Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

5,8-Bis(3-hydroxy-3-methylbut-1-yn-1-yl)-2,11-dithia[3.3]paracyclophane

Di Wu* and Jie Huang

Key Laboratory of Pesticide and Chemical Biology of the Ministry of Education, College of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China
Correspondence e-mail: wudi19871208@163.com

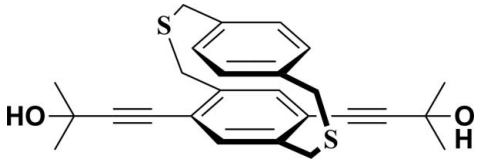
Received 24 October 2011; accepted 15 November 2011

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.066; wR factor = 0.149; data-to-parameter ratio = 16.8.

In the crystal structure of the title compound [systematic name: 2,2′-dimethyl-4,4′-(3,10-dithiatricyclo[10.2.2.2^{5,8}]octadeca-1(14),5,7,12,15,17-hexaen-6,17-diyl)dibut-3-yn-2-ol], $C_{26}H_{28}O_2S_2$, molecules are linked by O—H···O hydrogen bonds, forming a tubular chain which runs parallel to the b axis. The tubular structure is reinforced by π–π stacking interactions [centroid–centroid distance = 3.6332(16Å].

Related literature

For the preparation of the title compound, see: Jin & Lu (2010). For molecular building blocks associated with *para*-cyclophanes see: Xu *et al.* (2008).



Experimental

Crystal data

$C_{26}H_{28}O_2S_2$
M_r = 436.60
Monoclinic, $C2/c$
a = 17.1059 (5) Å
b = 11.8596 (4) Å
c = 24.5073 (10) Å
β = 108.113 (2)°
V = 4725.4 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 298 K
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.943, T_{max} = 0.976
14956 measured reflections
4646 independent reflections
2596 reflections with $I > 2\sigma(I)$
R_{int} = 0.080

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.149
S = 0.92
4646 reflections
277 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.82	1.99	2.777 (4)	161
O2—H2···O1^{ii}	0.82	2.03	2.808 (3)	158

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors are grateful to Professor Sheng-Hua Liu for technical assistance with the structure analysis and Dr Xiang-Gao Meng for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GO2035).

References

Bruker (2007). *APEX2*, *SADABS*, and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Jin, G. & Lu, Y. (2010). *Acta Cryst.* E**66**, o2144.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Xu, J. W., Wang, W. L., Lin, T. T., Sun, Z. & Lai, Y. H. (2008). *Supramol. Chem.* **20**, 723–730.

supporting information

Acta Cryst. (2011). E**67**, o3374 [https://doi.org/10.1107/S1600536811048446]

5,8-Bis(3-hydroxy-3-methylbut-1-yn-1-yl)-2,11-dithia[3.3]paracyclophane

Di Wu and Jie Huang

S1. Comment

The molecular building block associated with *para*-cyclophanes are widely used in chiral catalysis, the design of new optoelectronic (NLO) materials, electron transfer processes, and molecular electronics, polymer chemistry and materials science, and even organic solar cells.(Xu *et al.*, 2008)

Up to now, the dithia[3.3]paracyclophane building blocks, which are synthetically more accessible, have received less attention. Here we report the crystal structure of the title compound (Fig. 1).

The molecules are linked into pairs by the O1-H1···.O2 hydrogen bond, Table 1. These pairs are then linked together by the O2-H2···O1, Table 1, and a symmetry related hydrogen bond to form a tube which runs parallel to the *b*-axis.

This tubular structure is re-inforced by π–π stacking between the phenyl ring containing C1 and its symmetry related ring in the molecule at (5/2+x,1/2-y,1/2+z), centroid to centroid distance, 3.6332(16Å, perpendicular 3.4658 (12)Å and a slippage of 1.0901Å.

Within the molecule the two phenyl rings have a centroid to centoid distance of 3.2621 (18)Å, an average perpendicular spacing of 3.2402Å with a slippage of 0.3773Å.

S2. Experimental

To a stirred solution of appropriate 5,8-dibromo-2,11-dithia[3,3]paracyclophane and 2-methylbut-3-yn-2-ol (in the molecular ratio 1: 4) in THF, $^{i}Pr_2NH$, $Pd(PPh_3)_2Cl_2$(10 mol%) and CuI(10 mol%) was added under N_2, the mixture was refluxed for 48 h. The cooled reaction mixture was filtered, diluted with CH_2Cl_2 and washed with water. The organic phase was dried with Na_2S0_4, filtered, and the solvent was removed from the filtrate *in vacuo*. The crude products were purified by column chromatography on silica gel to yield diols (Jin and Lu 2010).

S3. Refinement

All the hydrogen atoms were located at their ideal positions with C—H=0.93Å (aromatic), *C*—*H*=0.96 Å(methyl), C—H=0.97Å (methylene) and O—H=0.82 Å. The thermal factors of these hydrogen atoms were set 1.2 (for aromatic and methylene) times or 1.5 (for methyl and hydroxyl) times of their carrier atoms.

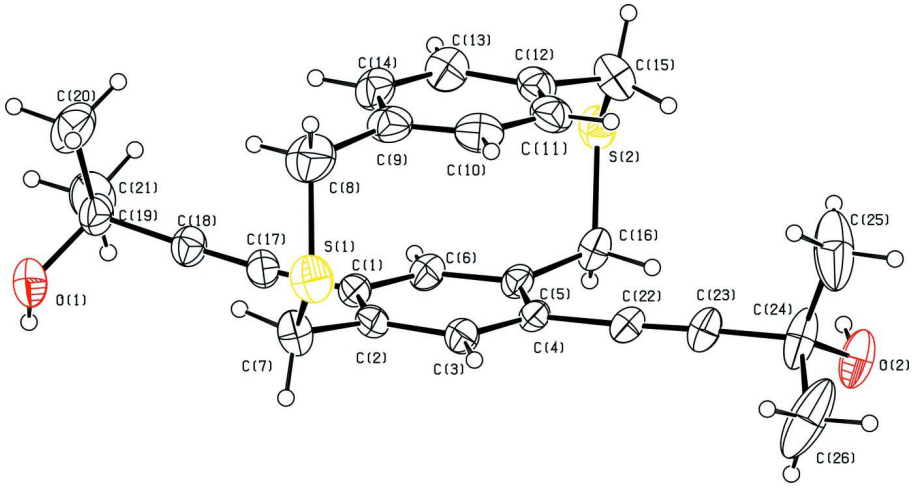


Figure 1

Molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

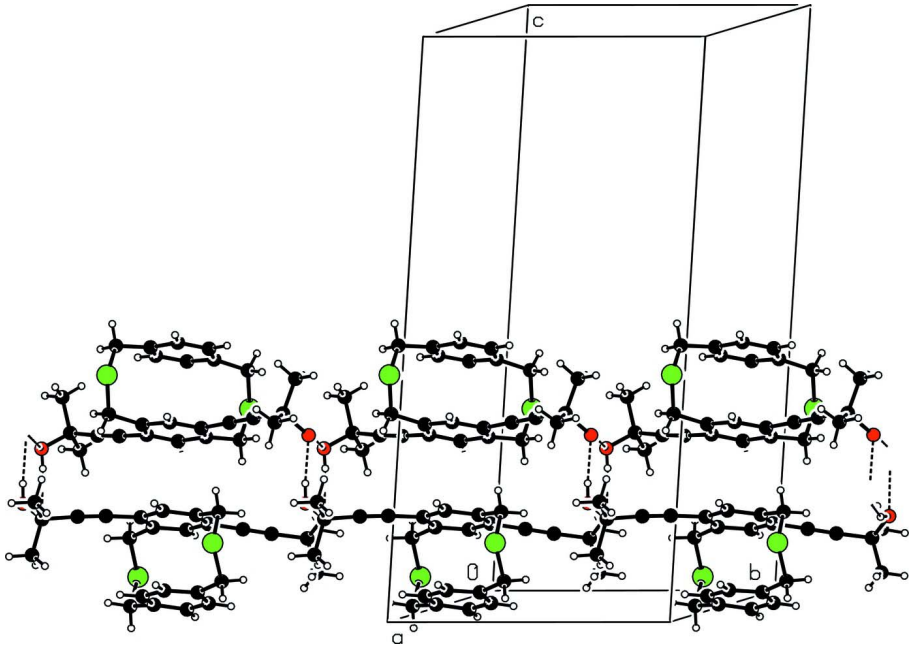


Figure 2

Part of the crystal structure of (I), showing the chains generated by the O—H···O hydrogen bonds running parallel to the b-axis.

2,2′-dimethyl-4,4′-(3,10-dithiatricyclo[10.2.2.2^{5,8}]octadeca- 1(14),5,7,12,15,17-hexaen-6,17-diyl)dibut-3-yn-2-ol

Crystal data

$C_{26}H_{28}O_2S_2$
M_r = 436.60
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 17.1059 (5) Å
b = 11.8596 (4) Å
c = 24.5073 (10) Å
β = 108.113 (2)°
V = 4725.4 (3) Å^3
Z = 8

$F(000) = 1856$
$D_x = 1.227$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1923 reflections
$\theta = 2.4$–$21.8°$
$\mu = 0.25$ mm^{-1}
$T = 298$ K
Block, colourless
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min} = 0.943$, $T_{max} = 0.976$
14956 measured reflections
4646 independent reflections
2596 reflections with $I > 2\sigma(I)$
$R_{int} = 0.080$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.8°$
$h = -21 \rightarrow 20$
$k = -12 \rightarrow 14$
$l = -30 \rightarrow 29$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.066$
$wR(F^2) = 0.149$
$S = 0.92$
4646 reflections
277 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
$w = 1/[\sigma^2(F_o^2) + (0.0638P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	1.00428 (17)	0.1057 (2)	0.17980 (12)	0.0432 (7)
C2	0.91906 (18)	0.1194 (2)	0.15785 (12)	0.0439 (7)
C3	0.88756 (18)	0.2274 (2)	0.15218 (12)	0.0467 (7)
H3	0.8308	0.2376	0.1396	0.056*
C4	0.93876 (18)	0.3215 (2)	0.16488 (12)	0.0427 (7)
C5	1.02399 (17)	0.3086 (2)	0.18464 (12)	0.0432 (7)
C6	1.05457 (18)	0.1999 (2)	0.19349 (12)	0.0479 (8)
H6	1.1110	0.1896	0.2092	0.057*
C7	0.86268 (19)	0.0188 (2)	0.13702 (14)	0.0607 (9)
H7A	0.8323	0.0059	0.1639	0.073*
H7B	0.8966	−0.0472	0.1380	0.073*
C8	0.8537 (3)	0.0327 (3)	0.01972 (17)	0.0937 (13)

H8A	0.8882	−0.0341	0.0274	0.112*
H8B	0.8182	0.0278	−0.0197	0.112*
C9	0.9086 (2)	0.1353 (3)	0.02529 (14)	0.0646 (9)
C10	0.8766 (2)	0.2425 (3)	0.01542 (15)	0.0699 (10)
H10	0.8201	0.2520	−0.0005	0.084*
C11	0.9268 (2)	0.3362 (3)	0.02867 (14)	0.0615 (9)
H11	0.9034	0.4077	0.0221	0.074*
C12	1.0111 (2)	0.3257 (3)	0.05155 (13)	0.0555 (8)
C13	1.0431 (2)	0.2181 (3)	0.05674 (14)	0.0658 (9)
H13	1.0999	0.2083	0.0691	0.079*
C14	0.9928 (2)	0.1248 (3)	0.04403 (14)	0.0644 (9)
H14	1.0162	0.0533	0.0482	0.077*
C15	1.0646 (2)	0.4279 (3)	0.07326 (15)	0.0728 (10)
H15A	1.0291	0.4911	0.0742	0.087*
H15B	1.0930	0.4460	0.0457	0.087*
C16	1.08110 (18)	0.4088 (2)	0.19252 (14)	0.0566 (9)
H16A	1.1188	0.4074	0.2314	0.068*
H16B	1.0486	0.4772	0.1885	0.068*
C17	1.04174 (18)	−0.0044 (2)	0.18399 (12)	0.0488 (8)
C18	1.07335 (18)	−0.0932 (3)	0.18470 (13)	0.0528 (8)
C19	1.1114 (2)	−0.2046 (3)	0.18242 (14)	0.0586 (9)
C20	1.0999 (3)	−0.2365 (3)	0.12062 (17)	0.1061 (15)
H20A	1.1261	−0.3076	0.1194	0.159*
H20B	1.1241	−0.1796	0.1030	0.159*
H20C	1.0423	−0.2424	0.1002	0.159*
C21	1.2026 (2)	−0.2005 (3)	0.21646 (18)	0.0865 (12)
H21A	1.2090	−0.1789	0.2554	0.130*
H21B	1.2297	−0.1465	0.1994	0.130*
H21C	1.2266	−0.2736	0.2161	0.130*
C22	0.90358 (18)	0.4331 (3)	0.15376 (13)	0.0492 (8)
C23	0.87791 (18)	0.5261 (3)	0.14457 (14)	0.0550 (8)
C24	0.8459 (2)	0.6417 (3)	0.13498 (17)	0.0758 (12)
C25	0.8404 (3)	0.6801 (3)	0.0756 (2)	0.140 (2)
H25A	0.8150	0.7531	0.0687	0.210*
H25B	0.8080	0.6273	0.0480	0.210*
H25C	0.8947	0.6843	0.0720	0.210*
C26	0.7637 (2)	0.6443 (4)	0.1460 (2)	0.135 (2)
H26A	0.7712	0.6261	0.1855	0.203*
H26B	0.7274	0.5902	0.1217	0.203*
H26C	0.7402	0.7183	0.1378	0.203*
O1	1.07259 (14)	−0.28867 (17)	0.20705 (10)	0.0672 (6)
H1	1.0921	−0.2870	0.2421	0.101*
O2	0.90016 (13)	0.71742 (18)	0.17522 (11)	0.0744 (7)
H2	0.9478	0.7048	0.1765	0.112*
S1	0.79017 (5)	0.03053 (7)	0.06626 (4)	0.0678 (3)
S2	1.14046 (5)	0.41556 (7)	0.14312 (4)	0.0590 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0508 (18)	0.0408 (18)	0.0387 (18)	0.0058 (14)	0.0149 (15)	0.0022 (13)
C2	0.0529 (19)	0.0422 (17)	0.0369 (17)	0.0019 (14)	0.0146 (15)	0.0054 (13)
C3	0.0460 (17)	0.0450 (19)	0.051 (2)	0.0045 (14)	0.0173 (16)	0.0028 (15)
C4	0.0547 (19)	0.0374 (17)	0.0399 (18)	0.0096 (14)	0.0202 (15)	−0.0001 (13)
C5	0.0491 (18)	0.0392 (17)	0.0419 (18)	0.0000 (14)	0.0148 (15)	−0.0077 (13)
C6	0.0467 (17)	0.0476 (19)	0.048 (2)	0.0069 (15)	0.0132 (15)	−0.0037 (14)
C7	0.057 (2)	0.0465 (19)	0.075 (2)	−0.0017 (16)	0.0148 (18)	0.0075 (17)
C8	0.109 (3)	0.088 (3)	0.088 (3)	−0.035 (2)	0.036 (3)	−0.036 (2)
C9	0.074 (3)	0.075 (3)	0.048 (2)	−0.011 (2)	0.0235 (19)	−0.0121 (18)
C10	0.059 (2)	0.089 (3)	0.065 (3)	−0.003 (2)	0.024 (2)	0.001 (2)
C11	0.067 (2)	0.068 (2)	0.052 (2)	0.0091 (19)	0.0225 (19)	0.0164 (18)
C12	0.063 (2)	0.058 (2)	0.045 (2)	0.0012 (17)	0.0159 (17)	0.0096 (16)
C13	0.062 (2)	0.071 (3)	0.058 (2)	0.004 (2)	0.0083 (19)	−0.0029 (19)
C14	0.084 (3)	0.058 (2)	0.046 (2)	0.003 (2)	0.013 (2)	−0.0098 (17)
C15	0.077 (2)	0.063 (2)	0.075 (3)	−0.0068 (19)	0.020 (2)	0.0167 (19)
C16	0.0585 (19)	0.0420 (18)	0.068 (2)	0.0066 (15)	0.0177 (18)	−0.0097 (16)
C17	0.0575 (19)	0.0392 (18)	0.0475 (19)	−0.0003 (15)	0.0131 (16)	0.0013 (15)
C18	0.0551 (19)	0.047 (2)	0.052 (2)	0.0068 (16)	0.0108 (16)	0.0014 (16)
C19	0.070 (2)	0.0448 (19)	0.059 (2)	0.0146 (16)	0.0179 (19)	0.0058 (16)
C20	0.170 (4)	0.077 (3)	0.074 (3)	0.028 (3)	0.042 (3)	−0.012 (2)
C21	0.061 (2)	0.083 (3)	0.115 (4)	0.020 (2)	0.028 (2)	0.027 (2)
C22	0.0521 (19)	0.0460 (19)	0.051 (2)	0.0065 (15)	0.0186 (16)	−0.0078 (15)
C23	0.0471 (18)	0.045 (2)	0.068 (2)	0.0087 (15)	0.0100 (17)	−0.0118 (16)
C24	0.069 (2)	0.044 (2)	0.083 (3)	0.0186 (17)	−0.022 (2)	−0.0229 (19)
C25	0.212 (6)	0.058 (3)	0.087 (4)	0.002 (3)	−0.046 (4)	−0.002 (2)
C26	0.056 (2)	0.111 (4)	0.201 (6)	0.028 (2)	−0.014 (3)	−0.088 (4)
O1	0.0762 (16)	0.0430 (13)	0.0763 (17)	0.0061 (11)	0.0145 (14)	0.0070 (12)
O2	0.0620 (14)	0.0477 (13)	0.0908 (19)	0.0060 (11)	−0.0093 (15)	−0.0242 (12)
S1	0.0540 (5)	0.0654 (6)	0.0772 (7)	−0.0130 (4)	0.0104 (5)	−0.0030 (5)
S2	0.0494 (5)	0.0500 (5)	0.0773 (7)	−0.0036 (4)	0.0194 (5)	−0.0010 (4)

Geometric parameters (Å, º)

C1—C6	1.386 (4)	C15—S2	1.804 (3)
C1—C2	1.397 (4)	C15—H15A	0.9700
C1—C17	1.445 (4)	C15—H15B	0.9700
C2—C3	1.381 (4)	C16—S2	1.808 (3)
C2—C7	1.519 (4)	C16—H16A	0.9700
C3—C4	1.393 (4)	C16—H16B	0.9700
C3—H3	0.9300	C17—C18	1.181 (4)
C4—C5	1.395 (4)	C18—C19	1.481 (4)
C4—C22	1.444 (4)	C19—O1	1.431 (4)
C5—C6	1.383 (4)	C19—C20	1.514 (5)
C5—C16	1.512 (4)	C19—C21	1.525 (4)
C6—H6	0.9300	C20—H20A	0.9600

C7—S1	1.797 (3)	C20—H20B	0.9600
C7—H7A	0.9700	C20—H20C	0.9600
C7—H7B	0.9700	C21—H21A	0.9600
C8—C9	1.517 (5)	C21—H21B	0.9600
C8—S1	1.804 (4)	C21—H21C	0.9600
C8—H8A	0.9700	C22—C23	1.183 (4)
C8—H8B	0.9700	C23—C24	1.467 (4)
C9—C14	1.375 (4)	C24—O2	1.440 (4)
C9—C10	1.376 (5)	C24—C25	1.500 (6)
C10—C11	1.379 (4)	C24—C26	1.512 (5)
C10—H10	0.9300	C25—H25A	0.9600
C11—C12	1.381 (4)	C25—H25B	0.9600
C11—H11	0.9300	C25—H25C	0.9600
C12—C13	1.380 (4)	C26—H26A	0.9600
C12—C15	1.512 (4)	C26—H26B	0.9600
C13—C14	1.377 (4)	C26—H26C	0.9600
C13—H13	0.9300	O1—H1	0.8200
C14—H14	0.9300	O2—H2	0.8200

C6—C1—C2	119.7 (3)	S2—C15—H15B	108.2
C6—C1—C17	118.9 (3)	H15A—C15—H15B	107.3
C2—C1—C17	121.2 (3)	C5—C16—S2	115.1 (2)
C3—C2—C1	118.3 (3)	C5—C16—H16A	108.5
C3—C2—C7	120.5 (3)	S2—C16—H16A	108.5
C1—C2—C7	121.1 (3)	C5—C16—H16B	108.5
C2—C3—C4	121.5 (3)	S2—C16—H16B	108.5
C2—C3—H3	119.2	H16A—C16—H16B	107.5
C4—C3—H3	119.2	C18—C17—C1	176.4 (3)
C3—C4—C5	120.4 (2)	C17—C18—C19	177.1 (3)
C3—C4—C22	119.7 (3)	O1—C19—C18	109.8 (3)
C5—C4—C22	119.7 (3)	O1—C19—C20	108.4 (3)
C6—C5—C4	117.4 (3)	C18—C19—C20	109.8 (3)
C6—C5—C16	121.0 (3)	O1—C19—C21	108.7 (3)
C4—C5—C16	121.5 (2)	C18—C19—C21	109.8 (3)
C5—C6—C1	122.5 (3)	C20—C19—C21	110.3 (3)
C5—C6—H6	118.8	C19—C20—H20A	109.5
C1—C6—H6	118.8	C19—C20—H20B	109.5
C2—C7—S1	116.0 (2)	H20A—C20—H20B	109.5
C2—C7—H7A	108.3	C19—C20—H20C	109.5
S1—C7—H7A	108.3	H20A—C20—H20C	109.5
C2—C7—H7B	108.3	H20B—C20—H20C	109.5
S1—C7—H7B	108.3	C19—C21—H21A	109.5
H7A—C7—H7B	107.4	C19—C21—H21B	109.5
C9—C8—S1	115.6 (2)	H21A—C21—H21B	109.5
C9—C8—H8A	108.4	C19—C21—H21C	109.5
S1—C8—H8A	108.4	H21A—C21—H21C	109.5
C9—C8—H8B	108.4	H21B—C21—H21C	109.5
S1—C8—H8B	108.4	C23—C22—C4	177.2 (3)

H8A—C8—H8B	107.4	C22—C23—C24	178.2 (4)
C14—C9—C10	117.4 (3)	O2—C24—C23	110.1 (3)
C14—C9—C8	120.8 (4)	O2—C24—C25	107.9 (3)
C10—C9—C8	121.7 (4)	C23—C24—C25	110.3 (3)
C9—C10—C11	121.3 (3)	O2—C24—C26	107.6 (3)
C9—C10—H10	119.4	C23—C24—C26	108.2 (3)
C11—C10—H10	119.4	C25—C24—C26	112.7 (4)
C10—C11—C12	121.2 (3)	C24—C25—H25A	109.5
C10—C11—H11	119.4	C24—C25—H25B	109.5
C12—C11—H11	119.4	H25A—C25—H25B	109.5
C13—C12—C11	117.1 (3)	C24—C25—H25C	109.5
C13—C12—C15	121.9 (3)	H25A—C25—H25C	109.5
C11—C12—C15	120.8 (3)	H25B—C25—H25C	109.5
C14—C13—C12	121.3 (3)	C24—C26—H26A	109.5
C14—C13—H13	119.3	C24—C26—H26B	109.5
C12—C13—H13	119.3	H26A—C26—H26B	109.5
C9—C14—C13	121.3 (3)	C24—C26—H26C	109.5
C9—C14—H14	119.3	H26A—C26—H26C	109.5
C13—C14—H14	119.3	H26B—C26—H26C	109.5
C12—C15—S2	116.6 (2)	C19—O1—H1	109.5
C12—C15—H15A	108.2	C24—O2—H2	109.5
S2—C15—H15A	108.2	C7—S1—C8	103.91 (18)
C12—C15—H15B	108.2	C15—S2—C16	104.56 (16)

C6—C1—C2—C3	−2.0 (4)	S1—C8—C9—C10	−59.7 (4)
C17—C1—C2—C3	−176.6 (3)	C14—C9—C10—C11	−5.7 (5)
C6—C1—C2—C7	174.1 (3)	C8—C9—C10—C11	170.3 (3)
C17—C1—C2—C7	−0.6 (4)	C9—C10—C11—C12	1.0 (5)
C1—C2—C3—C4	3.4 (4)	C10—C11—C12—C13	4.4 (5)
C7—C2—C3—C4	−172.6 (3)	C10—C11—C12—C15	−171.8 (3)
C2—C3—C4—C5	−0.9 (4)	C11—C12—C13—C14	−5.1 (5)
C2—C3—C4—C22	174.8 (3)	C15—C12—C13—C14	171.1 (3)
C3—C4—C5—C6	−3.0 (4)	C10—C9—C14—C13	5.0 (5)
C22—C4—C5—C6	−178.7 (3)	C8—C9—C14—C13	−171.0 (3)
C3—C4—C5—C16	173.2 (3)	C12—C13—C14—C9	0.4 (5)
C22—C4—C5—C16	−2.5 (4)	C13—C12—C15—S2	−43.9 (4)
C4—C5—C6—C1	4.5 (4)	C11—C12—C15—S2	132.2 (3)
C16—C5—C6—C1	−171.7 (3)	C6—C5—C16—S2	64.3 (3)
C2—C1—C6—C5	−2.1 (4)	C4—C5—C16—S2	−111.7 (3)
C17—C1—C6—C5	172.7 (3)	C2—C7—S1—C8	66.4 (3)
C3—C2—C7—S1	47.5 (4)	C9—C8—S1—C7	−66.4 (3)
C1—C2—C7—S1	−128.4 (3)	C12—C15—S2—C16	−68.5 (3)
S1—C8—C9—C14	116.1 (3)	C5—C16—S2—C15	62.2 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.82	1.99	2.777 (4)	161

O2—H2···O1^{ii}	0.82	2.03	2.808 (3)	158

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