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2,4-Dibenzoyl-1-phenyl-3,5-di-2-thienylcyclohexanol

Xian-Qiang Huang[a] and Jin-Xian Wang[b]*

[a]College of Chemistry and Chemical Engineering, Liaocheng University, Shandong 252059, People's Republic of China, and [b]Department of Chemistry, Northwest Normal University, Lanzhou Gansu Province 730072, People's Republic of China
Correspondence e-mail: hxqqxh2008@163.com

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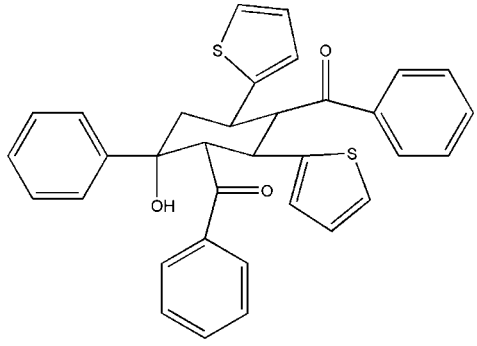
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.008 Å; R factor = 0.077; wR factor = 0.269; data-to-parameter ratio = 14.0.

The title compound, $C_{34}H_{28}O_3S_2$, was synthesized by the reaction of thiophene-2-carbaldehyde with acetophenone and NaOH under phase-transfer catalysis and solvent-free conditions. The central six-membered ring adopts a chair conformation and all the bulky side groups are located in equatorial positions. The hydroxyl group is involved in weak intramolecular hydrogen bonding.

Related literature

The crystal structure of 2,4-dibenzoyl-3,5-bis(4-methoxyphenyl)-1-phenylcyclohexanol was reported by Luo *et al.* (2006).



Experimental

Crystal data

$C_{34}H_{28}O_3S_2$
M_r = 548.68
Orthorhombic, *Pbca*
a = 19.477 (3) Å
b = 12.1666 (19) Å
c = 23.970 (4) Å
V = 5680.2 (16) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 298 (2) K
0.53 × 0.17 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.892, T_{max} = 0.983
26904 measured reflections
4916 independent reflections
2398 reflections with $I > 2\sigma(I)$
R_{int} = 0.080

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.077
$wR(F^2)$ = 0.269
S = 1.02
4916 reflections
352 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2	0.82	2.08	2.663 (5)	127

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2306).

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supplementary materials

Acta Cryst. (2007). E**63**, o4168 [**doi:10.1107/S1600536807046843**]

2,4-Dibenzoyl-1-phenyl-3,5-di2-thienylcyclohexanol

X.-Q. Huang and J.-X. Wang

Comment

In this paper, we present the title compound, (I), synthesized through the condensation and Micheal addition of thiophene-2-carbaldehyde with acetophenone under tetrabutyl ammonium bromide and solvent-free conditions.

In (I) (Fig. 1), the bond lengths and angles are normal and comparable to those observed in the related compound (Luo *et al.*, 2006). The hydroxyl group is involved in weak intramolecular hydrogen bonding (Table 1).

Experimental

Acetophenone (6.25 mmol), freshly distilled thiophene-2-carbaldehyde (3.125 mmol) and NaOH (6.25 mmol), tetrabutyl ammonium bromide (1 mmol), were aggregated with a glass paddle in an open flask. The resulting mixture was washed with water several times to remove NaOH and was recrystallized from ethanol, affording the title compound as a crystalline solid. Elemental analysis: calculated for $C_{34}H_{28}O_3S_2$: C 74.42, H 5.14%; found: C 74.38, H 5.22%.

Refinement

All H atoms were positioned geometrically (C—H 0.93–0.98 Å, O—H 0.82 Å) and refined using a riding model, with U_{iso}(H) = 1.2–1.5U_{eq} of the parent atom.

Figures

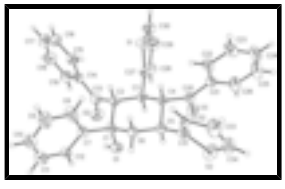


Fig. 1. *ORTEP* drawing of the title complex with atomic numbering scheme and displacement ellipsoids at 30% probability level.

2,4-Dibenzoyl-1-phenyl-3,5-di-2-thienylcyclohexanol

Crystal data

$C_{34}H_{28}O_3S_2$	D_x = 1.283 Mg m^{-3}
M_r = 548.68	Mo $K\alpha$ radiation λ = 0.71073 Å
Orthorhombic, *Pbca*	Cell parameters from 3335 reflections
a = 19.477 (3) Å	θ = 2.6–25.6º
b = 12.1666 (19) Å	μ = 0.22 mm^{-1}
c = 23.970 (4) Å	*T* = 298 (2) K

V = 5680.2 (16) Å^3	Stick, colourless
Z = 8	0.53 × 0.17 × 0.08 mm
F_{000} = 2304	

Data collection

Bruker SMART CCD area-detector diffractometer	4916 independent reflections
Radiation source: fine-focus sealed tube	2398 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.080
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −23→18
T_{min} = 0.892, T_{max} = 0.983	k = −14→14
26904 measured reflections	l = −28→27

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.077	H-atom parameters constrained
$wR(F^2)$ = 0.269	$w = 1/[\sigma^2(F_o^2) + (0.1283P)^2 + 5.0247P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max} < 0.001$
4916 reflections	$\Delta\rho_{max}$ = 0.77 e Å^{-3}
352 parameters	$\Delta\rho_{min}$ = −0.61 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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}
O1	0.28423 (19)	0.6427 (3)	0.03495 (16)	0.0698 (11)
H1	0.2465	0.6726	0.0334	0.105*

O2	0.15784 (18)	0.6294 (3)	0.07682 (17)	0.0677 (11)
O3	0.3657 (2)	0.5494 (3)	0.20752 (16)	0.0656 (10)
S1	0.20614 (8)	0.29648 (12)	0.17794 (6)	0.0693 (5)
S2	0.52146 (10)	0.51469 (18)	0.11031 (9)	0.0962 (7)
C1	0.2765 (2)	0.5261 (4)	0.02428 (19)	0.0477 (12)
C2	0.2313 (2)	0.4741 (4)	0.07074 (19)	0.0434 (11)
H2	0.2255	0.3958	0.0625	0.052*
C3	0.2641 (2)	0.4855 (4)	0.12933 (18)	0.0430 (11)
H3	0.2678	0.5643	0.1373	0.052*
C4	0.3367 (2)	0.4390 (4)	0.12956 (18)	0.0418 (11)
H4	0.3345	0.3598	0.1223	0.050*
C5	0.3822 (2)	0.4937 (4)	0.0843 (2)	0.0487 (12)
H5	0.3842	0.5727	0.0920	0.058*
C6	0.3487 (2)	0.4774 (4)	0.0277 (2)	0.0511 (12)
H6A	0.3462	0.3993	0.0198	0.061*
H6B	0.3772	0.5111	−0.0007	0.061*
C7	0.2462 (3)	0.5062 (4)	−0.0332 (2)	0.0514 (12)
C8	0.2346 (4)	0.3995 (5)	−0.0542 (3)	0.086 (2)
H8	0.2420	0.3388	−0.0314	0.103*
C9	0.2124 (4)	0.3843 (6)	−0.1082 (3)	0.092 (2)
H9	0.2057	0.3135	−0.1218	0.110*
C10	0.2006 (3)	0.4698 (6)	−0.1410 (3)	0.0753 (17)
H10	0.1858	0.4575	−0.1774	0.090*
C11	0.2092 (3)	0.5711 (7)	−0.1239 (3)	0.086 (2)
H11	0.2008	0.6292	−0.1482	0.103*
C12	0.2301 (3)	0.5915 (4)	−0.0712 (2)	0.0579 (14)
H12	0.2341	0.6641	−0.0594	0.069*
C13	0.1598 (3)	0.5287 (4)	0.0718 (2)	0.0493 (12)
C14	0.0959 (3)	0.4646 (4)	0.0683 (2)	0.0504 (12)
C15	0.0930 (3)	0.3540 (4)	0.0557 (2)	0.0605 (14)
H15	0.1334	0.3148	0.0499	0.073*
C16	0.0307 (3)	0.3015 (5)	0.0517 (3)	0.0740 (17)
H16	0.0296	0.2270	0.0431	0.089*
C17	−0.0284 (3)	0.3552 (6)	0.0599 (3)	0.0797 (18)
H17	−0.0701	0.3184	0.0569	0.096*
C18	−0.0271 (3)	0.4650 (7)	0.0727 (3)	0.0821 (19)
H18	−0.0682	0.5019	0.0786	0.099*
C19	0.0338 (3)	0.5217 (5)	0.0771 (2)	0.0641 (15)
H19	0.0339	0.5962	0.0857	0.077*
C20	0.3696 (2)	0.4576 (4)	0.1866 (2)	0.0472 (12)
C21	0.4073 (2)	0.3687 (4)	0.2159 (2)	0.0514 (12)
C22	0.4086 (3)	0.2613 (5)	0.1975 (3)	0.0751 (17)
H22	0.3836	0.2411	0.1660	0.090*
C23	0.4472 (4)	0.1832 (6)	0.2260 (3)	0.096 (2)
H23	0.4461	0.1102	0.2145	0.115*
C24	0.4863 (4)	0.2127 (7)	0.2703 (3)	0.092 (2)
H24	0.5139	0.1608	0.2879	0.111*
C25	0.4850 (4)	0.3185 (8)	0.2891 (3)	0.099 (2)
H25	0.5108	0.3377	0.3203	0.119*

C26	0.4461 (3)	0.3978 (6)	0.2624 (2)	0.0746 (17)
H26	0.4458	0.4698	0.2755	0.089*
C27	0.2211 (2)	0.4357 (4)	0.17447 (19)	0.0461 (11)
C28	0.1907 (3)	0.4878 (5)	0.2192 (2)	0.0691 (16)
H28	0.1918	0.5633	0.2254	0.083*
C29	0.1577 (4)	0.4108 (7)	0.2542 (3)	0.099 (2)
H29	0.1347	0.4313	0.2865	0.119*
C30	0.1620 (3)	0.3066 (6)	0.2374 (3)	0.0780 (18)
H30	0.1429	0.2473	0.2563	0.094*
C31	0.4541 (3)	0.4490 (4)	0.0861 (2)	0.0549 (13)
C32	0.4758 (2)	0.3415 (4)	0.0676 (2)	0.0520 (13)
H32	0.4477	0.2907	0.0498	0.062*
C33	0.5462 (4)	0.3241 (7)	0.0806 (3)	0.096 (2)
H33	0.5686	0.2576	0.0746	0.116*
C34	0.5765 (3)	0.4104 (8)	0.1017 (3)	0.098 (3)
H34	0.6228	0.4136	0.1108	0.118*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.077 (3)	0.052 (2)	0.080 (3)	−0.0065 (18)	−0.008 (2)	0.0067 (19)
O2	0.063 (2)	0.043 (2)	0.097 (3)	0.0091 (17)	0.002 (2)	−0.006 (2)
O3	0.075 (3)	0.050 (2)	0.072 (2)	0.0017 (18)	−0.0136 (19)	−0.0172 (19)
S1	0.0824 (11)	0.0493 (9)	0.0763 (10)	−0.0061 (7)	0.0135 (8)	0.0047 (7)
S2	0.0794 (13)	0.1066 (16)	0.1025 (15)	−0.0131 (11)	−0.0025 (10)	−0.0136 (11)
C1	0.055 (3)	0.043 (3)	0.045 (3)	0.000 (2)	0.000 (2)	0.001 (2)
C2	0.048 (3)	0.033 (2)	0.050 (3)	0.002 (2)	−0.001 (2)	−0.003 (2)
C3	0.045 (3)	0.037 (3)	0.047 (3)	0.000 (2)	−0.005 (2)	−0.004 (2)
C4	0.043 (3)	0.034 (2)	0.049 (3)	−0.0024 (19)	−0.002 (2)	−0.002 (2)
C5	0.053 (3)	0.043 (3)	0.050 (3)	−0.005 (2)	0.003 (2)	0.004 (2)
C6	0.049 (3)	0.056 (3)	0.048 (3)	0.004 (2)	0.001 (2)	0.005 (2)
C7	0.053 (3)	0.053 (3)	0.048 (3)	0.004 (2)	−0.004 (2)	0.005 (2)
C8	0.139 (6)	0.053 (4)	0.066 (4)	0.015 (4)	−0.026 (4)	0.001 (3)
C9	0.118 (6)	0.088 (5)	0.069 (4)	0.005 (4)	−0.020 (4)	−0.017 (4)
C10	0.078 (4)	0.093 (5)	0.055 (4)	0.002 (4)	−0.006 (3)	0.006 (4)
C11	0.089 (5)	0.089 (5)	0.079 (5)	−0.001 (4)	−0.014 (4)	0.029 (4)
C12	0.058 (3)	0.048 (3)	0.067 (4)	−0.003 (2)	−0.012 (3)	0.023 (3)
C13	0.054 (3)	0.037 (3)	0.057 (3)	0.008 (2)	0.000 (2)	−0.006 (2)
C14	0.053 (3)	0.043 (3)	0.055 (3)	0.005 (2)	−0.004 (2)	0.003 (2)
C15	0.055 (3)	0.052 (3)	0.074 (4)	0.000 (3)	−0.003 (3)	−0.001 (3)
C16	0.065 (4)	0.069 (4)	0.089 (4)	−0.014 (3)	−0.009 (3)	−0.002 (3)
C17	0.059 (4)	0.086 (5)	0.095 (5)	−0.011 (3)	−0.010 (3)	0.006 (4)
C18	0.053 (4)	0.099 (5)	0.094 (5)	0.015 (3)	0.003 (3)	0.015 (4)
C19	0.045 (3)	0.067 (4)	0.081 (4)	0.010 (3)	0.006 (3)	0.007 (3)
C20	0.045 (3)	0.046 (3)	0.051 (3)	−0.003 (2)	−0.002 (2)	0.000 (2)
C21	0.046 (3)	0.060 (3)	0.049 (3)	0.002 (2)	−0.004 (2)	0.007 (2)
C22	0.090 (4)	0.046 (3)	0.090 (4)	0.006 (3)	−0.032 (3)	0.003 (3)
C23	0.106 (5)	0.068 (4)	0.114 (6)	0.020 (4)	−0.023 (5)	0.025 (4)

C24	0.086 (5)	0.097 (6)	0.094 (5)	0.026 (4)	−0.018 (4)	0.031 (4)
C25	0.100 (5)	0.131 (7)	0.066 (4)	0.032 (5)	−0.027 (4)	0.004 (4)
C26	0.075 (4)	0.091 (5)	0.058 (4)	0.015 (3)	−0.011 (3)	−0.008 (3)
C27	0.046 (3)	0.043 (3)	0.049 (3)	0.002 (2)	0.002 (2)	−0.001 (2)
C28	0.089 (4)	0.055 (4)	0.063 (3)	−0.003 (3)	0.025 (3)	−0.009 (3)
C29	0.117 (6)	0.110 (6)	0.069 (4)	−0.020 (5)	0.043 (4)	−0.006 (4)
C30	0.074 (4)	0.089 (5)	0.071 (4)	−0.018 (3)	0.015 (3)	0.013 (4)
C31	0.054 (3)	0.057 (3)	0.054 (3)	0.002 (2)	0.007 (2)	0.004 (2)
C32	0.025 (2)	0.034 (2)	0.097 (4)	0.0049 (18)	0.004 (2)	−0.010 (2)
C33	0.076 (5)	0.106 (6)	0.107 (6)	0.035 (4)	−0.006 (4)	−0.004 (5)
C34	0.052 (4)	0.181 (9)	0.062 (4)	−0.005 (5)	0.000 (3)	0.022 (5)

Geometric parameters (Å, °)

O1—C1	1.450 (6)	C13—C14	1.471 (7)
O1—H1	0.8200	C14—C15	1.380 (7)
O2—C13	1.232 (6)	C14—C19	1.412 (7)
O3—C20	1.226 (6)	C15—C16	1.375 (8)
S1—C30	1.669 (6)	C15—H15	0.9300
S1—C27	1.721 (5)	C16—C17	1.338 (9)
S2—C31	1.643 (6)	C16—H16	0.9300
S2—C34	1.673 (9)	C17—C18	1.370 (9)
C1—C7	1.519 (7)	C17—H17	0.9300
C1—C6	1.527 (7)	C18—C19	1.375 (9)
C1—C2	1.554 (7)	C18—H18	0.9300
C2—C13	1.543 (7)	C19—H19	0.9300
C2—C3	1.549 (6)	C20—C21	1.484 (7)
C2—H2	0.9800	C21—C22	1.379 (7)
C3—C27	1.496 (6)	C21—C26	1.394 (7)
C3—C4	1.523 (6)	C22—C23	1.391 (8)
C3—H3	0.9800	C22—H22	0.9300
C4—C20	1.527 (6)	C23—C24	1.356 (10)
C4—C5	1.551 (6)	C23—H23	0.9300
C4—H4	0.9800	C24—C25	1.364 (10)
C5—C31	1.502 (7)	C24—H24	0.9300
C5—C6	1.519 (7)	C25—C26	1.383 (9)
C5—H5	0.9800	C25—H25	0.9300
C6—H6A	0.9700	C26—H26	0.9300
C6—H6B	0.9700	C27—C28	1.378 (7)
C7—C8	1.411 (8)	C28—C29	1.413 (8)
C7—C12	1.415 (7)	C28—H28	0.9300
C8—C9	1.378 (9)	C29—C30	1.332 (9)
C8—H8	0.9300	C29—H29	0.9300
C9—C10	1.323 (9)	C30—H30	0.9300
C9—H9	0.9300	C31—C32	1.444 (7)
C10—C11	1.309 (9)	C32—C33	1.422 (9)
C10—H10	0.9300	C32—H32	0.9300
C11—C12	1.352 (8)	C33—C34	1.307 (10)
C11—H11	0.9300	C33—H33	0.9300

C12—H12	0.9300	C34—H34	0.9300
C13—O2	1.232 (6)		
C1—O1—H1	109.5	C15—C14—C13	124.3 (5)
C30—S1—C27	93.2 (3)	C19—C14—C13	117.2 (5)
C31—S2—C34	95.7 (4)	C16—C15—C14	120.3 (5)
O1—C1—C7	110.9 (4)	C16—C15—H15	119.8
O1—C1—C6	106.0 (4)	C14—C15—H15	119.8
C7—C1—C6	110.2 (4)	C17—C16—C15	121.5 (6)
O1—C1—C2	109.3 (4)	C17—C16—H16	119.3
C7—C1—C2	111.4 (4)	C15—C16—H16	119.3
C6—C1—C2	109.0 (4)	C16—C17—C18	119.5 (6)
C13—C2—C3	108.6 (4)	C16—C17—H17	120.2
C13—C2—C1	110.4 (4)	C18—C17—H17	120.2
C3—C2—C1	112.3 (4)	C17—C18—C19	121.5 (6)
C13—C2—H2	108.5	C17—C18—H18	119.2
C3—C2—H2	108.5	C19—C18—H18	119.2
C1—C2—H2	108.5	C18—C19—C14	118.7 (6)
C27—C3—C4	111.5 (4)	C18—C19—H19	120.6
C27—C3—C2	112.8 (4)	C14—C19—H19	120.6
C4—C3—C2	110.7 (4)	O3—C20—C21	120.0 (4)
C27—C3—H3	107.1	O3—C20—C4	118.4 (4)
C4—C3—H3	107.1	C21—C20—C4	121.5 (4)
C2—C3—H3	107.1	C22—C21—C26	119.1 (5)
C3—C4—C20	109.7 (4)	C22—C21—C20	123.3 (5)
C3—C4—C5	111.6 (4)	C26—C21—C20	117.5 (5)
C20—C4—C5	108.8 (4)	C21—C22—C23	120.0 (6)
C3—C4—H4	108.9	C21—C22—H22	120.0
C20—C4—H4	108.9	C23—C22—H22	120.0
C5—C4—H4	108.9	C24—C23—C22	120.6 (7)
C31—C5—C6	112.2 (4)	C24—C23—H23	119.7
C31—C5—C4	111.0 (4)	C22—C23—H23	119.7
C6—C5—C4	108.8 (4)	C23—C24—C25	119.8 (6)
C31—C5—H5	108.2	C23—C24—H24	120.1
C6—C5—H5	108.2	C25—C24—H24	120.1
C4—C5—H5	108.2	C24—C25—C26	121.1 (7)
C5—C6—C1	113.1 (4)	C24—C25—H25	119.5
C5—C6—H6A	108.9	C26—C25—H25	119.5
C1—C6—H6A	108.9	C25—C26—C21	119.4 (6)
C5—C6—H6B	108.9	C25—C26—H26	120.3
C1—C6—H6B	108.9	C21—C26—H26	120.3
H6A—C6—H6B	107.8	C28—C27—C3	128.1 (4)
C8—C7—C12	114.3 (5)	C28—C27—S1	110.0 (4)
C8—C7—C1	122.2 (4)	C3—C27—S1	121.9 (3)
C12—C7—C1	123.5 (5)	C27—C28—C29	110.6 (5)
C9—C8—C7	120.6 (6)	C27—C28—H28	124.7
C9—C8—H8	119.7	C29—C28—H28	124.7
C7—C8—H8	119.7	C30—C29—C28	115.0 (6)
C10—C9—C8	120.5 (7)	C30—C29—H29	122.5
C10—C9—H9	119.8	C28—C29—H29	122.5

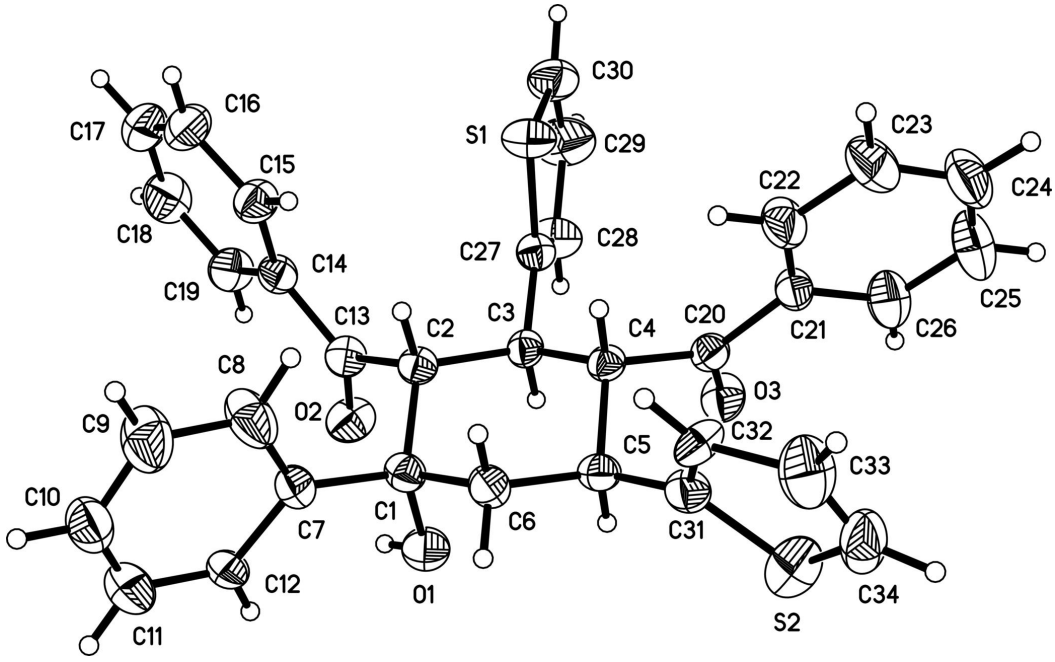
C8—C9—H9	119.8	C29—C30—S1	111.1 (5)
C11—C10—C9	122.1 (6)	C29—C30—H30	124.4
C11—C10—H10	118.9	S1—C30—H30	124.4
C9—C10—H10	118.9	C32—C31—C5	126.3 (5)
C10—C11—C12	120.3 (6)	C32—C31—S2	108.4 (4)
C10—C11—H11	119.8	C5—C31—S2	125.3 (4)
C12—C11—H11	119.8	C33—C32—C31	110.5 (5)
C11—C12—C7	122.2 (6)	C33—C32—H32	124.7
C11—C12—H12	118.9	C31—C32—H32	124.7
C7—C12—H12	118.9	C34—C33—C32	113.6 (7)
O2—C13—C14	120.4 (4)	C34—C33—H33	123.2
O2—C13—C14	120.4 (4)	C32—C33—H33	123.2
O2—C13—C2	117.2 (4)	C33—C34—S2	111.6 (5)
O2—C13—C2	117.2 (4)	C33—C34—H34	124.2
C14—C13—C2	122.3 (4)	S2—C34—H34	124.2
C15—C14—C19	118.5 (5)		
O1—C1—C2—C13	59.8 (5)	O2—C13—C14—C19	−6.8 (7)
C7—C1—C2—C13	−63.1 (5)	C2—C13—C14—C19	171.8 (5)
C6—C1—C2—C13	175.2 (4)	C19—C14—C15—C16	0.3 (8)
O1—C1—C2—C3	−61.6 (5)	C13—C14—C15—C16	−178.1 (5)
C7—C1—C2—C3	175.5 (4)	C14—C15—C16—C17	−0.2 (9)
C6—C1—C2—C3	53.8 (5)	C15—C16—C17—C18	−0.2 (10)
C13—C2—C3—C27	57.6 (5)	C16—C17—C18—C19	0.4 (10)
C1—C2—C3—C27	−180.0 (4)	C17—C18—C19—C14	−0.3 (9)
C13—C2—C3—C4	−176.6 (4)	C15—C14—C19—C18	−0.1 (8)
C1—C2—C3—C4	−54.2 (5)	C13—C14—C19—C18	178.4 (5)
C27—C3—C4—C20	−57.1 (5)	C3—C4—C20—O3	−48.0 (6)
C2—C3—C4—C20	176.4 (4)	C5—C4—C20—O3	74.4 (5)
C27—C3—C4—C5	−177.8 (4)	C3—C4—C20—C21	133.8 (4)
C2—C3—C4—C5	55.7 (5)	C5—C4—C20—C21	−103.8 (5)
C3—C4—C5—C31	178.5 (4)	O3—C20—C21—C22	174.0 (5)
C20—C4—C5—C31	57.3 (5)	C4—C20—C21—C22	−7.8 (8)
C3—C4—C5—C6	−57.5 (5)	O3—C20—C21—C26	−9.7 (7)
C20—C4—C5—C6	−178.7 (4)	C4—C20—C21—C26	168.5 (5)
C31—C5—C6—C1	−177.8 (4)	C26—C21—C22—C23	1.3 (9)
C4—C5—C6—C1	59.0 (5)	C20—C21—C22—C23	177.6 (6)
O1—C1—C6—C5	60.3 (5)	C21—C22—C23—C24	−3.1 (11)
C7—C1—C6—C5	−179.7 (4)	C22—C23—C24—C25	3.6 (12)
C2—C1—C6—C5	−57.2 (5)	C23—C24—C25—C26	−2.2 (12)
O1—C1—C7—C8	178.9 (5)	C24—C25—C26—C21	0.4 (11)
C6—C1—C7—C8	61.9 (7)	C22—C21—C26—C25	0.0 (9)
C2—C1—C7—C8	−59.2 (7)	C20—C21—C26—C25	−176.4 (6)
O1—C1—C7—C12	1.9 (7)	C4—C3—C27—C28	117.7 (6)
C6—C1—C7—C12	−115.1 (5)	C2—C3—C27—C28	−117.0 (6)
C2—C1—C7—C12	123.8 (5)	C4—C3—C27—S1	−59.4 (5)
C12—C7—C8—C9	2.7 (9)	C2—C3—C27—S1	66.0 (5)
C1—C7—C8—C9	−174.6 (6)	C30—S1—C27—C28	−0.8 (5)
C7—C8—C9—C10	−1.1 (11)	C30—S1—C27—C3	176.7 (4)
C8—C9—C10—C11	−0.2 (12)	C3—C27—C28—C29	−176.5 (5)

C9—C10—C11—C12	−0.5 (11)	S1—C27—C28—C29	0.8 (7)
C10—C11—C12—C7	2.5 (10)	C27—C28—C29—C30	−0.4 (9)
C8—C7—C12—C11	−3.5 (8)	C28—C29—C30—S1	−0.3 (9)
C1—C7—C12—C11	173.8 (5)	C27—S1—C30—C29	0.6 (6)
O2—O2—C13—C14	0.0 (17)	C6—C5—C31—C32	−48.9 (7)
O2—O2—C13—C2	0.0 (17)	C4—C5—C31—C32	73.0 (6)
C3—C2—C13—O2	68.3 (6)	C6—C5—C31—S2	131.9 (4)
C1—C2—C13—O2	−55.2 (6)	C4—C5—C31—S2	−106.1 (5)
C3—C2—C13—O2	68.3 (6)	C34—S2—C31—C32	−2.9 (4)
C1—C2—C13—O2	−55.2 (6)	C34—S2—C31—C5	176.4 (5)
C3—C2—C13—C14	−110.3 (5)	C5—C31—C32—C33	−174.4 (5)
C1—C2—C13—C14	126.2 (5)	S2—C31—C32—C33	4.9 (6)
O2—C13—C14—C15	171.6 (5)	C31—C32—C33—C34	−5.2 (9)
O2—C13—C14—C15	171.6 (5)	C32—C33—C34—S2	3.0 (8)
C2—C13—C14—C15	−9.8 (8)	C31—S2—C34—C33	0.0 (6)
O2—C13—C14—C19	−6.8 (7)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2	0.82	2.08	2.663 (5)	127

Fig. 1


C30
C16
C17
S1
C29
C23
C15
C22
C24
C18
C27
C28
C14
C19
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C13
C2
C3
C4
C20
C21
C26
C8
O3
O2
C9
C32
C5
C33
C10
C1
C6
C31
C7
C12
O1
C34
S2
C11