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## Structure Reports

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## 3,9'-Bi(9H-fluorene)

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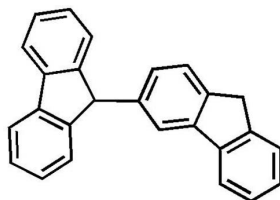
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 Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  
 R factor = 0.035; wR factor = 0.091; data-to-parameter ratio = 10.0.

The title compound [systematic name: 9-(9H-fluoren-3-yl)-9H-fluorene],  $\text{C}_{26}\text{H}_{18}$ , was obtained unintentionally as the product of the synthesis of a compound based on fluorene–thiophene units. The two fluorene rings are connected through C atoms in the 3- and 9'-positions, and the dihedral angle between the mean planes of the two fluorene units is  $78.57(6)^\circ$ .

## Related literature

For the crystal structures of related compounds, see: Dougherty *et al.* (1978); Sridevi *et al.* (2006). For the synthesis of the compound, see: Stille *et al.* (1993, 1998); Grasa & Nolan (2001). For the intermolecular C–H... $\pi$  interactions, see: Tsuzuki *et al.* (2000); Nishio (2004).



## Experimental

## Crystal data

 $\text{C}_{26}\text{H}_{18}$ 
 $M_r = 330.40$ 

 Orthorhombic,  $P2_12_12_1$ 
 $a = 6.22600(1)$  Å

 $b = 8.3968(2)$  Å

 $c = 33.5357(7)$  Å

 $V = 1753.20(6)$  Å<sup>3</sup>
 $Z = 4$ 

 Mo  $K\alpha$  radiation

 $\mu = 0.07$  mm<sup>-1</sup>
 $T = 293$  K

 $0.45 \times 0.22 \times 0.16$  mm

## Data collection

 Bruker APEXII CCD area-detector  
 diffractometer

Absorption correction: multi-scan

 (*APEX2*; Bruker, 2005)

 $T_{\min} = 0.969$ ,  $T_{\max} = 0.989$ 

15454 measured reflections

2352 independent reflections

 2014 reflections with  $I > 2\sigma(I)$ 
 $R_{\text{int}} = 0.032$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.035$ 
 $wR(F^2) = 0.091$ 
 $S = 1.04$ 

2352 reflections

235 parameters

H-atom parameters constrained

 $\Delta\rho_{\max} = 0.11$  e Å<sup>-3</sup>
 $\Delta\rho_{\min} = -0.14$  e Å<sup>-3</sup>

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *Mercury* (Macrae *et al.*, 2006).

The authors gratefully acknowledge the National Natural Science Foundation of China (grant No. 51021062) and the 973 program of the People's Republic of China (grant No. 2010CB630702).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZJ2080).

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## supporting information

*Acta Cryst.* (2012). E68, o2081 [https://doi.org/10.1107/S1600536812024841]

**3,9'-Bi(9*H*-fluorene)****Jie Liu and Wentao Yu****S1. Comment**

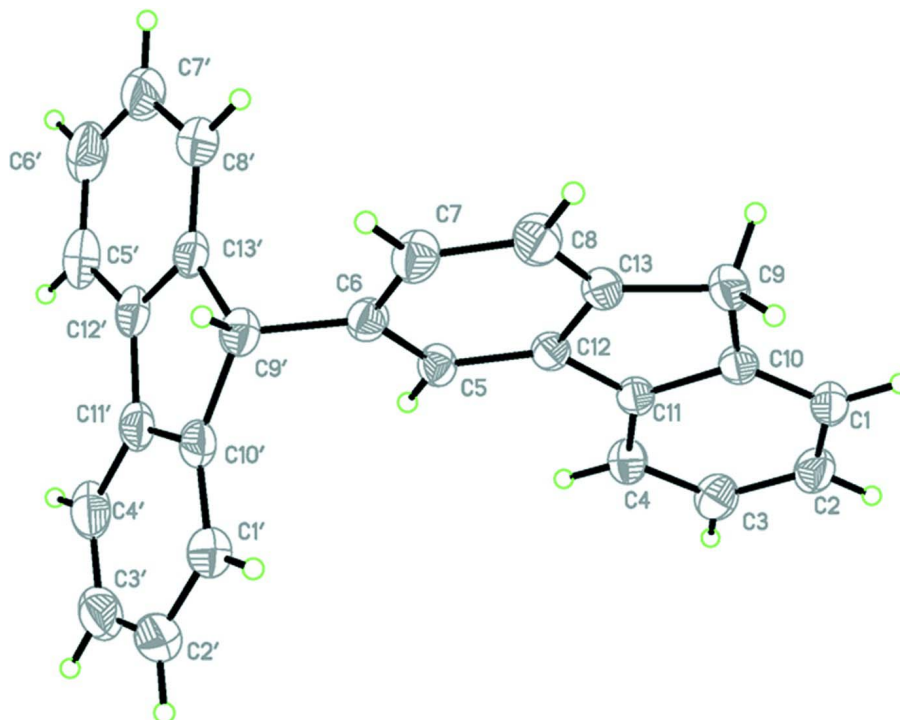
The molecule of the title compound (I) (Fig. 1) as the isomer of 9,9'-bi-9*H*-fluorene (9,9'-BF) is noncentrosymmetric, and the space group is  $P2_12_12_1$ . The two fluorene groups of the compound are like the letter 'T' in shape with a dihedral angle of 78.57 (6)°. Also, it is found that benzene rings of the fluorene units are not in the same plane, and the dihedral angles are 10.54 (6) and 5.84 (6)°, respectively. The crystal packing is stabilized by intermolecular C—H $\cdots$  $\pi$  interactions (Fig. 3).

**S2. Experimental**

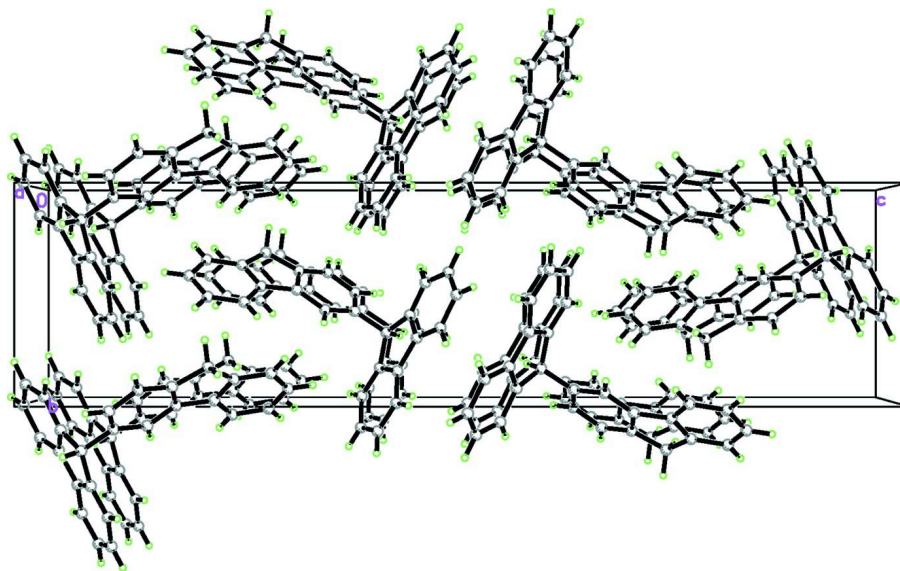
The title compound, 3,9'-BF, was obtained unintentionally as the product of an attempted synthesis of 2,5-bis(9*H*-fluoren-9-yl)thiophene through Still reaction method. *n*-Butyllithium (20 ml, 2.5 *M* in hexane, 50 mmol) was added dropwise at -78 °C into a consistently stirred mixture of thiophene (22 mmol, 1.8 ml) and dry THF (80 ml), and the mixture would be with further stirring for 2 h at room temperature under an atmosphere of dry argon. After cooling the reaction mixture to -78 °C tri-*n*-butyltin chloride (15 ml) was added drop-wise to the mixture system. Then, the mixture was stirred continuously over one night before being poured into saturated NH<sub>4</sub>Cl water solution (100 ml). After extraction with diethyl ether, the organic layer was dried over anhydrous MgSO<sub>4</sub> and the yellow fluid bis[tri-*n*-butyltin] thiophene (TBSB) was obtained. Furthermore, DMF (10 ml) was added to the mixture of TBSB (2.5 mmol, 1.654 g), 9-bromo-fluorene (6.25 mmol, 1.53 g) and potassium fluoride (2.5 mmol, 0.145 g) with stirring about 15 min. Appropriate amount of tetrakis (triphenylphosphine) palladium (0) was added to the stirring system and refluxed at 100 °C for 16 h under an atmosphere of dry argon. After extraction with dichloromethane (30 ml), the mixture was purified by silica-gel column chromatography to give 3,9'-BF, 9,9'-BF and 2,5-bis(9*H*-fluoren-9-yl)thiophene. Finally, single crystals of 3,9'-BF were obtained by recrystallizing from dichloromethane.

**S3. Refinement**

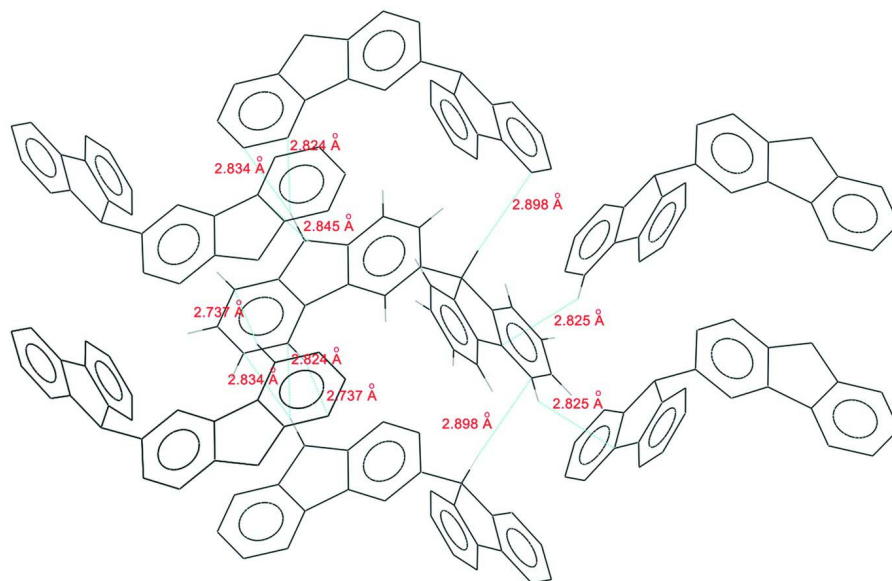
All the H atoms were positioned geometrically [C—H = 0.93, 0.96 and 0.98 Å] and refined using a riding model with  $U_{iso}(\text{H}) = 1.2 U_{eq}(\text{C})$ . In the absence of significant anomalous scattering, Friedel pairs were merged; the absolute configuration was not determined.

**Figure 1**

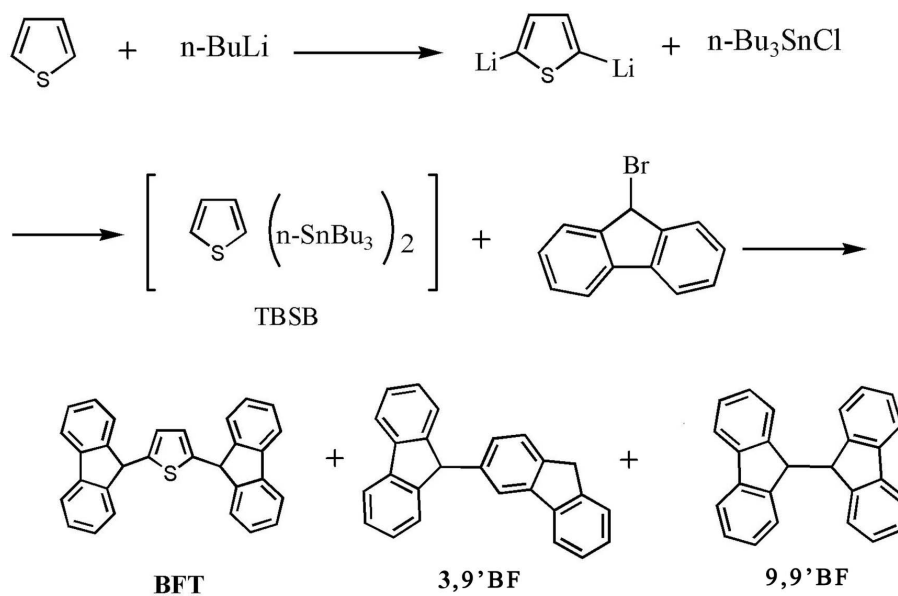
The molecular structure of the title compound with 30% probability displacement ellipsoids.

**Figure 2**

Part of the packing of the title compound, viewed down the *a* direction.


**Figure 3**

A view of the C—H ...  $\pi$  interactions (dotted lines) in the crystal structure of the title compound.


**Figure 4**

Reaction scheme showing the formation of 3,9'-BF, 9,9'-BF and 2,5-bis(9*H*-fluoren-9-yl)thiophene (BFT).

### 3,9'-Bi(9*H*-fluorene)

#### Crystal data

$C_{26}H_{18}$

$M_r = 330.40$

Orthorhombic,  $P2_12_12_1$

Hall symbol:  $P2ac2ab$

$a = 6.22600$  (1) Å

$b = 8.3968$  (2) Å

$c = 33.5357$  (7) Å

$V = 1753.20$  (6) Å<sup>3</sup>

$Z = 4$

$F(000) = 696$

$D_x = 1.252$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 5140 reflections  
 $\theta = 2.4\text{--}24.1^\circ$   
 $\mu = 0.07\text{ mm}^{-1}$

$T = 293\text{ K}$   
 Prism, colourless  
 $0.45 \times 0.22 \times 0.16\text{ mm}$

*Data collection*

Bruker APEXII CCD area-detector  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan  
 (APEX2; Bruker,2005)  
 $T_{\min} = 0.969, T_{\max} = 0.989$

15454 measured reflections  
 2352 independent reflections  
 2014 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.032$   
 $\theta_{\max} = 27.5^\circ, \theta_{\min} = 2.4^\circ$   
 $h = -8 \rightarrow 8$   
 $k = -10 \rightarrow 9$   
 $l = -43 \rightarrow 43$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.035$   
 $wR(F^2) = 0.091$   
 $S = 1.04$   
 2352 reflections  
 235 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0481P)^2 + 0.1328P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.11\text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.14\text{ e \AA}^{-3}$

*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.

**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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.6920 (3)	0.3409 (2)	0.20770 (5)	0.0533 (5)
H1	0.6063	0.2764	0.1917	0.064*
C2	0.8720 (4)	0.4144 (2)	0.19215 (5)	0.0578 (5)
H2	0.9063	0.4002	0.1654	0.069*
C3	1.0021 (3)	0.5087 (3)	0.21587 (5)	0.0581 (5)
H3	1.1234	0.5565	0.2050	0.070*
C4	0.9531 (3)	0.5326 (2)	0.25577 (5)	0.0503 (4)
H4	1.0414	0.5950	0.2718	0.060*
C5	0.7212 (3)	0.5705 (2)	0.34358 (4)	0.0424 (4)
H5	0.8501	0.6264	0.3441	0.051*
C6	0.5806 (3)	0.5777 (2)	0.37597 (5)	0.0451 (4)
C7	0.3899 (3)	0.4923 (3)	0.37462 (5)	0.0572 (5)
H7	0.2957	0.4980	0.3961	0.069*

C8	0.3361 (3)	0.3984 (3)	0.34195 (5)	0.0599 (5)
H8	0.2081	0.3413	0.3416	0.072*
C9	0.4518 (3)	0.3053 (2)	0.27093 (5)	0.0527 (5)
H9A	0.4584	0.1908	0.2746	0.063*
H9B	0.3175	0.3326	0.2579	0.063*
C10	0.6411 (3)	0.36460 (19)	0.24736 (5)	0.0445 (4)
C11	0.7703 (3)	0.46193 (19)	0.27133 (4)	0.0409 (4)
C12	0.6660 (3)	0.47883 (19)	0.31054 (4)	0.0394 (4)
C13	0.4749 (3)	0.3913 (2)	0.31014 (5)	0.0457 (4)
C1'	0.6708 (4)	0.9656 (3)	0.38487 (6)	0.0685 (6)
H1'	0.5425	0.9613	0.3707	0.082*
C2'	0.7935 (6)	1.1033 (3)	0.38502 (7)	0.0870 (9)
H2'	0.7461	1.1922	0.3710	0.104*
C3'	0.9840 (6)	1.1101 (3)	0.40558 (7)	0.0895 (9)
H3'	1.0644	1.2035	0.4051	0.107*
C4'	1.0581 (4)	0.9809 (3)	0.42685 (6)	0.0748 (7)
H4'	1.1876	0.9861	0.4406	0.090*
C5'	1.1220 (4)	0.6453 (3)	0.47611 (6)	0.0678 (6)
H5'	1.2371	0.7117	0.4821	0.081*
C6'	1.1042 (5)	0.4983 (3)	0.49389 (6)	0.0810 (7)
H6'	1.2075	0.4656	0.5122	0.097*
C7'	0.9355 (5)	0.3993 (3)	0.48493 (6)	0.0841 (8)
H7'	0.9269	0.2998	0.4970	0.101*
C8'	0.7779 (4)	0.4454 (3)	0.45821 (5)	0.0665 (6)
H8'	0.6643	0.3776	0.4522	0.080*
C9'	0.6353 (3)	0.6749 (2)	0.41279 (5)	0.0484 (4)
H9'	0.5018	0.6934	0.4276	0.058*
C10'	0.7422 (3)	0.8349 (2)	0.40610 (5)	0.0514 (5)
C11'	0.9357 (3)	0.8430 (2)	0.42730 (5)	0.0539 (5)
C12'	0.9652 (3)	0.6932 (2)	0.44908 (5)	0.0512 (5)
C13'	0.7921 (3)	0.5934 (2)	0.44068 (4)	0.0486 (4)

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0685 (12)	0.0461 (10)	0.0453 (9)	0.0044 (10)	-0.0133 (9)	-0.0061 (8)
C2	0.0726 (12)	0.0581 (11)	0.0425 (9)	0.0099 (11)	0.0001 (9)	-0.0040 (8)
C3	0.0576 (11)	0.0652 (12)	0.0515 (10)	0.0027 (11)	0.0064 (8)	-0.0017 (9)
C4	0.0454 (9)	0.0568 (10)	0.0487 (9)	-0.0012 (9)	-0.0007 (7)	-0.0064 (8)
C5	0.0395 (8)	0.0459 (9)	0.0418 (8)	-0.0055 (8)	-0.0037 (7)	-0.0027 (7)
C6	0.0460 (9)	0.0486 (10)	0.0406 (8)	-0.0027 (8)	-0.0032 (7)	0.0011 (7)
C7	0.0518 (10)	0.0723 (13)	0.0474 (9)	-0.0129 (11)	0.0049 (8)	-0.0008 (9)
C8	0.0533 (11)	0.0703 (13)	0.0560 (10)	-0.0224 (11)	-0.0015 (9)	0.0000 (9)
C9	0.0563 (10)	0.0489 (10)	0.0527 (9)	-0.0080 (9)	-0.0127 (9)	-0.0048 (8)
C10	0.0519 (9)	0.0358 (8)	0.0457 (8)	0.0059 (8)	-0.0106 (7)	0.0003 (7)
C11	0.0444 (8)	0.0365 (8)	0.0417 (8)	0.0053 (8)	-0.0071 (7)	-0.0017 (7)
C12	0.0402 (8)	0.0372 (8)	0.0409 (8)	0.0011 (7)	-0.0052 (6)	0.0010 (7)
C13	0.0477 (9)	0.0439 (9)	0.0456 (8)	-0.0082 (9)	-0.0078 (7)	0.0014 (7)

C1'	0.0966 (17)	0.0588 (12)	0.0499 (10)	0.0056 (14)	0.0028 (11)	-0.0061 (9)
C2'	0.148 (3)	0.0539 (13)	0.0587 (13)	-0.0025 (18)	0.0172 (16)	-0.0040 (11)
C3'	0.141 (3)	0.0634 (15)	0.0643 (13)	-0.0384 (18)	0.0314 (17)	-0.0150 (12)
C4'	0.0866 (15)	0.0826 (16)	0.0553 (11)	-0.0337 (15)	0.0164 (11)	-0.0219 (12)
C5'	0.0586 (11)	0.0961 (17)	0.0488 (10)	0.0035 (13)	-0.0035 (9)	-0.0247 (12)
C6'	0.0970 (17)	0.0944 (18)	0.0515 (11)	0.0283 (17)	-0.0225 (12)	-0.0155 (13)
C7'	0.130 (2)	0.0692 (14)	0.0530 (11)	0.0115 (17)	-0.0230 (14)	-0.0030 (11)
C8'	0.0916 (16)	0.0617 (12)	0.0463 (9)	-0.0063 (13)	-0.0088 (11)	-0.0038 (9)
C9'	0.0479 (9)	0.0566 (11)	0.0406 (8)	-0.0019 (9)	0.0039 (7)	-0.0064 (8)
C10'	0.0649 (12)	0.0515 (10)	0.0379 (8)	-0.0024 (10)	0.0085 (8)	-0.0105 (8)
C11'	0.0619 (11)	0.0610 (11)	0.0389 (8)	-0.0110 (10)	0.0108 (8)	-0.0151 (8)
C12'	0.0499 (10)	0.0679 (12)	0.0359 (7)	-0.0042 (10)	0.0060 (7)	-0.0145 (8)
C13'	0.0566 (10)	0.0562 (10)	0.0330 (7)	-0.0004 (9)	0.0022 (7)	-0.0087 (7)

*Geometric parameters (Å, °)*

C1—C2	1.382 (3)	C1'—C10'	1.382 (3)
C1—C10	1.382 (2)	C1'—C2'	1.385 (4)
C1—H1	0.9300	C1'—H1'	0.9300
C2—C3	1.384 (3)	C2'—C3'	1.374 (4)
C2—H2	0.9300	C2'—H2'	0.9300
C3—C4	1.387 (2)	C3'—C4'	1.378 (4)
C3—H3	0.9300	C3'—H3'	0.9300
C4—C11	1.386 (2)	C4'—C11'	1.387 (3)
C4—H4	0.9300	C4'—H4'	0.9300
C5—C12	1.392 (2)	C5'—C6'	1.375 (4)
C5—C6	1.396 (2)	C5'—C12'	1.392 (3)
C5—H5	0.9300	C5'—H5'	0.9300
C6—C7	1.388 (3)	C6'—C7'	1.373 (4)
C6—C9'	1.519 (2)	C6'—H6'	0.9300
C7—C8	1.391 (3)	C7'—C8'	1.384 (3)
C7—H7	0.9300	C7'—H7'	0.9300
C8—C13	1.374 (3)	C8'—C13'	1.378 (3)
C8—H8	0.9300	C8'—H8'	0.9300
C9—C10	1.504 (2)	C9'—C13'	1.515 (2)
C9—C13	1.507 (2)	C9'—C10'	1.516 (3)
C9—H9A	0.9700	C9'—H9'	0.9800
C9—H9B	0.9700	C10'—C11'	1.401 (3)
C10—C11	1.400 (2)	C11'—C12'	1.466 (3)
C11—C12	1.473 (2)	C12'—C13'	1.394 (3)
C12—C13	1.399 (2)		
C2—C1—C10	119.00 (17)	C10'—C1'—C2'	118.9 (2)
C2—C1—H1	120.5	C10'—C1'—H1'	120.5
C10—C1—H1	120.5	C2'—C1'—H1'	120.5
C1—C2—C3	120.87 (17)	C3'—C2'—C1'	120.9 (3)
C1—C2—H2	119.6	C3'—C2'—H2'	119.6
C3—C2—H2	119.6	C1'—C2'—H2'	119.6



C2—C3—C4	120.59 (18)	C2'—C3'—C4'	121.1 (2)
C2—C3—H3	119.7	C2'—C3'—H3'	119.5
C4—C3—H3	119.7	C4'—C3'—H3'	119.5
C11—C4—C3	118.81 (18)	C3'—C4'—C11'	118.6 (2)
C11—C4—H4	120.6	C3'—C4'—H4'	120.7
C3—C4—H4	120.6	C11'—C4'—H4'	120.7
C12—C5—C6	119.22 (15)	C6'—C5'—C12'	119.1 (2)
C12—C5—H5	120.4	C6'—C5'—H5'	120.5
C6—C5—H5	120.4	C12'—C5'—H5'	120.5
C7—C6—C5	119.27 (15)	C7'—C6'—C5'	120.7 (2)
C7—C6—C9'	119.73 (16)	C7'—C6'—H6'	119.7
C5—C6—C9'	120.99 (15)	C5'—C6'—H6'	119.7
C6—C7—C8	121.63 (17)	C6'—C7'—C8'	121.0 (2)
C6—C7—H7	119.2	C6'—C7'—H7'	119.5
C8—C7—H7	119.2	C8'—C7'—H7'	119.5
C13—C8—C7	119.00 (17)	C13'—C8'—C7'	118.9 (2)
C13—C8—H8	120.5	C13'—C8'—H8'	120.6
C7—C8—H8	120.5	C7'—C8'—H8'	120.6
C10—C9—C13	103.00 (14)	C13'—C9'—C10'	102.05 (15)
C10—C9—H9A	111.2	C13'—C9'—C6	113.82 (15)
C13—C9—H9A	111.2	C10'—C9'—C6	117.03 (14)
C10—C9—H9B	111.2	C13'—C9'—H9'	107.8
C13—C9—H9B	111.2	C10'—C9'—H9'	107.8
H9A—C9—H9B	109.1	C6—C9'—H9'	107.8
C1—C10—C11	120.33 (17)	C1'—C10'—C11'	120.0 (2)
C1—C10—C9	129.63 (17)	C1'—C10'—C9'	129.7 (2)
C11—C10—C9	109.98 (14)	C11'—C10'—C9'	110.21 (17)
C4—C11—C10	120.37 (15)	C4'—C11'—C10'	120.5 (2)
C4—C11—C12	131.06 (15)	C4'—C11'—C12'	130.8 (2)
C10—C11—C12	108.38 (15)	C10'—C11'—C12'	108.59 (17)
C5—C12—C13	120.54 (15)	C5'—C12'—C13'	120.0 (2)
C5—C12—C11	130.90 (15)	C5'—C12'—C11'	131.35 (19)
C13—C12—C11	108.41 (14)	C13'—C12'—C11'	108.56 (16)
C8—C13—C12	120.32 (16)	C8'—C13'—C12'	120.38 (19)
C8—C13—C9	129.64 (16)	C8'—C13'—C9'	128.99 (19)
C12—C13—C9	109.97 (15)	C12'—C13'—C9'	110.59 (16)
C10—C1—C2—C3	0.9 (3)	C12'—C5'—C6'—C7'	0.6 (3)
C1—C2—C3—C4	-0.6 (3)	C5'—C6'—C7'—C8'	-0.8 (4)
C2—C3—C4—C11	-0.7 (3)	C6'—C7'—C8'—C13'	-0.2 (3)
C12—C5—C6—C7	0.5 (3)	C7—C6—C9'—C13'	100.0 (2)
C12—C5—C6—C9'	179.39 (16)	C5—C6—C9'—C13'	-78.9 (2)
C5—C6—C7—C8	0.7 (3)	C7—C6—C9'—C10'	-141.21 (18)
C9'—C6—C7—C8	-178.28 (19)	C5—C6—C9'—C10'	39.9 (2)
C6—C7—C8—C13	-0.5 (3)	C2'—C1'—C10'—C11'	0.0 (3)
C2—C1—C10—C11	0.1 (3)	C2'—C1'—C10'—C9'	176.29 (18)
C2—C1—C10—C9	177.08 (18)	C13'—C9'—C10'—C1'	-176.25 (18)
C13—C9—C10—C1	-172.24 (18)	C6—C9'—C10'—C1'	58.8 (3)



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C13—C9—C10—C11	4.98 (19)	C13'—C9'—C10'—C11'	0.32 (17)
C3—C4—C11—C10	1.7 (3)	C6—C9'—C10'—C11'	-124.61 (17)
C3—C4—C11—C12	-172.68 (18)	C3'—C4'—C11'—C10'	0.8 (3)
C1—C10—C11—C4	-1.4 (2)	C3'—C4'—C11'—C12'	-175.29 (19)
C9—C10—C11—C4	-178.95 (15)	C1'—C10'—C11'—C4'	-0.7 (3)
C1—C10—C11—C12	174.13 (15)	C9'—C10'—C11'—C4'	-177.67 (16)
C9—C10—C11—C12	-3.39 (18)	C1'—C10'—C11'—C12'	176.20 (17)
C6—C5—C12—C13	-1.7 (2)	C9'—C10'—C11'—C12'	-0.76 (18)
C6—C5—C12—C11	173.23 (16)	C6'—C5'—C12'—C13'	0.6 (3)
C4—C11—C12—C5	-0.3 (3)	C6'—C5'—C12'—C11'	176.7 (2)
C10—C11—C12—C5	-175.22 (17)	C4'—C11'—C12'—C5'	1.0 (3)
C4—C11—C12—C13	175.13 (17)	C10'—C11'—C12'—C5'	-175.45 (17)
C10—C11—C12—C13	0.20 (18)	C4'—C11'—C12'—C13'	177.41 (18)
C7—C8—C13—C12	-0.8 (3)	C10'—C11'—C12'—C13'	0.92 (18)
C7—C8—C13—C9	-177.28 (19)	C7'—C8'—C13'—C12'	1.5 (3)
C5—C12—C13—C8	1.9 (2)	C7'—C8'—C13'—C9'	-175.90 (19)
C11—C12—C13—C8	-174.10 (17)	C5'—C12'—C13'—C8'	-1.7 (3)
C5—C12—C13—C9	179.04 (16)	C11'—C12'—C13'—C8'	-178.54 (17)
C11—C12—C13—C9	3.06 (18)	C5'—C12'—C13'—C9'	176.14 (15)
C10—C9—C13—C8	171.96 (19)	C11'—C12'—C13'—C9'	-0.72 (18)
C10—C9—C13—C12	-4.86 (19)	C10'—C9'—C13'—C8'	177.84 (18)
C10'—C1'—C2'—C3'	0.6 (3)	C6—C9'—C13'—C8'	-55.1 (2)
C1'—C2'—C3'—C4'	-0.4 (4)	C10'—C9'—C13'—C12'	0.26 (17)
C2'—C3'—C4'—C11'	-0.3 (3)	C6—C9'—C13'—C12'	127.29 (16)

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