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3-(Biphenyl-4-yl)-1-(4-fluorophenyl)-prop-2-en-1-one

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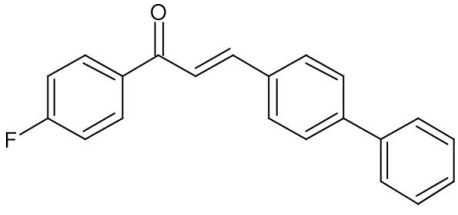
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.006 Å; R factor = 0.053; wR factor = 0.150; data-to-parameter ratio = 6.6.

The title compound, $C_{21}H_{15}FO$, crystallizes with two molecules in the asymmetric unit, which differ only in the signs of their torsion angles. Nevertheless, the two molecules are not related by any crystallographic symmetry element. The dihedral angles between the two phenyl rings of the biphenyl unit are 3.0 (2) and 2.1 (2)°.

Related literature

For related structures, see: Fischer *et al.* (2007*a*,*b*,*c*,*d*,*e*); Yathirajan *et al.* (2007). For related literature, see: Carlo *et al.* (1999); Fichou *et al.*, (1988); Goto *et al.*, (1991); Uchida *et al.* (1998); Zhao *et al.* (2000); Sarojini *et al.* (2006).



Experimental

Crystal data

$C_{21}H_{15}FO$
M_r = 302.33
Monoclinic, $P2_1$
a = 6.0095 (5) Å
b = 35.278 (3) Å
c = 7.2352 (6) Å
β = 90.018 (7)°
V = 1533.9 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 173 (2) K
0.24 × 0.23 × 0.07 mm

Data collection

Stoe IPDS II two-circle diffractometer
Absorption correction: none
11797 measured reflections
2748 independent reflections
2247 reflections with $I > 2\sigma(I)$
R_{int} = 0.078

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.150
S = 1.08
2748 reflections
416 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2013).

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supplementary materials

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3-(Biphenyl-4-yl)-1-(4-fluorophenyl)prop-2-en-1-one

B. K. Sarojini, H. S. Yathirajan, T. V. Sreevidya, B. Narayana and M. Bolte

Comment

Chalcones (1,3-diaryl-2-propen-1-ones), belonging to the flavonoid family is one of the major class of natural products which have been recently subjects of great interest for their interesting pharmacological activities. Chalcones have been reported to possess many useful properties, including anti-inflammatory, antimicrobial, antifungal, antioxidant, cytotoxic, antitumor and anticancer activities. Among several organic compounds reported for NLO property, chalcone derivatives are noticeable materials for their excellent blue light transmittance and good crystallizability. We have synthesized a new chalcone.

The title compound, $C_{21}H_{15}FO$, crystallized with two molecules in the asymmetric unit, which differ only in the sign of their torsion angles. A least-squares fit of all non H atoms of molecule one with the inverted molecule two gives an r.m.s. deviation of 0.022 Å. Nevertheless, the two molecules are not related by any crystallographic symmetry element (Fig. 2). The dihedral angle between the two phenyl rings of the biphenyl unit is 3.0 (2)% and 2.1 (2)°, respectively.

Experimental

A solution of potassium hydroxide (5%, 5 ml) was added slowly with stirring to a mixture of biphenyl aldehyde (1.8 g, 0.01 mol) and 4-fluoroacetophenone (1.38 g, 0.01 mol) in ethanol (15 ml). The mixture was stirred at room temperature for 6 h. The precipitated solid was filtered, washed with cold ethanol, dried and recrystallized from ethanol (yield: 83%; m.p.:405–407 K). Analysis for $C_{21}H_{15}FO$: Found (Calculated): C: 83.30 (83.42); H: 4.91% (5.00%).

Refinement

In the absence of any anomalous scatterer, the Flack (1983) parameter is meaningless and therefore, Friedel pairs had been merged prior to refinement. H atoms were found in a difference map, but they were refined using a riding model with C—H = 0.95Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

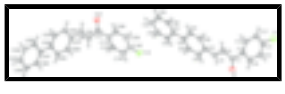

Fig. 1. Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level.

Fig. 2. Packing diagram of the title compound.

3-(biphenyl)-1-(4-fluorophenyl)prop-2-en-1-one

Crystal data

$C_{21}H_{15}FO$	$F_{000} = 632$
$M_r = 302.33$	$D_x = 1.309$ Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2yb	Cell parameters from 11222 reflections
$a = 6.0095$ (5) Å	$\theta = 2.4$–25.4º
$b = 35.278$ (3) Å	$\mu = 0.09$ mm^{-1}
$c = 7.2352$ (6) Å	$T = 173$ (2) K
$\beta = 90.018$ (7)º	Plate, colourless
$V = 1533.9$ (2) Å^3	0.24 × 0.23 × 0.07 mm
$Z = 4$	

Data collection

STOE IPDS II two-circle-diffractometer	2247 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.078$
Monochromator: graphite	$\theta_{max} = 25.1$º
$T = 173(2)$ K	$\theta_{min} = 2.3$º
ω scans	$h = -6\rightarrow7$
Absorption correction: none	$k = -41\rightarrow41$
11797 measured reflections	$l = -8\rightarrow7$
2748 independent reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0971P)^2 + 0.1253P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.053$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.150$	$\Delta\rho_{max} = 0.24$ e Å^{-3}
$S = 1.08$	$\Delta\rho_{min} = -0.21$ e Å^{-3}
2748 reflections	Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
416 parameters	Extinction coefficient: 0.029 (5)
1 restraint	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

Special details

Experimental. ;

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 $F^2 > 2\text{sigma}(F^2)$ 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}
F1	0.9293 (5)	0.05442 (9)	0.7455 (5)	0.0675 (9)
O1	0.3329 (5)	0.19910 (10)	0.6711 (5)	0.0543 (9)
C1	0.5359 (7)	0.19750 (14)	0.6794 (6)	0.0390 (10)
C2	0.6741 (8)	0.23236 (12)	0.6773 (6)	0.0400 (10)
H2	0.8271	0.2309	0.6453	0.048*
C3	0.5832 (7)	0.26574 (14)	0.7206 (6)	0.0391 (10)
H3	0.4313	0.2653	0.7570	0.047*
C11	0.6470 (7)	0.16017 (13)	0.6914 (6)	0.0356 (9)
C12	0.8594 (7)	0.15582 (14)	0.7682 (6)	0.0418 (11)
H12	0.9401	0.1775	0.8078	0.050*
C13	0.9530 (7)	0.12006 (15)	0.7871 (7)	0.0455 (11)
H13	1.0967	0.1171	0.8399	0.055*
C14	0.8367 (8)	0.08951 (14)	0.7293 (7)	0.0443 (11)
C15	0.6264 (7)	0.09220 (13)	0.6512 (7)	0.0437 (11)
H15	0.5489	0.0702	0.6110	0.052*
C16	0.5339 (7)	0.12755 (13)	0.6339 (6)	0.0398 (10)
H16	0.3895	0.1300	0.5817	0.048*
C21	0.6921 (7)	0.30301 (12)	0.7181 (6)	0.0333 (9)
C22	0.5779 (7)	0.33406 (12)	0.7906 (6)	0.0357 (10)
H22	0.4349	0.3304	0.8437	0.043*
C23	0.6694 (7)	0.37021 (12)	0.7867 (6)	0.0332 (9)
H23	0.5869	0.3908	0.8362	0.040*
C24	0.8798 (7)	0.37701 (12)	0.7115 (6)	0.0321 (9)
C25	0.9948 (7)	0.34561 (12)	0.6367 (6)	0.0360 (9)
H25	1.1370	0.3492	0.5821	0.043*
C26	0.9029 (7)	0.30978 (12)	0.6419 (6)	0.0356 (10)
H26	0.9848	0.2891	0.5924	0.043*
C31	0.9783 (7)	0.41586 (11)	0.7093 (5)	0.0313 (9)
C32	0.8697 (7)	0.44664 (13)	0.7904 (6)	0.0364 (10)
H32	0.7318	0.4425	0.8514	0.044*
C33	0.9562 (8)	0.48266 (13)	0.7848 (7)	0.0413 (10)

H33	0.8753	0.5031	0.8381	0.050*
C34	1.1616 (8)	0.48961 (13)	0.7018 (6)	0.0412 (10)
H34	1.2225	0.5145	0.6994	0.049*
C35	1.2753 (7)	0.45932 (12)	0.6224 (6)	0.0384 (10)
H35	1.4162	0.4634	0.5665	0.046*
C36	1.1845 (7)	0.42326 (12)	0.6245 (6)	0.0361 (9)
H36	1.2632	0.4031	0.5674	0.043*
F1A	0.5605 (5)	0.55587 (8)	0.8197 (5)	0.0630 (9)
O1A	1.1685 (5)	0.69972 (10)	0.7490 (5)	0.0533 (9)
C1A	0.9635 (7)	0.69835 (14)	0.7567 (6)	0.0386 (10)
C2A	0.8260 (8)	0.73304 (12)	0.7556 (6)	0.0396 (10)
H2A	0.6734	0.7317	0.7222	0.047*
C3A	0.9166 (7)	0.76640 (13)	0.8017 (6)	0.0378 (10)
H3A	1.0678	0.7659	0.8398	0.045*
C11A	0.8495 (7)	0.66086 (13)	0.7687 (6)	0.0371 (10)
C12A	0.6396 (7)	0.65722 (13)	0.8457 (6)	0.0378 (10)
H12A	0.5615	0.6792	0.8856	0.045*
C13A	0.5420 (7)	0.62161 (14)	0.8650 (7)	0.0426 (10)
H13A	0.3991	0.6190	0.9197	0.051*
C14A	0.6560 (8)	0.59074 (13)	0.8039 (7)	0.0428 (11)
C15A	0.8655 (8)	0.59300 (14)	0.7244 (7)	0.0440 (11)
H15A	0.9404	0.5709	0.6822	0.053*
C16A	0.9612 (7)	0.62829 (13)	0.7086 (6)	0.0390 (10)
H16A	1.1054	0.6306	0.6561	0.047*
C21A	0.8078 (7)	0.80367 (12)	0.7998 (6)	0.0327 (9)
C22A	0.9213 (7)	0.83501 (11)	0.8713 (6)	0.0344 (9)
H22A	1.0656	0.8315	0.9223	0.041*
C23A	0.8293 (7)	0.87083 (12)	0.8697 (6)	0.0342 (9)
H23A	0.9108	0.8913	0.9216	0.041*
C24A	0.6190 (7)	0.87784 (11)	0.7938 (6)	0.0306 (9)
C25A	0.5064 (7)	0.84613 (12)	0.7194 (6)	0.0319 (9)
H25A	0.3640	0.8497	0.6651	0.038*
C26A	0.5966 (8)	0.81006 (13)	0.7231 (6)	0.0369 (10)
H26A	0.5147	0.7894	0.6733	0.044*
C31A	0.5228 (7)	0.91661 (12)	0.7907 (6)	0.0319 (9)
C32A	0.6346 (7)	0.94764 (12)	0.8707 (6)	0.0370 (9)
H32A	0.7740	0.9435	0.9293	0.044*
C33A	0.5476 (7)	0.98384 (13)	0.8663 (7)	0.0412 (10)
H33A	0.6282	1.0042	0.9206	0.049*
C34A	0.3416 (7)	0.99082 (13)	0.7827 (6)	0.0379 (10)
H34A	0.2821	1.0158	0.7787	0.045*
C35A	0.2254 (7)	0.96054 (13)	0.7054 (6)	0.0387 (10)
H35A	0.0855	0.9648	0.6478	0.046*
C36A	0.3132 (7)	0.92418 (12)	0.7122 (6)	0.0337 (9)
H36A	0.2293	0.9038	0.6624	0.040*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0575 (19)	0.0508 (18)	0.094 (3)	0.0133 (15)	0.0044 (16)	0.0068 (16)
O1	0.0339 (18)	0.0486 (19)	0.081 (2)	−0.0034 (15)	−0.0018 (15)	0.0000 (18)
C1	0.032 (2)	0.046 (2)	0.040 (2)	−0.005 (2)	0.0027 (17)	−0.002 (2)
C2	0.039 (2)	0.040 (3)	0.041 (2)	−0.0042 (19)	0.0020 (18)	−0.0048 (19)
C3	0.036 (2)	0.046 (3)	0.035 (2)	−0.009 (2)	0.0007 (17)	−0.0007 (19)
C11	0.036 (2)	0.040 (2)	0.031 (2)	−0.0038 (19)	0.0032 (16)	0.0010 (18)
C12	0.033 (2)	0.053 (3)	0.039 (3)	−0.008 (2)	0.0027 (18)	−0.001 (2)
C13	0.031 (2)	0.061 (3)	0.044 (3)	0.003 (2)	0.0008 (19)	0.007 (2)
C14	0.041 (3)	0.039 (3)	0.052 (3)	0.004 (2)	0.013 (2)	0.006 (2)
C15	0.038 (2)	0.043 (3)	0.050 (3)	−0.005 (2)	0.0015 (19)	−0.001 (2)
C16	0.034 (2)	0.049 (3)	0.037 (2)	−0.007 (2)	0.0054 (18)	−0.002 (2)
C21	0.032 (2)	0.040 (2)	0.028 (2)	−0.0006 (18)	0.0016 (16)	−0.0004 (17)
C22	0.029 (2)	0.042 (2)	0.036 (3)	0.0038 (18)	−0.0011 (17)	−0.0003 (18)
C23	0.027 (2)	0.040 (2)	0.032 (2)	0.0038 (18)	−0.0002 (16)	−0.0028 (17)
C24	0.028 (2)	0.043 (2)	0.025 (2)	0.0016 (17)	−0.0009 (15)	0.0015 (16)
C25	0.031 (2)	0.042 (2)	0.035 (2)	0.0033 (18)	0.0082 (17)	0.0022 (18)
C26	0.034 (2)	0.033 (2)	0.040 (3)	0.0007 (17)	0.0046 (17)	−0.0046 (17)
C31	0.034 (2)	0.038 (2)	0.023 (2)	0.0014 (17)	−0.0002 (16)	0.0010 (15)
C32	0.030 (2)	0.042 (2)	0.037 (2)	0.0003 (18)	0.0030 (17)	0.0005 (19)
C33	0.046 (3)	0.033 (2)	0.044 (3)	0.0047 (19)	0.0063 (19)	−0.0032 (18)
C34	0.041 (2)	0.041 (2)	0.042 (3)	−0.003 (2)	−0.0002 (19)	0.0019 (19)
C35	0.034 (2)	0.044 (2)	0.036 (2)	−0.0019 (19)	0.0057 (17)	0.0011 (18)
C36	0.032 (2)	0.042 (2)	0.034 (2)	0.0036 (18)	0.0029 (17)	−0.0014 (18)
F1A	0.0545 (18)	0.0416 (16)	0.093 (2)	−0.0106 (13)	0.0007 (16)	0.0079 (15)
O1A	0.0342 (18)	0.0443 (19)	0.081 (3)	0.0014 (15)	0.0039 (15)	0.0009 (17)
C1A	0.034 (2)	0.044 (2)	0.037 (2)	0.008 (2)	0.0025 (16)	0.002 (2)
C2A	0.037 (2)	0.038 (2)	0.044 (3)	0.0031 (19)	−0.0032 (18)	0.0017 (19)
C3A	0.037 (2)	0.045 (2)	0.032 (2)	0.004 (2)	0.0060 (16)	0.0011 (19)
C11A	0.033 (2)	0.039 (2)	0.039 (3)	0.0030 (18)	−0.0036 (18)	0.0025 (19)
C12A	0.034 (2)	0.042 (2)	0.038 (2)	0.0061 (19)	0.0063 (17)	0.0002 (18)
C13A	0.034 (2)	0.050 (3)	0.044 (3)	−0.002 (2)	−0.0022 (18)	0.004 (2)
C14A	0.039 (2)	0.041 (3)	0.048 (3)	−0.004 (2)	0.000 (2)	0.005 (2)
C15A	0.043 (2)	0.043 (3)	0.046 (3)	0.007 (2)	−0.003 (2)	0.001 (2)
C16A	0.034 (2)	0.043 (2)	0.040 (2)	0.0044 (19)	0.0020 (17)	−0.0002 (19)
C21A	0.031 (2)	0.038 (2)	0.029 (2)	0.0011 (18)	0.0061 (16)	0.0029 (17)
C22A	0.026 (2)	0.042 (2)	0.035 (2)	0.0005 (18)	−0.0014 (16)	0.0031 (18)
C23A	0.035 (2)	0.039 (2)	0.029 (2)	−0.0048 (18)	0.0014 (16)	0.0000 (17)
C24A	0.029 (2)	0.037 (2)	0.026 (2)	−0.0008 (16)	0.0048 (16)	0.0012 (16)
C25A	0.026 (2)	0.038 (2)	0.031 (2)	−0.0011 (17)	−0.0020 (16)	−0.0018 (17)
C26A	0.039 (2)	0.038 (2)	0.034 (2)	−0.0029 (19)	−0.0025 (17)	−0.0026 (17)
C31A	0.032 (2)	0.037 (2)	0.027 (2)	−0.0029 (17)	0.0053 (16)	0.0024 (16)
C32A	0.034 (2)	0.042 (2)	0.035 (2)	0.0000 (19)	−0.0040 (17)	0.0011 (18)
C33A	0.043 (3)	0.039 (2)	0.042 (3)	−0.005 (2)	0.0036 (19)	−0.0006 (19)
C34A	0.040 (2)	0.036 (2)	0.037 (2)	0.0058 (19)	0.0068 (18)	0.0000 (18)

C35A	0.031 (2)	0.047 (3)	0.038 (2)	0.0063 (19)	0.0021 (18)	0.0028 (19)
C36A	0.027 (2)	0.040 (2)	0.034 (2)	−0.0006 (18)	0.0043 (16)	−0.0008 (17)

Geometric parameters (Å, °)

F1—C14	1.362 (5)	F1A—C14A	1.362 (5)
O1—C1	1.223 (5)	O1A—C1A	1.234 (5)
C1—C11	1.479 (7)	C1A—C2A	1.477 (6)
C1—C2	1.484 (6)	C1A—C11A	1.492 (6)
C2—C3	1.336 (6)	C2A—C3A	1.339 (6)
C2—H2	0.9500	C2A—H2A	0.9500
C3—C21	1.469 (6)	C3A—C21A	1.468 (6)
C3—H3	0.9500	C3A—H3A	0.9500
C11—C16	1.400 (6)	C11A—C12A	1.385 (6)
C11—C12	1.401 (6)	C11A—C16A	1.400 (6)
C12—C13	1.388 (7)	C12A—C13A	1.393 (7)
C12—H12	0.9500	C12A—H12A	0.9500
C13—C14	1.351 (7)	C13A—C14A	1.361 (7)
C13—H13	0.9500	C13A—H13A	0.9500
C14—C15	1.387 (7)	C14A—C15A	1.387 (7)
C15—C16	1.371 (7)	C15A—C16A	1.376 (7)
C15—H15	0.9500	C15A—H15A	0.9500
C16—H16	0.9500	C16A—H16A	0.9500
C21—C22	1.395 (6)	C21A—C22A	1.398 (6)
C21—C26	1.402 (6)	C21A—C26A	1.404 (6)
C22—C23	1.389 (6)	C22A—C23A	1.379 (6)
C22—H22	0.9500	C22A—H22A	0.9500
C23—C24	1.397 (6)	C23A—C24A	1.400 (6)
C23—H23	0.9500	C23A—H23A	0.9500
C24—C25	1.413 (6)	C24A—C25A	1.414 (6)
C24—C31	1.493 (6)	C24A—C31A	1.485 (5)
C25—C26	1.380 (6)	C25A—C26A	1.383 (6)
C25—H25	0.9500	C25A—H25A	0.9500
C26—H26	0.9500	C26A—H26A	0.9500
C31—C32	1.396 (6)	C31A—C36A	1.407 (6)
C31—C36	1.408 (6)	C31A—C32A	1.409 (6)
C32—C33	1.374 (6)	C32A—C33A	1.380 (6)
C32—H32	0.9500	C32A—H32A	0.9500
C33—C34	1.394 (7)	C33A—C34A	1.400 (7)
C33—H33	0.9500	C33A—H33A	0.9500
C34—C35	1.393 (6)	C34A—C35A	1.393 (6)
C34—H34	0.9500	C34A—H34A	0.9500
C35—C36	1.384 (6)	C35A—C36A	1.388 (6)
C35—H35	0.9500	C35A—H35A	0.9500
C36—H36	0.9500	C36A—H36A	0.9500
O1—C1—C11	119.6 (4)	O1A—C1A—C2A	121.7 (4)
O1—C1—C2	121.3 (4)	O1A—C1A—C11A	119.7 (4)
C11—C1—C2	119.1 (4)	C2A—C1A—C11A	118.5 (4)
C3—C2—C1	120.0 (4)	C3A—C2A—C1A	120.0 (4)

C3—C2—H2	120.0	C3A—C2A—H2A	120.0
C1—C2—H2	120.0	C1A—C2A—H2A	120.0
C2—C3—C21	127.2 (4)	C2A—C3A—C21A	127.2 (4)
C2—C3—H3	116.4	C2A—C3A—H3A	116.4
C21—C3—H3	116.4	C21A—C3A—H3A	116.4
C16—C11—C12	118.1 (4)	C12A—C11A—C16A	119.0 (4)
C16—C11—C1	119.7 (4)	C12A—C11A—C1A	121.6 (4)
C12—C11—C1	122.2 (4)	C16A—C11A—C1A	119.3 (4)
C13—C12—C11	120.5 (4)	C11A—C12A—C13A	120.5 (4)
C13—C12—H12	119.7	C11A—C12A—H12A	119.8
C11—C12—H12	119.7	C13A—C12A—H12A	119.8
C14—C13—C12	119.0 (4)	C14A—C13A—C12A	118.5 (4)
C14—C13—H13	120.5	C14A—C13A—H13A	120.8
C12—C13—H13	120.5	C12A—C13A—H13A	120.8
C13—C14—F1	119.1 (4)	C13A—C14A—F1A	118.9 (4)
C13—C14—C15	122.9 (4)	C13A—C14A—C15A	123.1 (4)
F1—C14—C15	118.0 (4)	F1A—C14A—C15A	118.0 (4)
C16—C15—C14	118.0 (4)	C16A—C15A—C14A	117.8 (4)
C16—C15—H15	121.0	C16A—C15A—H15A	121.1
C14—C15—H15	121.0	C14A—C15A—H15A	121.1
C15—C16—C11	121.6 (4)	C15A—C16A—C11A	121.1 (4)
C15—C16—H16	119.2	C15A—C16A—H16A	119.5
C11—C16—H16	119.2	C11A—C16A—H16A	119.5
C22—C21—C26	117.3 (4)	C22A—C21A—C26A	117.4 (4)
C22—C21—C3	118.6 (4)	C22A—C21A—C3A	119.2 (4)
C26—C21—C3	124.1 (4)	C26A—C21A—C3A	123.4 (4)
C23—C22—C21	121.2 (4)	C23A—C22A—C21A	121.7 (4)
C23—C22—H22	119.4	C23A—C22A—H22A	119.1
C21—C22—H22	119.4	C21A—C22A—H22A	119.1
C22—C23—C24	121.6 (4)	C22A—C23A—C24A	121.8 (4)
C22—C23—H23	119.2	C22A—C23A—H23A	119.1
C24—C23—H23	119.2	C24A—C23A—H23A	119.1
C23—C24—C25	117.2 (4)	C23A—C24A—C25A	116.2 (4)
C23—C24—C31	121.4 (4)	C23A—C24A—C31A	121.3 (4)
C25—C24—C31	121.4 (4)	C25A—C24A—C31A	122.4 (3)
C26—C25—C24	120.8 (4)	C26A—C25A—C24A	122.2 (4)
C26—C25—H25	119.6	C26A—C25A—H25A	118.9
C24—C25—H25	119.6	C24A—C25A—H25A	118.9
C25—C26—C21	121.9 (4)	C25A—C26A—C21A	120.6 (4)
C25—C26—H26	119.0	C25A—C26A—H26A	119.7
C21—C26—H26	119.0	C21A—C26A—H26A	119.7
C32—C31—C36	116.8 (4)	C36A—C31A—C32A	116.4 (4)
C32—C31—C24	121.6 (4)	C36A—C31A—C24A	122.0 (4)
C36—C31—C24	121.6 (3)	C32A—C31A—C24A	121.6 (3)
C33—C32—C31	122.0 (4)	C33A—C32A—C31A	121.9 (4)
C33—C32—H32	119.0	C33A—C32A—H32A	119.0
C31—C32—H32	119.0	C31A—C32A—H32A	119.0
C32—C33—C34	120.7 (4)	C32A—C33A—C34A	120.5 (4)
C32—C33—H33	119.7	C32A—C33A—H33A	119.8

C34—C33—H33	119.7	C34A—C33A—H33A	119.8
C35—C34—C33	118.5 (4)	C35A—C34A—C33A	118.8 (4)
C35—C34—H34	120.7	C35A—C34A—H34A	120.6
C33—C34—H34	120.7	C33A—C34A—H34A	120.6
C36—C35—C34	120.5 (4)	C36A—C35A—C34A	120.2 (4)
C36—C35—H35	119.8	C36A—C35A—H35A	119.9
C34—C35—H35	119.8	C34A—C35A—H35A	119.9
C35—C36—C31	121.5 (4)	C35A—C36A—C31A	122.0 (4)
C35—C36—H36	119.3	C35A—C36A—H36A	119.0
C31—C36—H36	119.3	C31A—C36A—H36A	119.0
O1—C1—C2—C3	19.7 (7)	O1A—C1A—C2A—C3A	−20.1 (7)
C11—C1—C2—C3	−160.4 (4)	C11A—C1A—C2A—C3A	159.5 (4)
C1—C2—C3—C21	−177.2 (4)	C1A—C2A—C3A—C21A	177.0 (4)
O1—C1—C11—C16	20.7 (6)	O1A—C1A—C11A—C12A	155.2 (4)
C2—C1—C11—C16	−159.1 (4)	C2A—C1A—C11A—C12A	−24.5 (6)
O1—C1—C11—C12	−155.7 (4)	O1A—C1A—C11A—C16A	−21.9 (6)
C2—C1—C11—C12	24.4 (6)	C2A—C1A—C11A—C16A	158.5 (4)
C16—C11—C12—C13	−0.3 (7)	C16A—C11A—C12A—C13A	0.7 (7)
C1—C11—C12—C13	176.2 (4)	C1A—C11A—C12A—C13A	−176.3 (4)
C11—C12—C13—C14	0.4 (7)	C11A—C12A—C13A—C14A	−1.1 (7)
C12—C13—C14—F1	179.2 (4)	C12A—C13A—C14A—F1A	−179.1 (4)
C12—C13—C14—C15	0.0 (7)	C12A—C13A—C14A—C15A	0.5 (7)
C13—C14—C15—C16	−0.4 (7)	C13A—C14A—C15A—C16A	0.4 (7)
F1—C14—C15—C16	−179.6 (4)	F1A—C14A—C15A—C16A	180.0 (4)
C14—C15—C16—C11	0.5 (7)	C14A—C15A—C16A—C11A	−0.8 (7)
C12—C11—C16—C15	−0.1 (7)	C12A—C11A—C16A—C15A	0.2 (7)
C1—C11—C16—C15	−176.7 (4)	C1A—C11A—C16A—C15A	177.3 (4)
C2—C3—C21—C22	−171.9 (4)	C2A—C3A—C21A—C22A	173.2 (4)
C2—C3—C21—C26	10.1 (7)	C2A—C3A—C21A—C26A	−9.2 (7)
C26—C21—C22—C23	0.2 (6)	C26A—C21A—C22A—C23A	0.9 (6)
C3—C21—C22—C23	−177.9 (4)	C3A—C21A—C22A—C23A	178.7 (4)
C21—C22—C23—C24	−0.5 (6)	C21A—C22A—C23A—C24A	−1.1 (6)
C22—C23—C24—C25	1.0 (6)	C22A—C23A—C24A—C25A	0.2 (6)
C22—C23—C24—C31	−179.4 (4)	C22A—C23A—C24A—C31A	−179.2 (4)
C23—C24—C25—C26	−1.3 (6)	C23A—C24A—C25A—C26A	0.8 (6)
C31—C24—C25—C26	179.2 (4)	C31A—C24A—C25A—C26A	−179.8 (4)
C24—C25—C26—C21	1.0 (6)	C24A—C25A—C26A—C21A	−0.9 (6)
C22—C21—C26—C25	−0.5 (6)	C22A—C21A—C26A—C25A	0.0 (6)
C3—C21—C26—C25	177.5 (4)	C3A—C21A—C26A—C25A	−177.6 (4)
C23—C24—C31—C32	3.4 (6)	C23A—C24A—C31A—C36A	179.0 (4)
C25—C24—C31—C32	−177.1 (4)	C25A—C24A—C31A—C36A	−0.4 (6)
C23—C24—C31—C36	−176.4 (4)	C23A—C24A—C31A—C32A	−2.7 (6)
C25—C24—C31—C36	3.2 (6)	C25A—C24A—C31A—C32A	178.0 (4)
C36—C31—C32—C33	1.5 (6)	C36A—C31A—C32A—C33A	−2.4 (6)
C24—C31—C32—C33	−178.3 (4)	C24A—C31A—C32A—C33A	179.2 (4)
C31—C32—C33—C34	−2.0 (7)	C31A—C32A—C33A—C34A	0.6 (7)
C32—C33—C34—C35	0.9 (7)	C32A—C33A—C34A—C35A	0.5 (7)
C33—C34—C35—C36	0.7 (6)	C33A—C34A—C35A—C36A	0.2 (6)
C34—C35—C36—C31	−1.3 (6)	C34A—C35A—C36A—C31A	−2.1 (6)

C32—C31—C36—C35	0.2 (6)	C32A—C31A—C36A—C35A	3.1 (6)
C24—C31—C36—C35	179.9 (4)	C24A—C31A—C36A—C35A	−178.5 (4)

Fig. 1

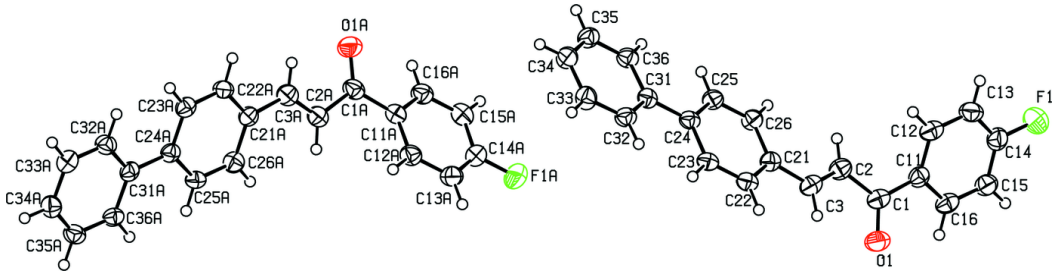

Fig. 2