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Triclinic polymorph of dibenzotetrathiafulvalene

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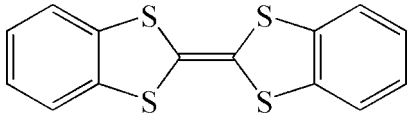
Key indicators: single-crystal X-ray study; T = 93 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.110; data-to-parameter ratio = 17.5.

Crystals of the title compound (DBTTF), $C_{14}H_8S_4$, feature a triclinic polymorph different from two known monoclinic polymorphs. In this form, there are two independent centrosymmetric half-molecules in the asymmetric unit. Although the molecular orientations are relatively similar to one of monoclinic polymorphs, the packing motif is different.

Related literature

For the synthesis, see: Nakayama *et al.* (1976). For the monoclinic polymorphs of DBTTF, see: Emge *et al.* (1982); Brillante *et al.* (2008). For the electronic properties of DBTTF, see: Jigami *et al.* (1998). For the characteristics of field-effect transistors based on DBTTF, see, for example: Mas-Torrent *et al.* (2005); Shibata *et al.* (2008). For related structures, see: Mas-Torrent *et al.* (2004); Naraso *et al.* (2006).



Experimental

Crystal data

$C_{14}H_8S_4$
M_r = 304.46
Triclinic, $P\overline{1}$
a = 8.6562 (4) Å
b = 9.4144 (5) Å
c = 9.5144 (4) Å
α = 74.0424 (15)°
β = 63.6158 (13)°
γ = 65.5653 (14)°
V = 628.43 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.73 mm^{-1}
T = 93 K
0.35 × 0.25 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.663, T_{max} = 0.896
6216 measured reflections
2871 independent reflections
2193 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.110
S = 1.12
2871 reflections
164 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5019).

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supplementary materials

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Triclinic polymorph of dibenzotetrathiafulvalene

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Comment

TTF and its derivatives have been well known as the most dominant electron donors (Jigami *et al.*, 1998). Recently, some TTF derivatives have been used as organic semiconductors for organic field-effect transistors (OFETs) (Mas-Torrent *et al.*, 2004; Naraso *et al.*, 2006), which show high hole mobilities in both the single crystals and thin films. The title compound, dibenzotetrathiafulvalene (**I**), has also exhibited high mobility (Mas-Torrent *et al.*, 2005; Shibata *et al.*, 2008). Since the strong intermolecular interactions between the molecules are necessary for carrier transportation in organic conductors and semiconductors, the investigation of crystal structures are very important. The crystal structure of compound (**I**) has been reported as two monoclinic polymorphs, which are space group $P2_1/c$ for α phase (Emge *et al.*, 1982) and *Cc* for β phase (Brillante *et al.*, 2008). These crystals were grown from solution and the existence of other two polymorphs has been found by means of lattice phonon confocal Raman microscopy and XRD. Herein, we report the single-crystal structure of compound (**I**) neither the α nor β phase.

The single-crystal of (**I**) which has been grown by vapour transport contains two crystallographically independent molecules with an inversion center. The molecules have chair-like structures which are slightly distorted from the molecular plane. The maximum deviations from the least-squares plane are 0.206 and 0.222 Å, and the average deviations are 0.085 and 0.111 Å. The molecular geometries in this phase are different from that in the α phase (average deviation: 0.037 Å) and similar to that in the β phase (maximum deviation: 0.235 Å, average deviation: 0.085 Å). The packing structure in this phase is a herringbone type with a tilt angle of 51.11° (Fig. 2), which is also similar to the β phase. However, the long axis is observed to be sliding and the number of intermolecular short contacts between the molecules is increased and the contact distances are shorter compared with the α and the β phase.

Experimental

To a stirred solution of 1,3-benzodithiolylium tetrafluoroborate (0.83 g, 3.5 mmol) in dichloromethane (30 ml) was added dropwise 1,8-diazabicyclo[5.4.0]undec-7-ene (1 ml) at room temperature. After being stirred for 4 h, the resulting precipitate was filtered, washed with dichloromethane and dried to give 0.30 g (58%) of the title compound. Yellow crystals of (**I**) suitable for X-ray analysis were obtained from slow vacuum sublimation in a gradient-temperature horizontal glass tube. A temperature of the source material was maintained at 480 K.

Refinement

H atoms were placed in calculated positions and refined in the riding model, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C) for CH groups.

Figures

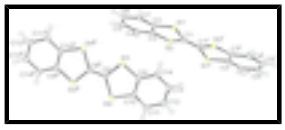


Fig. 1. The molecular structure of (**I**), showing 50% probability displacement ellipsoids. [symmetry codes: (i) 1 - *x*, 1 - *y*, 1 - *z*, (ii) -*x*, -*y*, 1 - *z*.]

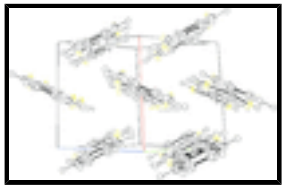


Fig. 2. A packing diagram for (**I**) viewed along the molecular long axis.

dibenzotetrathiafulvalene

Crystal data

$C_{14}H_8S_4$	$Z = 2$
$M_r = 304.46$	$F_{000} = 312.00$
Triclinic, $P\overline{1}$	$D_x = 1.609$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
$a = 8.6562$ (4) Å	Cell parameters from 4982 reflections
$b = 9.4144$ (5) Å	$\theta = 3.0$–27.5°
$c = 9.5144$ (4) Å	$\mu = 0.73$ mm^{-1}
$\alpha = 74.0424$ (15)°	$T = 93$ K
$\beta = 63.6158$ (13)°	Platelet, yellow
$\gamma = 65.5653$ (14)°	0.35 × 0.25 × 0.15 mm
$V = 628.43$ (5) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	2193 reflections with $F^2 > 2\sigma(F^2)$
Detector resolution: 10.00 pixels mm^{-1}	$R_{int} = 0.028$
ω scans	$\theta_{max} = 27.5^\circ$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -11 \rightarrow 11$
$T_{min} = 0.663$, $T_{max} = 0.896$	$k = -12 \rightarrow 12$
6216 measured reflections	$l = -12 \rightarrow 11$
2871 independent reflections	

Refinement

Refinement on F^2	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)] = 0.037$	$w = 1/[\sigma^2(F_o^2) + (0.0363P)^2 + 1.1654P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.110$	$(\Delta/\sigma)_{max} < 0.001$

S = 1.12	$\Delta\rho_{max}$ = 0.56 e Å^{-3}
2871 reflections	$\Delta\rho_{min}$ = −0.46 e Å^{-3}
164 parameters	Extinction correction: none

Special details

Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY

Refinement. Refinement was performed using all reflections. The weighted *R*-factor (*wR*) and goodness of fit (*S*) are based on F^2. *R*-factor (gt) are based on *F*. The threshold expression of $F^2 > 2.0\ \sigma(F^2)$ is used only for calculating *R*-factor (gt).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S(1)	0.43963 (10)	0.53797 (9)	0.28891 (8)	0.01843 (17)
S(2)	0.60882 (10)	0.24998 (8)	0.46970 (9)	0.02064 (17)
S(3)	0.07081 (10)	0.20979 (9)	0.46015 (9)	0.01946 (17)
S(4)	−0.11044 (10)	0.02886 (9)	0.75183 (8)	0.01913 (17)
C(1)	0.5095 (3)	0.4558 (3)	0.4497 (3)	0.0156 (5)
C(2)	0.4701 (3)	0.3575 (3)	0.2425 (3)	0.0172 (5)
C(3)	0.5503 (3)	0.2223 (3)	0.3267 (3)	0.0193 (5)
C(4)	0.5830 (4)	0.0743 (3)	0.2954 (4)	0.0241 (6)
C(5)	0.5339 (4)	0.0630 (4)	0.1786 (4)	0.0297 (7)
C(6)	0.4545 (4)	0.1975 (4)	0.0947 (3)	0.0291 (7)
C(7)	0.4203 (4)	0.3460 (4)	0.1263 (3)	0.0232 (6)
C(8)	−0.0073 (3)	0.0491 (3)	0.5443 (3)	0.0161 (5)
C(9)	0.0398 (3)	0.2558 (3)	0.6390 (3)	0.0181 (5)
C(10)	−0.0446 (3)	0.1709 (3)	0.7768 (3)	0.0173 (5)
C(11)	−0.0710 (4)	0.1986 (3)	0.9235 (3)	0.0222 (6)
C(12)	−0.0092 (4)	0.3109 (4)	0.9306 (4)	0.0270 (7)
C(13)	0.0748 (4)	0.3954 (3)	0.7934 (4)	0.0265 (6)
C(14)	0.0984 (4)	0.3703 (3)	0.6477 (3)	0.0211 (6)
H(1)	0.6380	−0.0176	0.3526	0.029*
H(2)	0.5550	−0.0373	0.1565	0.036*
H(3)	0.4231	0.1883	0.0147	0.035*
H(4)	0.3641	0.4378	0.0697	0.028*
H(5)	−0.1302	0.1420	1.0174	0.027*
H(6)	−0.0247	0.3296	1.0299	0.032*
H(7)	0.1166	0.4713	0.7998	0.032*
H(8)	0.1536	0.4299	0.5544	0.025*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S(1)	0.0239 (3)	0.0176 (3)	0.0167 (3)	−0.0073 (2)	−0.0113 (2)	0.0003 (2)
S(2)	0.0255 (3)	0.0145 (3)	0.0260 (3)	−0.0040 (2)	−0.0158 (3)	−0.0021 (3)
S(3)	0.0250 (3)	0.0186 (3)	0.0157 (3)	−0.0117 (3)	−0.0055 (2)	0.0000 (2)
S(4)	0.0247 (3)	0.0210 (3)	0.0144 (3)	−0.0139 (3)	−0.0053 (2)	0.0002 (2)

C(1)	0.0180 (13)	0.0138 (12)	0.0156 (12)	−0.0057 (11)	−0.0079 (10)	0.0008 (11)
C(2)	0.0152 (12)	0.0240 (14)	0.0145 (12)	−0.0101 (11)	−0.0017 (10)	−0.0065 (11)
C(3)	0.0177 (13)	0.0227 (14)	0.0187 (13)	−0.0077 (11)	−0.0043 (11)	−0.0069 (12)
C(4)	0.0185 (14)	0.0227 (15)	0.0308 (16)	−0.0098 (12)	−0.0042 (12)	−0.0068 (13)
C(5)	0.0276 (16)	0.0363 (18)	0.0293 (16)	−0.0187 (15)	−0.0003 (13)	−0.0150 (15)
C(6)	0.0311 (16)	0.048 (2)	0.0188 (14)	−0.0263 (16)	−0.0015 (13)	−0.0121 (15)
C(7)	0.0245 (15)	0.0366 (18)	0.0138 (13)	−0.0180 (14)	−0.0046 (11)	−0.0031 (13)
C(8)	0.0163 (12)	0.0164 (13)	0.0155 (12)	−0.0058 (11)	−0.0077 (10)	0.0017 (11)
C(9)	0.0156 (12)	0.0167 (13)	0.0223 (14)	−0.0043 (11)	−0.0079 (11)	−0.0032 (12)
C(10)	0.0164 (12)	0.0151 (13)	0.0192 (13)	−0.0036 (10)	−0.0058 (11)	−0.0046 (11)
C(11)	0.0209 (14)	0.0243 (15)	0.0194 (14)	−0.0075 (12)	−0.0046 (12)	−0.0049 (13)
C(12)	0.0293 (16)	0.0291 (17)	0.0252 (16)	−0.0077 (14)	−0.0083 (13)	−0.0135 (14)
C(13)	0.0271 (15)	0.0256 (16)	0.0305 (16)	−0.0112 (13)	−0.0073 (13)	−0.0109 (14)
C(14)	0.0193 (13)	0.0197 (14)	0.0253 (15)	−0.0101 (12)	−0.0061 (12)	−0.0024 (12)

Geometric parameters (Å, °)

S(1)—C(1)	1.758 (3)	C(8)—C(8)^{ii}	1.350 (5)
S(1)—C(2)	1.757 (3)	C(9)—C(10)	1.395 (3)
S(2)—C(1)	1.759 (2)	C(9)—C(14)	1.401 (5)
S(2)—C(3)	1.759 (4)	C(10)—C(11)	1.391 (5)
S(3)—C(8)	1.756 (3)	C(11)—C(12)	1.395 (6)
S(3)—C(9)	1.748 (3)	C(12)—C(13)	1.389 (4)
S(4)—C(8)	1.760 (2)	C(13)—C(14)	1.382 (5)
S(4)—C(10)	1.759 (4)	C(4)—H(1)	0.950
C(1)—C(1)^{i}	1.349 (5)	C(5)—H(2)	0.950
C(2)—C(3)	1.395 (4)	C(6)—H(3)	0.950
C(2)—C(7)	1.396 (5)	C(7)—H(4)	0.950
C(3)—C(4)	1.391 (5)	C(11)—H(5)	0.950
C(4)—C(5)	1.396 (6)	C(12)—H(6)	0.950
C(5)—C(6)	1.388 (4)	C(13)—H(7)	0.950
C(6)—C(7)	1.393 (6)	C(14)—H(8)	0.950
S(1)···C(7)^{iii}	3.568 (3)	H(1)···C(9)^{vi}	2.782
S(1)···C(10)^{iv}	3.578 (2)	H(1)···C(10)^{vi}	2.985
S(2)···C(8)^{v}	3.359 (3)	H(1)···C(11)^{vi}	3.504
S(2)···C(8)^{vi}	3.407 (2)	H(1)···C(14)^{vi}	3.156
S(3)···C(6)	3.574 (2)	H(1)···H(1)^{vi}	2.754
C(1)···C(14)	3.527 (4)	H(1)···H(5)^{x}	3.260
C(4)···C(4)^{vi}	3.589 (4)	H(1)···H(8)^{vi}	3.583
C(4)···C(10)^{vi}	3.545 (3)	H(2)···S(2)^{vi}	3.552
C(6)···S(3)	3.574 (2)	H(2)···S(4)^{ii}	3.518
C(7)···S(1)^{iii}	3.568 (3)	H(2)···C(6)^{xi}	3.202
C(7)···C(7)^{iii}	3.552 (5)	H(2)···C(12)^{vi}	3.561
C(8)···S(2)^{vii}	3.359 (3)	H(2)···H(2)^{xi}	3.329
C(8)···S(2)^{vi}	3.407 (2)	H(2)···H(3)^{xi}	2.341
C(10)···S(1)^{iv}	3.578 (2)	H(2)···H(5)^{x}	3.376

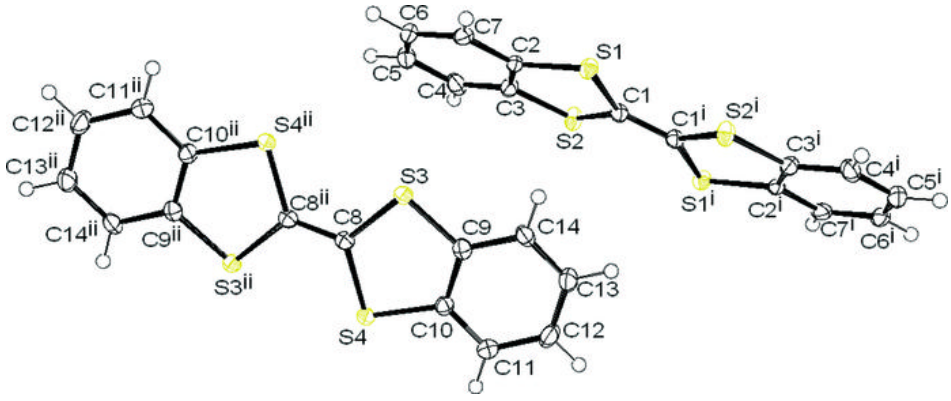
C(10)···C(4)^{vi}	3.545 (3)	H(3)···S(1)^{iii}	3.433
C(11)···C(11)^{viii}	3.523 (4)	H(3)···S(4)^{x}	3.590
C(14)···C(1)	3.527 (4)	H(3)···C(5)^{xi}	3.189
S(1)···H(3)^{iii}	3.433	H(3)···H(2)^{xi}	2.341
S(1)···H(4)^{iii}	3.053	H(3)···H(3)^{xi}	3.275
S(1)···H(7)^{i}	3.515	H(3)···H(6)^{xiii}	3.486
S(1)···H(8)	2.942	H(4)···S(1)^{iii}	3.053
S(2)···H(1)^{vi}	3.291	H(4)···C(2)^{iii}	3.154
S(2)···H(2)^{vi}	3.552	H(4)···C(7)^{iii}	3.010
S(2)···H(8)	3.384	H(4)···C(11)^{iv}	3.309
S(3)···H(1)^{vi}	3.354	H(4)···C(12)^{iv}	3.004
S(3)···H(8)^{iv}	3.135	H(4)···C(13)^{iv}	3.223
S(4)···H(2)^{ii}	3.518	H(4)···H(4)^{iii}	2.705
S(4)···H(3)^{ix}	3.590	H(4)···H(6)^{iv}	3.215
S(4)···H(5)^{viii}	3.332	H(4)···H(7)^{iv}	3.555
S(4)···H(6)^{viii}	3.480	H(5)···S(4)^{viii}	3.332
C(1)···H(7)	3.532	H(5)···C(2)^{ix}	3.267
C(1)···H(7)^{i}	3.271	H(5)···C(3)^{ix}	3.024
C(1)···H(8)	2.881	H(5)···C(4)^{ix}	2.848
C(1)···H(8)^{i}	3.484	H(5)···C(5)^{ix}	2.925
C(2)···H(4)^{iii}	3.154	H(5)···C(6)^{ix}	3.169
C(2)···H(5)^{x}	3.267	H(5)···C(7)^{ix}	3.351
C(2)···H(8)	3.019	H(5)···C(10)^{viii}	3.252
C(3)···H(1)^{vi}	3.259	H(5)···C(11)^{viii}	2.982
C(3)···H(5)^{x}	3.024	H(5)···H(1)^{ix}	3.260
C(3)···H(8)	3.235	H(5)···H(2)^{ix}	3.376
C(4)···H(1)^{vi}	3.055	H(5)···H(5)^{viii}	2.679
C(4)···H(5)^{x}	2.848	H(6)···S(4)^{viii}	3.480
C(5)···H(3)^{xi}	3.189	H(6)···C(13)^{xii}	3.245
C(5)···H(5)^{x}	2.925	H(6)···H(3)^{xiv}	3.486
C(6)···H(2)^{xi}	3.202	H(6)···H(4)^{iv}	3.215
C(6)···H(5)^{x}	3.169	H(6)···H(6)^{xii}	3.273
C(7)···H(4)^{iii}	3.010	H(6)···H(7)^{xii}	2.461
C(7)···H(5)^{x}	3.351	H(7)···S(1)^{i}	3.515
C(9)···H(1)^{vi}	2.782	H(7)···C(1)	3.532
C(9)···H(8)^{iv}	3.254	H(7)···C(1)^{i}	3.271
C(10)···H(1)^{vi}	2.985	H(7)···C(12)^{xii}	3.293
C(10)···H(5)^{viii}	3.252	H(7)···H(4)^{iv}	3.555
C(11)···H(1)^{vi}	3.504	H(7)···H(6)^{xii}	2.461
C(11)···H(4)^{iv}	3.309	H(7)···H(7)^{xii}	3.503
C(11)···H(5)^{viii}	2.982	H(8)···S(1)	2.942

C(12)···H(2)^{vi}	3.561	H(8)···S(2)	3.384
C(12)···H(4)^{iv}	3.004	H(8)···S(3)^{iv}	3.135
C(12)···H(7)^{xii}	3.293	H(8)···C(1)	2.881
C(13)···H(4)^{iv}	3.223	H(8)···C(1)^{i}	3.484
C(13)···H(6)^{xii}	3.245	H(8)···C(2)	3.019
C(14)···H(1)^{vi}	3.156	H(8)···C(3)	3.235
C(14)···H(8)^{iv}	3.215	H(8)···C(9)^{iv}	3.254
H(1)···S(2)^{vi}	3.291	H(8)···C(14)^{iv}	3.215
H(1)···S(3)^{vi}	3.354	H(8)···H(1)^{vi}	3.583
H(1)···C(3)^{vi}	3.259	H(8)···H(8)^{iv}	2.946
H(1)···C(4)^{vi}	3.055		
C(1)—S(1)—C(2)	95.02 (15)	S(4)—C(10)—C(9)	116.1 (2)
C(1)—S(2)—C(3)	95.06 (16)	S(4)—C(10)—C(11)	123.3 (2)
C(8)—S(3)—C(9)	95.27 (15)	C(9)—C(10)—C(11)	120.5 (3)
C(8)—S(4)—C(10)	95.27 (16)	C(10)—C(11)—C(12)	119.0 (2)
S(1)—C(1)—S(2)	115.5 (2)	C(11)—C(12)—C(13)	120.5 (3)
S(1)—C(1)—C(1)^{i}	122.5 (2)	C(12)—C(13)—C(14)	120.7 (4)
S(2)—C(1)—C(1)^{i}	122.0 (2)	C(9)—C(14)—C(13)	119.3 (2)
S(1)—C(2)—C(3)	116.8 (3)	C(3)—C(4)—H(1)	120.5
S(1)—C(2)—C(7)	122.9 (2)	C(5)—C(4)—H(1)	120.5
C(3)—C(2)—C(7)	120.3 (3)	C(4)—C(5)—H(2)	119.8
S(2)—C(3)—C(2)	116.6 (2)	C(6)—C(5)—H(2)	119.8
S(2)—C(3)—C(4)	122.8 (2)	C(5)—C(6)—H(3)	119.6
C(2)—C(3)—C(4)	120.6 (3)	C(7)—C(6)—H(3)	119.5
C(3)—C(4)—C(5)	119.0 (3)	C(2)—C(7)—H(4)	120.6
C(4)—C(5)—C(6)	120.3 (4)	C(6)—C(7)—H(4)	120.6
C(5)—C(6)—C(7)	120.9 (4)	C(10)—C(11)—H(5)	120.5
C(2)—C(7)—C(6)	118.8 (3)	C(12)—C(11)—H(5)	120.5
S(3)—C(8)—S(4)	115.1 (2)	C(11)—C(12)—H(6)	119.8
S(3)—C(8)—C(8)^{ii}	122.2 (2)	C(13)—C(12)—H(6)	119.8
S(4)—C(8)—C(8)^{ii}	122.6 (2)	C(12)—C(13)—H(7)	119.6
S(3)—C(9)—C(10)	117.1 (3)	C(14)—C(13)—H(7)	119.7
S(3)—C(9)—C(14)	122.9 (2)	C(9)—C(14)—H(8)	120.4
C(10)—C(9)—C(14)	120.0 (3)	C(13)—C(14)—H(8)	120.4
C(1)—S(1)—C(2)—C(3)	−6.4 (2)	C(3)—C(2)—C(7)—C(6)	−0.9 (4)
C(1)—S(1)—C(2)—C(7)	174.5 (2)	C(7)—C(2)—C(3)—S(2)	179.7 (2)
C(2)—S(1)—C(1)—S(2)	10.26 (18)	C(7)—C(2)—C(3)—C(4)	0.5 (4)
C(2)—S(1)—C(1)—C(1)^{i}	−170.5 (2)	S(2)—C(3)—C(4)—C(5)	−179.3 (2)
C(1)—S(2)—C(3)—C(2)	5.7 (2)	C(2)—C(3)—C(4)—C(5)	−0.2 (4)
C(1)—S(2)—C(3)—C(4)	−175.2 (2)	C(3)—C(4)—C(5)—C(6)	0.3 (4)
C(3)—S(2)—C(1)—S(1)	−10.05 (18)	C(4)—C(5)—C(6)—C(7)	−0.8 (4)
C(3)—S(2)—C(1)—C(1)^{i}	170.7 (2)	C(5)—C(6)—C(7)—C(2)	1.0 (4)
C(8)—S(3)—C(9)—C(10)	−5.7 (2)	S(3)—C(8)—C(8)^{ii}—S(4)^{ii}	1.6 (3)
C(8)—S(3)—C(9)—C(14)	173.1 (2)	S(4)—C(8)—C(8)^{ii}—S(3)^{ii}	−1.6 (3)
C(9)—S(3)—C(8)—S(4)	10.05 (18)	S(3)—C(9)—C(10)—S(4)	−0.5 (2)

C(9)—S(3)—C(8)—C(8)^{ii}	−171.4 (2)	S(3)—C(9)—C(10)—C(11)	178.8 (2)
C(8)—S(4)—C(10)—C(9)	6.4 (2)	S(3)—C(9)—C(14)—C(13)	−177.6 (2)
C(8)—S(4)—C(10)—C(11)	−172.8 (2)	C(10)—C(9)—C(14)—C(13)	1.3 (4)
C(10)—S(4)—C(8)—S(3)	−10.26 (18)	C(14)—C(9)—C(10)—S(4)	−179.4 (2)
C(10)—S(4)—C(8)—C(8)^{ii}	171.2 (2)	C(14)—C(9)—C(10)—C(11)	−0.1 (3)
S(1)—C(1)—C(1)^{i}—S(2)^{i}	0.8 (3)	S(4)—C(10)—C(11)—C(12)	178.2 (2)
S(2)—C(1)—C(1)^{i}—S(1)^{i}	−0.8 (3)	C(9)—C(10)—C(11)—C(12)	−1.0 (4)
S(1)—C(2)—C(3)—S(2)	0.5 (2)	C(10)—C(11)—C(12)—C(13)	1.0 (4)
S(1)—C(2)—C(3)—C(4)	−178.7 (2)	C(11)—C(12)—C(13)—C(14)	0.2 (3)
S(1)—C(2)—C(7)—C(6)	178.2 (2)	C(12)—C(13)—C(14)—C(9)	−1.3 (4)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*, −*y*, −*z*+1; (iii) −*x*+1, −*y*+1, −*z*; (iv) −*x*, −*y*+1, −*z*+1; (v) *x*+1, *y*, *z*; (vi) −*x*+1, −*y*, −*z*+1; (vii) *x*−1, *y*, *z*; (viii) −*x*, −*y*, −*z*+2; (ix) *x*−1, *y*, *z*+1; (x) *x*+1, *y*, *z*−1; (xi) −*x*+1, −*y*, −*z*; (xii) −*x*, −*y*+1, −*z*+2; (xiii) *x*, *y*, *z*−1; (xiv) *x*, *y*, *z*+1.

Fig. 1


C6
C7
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S1
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C2i
C7i
C6i
C11ii
C12ii
C10ii
S4ii
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C11

Fig. 2