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

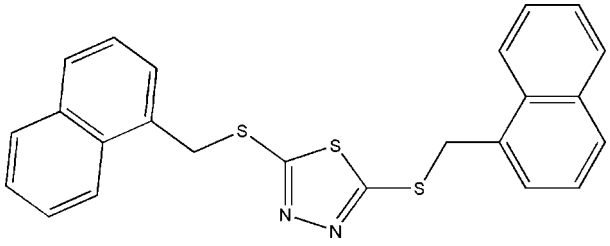
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.002 Å; R factor = 0.034; wR factor = 0.072; data-to-parameter ratio = 18.1.

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, π-π 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
β = 93.2975 (7)°
V = 1999.62 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 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.

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

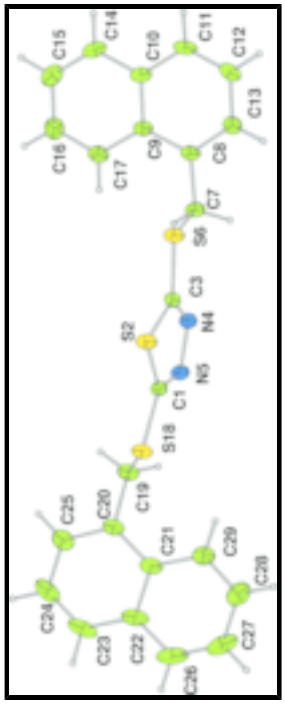


Fig. 1. The molecular structure of title compound with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitary radius.

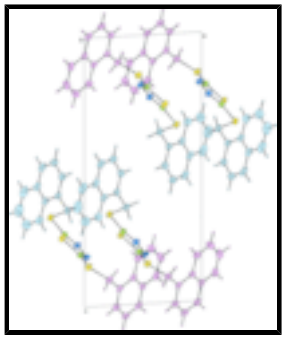


Fig. 2. The packing of the molecules viewed along the *b* axis.

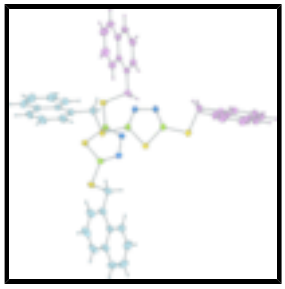


Fig. 3. The π-π interaction between atom S18 and a symmetry related 5 membered ring.

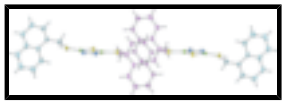


Fig. 4. The π-π interaction between a C8—C17 ring and a symmetry related C8—C17 ring.

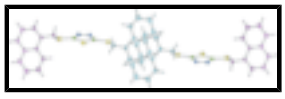


Fig. 5. The π-π interaction between a C20—C29 ring with a symmetry related C20—C29 ring.

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 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	θ_{max} = 27.9º
ω scans	θ_{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

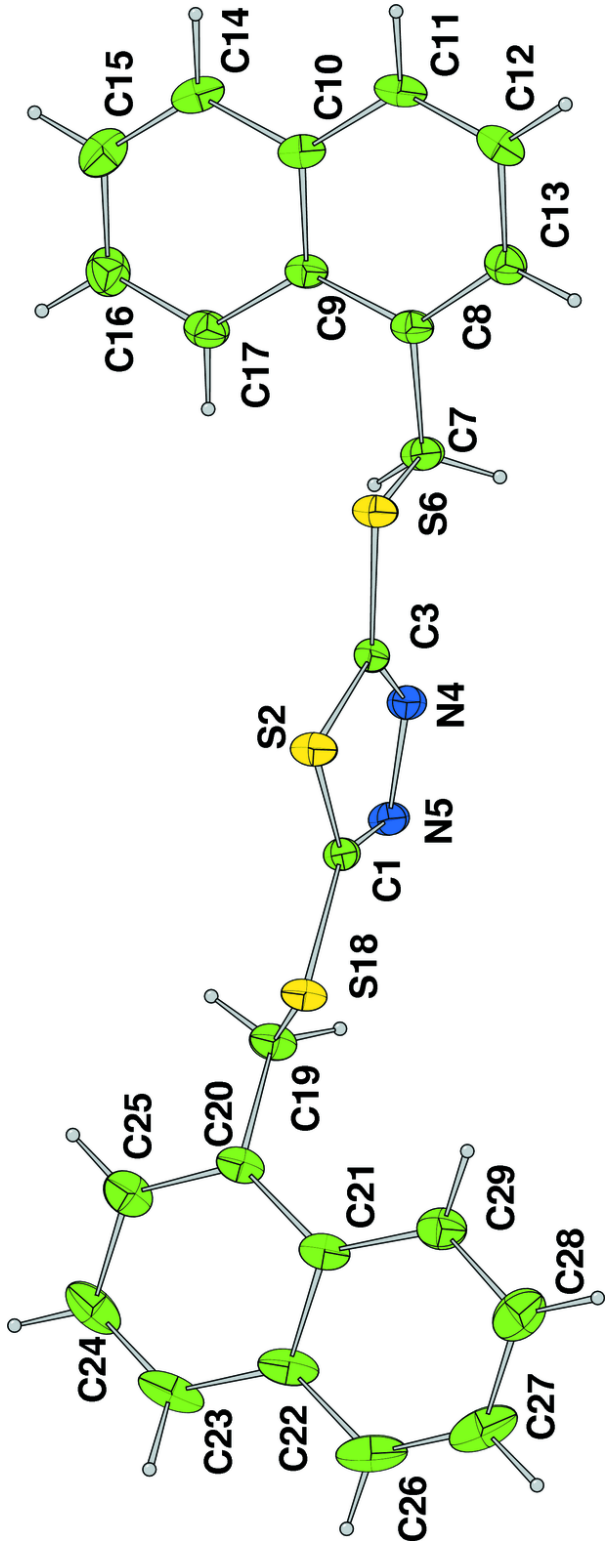

C15
C14
C10
C11
C12
C13
C16
C17
C9
C8
C7
S6
C3
N4
S2
N5
C1
S18
C19
C20
C25
C21
C29
C28
C24
C23
C22
C27
C26

Fig. 2

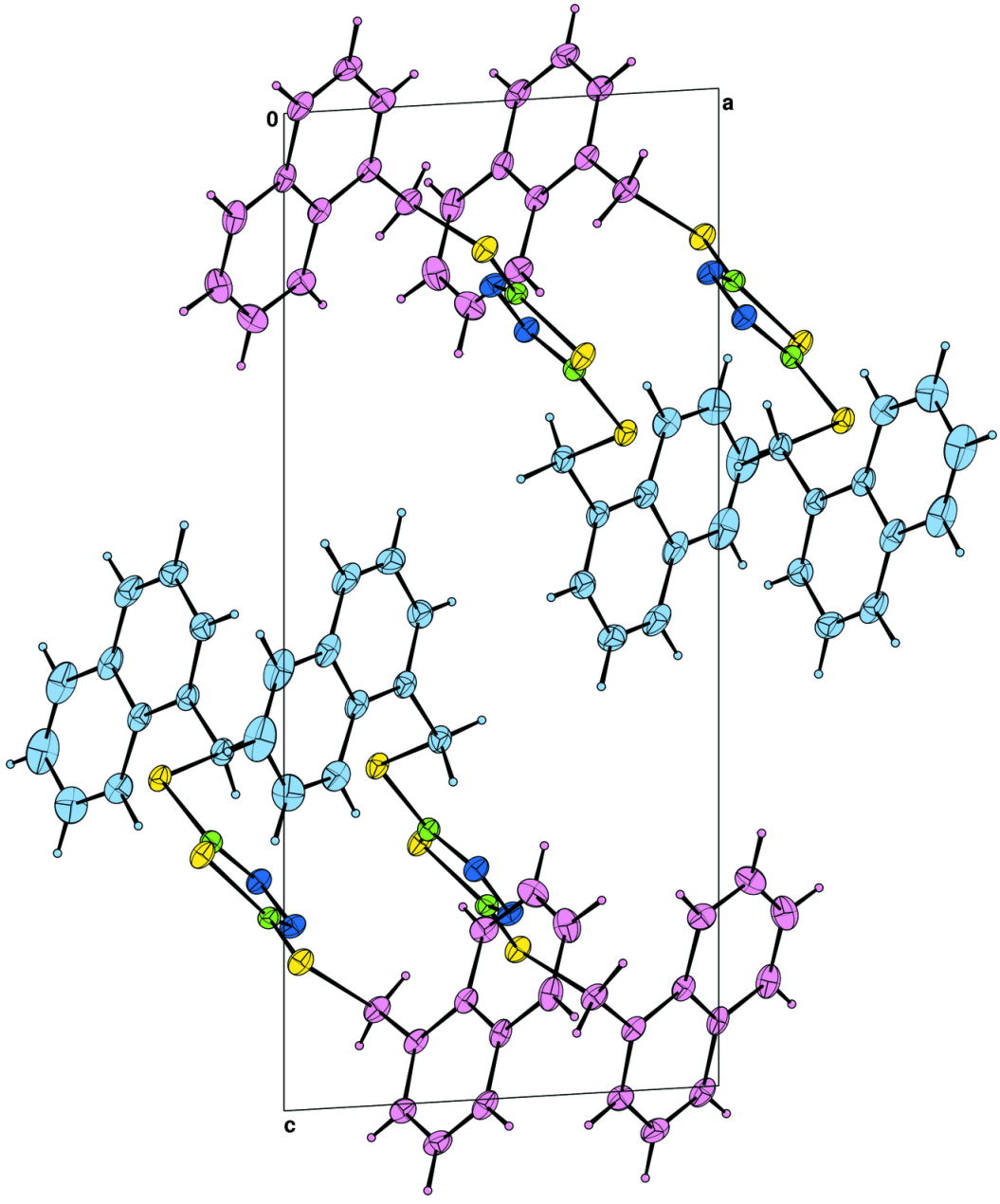


Fig. 3

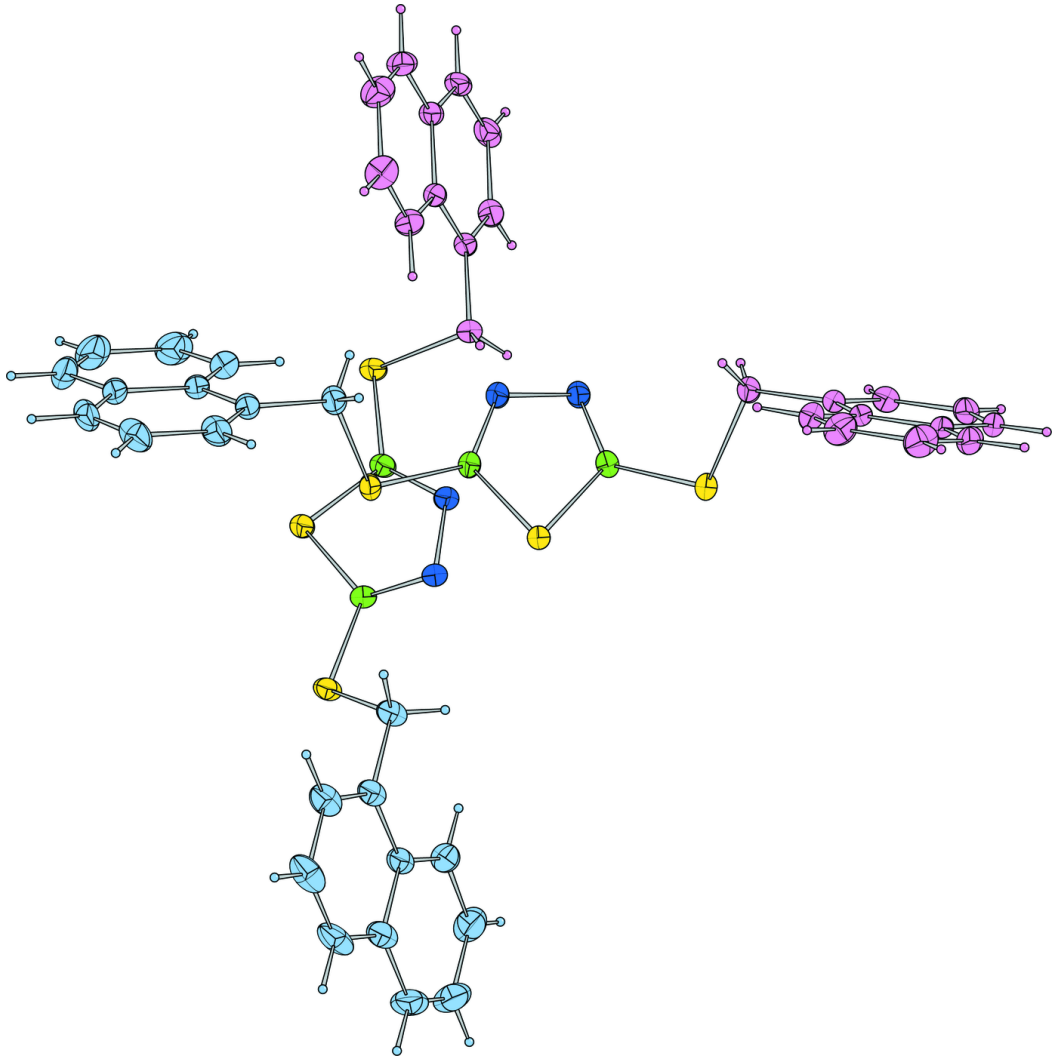


Fig. 4

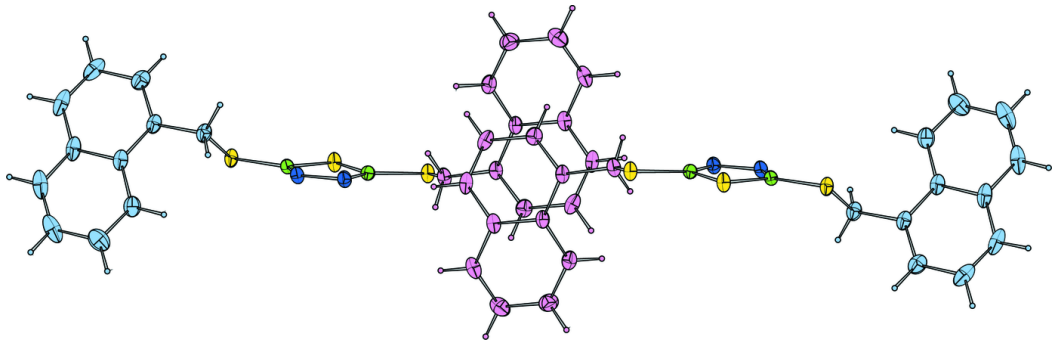


Fig. 5