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# *rac*-2,2′-(Thiane-2,6-diyl)bis[1-(4-bromophenyl)ethanone]

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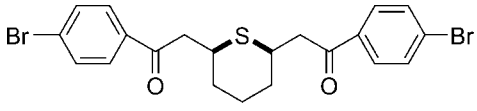
Key indicators: single-crystal X-ray study; $T$ = 295 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.055; $wR$ factor = 0.112; data-to-parameter ratio = 15.1.

In the title compound, $C_{21}H_{20}Br_2O_2S$, prepared by the reaction of 1,9-bis(4-bromophenyl)nona-2,7-diene-1,9-dione with sodium sulfide nonahydrate in acetonitrile, the six-membered thiopyran ring has a chair conformation while the H atoms *ortho* to the S atom adopt a *cis* configuration. The dihedral angle between the two benzene rings is 2.59 (8)°.

## Related literature

For the synthesis of 1,9-bis(4-bromophenyl)nona-2,7-diene-1,9-dione, see: Yang, Cauble *et al.* (2004); Yang, Felton *et al.* (2004). For the synthesis of compounds containing sulfur, see: Knapp *et al.* (2002); Yao *et al.* (2003); Oliveira *et al.* (1999). For applications of natural products containing sulfur, see: Qi *et al.* (2004); Zhang & Zhang (2006); Barco *et al.* (2006).




## Experimental

### *Crystal data*

$C_{21}H_{20}Br_2O_2S$
$M_r$ = 496.25
Triclinic, $P\overline{1}$
$a$ = 6.484 (4) Å
$b$ = 12.970 (5) Å
$c$ = 13.076 (4) Å
$\alpha$ = 71.14 (3)°
$\beta$ = 79.45 (4)°
$\gamma$ = 79.52 (4)°
$V$ = 1014.1 (7) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 4.11 mm$^{-1}$
$T$ = 295 K
0.40 × 0.30 × 0.20 mm

### *Data collection*

Siemens P4 four-circle diffractometer
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.381, $T_{max}$ = 0.459
4549 measured reflections
3548 independent reflections
2220 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.032
3 standard reflections every 97 reflections
intensity decay: none

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.112
$S$ = 1.07
3548 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.41 e Å$^{-3}$

Data collection: *XSCANS* (Bruker, 1997); cell refinement: *XSCANS*; data reduction: *XSCANS*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2103).

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# supplementary materials

*Acta Cryst.* (2011). E**67**, o1047 [ **doi:10.1107/S1600536811011792** ]

# *rac*-2,2'-(Thiane-2,6-diyl)bis[1-(4-bromophenyl)ethanone]

**L.-Q. Liu and J.-K. Yang**

## Comment

The mothods for the synthesis of compounds containing sulfur have been described (Knapp *et al.*, 2002; Yao *et al.*, 2003; Oliveira *et al.* 1999). Natural products containing sulfur often have biological activity, so that the methods for their synthesis have received considerable attention among researchers. In this paper, we report the structure of the title compound $C_{21}H_{20}Br_2O_2S$ (I), prepared by the reaction of 1,9-bis(4-bromophenyl)nona-2,7-diene-1,9-dione with sodium sulfide nonahydrate in acetonitrile. In the crystal, the six-membered thiopyran ring has a chair conformation with the H atoms *ortho* to the S (H9 and H13) adopting a *cis* configuration (Fig. 1). The dihedral angle between the benzene rings on the substituent chains is 2.59 (8)°.

## Experimental

The reaction mixture of 1,9-bis(4-bromophenyl)nona-2,7-diene-1,9-dione (100 mg, 0.20 mmol) with sodium sulfide nonahydrate (67 mg, 0.28 mmol) in 50 ml of acetonitrile was stirred for 11 days at room temperature, affording the title compound (20 mg; yield 32%). Colorless single crystals were obtained by slow evaporation of an ethyl acetate solution in air.

## Refinement

All hydrogen atoms were generated geometically with C—H bond distances of 0.93–0.98 Å according to criteria described in the *SHELXTL* manual (Bruker, 1997). These were included in the refinement with $U_{iso}(H) = 1.2U_{eq}(C)$.

## Figures

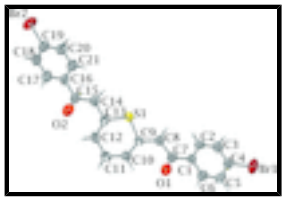


Fig. 1. The molecular conformation of the title compound showing 35% probability displacement ellipsoids and the atom numbering scheme

## *rac*-2,2'-(Thiane-2,6-diyl)bis[1-(4-bromophenyl)ethanone]

*Crystal data*

| | |
|---|---|
| $C_{21}H_{20}Br_2O_2S$ | $Z = 2$ |
| $M_r = 496.25$ | $F(000) = 496$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.625$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 6.484$ (4) Å | Cell parameters from 45 reflections |

| | |
|---|---|
| $b$ = 12.970 (5) Å | θ = 5.6–12.4° |
| $c$ = 13.076 (4) Å | μ = 4.11 mm$^{-1}$ |
| α = 71.14 (3)° | $T$ = 295 K |
| β = 79.45 (4)° | Prism, colorless |
| γ = 79.52 (4)° | 0.40 × 0.30 × 0.20 mm |
| $V$ = 1014.1 (7) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Siemens P4 four-circle diffractometer | 2220 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{int}$ = 0.032 |
| graphite | $\theta_{max}$ = 25.1°, $\theta_{min}$ = 2.0° |
| ω scans | $h = -1 \rightarrow 7$ |
| Absorption correction: ψ scan (North *et al.*, 1968) | $k = -14 \rightarrow 14$ |
| $T_{min}$ = 0.381, $T_{max}$ = 0.459 | $l = -15 \rightarrow 15$ |
| 4549 measured reflections | 3 standard reflections every 97 reflections |
| 3548 independent reflections | intensity decay: none |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)]$ = 0.055 | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2)$ = 0.112 | H-atom parameters constrained |
| $S$ = 1.07 | $w = 1/[\sigma^2(F_o^2) + (0.001P)^2 + 2.0P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 3548 reflections | $(\Delta/\sigma)_{max}$ = 0.001 |
| 235 parameters | $\Delta\rho_{max}$ = 0.51 e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min}$ = −0.41 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 ($Å^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Br1 | 0.47955 (9) | 1.39832 (4) | 0.65329 (4) | 0.08336 (16) |
| Br2 | 0.87756 (10) | 0.46636 (4) | −0.19734 (4) | 0.09195 (19) |
| S1 | 0.35503 (17) | 0.97967 (9) | 0.19248 (8) | 0.0594 (3) |
| O1 | −0.0519 (5) | 1.2370 (2) | 0.3377 (2) | 0.0755 (9) |
| O2 | 0.0963 (5) | 0.8256 (2) | −0.0195 (2) | 0.0740 (9) |
| C1 | 0.2190 (6) | 1.2490 (3) | 0.4300 (3) | 0.0477 (10) |
| C2 | 0.4267 (6) | 1.2193 (3) | 0.4523 (3) | 0.0596 (12) |
| H2A | 0.5153 | 1.1687 | 0.4220 | 0.071* |
| C3 | 0.5051 (7) | 1.2633 (3) | 0.5185 (3) | 0.0673 (13) |
| H3A | 0.6453 | 1.2438 | 0.5316 | 0.081* |
| C4 | 0.3711 (6) | 1.3365 (3) | 0.5645 (3) | 0.0559 (11) |
| C5 | 0.1643 (7) | 1.3678 (3) | 0.5447 (3) | 0.0597 (12) |
| H5A | 0.0760 | 1.4175 | 0.5764 | 0.072* |
| C6 | 0.0894 (7) | 1.3245 (3) | 0.4772 (3) | 0.0568 (12) |
| H6A | −0.0499 | 1.3460 | 0.4630 | 0.068* |
| C7 | 0.1259 (7) | 1.2030 (3) | 0.3601 (3) | 0.0543 (11) |
| C8 | 0.2614 (6) | 1.1124 (3) | 0.3196 (3) | 0.0557 (11) |
| H8A | 0.3138 | 1.0552 | 0.3815 | 0.067* |
| H8B | 0.3829 | 1.1420 | 0.2711 | 0.067* |
| C9 | 0.1493 (6) | 1.0605 (3) | 0.2598 (3) | 0.0494 (10) |
| H9A | 0.0776 | 1.1190 | 0.2042 | 0.059* |
| C10 | −0.0111 (6) | 0.9885 (3) | 0.3336 (3) | 0.0601 (12) |
| H10A | −0.1162 | 1.0322 | 0.3709 | 0.072* |
| H10B | 0.0599 | 0.9303 | 0.3884 | 0.072* |
| C11 | −0.1229 (6) | 0.9372 (3) | 0.2727 (3) | 0.0650 (13) |
| H11A | −0.2286 | 0.8956 | 0.3238 | 0.078* |
| H11B | −0.1954 | 0.9953 | 0.2184 | 0.078* |
| C12 | 0.0287 (6) | 0.8618 (3) | 0.2168 (3) | 0.0588 (12) |
| H12A | −0.0519 | 0.8293 | 0.1826 | 0.071* |
| H12B | 0.0979 | 0.8027 | 0.2717 | 0.071* |
| C13 | 0.1970 (6) | 0.9190 (3) | 0.1311 (3) | 0.0517 (11) |
| H13A | 0.1284 | 0.9771 | 0.0739 | 0.062* |
| C14 | 0.3569 (6) | 0.8426 (3) | 0.0794 (3) | 0.0561 (12) |
| H14A | 0.4755 | 0.8815 | 0.0400 | 0.067* |
| H14B | 0.4100 | 0.7805 | 0.1374 | 0.067* |
| C15 | 0.2757 (7) | 0.7987 (3) | 0.0020 (3) | 0.0543 (12) |
| C16 | 0.4289 (6) | 0.7209 (3) | −0.0478 (3) | 0.0530 (11) |
| C17 | 0.3596 (7) | 0.6792 (3) | −0.1196 (3) | 0.0645 (13) |
| H17A | 0.2225 | 0.7017 | −0.1372 | 0.077* |
| C18 | 0.4938 (7) | 0.6047 (3) | −0.1650 (3) | 0.0667 (13) |
| H18A | 0.4479 | 0.5780 | −0.2137 | 0.080* |
| C19 | 0.6922 (7) | 0.5709 (3) | −0.1379 (3) | 0.0646 (13) |
| C20 | 0.7680 (8) | 0.6127 (3) | −0.0700 (3) | 0.0719 (14) |
| H20A | 0.9069 | 0.5912 | −0.0550 | 0.086* |
| C21 | 0.6352 (7) | 0.6872 (3) | −0.0241 (3) | 0.0657 (13) |

| | | | | |
|---|---|---|---|---|
| H21A | 0.6846 | 0.7148 | 0.0229 | 0.079* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.1169 (4) | 0.0718 (3) | 0.0768 (3) | −0.0107 (3) | −0.0346 (3) | −0.0323 (2) |
| Br2 | 0.1217 (5) | 0.0730 (3) | 0.0745 (3) | 0.0071 (3) | 0.0042 (3) | −0.0334 (2) |
| S1 | 0.0517 (6) | 0.0715 (6) | 0.0667 (6) | −0.0140 (5) | −0.0006 (5) | −0.0374 (5) |
| O1 | 0.0630 (18) | 0.0824 (17) | 0.0972 (18) | 0.0060 (16) | −0.0260 (15) | −0.0490 (15) |
| O2 | 0.0769 (19) | 0.0751 (17) | 0.0793 (17) | 0.0154 (16) | −0.0348 (15) | −0.0364 (14) |
| C1 | 0.051 (2) | 0.0488 (19) | 0.0465 (19) | −0.0129 (18) | −0.0055 (17) | −0.0160 (16) |
| C2 | 0.049 (2) | 0.067 (2) | 0.067 (2) | −0.004 (2) | 0.000 (2) | −0.0335 (19) |
| C3 | 0.063 (3) | 0.075 (3) | 0.074 (3) | −0.010 (2) | −0.014 (2) | −0.033 (2) |
| C4 | 0.070 (3) | 0.053 (2) | 0.050 (2) | −0.016 (2) | −0.013 (2) | −0.0154 (17) |
| C5 | 0.076 (3) | 0.050 (2) | 0.052 (2) | 0.003 (2) | −0.011 (2) | −0.0193 (17) |
| C6 | 0.058 (3) | 0.055 (2) | 0.056 (2) | −0.001 (2) | −0.012 (2) | −0.0159 (18) |
| C7 | 0.055 (2) | 0.055 (2) | 0.053 (2) | −0.007 (2) | −0.0016 (19) | −0.0191 (17) |
| C8 | 0.056 (2) | 0.060 (2) | 0.058 (2) | −0.013 (2) | −0.0022 (19) | −0.0272 (17) |
| C9 | 0.043 (2) | 0.057 (2) | 0.0519 (19) | −0.0110 (18) | −0.0026 (17) | −0.0212 (17) |
| C10 | 0.056 (2) | 0.064 (2) | 0.061 (2) | −0.012 (2) | 0.004 (2) | −0.0246 (19) |
| C11 | 0.052 (2) | 0.070 (3) | 0.072 (3) | −0.017 (2) | 0.000 (2) | −0.019 (2) |
| C12 | 0.063 (3) | 0.058 (2) | 0.059 (2) | −0.024 (2) | −0.005 (2) | −0.0159 (19) |
| C13 | 0.057 (2) | 0.051 (2) | 0.0507 (19) | −0.0033 (19) | −0.0162 (18) | −0.0179 (16) |
| C14 | 0.063 (3) | 0.055 (2) | 0.055 (2) | −0.010 (2) | −0.011 (2) | −0.0196 (18) |
| C15 | 0.072 (3) | 0.0383 (19) | 0.052 (2) | −0.006 (2) | −0.013 (2) | −0.0118 (16) |
| C16 | 0.066 (3) | 0.0443 (19) | 0.051 (2) | −0.0110 (19) | −0.0120 (19) | −0.0125 (17) |
| C17 | 0.074 (3) | 0.065 (2) | 0.060 (2) | −0.010 (2) | −0.016 (2) | −0.0232 (19) |
| C18 | 0.080 (3) | 0.068 (2) | 0.064 (2) | −0.016 (2) | −0.011 (2) | −0.0317 (19) |
| C19 | 0.083 (3) | 0.054 (2) | 0.053 (2) | −0.007 (2) | 0.001 (2) | −0.0183 (19) |
| C20 | 0.078 (3) | 0.063 (2) | 0.074 (3) | 0.004 (2) | −0.013 (2) | −0.026 (2) |
| C21 | 0.075 (3) | 0.068 (2) | 0.061 (2) | −0.007 (2) | −0.015 (2) | −0.0262 (19) |

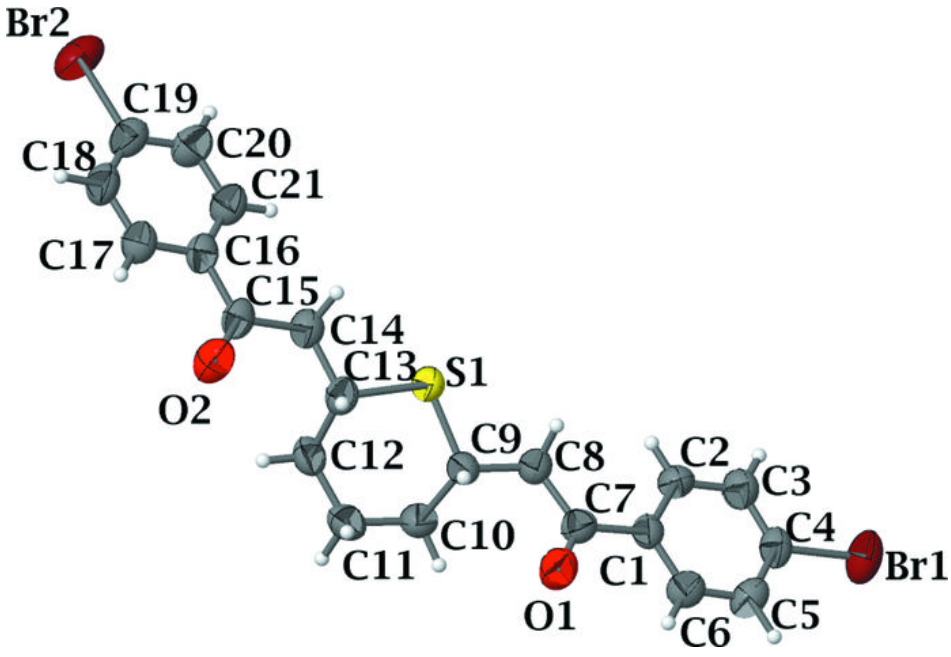
*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Br1—C4 | 1.895 (4) | C10—H10A | 0.9700 |
| Br2—C19 | 1.906 (4) | C10—H10B | 0.9700 |
| S1—C9 | 1.819 (4) | C11—C12 | 1.518 (6) |
| S1—C13 | 1.820 (4) | C11—H11A | 0.9700 |
| O1—C7 | 1.210 (5) | C11—H11B | 0.9700 |
| O2—C15 | 1.209 (5) | C12—C13 | 1.518 (5) |
| C1—C2 | 1.389 (5) | C12—H12A | 0.9700 |
| C1—C6 | 1.395 (5) | C12—H12B | 0.9700 |
| C1—C7 | 1.497 (6) | C13—C14 | 1.523 (5) |
| C2—C3 | 1.386 (6) | C13—H13A | 0.9800 |
| C2—H2A | 0.9300 | C14—C15 | 1.517 (6) |
| C3—C4 | 1.377 (6) | C14—H14A | 0.9700 |
| C3—H3A | 0.9300 | C14—H14B | 0.9700 |
| C4—C5 | 1.375 (6) | C15—C16 | 1.500 (5) |
| C5—C6 | 1.381 (6) | C16—C21 | 1.389 (6) |

| | | | |
|---|---|---|---|
| C5—H5A | 0.9300 | C16—C17 | 1.396 (6) |
| C6—H6A | 0.9300 | C17—C18 | 1.385 (6) |
| C7—C8 | 1.513 (5) | C17—H17A | 0.9300 |
| C8—C9 | 1.523 (6) | C18—C19 | 1.354 (6) |
| C8—H8A | 0.9700 | C18—H18A | 0.9300 |
| C8—H8B | 0.9700 | C19—C20 | 1.376 (7) |
| C9—C10 | 1.512 (5) | C20—C21 | 1.385 (6) |
| C9—H9A | 0.9800 | C20—H20A | 0.9300 |
| C10—C11 | 1.528 (6) | C21—H21A | 0.9300 |
| C9—S1—C13 | 101.01 (18) | C12—C11—H11B | 109.1 |
| C2—C1—C6 | 117.9 (4) | C10—C11—H11B | 109.1 |
| C2—C1—C7 | 123.7 (4) | H11A—C11—H11B | 107.8 |
| C6—C1—C7 | 118.4 (4) | C11—C12—C13 | 114.0 (3) |
| C3—C2—C1 | 121.6 (4) | C11—C12—H12A | 108.8 |
| C3—C2—H2A | 119.2 | C13—C12—H12A | 108.8 |
| C1—C2—H2A | 119.2 | C11—C12—H12B | 108.8 |
| C4—C3—C2 | 118.6 (4) | C13—C12—H12B | 108.8 |
| C4—C3—H3A | 120.7 | H12A—C12—H12B | 107.7 |
| C2—C3—H3A | 120.7 | C12—C13—C14 | 114.1 (3) |
| C5—C4—C3 | 121.6 (4) | C12—C13—S1 | 110.2 (3) |
| C5—C4—Br1 | 119.8 (3) | C14—C13—S1 | 104.6 (3) |
| C3—C4—Br1 | 118.6 (3) | C12—C13—H13A | 109.2 |
| C4—C5—C6 | 119.1 (4) | C14—C13—H13A | 109.2 |
| C4—C5—H5A | 120.5 | S1—C13—H13A | 109.2 |
| C6—C5—H5A | 120.5 | C15—C14—C13 | 116.0 (3) |
| C5—C6—C1 | 121.2 (4) | C15—C14—H14A | 108.3 |
| C5—C6—H6A | 119.4 | C13—C14—H14A | 108.3 |
| C1—C6—H6A | 119.4 | C15—C14—H14B | 108.3 |
| O1—C7—C1 | 120.8 (4) | C13—C14—H14B | 108.3 |
| O1—C7—C8 | 121.6 (4) | H14A—C14—H14B | 107.4 |
| C1—C7—C8 | 117.6 (3) | O2—C15—C16 | 121.3 (4) |
| C7—C8—C9 | 114.9 (3) | O2—C15—C14 | 121.8 (4) |
| C7—C8—H8A | 108.5 | C16—C15—C14 | 117.0 (4) |
| C9—C8—H8A | 108.5 | C21—C16—C17 | 118.6 (4) |
| C7—C8—H8B | 108.5 | C21—C16—C15 | 122.9 (4) |
| C9—C8—H8B | 108.5 | C17—C16—C15 | 118.5 (4) |
| H8A—C8—H8B | 107.5 | C18—C17—C16 | 120.4 (4) |
| C10—C9—C8 | 113.7 (3) | C18—C17—H17A | 119.8 |
| C10—C9—S1 | 110.1 (3) | C16—C17—H17A | 119.8 |
| C8—C9—S1 | 106.4 (3) | C19—C18—C17 | 119.6 (4) |
| C10—C9—H9A | 108.8 | C19—C18—H18A | 120.2 |
| C8—C9—H9A | 108.8 | C17—C18—H18A | 120.2 |
| S1—C9—H9A | 108.8 | C18—C19—C20 | 121.5 (4) |
| C9—C10—C11 | 113.2 (3) | C18—C19—Br2 | 120.3 (4) |
| C9—C10—H10A | 108.9 | C20—C19—Br2 | 118.1 (4) |
| C11—C10—H10A | 108.9 | C19—C20—C21 | 119.3 (5) |
| C9—C10—H10B | 108.9 | C19—C20—H20A | 120.4 |
| C11—C10—H10B | 108.9 | C21—C20—H20A | 120.4 |
| H10A—C10—H10B | 107.7 | C20—C21—C16 | 120.5 (4) |

| | | | |
|---|---|---|---|
| C12—C11—C10 | 112.6 (3) | C20—C21—H21A | 119.8 |
| C12—C11—H11A | 109.1 | C16—C21—H21A | 119.8 |
| C10—C11—H11A | 109.1 | | |

Fig. 1


Br2
C19
C18
C20
C21
C17
C16
C15
C14
C13
S1
O2
C12
C9
C8
C2
C3
C7
C4
Br1
C10
C11
O1
C1
C6
C5