

# A second orthorhombic polymorph of (Z)-3-(9-anthryl)-1-(2-thienyl)prop-2-en-1-one<sup>1</sup>

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Received 19 December 2009; accepted 1 January 2010

Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.042;  $wR$  factor = 0.108; data-to-parameter ratio = 17.1.

The title heteroaryl chalcone,  $\text{C}_{21}\text{H}_{14}\text{OS}$ , is a second orthorhombic polymorph which crystallizes in the space group  $P2_12_12_1$ . The structure was previously reported [Fun *et al.* (2009). *Acta Cryst. E* **65**, o2168–o2169] in the space group  $Pna2_1$ . The bond distances and angles are similar in both structures. In contrast, the overall crystal packing is different from that in the first orthorhombic  $Pna2_1$  polymorph in which molecules were stacked into columns along the  $b$  axis and the thiophene units of two adjacent columns were stacked in a head to tail fashion. In the present polymorph, molecules are found to dimerize through a weak  $\text{S}\cdots\text{S}$  interaction [3.6513 (7) Å] and these dimers are arranged into sheets parallel to the  $bc$  plane. There are no classical hydrogen bonds in the packing which features short  $\text{C}\cdots\text{O}$  [3.2832 (2)–3.6251 (9) Å],  $\text{C}\cdots\text{S}$  [3.4879 (17)–3.6251 (19) Å] and  $\text{S}\cdots\text{O}$  [2.9948 (16) Å] contacts, together with  $\text{C}-\text{H}\cdots\pi$  interactions. Similar contacts were found in the other polymorph.

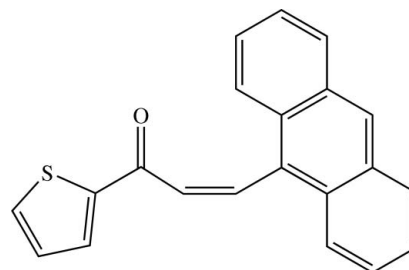
## Related literature

For bond-length data, see: Allen *et al.* (1987). For the structure of the first polymorph, see: Fun *et al.* (2009). For background to and applications of chalcones, see: Chantrapromma *et al.* (2009); Patil & Dharmaparakash (2008); Saydam *et al.* (2003); Suwunwong *et al.* (2009); Svetlichny *et al.* (2007). For the stability of the temperature controller used in the data collection, see Cosier & Glazer, (1986).

<sup>1</sup>This paper is dedicated to His Majesty King Bhumibol Adulyadej of Thailand (King Rama IX) for his sustainable development of the country.

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## Experimental

### Crystal data

$\text{C}_{21}\text{H}_{14}\text{OS}$   
 $M_r = 314.38$   
Orthorhombic,  $P2_12_12_1$   
 $a = 5.5116$  (1) Å  
 $b = 14.8497$  (2) Å  
 $c = 18.3625$  (3) Å  
 $V = 1502.89$  (4) Å<sup>3</sup>  
 $Z = 4$   
Mo  $K\alpha$  radiation  
 $\mu = 0.22$  mm<sup>-1</sup>  
 $T = 100$  K  
 $0.50 \times 0.19 \times 0.11$  mm

### Data collection

Bruker APEXII CCD area-detector diffractometer  
Absorption correction: multi-scan (SADABS; Bruker, 2005)  
 $T_{\min} = 0.900$ ,  $T_{\max} = 0.977$   
14062 measured reflections  
4354 independent reflections  
4035 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.025$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$   
 $wR(F^2) = 0.108$   
 $S = 1.05$   
4354 reflections  
254 parameters  
H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\max} = 0.79$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.62$  e Å<sup>-3</sup>  
Absolute structure: Flack (1983), 1830 Friedel pairs  
Flack parameter: 0.04 (8)

**Table 1**

Hydrogen-bond geometry (Å, °).

$Cg_1$ ,  $Cg_2$  and  $Cg_3$  are the centroids of the S1/C18–C21, C1–C6 and C8–C13 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C5-H5A\cdots Cg1^i$	0.91 (3)	2.64 (3)	3.443 (2)	149 (2)
$C15-H15A\cdots Cg2^{ii}$	0.95 (2)	2.74 (2)	3.565 (2)	146.4 (17)
$C21-H21A\cdots Cg3^{iii}$	1.04 (3)	2.91 (3)	3.711 (2)	134.4 (19)

Symmetry codes: (i)  $x + \frac{3}{2}, -y - \frac{1}{2}, -z + 1$ ; (ii)  $x + 1, y, z$ ; (iii)  $-x, y + \frac{3}{2}, -z + \frac{5}{2}$ .

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT (Bruker, 2005); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL software used to prepare material for publication: SHELXTL and PLATON (Spek, 2009).

The authors thank the Thailand Research Fund (TRF) for research grant (RSA 5280033) and the Prince of Songkla University for financial support through the Crystal Materials Research Unit. The authors also thank Universiti Sains Malaysia for the Research University Golden Goose grant No. 1001/PFIZIK/811012.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2716).

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## supporting information

*Acta Cryst.* (2010). E66, o312–o313 [https://doi.org/10.1107/S1600536810000061]

## A second orthorhombic polymorph of (Z)-3-(9-anthryl)-1-(2-thienyl)prop-2-en-1-one

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### S1. Comment

In continuation of our study of chalcone derivatives (Chantrapromma *et al.*, 2009; Fun *et al.*, 2009; Suwunwong *et al.*, 2009) which can be used for non-linear optical (NLO) materials (Patil & Dharmaprasadh, 2008), fluorescent materials (Svetlichny *et al.*, 2007) and bioactive compounds (Saydam *et al.*, 2003), the title heteroaryl chalcone (I) was synthesized and its crystal structure was previously reported in the orthorhombic space group  $Pna2_1$  (Fun *et al.*, 2009). In the present work, the compound crystallized in the orthorhombic space group  $P2_12_12_1$  from an ethanol/acetone (1:1) solvent mixture, while the crystal of the  $Pna2_1$  form crystallized from hot ethanol. (I) exhibits fluorescence with the maximum emission at 402 nm when the compound is excited at 335 nm.

The molecule of (I) (Fig. 1) exists in an *Z* configuration with respect to the C15=C16 double bond and the torsion angle C14–C15–C16–C17 =  $-2.9$  (3)° [compared to  $-3.7$  (7)° in one molecule and  $-4.0$  (7)° in the other in the  $Pna2_1$  polymorph which contains two molecules in an asymmetric unit]. The molecule of the present polymorph is less twisted as indicated by the interplanar angles between thiophene and anthracene rings being  $56.36$  (7)° and the least squares plane through the prop-2-en-1-one unit (C15–C17/O1) makes interplanar angles of  $12.2$  and  $68.00$  (11)° with the thiophene and anthracene rings, respectively [the corresponding values are  $75.07$  (17),  $13.1$  (3) and  $71.2$  (3)° in one molecule and  $76.32$  (17),  $15.2$  (3) and  $72.3$  (3)° in the other for the  $Pna2_1$  polymorph]. Bond distances are within normal ranges (Allen *et al.*, 1987).

In the crystal packing (Fig. 2), molecules are found to dimerize through a non-bonding S⋯S interaction [S⋯S =  $3.6513$  (7) Å]. The dimers are arranged into sheets parallel to the *bc* plane. These sheets are stacked along the *a* axis. The intermolecular interactions and short contacts are almost similar in both polymorph. There is no classic hydrogen bond and the crystal is consolidated by short C⋯O [ $3.2832$  (2)– $3.6251$  (9) Å], C⋯S [ $3.4879$  (17)– $3.6251$  (19) Å] and S⋯O [ $2.9948$  (16) Å] contacts, as well as C–H⋯ $\pi$  interactions (Table 1);  $Cg_1$ ,  $Cg_2$  and  $Cg_3$  are the centroids of the S1/C18–C21, C1–C6 and C8–C13 rings, respectively.

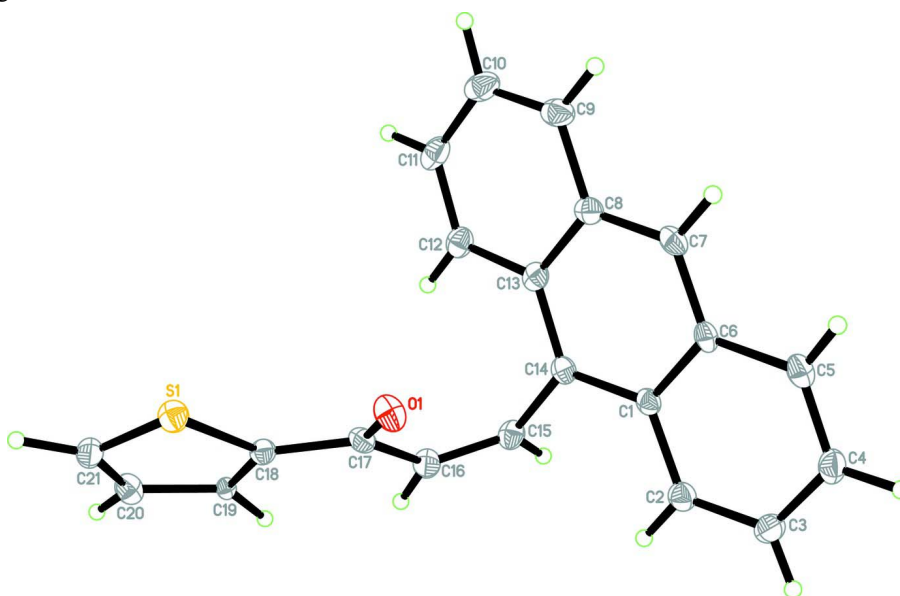
### S2. Experimental

The title compound was synthesized as reported by Fun *et al.* (2009). Yellow block-shaped single crystals of the title compound suitable for *x*-ray structure determination were recrystallized from ethanol/acetone (1:1 *v/v*) by slow evaporation of the solvent at room temperature over several days, Mp. 400–401 K.

### S3. Refinement

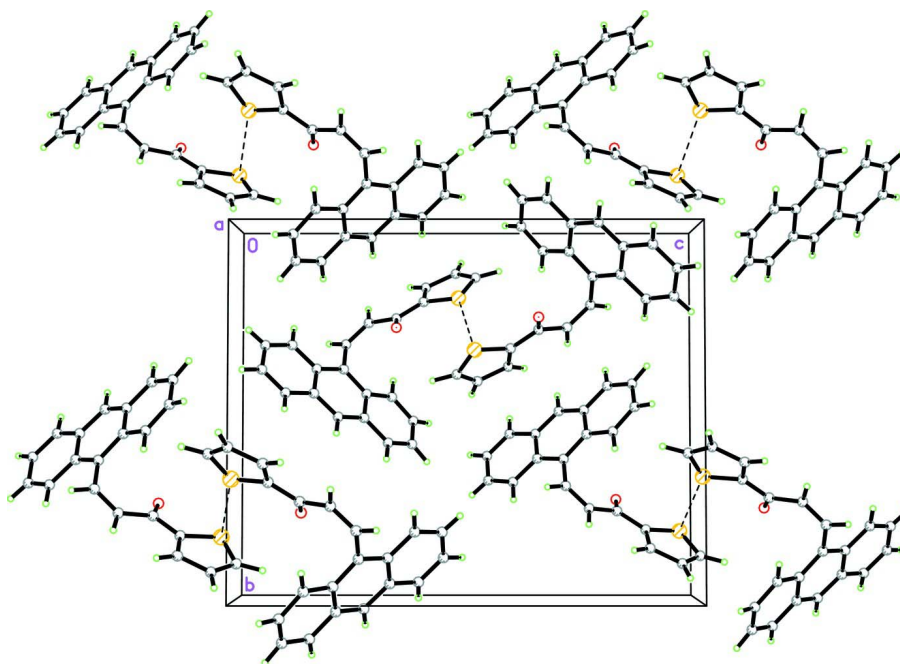
The H atom attached to C19 was placed in a calculated position, with  $d(C-H) = 0.93$  Å,  $U_{iso} = 1.2U_{eq}(C)$ . The remaining H atoms were located from the difference maps and refined isotropically. The highest residual electron density peak is located at  $0.04$  Å from C19 and the deepest hole is  $0.07$  Å from C20. A total of 1830 Friedel pairs were used to determine

the absolute configuration.



**Figure 1**

The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.



**Figure 2**

The crystal packing of the title compound viewed along the *a* axis. S...S contacts are shown as dashed lines.

**(Z)-3-(9-anthryl)-1-(2-thienyl)prop-2-en-1-one***Crystal data*C<sub>21</sub>H<sub>14</sub>OS $M_r = 314.38$ Orthorhombic,  $P2_12_12_1$ 

Hall symbol: P 2ac 2ab

 $a = 5.5116$  (1) Å $b = 14.8497$  (2) Å $c = 18.3625$  (3) Å $V = 1502.89$  (4) Å<sup>3</sup> $Z = 4$  $F(000) = 656$  $D_x = 1.390$  Mg m<sup>-3</sup>

Melting point = 400–401 K

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

Cell parameters from 4354 reflections

 $\theta = 1.8$ – $30.0^\circ$  $\mu = 0.22$  mm<sup>-1</sup> $T = 100$  K

Block, yellow

 $0.50 \times 0.19 \times 0.11$  mm*Data collection*Bruker APEXII CCD area-detector  
diffractometer

Radiation source: sealed tube

Graphite monochromator

 $\varphi$  and  $\omega$  scansAbsorption correction: multi-scan  
(SADABS; Bruker, 2005) $T_{\min} = 0.900$ ,  $T_{\max} = 0.977$ 

14062 measured reflections

4354 independent reflections

4035 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.025$  $\theta_{\max} = 30.0^\circ$ ,  $\theta_{\min} = 1.8^\circ$  $h = -7 \rightarrow 5$  $k = -17 \rightarrow 20$  $l = -25 \rightarrow 18$ *Refinement*Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.042$  $wR(F^2) = 0.108$  $S = 1.05$ 

4354 reflections

254 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methodsSecondary atom site location: difference Fourier  
mapHydrogen site location: inferred from  
neighbouring sitesH atoms treated by a mixture of independent  
and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 0.8977P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} = 0.001$  $\Delta\rho_{\max} = 0.79$  e Å<sup>-3</sup> $\Delta\rho_{\min} = -0.62$  e Å<sup>-3</sup>Absolute structure: Flack (1983), 1830 Friedel  
pairs

Absolute structure parameter: 0.04 (8)

*Special details***Experimental.** The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 120.0 (1) K.**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 (Å<sup>2</sup>)*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.79023 (9)	0.82740 (3)	0.98167 (3)	0.01920 (11)

O1	0.6379 (3)	0.74101 (10)	0.84157 (8)	0.0208 (3)
C1	0.6215 (3)	0.62511 (12)	0.66251 (10)	0.0142 (3)
C2	0.6199 (4)	0.69201 (13)	0.60656 (10)	0.0176 (4)
H2A	0.747 (4)	0.7404 (15)	0.6071 (12)	0.019 (6)*
C3	0.4549 (4)	0.68828 (13)	0.55096 (10)	0.0193 (4)
H3A	0.459 (4)	0.7304 (16)	0.5132 (14)	0.022 (6)*
C4	0.2761 (4)	0.61930 (13)	0.54827 (11)	0.0198 (4)
H4A	0.150 (5)	0.6169 (17)	0.5090 (13)	0.026 (6)*
C5	0.2685 (4)	0.55527 (13)	0.60124 (10)	0.0184 (4)
H5A	0.155 (5)	0.5111 (18)	0.6021 (14)	0.033 (7)*
C6	0.4394 (3)	0.55565 (12)	0.65992 (10)	0.0146 (3)
C7	0.4332 (4)	0.49043 (12)	0.71450 (10)	0.0169 (4)
H7A	0.311 (4)	0.4456 (14)	0.7129 (11)	0.010 (5)*
C8	0.6064 (4)	0.48855 (12)	0.76949 (10)	0.0159 (4)
C9	0.6059 (4)	0.41897 (13)	0.82390 (11)	0.0213 (4)
H9A	0.479 (4)	0.3744 (16)	0.8218 (13)	0.019 (6)*
C10	0.7811 (4)	0.41528 (14)	0.87607 (11)	0.0240 (4)
H10A	0.788 (5)	0.3656 (16)	0.9099 (13)	0.022 (6)*
C11	0.9682 (4)	0.48106 (15)	0.87753 (11)	0.0222 (4)
H11A	1.103 (5)	0.4744 (16)	0.9123 (13)	0.023 (6)*
C12	0.9731 (4)	0.54951 (14)	0.82813 (10)	0.0189 (4)
H12A	1.091 (5)	0.5966 (17)	0.8299 (13)	0.027 (7)*
C13	0.7917 (4)	0.55659 (12)	0.77254 (9)	0.0156 (3)
C14	0.7917 (3)	0.62627 (12)	0.72009 (9)	0.0143 (3)
C15	0.9746 (4)	0.69969 (13)	0.72208 (10)	0.0172 (4)
H15A	1.077 (4)	0.7024 (15)	0.6807 (12)	0.016 (6)*
C16	1.0028 (4)	0.76158 (13)	0.77411 (10)	0.0178 (4)
H16A	1.138 (5)	0.8035 (17)	0.7711 (13)	0.026 (6)*
C17	0.8452 (3)	0.77098 (12)	0.83955 (10)	0.0153 (3)
C18	0.9491 (3)	0.82083 (12)	0.90132 (9)	0.0146 (3)
C19	1.1727 (3)	0.86783 (12)	0.90518 (10)	0.0146 (2)
H19A	1.2863	0.8714	0.8678	0.018*
C20	1.1971 (3)	0.90888 (11)	0.97520 (10)	0.0146 (2)
H20A	1.351 (5)	0.9445 (17)	0.9876 (14)	0.031 (7)*
C21	1.0083 (4)	0.89174 (13)	1.02086 (11)	0.0198 (4)
H21A	0.993 (5)	0.9095 (18)	1.0753 (15)	0.034 (7)*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0185 (2)	0.0204 (2)	0.0188 (2)	-0.00094 (17)	0.00214 (18)	-0.00059 (18)
O1	0.0163 (6)	0.0219 (7)	0.0243 (7)	-0.0038 (6)	0.0037 (6)	-0.0053 (6)
C1	0.0159 (8)	0.0132 (8)	0.0136 (8)	0.0006 (7)	0.0018 (6)	-0.0028 (6)
C2	0.0200 (9)	0.0167 (8)	0.0162 (8)	0.0000 (7)	0.0013 (7)	-0.0014 (7)
C3	0.0234 (9)	0.0181 (9)	0.0163 (8)	0.0033 (7)	-0.0002 (7)	0.0009 (7)
C4	0.0211 (9)	0.0210 (9)	0.0174 (8)	0.0038 (8)	-0.0038 (8)	-0.0049 (7)
C5	0.0182 (9)	0.0167 (8)	0.0204 (8)	0.0001 (7)	-0.0007 (8)	-0.0057 (7)
C6	0.0140 (8)	0.0143 (8)	0.0155 (8)	0.0007 (7)	-0.0001 (7)	-0.0056 (7)

C7	0.0187 (9)	0.0131 (8)	0.0188 (8)	-0.0010 (7)	0.0030 (7)	-0.0038 (7)
C8	0.0192 (9)	0.0142 (8)	0.0143 (8)	0.0023 (7)	0.0050 (7)	-0.0007 (7)
C9	0.0279 (11)	0.0152 (9)	0.0208 (9)	0.0012 (8)	0.0065 (8)	0.0002 (7)
C10	0.0325 (11)	0.0215 (9)	0.0179 (8)	0.0078 (9)	0.0061 (9)	0.0032 (7)
C11	0.0254 (10)	0.0262 (10)	0.0149 (8)	0.0088 (9)	0.0012 (8)	0.0007 (8)
C12	0.0182 (9)	0.0219 (9)	0.0166 (8)	0.0029 (8)	0.0016 (7)	-0.0013 (7)
C13	0.0164 (8)	0.0170 (8)	0.0133 (7)	0.0038 (7)	0.0036 (7)	-0.0019 (6)
C14	0.0146 (7)	0.0144 (8)	0.0141 (7)	0.0014 (7)	0.0019 (7)	-0.0028 (6)
C15	0.0163 (8)	0.0213 (9)	0.0141 (8)	-0.0014 (7)	0.0026 (7)	0.0002 (7)
C16	0.0170 (9)	0.0198 (9)	0.0165 (8)	-0.0033 (7)	0.0013 (7)	0.0000 (7)
C17	0.0173 (9)	0.0118 (8)	0.0167 (8)	-0.0001 (7)	0.0011 (7)	-0.0010 (6)
C18	0.0161 (8)	0.0151 (8)	0.0125 (7)	0.0021 (7)	0.0022 (6)	0.0003 (7)
C19	0.0125 (5)	0.0149 (5)	0.0164 (6)	0.0005 (5)	-0.0024 (5)	-0.0019 (5)
C20	0.0125 (5)	0.0149 (5)	0.0164 (6)	0.0005 (5)	-0.0024 (5)	-0.0019 (5)
C21	0.0243 (9)	0.0190 (8)	0.0161 (8)	0.0040 (7)	-0.0012 (8)	-0.0017 (7)

*Geometric parameters (Å, °)*

S1—C21	1.696 (2)	C9—H9A	0.96 (3)
S1—C18	1.7184 (18)	C10—C11	1.421 (3)
O1—C17	1.227 (2)	C10—H10A	0.97 (2)
C1—C14	1.414 (3)	C11—C12	1.363 (3)
C1—C2	1.429 (3)	C11—H11A	0.98 (3)
C1—C6	1.440 (3)	C12—C13	1.433 (3)
C2—C3	1.368 (3)	C12—H12A	0.96 (3)
C2—H2A	1.00 (2)	C13—C14	1.414 (2)
C3—C4	1.422 (3)	C14—C15	1.485 (3)
C3—H3A	0.93 (2)	C15—C16	1.335 (3)
C4—C5	1.361 (3)	C15—H15A	0.95 (2)
C4—H4A	1.00 (3)	C16—C17	1.489 (3)
C5—C6	1.431 (3)	C16—H16A	0.97 (3)
C5—H5A	0.91 (3)	C17—C18	1.470 (3)
C6—C7	1.394 (3)	C18—C19	1.418 (3)
C7—C8	1.390 (3)	C19—C20	1.429 (2)
C7—H7A	0.95 (2)	C19—H19A	0.9300
C8—C9	1.437 (3)	C20—C21	1.360 (3)
C8—C13	1.438 (3)	C20—H20A	1.02 (3)
C9—C10	1.361 (3)	C21—H21A	1.04 (3)
C21—S1—C18	92.02 (10)	C12—C11—H11A	119.5 (15)
C14—C1—C2	122.21 (17)	C10—C11—H11A	119.4 (14)
C14—C1—C6	119.73 (17)	C11—C12—C13	121.0 (2)
C2—C1—C6	118.05 (17)	C11—C12—H12A	122.4 (16)
C3—C2—C1	120.81 (18)	C13—C12—H12A	116.5 (16)
C3—C2—H2A	120.0 (13)	C14—C13—C12	122.62 (18)
C1—C2—H2A	119.1 (13)	C14—C13—C8	119.20 (17)
C2—C3—C4	121.04 (18)	C12—C13—C8	118.16 (17)
C2—C3—H3A	120.8 (15)	C13—C14—C1	120.04 (17)

C4—C3—H3A	118.2 (15)	C13—C14—C15	121.37 (16)
C5—C4—C3	119.99 (18)	C1—C14—C15	118.55 (16)
C5—C4—H4A	118.0 (15)	C16—C15—C14	127.01 (17)
C3—C4—H4A	122.0 (15)	C16—C15—H15A	118.3 (14)
C4—C5—C6	120.99 (19)	C14—C15—H15A	114.7 (14)
C4—C5—H5A	122.6 (17)	C15—C16—C17	125.05 (17)
C6—C5—H5A	116.4 (17)	C15—C16—H16A	119.3 (15)
C7—C6—C5	121.47 (17)	C17—C16—H16A	115.6 (15)
C7—C6—C1	119.43 (17)	O1—C17—C18	121.46 (17)
C5—C6—C1	119.10 (17)	O1—C17—C16	122.25 (17)
C8—C7—C6	121.27 (17)	C18—C17—C16	116.26 (16)
C8—C7—H7A	119.8 (13)	C19—C18—C17	128.65 (16)
C6—C7—H7A	118.9 (13)	C19—C18—S1	111.83 (13)
C7—C8—C9	121.21 (18)	C17—C18—S1	119.51 (14)
C7—C8—C13	120.14 (17)	C18—C19—C20	109.67 (16)
C9—C8—C13	118.65 (18)	C18—C19—H19A	125.2
C10—C9—C8	121.1 (2)	C20—C19—H19A	125.2
C10—C9—H9A	121.0 (14)	C21—C20—C19	113.75 (16)
C8—C9—H9A	117.8 (14)	C21—C20—H20A	126.4 (15)
C9—C10—C11	120.04 (18)	C19—C20—H20A	119.8 (15)
C9—C10—H10A	120.8 (16)	C20—C21—S1	112.71 (15)
C11—C10—H10A	119.0 (16)	C20—C21—H21A	127.5 (16)
C12—C11—C10	121.0 (2)	S1—C21—H21A	119.7 (16)
C14—C1—C2—C3	179.06 (17)	C9—C8—C13—C12	2.5 (3)
C6—C1—C2—C3	-2.1 (3)	C12—C13—C14—C1	174.11 (17)
C1—C2—C3—C4	1.7 (3)	C8—C13—C14—C1	-4.4 (3)
C2—C3—C4—C5	-0.5 (3)	C12—C13—C14—C15	-3.3 (3)
C3—C4—C5—C6	-0.4 (3)	C8—C13—C14—C15	178.18 (16)
C4—C5—C6—C7	179.95 (18)	C2—C1—C14—C13	-177.53 (17)
C4—C5—C6—C1	0.0 (3)	C6—C1—C14—C13	3.6 (3)
C14—C1—C6—C7	0.2 (3)	C2—C1—C14—C15	0.0 (3)
C2—C1—C6—C7	-178.75 (17)	C6—C1—C14—C15	-178.90 (16)
C14—C1—C6—C5	-179.92 (16)	C13—C14—C15—C16	-64.2 (3)
C2—C1—C6—C5	1.2 (3)	C1—C14—C15—C16	118.4 (2)
C5—C6—C7—C8	176.94 (17)	C14—C15—C16—C17	-2.9 (3)
C1—C6—C7—C8	-3.1 (3)	C15—C16—C17—O1	-21.8 (3)
C6—C7—C8—C9	-177.26 (17)	C15—C16—C17—C18	160.02 (19)
C6—C7—C8—C13	2.3 (3)	O1—C17—C18—C19	-172.54 (18)
C7—C8—C9—C10	177.47 (19)	C16—C17—C18—C19	5.7 (3)
C13—C8—C9—C10	-2.1 (3)	O1—C17—C18—S1	6.9 (2)
C8—C9—C10—C11	0.2 (3)	C16—C17—C18—S1	-174.86 (13)
C9—C10—C11—C12	1.3 (3)	C21—S1—C18—C19	0.62 (15)
C10—C11—C12—C13	-0.9 (3)	C21—S1—C18—C17	-178.93 (15)
C11—C12—C13—C14	-179.56 (18)	C17—C18—C19—C20	178.21 (17)
C11—C12—C13—C8	-1.0 (3)	S1—C18—C19—C20	-1.30 (19)
C7—C8—C13—C14	1.5 (3)	C18—C19—C20—C21	1.5 (2)
C9—C8—C13—C14	-178.92 (17)	C19—C20—C21—S1	-1.1 (2)



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C7—C8—C13—C12                      -177.10 (17)                      C18—S1—C21—C20                      0.27 (15)

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*Hydrogen-bond geometry (Å, °)*

*Cg*<sub>1</sub>, *Cg*<sub>2</sub> and *Cg*<sub>3</sub> are the centroids of the S1/C18—C21, C1—C6 and C8—C13 rings, respectively.

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<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C5—H5 <i>A</i> ··· <i>Cg</i> 1 <sup>i</sup>	0.91 (3)	2.64 (3)	3.443 (2)	149 (2)
C15—H15 <i>A</i> ··· <i>Cg</i> 2 <sup>ii</sup>	0.95 (2)	2.74 (2)	3.565 (2)	146.4 (17)
C21—H21 <i>A</i> ··· <i>Cg</i> 3 <sup>iii</sup>	1.04 (3)	2.91 (3)	3.711 (2)	134.4 (19)

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Symmetry codes: (i)  $x+3/2, -y-1/2, -z+1$ ; (ii)  $x+1, y, z$ ; (iii)  $-x, y+3/2, -z+5/2$ .