364 (10)	0.6844 (16)
H3CA	0.4400	0.0399	−0.2047	0.044*	0.6844 (16)
C4C	0.43317 (2)	0.3416 (5)	−0.3161 (4)	0.0306 (9)	0.6844 (16)
C5C	0.42076 (3)	0.4759 (4)	−0.3539 (4)	0.0279 (8)	0.6844 (16)
H5CA	0.4219	0.6193	−0.4124	0.034*	0.6844 (16)
C6C	0.40672 (2)	0.4003 (3)	−0.3063 (3)	0.0253 (8)	0.6844 (16)
H6CA	0.3982	0.4921	−0.3322	0.030*	0.6844 (16)
C1CD	0.40875 (5)	0.1069 (7)	−0.2267 (6)	0.0276 (8)	0.32

C2CD	0.42367 (5)	0.0520 (8)	−0.2028 (7)	0.0289 (9)	0.32
H2CB	0.4264	−0.0918	−0.1527	0.035*	0.3156 (16)
C3CD	0.43457 (4)	0.2075 (10)	−0.2523 (9)	0.0364 (10)	0.32
H3CB	0.4448	0.1700	−0.2360	0.044*	0.3156 (16)
C4CD	0.43054 (6)	0.4180 (10)	−0.3256 (9)	0.0306 (9)	0.32
C5CD	0.41561 (6)	0.4729 (8)	−0.3495 (9)	0.0279 (8)	0.32
H5CB	0.4129	0.6168	−0.3996	0.034*	0.3156 (16)
C6CD	0.40472 (5)	0.3174 (7)	−0.3000 (7)	0.0253 (8)	0.32
H6CB	0.3945	0.3549	−0.3163	0.030*	0.3156 (16)
C9C	0.37021 (4)	−0.1462 (4)	−0.0794 (5)	0.0342 (5)	
C7CA	0.38965 (4)	0.1354 (7)	−0.1664 (5)	0.0314 (8)	0.6844 (16)
H7CA	0.3827	0.2576	−0.1600	0.038*	0.6844 (16)
C8CA	0.38508 (4)	−0.0754 (8)	−0.1261 (6)	0.0346 (10)	0.6844 (16)
H8CA	0.3924	−0.1928	−0.1283	0.042*	0.6844 (16)
C10C	0.35928 (4)	0.0388 (6)	−0.0231 (5)	0.0273 (8)	0.6844 (16)
H10C	0.3623	0.1935	−0.0067	0.033*	0.6844 (16)
C11C	0.34513 (4)	−0.0255 (6)	0.0025 (5)	0.0260 (7)	0.6844 (16)
H11C	0.3426	−0.1827	−0.0133	0.031*	0.6844 (16)
C7CB	0.39565 (10)	−0.0167 (16)	−0.1759 (11)	0.0314 (8)	0.32
H7CB	0.3981	−0.1737	−0.1569	0.038*	0.3156 (16)
C8CB	0.38114 (10)	0.0166 (18)	−0.1467 (13)	0.0346 (10)	0.32
H8CB	0.3775	0.1659	−0.1732	0.042*	0.3156 (16)
C10D	0.35532 (10)	−0.0780 (15)	−0.0381 (11)	0.0273 (8)	0.32
H10D	0.3479	−0.1931	−0.0349	0.033*	0.3156 (16)
C11D	0.35145 (9)	0.1373 (14)	−0.0040 (11)	0.0260 (7)	0.32
H11D	0.3589	0.2513	−0.0197	0.031*	0.3156 (16)
C12C	0.333494 (17)	0.1331 (3)	0.0532 (2)	0.0227 (8)	0.6844 (16)
C13C	0.319100 (19)	0.0514 (3)	0.0286 (3)	0.0256 (8)	0.6844 (16)
H13C	0.3175	−0.0940	−0.0255	0.031*	0.6844 (16)
C14C	0.307097 (17)	0.1826 (4)	0.0830 (4)	0.0325 (9)	0.6844 (16)
H14C	0.2973	0.1268	0.0662	0.039*	0.6844 (16)
C15C	0.30949 (2)	0.3954 (4)	0.1621 (4)	0.0267 (9)	0.6844 (16)
C16C	0.32388 (3)	0.4770 (4)	0.1867 (4)	0.0288 (9)	0.6844 (16)
H16C	0.3255	0.6225	0.2407	0.035*	0.6844 (16)
C17C	0.33589 (2)	0.3459 (3)	0.1322 (3)	0.0242 (8)	0.6844 (16)
H17C	0.3457	0.4017	0.1491	0.029*	0.6844 (16)
C12D	0.33677 (4)	0.2175 (7)	0.0559 (6)	0.0227 (8)	0.32
C13D	0.32559 (5)	0.0627 (8)	0.0101 (7)	0.0256 (8)	0.32
H13D	0.3280	−0.0762	−0.0491	0.031*	0.3156 (16)
C14D	0.31092 (4)	0.1112 (10)	0.0510 (8)	0.0325 (9)	0.32
H14D	0.3033	0.0055	0.0198	0.039*	0.3156 (16)
C15D	0.30742 (4)	0.3145 (11)	0.1377 (8)	0.0267 (9)	0.32
C16D	0.31859 (6)	0.4692 (10)	0.1834 (9)	0.0288 (9)	0.32
H16D	0.3162	0.6082	0.2427	0.035*	0.3156 (16)
C17D	0.33327 (5)	0.4207 (8)	0.1425 (8)	0.0242 (8)	0.32
H17D	0.3409	0.5265	0.1738	0.029*	0.3156 (16)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1A	0.0356 (9)	0.0683 (13)	0.0826 (15)	−0.0186 (9)	0.0055 (9)	0.0110 (12)
F2A	0.0407 (9)	0.0771 (14)	0.0639 (12)	0.0103 (10)	0.0235 (8)	−0.0040 (11)
O1A	0.0467 (11)	0.0380 (12)	0.0679 (15)	0.0046 (10)	0.0145 (10)	0.0030 (11)
C1A	0.0286 (11)	0.0370 (13)	0.0233 (11)	0.0004 (10)	0.0032 (9)	−0.0070 (10)
C2A	0.0576 (17)	0.0244 (12)	0.0377 (15)	0.0124 (12)	−0.0068 (13)	−0.0056 (11)
C3A	0.0292 (12)	0.0463 (16)	0.0497 (17)	0.0055 (12)	0.0006 (12)	0.0048 (14)
C4A	0.0349 (12)	0.0496 (16)	0.0273 (13)	−0.0104 (12)	0.0049 (10)	−0.0032 (12)
C5A	0.0392 (13)	0.0261 (12)	0.0294 (13)	−0.0065 (10)	0.0025 (10)	−0.0001 (10)
C6A	0.0278 (11)	0.0394 (14)	0.0257 (12)	0.0039 (11)	−0.0009 (9)	−0.0016 (11)
C7A	0.0507 (16)	0.0369 (14)	0.0297 (14)	−0.0046 (12)	0.0004 (12)	0.0024 (11)
C8A	0.0312 (12)	0.0361 (13)	0.0352 (14)	0.0015 (11)	0.0002 (10)	−0.0067 (11)
C9A	0.0418 (14)	0.0324 (14)	0.0314 (14)	0.0032 (11)	−0.0072 (11)	−0.0051 (11)
C10A	0.0445 (15)	0.0317 (13)	0.0392 (14)	−0.0131 (11)	−0.0057 (12)	0.0144 (11)
C11A	0.0233 (10)	0.0400 (14)	0.0301 (12)	−0.0008 (10)	0.0012 (9)	−0.0071 (11)
C12A	0.0280 (11)	0.0304 (12)	0.0265 (12)	−0.0001 (10)	−0.0017 (9)	0.0055 (10)
C13A	0.0275 (11)	0.0338 (13)	0.0288 (12)	−0.0002 (10)	0.0014 (9)	−0.0027 (11)
C14A	0.0247 (11)	0.0396 (14)	0.0400 (14)	−0.0037 (11)	−0.0002 (10)	0.0097 (12)
C15A	0.0416 (14)	0.0482 (16)	0.0271 (13)	0.0147 (12)	0.0092 (11)	0.0026 (12)
C16A	0.0495 (15)	0.0321 (13)	0.0280 (13)	0.0050 (12)	0.0061 (11)	0.0027 (11)
C17A	0.0405 (13)	0.0239 (11)	0.0253 (11)	−0.0048 (10)	−0.0006 (10)	−0.0052 (10)
F1B	0.0345 (9)	0.0549 (11)	0.0748 (14)	−0.0174 (9)	0.0101 (9)	0.0090 (10)
F2B	0.0378 (9)	0.0656 (12)	0.0569 (12)	0.0209 (9)	0.0065 (8)	−0.0092 (10)
O1B	0.0501 (12)	0.0207 (9)	0.0663 (15)	0.0024 (9)	0.0086 (11)	0.0016 (10)
C1B	0.0268 (11)	0.0370 (13)	0.0178 (11)	−0.0028 (10)	0.0050 (9)	−0.0005 (10)
C2B	0.0401 (13)	0.0184 (11)	0.0289 (13)	0.0015 (10)	−0.0021 (10)	−0.0008 (10)
C3B	0.0330 (13)	0.0378 (15)	0.0338 (14)	0.0066 (12)	0.0064 (11)	0.0021 (12)
C4B	0.0225 (11)	0.0398 (15)	0.0447 (16)	−0.0039 (11)	0.0065 (11)	−0.0066 (13)
C5B	0.0517 (16)	0.0265 (13)	0.0290 (13)	−0.0072 (12)	0.0035 (12)	0.0037 (11)
C6B	0.0354 (13)	0.0369 (14)	0.0289 (13)	0.0106 (11)	−0.0032 (10)	−0.0119 (11)
C7B	0.0323 (12)	0.0256 (12)	0.0269 (12)	0.0093 (10)	0.0024 (10)	−0.0069 (10)
C8B	0.0199 (10)	0.0421 (14)	0.0262 (11)	−0.0023 (10)	0.0113 (9)	0.0048 (11)
C9B	0.0204 (9)	0.0256 (11)	0.0323 (12)	0.0037 (9)	0.0096 (9)	−0.0056 (10)
C10B	0.0308 (12)	0.0289 (13)	0.0386 (14)	0.0013 (10)	0.0086 (11)	−0.0116 (11)
C11B	0.0218 (10)	0.0242 (11)	0.0291 (12)	−0.0032 (9)	0.0061 (9)	0.0013 (10)
C12B	0.0273 (11)	0.0279 (12)	0.0311 (13)	0.0072 (10)	0.0033 (10)	−0.0021 (10)
C13B	0.0245 (11)	0.0293 (12)	0.0276 (12)	−0.0002 (10)	0.0059 (9)	−0.0040 (10)
C14B	0.0251 (11)	0.0477 (16)	0.0331 (14)	−0.0032 (12)	0.0006 (10)	0.0069 (13)
C15B	0.0270 (12)	0.0405 (15)	0.0406 (15)	0.0102 (11)	0.0079 (11)	−0.0010 (13)
C16B	0.0427 (15)	0.0309 (14)	0.0301 (14)	−0.0022 (12)	0.0014 (11)	−0.0019 (11)
C17B	0.0279 (12)	0.0348 (14)	0.0309 (13)	−0.0037 (11)	0.0033 (10)	0.0031 (11)
F1CA	0.0393 (12)	0.083 (2)	0.0649 (14)	−0.0235 (13)	0.0191 (11)	−0.0180 (17)
F2CA	0.0422 (13)	0.0632 (18)	0.0680 (16)	0.0179 (13)	0.0017 (12)	−0.0168 (15)
O1CA	0.0414 (17)	0.0303 (10)	0.0809 (17)	−0.0108 (16)	0.0130 (17)	−0.0017 (18)
F1CB	0.0393 (12)	0.083 (2)	0.0649 (14)	−0.0235 (13)	0.0191 (11)	−0.0180 (17)

F2CB	0.0422 (13)	0.0632 (18)	0.0680 (16)	0.0179 (13)	0.0017 (12)	−0.0168 (15)
O1CB	0.0414 (17)	0.0303 (10)	0.0809 (17)	−0.0108 (16)	0.0130 (17)	−0.0017 (18)
C1C	0.0400 (17)	0.0231 (19)	0.0196 (13)	−0.0020 (14)	−0.0004 (12)	−0.0015 (13)
C2C	0.028 (2)	0.0340 (15)	0.0244 (14)	0.0012 (16)	−0.0020 (14)	0.0006 (12)
C3C	0.0444 (19)	0.030 (2)	0.0345 (17)	0.0000 (17)	0.0019 (15)	−0.0008 (16)
C4C	0.0306 (15)	0.025 (2)	0.0364 (16)	−0.0028 (14)	0.0039 (12)	−0.0045 (15)
C5C	0.027 (2)	0.0336 (14)	0.0235 (13)	−0.0114 (15)	0.0017 (13)	0.0035 (11)
C6C	0.0295 (14)	0.0172 (19)	0.0290 (14)	−0.0061 (14)	−0.0007 (11)	−0.0018 (14)
C1CD	0.0400 (17)	0.0231 (19)	0.0196 (13)	−0.0020 (14)	−0.0004 (12)	−0.0015 (13)
C2CD	0.028 (2)	0.0340 (15)	0.0244 (14)	0.0012 (16)	−0.0020 (14)	0.0006 (12)
C3CD	0.0444 (19)	0.030 (2)	0.0345 (17)	0.0000 (17)	0.0019 (15)	−0.0008 (16)
C4CD	0.0306 (15)	0.025 (2)	0.0364 (16)	−0.0028 (14)	0.0039 (12)	−0.0045 (15)
C5CD	0.027 (2)	0.0336 (14)	0.0235 (13)	−0.0114 (15)	0.0017 (13)	0.0035 (11)
C6CD	0.0295 (14)	0.0172 (19)	0.0290 (14)	−0.0061 (14)	−0.0007 (11)	−0.0018 (14)
C9C	0.0316 (10)	0.0308 (10)	0.0403 (12)	−0.0035 (15)	−0.0008 (9)	0.0014 (16)
C7CA	0.0360 (17)	0.0346 (16)	0.0236 (15)	0.0085 (13)	−0.0015 (13)	−0.0059 (14)
C8CA	0.0253 (16)	0.040 (2)	0.0391 (17)	0.0028 (15)	0.0026 (14)	−0.0049 (18)
C10C	0.0328 (16)	0.0210 (16)	0.0282 (15)	−0.0005 (13)	0.0042 (13)	0.0019 (14)
C11C	0.0266 (15)	0.0231 (14)	0.0283 (16)	0.0018 (12)	−0.0021 (12)	−0.0070 (13)
C7CB	0.0360 (17)	0.0346 (16)	0.0236 (15)	0.0085 (13)	−0.0015 (13)	−0.0059 (14)
C8CB	0.0253 (16)	0.040 (2)	0.0391 (17)	0.0028 (15)	0.0026 (14)	−0.0049 (18)
C10D	0.0328 (16)	0.0210 (16)	0.0282 (15)	−0.0005 (13)	0.0042 (13)	0.0019 (14)
C11D	0.0266 (15)	0.0231 (14)	0.0283 (16)	0.0018 (12)	−0.0021 (12)	−0.0070 (13)
C12C	0.0214 (14)	0.0251 (19)	0.0214 (12)	−0.0034 (13)	−0.0077 (10)	0.0012 (14)
C13C	0.0082 (14)	0.0335 (16)	0.0351 (16)	0.0028 (14)	−0.0035 (14)	0.0026 (13)
C14C	0.0238 (16)	0.042 (2)	0.0316 (16)	−0.0044 (15)	−0.0074 (13)	0.0026 (16)
C15C	0.0240 (14)	0.026 (2)	0.0296 (15)	−0.0017 (14)	−0.0015 (12)	−0.0079 (15)
C16C	0.018 (2)	0.0306 (15)	0.0371 (16)	−0.0057 (15)	−0.0082 (15)	0.0037 (12)
C17C	0.0299 (15)	0.0127 (17)	0.0299 (14)	0.0041 (13)	−0.0044 (12)	0.0005 (14)
C12D	0.0214 (14)	0.0251 (19)	0.0214 (12)	−0.0034 (13)	−0.0077 (10)	0.0012 (14)
C13D	0.0082 (14)	0.0335 (16)	0.0351 (16)	0.0028 (14)	−0.0035 (14)	0.0026 (13)
C14D	0.0238 (16)	0.042 (2)	0.0316 (16)	−0.0044 (15)	−0.0074 (13)	0.0026 (16)
C15D	0.0240 (14)	0.026 (2)	0.0296 (15)	−0.0017 (14)	−0.0015 (12)	−0.0079 (15)
C16D	0.018 (2)	0.0306 (15)	0.0371 (16)	−0.0057 (15)	−0.0082 (15)	0.0037 (12)
C17D	0.0299 (15)	0.0127 (17)	0.0299 (14)	0.0041 (13)	−0.0044 (12)	0.0005 (14)

Geometric parameters (Å, °)

F1A—C4A	1.354 (3)	F1CA—C4C	1.313 (3)
F2A—C15A	1.379 (3)	F2CA—C15C	1.343 (3)
O1A—C9A	1.233 (4)	O1CA—C9C	1.197 (4)
C1A—C2A	1.397 (4)	F1CB—C4CD	1.348 (8)
C1A—C6A	1.397 (4)	F2CB—C15D	1.356 (7)
C1A—C7A	1.482 (4)	O1CB—C9C	1.331 (8)
C2A—C3A	1.360 (4)	C1C—C2C	1.3900
C2A—H2AA	0.9500	C1C—C6C	1.3900
C3A—C4A	1.395 (4)	C1C—C7CA	1.491 (4)
C3A—H3AA	0.9500	C2C—C3C	1.3900
C4A—C5A	1.360 (4)	C2C—H2CA	0.9500

C5A—C6A	1.372 (4)	C3C—C4C	1.3900
C5A—H5AA	0.9500	C3C—H3CA	0.9500
C6A—H6AA	0.9500	C4C—C5C	1.3900
C7A—C8A	1.293 (4)	C5C—C6C	1.3900
C7A—H7AA	0.9500	C5C—H5CA	0.9500
C8A—C9A	1.486 (4)	C6C—H6CA	0.9500
C8A—H8AA	0.9500	C1CD—C2CD	1.3900
C9A—C10A	1.491 (4)	C1CD—C6CD	1.3900
C10A—C11A	1.309 (4)	C1CD—C7CB	1.438 (10)
C10A—H10A	0.9500	C2CD—C3CD	1.3900
C11A—C12A	1.473 (4)	C2CD—H2CB	0.9500
C11A—H11A	0.9500	C3CD—C4CD	1.3900
C12A—C17A	1.399 (4)	C3CD—H3CB	0.9500
C12A—C13A	1.417 (4)	C4CD—C5CD	1.3900
C13A—C14A	1.399 (4)	C5CD—C6CD	1.3900
C13A—H13A	0.9500	C5CD—H5CB	0.9500
C14A—C15A	1.376 (4)	C6CD—H6CB	0.9500
C14A—H14A	0.9500	C9C—C10D	1.437 (9)
C15A—C16A	1.356 (4)	C9C—C8CA	1.449 (5)
C16A—C17A	1.389 (4)	C9C—C8CB	1.462 (10)
C16A—H16A	0.9500	C9C—C10C	1.523 (5)
C17A—H17A	0.9500	C7CA—C8CA	1.331 (6)
F1B—C4B	1.342 (3)	C7CA—H7CA	0.9500
F2B—C15B	1.367 (3)	C8CA—H8CA	0.9500
O1B—C9B	1.220 (3)	C10C—C11C	1.344 (5)
C1B—C2B	1.385 (4)	C10C—H10C	0.9500
C1B—C6B	1.389 (4)	C11C—C12C	1.452 (4)
C1B—C7B	1.471 (4)	C11C—H11C	0.9500
C2B—C3B	1.363 (4)	C7CB—C8CB	1.342 (12)
C2B—H2BA	0.9500	C7CB—H7CB	0.9500
C3B—C4B	1.368 (4)	C8CB—H8CB	0.9500
C3B—H3BA	0.9500	C10D—C11D	1.327 (12)
C4B—C5B	1.385 (4)	C10D—H10D	0.9500
C5B—C6B	1.392 (4)	C11D—C12D	1.479 (9)
C5B—H5BA	0.9500	C11D—H11D	0.9500
C6B—H6BA	0.9500	C12C—C13C	1.3900
C7B—C8B	1.338 (4)	C12C—C17C	1.3900
C7B—H7BA	0.9500	C13C—C14C	1.3900
C8B—C9B	1.457 (3)	C13C—H13C	0.9500
C8B—H8BA	0.9500	C14C—C15C	1.3900
C9B—C10B	1.485 (4)	C14C—H14C	0.9500
C10B—C11B	1.349 (4)	C15C—C16C	1.3900
C10B—H10B	0.9500	C16C—C17C	1.3900
C11B—C12B	1.470 (4)	C16C—H16C	0.9500
C11B—H11B	0.9500	C17C—H17C	0.9500
C12B—C13B	1.389 (4)	C12D—C13D	1.3900
C12B—C17B	1.404 (4)	C12D—C17D	1.3900
C13B—C14B	1.403 (4)	C13D—C14D	1.3900
C13B—H13B	0.9500	C13D—H13D	0.9500

C14B—C15B	1.349 (4)	C14D—C15D	1.3900
C14B—H14B	0.9500	C14D—H14D	0.9500
C15B—C16B	1.403 (4)	C15D—C16D	1.3900
C16B—C17B	1.392 (4)	C16D—C17D	1.3900
C16B—H16B	0.9500	C16D—H16D	0.9500
C17B—H17B	0.9500	C17D—H17D	0.9500
C2A—C1A—C6A	116.9 (2)	C1C—C2C—H2CA	120.0
C2A—C1A—C7A	119.2 (3)	C2C—C3C—C4C	120.0
C6A—C1A—C7A	123.9 (2)	C2C—C3C—H3CA	120.0
C3A—C2A—C1A	123.4 (3)	C4C—C3C—H3CA	120.0
C3A—C2A—H2AA	118.3	F1CA—C4C—C3C	119.7 (2)
C1A—C2A—H2AA	118.3	F1CA—C4C—C5C	120.3 (2)
C2A—C3A—C4A	117.0 (3)	C3C—C4C—C5C	120.0
C2A—C3A—H3AA	121.5	C6C—C5C—C4C	120.0
C4A—C3A—H3AA	121.5	C6C—C5C—H5CA	120.0
F1A—C4A—C5A	119.2 (3)	C4C—C5C—H5CA	120.0
F1A—C4A—C3A	118.7 (3)	C5C—C6C—C1C	120.0
C5A—C4A—C3A	122.0 (3)	C5C—C6C—H6CA	120.0
C4A—C5A—C6A	119.7 (3)	C1C—C6C—H6CA	120.0
C4A—C5A—H5AA	120.2	C2CD—C1CD—C6CD	120.0
C6A—C5A—H5AA	120.2	C2CD—C1CD—C7CB	130.2 (4)
C5A—C6A—C1A	120.9 (2)	C6CD—C1CD—C7CB	109.7 (4)
C5A—C6A—H6AA	119.6	C3CD—C2CD—C1CD	120.0
C1A—C6A—H6AA	119.6	C3CD—C2CD—H2CB	120.0
C8A—C7A—C1A	126.1 (3)	C1CD—C2CD—H2CB	120.0
C8A—C7A—H7AA	116.9	C4CD—C3CD—C2CD	120.0
C1A—C7A—H7AA	116.9	C4CD—C3CD—H3CB	120.0
C7A—C8A—C9A	118.9 (3)	C2CD—C3CD—H3CB	120.0
C7A—C8A—H8AA	120.6	F1CB—C4CD—C3CD	111.7 (5)
C9A—C8A—H8AA	120.6	F1CB—C4CD—C5CD	128.2 (5)
O1A—C9A—C8A	122.8 (3)	C3CD—C4CD—C5CD	120.0
O1A—C9A—C10A	117.8 (3)	C6CD—C5CD—C4CD	120.0
C8A—C9A—C10A	119.4 (2)	C6CD—C5CD—H5CB	120.0
C11A—C10A—C9A	126.5 (3)	C4CD—C5CD—H5CB	120.0
C11A—C10A—H10A	116.8	C5CD—C6CD—C1CD	120.0
C9A—C10A—H10A	116.8	C5CD—C6CD—H6CB	120.0
C10A—C11A—C12A	124.1 (3)	C1CD—C6CD—H6CB	120.0
C10A—C11A—H11A	118.0	O1CA—C9C—O1CB	32.6 (3)
C12A—C11A—H11A	118.0	O1CA—C9C—C10D	95.0 (4)
C17A—C12A—C13A	118.5 (2)	O1CB—C9C—C10D	127.5 (5)
C17A—C12A—C11A	120.7 (2)	O1CA—C9C—C8CA	117.7 (3)
C13A—C12A—C11A	120.8 (2)	O1CB—C9C—C8CA	85.1 (4)
C14A—C13A—C12A	119.5 (2)	C10D—C9C—C8CA	147.4 (4)
C14A—C13A—H13A	120.3	O1CA—C9C—C8CB	141.4 (5)
C12A—C13A—H13A	120.2	O1CB—C9C—C8CB	109.6 (6)
C15A—C14A—C13A	118.2 (3)	C10D—C9C—C8CB	122.1 (6)
C15A—C14A—H14A	120.9	C8CA—C9C—C8CB	26.2 (4)
C13A—C14A—H14A	120.9	O1CA—C9C—C10C	123.9 (4)
C16A—C15A—C14A	124.7 (3)	O1CB—C9C—C10C	155.5 (5)

C16A—C15A—F2A	117.9 (3)	C10D—C9C—C10C	30.2 (4)
C14A—C15A—F2A	117.4 (3)	C8CA—C9C—C10C	118.0 (3)
C15A—C16A—C17A	117.1 (3)	C8CB—C9C—C10C	94.5 (4)
C15A—C16A—H16A	121.5	C8CA—C7CA—C1C	123.6 (3)
C17A—C16A—H16A	121.5	C8CA—C7CA—H7CA	118.2
C16A—C17A—C12A	122.0 (2)	C1C—C7CA—H7CA	118.2
C16A—C17A—H17A	119.0	C7CA—C8CA—C9C	127.4 (4)
C12A—C17A—H17A	119.0	C7CA—C8CA—H8CA	116.3
C2B—C1B—C6B	118.6 (2)	C9C—C8CA—H8CA	116.3
C2B—C1B—C7B	124.2 (2)	C11C—C10C—C9C	117.4 (3)
C6B—C1B—C7B	117.2 (2)	C11C—C10C—H10C	121.3
C3B—C2B—C1B	122.1 (3)	C9C—C10C—H10C	121.3
C3B—C2B—H2BA	118.9	C10C—C11C—C12C	123.3 (3)
C1B—C2B—H2BA	119.0	C10C—C11C—H11C	118.3
C2B—C3B—C4B	118.8 (3)	C12C—C11C—H11C	118.3
C2B—C3B—H3BA	120.6	C8CB—C7CB—C1CD	140.8 (9)
C4B—C3B—H3BA	120.6	C8CB—C7CB—H7CB	109.6
F1B—C4B—C3B	119.0 (3)	C1CD—C7CB—H7CB	109.6
F1B—C4B—C5B	119.4 (3)	C7CB—C8CB—C9C	128.7 (9)
C3B—C4B—C5B	121.5 (3)	C7CB—C8CB—H8CB	115.7
C4B—C5B—C6B	118.9 (3)	C9C—C8CB—H8CB	115.7
C4B—C5B—H5BA	120.5	C11D—C10D—C9C	123.5 (7)
C6B—C5B—H5BA	120.5	C11D—C10D—H10D	118.3
C1B—C6B—C5B	120.0 (3)	C9C—C10D—H10D	118.3
C1B—C6B—H6BA	120.0	C10D—C11D—C12D	126.6 (7)
C5B—C6B—H6BA	120.0	C10D—C11D—H11D	116.7
C8B—C7B—C1B	124.2 (2)	C12D—C11D—H11D	116.7
C8B—C7B—H7BA	117.9	C13C—C12C—C17C	120.0
C1B—C7B—H7BA	117.9	C13C—C12C—C11C	114.99 (17)
C7B—C8B—C9B	128.6 (3)	C17C—C12C—C11C	124.87 (17)
C7B—C8B—H8BA	115.7	C12C—C13C—C14C	120.0
C9B—C8B—H8BA	115.7	C12C—C13C—H13C	120.0
O1B—C9B—C8B	119.5 (2)	C14C—C13C—H13C	120.0
O1B—C9B—C10B	121.3 (2)	C15C—C14C—C13C	120.0
C8B—C9B—C10B	119.2 (2)	C15C—C14C—H14C	120.0
C11B—C10B—C9B	120.5 (2)	C13C—C14C—H14C	120.0
C11B—C10B—H10B	119.7	F2CA—C15C—C16C	118.8 (2)
C9B—C10B—H10B	119.7	F2CA—C15C—C14C	121.1 (2)
C10B—C11B—C12B	127.5 (2)	C16C—C15C—C14C	120.0
C10B—C11B—H11B	116.2	C15C—C16C—C17C	120.0
C12B—C11B—H11B	116.2	C15C—C16C—H16C	120.0
C13B—C12B—C17B	120.9 (2)	C17C—C16C—H16C	120.0
C13B—C12B—C11B	117.4 (2)	C16C—C17C—C12C	120.0
C17B—C12B—C11B	121.6 (2)	C16C—C17C—H17C	120.0
C12B—C13B—C14B	119.2 (3)	C12C—C17C—H17C	120.0
C12B—C13B—H13B	120.4	C13D—C12D—C17D	120.0
C14B—C13B—H13B	120.4	C13D—C12D—C11D	111.5 (4)
C15B—C14B—C13B	118.8 (3)	C17D—C12D—C11D	128.5 (4)
C15B—C14B—H14B	120.6	C14D—C13D—C12D	120.0

C13B—C14B—H14B	120.6	C14D—C13D—H13D	120.0
C14B—C15B—F2B	119.4 (3)	C12D—C13D—H13D	120.0
C14B—C15B—C16B	124.2 (3)	C13D—C14D—C15D	120.0
F2B—C15B—C16B	116.3 (3)	C13D—C14D—H14D	120.0
C17B—C16B—C15B	116.9 (3)	C15D—C14D—H14D	120.0
C17B—C16B—H16B	121.6	F2CB—C15D—C14D	129.0 (5)
C15B—C16B—H16B	121.6	F2CB—C15D—C16D	111.0 (5)
C16B—C17B—C12B	120.0 (2)	C14D—C15D—C16D	120.0
C16B—C17B—H17B	120.0	C17D—C16D—C15D	120.0
C12B—C17B—H17B	120.0	C17D—C16D—H16D	120.0
C2C—C1C—C6C	120.0	C15D—C16D—H16D	120.0
C2C—C1C—C7CA	124.98 (18)	C16D—C17D—C12D	120.0
C6C—C1C—C7CA	114.90 (18)	C16D—C17D—H17D	120.0
C3C—C2C—C1C	120.0	C12D—C17D—H17D	120.0
C3C—C2C—H2CA	120.0		
C6A—C1A—C2A—C3A	1.8 (4)	C3C—C4C—C5C—C6C	0.0
C7A—C1A—C2A—C3A	−179.6 (3)	C4C—C5C—C6C—C1C	0.0
C1A—C2A—C3A—C4A	−1.4 (4)	C2C—C1C—C6C—C5C	0.0
C2A—C3A—C4A—F1A	−179.8 (2)	C7CA—C1C—C6C—C5C	176.26 (19)
C2A—C3A—C4A—C5A	−1.5 (4)	C6CD—C1CD—C2CD—C3CD	0.0
F1A—C4A—C5A—C6A	−177.7 (2)	C7CB—C1CD—C2CD—C3CD	−175.4 (6)
C3A—C4A—C5A—C6A	4.0 (4)	C1CD—C2CD—C3CD—C4CD	0.0
C4A—C5A—C6A—C1A	−3.7 (4)	C2CD—C3CD—C4CD—F1CB	−177.0 (6)
C2A—C1A—C6A—C5A	0.8 (4)	C2CD—C3CD—C4CD—C5CD	0.0
C7A—C1A—C6A—C5A	−177.7 (2)	F1CB—C4CD—C5CD—C6CD	176.5 (7)
C2A—C1A—C7A—C8A	160.4 (3)	C3CD—C4CD—C5CD—C6CD	0.0
C6A—C1A—C7A—C8A	−21.0 (4)	C4CD—C5CD—C6CD—C1CD	0.0
C1A—C7A—C8A—C9A	179.3 (2)	C2CD—C1CD—C6CD—C5CD	0.0
C7A—C8A—C9A—O1A	−8.8 (4)	C7CB—C1CD—C6CD—C5CD	176.2 (5)
C7A—C8A—C9A—C10A	170.4 (3)	C2C—C1C—C7CA—C8CA	−22.0 (5)
O1A—C9A—C10A—C11A	166.4 (3)	C6C—C1C—C7CA—C8CA	161.9 (3)
C8A—C9A—C10A—C11A	−12.9 (4)	C1C—C7CA—C8CA—C9C	−177.2 (3)
C9A—C10A—C11A—C12A	−179.3 (2)	O1CA—C9C—C8CA—C7CA	170.8 (4)
C10A—C11A—C12A—C17A	162.1 (3)	O1CB—C9C—C8CA—C7CA	171.6 (6)
C10A—C11A—C12A—C13A	−18.7 (4)	C10D—C9C—C8CA—C7CA	−7.3 (12)
C17A—C12A—C13A—C14A	−1.0 (4)	C8CB—C9C—C8CA—C7CA	11.5 (9)
C11A—C12A—C13A—C14A	179.8 (2)	C10C—C9C—C8CA—C7CA	−17.0 (6)
C12A—C13A—C14A—C15A	1.2 (4)	O1CA—C9C—C10C—C11C	−14.9 (6)
C13A—C14A—C15A—C16A	−1.1 (4)	O1CB—C9C—C10C—C11C	−27.6 (14)
C13A—C14A—C15A—F2A	179.8 (2)	C10D—C9C—C10C—C11C	3.9 (7)
C14A—C15A—C16A—C17A	0.7 (4)	C8CA—C9C—C10C—C11C	173.4 (4)
F2A—C15A—C16A—C17A	179.8 (2)	C8CB—C9C—C10C—C11C	161.2 (5)
C15A—C16A—C17A—C12A	−0.5 (4)	C9C—C10C—C11C—C12C	−178.9 (3)
C13A—C12A—C17A—C16A	0.7 (4)	C2CD—C1CD—C7CB—C8CB	159.8 (10)
C11A—C12A—C17A—C16A	179.9 (2)	C6CD—C1CD—C7CB—C8CB	−15.9 (13)
C6B—C1B—C2B—C3B	−0.2 (4)	C1CD—C7CB—C8CB—C9C	−174.4 (8)
C7B—C1B—C2B—C3B	−179.3 (2)	O1CA—C9C—C8CB—C7CB	−24.8 (16)
C1B—C2B—C3B—C4B	−0.4 (4)	O1CB—C9C—C8CB—C7CB	−15.8 (12)
C2B—C3B—C4B—F1B	−179.2 (3)	C10D—C9C—C8CB—C7CB	173.5 (9)

C2B—C3B—C4B—C5B	0.6 (4)	C8CA—C9C—C8CB—C7CB	5.4 (6)
F1B—C4B—C5B—C6B	179.6 (3)	C10C—C9C—C8CB—C7CB	160.3 (10)
C3B—C4B—C5B—C6B	−0.2 (4)	O1CA—C9C—C10D—C11D	169.9 (8)
C2B—C1B—C6B—C5B	0.6 (4)	O1CB—C9C—C10D—C11D	169.7 (8)
C7B—C1B—C6B—C5B	179.8 (2)	C8CA—C9C—C10D—C11D	−11.8 (15)
C4B—C5B—C6B—C1B	−0.5 (4)	C8CB—C9C—C10D—C11D	−21.4 (11)
C2B—C1B—C7B—C8B	−18.2 (4)	C10C—C9C—C10D—C11D	5.5 (5)
C6B—C1B—C7B—C8B	162.7 (3)	C9C—C10D—C11D—C12D	−173.8 (6)
C1B—C7B—C8B—C9B	−178.7 (2)	C10C—C11C—C12C—C13C	163.8 (3)
C7B—C8B—C9B—O1B	169.0 (3)	C10C—C11C—C12C—C17C	−20.5 (4)
C7B—C8B—C9B—C10B	−12.9 (4)	C17C—C12C—C13C—C14C	0.0
O1B—C9B—C10B—C11B	−10.4 (4)	C11C—C12C—C13C—C14C	175.9 (2)
C8B—C9B—C10B—C11B	171.5 (2)	C12C—C13C—C14C—C15C	0.0
C9B—C10B—C11B—C12B	179.5 (2)	C13C—C14C—C15C—F2CA	176.7 (3)
C10B—C11B—C12B—C13B	158.1 (3)	C13C—C14C—C15C—C16C	0.0
C10B—C11B—C12B—C17B	−21.8 (4)	F2CA—C15C—C16C—C17C	−176.7 (3)
C17B—C12B—C13B—C14B	−0.3 (4)	C14C—C15C—C16C—C17C	0.0
C11B—C12B—C13B—C14B	179.8 (2)	C15C—C16C—C17C—C12C	0.0
C12B—C13B—C14B—C15B	−0.6 (4)	C13C—C12C—C17C—C16C	0.0
C13B—C14B—C15B—F2B	179.4 (2)	C11C—C12C—C17C—C16C	−175.4 (2)
C13B—C14B—C15B—C16B	1.6 (5)	C10D—C11D—C12D—C13D	−23.1 (10)
C14B—C15B—C16B—C17B	−1.7 (5)	C10D—C11D—C12D—C17D	158.8 (7)
F2B—C15B—C16B—C17B	−179.6 (2)	C17D—C12D—C13D—C14D	0.0
C15B—C16B—C17B—C12B	0.8 (4)	C11D—C12D—C13D—C14D	−178.3 (4)
C13B—C12B—C17B—C16B	0.1 (4)	C12D—C13D—C14D—C15D	0.0
C11B—C12B—C17B—C16B	−180.0 (3)	C13D—C14D—C15D—F2CB	179.2 (7)
C6C—C1C—C2C—C3C	0.0	C13D—C14D—C15D—C16D	0.0
C7CA—C1C—C2C—C3C	−175.9 (2)	F2CB—C15D—C16D—C17D	−179.3 (5)
C1C—C2C—C3C—C4C	0.0	C14D—C15D—C16D—C17D	0.0
C2C—C3C—C4C—F1CA	178.6 (3)	C15D—C16D—C17D—C12D	0.0
C2C—C3C—C4C—C5C	0.0	C13D—C12D—C17D—C16D	0.0
F1CA—C4C—C5C—C6C	−178.6 (3)	C11D—C12D—C17D—C16D	178.0 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7CA—H7CA···O1CB^{i}	0.95	2.38	3.260 (8)	153
C11D—H11D···O1CA^{i}	0.95	2.50	3.379 (9)	154

Symmetry codes: (i) *x*, *y*+1, *z*.

Fig. 1

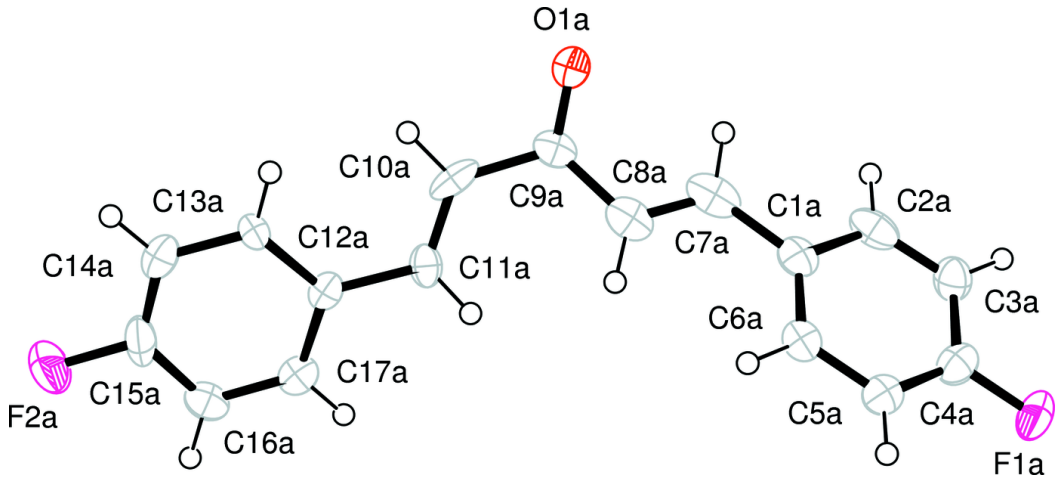
O1a
C10a
C9a
C8a
C1a
C2a
C13a
C12a
C7a
C14a
C11a
C3a
C6a
C17a
C15a
F2a
C5a
C4a
C16a
F1a

Fig. 2

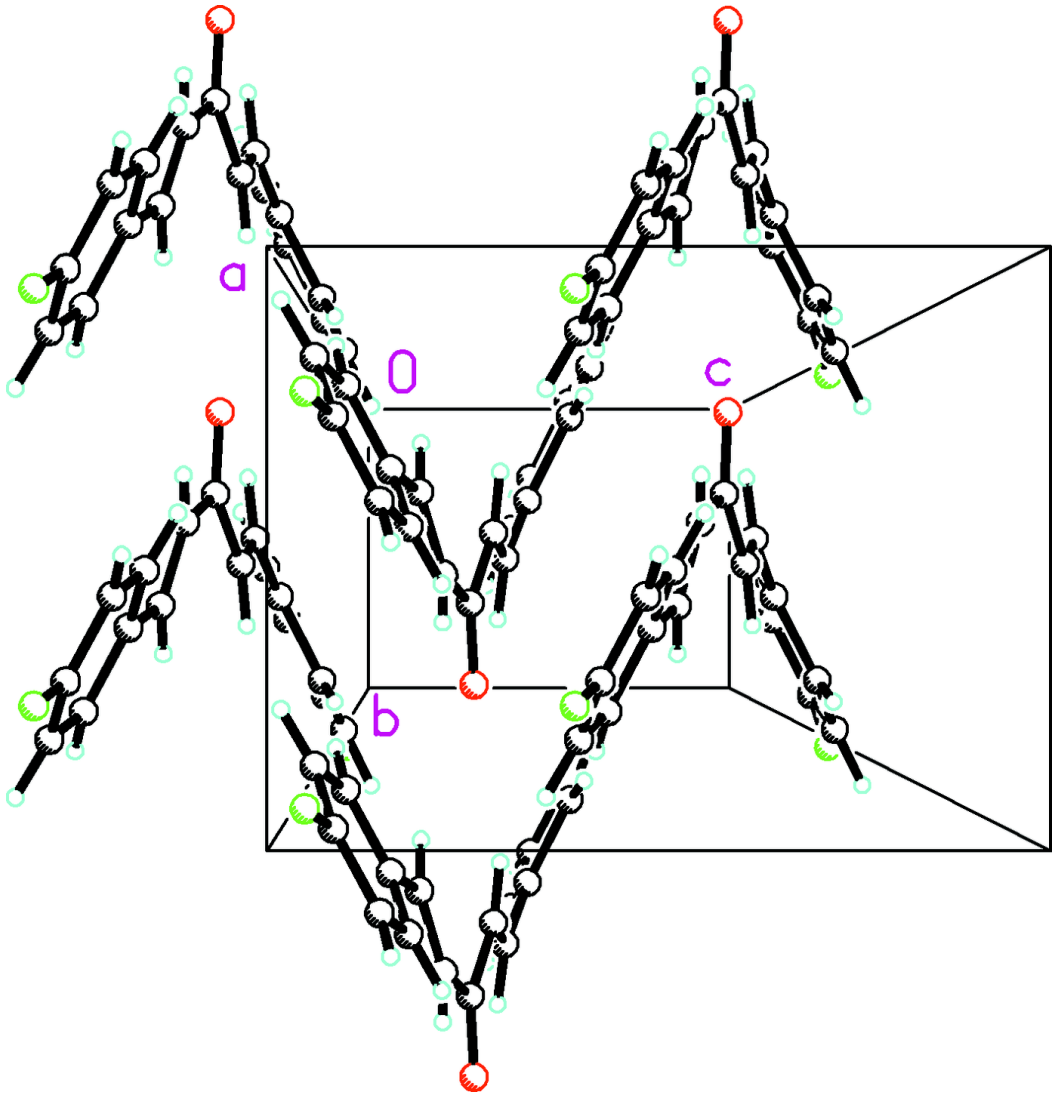

Fig. 3