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# 2,4,5,7,9,10-Hexathia-1,3,6,8(1,4)-tetrabenzenacyclodecaphane

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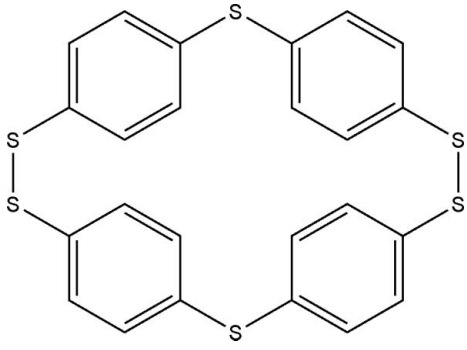
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.034; $wR$ factor = 0.089; data-to-parameter ratio = 14.0.

In the title macrocyclic molecule, $C_{24}H_{16}S_6$, the S—S bond lengths are 2.0600 (11) and 2.0589 (12) Å. The crystal packing exhibits no classical intermolecular interactions.

## Related literature

For S—S bond lengths, see: Ogawa *et al.* (1999).




## Experimental

### Crystal data

$C_{24}H_{16}S_6$
$M_r$ = 496.73
Orthorhombic, $Pna2_1$
$a$ = 14.6300 (15) Å
$b$ = 25.025 (3) Å
$c$ = 5.9754 (6) Å
$V$ = 2187.7 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.64 mm$^{-1}$
$T$ = 298 (2) K
0.33 × 0.11 × 0.08 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.818, $T_{max}$ = 0.951
11286 measured reflections
3815 independent reflections
3452 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.089
$S$ = 1.00
3815 reflections
272 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$
Absolute structure: Flack (1983), 1683 Friedel pairs
Flack parameter: 0.02 (8)

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: CV2323).

## References

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# supplementary materials

*Acta Cryst.* (2007). E**63**, o4465 [ **doi:10.1107/S1600536807052567** ]

# 2,4,5,7,9,10-Hexathia-1,3,6,8(1,4)-tetrabenzenacyclodecaphane

**Z. Guo and R. Zhang**

## Comment

In the title compound (Fig. 1), the S—S bond lengths are 2.0600 (11) Å [S2—S5] and 2.0589 (12) Å [S3—S6], which are consistent with the reported values (Ogawa *et al.*, 1999). The intramolecular distances C2···C20 and C8···C18 are 4.418 (5) and 7.281 (7) Å, respectively.

## Experimental

To an ethanol (10 ml) solution of 4,4'-thiodibenzenethiol (1 mmol) was added an ethanol (5 ml) solution of iodine (2 mmol). The mixture was stirred for 4 h at room temperature, and a pale yellow solution was obtained and filtered. The filtrate was left undisturbed at room temperature for two weeks. Crystals of the title compound suitable for X-ray analysis were grown from an ethanol solution (yield 63%).

## Refinement

All H atoms were placed in geometrically idealized positions (C—H = 0.93 Å) and treated as riding on their parent atoms, with $U_{iso}$(H)=1.2$U_{eq}$(C).

## Figures

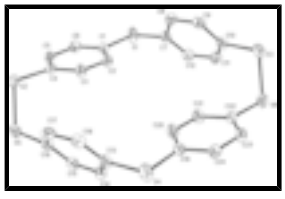


Fig. 1. The molecular structure of the title compound, showing 30% probability displacement ellipsoids and atomic numbering. H atoms have been omited for clarity.

## 2,4,5,7,9,10-Hexathia-1,3,6,8(1,4)-tetrabenzenacyclodecaphane

*Crystal data*

| | |
|---|---|
| $C_{24}H_{16}S_6$ | $F_{000}$ = 1024 |
| $M_r$ = 496.73 | $D_x$ = 1.508 Mg m$^{-3}$ |
| Orthorhombic, *Pna*2$_1$ | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: P 2c -2n | Cell parameters from 5516 reflections |
| *a* = 14.6300 (15) Å | θ = 2.8–28.2º |
| *b* = 25.025 (3) Å | μ = 0.64 mm$^{-1}$ |
| *c* = 5.9754 (6) Å | *T* = 298 (2) K |

| | |
|---|---|
| $V$ = 2187.7 (4) Å$^3$ | Block, colourless |
| $Z$ = 4 | 0.33 × 0.11 × 0.08 mm |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 3815 independent reflections |
| Radiation source: fine-focus sealed tube | 3452 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.029 |
| $T$ = 298(2) K | $\theta_{max}$ = 25.0º |
| φ and ω scans | $\theta_{min}$ = 1.6º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h$ = −17→12 |
| $T_{min}$ = 0.818, $T_{max}$ = 0.951 | $k$ = −29→29 |
| 11286 measured reflections | $l$ = −7→6 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)]$ = 0.034 | $w = 1/[\sigma^2(F_o^2) + (0.051P)^2 + 0.7742P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2)$ = 0.089 | $(\Delta/\sigma)_{max}$ = 0.001 |
| $S$ = 1.00 | $\Delta\rho_{max}$ = 0.25 e Å$^{-3}$ |
| 3815 reflections | $\Delta\rho_{min}$ = −0.21 e Å$^{-3}$ |
| 272 parameters | Extinction correction: none |
| 1 restraint | Absolute structure: Flack (1983) |
| Primary atom site location: structure-invariant direct methods | Flack parameter: 0.02 (8) |
| Secondary atom site location: difference Fourier map | |

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.04551 (7) | 0.61284 (3) | −0.25432 (16) | 0.0556 (3) |

| | | | | |
|---|---|---|---|---|
| S2 | 0.19406 (5) | 0.42222 (3) | 0.33953 (16) | 0.04216 (19) |
| S3 | 0.10998 (5) | 0.81877 (3) | 0.33467 (17) | 0.0505 (2) |
| S4 | 0.42460 (7) | 0.63478 (3) | 0.83251 (19) | 0.0586 (2) |
| S5 | 0.33401 (5) | 0.42247 (3) | 0.30183 (15) | 0.0479 (2) |
| S6 | 0.24892 (6) | 0.82644 (3) | 0.29017 (17) | 0.0495 (2) |
| C1 | 0.09121 (19) | 0.56196 (11) | −0.0797 (5) | 0.0373 (7) |
| C2 | 0.1331 (2) | 0.57092 (12) | 0.1244 (6) | 0.0428 (8) |
| H2 | 0.1401 | 0.6057 | 0.1765 | 0.051* |
| C3 | 0.1646 (2) | 0.52860 (11) | 0.2518 (6) | 0.0393 (7) |
| H3 | 0.1903 | 0.5349 | 0.3916 | 0.047* |
| C4 | 0.15771 (19) | 0.47662 (11) | 0.1706 (5) | 0.0355 (7) |
| C5 | 0.1188 (2) | 0.46789 (11) | −0.0373 (5) | 0.0373 (7) |
| H5 | 0.1156 | 0.4333 | −0.0940 | 0.045* |
| C6 | 0.08465 (19) | 0.50999 (11) | −0.1612 (6) | 0.0400 (6) |
| H6 | 0.0573 | 0.5036 | −0.2992 | 0.048* |
| C7 | 0.0574 (2) | 0.67187 (12) | −0.0927 (5) | 0.0400 (7) |
| C8 | 0.0130 (2) | 0.67842 (12) | 0.1109 (6) | 0.0441 (8) |
| H8 | −0.0272 | 0.6523 | 0.1620 | 0.053* |
| C9 | 0.0283 (2) | 0.72354 (12) | 0.2371 (6) | 0.0415 (7) |
| H9 | 0.0011 | 0.7270 | 0.3771 | 0.050* |
| C10 | 0.0843 (2) | 0.76392 (12) | 0.1554 (5) | 0.0385 (7) |
| C11 | 0.1210 (2) | 0.75951 (13) | −0.0562 (5) | 0.0425 (7) |
| H11 | 0.1532 | 0.7880 | −0.1178 | 0.051* |
| C12 | 0.11021 (19) | 0.71307 (11) | −0.1764 (6) | 0.0418 (7) |
| H12 | 0.1386 | 0.7094 | −0.3148 | 0.050* |
| C13 | 0.4031 (2) | 0.57457 (12) | 0.6845 (6) | 0.0404 (7) |
| C14 | 0.4422 (2) | 0.56461 (12) | 0.4793 (6) | 0.0431 (8) |
| H14 | 0.4823 | 0.5893 | 0.4168 | 0.052* |
| C15 | 0.42192 (19) | 0.51778 (11) | 0.3656 (6) | 0.0394 (7) |
| H15 | 0.4460 | 0.5119 | 0.2237 | 0.047* |
| C16 | 0.3658 (2) | 0.47972 (11) | 0.4632 (5) | 0.0378 (7) |
| C17 | 0.3322 (2) | 0.48796 (13) | 0.6754 (6) | 0.0451 (8) |
| H17 | 0.2985 | 0.4613 | 0.7457 | 0.054* |
| C18 | 0.3483 (2) | 0.53591 (12) | 0.7850 (6) | 0.0436 (7) |
| H18 | 0.3226 | 0.5422 | 0.9249 | 0.052* |
| C19 | 0.3718 (2) | 0.68490 (12) | 0.6690 (6) | 0.0392 (7) |
| C20 | 0.3303 (2) | 0.67732 (12) | 0.4636 (6) | 0.0462 (8) |
| H20 | 0.3279 | 0.6433 | 0.4016 | 0.055* |
| C21 | 0.2923 (2) | 0.72005 (11) | 0.3493 (6) | 0.0446 (7) |
| H21 | 0.2652 | 0.7145 | 0.2104 | 0.053* |
| C22 | 0.2943 (2) | 0.77105 (11) | 0.4405 (5) | 0.0378 (7) |
| C23 | 0.3359 (2) | 0.77856 (12) | 0.6463 (6) | 0.0414 (7) |
| H23 | 0.3380 | 0.8126 | 0.7088 | 0.050* |
| C24 | 0.37435 (19) | 0.73607 (11) | 0.7594 (6) | 0.0410 (7) |
| H24 | 0.4022 | 0.7417 | 0.8973 | 0.049* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0788 (6) | 0.0384 (4) | 0.0496 (5) | 0.0030 (4) | −0.0241 (5) | 0.0010 (4) |
| S2 | 0.0472 (4) | 0.0278 (3) | 0.0515 (5) | −0.0022 (3) | −0.0025 (4) | 0.0039 (4) |
| S3 | 0.0544 (4) | 0.0424 (4) | 0.0547 (5) | 0.0143 (3) | −0.0033 (5) | −0.0102 (4) |
| S4 | 0.0803 (6) | 0.0408 (4) | 0.0545 (5) | 0.0112 (4) | −0.0296 (5) | −0.0075 (5) |
| S5 | 0.0467 (4) | 0.0367 (4) | 0.0603 (6) | 0.0083 (3) | −0.0029 (4) | −0.0104 (4) |
| S6 | 0.0575 (5) | 0.0309 (4) | 0.0602 (6) | −0.0033 (3) | −0.0076 (4) | 0.0049 (4) |
| C1 | 0.0365 (15) | 0.0324 (15) | 0.0430 (19) | 0.0011 (12) | −0.0013 (13) | 0.0013 (13) |
| C2 | 0.0506 (19) | 0.0294 (15) | 0.048 (2) | 0.0001 (13) | −0.0111 (16) | −0.0056 (14) |
| C3 | 0.0466 (16) | 0.0314 (15) | 0.0399 (18) | 0.0009 (12) | −0.0067 (15) | −0.0029 (13) |
| C4 | 0.0340 (15) | 0.0303 (15) | 0.0423 (18) | 0.0009 (12) | 0.0043 (14) | 0.0008 (13) |
| C5 | 0.0396 (16) | 0.0292 (15) | 0.0431 (18) | −0.0018 (12) | 0.0027 (14) | −0.0050 (13) |
| C6 | 0.0436 (15) | 0.0404 (15) | 0.0361 (16) | −0.0034 (12) | −0.0025 (15) | −0.0047 (16) |
| C7 | 0.0420 (16) | 0.0339 (15) | 0.0442 (19) | 0.0049 (12) | −0.0109 (14) | 0.0035 (13) |
| C8 | 0.0432 (18) | 0.0398 (18) | 0.049 (2) | −0.0031 (14) | 0.0014 (15) | 0.0115 (15) |
| C9 | 0.0381 (15) | 0.0490 (18) | 0.0374 (17) | 0.0071 (13) | 0.0047 (14) | 0.0066 (15) |
| C10 | 0.0391 (16) | 0.0332 (15) | 0.0431 (19) | 0.0098 (13) | −0.0050 (14) | 0.0022 (14) |
| C11 | 0.0466 (18) | 0.0396 (17) | 0.0414 (18) | −0.0044 (13) | 0.0014 (15) | 0.0039 (14) |
| C12 | 0.0454 (15) | 0.0447 (16) | 0.0353 (17) | 0.0023 (12) | 0.0015 (16) | 0.0020 (15) |
| C13 | 0.0436 (17) | 0.0351 (16) | 0.0425 (18) | 0.0078 (13) | −0.0116 (14) | −0.0011 (14) |
| C14 | 0.0453 (17) | 0.0351 (16) | 0.049 (2) | 0.0006 (13) | 0.0002 (15) | 0.0065 (15) |
| C15 | 0.0399 (15) | 0.0384 (15) | 0.0398 (18) | 0.0071 (12) | 0.0025 (14) | 0.0014 (15) |
| C16 | 0.0365 (16) | 0.0359 (16) | 0.0411 (18) | 0.0043 (12) | −0.0040 (14) | 0.0018 (14) |
| C17 | 0.0402 (18) | 0.049 (2) | 0.046 (2) | −0.0048 (14) | 0.0010 (15) | 0.0024 (16) |
| C18 | 0.0414 (15) | 0.0526 (18) | 0.0368 (18) | 0.0068 (13) | −0.0003 (14) | −0.0012 (16) |
| C19 | 0.0378 (16) | 0.0340 (15) | 0.0458 (19) | 0.0053 (13) | −0.0046 (14) | −0.0050 (14) |
| C20 | 0.058 (2) | 0.0341 (16) | 0.046 (2) | 0.0079 (14) | −0.0123 (16) | −0.0108 (15) |
| C21 | 0.0536 (17) | 0.0387 (15) | 0.0413 (17) | 0.0072 (13) | −0.0118 (17) | −0.0070 (16) |
| C22 | 0.0383 (16) | 0.0288 (14) | 0.0464 (18) | 0.0001 (12) | 0.0010 (14) | −0.0018 (13) |
| C23 | 0.0432 (17) | 0.0324 (16) | 0.049 (2) | −0.0024 (13) | 0.0013 (15) | −0.0109 (14) |
| C24 | 0.0420 (16) | 0.0383 (16) | 0.0428 (18) | −0.0012 (12) | −0.0057 (15) | −0.0081 (14) |

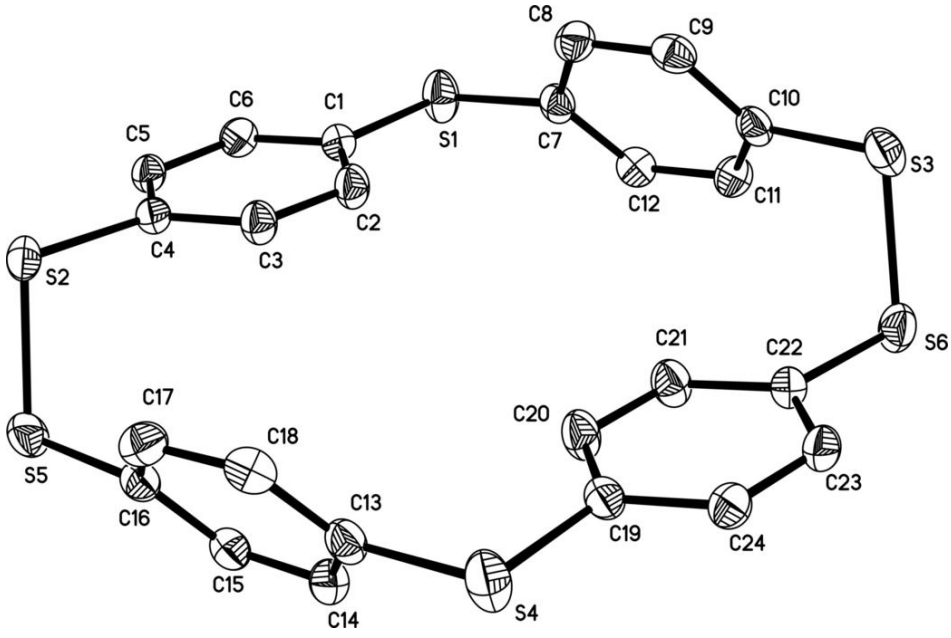
*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| S1—C7 | 1.773 (3) | C9—H9 | 0.9300 |
| S1—C1 | 1.777 (3) | C10—C11 | 1.379 (5) |
| S2—C4 | 1.776 (3) | C11—C12 | 1.376 (4) |
| S2—S5 | 2.0600 (11) | C11—H11 | 0.9300 |
| S3—C10 | 1.781 (3) | C12—H12 | 0.9300 |
| S3—S6 | 2.0589 (12) | C13—C14 | 1.376 (5) |
| S4—C19 | 1.768 (3) | C13—C18 | 1.393 (4) |
| S4—C13 | 1.775 (3) | C14—C15 | 1.387 (4) |
| S5—C16 | 1.789 (3) | C14—H14 | 0.9300 |
| S6—C22 | 1.780 (3) | C15—C16 | 1.386 (4) |
| C1—C2 | 1.383 (4) | C15—H15 | 0.9300 |
| C1—C6 | 1.392 (4) | C16—C17 | 1.376 (5) |

| | | | |
|---|---|---|---|
| C2—C3 | 1.383 (4) | C17—C18 | 1.387 (4) |
| C2—H2 | 0.9300 | C17—H17 | 0.9300 |
| C3—C4 | 1.392 (4) | C18—H18 | 0.9300 |
| C3—H3 | 0.9300 | C19—C20 | 1.382 (4) |
| C4—C5 | 1.384 (4) | C19—C24 | 1.390 (4) |
| C5—C6 | 1.381 (4) | C20—C21 | 1.386 (4) |
| C5—H5 | 0.9300 | C20—H20 | 0.9300 |
| C6—H6 | 0.9300 | C21—C22 | 1.388 (4) |
| C7—C12 | 1.383 (4) | C21—H21 | 0.9300 |
| C7—C8 | 1.389 (5) | C22—C23 | 1.385 (5) |
| C8—C9 | 1.376 (5) | C23—C24 | 1.380 (4) |
| C8—H8 | 0.9300 | C23—H23 | 0.9300 |
| C9—C10 | 1.390 (4) | C24—H24 | 0.9300 |
| C7—S1—C1 | 103.91 (14) | C11—C12—C7 | 120.4 (3) |
| C4—S2—S5 | 103.48 (10) | C11—C12—H12 | 119.8 |
| C10—S3—S6 | 101.69 (11) | C7—C12—H12 | 119.8 |
| C19—S4—C13 | 104.44 (15) | C14—C13—C18 | 119.9 (3) |
| C16—S5—S2 | 101.66 (10) | C14—C13—S4 | 121.6 (3) |
| C22—S6—S3 | 103.33 (11) | C18—C13—S4 | 118.5 (3) |
| C2—C1—C6 | 119.4 (3) | C13—C14—C15 | 120.0 (3) |
| C2—C1—S1 | 124.6 (2) | C13—C14—H14 | 120.0 |
| C6—C1—S1 | 116.0 (2) | C15—C14—H14 | 120.0 |
| C3—C2—C1 | 120.6 (3) | C16—C15—C14 | 120.1 (3) |
| C3—C2—H2 | 119.7 | C16—C15—H15 | 119.9 |
| C1—C2—H2 | 119.7 | C14—C15—H15 | 119.9 |
| C2—C3—C4 | 120.0 (3) | C17—C16—C15 | 119.8 (3) |
| C2—C3—H3 | 120.0 | C17—C16—S5 | 121.6 (2) |
| C4—C3—H3 | 120.0 | C15—C16—S5 | 118.5 (3) |
| C5—C4—C3 | 119.3 (3) | C16—C17—C18 | 120.3 (3) |
| C5—C4—S2 | 120.8 (2) | C16—C17—H17 | 119.9 |
| C3—C4—S2 | 119.8 (2) | C18—C17—H17 | 119.9 |
| C6—C5—C4 | 120.6 (3) | C17—C18—C13 | 119.7 (3) |
| C6—C5—H5 | 119.7 | C17—C18—H18 | 120.2 |
| C4—C5—H5 | 119.7 | C13—C18—H18 | 120.2 |
| C5—C6—C1 | 120.0 (3) | C20—C19—C24 | 118.9 (3) |
| C5—C6—H6 | 120.0 | C20—C19—S4 | 125.8 (2) |
| C1—C6—H6 | 120.0 | C24—C19—S4 | 115.3 (2) |
| C12—C7—C8 | 119.4 (3) | C19—C20—C21 | 120.5 (3) |
| C12—C7—S1 | 118.6 (3) | C19—C20—H20 | 119.7 |
| C8—C7—S1 | 122.0 (2) | C21—C20—H20 | 119.7 |
| C9—C8—C7 | 120.0 (3) | C20—C21—C22 | 120.5 (3) |
| C9—C8—H8 | 120.0 | C20—C21—H21 | 119.8 |
| C7—C8—H8 | 120.0 | C22—C21—H21 | 119.8 |
| C8—C9—C10 | 120.0 (3) | C23—C22—C21 | 118.9 (3) |
| C8—C9—H9 | 120.0 | C23—C22—S6 | 120.4 (2) |
| C10—C9—H9 | 120.0 | C21—C22—S6 | 120.6 (2) |
| C11—C10—C9 | 119.6 (3) | C24—C23—C22 | 120.6 (3) |
| C11—C10—S3 | 122.1 (2) | C24—C23—H23 | 119.7 |
| C9—C10—S3 | 118.3 (2) | C22—C23—H23 | 119.7 |

| | | | |
|---|---|---|---|
| C12—C11—C10 | 120.1 (3) | C23—C24—C19 | 120.6 (3) |
| C12—C11—H11 | 119.9 | C23—C24—H24 | 119.7 |
| C10—C11—H11 | 119.9 | C19—C24—H24 | 119.7 |
| C4—S2—S5—C16 | 73.11 (15) | S1—C7—C12—C11 | 180.0 (2) |
| C10—S3—S6—C22 | −73.89 (15) | C19—S4—C13—C14 | 67.7 (3) |
| C7—S1—C1—C2 | −5.4 (3) | C19—S4—C13—C18 | −115.1 (3) |
| C7—S1—C1—C6 | 175.8 (2) | C18—C13—C14—C15 | 4.6 (5) |
| C6—C1—C2—C3 | −2.9 (5) | S4—C13—C14—C15 | −178.2 (2) |
| S1—C1—C2—C3 | 178.3 (3) | C13—C14—C15—C16 | −3.2 (4) |
| C1—C2—C3—C4 | 2.7 (5) | C14—C15—C16—C17 | −1.6 (4) |
| C2—C3—C4—C5 | −0.3 (4) | C14—C15—C16—S5 | 175.0 (2) |
| C2—C3—C4—S2 | −177.5 (2) | S2—S5—C16—C17 | 47.7 (3) |
| S5—S2—C4—C5 | 103.3 (2) | S2—S5—C16—C15 | −128.9 (2) |
| S5—S2—C4—C3 | −79.6 (2) | C15—C16—C17—C18 | 5.0 (5) |
| C3—C4—C5—C6 | −1.8 (4) | S5—C16—C17—C18 | −171.5 (2) |
| S2—C4—C5—C6 | 175.3 (2) | C16—C17—C18—C13 | −3.7 (5) |
| C4—C5—C6—C1 | 1.6 (4) | C14—C13—C18—C17 | −1.2 (5) |
| C2—C1—C6—C5 | 0.8 (4) | S4—C13—C18—C17 | −178.4 (2) |
| S1—C1—C6—C5 | 179.7 (2) | C13—S4—C19—C20 | −4.6 (3) |
| C1—S1—C7—C12 | 119.6 (2) | C13—S4—C19—C24 | 176.0 (2) |
| C1—S1—C7—C8 | −62.4 (3) | C24—C19—C20—C21 | 0.3 (5) |
| C12—C7—C8—C9 | −5.9 (5) | S4—C19—C20—C21 | −179.0 (3) |
| S1—C7—C8—C9 | 176.2 (2) | C19—C20—C21—C22 | −0.8 (5) |
| C7—C8—C9—C10 | 3.5 (5) | C20—C21—C22—C23 | 0.8 (5) |
| C8—C9—C10—C11 | 2.8 (4) | C20—C21—C22—S6 | 177.9 (3) |
| C8—C9—C10—S3 | −174.6 (2) | S3—S6—C22—C23 | −104.9 (2) |
| S6—S3—C10—C11 | −43.3 (3) | S3—S6—C22—C21 | 78.0 (3) |
| S6—S3—C10—C9 | 134.0 (2) | C21—C22—C23—C24 | −0.4 (5) |
| C9—C10—C11—C12 | −6.7 (5) | S6—C22—C23—C24 | −177.5 (2) |
| S3—C10—C11—C12 | 170.6 (2) | C22—C23—C24—C19 | −0.1 (5) |
| C10—C11—C12—C7 | 4.3 (5) | C20—C19—C24—C23 | 0.1 (5) |
| C8—C7—C12—C11 | 2.0 (5) | S4—C19—C24—C23 | 179.5 (2) |

**Fig. 1**


C8
C9
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C1
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C14