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2-[3,5-Bis(5,6-dihydro-4*H*-1,3-thiazin-2-ylsulfanylmethyl)-2,4,6-trimethylbenzylsulfanyl]-5,6-dihydro-4*H*-1,3-thiazine

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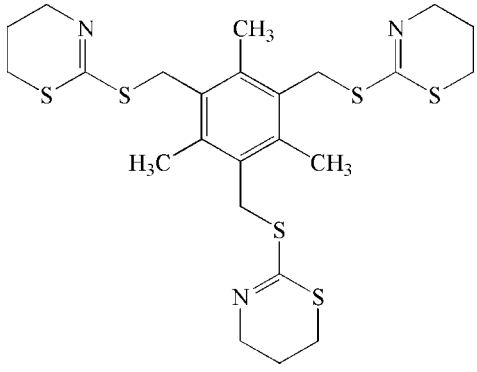
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.055; wR factor = 0.139; data-to-parameter ratio = 15.7.

The title compound, $C_{24}H_{33}N_3S_6$, contains three 1,3-thiazin-2-ylsulfanyl groups. Two are located on the same side of the planar benzene ring and the other is on the opposite side. The three C atoms in one of the heterocyclic rings are disordered over two sites in an approximately 0.54:0.46 ratio.

Related literature

For bond-length data, see: Allen *et al.* (1987). For related literature, see: Wang *et al.* (2004, 2005); Jacobson (1998).



Experimental

Crystal data

$C_{24}H_{33}N_3S_6$
M_r = 555.89
Monoclinic, $P2_1/c$
a = 17.146 (3) Å
b = 10.123 (2) Å
c = 17.408 (4) Å
β = 119.20 (3)°
V = 2637.6 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.58 mm^{-1}
T = 113 (2) K
0.20 × 0.18 × 0.02 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.900, T_{max} = 0.989
17102 measured reflections
5178 independent reflections
4350 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.139
S = 1.08
5178 reflections
329 parameters
7 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 1999); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); 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: BV2058).

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.
Bruker (1997). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Jacobson, R. (1998). REQAB. Private communication to the Rigaku Corporation, Tokyo, Japan.
Molecular Structure Corporation & Rigaku (1999). *CrystalClear*. Version 1.3.6. MSC, The Woodlands, Texas, USA, and Rigaku, Tokyo, Japan.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Wang, W., Liu, H.-M., Zheng, Y. & Zhang, W.-Q. (2004). *Acta Cryst.* E**60**, o1279–o1280.
Wang, W., Zhao, B., Zheng, P.-W. & Duan, X.-M. (2005). *Acta Cryst.* E**61**, o1163–o1164.

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supplementary materials

Acta Cryst. (2007). E**63**, o3370 [**doi:10.1107/S1600536807029157**]

2-[3,5-Bis(5,6-dihydro-4*H*-1,3-thiazin-2-ylsulfanylmethyl)-2,4,6-trimethylbenzylsulfanyl]-5,6-dihydro-4*H*-1,3-thiazine

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Comment

Thioethers are often used as bridging ligands in construction of coordination polymers with soft metal ions. Now, we have a new thiazinyl derivative and present here the crystal structure of 2-(3,5-bis((5,6-dihydro-4*H*-1,3-thiazin-2-ylthio)methyl)-2,4,6- trimethylbenzylthio)-5,6-dihydro-4*H*-1,3-thiazine, (I).

There are three 1,3-thiazinyl sulfanyl groups in this molecule. Two 1,3-thiazinyl sulfanyl groups are located on the same side of the planar benzene ring and the other is on the opposite side. In the thiazinyl ring, the C11 atom has an distorted trigonal geometry, with S2—C11—S1 = 108.22 (2) and N1—C11—S2 = 130.7 (2)° deviating significantly from the ideal sp^2 value of 120°. The similar results are observed in the other two thiazinyl rings. The C22, C23 and C24 atoms in the thiazinyl ring attached to the S5 atom are disordered over two sites [occupancies 0.462 (2) and 0.538 (2)]. The three methyl groups are almost coplanar with the benzene ring, with an r. m. s. derivation of 0.0272 Å.

Due to π-π conjugation, the Csp^2—S bonds distances[S2—C11 = 1.764 (3) Å, S4—C16 = 1.773 (3)Å and S5—C21 = 1.759 (3) Å] are significantly shorter than the Csp^3—S bonds distances [S1—C10 = 1.824 (3) Å, S3—C15 = 1.828 (3)Å and S5—C20 = 1.822 (3) Å]. These values are comparable with those in the literature (Wang *et al.*, 2004, 2005). The other bond distances are within normal ranges (Allen *et al.*, 1987).

Experimental

A solution of 1-bromo-3,5-bis(bromomethyl)-2,4,6-trimethylbenzene (0.45 g, 1 mmol) in ethanol (5 ml) was added dropwise to a mixture of 5,6-dihydro-4*H*-1,3-thiazine-2-thiol (0.45 g, 3.4 mmol), KOH (0.19 g, 3.4 mmol) and ethanol (15 ml). The reaction mixture was then stirred for 48 h at room temperature. Then the precipitate was filtered off, washed with water and recrystallized from ethanol and water (yield 62%, m.p. 455–457 K). Crystals of (I) suitable for single-crystal X-ray analysis were grown by slow evaporation of a CH_2Cl_2 solution.

Refinement

All H atoms were positioned geometrically and refined as riding with C—H = 0.98 and 0.99 Å). For the CH groups, U_{iso}(H) values are set equal to 1.2U_{eq} (carrier atom) and for the methyl groups they are set equal to 1.5U_{eq} (carrier atom). The C22, C23 and C24 atoms in the thiazinyl ring attached to the S5 atom are disordered over two sites [occupancies 0.462 (2) and 0.538 (2)].

Figures

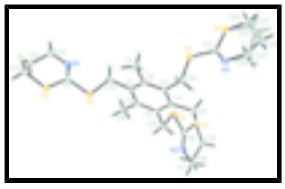


Fig. 1. View of the molecule of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

2-[3,5-Bis(5,6-dihydro-4*H*-1,3-thiazin-2-ylsulfanylmethyl)-2,4,6- trimethylbenzylsulfanyl]-5,6-dihydro-4*H*-1,3-thiazine

Crystal data

$C_{24}H_{33}N_3S_6$	F_{000} = 1176
M_r = 555.89	D_x = 1.400 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 455 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 17.146 (3) Å	Cell parameters from 5347 reflections
b = 10.123 (2) Å	θ = 2.3–24.5º
c = 17.408 (4) Å	μ = 0.58 mm^{-1}
β = 119.20 (3)º	T = 113 (2) K
V = 2637.6 (9) Å^3	Block, colourless
Z = 4	0.20 × 0.18 × 0.02 mm

Data collection

Rigaku Saturn diffractometer	R_{int} = 0.043
Radiation source: rotating anode	θ_{max} = 26.0º
Monochromator: confocal	θ_{min} = 1.4º
T = 113(2) K	h = −21→20
ω scans	k = −12→12
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	l = −13→21
T_{min} = 0.900, T_{max} = 0.989	Standard reflections: .;
17102 measured reflections	every . reflections
5178 independent reflections	intensity decay: .
4350 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.055	H-atom parameters constrained
$wR(F^2)$ = 0.139	$w = 1/[\sigma^2(F_o^2) + (0.0604P)^2 + 3.1576P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} = 0.002$
5178 reflections	$\Delta\rho_{max} = 1.17$ e Å^{-3}
329 parameters	$\Delta\rho_{min} = -0.42$ e Å^{-3}
7 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}	Occ. (<1)
S1	0.22603 (7)	0.49261 (8)	1.16480 (5)	0.0391 (2)	
S2	0.21116 (6)	0.41297 (8)	1.31502 (5)	0.0341 (2)	
S3	0.40459 (7)	0.67273 (8)	0.89432 (7)	0.0443 (3)	
S4	0.51695 (7)	0.75283 (8)	0.82245 (6)	0.0389 (2)	
S5	0.04801 (6)	0.40067 (8)	0.72402 (5)	0.0414 (3)	
S6	−0.01276 (6)	0.28553 (9)	0.55715 (6)	0.0378 (2)	
N1	0.2901 (2)	0.2620 (3)	1.24070 (19)	0.0378 (7)	
N2	0.44422 (17)	0.9257 (2)	0.89238 (17)	0.0272 (6)	
N3	−0.09428 (18)	0.5017 (3)	0.58476 (16)	0.0305 (6)	
C1	0.2251 (2)	0.5004 (3)	1.00786 (18)	0.0262 (7)	
C2	0.2894 (2)	0.5851 (3)	1.00776 (19)	0.0265 (7)	
C3	0.2683 (2)	0.6612 (3)	0.93296 (19)	0.0242 (6)	
C4	0.1851 (2)	0.6473 (3)	0.85736 (18)	0.0229 (6)	
C5	0.1201 (2)	0.5656 (3)	0.85905 (18)	0.0220 (6)	
C6	0.1388 (2)	0.4930 (3)	0.93487 (19)	0.0247 (6)	
C7	0.0681 (2)	0.4062 (3)	0.9370 (2)	0.0365 (8)	
H7A	0.0677	0.3200	0.9112	0.055*	
H7B	0.0095	0.4481	0.9032	0.055*	
H7C	0.0815	0.3943	0.9981	0.055*	
C8	0.3816 (2)	0.5939 (4)	1.0879 (2)	0.0440 (9)	
H8A	0.3761	0.6214	1.1391	0.066*	
H8B	0.4176	0.6586	1.0771	0.066*	
H8C	0.4106	0.5072	1.0994	0.066*	
C9	0.1652 (3)	0.7181 (3)	0.7734 (2)	0.0372 (8)	
H9A	0.1291	0.7968	0.7666	0.056*	

H9B	0.1322	0.6590	0.7231	0.056*	
H9C	0.2214	0.7445	0.7759	0.056*	
C10	0.2502 (2)	0.4094 (3)	1.0858 (2)	0.0327 (7)	
H10A	0.3145	0.3872	1.1139	0.039*	
H10B	0.2155	0.3263	1.0657	0.039*	
C11	0.2507 (2)	0.3647 (3)	1.24276 (19)	0.0278 (7)	
C12	0.3113 (3)	0.1601 (4)	1.3058 (3)	0.0510 (11)	
H12A	0.3651	0.1125	1.3137	0.061*	
H12B	0.2614	0.0959	1.2831	0.061*	
C13	0.3284 (3)	0.2093 (4)	1.3963 (2)	0.0487 (10)	
H13A	0.3445	0.1331	1.4368	0.058*	
H13B	0.3799	0.2707	1.4205	0.058*	
C14	0.2501 (2)	0.2779 (3)	1.3929 (2)	0.0352 (8)	
H14A	0.2667	0.3123	1.4521	0.042*	
H14B	0.2010	0.2135	1.3762	0.042*	
C15	0.3350 (2)	0.7569 (3)	0.9320 (2)	0.0351 (8)	
H15A	0.3731	0.7927	0.9918	0.042*	
H15B	0.3033	0.8316	0.8922	0.042*	
C16	0.4551 (2)	0.8098 (3)	0.8730 (2)	0.0264 (6)	
C17	0.4867 (2)	1.0354 (3)	0.8727 (2)	0.0298 (7)	
H17A	0.4925	1.1106	0.9115	0.036*	
H17B	0.4474	1.0639	0.8112	0.036*	
C18	0.5787 (2)	1.0031 (3)	0.8843 (2)	0.0288 (7)	
H18A	0.6060	1.0848	0.8768	0.035*	
H18B	0.6175	0.9699	0.9447	0.035*	
C19	0.5739 (2)	0.9015 (3)	0.8193 (2)	0.0318 (7)	
H19A	0.6352	0.8786	0.8322	0.038*	
H19B	0.5421	0.9395	0.7593	0.038*	
C20	0.0312 (2)	0.5463 (3)	0.77578 (19)	0.0298 (7)	
H20A	0.0162	0.6243	0.7367	0.036*	
H20B	−0.0174	0.5315	0.7900	0.036*	
C21	−0.0352 (2)	0.4136 (3)	0.61307 (19)	0.0249 (6)	
C22	−0.1721 (8)	0.5025 (18)	0.4950 (7)	0.029 (3)	0.462 (15)
H22A	−0.1877	0.5951	0.4752	0.035*	0.462 (15)
H22B	−0.2238	0.4623	0.4968	0.035*	0.462 (15)
C23	−0.1552 (8)	0.4282 (10)	0.4290 (6)	0.038 (3)	0.462 (15)
H23A	−0.2119	0.4218	0.3727	0.046*	0.462 (15)
H23B	−0.1123	0.4789	0.4179	0.046*	0.462 (15)
C24	−0.1187 (7)	0.2907 (10)	0.4594 (6)	0.048 (3)	0.462 (15)
H24A	−0.1134	0.2460	0.4116	0.058*	0.462 (15)
H24B	−0.1622	0.2402	0.4696	0.058*	0.462 (15)
C22'	−0.1523 (9)	0.5088 (14)	0.4878 (7)	0.035 (3)	0.538 (15)
H22C	−0.1216	0.5628	0.4631	0.042*	0.538 (15)
H22D	−0.2082	0.5552	0.4749	0.042*	0.538 (15)
C23'	−0.1763 (5)	0.3763 (11)	0.4411 (6)	0.037 (2)	0.538 (15)
H23C	−0.2009	0.3173	0.4694	0.045*	0.538 (15)
H23D	−0.2226	0.3887	0.3789	0.045*	0.538 (15)
C24'	−0.0947 (6)	0.3143 (11)	0.4453 (4)	0.039 (2)	0.538 (15)
H24C	−0.0699	0.3736	0.4173	0.046*	0.538 (15)

H24D	−0.1111	0.2297	0.4126	0.046*	0.538 (15)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0654 (6)	0.0283 (4)	0.0286 (4)	0.0160 (4)	0.0268 (4)	0.0070 (3)
S2	0.0400 (5)	0.0332 (4)	0.0363 (4)	0.0023 (4)	0.0244 (4)	0.0006 (3)
S3	0.0469 (6)	0.0207 (4)	0.0842 (7)	−0.0071 (4)	0.0468 (5)	−0.0085 (4)
S4	0.0542 (6)	0.0262 (4)	0.0516 (5)	0.0010 (4)	0.0378 (5)	−0.0066 (4)
S5	0.0462 (6)	0.0280 (4)	0.0292 (4)	0.0092 (4)	0.0021 (4)	−0.0067 (3)
S6	0.0474 (6)	0.0332 (5)	0.0387 (5)	0.0019 (4)	0.0258 (4)	−0.0067 (3)
N1	0.0500 (19)	0.0335 (16)	0.0406 (16)	0.0104 (14)	0.0305 (14)	0.0115 (12)
N2	0.0223 (14)	0.0218 (13)	0.0410 (15)	−0.0026 (10)	0.0183 (11)	−0.0038 (10)
N3	0.0304 (15)	0.0355 (15)	0.0217 (12)	0.0004 (12)	0.0098 (11)	−0.0069 (10)
C1	0.0358 (18)	0.0241 (15)	0.0212 (14)	0.0040 (13)	0.0158 (13)	0.0007 (11)
C2	0.0299 (17)	0.0197 (14)	0.0250 (15)	−0.0009 (12)	0.0095 (13)	−0.0038 (11)
C3	0.0250 (16)	0.0161 (14)	0.0330 (16)	−0.0027 (12)	0.0154 (13)	−0.0032 (11)
C4	0.0330 (17)	0.0174 (14)	0.0240 (14)	0.0023 (12)	0.0184 (13)	0.0017 (11)
C5	0.0243 (16)	0.0211 (14)	0.0210 (14)	0.0000 (12)	0.0113 (12)	−0.0019 (11)
C6	0.0323 (17)	0.0219 (15)	0.0258 (15)	−0.0012 (13)	0.0188 (13)	−0.0018 (11)
C7	0.038 (2)	0.0372 (19)	0.0442 (19)	−0.0047 (15)	0.0281 (16)	0.0030 (15)
C8	0.038 (2)	0.0313 (19)	0.042 (2)	−0.0040 (16)	0.0031 (16)	0.0008 (15)
C9	0.054 (2)	0.0321 (18)	0.0286 (16)	−0.0043 (16)	0.0223 (16)	0.0048 (13)
C10	0.044 (2)	0.0265 (16)	0.0309 (16)	0.0085 (15)	0.0208 (15)	0.0032 (12)
C11	0.0289 (17)	0.0292 (16)	0.0263 (15)	−0.0002 (13)	0.0144 (13)	0.0039 (12)
C12	0.069 (3)	0.0296 (19)	0.078 (3)	0.0285 (19)	0.053 (2)	0.0235 (18)
C13	0.044 (2)	0.065 (3)	0.043 (2)	0.013 (2)	0.0264 (18)	0.0299 (19)
C14	0.044 (2)	0.0371 (19)	0.0273 (16)	−0.0063 (16)	0.0199 (15)	−0.0015 (13)
C15	0.0375 (19)	0.0236 (16)	0.053 (2)	−0.0064 (14)	0.0288 (17)	−0.0063 (14)
C16	0.0228 (16)	0.0238 (16)	0.0330 (16)	−0.0010 (12)	0.0140 (13)	−0.0026 (12)
C17	0.0305 (17)	0.0217 (15)	0.0411 (18)	0.0007 (13)	0.0206 (14)	−0.0002 (13)
C18	0.0281 (17)	0.0263 (16)	0.0354 (17)	0.0023 (13)	0.0182 (14)	0.0026 (12)
C19	0.0309 (18)	0.0360 (18)	0.0352 (17)	0.0037 (14)	0.0213 (14)	0.0031 (13)
C20	0.0282 (17)	0.0282 (16)	0.0286 (16)	0.0021 (13)	0.0105 (13)	−0.0027 (12)
C21	0.0254 (16)	0.0256 (15)	0.0264 (15)	−0.0055 (13)	0.0146 (13)	−0.0041 (11)
C22	0.018 (6)	0.049 (6)	0.018 (4)	0.008 (4)	0.008 (4)	−0.007 (4)
C23	0.051 (6)	0.035 (5)	0.030 (4)	−0.009 (4)	0.020 (4)	−0.011 (4)
C24	0.097 (9)	0.036 (5)	0.030 (5)	0.007 (6)	0.045 (6)	0.002 (4)
C22'	0.025 (6)	0.050 (5)	0.031 (5)	0.008 (4)	0.015 (4)	−0.003 (4)
C23'	0.028 (4)	0.049 (6)	0.032 (4)	−0.012 (4)	0.012 (3)	−0.007 (4)
C24'	0.059 (5)	0.049 (5)	0.010 (3)	0.001 (4)	0.019 (3)	−0.006 (3)

Geometric parameters (Å, °)

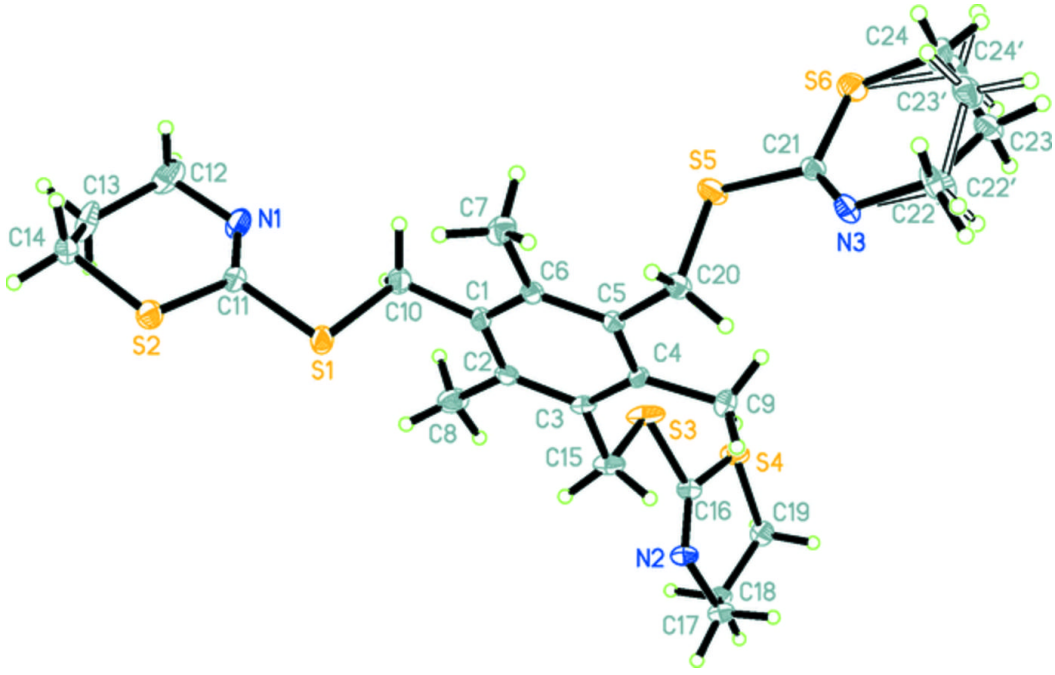
S1—C11	1.772 (3)	C9—H9C	0.9800
S1—C10	1.824 (3)	C10—H10A	0.9900
S2—C11	1.764 (3)	C10—H10B	0.9900
S2—C14	1.808 (3)	C12—C13	1.537 (6)
S3—C16	1.768 (3)	C12—H12A	0.9900

S3—C15	1.828 (3)	C12—H12B	0.9900
S4—C16	1.773 (3)	C13—C14	1.487 (5)
S4—C19	1.809 (3)	C13—H13A	0.9900
S5—C21	1.759 (3)	C13—H13B	0.9900
S5—C20	1.822 (3)	C14—H14A	0.9900
S6—C21	1.773 (3)	C14—H14B	0.9900
S6—C24	1.784 (8)	C15—H15A	0.9900
S6—C24'	1.784 (6)	C15—H15B	0.9900
N1—C11	1.250 (4)	C17—C18	1.525 (4)
N1—C12	1.442 (4)	C17—H17A	0.9900
N2—C16	1.259 (4)	C17—H17B	0.9900
N2—C17	1.458 (4)	C18—C19	1.502 (4)
N3—C21	1.256 (4)	C18—H18A	0.9900
N3—C22	1.478 (11)	C18—H18B	0.9900
N3—C22'	1.486 (10)	C19—H19A	0.9900
C1—C2	1.397 (4)	C19—H19B	0.9900
C1—C6	1.406 (4)	C20—H20A	0.9900
C1—C10	1.519 (4)	C20—H20B	0.9900
C2—C3	1.400 (4)	C22—C23	1.515 (9)
C2—C8	1.517 (4)	C22—H22A	0.9900
C3—C4	1.398 (4)	C22—H22B	0.9900
C3—C15	1.506 (4)	C23—C24	1.511 (9)
C4—C5	1.399 (4)	C23—H23A	0.9900
C4—C9	1.511 (4)	C23—H23B	0.9900
C5—C6	1.405 (4)	C24—H24A	0.9900
C5—C20	1.519 (4)	C24—H24B	0.9900
C6—C7	1.511 (4)	C22'—C23'	1.518 (9)
C7—H7A	0.9800	C22'—H22C	0.9900
C7—H7B	0.9800	C22'—H22D	0.9900
C7—H7C	0.9800	C23'—C24'	1.502 (8)
C8—H8A	0.9800	C23'—H23C	0.9900
C8—H8B	0.9800	C23'—H23D	0.9900
C8—H8C	0.9800	C24'—H24C	0.9900
C9—H9A	0.9800	C24'—H24D	0.9900
C9—H9B	0.9800		
C11—S1—C10	100.53 (15)	S2—C14—H14B	109.1
C11—S2—C14	101.23 (15)	H14A—C14—H14B	107.9
C16—S3—C15	100.44 (15)	C3—C15—S3	109.7 (2)
C16—S4—C19	101.96 (15)	C3—C15—H15A	109.7
C21—S5—C20	104.09 (14)	S3—C15—H15A	109.7
C21—S6—C24	96.3 (4)	C3—C15—H15B	109.7
C21—S6—C24'	102.3 (3)	S3—C15—H15B	109.7
C24—S6—C24'	20.1 (3)	H15A—C15—H15B	108.2
C11—N1—C12	120.4 (3)	N2—C16—S3	121.6 (2)
C16—N2—C17	119.4 (3)	N2—C16—S4	129.7 (2)
C21—N3—C22	123.9 (6)	S3—C16—S4	108.78 (16)
C21—N3—C22'	116.4 (6)	N2—C17—C18	114.1 (3)
C22—N3—C22'	16.3 (8)	N2—C17—H17A	108.7
C2—C1—C6	121.0 (3)	C18—C17—H17A	108.7

C2—C1—C10	119.6 (3)	N2—C17—H17B	108.7
C6—C1—C10	119.3 (3)	C18—C17—H17B	108.7
C1—C2—C3	119.5 (3)	H17A—C17—H17B	107.6
C1—C2—C8	120.2 (3)	C19—C18—C17	112.0 (3)
C3—C2—C8	120.3 (3)	C19—C18—H18A	109.2
C4—C3—C2	120.1 (3)	C17—C18—H18A	109.2
C4—C3—C15	119.1 (3)	C19—C18—H18B	109.2
C2—C3—C15	120.8 (3)	C17—C18—H18B	109.2
C3—C4—C5	119.8 (3)	H18A—C18—H18B	107.9
C3—C4—C9	120.5 (3)	C18—C19—S4	112.3 (2)
C5—C4—C9	119.7 (3)	C18—C19—H19A	109.1
C4—C5—C6	120.7 (3)	S4—C19—H19A	109.1
C4—C5—C20	119.6 (3)	C18—C19—H19B	109.1
C6—C5—C20	119.4 (3)	S4—C19—H19B	109.1
C5—C6—C1	118.5 (3)	H19A—C19—H19B	107.9
C5—C6—C7	120.7 (3)	C5—C20—S5	104.4 (2)
C1—C6—C7	120.8 (3)	C5—C20—H20A	110.9
C6—C7—H7A	109.5	S5—C20—H20A	110.9
C6—C7—H7B	109.5	C5—C20—H20B	110.9
H7A—C7—H7B	109.5	S5—C20—H20B	110.9
C6—C7—H7C	109.5	H20A—C20—H20B	108.9
H7A—C7—H7C	109.5	N3—C21—S5	123.4 (2)
H7B—C7—H7C	109.5	N3—C21—S6	130.8 (2)
C2—C8—H8A	109.5	S5—C21—S6	105.75 (17)
C2—C8—H8B	109.5	N3—C22—C23	113.0 (9)
H8A—C8—H8B	109.5	N3—C22—H22A	109.0
C2—C8—H8C	109.5	C23—C22—H22A	109.0
H8A—C8—H8C	109.5	N3—C22—H22B	109.0
H8B—C8—H8C	109.5	C23—C22—H22B	109.0
C4—C9—H9A	109.5	H22A—C22—H22B	107.8
C4—C9—H9B	109.5	C24—C23—C22	113.0 (14)
H9A—C9—H9B	109.5	C24—C23—H23A	109.0
C4—C9—H9C	109.5	C22—C23—H23A	109.0
H9A—C9—H9C	109.5	C24—C23—H23B	109.0
H9B—C9—H9C	109.5	C22—C23—H23B	109.0
C1—C10—S1	108.9 (2)	H23A—C23—H23B	107.8
C1—C10—H10A	109.9	C23—C24—S6	114.6 (7)
S1—C10—H10A	109.9	C23—C24—H24A	108.6
C1—C10—H10B	109.9	S6—C24—H24A	108.6
S1—C10—H10B	109.9	C23—C24—H24B	108.6
H10A—C10—H10B	108.3	S6—C24—H24B	108.6
N1—C11—S2	130.7 (2)	H24A—C24—H24B	107.6
N1—C11—S1	121.1 (2)	N3—C22'—C23'	115.0 (9)
S2—C11—S1	108.22 (17)	N3—C22'—H22C	108.5
N1—C12—C13	115.0 (3)	C23'—C22'—H22C	108.5
N1—C12—H12A	108.5	N3—C22'—H22D	108.5
C13—C12—H12A	108.5	C23'—C22'—H22D	108.5
N1—C12—H12B	108.5	H22C—C22'—H22D	107.5
C13—C12—H12B	108.5	C24'—C23'—C22'	109.9 (11)

H12A—C12—H12B	107.5	C24'—C23'—H23C	109.7
C14—C13—C12	113.1 (3)	C22'—C23'—H23C	109.7
C14—C13—H13A	108.9	C24'—C23'—H23D	109.7
C12—C13—H13A	108.9	C22'—C23'—H23D	109.7
C14—C13—H13B	108.9	H23C—C23'—H23D	108.2
C12—C13—H13B	108.9	C23'—C24'—S6	109.9 (6)
H13A—C13—H13B	107.8	C23'—C24'—H24C	109.7
C13—C14—S2	112.3 (2)	S6—C24'—H24C	109.7
C13—C14—H14A	109.1	C23'—C24'—H24D	109.7
S2—C14—H14A	109.1	S6—C24'—H24D	109.7
C13—C14—H14B	109.1	H24C—C24'—H24D	108.2
C6—C1—C2—C3	−1.7 (4)	C2—C3—C15—S3	89.1 (3)
C10—C1—C2—C3	174.9 (3)	C16—S3—C15—C3	166.1 (2)
C6—C1—C2—C8	178.7 (3)	C17—N2—C16—S3	−179.5 (2)
C10—C1—C2—C8	−4.7 (4)	C17—N2—C16—S4	−0.1 (5)
C1—C2—C3—C4	−3.3 (4)	C15—S3—C16—N2	6.4 (3)
C8—C2—C3—C4	176.2 (3)	C15—S3—C16—S4	−173.11 (17)
C1—C2—C3—C15	177.9 (3)	C19—S4—C16—N2	7.6 (3)
C8—C2—C3—C15	−2.5 (4)	C19—S4—C16—S3	−172.93 (16)
C2—C3—C4—C5	5.5 (4)	C16—N2—C17—C18	−36.0 (4)
C15—C3—C4—C5	−175.7 (3)	N2—C17—C18—C19	65.7 (3)
C2—C3—C4—C9	−173.6 (3)	C17—C18—C19—S4	−54.5 (3)
C15—C3—C4—C9	5.2 (4)	C16—S4—C19—C18	20.3 (3)
C3—C4—C5—C6	−2.6 (4)	C4—C5—C20—S5	91.8 (3)
C9—C4—C5—C6	176.5 (3)	C6—C5—C20—S5	−83.3 (3)
C3—C4—C5—C20	−177.6 (3)	C21—S5—C20—C5	−158.9 (2)
C9—C4—C5—C20	1.5 (4)	C22—N3—C21—S5	−170.7 (8)
C4—C5—C6—C1	−2.4 (4)	C22'—N3—C21—S5	172.5 (6)
C20—C5—C6—C1	172.6 (3)	C22—N3—C21—S6	11.8 (9)
C4—C5—C6—C7	179.1 (3)	C22'—N3—C21—S6	−5.0 (7)
C20—C5—C6—C7	−5.9 (4)	C20—S5—C21—N3	−5.3 (3)
C2—C1—C6—C5	4.6 (4)	C20—S5—C21—S6	172.78 (16)
C10—C1—C6—C5	−172.1 (3)	C24—S6—C21—N3	−17.4 (5)
C2—C1—C6—C7	−176.9 (3)	C24'—S6—C21—N3	2.0 (5)
C10—C1—C6—C7	6.4 (4)	C24—S6—C21—S5	164.7 (4)
C2—C1—C10—S1	91.8 (3)	C24'—S6—C21—S5	−175.9 (4)
C6—C1—C10—S1	−91.5 (3)	C21—N3—C22—C23	−25.6 (18)
C11—S1—C10—C1	175.1 (2)	C22'—N3—C22—C23	42 (3)
C12—N1—C11—S2	−1.0 (5)	N3—C22—C23—C24	51 (2)
C12—N1—C11—S1	178.6 (3)	C22—C23—C24—S6	−62.3 (19)
C14—S2—C11—N1	4.1 (4)	C21—S6—C24—C23	40.2 (12)
C14—S2—C11—S1	−175.66 (17)	C24'—S6—C24—C23	−68.8 (15)
C10—S1—C11—N1	11.6 (3)	C21—N3—C22'—C23'	36.9 (13)
C10—S1—C11—S2	−168.71 (17)	C22—N3—C22'—C23'	−84 (4)
C11—N1—C12—C13	−30.1 (5)	N3—C22'—C23'—C24'	−68.7 (16)
N1—C12—C13—C14	60.7 (5)	C22'—C23'—C24'—S6	61.7 (13)
C12—C13—C14—S2	−55.0 (4)	C21—S6—C24'—C23'	−29.7 (11)
C11—S2—C14—C13	24.1 (3)	C24—S6—C24'—C23'	44.4 (12)
C4—C3—C15—S3	−89.7 (3)		

Fig. 1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