

1,3-Bis{[(2,6-dimethylphenyl)sulfanyl]methyl}-benzene

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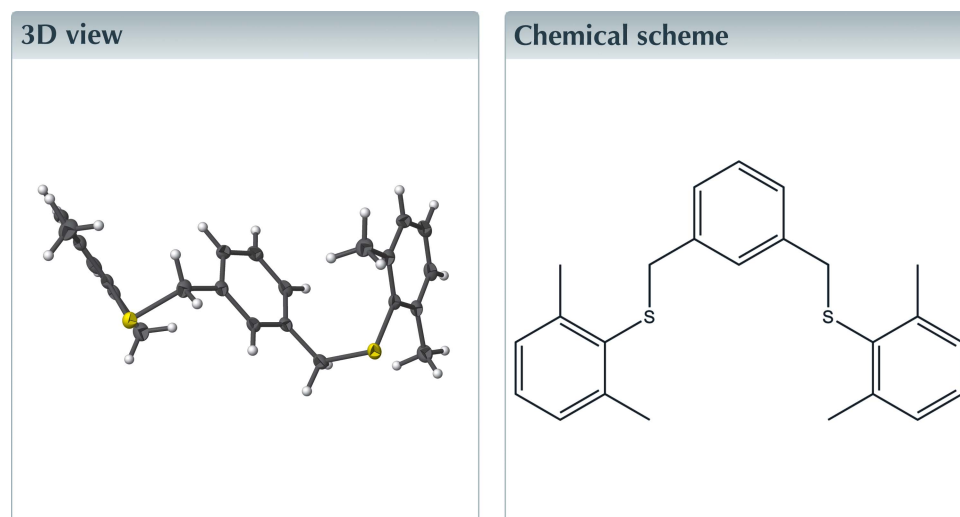
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Structural data: full structural data are available from iucrdata.iucr.org

The structure of the title compound, C₂₄H₂₆S₂, an example of a pincer ligand with an SCS-chelation motif, illustrates the steric effects of the methyl groups in the thiophenyl rings at the 2- and 6-positions, forcing a dissimilar spatial orientation of the thiophenyl rings relative to the central aryl group [dihedral angles = 33.58 (7) and 40.49 (7)^o]. In the crystal, weak S⋯S contacts [3.4009 (7) Å] link the molecules into inversion dimers.



Structure description

Thermodynamic and kinetic stabilization are widely used synthetic concepts for the molecular design of highly reactive species. While the first approach harnesses the mesomeric effect of neighboring heteroatoms, the attachment of electron-donating or -withdrawing substituents or complexation with a transition metal, the second technique takes advantage of steric protection by bulky groups (Tokitoh & Okazaki, 2001; Albrecht *et al.*, 2001). In this context, pincer-type ligands consisting of a planar aryl backbone (common framework) and two neutral donor groups, result in an *ECE* chelating environment (*E* = 2-electron donor atom; *C* = *ipso* carbon atom of the aromatic scaffold). Such tridentate ligands have been commonly employed to generate versatile organic and organometallic systems rich in electrons with tunable features, leading to several applications in homogeneous catalysis, activation of strong bonds or as potential therapeutic and pharmaceutical agents (Morales-Morales & Jensen, 2007). For instance, monoanionic aromatic ligands containing one or two *ortho*-pendant functional group(s), bearing intramolecularly coordinating chelating ligands (Dostál *et al.*, 2006) (*E* = N, P, O, S, Se) and bonded with aryl or aliphatic substituents, stabilized both transition-metal and main-group complexes affording direct metal-to-carbon σ -bonds, and delivering hypervalent or hypercoordinated compounds (Jambor *et al.*, 2002). In effect, the modification of the

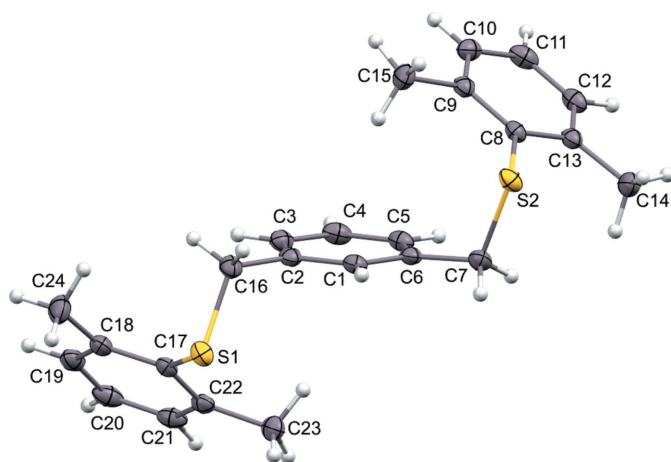


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

electronic properties by donor atoms enhances the nucleophilicity significantly, along with changes in the spatial arrangement by the stereochemical configuration and rigidity of the carbon chain connecting these donor atoms (van Koten *et al.*, 1989), as well the solubility (Šimon *et al.*, 2010). As part of our studies in this area, we now report the synthesis and structure of the title compound, $C_{24}H_{26}S_2$.

The crystal structure of the title compound has monoclinic symmetry with one molecule in the asymmetric unit: the central phenyl ring (C1–C6) is bonded to methylene moieties (C7 and C16) at the 2- and 6-positions and these latter fragments further act as bridges to the thiophenyl rings (Fig. 1). The thiophenyl rings are each flanked by a pair of methyl groups (C14, C15, C23, and C24) at the 2- and 6-positions, and show dissimilar spatial orientations, being farther away from each other in relation to the central aryl backbone. Such an arrangement is likely due to steric effects of the methyl groups and the rotation around the C_m-S ($m = \text{methylene}$) bond. The bond lengths C7–S2 and C16–S1 are 1.839 (2) and 1.834 (2) Å, respectively. The corresponding methylene/thiophenyl units (C7–S2–C8 and C16–S1–C17) exhibit bond angles of 100.76 (7) and 101.96 (7)°, respectively. In the

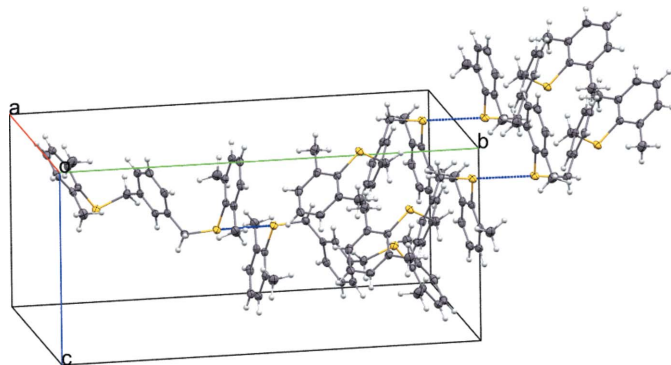


Figure 2
Partial packing diagram for the title compound. S2...S2 interactions are shown as blue dashed lines.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{26}S_2$
M_r	378.57
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	8.4487 (2), 23.7284 (5), 10.4078 (2)
β (°)	104.698 (1)
V (Å ³)	2018.22 (8)
Z	4
Radiation type	Cu $K\alpha$
μ (mm ⁻¹)	2.40
Crystal size (mm)	0.25 × 0.15 × 0.10
Data collection	
Diffractometer	Bruker D8 Venture
Absorption correction	Multi-scan (SADABS; Bruker, 2015)
T_{\min}, T_{\max}	0.630, 0.753
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	30031, 3679, 3342
R_{int}	0.038
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.030, 0.077, 1.05
No. of reflections	3679
No. of parameters	239
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.25, -0.26

Computer programs: APEX3 and SAINT (Bruker, 2015), SHELXT (Sheldrick, 2015a), SHELXL2014 (Sheldrick, 2015b), shelXle (Hübschle *et al.*, 2011 and Mercury (Macrae *et al.*, 2006).

crystal, weak S2...S2ⁱ contacts [3.4009 (7) Å; symmetry code: (i) 1 - x, 1 - y, 1 - z] are observed between the molecules, leading to the formation of inversion dimers (Fig. 2).

Synthesis and crystallization

All manipulations were carried out using standard Schlenk techniques or in a glovebox (Lab MBraun workstation) under a nitrogen atmosphere. All reagents and solvents were procured from commercial sources. Anhydrous solvents were dried as reported in the literature.

The title compound was synthesized according to a literature procedure (Romero *et al.*, 1996) with some modifications. In a three-neck flask, a solution of 85% KOH solution in *n*-butanol (100 mL) [KOH (1.88 g, 28.50 mmol) as pellets was dried under vacuum for 1 h and dissolved in *n*-butanol (100 mL)] and 2,6-dimethylthiophenol (3.80 mL, 28.50 mmol) were mixed and refluxed for 30 min under nitrogen protection, giving a light-yellow solution. While the reaction mixture was still hot, a colourless solution of 1,3-bis(bromomethyl)benzene (3.75 g, 14.25 mmol) in *n*-butanol (90 mL) was added, and it was further refluxed for 1 h. At this stage, the reaction mixture turned off-white due to the formation of KBr, which was afterward filtered off while still hot. The resulting filtrate was allowed to stand in a water bath at ambient temperature to crystallize slowly. On cooling, after 2 d a white crystalline solid of the title compound was precipitated. It was filtered off, washed with distilled water to dissolve any remaining KBr

(2 × 100 mL) and cold *n*-butanol (2 × 20 mL), and dried under vacuum. Yield: 2.42 g (45%) m.p. 357–358 K, ¹H NMR (400 MHz, CDCl₃, 298 K): δ 7.08–7.15 (*m*, 7H), 6.96 (*d*, 2H), 6.69 (*s*, 1H), (3.70 (*s*, 4H), 2.40 p.p.m. (*s*, 6H). ¹³C NMR (400 MHz, CDCl₃, 298 K): δ 143.5, 138.3, 132.9, 129.3, 128.4, 128.3, 128.0, 127.3, 39.6, 21.8 p.p.m. ¹H NMR and ¹³C NMR are given in the supporting information Colourless blocks of the title compound were grown from a warm saturated *n*-butanol solution upon cooling in a water bath at ambient temperature.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

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full crystallographic data

IUCrData (2019). 4, x190677 [https://doi.org/10.1107/S2414314619006771]

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Crystal data

$C_{24}H_{26}S_2$	$F(000) = 808$
$M_r = 378.57$	$D_x = 1.246 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Cu $K\alpha$ radiation, $\lambda = 1.54178 \text{ \AA}$
$a = 8.4487 (2) \text{ \AA}$	Cell parameters from 9984 reflections
$b = 23.7284 (5) \text{ \AA}$	$\theta = 3.7\text{--}68.2^\circ$
$c = 10.4078 (2) \text{ \AA}$	$\mu = 2.40 \text{ mm}^{-1}$
$\beta = 104.698 (1)^\circ$	$T = 100 \text{ K}$
$V = 2018.22 (8) \text{ \AA}^3$	Block, colourless
$Z = 4$	$0.25 \times 0.15 \times 0.10 \text{ mm}$

Data collection

Bruker D8 Venture diffractometer	30031 measured reflections
Radiation source: Incoatec microsource	3679 independent reflections
Mirrors monochromator	3342 reflections with $I > 2\sigma(I)$
Detector resolution: $10.4167 \text{ pixels mm}^{-1}$	$R_{\text{int}} = 0.038$
ω scans	$\theta_{\text{max}} = 68.3^\circ$, $\theta_{\text{min}} = 3.7^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2015)	$h = -10 \rightarrow 10$
$T_{\text{min}} = 0.630$, $T_{\text{max}} = 0.753$	$k = -28 \rightarrow 28$
	$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.030$	H-atom parameters constrained
$wR(F^2) = 0.077$	$w = 1/[\sigma^2(F_o^2) + (0.036P)^2 + 0.9617P]$
$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
3679 reflections	$(\Delta/\sigma)_{\text{max}} = 0.002$
239 parameters	$\Delta\rho_{\text{max}} = 0.25 \text{ e \AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.26 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

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. All hydrogen atoms were placed geometrically and refined using a riding-atom model approximation, with C—H = 0.95–1.00 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. A rotating model was used for the methyl groups.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	−0.05299 (4)	0.78989 (2)	0.46396 (3)	0.02099 (10)
C1	0.26784 (17)	0.68696 (6)	0.52695 (14)	0.0184 (3)
H1	0.2166	0.6767	0.4379	0.022*
S2	0.52713 (4)	0.57105 (2)	0.50641 (3)	0.02155 (10)
C2	0.17461 (17)	0.71129 (6)	0.60489 (14)	0.0192 (3)
C5	0.50961 (18)	0.69337 (6)	0.70751 (15)	0.0215 (3)
H5	0.6237	0.6877	0.7426	0.026*
C4	0.41787 (19)	0.71745 (6)	0.78570 (15)	0.0237 (3)
H4	0.4695	0.7283	0.8743	0.028*
C3	0.25039 (19)	0.72598 (6)	0.73568 (15)	0.0223 (3)
H3	0.1878	0.7418	0.7907	0.027*
C6	0.43510 (17)	0.67737 (6)	0.57694 (14)	0.0188 (3)
C7	0.53111 (18)	0.64828 (6)	0.49341 (15)	0.0223 (3)
H7A	0.6461	0.6613	0.5209	0.027*
H7B	0.4863	0.6592	0.3994	0.027*
C8	0.63461 (17)	0.56138 (6)	0.67620 (14)	0.0182 (3)
C9	0.54664 (17)	0.55204 (6)	0.77163 (15)	0.0201 (3)
C10	0.63401 (19)	0.54523 (6)	0.90400 (15)	0.0238 (3)
H10	0.5763	0.5393	0.9702	0.029*
C11	0.80332 (19)	0.54693 (6)	0.94022 (15)	0.0253 (3)
H11	0.8608	0.5423	1.0307	0.03*
C12	0.88842 (18)	0.55536 (6)	0.84522 (15)	0.0235 (3)
H12	1.0046	0.5563	0.8709	0.028*
C13	0.80697 (17)	0.56250 (6)	0.71206 (15)	0.0199 (3)
C14	0.90487 (19)	0.57030 (7)	0.61095 (17)	0.0291 (4)
H14A	0.8624	0.5452	0.5352	0.044*
H14B	1.0199	0.5613	0.6514	0.044*
H14C	0.896	0.6095	0.5804	0.044*
C15	0.36202 (18)	0.54935 (7)	0.73663 (17)	0.0275 (3)
H15A	0.3168	0.586	0.7022	0.041*
H15B	0.3255	0.54	0.8162	0.041*
H15C	0.324	0.5203	0.6688	0.041*
C16	−0.00542 (18)	0.72194 (6)	0.54890 (15)	0.0222 (3)
H16A	−0.0605	0.7202	0.6222	0.027*
H16B	−0.0512	0.6914	0.4854	0.027*
C17	−0.00375 (17)	0.83831 (6)	0.59923 (14)	0.0180 (3)
C18	−0.11909 (17)	0.84889 (6)	0.67253 (14)	0.0206 (3)
C19	−0.0832 (2)	0.88954 (6)	0.77240 (15)	0.0248 (3)
H19	−0.1594	0.8968	0.8236	0.03*
C20	0.0622 (2)	0.91949 (7)	0.79792 (15)	0.0277 (4)
H20	0.0854	0.9469	0.8666	0.033*
C21	0.17354 (19)	0.90944 (6)	0.72361 (15)	0.0250 (3)
H21	0.272	0.9307	0.7408	0.03*
C22	0.14412 (17)	0.86870 (6)	0.62377 (14)	0.0202 (3)
C23	0.26849 (18)	0.85884 (7)	0.54506 (17)	0.0275 (4)

H23A	0.2162	0.8632	0.4502	0.041*
H23B	0.3127	0.8206	0.5619	0.041*
H23C	0.3575	0.8863	0.5719	0.041*
C24	-0.28224 (19)	0.81941 (7)	0.64360 (18)	0.0321 (4)
H24A	-0.3467	0.8298	0.5545	0.048*
H24B	-0.3411	0.8307	0.7094	0.048*
H24C	-0.2651	0.7785	0.6481	0.048*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.02004 (18)	0.02104 (19)	0.01986 (18)	0.00211 (13)	0.00130 (14)	-0.00266 (14)
C1	0.0220 (7)	0.0146 (7)	0.0173 (7)	-0.0007 (5)	0.0023 (6)	0.0011 (5)
S2	0.02313 (19)	0.02071 (19)	0.01796 (18)	0.00424 (14)	-0.00004 (14)	-0.00098 (14)
C2	0.0221 (7)	0.0133 (7)	0.0223 (7)	-0.0008 (5)	0.0057 (6)	0.0014 (6)
C5	0.0212 (7)	0.0170 (7)	0.0234 (7)	-0.0019 (6)	0.0001 (6)	0.0029 (6)
C4	0.0324 (8)	0.0190 (8)	0.0166 (7)	-0.0020 (6)	0.0003 (6)	-0.0006 (6)
C3	0.0304 (8)	0.0173 (7)	0.0206 (7)	0.0007 (6)	0.0091 (6)	-0.0010 (6)
C6	0.0219 (7)	0.0142 (7)	0.0205 (7)	-0.0001 (5)	0.0056 (6)	0.0037 (5)
C7	0.0226 (7)	0.0225 (8)	0.0215 (7)	0.0028 (6)	0.0049 (6)	0.0050 (6)
C8	0.0186 (7)	0.0145 (7)	0.0198 (7)	0.0015 (5)	0.0019 (6)	-0.0014 (6)
C9	0.0207 (7)	0.0149 (7)	0.0248 (7)	0.0006 (5)	0.0059 (6)	-0.0008 (6)
C10	0.0340 (8)	0.0189 (8)	0.0205 (7)	0.0004 (6)	0.0106 (6)	-0.0005 (6)
C11	0.0327 (8)	0.0185 (8)	0.0199 (7)	0.0019 (6)	-0.0023 (6)	-0.0012 (6)
C12	0.0196 (7)	0.0182 (7)	0.0283 (8)	-0.0001 (6)	-0.0019 (6)	-0.0003 (6)
C13	0.0192 (7)	0.0147 (7)	0.0253 (8)	0.0008 (5)	0.0045 (6)	0.0010 (6)
C14	0.0222 (8)	0.0301 (9)	0.0368 (9)	0.0034 (6)	0.0109 (7)	0.0082 (7)
C15	0.0209 (8)	0.0289 (9)	0.0349 (9)	-0.0004 (6)	0.0110 (7)	0.0003 (7)
C16	0.0216 (7)	0.0168 (7)	0.0281 (8)	-0.0015 (6)	0.0064 (6)	-0.0030 (6)
C17	0.0184 (7)	0.0165 (7)	0.0174 (7)	0.0026 (5)	0.0014 (6)	0.0018 (5)
C18	0.0214 (7)	0.0182 (7)	0.0219 (7)	0.0034 (6)	0.0048 (6)	0.0037 (6)
C19	0.0346 (8)	0.0220 (8)	0.0189 (7)	0.0062 (6)	0.0088 (6)	0.0031 (6)
C20	0.0422 (9)	0.0184 (8)	0.0185 (7)	0.0012 (7)	0.0006 (7)	0.0001 (6)
C21	0.0261 (8)	0.0197 (8)	0.0237 (8)	-0.0033 (6)	-0.0038 (6)	0.0046 (6)
C22	0.0187 (7)	0.0184 (7)	0.0213 (7)	0.0017 (6)	0.0007 (6)	0.0059 (6)
C23	0.0187 (7)	0.0276 (9)	0.0359 (9)	-0.0005 (6)	0.0066 (7)	0.0040 (7)
C24	0.0234 (8)	0.0324 (9)	0.0443 (10)	-0.0013 (7)	0.0155 (7)	-0.0036 (8)

Geometric parameters (Å, °)

S1—C17	1.7827 (14)	C12—H12	0.95
S1—C16	1.8337 (15)	C13—C14	1.506 (2)
C1—C2	1.391 (2)	C14—H14A	0.98
C1—C6	1.395 (2)	C14—H14B	0.98
C1—H1	0.95	C14—H14C	0.98
S2—C8	1.7848 (14)	C15—H15A	0.98
S2—C7	1.8385 (15)	C15—H15B	0.98
C2—C3	1.394 (2)	C15—H15C	0.98

C2—C16	1.506 (2)	C16—H16A	0.99
C5—C4	1.382 (2)	C16—H16B	0.99
C5—C6	1.398 (2)	C17—C18	1.404 (2)
C5—H5	0.95	C17—C22	1.409 (2)
C4—C3	1.393 (2)	C18—C19	1.394 (2)
C4—H4	0.95	C18—C24	1.506 (2)
C3—H3	0.95	C19—C20	1.385 (2)
C6—C7	1.499 (2)	C19—H19	0.95
C7—H7A	0.99	C20—C21	1.381 (2)
C7—H7B	0.99	C20—H20	0.95
C8—C9	1.401 (2)	C21—C22	1.395 (2)
C8—C13	1.409 (2)	C21—H21	0.95
C9—C10	1.397 (2)	C22—C23	1.506 (2)
C9—C15	1.510 (2)	C23—H23A	0.98
C10—C11	1.384 (2)	C23—H23B	0.98
C10—H10	0.95	C23—H23C	0.98
C11—C12	1.377 (2)	C24—H24A	0.98
C11—H11	0.95	C24—H24B	0.98
C12—C13	1.392 (2)	C24—H24C	0.98
C17—S1—C16	101.96 (7)	H14A—C14—H14B	109.5
C2—C1—C6	121.33 (13)	C13—C14—H14C	109.5
C2—C1—H1	119.3	H14A—C14—H14C	109.5
C6—C1—H1	119.3	H14B—C14—H14C	109.5
C8—S2—C7	100.76 (7)	C9—C15—H15A	109.5
C1—C2—C3	119.04 (13)	C9—C15—H15B	109.5
C1—C2—C16	120.64 (13)	H15A—C15—H15B	109.5
C3—C2—C16	120.31 (13)	C9—C15—H15C	109.5
C4—C5—C6	120.23 (14)	H15A—C15—H15C	109.5
C4—C5—H5	119.9	H15B—C15—H15C	109.5
C6—C5—H5	119.9	C2—C16—S1	114.23 (10)
C5—C4—C3	120.55 (14)	C2—C16—H16A	108.7
C5—C4—H4	119.7	S1—C16—H16A	108.7
C3—C4—H4	119.7	C2—C16—H16B	108.7
C4—C3—C2	120.01 (14)	S1—C16—H16B	108.7
C4—C3—H3	120.0	H16A—C16—H16B	107.6
C2—C3—H3	120.0	C18—C17—C22	121.05 (13)
C1—C6—C5	118.82 (14)	C18—C17—S1	119.29 (11)
C1—C6—C7	120.31 (13)	C22—C17—S1	119.45 (11)
C5—C6—C7	120.82 (13)	C19—C18—C17	118.62 (14)
C6—C7—S2	113.18 (10)	C19—C18—C24	119.04 (14)
C6—C7—H7A	108.9	C17—C18—C24	122.30 (14)
S2—C7—H7A	108.9	C20—C19—C18	120.84 (15)
C6—C7—H7B	108.9	C20—C19—H19	119.6
S2—C7—H7B	108.9	C18—C19—H19	119.6
H7A—C7—H7B	107.8	C21—C20—C19	120.05 (14)
C9—C8—C13	120.92 (13)	C21—C20—H20	120.0
C9—C8—S2	119.61 (11)	C19—C20—H20	120.0

C13—C8—S2	119.47 (11)	C20—C21—C22	121.25 (14)
C10—C9—C8	118.34 (13)	C20—C21—H21	119.4
C10—C9—C15	119.19 (14)	C22—C21—H21	119.4
C8—C9—C15	122.47 (13)	C21—C22—C17	118.17 (14)
C11—C10—C9	121.07 (14)	C21—C22—C23	119.73 (14)
C11—C10—H10	119.5	C17—C22—C23	122.09 (13)
C9—C10—H10	119.5	C22—C23—H23A	109.5
C12—C11—C10	120.03 (14)	C22—C23—H23B	109.5
C12—C11—H11	120.0	H23A—C23—H23B	109.5
C10—C11—H11	120.0	C22—C23—H23C	109.5
C11—C12—C13	121.08 (14)	H23A—C23—H23C	109.5
C11—C12—H12	119.5	H23B—C23—H23C	109.5
C13—C12—H12	119.5	C18—C24—H24A	109.5
C12—C13—C8	118.55 (14)	C18—C24—H24B	109.5
C12—C13—C14	119.35 (13)	H24A—C24—H24B	109.5
C8—C13—C14	122.09 (13)	C18—C24—H24C	109.5
C13—C14—H14A	109.5	H24A—C24—H24C	109.5
C13—C14—H14B	109.5	H24B—C24—H24C	109.5
C6—C1—C2—C3	-0.4 (2)	C11—C12—C13—C14	-178.63 (14)
C6—C1—C2—C16	179.32 (13)	C9—C8—C13—C12	-1.4 (2)
C6—C5—C4—C3	0.1 (2)	S2—C8—C13—C12	179.45 (11)
C5—C4—C3—C2	-1.4 (2)	C9—C8—C13—C14	177.68 (14)
C1—C2—C3—C4	1.5 (2)	S2—C8—C13—C14	-1.43 (19)
C16—C2—C3—C4	-178.22 (13)	C1—C2—C16—S1	-87.22 (15)
C2—C1—C6—C5	-0.8 (2)	C3—C2—C16—S1	92.49 (15)
C2—C1—C6—C7	176.71 (13)	C17—S1—C16—C2	-70.83 (12)
C4—C5—C6—C1	1.0 (2)	C16—S1—C17—C18	-82.68 (12)
C4—C5—C6—C7	-176.56 (13)	C16—S1—C17—C22	102.54 (12)
C1—C6—C7—S2	-86.79 (15)	C22—C17—C18—C19	-1.2 (2)
C5—C6—C7—S2	90.70 (15)	S1—C17—C18—C19	-175.88 (11)
C8—S2—C7—C6	-65.52 (12)	C22—C17—C18—C24	176.53 (14)
C7—S2—C8—C9	99.48 (12)	S1—C17—C18—C24	1.8 (2)
C7—S2—C8—C13	-81.39 (12)	C17—C18—C19—C20	0.8 (2)
C13—C8—C9—C10	1.6 (2)	C24—C18—C19—C20	-176.95 (14)
S2—C8—C9—C10	-179.31 (11)	C18—C19—C20—C21	0.3 (2)
C13—C8—C9—C15	-178.71 (14)	C19—C20—C21—C22	-1.1 (2)
S2—C8—C9—C15	0.41 (19)	C20—C21—C22—C17	0.8 (2)
C8—C9—C10—C11	-0.8 (2)	C20—C21—C22—C23	-179.86 (14)
C15—C9—C10—C11	179.46 (14)	C18—C17—C22—C21	0.4 (2)
C9—C10—C11—C12	-0.1 (2)	S1—C17—C22—C21	175.08 (11)
C10—C11—C12—C13	0.2 (2)	C18—C17—C22—C23	-178.95 (13)
C11—C12—C13—C8	0.5 (2)	S1—C17—C22—C23	-4.27 (19)