Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(benzylsulfanyl)methane

Hojin Yang,[a] Tae Ho Kim,[a]* Suk-Hee Moon[b] and Jineun Kim[a]*

[a]Department of Chemistry and Research Institute of Natural Sciences, Gyeongsang National University, Jinju 660-701, Republic of Korea, and [b]Subdivision of Food Science, Kyungnam College of Information and Technology, Busan 616-701, Republic of Korea
Correspondence e-mail: thkim@gnu.ac.kr, jekim@gnu.ac.kr

Received 14 May 2010; accepted 25 May 2010

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.031; wR factor = 0.082; data-to-parameter ratio = 21.5.

In the title compound, $C_{15}H_{16}S_2$, the structure of the dithioalkyl chain is a helix with an all-*cis* conformation. The dihedral angle between the mean planes of the terminal aromatic rings is 74.60 (4)°. In the crystal structure, weak C—H$\cdots\pi$ interactions contribute to the stabilization of the packing.

Related literature

For the synthesis of the title ligand, see: Cohen *et al.* (1980). For related structures, see: Li *et al.* (2005); Tanaka & Ajiki (2005).

Experimental

Crystal data

$C_{15}H_{16}S_2$
M_r = 260.40
Monoclinic, $P2_1/c$
a = 5.5146 (1) Å
b = 12.2628 (3) Å
c = 20.0128 (5) Å
β = 101.156 (1)°
V = 1327.78 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.38 mm^{-1}
T = 173 K
0.22 × 0.15 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.922, T_{max} = 0.946
12942 measured reflections
3335 independent reflections
2977 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.082
S = 1.04
3335 reflections
155 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

Cg is the centroid of the C1–C6 ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C13—H13$\cdots Cg^{i}$	0.95	2.85	3.71	151

Symmetry code: (i) $x, y-1, z$.

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXTL*.

This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (No. 2010-0016386).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5008).

References

Brandenburg, K. (1998). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2006). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cohen, T., Ruffner, R. J., Shull, D. W., Fogel, E. R. & Falck, J. R. (1980). *Org. Synth.* **59**, 202–212.
Li, J.-R., Bu, X.-H., Jiao, J., Du, X.-H. & Zhang, R.-H. (2005). *Dalton Trans*. pp. 464–474.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Tanaka, K. & Ajiki, K. (2005). *Org. Lett.* **7**, 1537–1539.

supporting information

Acta Cryst. (2010). E**66**, o1519 [https://doi.org/10.1107/S1600536810019641]

Bis(benzylsulfanyl)methane

Hojin Yang, Tae Ho Kim, Suk-Hee Moon and Jineun Kim

S1. Comment

Dithio acetals ($RSCH_2SR$) have received considerable attention in the literature (Li *et al.*, 2005; Tanaka & Ajiki, 2005). We report herein the crystal structure of the title compound. In asymmetric unit, the conformation of dithioalkyl chain is all *cis* and the dihedral angle between the aromatic rings is 74.60 (4)°. In the crystal structure (Fig. 1), the bond lengths and angles are within normal ranges.

A weak C13—H13···Cg = 2.85 Å interaction (Cg is the centroid of the C1···C6 ring) is observed, Table 1. Weak intermolecular S···S interactions with 3.4732 (6)Å also exist. These intermolecular interactions may be effective in the stabilization of the structure, Fig. 2.

S2. Experimental

The title compound was synthesised according to the published procedure (Cohen *et al.*, 1980) and recrystallized from petroleum ether.

S3. Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.95 Å, U_{iso} =1.2U_{eq}(C) for aromatic and 0.99 Å, U_{iso} = 1.2U_{eq}(C) for the CH_2 atoms.

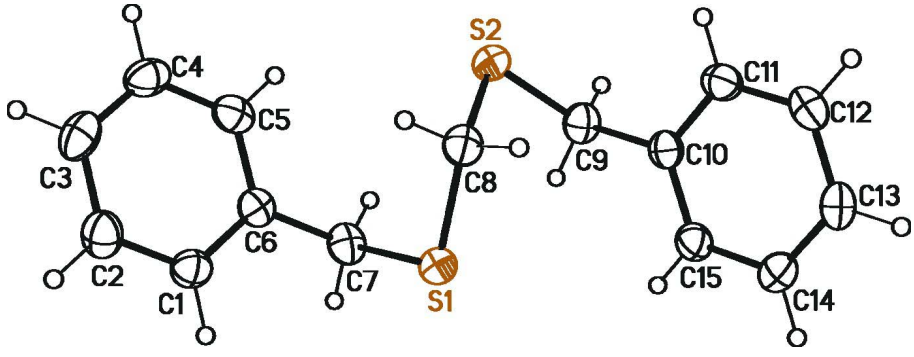

Figure 1

The molecular structure of the title compound, showing displacement ellipsoids drawn at the 50% probability level.

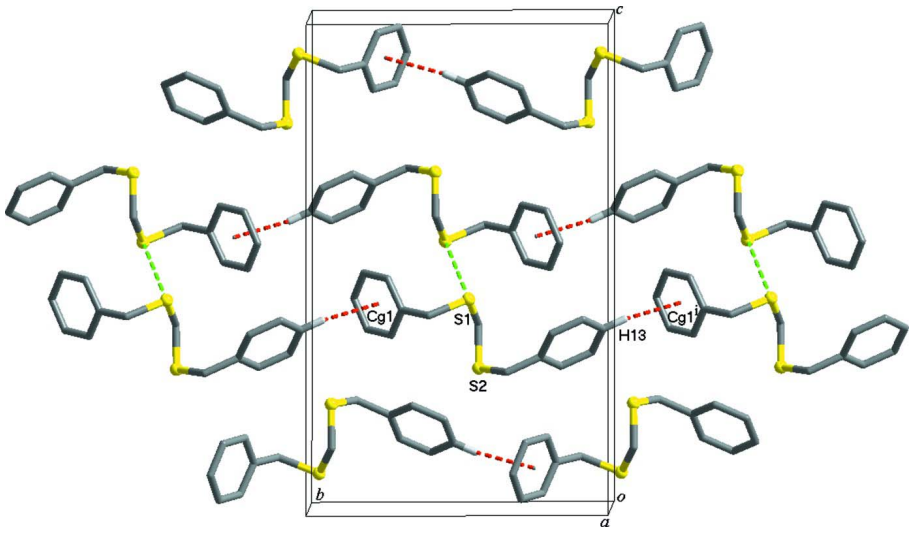

Figure 2

Intermolecular C—H···π (red dotted lines) and S···S (green dotted lines) interactions in the title compound. All H atoms except those related to intermolecular interactions have been omitted for clarity. *Cg* is the centroid of the C1/C2/C3/C4/C5/C6 ring. [Symmetry codes: (i) x, -1+y, z]

Bis(benzylsulfanyl)methane

Crystal data

$C_{15}H_{16}S_2$
$M_r = 260.40$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 5.5146\ (1)$ Å
$b = 12.2628\ (3)$ Å
$c = 20.0128\ (5)$ Å
$\beta = 101.156\ (1)°$
$V = 1327.78\ (5)$ Å^3
$Z = 4$
$F(000) = 552$
$D_x = 1.303$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7825 reflections
$\theta = 2.7–28.4°$
$\mu = 0.38$ mm^{-1}
$T = 173$ K
Block, colourless
0.22 × 0.15 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.0 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.922$, $T_{max} = 0.946$
12942 measured reflections
3335 independent reflections
2977 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 28.4°$, $\theta_{min} = 2.0°$
$h = -7\rightarrow7$
$k = -12\rightarrow16$
$l = -24\rightarrow26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.082$
$S = 1.04$
3335 reflections
155 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
$w = 1/[\sigma^2(F_o^2) + (0.0369P)^2 + 0.4363P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.030 (2)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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}
S1	0.63212 (6)	0.46872 (3)	0.430321 (16)	0.03123 (10)
S2	0.80471 (6)	0.43167 (3)	0.294901 (16)	0.03327 (11)
C1	0.7958 (2)	0.73297 (11)	0.47700 (6)	0.0318 (3)
H1	0.6990	0.7130	0.5095	0.038*
C2	0.9857 (3)	0.80750 (11)	0.49456 (7)	0.0369 (3)
H2	1.0197	0.8377	0.5391	0.044*
C3	1.1262 (3)	0.83815 (11)	0.44745 (8)	0.0376 (3)
H3	1.2579	0.8887	0.4597	0.045*
C4	1.0740 (3)	0.79496 (11)	0.38253 (7)	0.0371 (3)
H4	1.1678	0.8170	0.3498	0.045*
C5	0.8848 (2)	0.71936 (11)	0.36495 (6)	0.0324 (3)
H5	0.8508	0.6897	0.3203	0.039*
C6	0.7447 (2)	0.68671 (10)	0.41215 (6)	0.0269 (2)
C7	0.5451 (2)	0.60237 (11)	0.39470 (7)	0.0319 (3)
H7A	0.4995	0.5959	0.3445	0.038*
H7B	0.3970	0.6276	0.4114	0.038*
C8	0.8761 (2)	0.43180 (11)	0.38662 (7)	0.0303 (3)
H8A	0.9344	0.3579	0.4019	0.036*
H8B	1.0158	0.4826	0.4014	0.036*
C9	0.5351 (2)	0.34398 (11)	0.27868 (6)	0.0320 (3)
H9A	0.3992	0.3808	0.2956	0.038*
H9B	0.4822	0.3351	0.2288	0.038*
C10	0.5717 (2)	0.23235 (10)	0.31064 (6)	0.0263 (2)
C11	0.7532 (2)	0.16136 (11)	0.29690 (6)	0.0309 (3)
H11	0.8598	0.1839	0.2675	0.037*
C12	0.7799 (2)	0.05829 (11)	0.32574 (7)	0.0327 (3)
H12	0.9041	0.0106	0.3158	0.039*
C13	0.6268 (2)	0.02439 (11)	0.36880 (7)	0.0324 (3)
H13	0.6452	−0.0463	0.3885	0.039*

C14	0.4464 (3)	0.09429 (11)	0.38292 (7)	0.0344 (3)
H14	0.3406	0.0716	0.4125	0.041*
C15	0.4196 (2)	0.19762 (11)	0.35389 (7)	0.0307 (3)
H15	0.2951	0.2451	0.3639	0.037*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.03604 (18)	0.02830 (18)	0.03133 (17)	−0.00231 (12)	0.01147 (13)	−0.00010 (12)
S2	0.04070 (19)	0.02943 (18)	0.03283 (17)	−0.00462 (13)	0.01497 (13)	0.00064 (12)
C1	0.0353 (6)	0.0333 (7)	0.0270 (6)	−0.0013 (5)	0.0064 (5)	0.0029 (5)
C2	0.0422 (7)	0.0336 (7)	0.0322 (6)	−0.0033 (6)	0.0008 (5)	0.0007 (5)
C3	0.0336 (7)	0.0275 (7)	0.0505 (8)	−0.0018 (5)	0.0048 (6)	0.0079 (6)
C4	0.0395 (7)	0.0316 (7)	0.0445 (7)	0.0056 (6)	0.0185 (6)	0.0113 (6)
C5	0.0390 (7)	0.0293 (6)	0.0299 (6)	0.0089 (5)	0.0093 (5)	0.0039 (5)
C6	0.0270 (6)	0.0240 (6)	0.0285 (5)	0.0060 (5)	0.0026 (4)	0.0028 (4)
C7	0.0269 (6)	0.0302 (6)	0.0368 (6)	0.0046 (5)	0.0018 (5)	−0.0015 (5)
C8	0.0263 (6)	0.0291 (6)	0.0349 (6)	0.0019 (5)	0.0042 (5)	0.0005 (5)
C9	0.0345 (6)	0.0295 (6)	0.0302 (6)	−0.0001 (5)	0.0019 (5)	0.0020 (5)
C10	0.0264 (5)	0.0257 (6)	0.0251 (5)	−0.0019 (5)	0.0009 (4)	−0.0029 (4)
C11	0.0309 (6)	0.0340 (7)	0.0288 (6)	−0.0006 (5)	0.0085 (5)	−0.0032 (5)
C12	0.0320 (6)	0.0297 (6)	0.0359 (6)	0.0043 (5)	0.0051 (5)	−0.0072 (5)
C13	0.0355 (6)	0.0231 (6)	0.0364 (6)	−0.0019 (5)	0.0011 (5)	−0.0015 (5)
C14	0.0347 (7)	0.0305 (7)	0.0399 (7)	−0.0041 (5)	0.0120 (5)	0.0012 (5)
C15	0.0277 (6)	0.0281 (6)	0.0374 (6)	0.0011 (5)	0.0087 (5)	−0.0027 (5)

Geometric parameters (Å, º)

S1—C8	1.7988 (13)	C7—H7B	0.9900
S1—C7	1.8144 (14)	C8—H8A	0.9900
S2—C8	1.8013 (13)	C8—H8B	0.9900
S2—C9	1.8125 (14)	C9—C10	1.5079 (17)
C1—C2	1.3831 (19)	C9—H9A	0.9900
C1—C6	1.3942 (17)	C9—H9B	0.9900
C1—H1	0.9500	C10—C15	1.3841 (18)
C2—C3	1.383 (2)	C10—C11	1.3934 (18)
C2—H2	0.9500	C11—C12	1.3854 (19)
C3—C4	1.381 (2)	C11—H11	0.9500
C3—H3	0.9500	C12—C13	1.382 (2)
C4—C5	1.389 (2)	C12—H12	0.9500
C4—H4	0.9500	C13—C14	1.383 (2)
C5—C6	1.3898 (18)	C13—H13	0.9500
C5—H5	0.9500	C14—C15	1.3899 (19)
C6—C7	1.5016 (18)	C14—H14	0.9500
C7—H7A	0.9900	C15—H15	0.9500
C8—S1—C7	101.67 (6)	S2—C8—H8A	108.0
C8—S2—C9	101.13 (6)	S1—C8—H8B	108.0

C2—C1—C6	120.80 (12)	S2—C8—H8B	108.0
C2—C1—H1	119.6	H8A—C8—H8B	107.2
C6—C1—H1	119.6	C10—C9—S2	115.14 (9)
C1—C2—C3	120.19 (13)	C10—C9—H9A	108.5
C1—C2—H2	119.9	S2—C9—H9A	108.5
C3—C2—H2	119.9	C10—C9—H9B	108.5
C4—C3—C2	119.65 (13)	S2—C9—H9B	108.5
C4—C3—H3	120.2	H9A—C9—H9B	107.5
C2—C3—H3	120.2	C15—C10—C11	118.46 (12)
C3—C4—C5	120.26 (13)	C15—C10—C9	119.80 (11)
C3—C4—H4	119.9	C11—C10—C9	121.73 (11)
C5—C4—H4	119.9	C12—C11—C10	120.68 (12)
C4—C5—C6	120.61 (12)	C12—C11—H11	119.7
C4—C5—H5	119.7	C10—C11—H11	119.7
C6—C5—H5	119.7	C13—C12—C11	120.38 (12)
C5—C6—C1	118.46 (12)	C13—C12—H12	119.8
C5—C6—C7	121.28 (11)	C11—C12—H12	119.8
C1—C6—C7	120.25 (12)	C12—C13—C14	119.43 (12)
C6—C7—S1	113.86 (8)	C12—C13—H13	120.3
C6—C7—H7A	108.8	C14—C13—H13	120.3
S1—C7—H7A	108.8	C13—C14—C15	120.14 (13)
C6—C7—H7B	108.8	C13—C14—H14	119.9
S1—C7—H7B	108.8	C15—C14—H14	119.9
H7A—C7—H7B	107.7	C10—C15—C14	120.91 (12)
S1—C8—S2	117.33 (7)	C10—C15—H15	119.5
S1—C8—H8A	108.0	C14—C15—H15	119.5

C6—C1—C2—C3	0.7 (2)	C9—S2—C8—S1	−53.62 (9)
C1—C2—C3—C4	0.8 (2)	C8—S2—C9—C10	−55.87 (11)
C2—C3—C4—C5	−1.4 (2)	S2—C9—C10—C15	123.62 (11)
C3—C4—C5—C6	0.4 (2)	S2—C9—C10—C11	−57.57 (14)
C4—C5—C6—C1	1.09 (18)	C15—C10—C11—C12	0.22 (18)
C4—C5—C6—C7	−177.97 (12)	C9—C10—C11—C12	−178.61 (11)
C2—C1—C6—C5	−1.67 (19)	C10—C11—C12—C13	−0.15 (19)
C2—C1—C6—C7	177.40 (12)	C11—C12—C13—C14	0.00 (19)
C5—C6—C7—S1	103.14 (12)	C12—C13—C14—C15	0.1 (2)
C1—C6—C7—S1	−75.91 (14)	C11—C10—C15—C14	−0.12 (18)
C8—S1—C7—C6	−64.96 (10)	C9—C10—C15—C14	178.72 (12)
C7—S1—C8—S2	−56.40 (9)	C13—C14—C15—C10	0.0 (2)

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···*Cg*^{i}	0.95	2.85	3.71	151

Symmetry code: (i) *x*, *y*−1, *z*.