Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 2,5-Bis(2-naphthylmethylsulfanyl)-1-thia-3,4-diazacyclopenta-2,5-diene

**Fiona N.-F. How,[a]*‡ David J. Watkin,[b] Karen A. Crouse[a] and M. Ibrahim M. Tahir[a]**

[a]Department of Chemistry, Universiti Putra Malaysia, 43400 UPM, Selangor, Malaysia, and [b]Chemical Crystallography, Chemistry Research Laboratory, 12 Mansfield Road, Oxford OX1 3TA, England
Correspondence e-mail: howfiona@gmail.com

Received 11 May 2007; accepted 16 May 2007

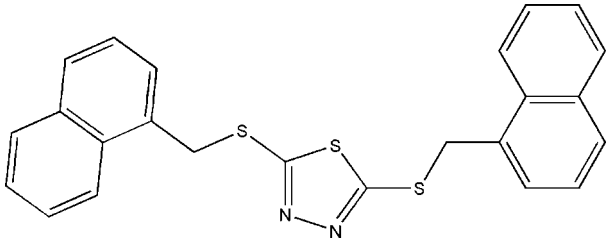
Key indicators: single-crystal X-ray study; $T$ = 150 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.034; $wR$ factor = 0.072; data-to-parameter ratio = 18.1.

The title molecule, $C_{24}H_{18}N_2S_3$, consists of three essentially planar fragments *viz.* two methylnaphthalene groups and a five-membered thiadiazole ring. The dihedral angles between the two methylnaphthalene groups and the central 1-thia-3,4-diazacyclopenta-2,5-diene group are 78.9 (1) and 68.8 (1)°. In the crystal structure, $\pi$-$\pi$ stacking interactions exist between pairs of symmetry-related naphthalene fragments with an interplanar separation of 3.35 Å. All bond lengths and angles are comparable with previous reports except that both C—S bond lengths are slightly longer than normal. In addition, the C—S—C and S—C—C bond angles appear to be smaller than normal and this could be due to the steric hindrance of the methylnaphthalene fragments.

## Related literature

Similar compounds have been discovered unintentionally by crystallization of dithiocarbazate compounds (Tarafder, Azahari *et al.*, 2000; Tarafder, Saravanan *et al.*, 2000).

For related literature, see: Allen *et al.* (1987); Görbitz (1999); Shanmuga Sundara Raj *et al.* (2000).



## Experimental

### Crystal data

$C_{24}H_{18}N_2S_3$
$M_r$ = 430.62
Monoclinic, $P2_1/a$
$a$ = 8.2095 (1) Å
$b$ = 12.9738 (2) Å
$c$ = 18.8054 (3) Å
$\beta$ = 93.2975 (7)°
$V$ = 1999.62 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.39 mm$^{-1}$
$T$ = 150 K
0.62 × 0.60 × 0.45 mm

### Data collection

Bruker-Nonius KappaCCD diffractometer
Absorption correction: multi-scan *DENZO/SCALEPACK* (Otwinowski & Minor, 1997)
$T_{min}$ = 0.56, $T_{max}$ = 0.84
23179 measured reflections
4734 independent reflections
4734 reflections with $I > -3\sigma(I)$
$R_{int}$ = 0.013

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.072
$S$ = 0.98
4734 reflections
262 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.26 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| S6—C7 | 1.8360 (13) | S18—C19 | 1.8339 (13) |
| S6—C7—C8 | 106.47 (8) | C1—S18—C19 | 99.93 (6) |

Data collection: *COLLECT* (Nonius, 2001); cell refinement: *DENZO/SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO/SCALEPACK*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *CRYSTALS*.

FNHF gratefully acknowledges MOSTI, Malaysia for an attachment grant under an NSF scholarship and the Chemical Crystallography Laboratory, Oxford University for instrumental facilities.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2391).

## References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Altomare, A., Cascarano, G., Giacovazzo, G., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, K. & Watkin, D. J. (2003). *J. Appl. Cryst.* **36**, 1487.
Görbitz, C. H. (1999). *Acta Cryst.* B**55**, 1090–1098.
Nonius (2001). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. **276**, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Shanmuga Sundara Raj, S., Yamin, B. M., Yussof, Y. A., Tarafder, M. T. H., Fun, H.-K. & Grouse, K. A. (2000). *Acta Cryst.* C**56**, 1236–1237.
Tarafder, M. T. H., Azahari, K., Crouse, K. A., Yamin, B. M., Sundara Raj, S. S., Ibrahim, A. R. & Fun, H.-K. (2000). *Z. Kristallogr. New Cryst. Struct.* **215**, 487–488.
Tarafder, M. T. H., Saravanan, N., Yamin, B. M., Sundara Raj, S. S., Ibrahim, A. R. & Fun, H.-K. (2000). *Z. Kristallogr. New Cryst. Struct.* **215**, 485–486.
Watkin, D. J., Prout, C. K. & Pearce, L. J. (1996). *CAMERON*. Chemical Crystallography Laboratory, Oxford, England.

‡ Current address: Chemical Crystallography, Chemistry Research Laboratory, 12 Mansfield Road, Oxford OX1 3TA, England.

 © 2007 International Union of Crystallography 

# supplementary materials

*Acta Cryst.* (2007). E**63**, o2913 [ **doi:10.1107/S1600536807024257** ]

## 2,5-Bis(2-naphthylmethylsulfanyl)-1-thia-3,4-diazacyclopenta-2,5-diene

**F. N.-F. How, D. J. Watkin, K. A. Crouse and M. I. M. Tahir**

### Comment

Crystallization of S-substituted dithiocarbazate or its derivatives may sometimes lead to unexpected compounds (Tarafder, Azahari *et al.*, 2000; Tarafder, Saravanan *et al.*, 2000]. These unexpected products are usually cyclized with the formation of a 5-membered thiazole-like ring. This could be due to either that solvent used for crystallization interacts with the dithiocarbzate compound or the compounds are simply unstable and tend to cyclize in solution. The title compound (see Fig. 1 for the molecular structure) was obtained unintensionally upon crystallization.

The bond length of N4—N5 [1.3929 (14) Å] is comparable to another similar compound derived from *S*-benzyldithiocarbazate (1.391 (3) Å; Tarafder, Saravanan *et al.*, 2000). The bond length of N5—C1[1.2981 (16) Å] and N4—C3[1.3013 (16) Å] are characteristic of a normal C=N bond (Allen *et al.*, 1987). Bond distances of C19—S18 [1.8339 (13) Å] and S6—C7 [1.8360 (13) Å] are slightly longer than previous literature values [1.816 (2)Å and 1.813 (3) Å; Tarafder, Saravanan *et al.*, 2000].

The bond angles of the central 5-membered ring are comparable to the previous literature values (Tarafder, Saravanan *et al.*, 2000). The smaller angles of C1—S18—C19 [99.93 (6)°] and S6—C7—C8 [106.47 (8)°] compared to literature values [101.04 (10)° and 109.31 (18)°; Tarafder, Saravanan *et al.*, 2000) may be due to steric hindrance of the methyl naphthalene rings.

A TLS analysis of the anisotropic atomic displacement parameters for the naphthalene fragment C19 to C29 show that it is undergoing substantial libration about the bond S18—C19 (mean square displacement 11.7 $Å^2$).

Molecules of the title compound are packed in diagonal layers along the *b* axis [Fig. 2]. Atom S18 overlaps a 5 membered thiazole-liked ring with a distance of 3.28 Å, leading to a π-π stacking interaction between S18 with the 5-membered ring situated in the middle of the two symmetry related methyl naphthalene fragments of an adjacent molecule [Fig. 3].

The naphthalene fragments at each end of the molecule are parallel to and overlap with the corresponding napthalene fragments in symmetry realted molecules, with an interplanar separation of 3.35Å [Fig. 4 and Fig. 5].

### Experimental

The peparative procedure is modified from that previously reported for S-substituted dithiocarbazates (Shanmuga Sundara Raj *et al.*, 2000), except substitution of benzyl chloride with 1-(chloromethyl) naphthalene (29.9 ml, 0.2 mol). The product expected to form was *S*-napthalen-2-ylmethyldithiocarbazate. Light pinkish crystals were obtained in acetonitrile solution. It was expected that the compound had cyclized in solution forming the title compound.

### Refinement

The relatively large ratio of minimum to maximum corrections applied in the multiscan process (1:1.51) reflect changes in the illuminated volume of the crystal, which were kept to a minimum, and were taken into account (Görbitz, 1999) by the inter-frame scaling (*DENZO*/*SCALEPACK*, Otwinowski & Minor, 1997).

The H atoms were all located in a difference map, but those attached to carbon atoms were repositioned geometrically. The H atoms were initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C—H in the range 0.93–0.98 Å) and $U_{iso}$(H) (in the range 1.2–1.5 times $U_{eq}$ of the parent atom), after which the positions were refined with riding constraints.

### Figures

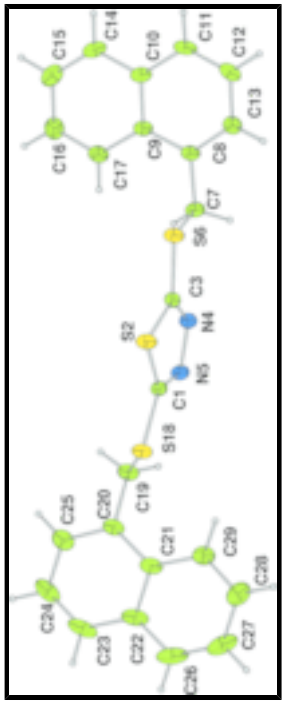



Fig. 1. The molecular structure of title compound with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitary radius.

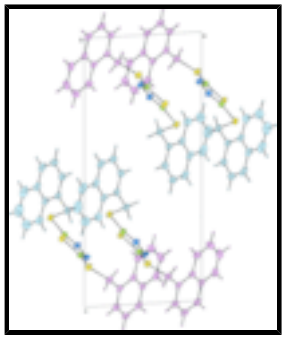


Fig. 2. The packing of the molecules viewed along the *b* axis.

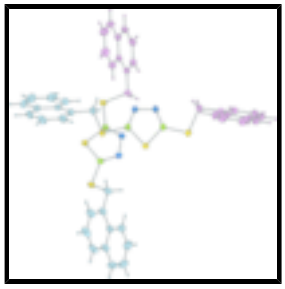


Fig. 3. The π-π interaction between atom S18 and a symmetry related 5 membered ring.

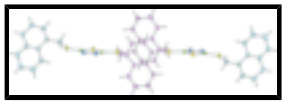


Fig. 4. The π-π interaction between a C8—C17 ring and a symmetry related C8—C17 ring.

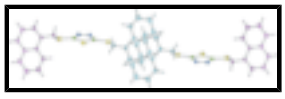


Fig. 5. The π-π interaction between a C20—C29 ring with a symmetry related C20—C29 ring.

**2,5-Bis(2-naphthylmethylsulfanyl)-1-thia-3,4-diazacyclopenta-2,5-diene**

*Crystal data*

| | |
|---|---|
| $C_{24}H_{18}N_2S_3$ | $F_{000}$ = 896 |
| $M_r$ = 430.62 | $D_x$ = 1.430 Mg m$^{-3}$ |
| Monoclinic, $P2_1/a$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| $a$ = 8.20950 (10) Å | Cell parameters from 4829 reflections |
| $b$ = 12.9738 (2) Å | θ = 5–28º |
| $c$ = 18.8054 (3) Å | μ = 0.39 mm$^{-1}$ |
| β = 93.2975 (7)º | $T$ = 150 K |
| $V$ = 1999.62 (5) Å$^3$ | Block, pink |
| $Z$ = 4 | 0.62 × 0.60 × 0.45 mm |

*Data collection*

| | |
|---|---|
| Bruker-Nonius KappaCCD diffractometer | 4734 reflections with $I > -3.0\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.013 |
| $T$ = 150 K | $\theta_{max}$ = 27.9º |
| ω scans | $\theta_{min}$ = 5.1º |
| Absorption correction: multi-scan DENZO/SCALEPACK (Otwinowski & Minor, 1997) | $h$ = −10→10 |
| $T_{min}$ = 0.56, $T_{max}$ = 0.84 | $k$ = −17→12 |
| 23179 measured reflections | $l$ = −24→24 |
| 4734 independent reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.034$ | Method = Modified Sheldrick $w = 1/[\sigma^2(F^2) + (0.02P)^2 + 1.34P]$, where $P = (\max(F_o^2,0) + 2F_c^2)/3$ |
| $wR(F^2) = 0.072$ | $(\Delta/\sigma)_{max} = 0.001$ |
| $S = 0.98$ | $\Delta\rho_{max} = 0.37$ e Å$^{-3}$ |
| 4734 reflections | $\Delta\rho_{min} = -0.26$ e Å$^{-3}$ |
| 262 parameters | Extinction correction: None |
| Primary atom site location: structure-invariant direct methods | |

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.66751 (15) | 0.75552 (9) | 0.27352 (6) | 0.0190 |
| S2 | 0.68740 (4) | 0.88721 (2) | 0.261136 (17) | 0.0231 |
| C3 | 0.53408 (15) | 0.87515 (10) | 0.19411 (6) | 0.0197 |
| N4 | 0.47998 (13) | 0.78163 (8) | 0.18438 (6) | 0.0219 |
| N5 | 0.55794 (13) | 0.71174 (8) | 0.23113 (6) | 0.0216 |
| S6 | 0.46202 (4) | 0.98431 (2) | 0.148072 (17) | 0.0235 |
| C7 | 0.28616 (16) | 0.93037 (10) | 0.09599 (7) | 0.0236 |
| C8 | 0.19611 (15) | 1.02049 (9) | 0.06172 (7) | 0.0208 |
| C9 | 0.08118 (15) | 1.07858 (9) | 0.09984 (7) | 0.0201 |
| C10 | 0.00184 (15) | 1.16412 (9) | 0.06500 (7) | 0.0219 |
| C11 | 0.03773 (16) | 1.18887 (10) | −0.00596 (7) | 0.0254 |
| C12 | 0.14673 (17) | 1.13191 (11) | −0.04135 (7) | 0.0268 |
| C13 | 0.22634 (16) | 1.04754 (10) | −0.00684 (7) | 0.0246 |
| C14 | −0.11338 (17) | 1.22204 (10) | 0.10167 (8) | 0.0287 |
| C15 | −0.15069 (18) | 1.19678 (12) | 0.16931 (9) | 0.0341 |
| C16 | −0.07261 (19) | 1.11184 (12) | 0.20385 (8) | 0.0323 |
| C17 | 0.03962 (17) | 1.05441 (10) | 0.17013 (7) | 0.0260 |
| S18 | 0.78546 (4) | 0.69146 (2) | 0.340331 (17) | 0.0223 |
| C19 | 0.64192 (16) | 0.59002 (11) | 0.36317 (7) | 0.0251 |
| C20 | 0.72179 (15) | 0.52241 (10) | 0.42019 (7) | 0.0236 |
| C21 | 0.83252 (16) | 0.44238 (10) | 0.40272 (7) | 0.0244 |
| C22 | 0.89975 (17) | 0.37824 (11) | 0.45879 (8) | 0.0305 |
| C23 | 0.85668 (19) | 0.39678 (13) | 0.52956 (8) | 0.0373 |
| C24 | 0.75468 (19) | 0.47467 (14) | 0.54493 (8) | 0.0376 |
| C25 | 0.68700 (17) | 0.53818 (12) | 0.48984 (8) | 0.0304 |
| C26 | 1.0115 (2) | 0.29975 (12) | 0.44187 (11) | 0.0423 |
| C27 | 1.0555 (2) | 0.28529 (13) | 0.37410 (12) | 0.0480 |
| C28 | 0.9898 (2) | 0.34872 (12) | 0.31864 (10) | 0.0405 |
| C29 | 0.88061 (18) | 0.42487 (11) | 0.33260 (8) | 0.0294 |
| H71 | 0.2205 | 0.8932 | 0.1284 | 0.0285* |
| H72 | 0.3267 | 0.8841 | 0.0610 | 0.0293* |
| H111 | −0.0173 | 1.2450 | −0.0283 | 0.0310* |
| H121 | 0.1690 | 1.1490 | −0.0883 | 0.0323* |
| H131 | 0.2991 | 1.0088 | −0.0319 | 0.0288* |
| H141 | −0.1678 | 1.2785 | 0.0776 | 0.0339* |

| | | | | |
|---|---|---|---|---|
| H151 | −0.2304 | 1.2365 | 0.1927 | 0.0414* |
| H161 | −0.0988 | 1.0958 | 0.2507 | 0.0388* |
| H171 | 0.0887 | 0.9967 | 0.1941 | 0.0308* |
| H191 | 0.5451 | 0.6233 | 0.3802 | 0.0303* |
| H192 | 0.6112 | 0.5516 | 0.3200 | 0.0304* |
| H231 | 0.9061 | 0.3540 | 0.5661 | 0.0446* |
| H241 | 0.7298 | 0.4877 | 0.5929 | 0.0460* |
| H251 | 0.6141 | 0.5924 | 0.5007 | 0.0368* |
| H261 | 1.0547 | 0.2582 | 0.4791 | 0.0508* |
| H271 | 1.1292 | 0.2343 | 0.3634 | 0.0573* |
| H281 | 1.0207 | 0.3378 | 0.2712 | 0.0485* |
| H291 | 0.8351 | 0.4674 | 0.2941 | 0.0348* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0188 (6) | 0.0181 (5) | 0.0200 (6) | 0.0025 (4) | 0.0010 (5) | 0.0018 (4) |
| S2 | 0.02330 (16) | 0.01779 (15) | 0.02724 (17) | −0.00106 (11) | −0.00687 (12) | 0.00231 (11) |
| C3 | 0.0196 (6) | 0.0220 (6) | 0.0175 (5) | 0.0032 (5) | 0.0000 (4) | 0.0007 (4) |
| N4 | 0.0255 (5) | 0.0193 (5) | 0.0205 (5) | 0.0034 (4) | −0.0035 (4) | −0.0006 (4) |
| N5 | 0.0232 (5) | 0.0178 (5) | 0.0233 (5) | 0.0028 (4) | −0.0030 (4) | 0.0005 (4) |
| S6 | 0.02495 (17) | 0.01913 (15) | 0.02580 (16) | 0.00140 (12) | −0.00453 (12) | 0.00427 (12) |
| C7 | 0.0264 (6) | 0.0184 (6) | 0.0253 (6) | 0.0035 (5) | −0.0057 (5) | −0.0002 (5) |
| C8 | 0.0221 (6) | 0.0165 (5) | 0.0230 (6) | −0.0011 (5) | −0.0057 (5) | 0.0009 (5) |
| C9 | 0.0203 (6) | 0.0157 (5) | 0.0237 (6) | −0.0021 (5) | −0.0041 (5) | 0.0015 (5) |
| C10 | 0.0184 (6) | 0.0167 (5) | 0.0299 (6) | −0.0026 (5) | −0.0055 (5) | 0.0026 (5) |
| C11 | 0.0251 (7) | 0.0191 (6) | 0.0308 (7) | −0.0035 (5) | −0.0095 (5) | 0.0075 (5) |
| C12 | 0.0304 (7) | 0.0272 (7) | 0.0220 (6) | −0.0069 (5) | −0.0056 (5) | 0.0063 (5) |
| C13 | 0.0262 (7) | 0.0235 (6) | 0.0235 (6) | −0.0016 (5) | −0.0024 (5) | −0.0006 (5) |
| C14 | 0.0223 (6) | 0.0210 (6) | 0.0422 (8) | 0.0030 (5) | −0.0040 (6) | 0.0021 (6) |
| C15 | 0.0284 (7) | 0.0299 (7) | 0.0447 (9) | 0.0030 (6) | 0.0070 (6) | −0.0028 (6) |
| C16 | 0.0356 (8) | 0.0314 (7) | 0.0307 (7) | −0.0021 (6) | 0.0084 (6) | 0.0015 (6) |
| C17 | 0.0306 (7) | 0.0207 (6) | 0.0263 (6) | −0.0003 (5) | −0.0012 (5) | 0.0039 (5) |
| S18 | 0.01965 (15) | 0.02174 (15) | 0.02509 (16) | 0.00028 (11) | −0.00367 (12) | 0.00625 (12) |
| C19 | 0.0203 (6) | 0.0272 (6) | 0.0275 (7) | −0.0015 (5) | −0.0013 (5) | 0.0076 (5) |
| C20 | 0.0193 (6) | 0.0244 (6) | 0.0265 (6) | −0.0049 (5) | −0.0026 (5) | 0.0078 (5) |
| C21 | 0.0209 (6) | 0.0213 (6) | 0.0301 (7) | −0.0058 (5) | −0.0052 (5) | 0.0067 (5) |
| C22 | 0.0245 (7) | 0.0255 (7) | 0.0402 (8) | −0.0082 (5) | −0.0099 (6) | 0.0130 (6) |
| C23 | 0.0303 (8) | 0.0433 (9) | 0.0367 (8) | −0.0142 (7) | −0.0125 (6) | 0.0226 (7) |
| C24 | 0.0316 (8) | 0.0547 (10) | 0.0259 (7) | −0.0142 (7) | −0.0028 (6) | 0.0130 (7) |
| C25 | 0.0243 (7) | 0.0377 (8) | 0.0291 (7) | −0.0058 (6) | 0.0004 (5) | 0.0066 (6) |
| C26 | 0.0357 (8) | 0.0253 (7) | 0.0640 (11) | −0.0010 (6) | −0.0131 (8) | 0.0152 (7) |
| C27 | 0.0406 (9) | 0.0253 (8) | 0.0768 (13) | 0.0082 (7) | −0.0075 (9) | −0.0022 (8) |
| C28 | 0.0398 (9) | 0.0309 (8) | 0.0507 (10) | 0.0020 (7) | 0.0015 (7) | −0.0079 (7) |
| C29 | 0.0301 (7) | 0.0241 (6) | 0.0335 (7) | −0.0026 (5) | −0.0029 (6) | 0.0021 (5) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—S2 | 1.7332 (13) | C16—C17 | 1.369 (2) |

| | | | |
|---|---|---|---|
| C1—N5 | 1.2981 (16) | C16—H161 | 0.942 |
| C1—S18 | 1.7512 (12) | C17—H171 | 0.952 |
| S2—C3 | 1.7364 (12) | S18—C19 | 1.8339 (13) |
| C3—N4 | 1.3013 (16) | C19—C20 | 1.5061 (17) |
| C3—S6 | 1.7453 (12) | C19—H191 | 0.974 |
| N4—N5 | 1.3929 (14) | C19—H192 | 0.973 |
| S6—C7 | 1.8360 (13) | C20—C21 | 1.4306 (19) |
| C7—C8 | 1.5080 (17) | C20—C25 | 1.372 (2) |
| C7—H71 | 0.966 | C21—C22 | 1.4290 (18) |
| C7—H72 | 0.964 | C21—C29 | 1.416 (2) |
| C8—C9 | 1.4317 (18) | C22—C23 | 1.417 (2) |
| C8—C13 | 1.3725 (18) | C22—C26 | 1.419 (2) |
| C9—C10 | 1.4269 (17) | C23—C24 | 1.354 (3) |
| C9—C17 | 1.4192 (18) | C23—H231 | 0.956 |
| C10—C11 | 1.4198 (19) | C24—C25 | 1.412 (2) |
| C10—C14 | 1.4178 (19) | C24—H241 | 0.952 |
| C11—C12 | 1.363 (2) | C25—H251 | 0.953 |
| C11—H111 | 0.942 | C26—C27 | 1.357 (3) |
| C12—C13 | 1.4133 (18) | C26—H261 | 0.937 |
| C12—H121 | 0.939 | C27—C28 | 1.411 (3) |
| C13—H131 | 0.929 | C27—H271 | 0.927 |
| C14—C15 | 1.365 (2) | C28—C29 | 1.370 (2) |
| C14—H141 | 0.958 | C28—H281 | 0.951 |
| C15—C16 | 1.414 (2) | C29—H291 | 0.968 |
| C15—H151 | 0.959 | | |
| S2—C1—N5 | 114.59 (9) | C17—C16—H161 | 120.6 |
| S2—C1—S18 | 120.78 (7) | C9—C17—C16 | 121.04 (12) |
| N5—C1—S18 | 124.61 (10) | C9—C17—H171 | 119.8 |
| C1—S2—C3 | 86.49 (6) | C16—C17—H171 | 119.2 |
| S2—C3—N4 | 114.42 (9) | C1—S18—C19 | 99.93 (6) |
| S2—C3—S6 | 119.86 (7) | S18—C19—C20 | 108.99 (9) |
| N4—C3—S6 | 125.70 (10) | S18—C19—H191 | 107.9 |
| C3—N4—N5 | 112.18 (10) | C20—C19—H191 | 110.7 |
| N4—N5—C1 | 112.32 (10) | S18—C19—H192 | 108.1 |
| C3—S6—C7 | 100.90 (6) | C20—C19—H192 | 112.1 |
| S6—C7—C8 | 106.47 (8) | H191—C19—H192 | 108.9 |
| S6—C7—H71 | 107.7 | C19—C20—C21 | 121.03 (12) |
| C8—C7—H71 | 112.3 | C19—C20—C25 | 119.13 (13) |
| S6—C7—H72 | 108.0 | C21—C20—C25 | 119.84 (12) |
| C8—C7—H72 | 111.8 | C20—C21—C22 | 118.47 (13) |
| H71—C7—H72 | 110.3 | C20—C21—C29 | 123.03 (12) |
| C7—C8—C9 | 121.01 (11) | C22—C21—C29 | 118.49 (13) |
| C7—C8—C13 | 119.27 (12) | C21—C22—C23 | 119.18 (14) |
| C9—C8—C13 | 119.71 (11) | C21—C22—C26 | 118.66 (15) |
| C8—C9—C10 | 118.43 (12) | C23—C22—C26 | 122.14 (14) |
| C8—C9—C17 | 123.42 (11) | C22—C23—C24 | 121.19 (13) |
| C10—C9—C17 | 118.14 (12) | C22—C23—H231 | 117.3 |
| C9—C10—C11 | 119.57 (12) | C24—C23—H231 | 121.4 |
| C9—C10—C14 | 119.25 (12) | C23—C24—C25 | 120.05 (15) |

| | | | |
|---|---|---|---|
| C11—C10—C14 | 121.17 (12) | C23—C24—H241 | 120.2 |
| C10—C11—C12 | 120.92 (12) | C25—C24—H241 | 119.7 |
| C10—C11—H111 | 118.3 | C24—C25—C20 | 121.24 (15) |
| C12—C11—H111 | 120.8 | C24—C25—H251 | 119.9 |
| C11—C12—C13 | 119.66 (12) | C20—C25—H251 | 118.9 |
| C11—C12—H121 | 120.0 | C22—C26—C27 | 121.34 (15) |
| C13—C12—H121 | 120.4 | C22—C26—H261 | 117.9 |
| C12—C13—C8 | 121.71 (13) | C27—C26—H261 | 120.8 |
| C12—C13—H131 | 118.7 | C26—C27—C28 | 120.16 (16) |
| C8—C13—H131 | 119.6 | C26—C27—H271 | 121.0 |
| C10—C14—C15 | 121.17 (13) | C28—C27—H271 | 118.8 |
| C10—C14—H141 | 118.8 | C27—C28—C29 | 120.37 (17) |
| C15—C14—H141 | 120.0 | C27—C28—H281 | 119.7 |
| C14—C15—C16 | 119.67 (14) | C29—C28—H281 | 119.9 |
| C14—C15—H151 | 119.6 | C21—C29—C28 | 120.98 (14) |
| C16—C15—H151 | 120.8 | C21—C29—H291 | 119.2 |
| C15—C16—C17 | 120.73 (14) | C28—C29—H291 | 119.8 |
| C15—C16—H161 | 118.7 | | |

**Fig. 1**

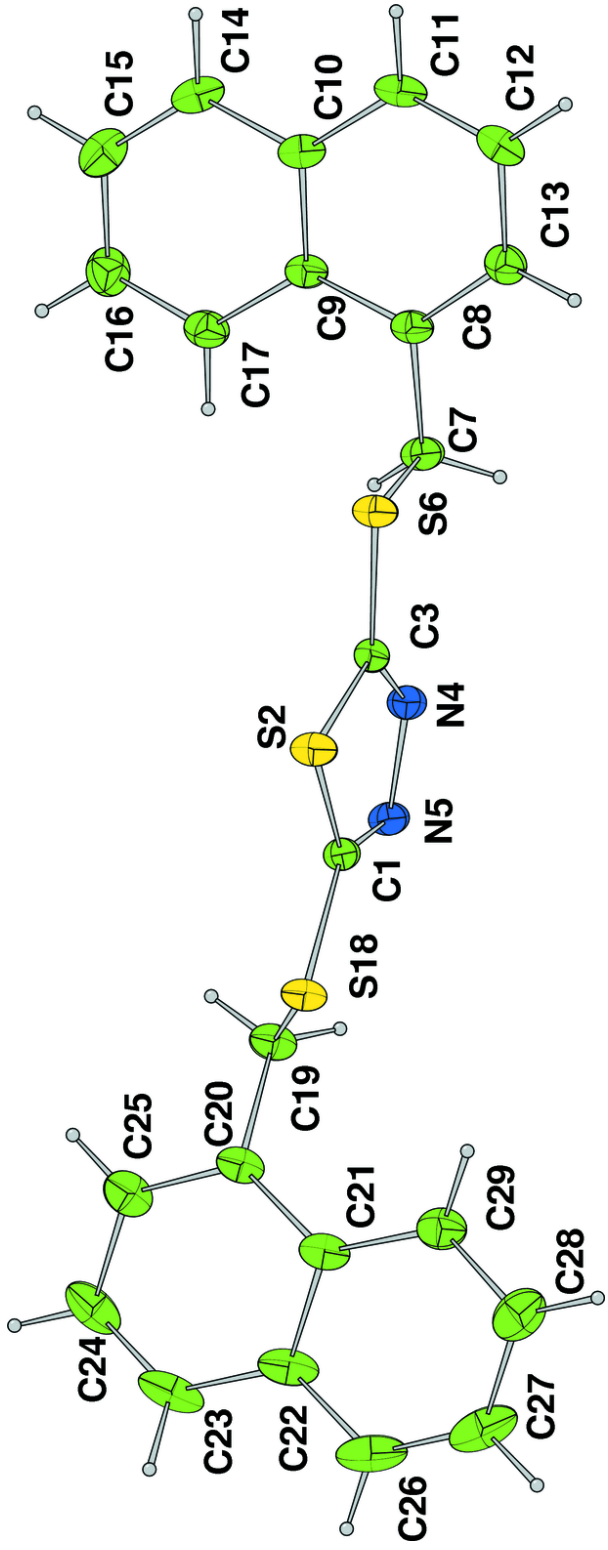

C15
C14
C10
C11
C12
C13
C16
C17
C9
C8
C7
S6
C3
N4
S2
N5
C1
S18
C19
C20
C25
C21
C29
C28
C24
C23
C22
C27
C26

**Fig. 2**

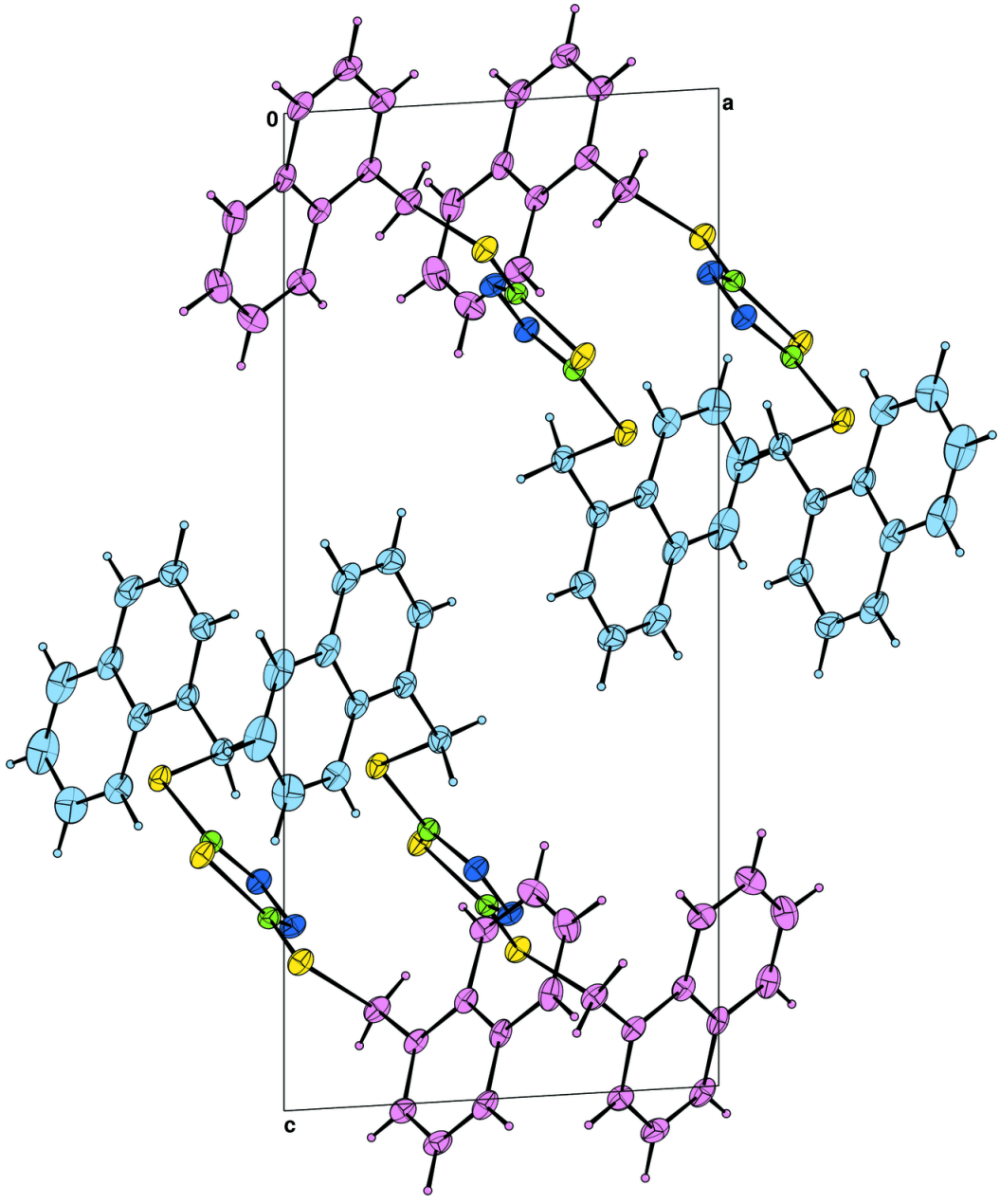


**Fig. 3**

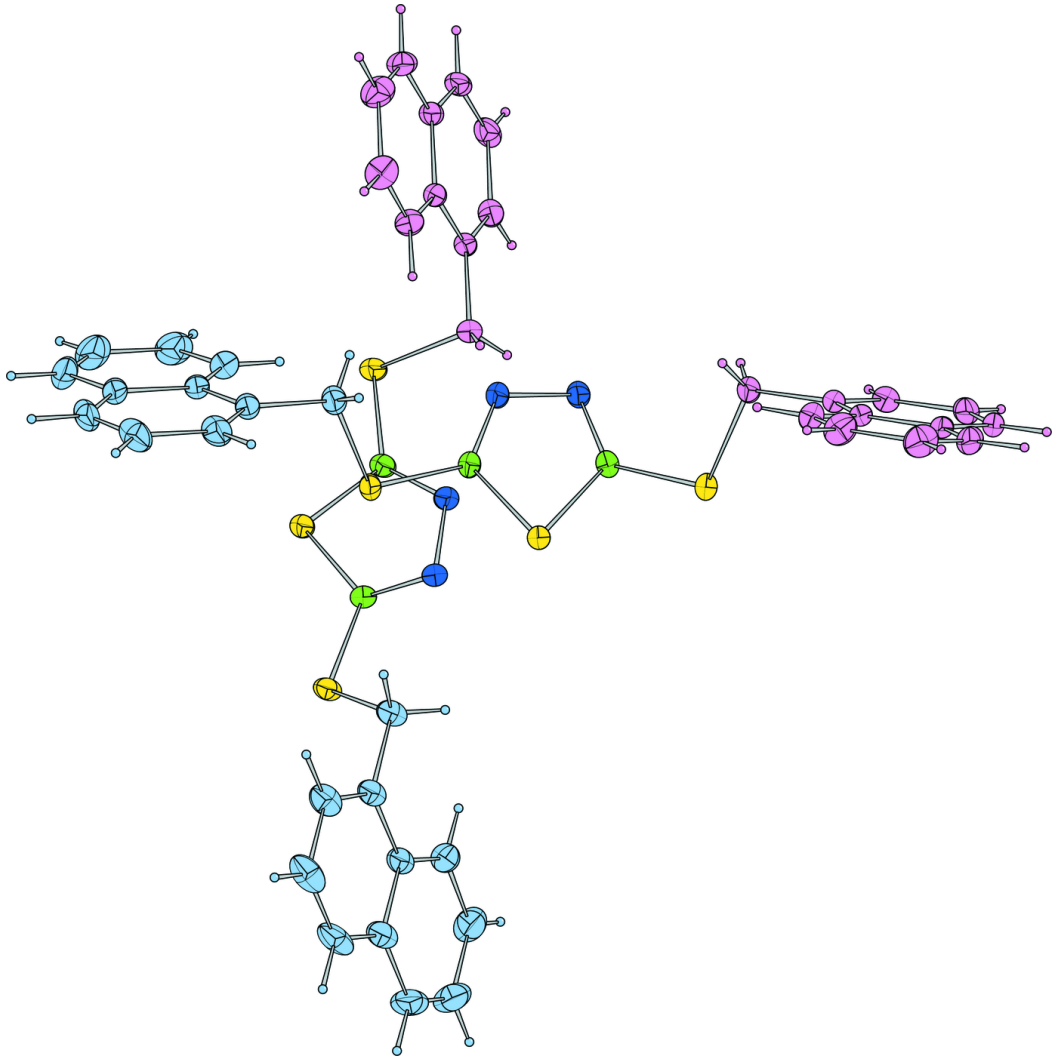


**Fig. 4**

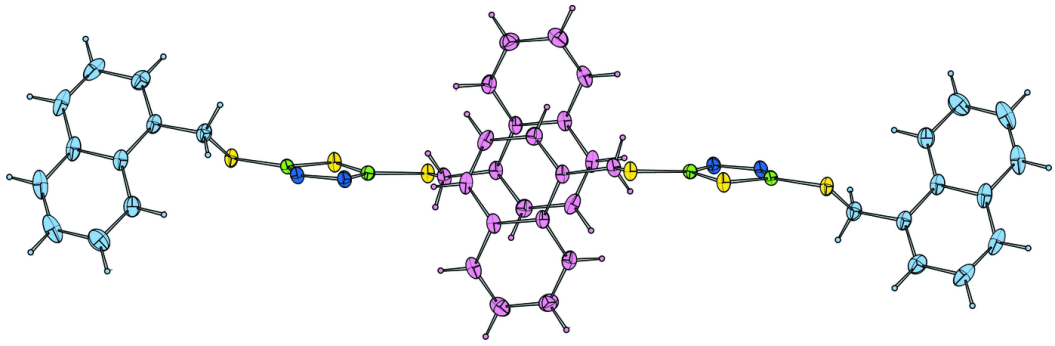


**Fig. 5**