

4-Phenyl-2-(2-pyridylmethylsulfanyl)-3H-1,5-benzodiazepine

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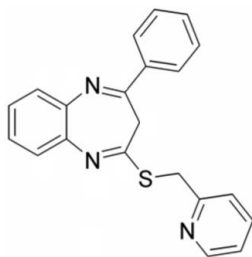
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.044; wR factor = 0.152; data-to-parameter ratio = 25.8.

The title compound, $\text{C}_{21}\text{H}_{17}\text{N}_3\text{S}$, is a new heterocyclic system derived from 1,5-benzodiazepine. The molecule is built up from two fused six- and seven-membered rings with phenyl and picolylsulfanyl side groups. The seven-membered ring displays a twist-chair conformation. The cohesion of the crystal structure is ensured by weak slipped $\pi-\pi$ stacking between the pyridine rings of symmetry-related molecules [interplanar distance = 3.42 Å and centroid-to-centroid vector = 3.784 (1) Å] and weak $\text{C}-\text{H}\cdots\text{N}$ hydrogen-bond interactions.

Related literature

A comparative study of the crystal structure of this molecule and that of the related molecule containing benzylsulfanyl instead of picolylsulfanyl has been carried out (Doubia *et al.*, 2007). For related literature, see: Atack *et al.* (2006); Cremer & Pople (1975); Doubia *et al.* (2007); Dourlat *et al.* (2007); El Azzaoui *et al.* (2006); Ghomsi *et al.* (2004); Kumar *et al.* (2006); Zellou *et al.* (1999).



Experimental

Crystal data

$\text{C}_{21}\text{H}_{17}\text{N}_3\text{S}$	$V = 1741.40$ (7) Å ³
$M_r = 343.44$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 14.2995$ (3) Å	$\mu = 0.19$ mm ⁻¹
$b = 8.7004$ (2) Å	$T = 296$ (2) K
$c = 14.3851$ (4) Å	$0.38 \times 0.22 \times 0.12$ mm
$\beta = 103.337$ (1)°	

Data collection

Bruker X8 APEXII diffractometer	5841 independent reflections
Absorption correction: none	4115 reflections with $I > 2\sigma(I)$
25788 measured reflections	$R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$	226 parameters
$wR(F^2) = 0.152$	H-atom parameters constrained
$S = 1.11$	$\Delta\rho_{\text{max}} = 0.44$ e Å ⁻³
5841 reflections	$\Delta\rho_{\text{min}} = -0.23$ e Å ⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C21}-\text{H21}\cdots\text{N3}^i$	0.93	2.56	3.411 (2)	152
$\text{C13}-\text{H13}\cdots\text{N1}^{ii}$	0.93	2.67	3.554 (2)	160

Symmetry codes: (i) $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$; (ii) $x, y + 1, z$.

Data collection, cell refinement and data reduction: *APEX2* (Bruker, 2005); structure solution: *SHELXS97* (Sheldrick, 1997); structure refinement: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2192).

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supplementary materials

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4-Phenyl-2-(2-pyridylmethylsulfanyl)-3H-1,5-benzodiazepine

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Comment

Many benzodiazepines and their derivatives reveal very interesting biological and pharmacological activities (Dourlat *et al.*, 2007, Zellou *et al.*, 1999). Furthermore, it has been shown that the introduction of one or several nitrogenous heterocycles on the different positions of the diazepinic cycle increases the biological activity considerably (Atack *et al.*, 2006, Kumar *et al.*, 2006). In this context, our team has been interested in the synthesis of new heterocyclic systems deriving from 1,5-benzodiazepine (Ghomsi *et al.*, 2004, El Azzaoui *et al.*, 2006).

The 2-(benzylsulfanyl)-4-phenyl-3H-1,5-benzodiazepine (II) (Doubia *et al.* 2007) and 2-(picolylsulfanyl)-4-phenyl-3H-1,5-benzodiazepine (I) are two almost identical molecules as shown in scheme 1. In fact, each molecule is built up from two fused six-membered and seven-membered rings linked to benzylsulfanyl and phenyl for (II) or picolylsulfanyl and phenyl for (I) (Fig. 1). The seven-membered ring displays a twist-chair conformation in both molecules (I) and (II), as indicated by the total puckering amplitude $Q_T=0.859$ (2) Å and spherical polar angle $\theta_2=74.83$ (9)° with $\varphi_2=-48.0$ (2)° and $\varphi_3=103.0$ (4)° for (II) and $Q_T=0.860$ (2) Å $\theta_2=74.45$ (8)° with $\varphi_2=-48.4$ (2)° and $\varphi_3=103.1$ (3)° for (I) (Cremer & Pople, 1975). However, slightly geometrical differences exist between the torsion angles of the two molecules, especially: C9—S1—C10—C11 = -87.07°, C8—C7—C17—C22 = 3.36° and C8—C7—C17—C18 = -177.46° in molecule (II) differ from that observed in molecule (I), respectively: -90.23°, 10.04° and -170.26°. But the most important difference resides in the measurements of the crystal unit cell. This difference can be explained by the intermolecular hydrogen bonds (H...N3) that influence the orientation of the molecules in the crystals. The crystal structure is stabilized by weak C—H...N hydrogen bonds (Table 1) and also by weak slipped π - π stacking between symmetry related molecules (C16 to C21 ring) with interplanar distance of 3.42 Å and centroid to centroid vector of 3.784 (1) Å.

Experimental

To a solution of 4-phenyl-1,5-benzodiazepine-2-thione (1 g, 3.96 mmol) and benzylbromide (0.70 ml, 4.36 mmol) or picolychloride (0.51 g, 3.96 mmol) in DMF (20 ml), 0.5 mmol of tetra-*n*-butylammonium bromide and 4.36 mmol (0.60 g) of anhydrous potassium carbonate were added. After filtration, the solvent was evaporated under reduced pressure and the crude residue was recrystallized from ethanol giving compound II in 76% yield.

Refinement

All H atoms were fixed geometrically and treated as riding with C—H = 0.93 Å (aromatic) or 0.97 Å (methylene) with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

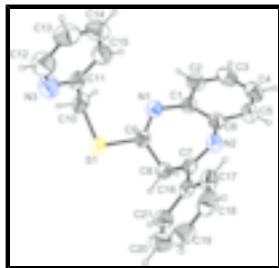


Fig. 1. Molecular view of compound (I) with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

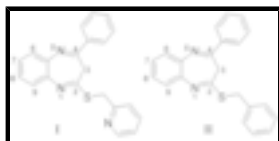


Fig. 2. Schematic representations of the structures of (I) and (II).

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Crystal data

$C_{21}H_{17}N_3S$

$M_r = 343.44$

Monoclinic, $P2_1/n$

Hall symbol: $-p\ 2yn$

$a = 14.2995\ (3)\ \text{\AA}$

$b = 8.7004\ (2)\ \text{\AA}$

$c = 14.3851\ (4)\ \text{\AA}$

$\beta = 103.337\ (1)^\circ$

$V = 1741.40\ (7)\ \text{\AA}^3$

$Z = 4$

$F_{000} = 720$

$D_x = 1.310\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 5841 reflections

$\theta = 2.8\text{--}31.6^\circ$

$\mu = 0.19\ \text{mm}^{-1}$

$T = 296\ (2)\ \text{K}$

Parallelepiped, pale yellow

$0.38 \times 0.22 \times 0.12\ \text{mm}$

Data collection

Bruker X8 APEXII KappaCCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 296\ (2)\ \text{K}$

φ scans, and ω scans with κ offsets

Absorption correction: none

25788 measured reflections

5841 independent reflections

4115 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\text{max}} = 31.6^\circ$

$\theta_{\text{min}} = 2.8^\circ$

$h = -21 \rightarrow 21$

$k = -12 \rightarrow 11$

$l = -21 \rightarrow 21$

Refinement

Refinement on F^2

Secondary atom site location: difference Fourier map

Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.044$$

$$wR(F^2) = 0.152$$

$$S = 1.11$$

5841 reflections

226 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0656P)^2 + 0.3072P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.44 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.23 \text{ e } \text{\AA}^{-3}$$

Extinction correction: none

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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.67517 (3)	0.23757 (5)	0.79695 (3)	0.04864 (13)
N1	0.49783 (9)	0.16662 (14)	0.81086 (8)	0.0431 (3)
N2	0.38145 (8)	0.15159 (13)	0.60681 (8)	0.0407 (2)
N3	0.69778 (11)	0.59718 (18)	0.88759 (13)	0.0654 (4)
C1	0.40814 (10)	0.09371 (15)	0.78066 (10)	0.0409 (3)
C2	0.36691 (12)	0.0369 (2)	0.85337 (12)	0.0529 (4)
H2	0.3993	0.0496	0.9168	0.064*
C3	0.27984 (14)	-0.0371 (2)	0.83291 (15)	0.0611 (4)
H3	0.2555	-0.0789	0.8820	0.073*
C4	0.22823 (12)	-0.0495 (2)	0.73931 (14)	0.0592 (4)
H4	0.1695	-0.1004	0.7252	0.071*
C5	0.26406 (11)	0.01364 (19)	0.66732 (12)	0.0509 (3)
H5	0.2272	0.0102	0.6050	0.061*
C6	0.35536 (10)	0.08363 (15)	0.68549 (10)	0.0401 (3)
C7	0.46882 (9)	0.14973 (14)	0.59740 (9)	0.0355 (2)
C8	0.54617 (10)	0.06568 (15)	0.66913 (9)	0.0389 (3)
H8A	0.5260	-0.0386	0.6781	0.047*
H8B	0.6054	0.0618	0.6471	0.047*
C9	0.56080 (9)	0.15465 (14)	0.76107 (9)	0.0379 (3)
C10	0.66896 (12)	0.32930 (18)	0.90820 (11)	0.0504 (3)
H10A	0.6265	0.2700	0.9382	0.060*
H10B	0.7324	0.3278	0.9507	0.060*

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C11	0.63335 (10)	0.49434 (17)	0.89685 (9)	0.0442 (3)
C12	0.66942 (17)	0.7437 (2)	0.88149 (18)	0.0729 (6)
H12	0.7137	0.8185	0.8744	0.087*
C13	0.57906 (17)	0.7904 (2)	0.88511 (14)	0.0682 (5)
H13	0.5633	0.8942	0.8829	0.082*
C14	0.51236 (16)	0.6808 (3)	0.89215 (16)	0.0704 (5)
H14	0.4496	0.7083	0.8926	0.085*
C15	0.54042 (14)	0.5277 (2)	0.89861 (13)	0.0597 (4)
H15	0.4972	0.4502	0.9040	0.072*
C16	0.49184 (10)	0.23272 (14)	0.51568 (9)	0.0375 (3)
C17	0.42283 (11)	0.32813 (18)	0.45926 (10)	0.0475 (3)
H17	0.3633	0.3398	0.4742	0.057*
C18	0.44150 (14)	0.4053 (2)	0.38182 (12)	0.0602 (4)
H18	0.3945	0.4671	0.3443	0.072*
C19	0.53019 (16)	0.3904 (2)	0.36022 (12)	0.0637 (5)
H19	0.5433	0.4438	0.3087	0.076*
C20	0.59865 (15)	0.2978 (2)	0.41406 (14)	0.0617 (4)
H20	0.6580	0.2876	0.3986	0.074*
C21	0.58049 (12)	0.21835 (18)	0.49195 (12)	0.0490 (3)
H21	0.6277	0.1555	0.5283	0.059*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.03589 (19)	0.0547 (2)	0.0509 (2)	-0.00153 (14)	0.00101 (15)	-0.00703 (15)
N1	0.0428 (6)	0.0460 (6)	0.0390 (5)	0.0000 (5)	0.0065 (5)	-0.0043 (5)
N2	0.0355 (5)	0.0435 (6)	0.0409 (6)	-0.0012 (4)	0.0041 (4)	0.0013 (4)
N3	0.0542 (8)	0.0557 (8)	0.0854 (11)	0.0004 (7)	0.0145 (8)	-0.0003 (8)
C1	0.0408 (6)	0.0385 (6)	0.0441 (6)	0.0025 (5)	0.0111 (5)	-0.0016 (5)
C2	0.0528 (8)	0.0610 (9)	0.0478 (8)	0.0040 (7)	0.0176 (7)	0.0024 (7)
C3	0.0577 (10)	0.0629 (10)	0.0707 (11)	0.0019 (8)	0.0313 (9)	0.0125 (8)
C4	0.0445 (8)	0.0587 (9)	0.0776 (12)	-0.0074 (7)	0.0204 (8)	0.0048 (8)
C5	0.0403 (7)	0.0546 (8)	0.0558 (9)	-0.0051 (6)	0.0068 (6)	0.0009 (7)
C6	0.0372 (6)	0.0379 (6)	0.0447 (7)	-0.0003 (5)	0.0084 (5)	-0.0004 (5)
C7	0.0353 (6)	0.0347 (5)	0.0340 (5)	-0.0004 (4)	0.0028 (4)	-0.0042 (4)
C8	0.0386 (6)	0.0382 (6)	0.0381 (6)	0.0051 (5)	0.0050 (5)	-0.0020 (5)
C9	0.0369 (6)	0.0355 (5)	0.0374 (6)	0.0027 (4)	0.0009 (5)	-0.0004 (4)
C10	0.0491 (8)	0.0498 (8)	0.0428 (7)	0.0012 (6)	-0.0088 (6)	-0.0035 (6)
C11	0.0421 (7)	0.0517 (7)	0.0333 (6)	0.0009 (6)	-0.0026 (5)	-0.0029 (5)
C12	0.0766 (14)	0.0537 (10)	0.0908 (15)	-0.0020 (9)	0.0245 (12)	0.0067 (9)
C13	0.0884 (15)	0.0552 (9)	0.0604 (10)	0.0209 (10)	0.0163 (10)	0.0067 (8)
C14	0.0641 (11)	0.0749 (12)	0.0742 (12)	0.0199 (10)	0.0199 (9)	0.0035 (10)
C15	0.0538 (9)	0.0651 (10)	0.0602 (10)	0.0003 (8)	0.0130 (8)	0.0002 (8)
C16	0.0398 (6)	0.0368 (6)	0.0340 (6)	-0.0048 (5)	0.0046 (5)	-0.0054 (4)
C17	0.0446 (7)	0.0493 (7)	0.0438 (7)	-0.0062 (6)	0.0003 (6)	0.0046 (6)
C18	0.0683 (11)	0.0607 (9)	0.0443 (8)	-0.0104 (8)	-0.0020 (7)	0.0103 (7)
C19	0.0897 (14)	0.0609 (10)	0.0424 (8)	-0.0158 (9)	0.0194 (8)	0.0021 (7)
C20	0.0710 (11)	0.0592 (9)	0.0649 (10)	-0.0070 (8)	0.0366 (9)	-0.0054 (8)

C21 0.0491 (8) 0.0475 (7) 0.0525 (8) 0.0030 (6) 0.0163 (6) -0.0025 (6)

Geometric parameters (Å, °)

S1—C9	1.7527 (14)	C10—C11	1.520 (2)
S1—C10	1.8088 (16)	C10—H10A	0.9700
N1—C9	1.2776 (18)	C10—H10B	0.9700
N1—C1	1.4067 (18)	C11—C15	1.366 (2)
N2—C7	1.2875 (17)	C12—C13	1.367 (3)
N2—C6	1.4016 (17)	C12—H12	0.9300
N3—C11	1.313 (2)	C13—C14	1.369 (3)
N3—C12	1.335 (2)	C13—H13	0.9300
C1—C2	1.404 (2)	C14—C15	1.388 (3)
C1—C6	1.405 (2)	C14—H14	0.9300
C2—C3	1.372 (3)	C15—H15	0.9300
C2—H2	0.9300	C16—C21	1.392 (2)
C3—C4	1.382 (3)	C16—C17	1.397 (2)
C3—H3	0.9300	C17—C18	1.378 (2)
C4—C5	1.372 (2)	C17—H17	0.9300
C4—H4	0.9300	C18—C19	1.380 (3)
C5—C6	1.409 (2)	C18—H18	0.9300
C5—H5	0.9300	C19—C20	1.363 (3)
C7—C16	1.4798 (18)	C19—H19	0.9300
C7—C8	1.5153 (18)	C20—C21	1.391 (2)
C8—C9	1.5048 (18)	C20—H20	0.9300
C8—H8A	0.9700	C21—H21	0.9300
C8—H8B	0.9700		
C9—S1—C10	102.08 (7)	C11—C10—H10B	108.8
C9—N1—C1	120.03 (12)	S1—C10—H10B	108.8
C7—N2—C6	121.68 (12)	H10A—C10—H10B	107.7
C11—N3—C12	116.61 (17)	N3—C11—C15	124.42 (16)
C2—C1—C6	118.71 (13)	N3—C11—C10	115.42 (14)
C2—C1—N1	116.01 (13)	C15—C11—C10	120.15 (15)
C6—C1—N1	125.13 (12)	N3—C12—C13	123.8 (2)
C3—C2—C1	121.45 (16)	N3—C12—H12	118.1
C3—C2—H2	119.3	C13—C12—H12	118.1
C1—C2—H2	119.3	C12—C13—C14	118.48 (18)
C2—C3—C4	119.99 (15)	C12—C13—H13	120.8
C2—C3—H3	120.0	C14—C13—H13	120.8
C4—C3—H3	120.0	C13—C14—C15	118.54 (19)
C5—C4—C3	119.71 (16)	C13—C14—H14	120.7
C5—C4—H4	120.1	C15—C14—H14	120.7
C3—C4—H4	120.1	C11—C15—C14	118.06 (18)
C4—C5—C6	121.63 (16)	C11—C15—H15	121.0
C4—C5—H5	119.2	C14—C15—H15	121.0
C6—C5—H5	119.2	C21—C16—C17	118.15 (13)
N2—C6—C1	125.25 (12)	C21—C16—C7	122.20 (13)
N2—C6—C5	116.12 (13)	C17—C16—C7	119.65 (12)
C1—C6—C5	118.29 (13)	C18—C17—C16	121.08 (16)

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N2—C7—C16	118.45 (12)	C18—C17—H17	119.5
N2—C7—C8	120.53 (12)	C16—C17—H17	119.5
C16—C7—C8	121.02 (11)	C17—C18—C19	119.72 (17)
C9—C8—C7	106.37 (10)	C17—C18—H18	120.1
C9—C8—H8A	110.5	C19—C18—H18	120.1
C7—C8—H8A	110.5	C20—C19—C18	120.30 (16)
C9—C8—H8B	110.5	C20—C19—H19	119.9
C7—C8—H8B	110.5	C18—C19—H19	119.9
H8A—C8—H8B	108.6	C19—C20—C21	120.55 (17)
N1—C9—C8	124.16 (12)	C19—C20—H20	119.7
N1—C9—S1	122.13 (10)	C21—C20—H20	119.7
C8—C9—S1	113.68 (10)	C20—C21—C16	120.18 (16)
C11—C10—S1	113.92 (10)	C20—C21—H21	119.9
C11—C10—H10A	108.8	C16—C21—H21	119.9
S1—C10—H10A	108.8		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C21—H21 \cdots N3 ⁱ	0.93	2.56	3.411 (2)	152
C13—H13 \cdots N1 ⁱⁱ	0.93	2.67	3.554 (2)	160

Symmetry codes: (i) $-x+3/2, y-1/2, -z+3/2$; (ii) $x, y+1, z$.

Fig. 1

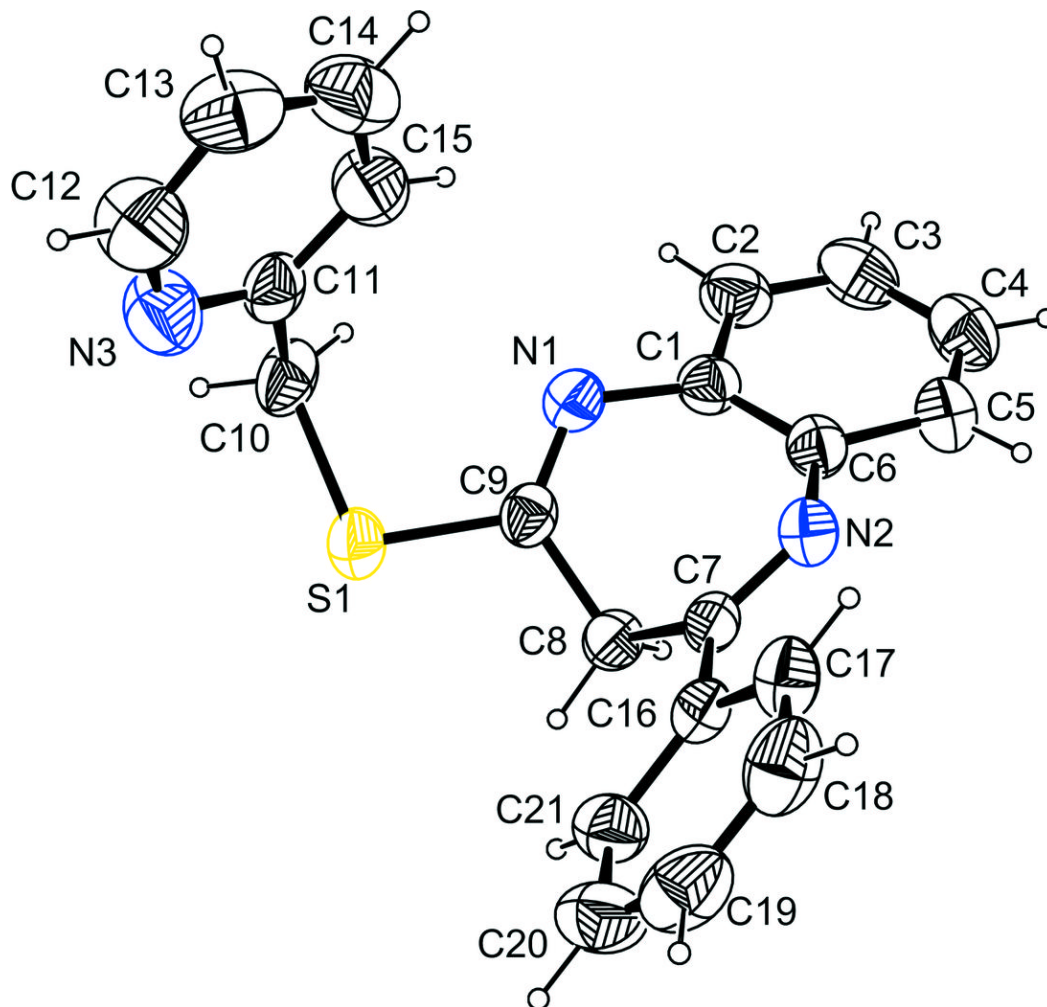


Fig. 2

