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3-[5,6-Dimethyl-1,3-benzothiazol-2-yl)-diazenyl]-1-methyl-2-phenyl-1*H*-indole

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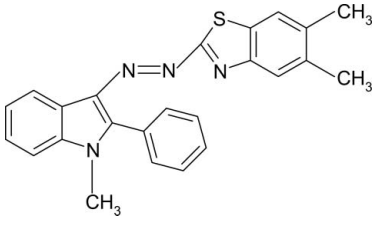
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.060; wR factor = 0.159; data-to-parameter ratio = 18.5.

In the title compound, $C_{24}H_{20}N_4S$, the phenyl ring forms a dihedral angle of 49.22 (7)° with the indole ring system. The indole and benzothiazole ring systems are both approximately planar, with dihedral angles between the five- and six-membered rings of 0.98 (7) and 1.28 (5)°, respectively. They are also oriented relative to the central N=N double bond at angles of 3.12 (14) and 3.82 (10)°, respectively.

Related literature

For general background, see: Zabriskie *et al.* (1988); Metzger (1984); Florin *et al.* (1980); Rau (1990); Bach *et al.* (1996); Biswas & Umapathy (2000); Ochiai *et al.* (1986); Tsuda *et al.* (2000); Allen *et al.* (1987). For related literature, see: Bruni *et al.* (1995); Seferoğlu *et al.* (2006, 2006*a*,*b*,*c*, 2007*a*,*b*,*c*); Hökelek *et al.* (2007).



Experimental

Crystal data

$C_{24}H_{20}N_4S$
M_r = 396.50
Monoclinic, $P2_1/n$
a = 13.171 (5) Å
b = 9.815 (2) Å
c = 17.257 (4) Å
β = 112.31 (2)°
V = 2063.9 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.17 mm^{-1}
T = 294 (2) K
0.35 × 0.20 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID-S diffractometer
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.959, T_{max} = 0.974
59779 measured reflections
6324 independent reflections
3982 reflections with $I > 2\sigma(I)$
R_{int} = 0.072

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.159
S = 1.03
6324 reflections
342 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Data collection: *CrystalClear* (Rigaku/MSC, 2005); 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: *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: CI2395).

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supplementary materials

Acta Cryst. (2007). E**63**, o3170 [**doi:10.1107/S1600536807028310**]

3-[5,6-Dimethyl-1,3-benzothiazol-2-yl)diazenyl]-1-methyl-2-phenyl-1*H*-indole

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Comment

Heterocycles containing the 1,3-thiazole ring system exhibit a wide spectrum of biological activities, including antiviral and antifungal. 1,3-thiazole ring system has been identified as a central structural element of a number of biologically active natural products (Zabriskie et al., 1988) and of pharmacologically active compounds (Metzger, 1984). Indole and its derivatives form a class of toxic recalcitrant N-heterocyclic compounds that are considered as pollutants (Florin et al., 1980). Azo derivatives are used extensively in analytical chemistry and in dyestuff industry as metallochromic and acid-base indicators (Rau, 1990). They are also used in the fields of non-linear optics and optical data storage (Bach et al., 1996). Azo dyes have wide applicability as optical materials and their structures have also attracted considerable attention (Biswas & Umapathy, 2000). Many azo-dye breakdown products are carcinogenic, toxic or mutagenic to life (Ochiai et al., 1986). Although there are many publications on the industrial applications of azo dyes (Tsuda et al., 2000), to the best of our knowledge, few structures of azoindole derivatives have been reported to date (Bruni et al., 1995; Seferoğlu et al., 2006, 2006a,b,c, 2007a,b,c; Hökelek et al., 2007). The present study was undertaken in order to ascertain the crystal structure of the title compound, (I).

The molecular structure of (I), is shown in Fig. 1. The bond lengths and angles are in normal ranges (Allen et al., 1987). An examination of the deviations from the least-squares planes through the individual rings shows that the indole and benzothiazole ring systems are both virtually planar, with dihedral angles between the fused five- and six-membered rings of 0.98 (7) and 1.28 (5)°, respectively. The phenyl ring forms a dihedral angle of 49.22 (7)° with the indole ring system.

As can be seen from the packing diagram (Fig. 2), the molecules of (I) are stacked along the b axis and elongated along the a</i axis. Dipole-dipole and van der Waals interactions are effective in the molecular packing.

Experimental

For the preparation of the title compound, 2-amino-5,6-dimethylbenzothiazole (360 mg, 2 mmol) was dissolved in a hot glacial acetic acid-propionic acid mixture (2:1, 6 ml). The solution was rapidly cooled in an ice-salt bath and then added dropwise with stirring to a cold solution of nitrosylsulfuric acid (3 ml) over a period 30 min. The mixture was stirred for an additional 2 h at 273 K. The resulting diazonium salt was cooled in an ice-salt bath and then added dropwise with stirring to 1-methyl-2-phenylindole (414 mg, 2 mmol) in an acetic acid-propionic acid mixture (3:1, 8 ml). The solution was stirred at 273–278 K for 2 h and the pH of the reaction mixture was maintained at 4–6 by the simultaneous addition of a saturated sodium carbonate solution (40 ml). The mixture was stirred for a further 1 h. The resulting solid was filtered, washed with cold water and crystallized from acetic acid (yield: 610 mg, 71%; m.p: 543–544 K).

Refinement

H atoms were located in a difference map and refined isotropically (C—H = 0.93 (2)–1.10 (4) Å and U_{iso}(H) = 0.068 (6)–0.188 (19) Å^2).

Figures

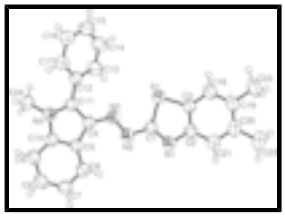

Fig. 1. The title molecular structure, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

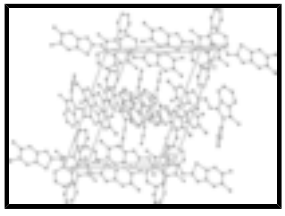

Fig. 2. A packing diagram of (I). H atoms have been omitted.

3-[5,6-Dimethyl-1,3-benzothiazol-2-yl)diazenyl]-1-methyl-2-phenyl- 1*H*-indole

Crystal data

$C_{24}H_{20}N_4S$	F_{000} = 832
M_r = 396.50	D_x = 1.276 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 9003 reflections
a = 13.171 (5) Å	θ = 2.4–30.7º
b = 9.815 (2) Å	μ = 0.17 mm^{-1}
c = 17.257 (4) Å	T = 294 (2) K
β = 112.31 (2)º	Rod, red
V = 2063.9 (10) Å^3	0.35 × 0.20 × 0.15 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID-S diffractometer	6324 independent reflections
Radiation source: fine-focus sealed tube	3982 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.072
T = 294(2) K	θ_{max} = 30.7º
ω scans	θ_{min} = 2.4º
Absorption correction: multi-scan (Blessing, 1995)	h = −18→18
T_{min} = 0.959, T_{max} = 0.974	k = −14→14
59779 measured reflections	l = −24→24

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.060$	All H-atom parameters refined
$wR(F^2) = 0.159$	$w = 1/[\sigma^2(F_o^2) + (0.0629P)^2 + 0.3279P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
6324 reflections	$\Delta\rho_{max} = 0.15$ e Å^{-3}
342 parameters	$\Delta\rho_{min} = -0.31$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.81333 (4)	−0.07830 (5)	0.48177 (3)	0.06181 (16)
N1	0.91361 (12)	0.02065 (16)	0.63292 (9)	0.0586 (4)
N2	0.73876 (13)	0.11429 (16)	0.56438 (10)	0.0601 (4)
N3	0.65949 (13)	0.10981 (16)	0.49199 (9)	0.0570 (4)
N4	0.39938 (12)	0.26821 (16)	0.41814 (9)	0.0573 (4)
C1	0.82355 (15)	0.02774 (18)	0.56648 (11)	0.0549 (4)
C2	0.98359 (14)	−0.07440 (17)	0.61996 (11)	0.0531 (4)
C3	0.94328 (15)	−0.13949 (19)	0.54207 (11)	0.0556 (4)
C4	0.57045 (14)	0.18717 (19)	0.48424 (11)	0.0543 (4)
C5	0.54789 (14)	0.27815 (18)	0.54149 (11)	0.0538 (4)
C6	0.60663 (18)	0.3234 (2)	0.62308 (12)	0.0623 (5)
C7	0.5564 (2)	0.4142 (2)	0.65846 (13)	0.0682 (5)
C8	0.4500 (2)	0.4592 (2)	0.61468 (14)	0.0717 (6)
C9	0.38999 (19)	0.4161 (2)	0.53410 (14)	0.0667 (5)
C10	0.44060 (15)	0.32548 (19)	0.49855 (11)	0.0564 (4)
C11	0.47722 (14)	0.18636 (18)	0.40882 (11)	0.0544 (4)
C12	0.46606 (14)	0.11818 (19)	0.33031 (11)	0.0548 (4)
C13	0.4977 (2)	−0.0171 (2)	0.33090 (15)	0.0699 (5)
C14	0.4947 (2)	−0.0781 (2)	0.25804 (16)	0.0793 (6)
C15	0.4605 (2)	−0.0063 (3)	0.18446 (15)	0.0772 (6)
C16	0.42920 (19)	0.1273 (3)	0.18264 (14)	0.0721 (6)
C17	0.43107 (16)	0.1896 (2)	0.25516 (12)	0.0616 (5)

C18	1.00534 (18)	−0.2391 (2)	0.52295 (13)	0.0644 (5)
C19	1.10791 (17)	−0.2730 (2)	0.58150 (13)	0.0653 (5)
C20	1.15065 (16)	−0.2050 (2)	0.65919 (14)	0.0672 (5)
C21	1.08800 (16)	−0.1070 (2)	0.67762 (13)	0.0634 (5)
C22	1.2636 (3)	−0.2388 (5)	0.7231 (2)	0.1067 (10)
C23	1.1731 (3)	−0.3838 (3)	0.5606 (2)	0.0917 (8)
C24	0.28592 (18)	0.2857 (3)	0.35983 (16)	0.0735 (6)
H6	0.6801 (17)	0.295 (2)	0.6518 (12)	0.069 (6)*
H7	0.5988 (17)	0.447 (2)	0.7159 (14)	0.072 (6)*
H8	0.4213 (18)	0.522 (2)	0.6415 (14)	0.082 (7)*
H9	0.3158 (18)	0.446 (2)	0.5029 (13)	0.075 (6)*
H13	0.5245 (19)	−0.065 (2)	0.3812 (14)	0.081 (7)*
H14	0.519 (2)	−0.171 (3)	0.2621 (14)	0.095 (8)*
H15	0.457 (2)	−0.049 (3)	0.1348 (16)	0.097 (8)*
H16	0.408 (2)	0.181 (3)	0.1325 (16)	0.097 (8)*
H17	0.4136 (17)	0.288 (2)	0.2556 (12)	0.074 (6)*
H18	0.9754 (18)	−0.286 (2)	0.4685 (14)	0.081 (7)*
H21	1.1188 (16)	−0.058 (2)	0.7329 (13)	0.068 (6)*
H221	1.286 (3)	−0.174 (4)	0.773 (2)	0.145 (13)*
H222	1.268 (4)	−0.331 (5)	0.741 (3)	0.188 (19)*
H223	1.314 (3)	−0.231 (4)	0.697 (2)	0.154 (15)*
H231	1.193 (2)	−0.453 (3)	0.6034 (18)	0.105 (9)*
H232	1.242 (3)	−0.349 (3)	0.564 (2)	0.141 (13)*
H233	1.122 (3)	−0.435 (4)	0.502 (2)	0.155 (14)*
H241	0.239 (2)	0.277 (3)	0.3919 (16)	0.102 (8)*
H242	0.275 (2)	0.374 (3)	0.3315 (19)	0.126 (11)*
H243	0.267 (2)	0.222 (3)	0.317 (2)	0.122 (10)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0630 (3)	0.0667 (3)	0.0526 (3)	0.0138 (2)	0.0185 (2)	0.0013 (2)
N1	0.0596 (9)	0.0595 (9)	0.0546 (8)	0.0122 (7)	0.0193 (7)	0.0013 (7)
N2	0.0593 (9)	0.0613 (9)	0.0582 (9)	0.0152 (7)	0.0209 (7)	0.0037 (7)
N3	0.0565 (8)	0.0579 (8)	0.0567 (9)	0.0096 (7)	0.0214 (7)	0.0051 (7)
N4	0.0514 (8)	0.0649 (9)	0.0548 (8)	0.0105 (7)	0.0191 (7)	0.0036 (7)
C1	0.0578 (10)	0.0549 (9)	0.0525 (9)	0.0088 (8)	0.0214 (8)	0.0038 (8)
C2	0.0532 (9)	0.0516 (9)	0.0559 (10)	0.0067 (7)	0.0224 (8)	0.0068 (7)
C3	0.0585 (10)	0.0586 (10)	0.0532 (10)	0.0088 (8)	0.0252 (8)	0.0076 (8)
C4	0.0535 (9)	0.0558 (10)	0.0535 (9)	0.0113 (8)	0.0203 (8)	0.0044 (8)
C5	0.0557 (10)	0.0554 (10)	0.0520 (9)	0.0073 (8)	0.0223 (8)	0.0043 (7)
C6	0.0679 (12)	0.0643 (11)	0.0533 (10)	0.0094 (10)	0.0215 (9)	0.0042 (9)
C7	0.0826 (14)	0.0691 (13)	0.0540 (11)	0.0079 (10)	0.0272 (10)	−0.0011 (9)
C8	0.0853 (15)	0.0720 (13)	0.0686 (13)	0.0187 (11)	0.0414 (12)	0.0003 (10)
C9	0.0668 (12)	0.0728 (13)	0.0669 (12)	0.0177 (10)	0.0327 (10)	0.0032 (10)
C10	0.0572 (10)	0.0603 (10)	0.0541 (10)	0.0092 (8)	0.0239 (8)	0.0043 (8)
C11	0.0560 (10)	0.0536 (9)	0.0547 (10)	0.0074 (8)	0.0222 (8)	0.0043 (8)
C12	0.0534 (9)	0.0548 (10)	0.0565 (10)	−0.0001 (8)	0.0212 (8)	−0.0021 (8)

C13	0.0875 (15)	0.0538 (11)	0.0694 (13)	0.0013 (10)	0.0311 (11)	0.0029 (10)
C14	0.0962 (17)	0.0578 (12)	0.0843 (16)	0.0036 (12)	0.0347 (13)	−0.0121 (11)
C15	0.0819 (15)	0.0839 (16)	0.0678 (13)	−0.0034 (12)	0.0308 (11)	−0.0202 (12)
C16	0.0769 (14)	0.0805 (15)	0.0573 (12)	0.0068 (11)	0.0239 (10)	−0.0017 (11)
C17	0.0628 (11)	0.0621 (11)	0.0572 (10)	0.0080 (9)	0.0197 (9)	0.0009 (9)
C18	0.0725 (13)	0.0646 (12)	0.0634 (12)	0.0129 (10)	0.0340 (10)	0.0047 (9)
C19	0.0661 (11)	0.0647 (11)	0.0752 (13)	0.0172 (9)	0.0381 (10)	0.0139 (10)
C20	0.0553 (10)	0.0709 (12)	0.0760 (13)	0.0122 (9)	0.0254 (10)	0.0138 (10)
C21	0.0578 (11)	0.0665 (12)	0.0626 (11)	0.0075 (9)	0.0190 (9)	0.0026 (9)
C22	0.0652 (16)	0.126 (3)	0.110 (2)	0.0323 (17)	0.0120 (16)	0.001 (2)
C23	0.094 (2)	0.0920 (18)	0.101 (2)	0.0403 (16)	0.0512 (17)	0.0148 (17)
C24	0.0511 (11)	0.0968 (18)	0.0682 (14)	0.0103 (11)	0.0177 (10)	0.0015 (13)

Geometric parameters (Å, °)

S1—C1	1.7575 (19)	C12—C17	1.390 (3)
S1—C3	1.7382 (19)	C13—H13	0.93 (2)
N1—C1	1.301 (2)	C13—C14	1.380 (3)
N1—C2	1.388 (2)	C14—H14	0.96 (3)
N2—C1	1.393 (2)	C14—C15	1.371 (3)
N3—N2	1.289 (2)	C15—H15	0.94 (3)
N3—C4	1.360 (2)	C16—C15	1.371 (3)
N4—C10	1.401 (2)	C16—H16	0.96 (2)
N4—C11	1.359 (2)	C17—C16	1.385 (3)
N4—C24	1.461 (3)	C17—H17	1.00 (2)
C2—C3	1.398 (3)	C18—C19	1.386 (3)
C2—C21	1.395 (3)	C18—H18	0.99 (2)
C3—C18	1.392 (3)	C19—C23	1.512 (3)
C5—C4	1.444 (2)	C20—C21	1.381 (3)
C5—C6	1.397 (3)	C20—C19	1.410 (3)
C6—H6	0.95 (2)	C20—C22	1.514 (3)
C6—C7	1.382 (3)	C21—H21	1.01 (2)
C7—H7	0.99 (2)	C22—H221	1.02 (4)
C8—C7	1.388 (3)	C22—H222	0.95 (5)
C8—H8	0.93 (2)	C22—H223	0.94 (4)
C8—C9	1.380 (3)	C23—H231	0.96 (3)
C9—H9	0.97 (2)	C23—H232	0.95 (4)
C10—C5	1.402 (2)	C23—H233	1.10 (4)
C10—C9	1.386 (3)	C24—H241	0.98 (3)
C11—C4	1.410 (2)	C24—H242	0.98 (3)
C11—C12	1.468 (2)	C24—H243	0.94 (3)
C12—C13	1.390 (3)		
C3—S1—C1	87.68 (9)	C14—C13—H13	119.7 (14)
C1—N1—C2	109.45 (15)	C12—C13—H13	120.0 (14)
N3—N2—C1	110.54 (15)	C15—C14—C13	120.4 (2)
N2—N3—C4	115.28 (15)	C15—C14—H14	122.7 (15)
C11—N4—C10	109.16 (14)	C13—C14—H14	116.9 (15)
C11—N4—C24	127.48 (18)	C14—C15—C16	120.2 (2)
C10—N4—C24	123.04 (17)	C14—C15—H15	120.3 (15)

N1—C1—N2	120.62 (16)	C16—C15—H15	119.5 (15)
N1—C1—S1	117.23 (13)	C15—C16—C17	120.0 (2)
N2—C1—S1	122.14 (14)	C15—C16—H16	121.8 (15)
N1—C2—C21	125.07 (17)	C17—C16—H16	118.1 (15)
N1—C2—C3	115.41 (15)	C16—C17—C12	120.4 (2)
C21—C2—C3	119.52 (17)	C16—C17—H17	120.8 (12)
C18—C3—C2	120.40 (17)	C12—C17—H17	118.7 (12)
C18—C3—S1	129.36 (16)	C19—C18—C3	119.56 (19)
C2—C3—S1	110.24 (13)	C19—C18—H18	120.6 (13)
N3—C4—C11	120.25 (16)	C3—C18—H18	119.8 (13)
N3—C4—C5	132.18 (17)	C18—C19—C20	120.44 (18)
C11—C4—C5	107.57 (15)	C18—C19—C23	118.9 (2)
C6—C5—C10	119.25 (17)	C20—C19—C23	120.7 (2)
C6—C5—C4	135.02 (17)	C21—C20—C19	119.42 (18)
C10—C5—C4	105.73 (15)	C21—C20—C22	119.5 (2)
C7—C6—C5	118.40 (19)	C19—C20—C22	121.1 (2)
C7—C6—H6	121.7 (12)	C20—C21—C2	120.61 (19)
C5—C6—H6	119.8 (12)	C20—C21—H21	119.4 (11)
C6—C7—C8	121.2 (2)	C2—C21—H21	119.9 (11)
C6—C7—H7	118.1 (12)	C20—C22—H221	111.4 (19)
C8—C7—H7	120.7 (12)	C20—C22—H222	111 (3)
C9—C8—C7	121.7 (2)	H221—C22—H222	111 (3)
C9—C8—H8	121.2 (14)	C20—C22—H223	108 (2)
C7—C8—H8	117.1 (14)	H221—C22—H223	109 (3)
C8—C9—C10	117.1 (2)	H222—C22—H223	106 (4)
C8—C9—H9	122.6 (13)	C19—C23—H231	109.8 (17)
C10—C9—H9	120.4 (13)	C19—C23—H233	109.8 (19)
C9—C10—N4	128.67 (17)	H231—C23—H233	106 (2)
C9—C10—C5	122.41 (18)	C19—C23—H232	110 (2)
N4—C10—C5	108.92 (15)	H231—C23—H232	103 (3)
N4—C11—C4	108.61 (15)	H233—C23—H232	117 (3)
N4—C11—C12	124.26 (16)	N4—C24—H241	107.6 (15)
C4—C11—C12	126.99 (16)	N4—C24—H243	111.2 (18)
C13—C12—C17	118.75 (18)	H241—C24—H243	111 (2)
C13—C12—C11	120.26 (17)	N4—C24—H242	111.6 (18)
C17—C12—C11	120.84 (17)	H241—C24—H242	111 (2)
C14—C13—C12	120.2 (2)	H243—C24—H242	105 (2)
C3—S1—C1—N1	0.40 (16)	C4—C5—C6—C7	179.7 (2)
C3—S1—C1—N2	−178.29 (17)	C5—C6—C7—C8	0.4 (3)
C1—S1—C3—C18	178.5 (2)	C9—C8—C7—C6	−0.3 (4)
C1—S1—C3—C2	−0.63 (14)	C7—C8—C9—C10	0.0 (3)
C2—N1—C1—N2	178.68 (16)	N4—C10—C9—C8	−178.78 (19)
C2—N1—C1—S1	0.0 (2)	C9—C10—C5—C6	−0.1 (3)
N3—N2—C1—N1	177.38 (17)	N4—C10—C5—C6	179.06 (17)
N3—N2—C1—S1	−4.0 (2)	C9—C10—C5—C4	−179.99 (18)
C1—N1—C2—C21	179.13 (18)	N4—C10—C5—C4	−0.9 (2)
C1—N1—C2—C3	−0.5 (2)	C5—C10—C9—C8	0.1 (3)
C4—N3—N2—C1	177.68 (16)	N4—C11—C4—N3	178.22 (16)
N2—N3—C4—C11	−177.71 (17)	C12—C11—C4—N3	−6.0 (3)

N2—N3—C4—C5	2.0 (3)	N4—C11—C4—C5	−1.6 (2)
C10—N4—C11—C4	1.1 (2)	C12—C11—C4—C5	174.21 (17)
C24—N4—C11—C4	−172.5 (2)	N4—C11—C12—C13	−136.4 (2)
C10—N4—C11—C12	−174.88 (17)	C4—C11—C12—C13	48.4 (3)
C24—N4—C11—C12	11.5 (3)	N4—C11—C12—C17	48.1 (3)
C11—N4—C10—C9	178.9 (2)	C4—C11—C12—C17	−127.1 (2)
C24—N4—C10—C9	−7.1 (3)	C17—C12—C13—C14	0.4 (3)
C11—N4—C10—C5	−0.1 (2)	C11—C12—C13—C14	−175.2 (2)
C24—N4—C10—C5	173.8 (2)	C13—C12—C17—C16	−0.8 (3)
N1—C2—C3—C18	−178.45 (17)	C11—C12—C17—C16	174.81 (18)
C21—C2—C3—C18	1.9 (3)	C12—C13—C14—C15	−0.1 (4)
N1—C2—C3—S1	0.8 (2)	C13—C14—C15—C16	0.2 (4)
C21—C2—C3—S1	−178.86 (15)	C17—C16—C15—C14	−0.6 (4)
N1—C2—C21—C20	178.91 (18)	C12—C17—C16—C15	0.9 (3)
C3—C2—C21—C20	−1.5 (3)	C3—C18—C19—C20	−1.6 (3)
C2—C3—C18—C19	−0.4 (3)	C3—C18—C19—C23	178.6 (2)
S1—C3—C18—C19	−179.45 (16)	C21—C20—C19—C18	2.0 (3)
C6—C5—C4—N3	1.8 (4)	C22—C20—C19—C18	−178.7 (3)
C10—C5—C4—N3	−178.29 (19)	C21—C20—C19—C23	−178.1 (2)
C6—C5—C4—C11	−178.4 (2)	C22—C20—C19—C23	1.1 (4)
C10—C5—C4—C11	1.5 (2)	C19—C20—C21—C2	−0.4 (3)
C10—C5—C6—C7	−0.2 (3)	C22—C20—C21—C2	−179.7 (3)

Fig. 1

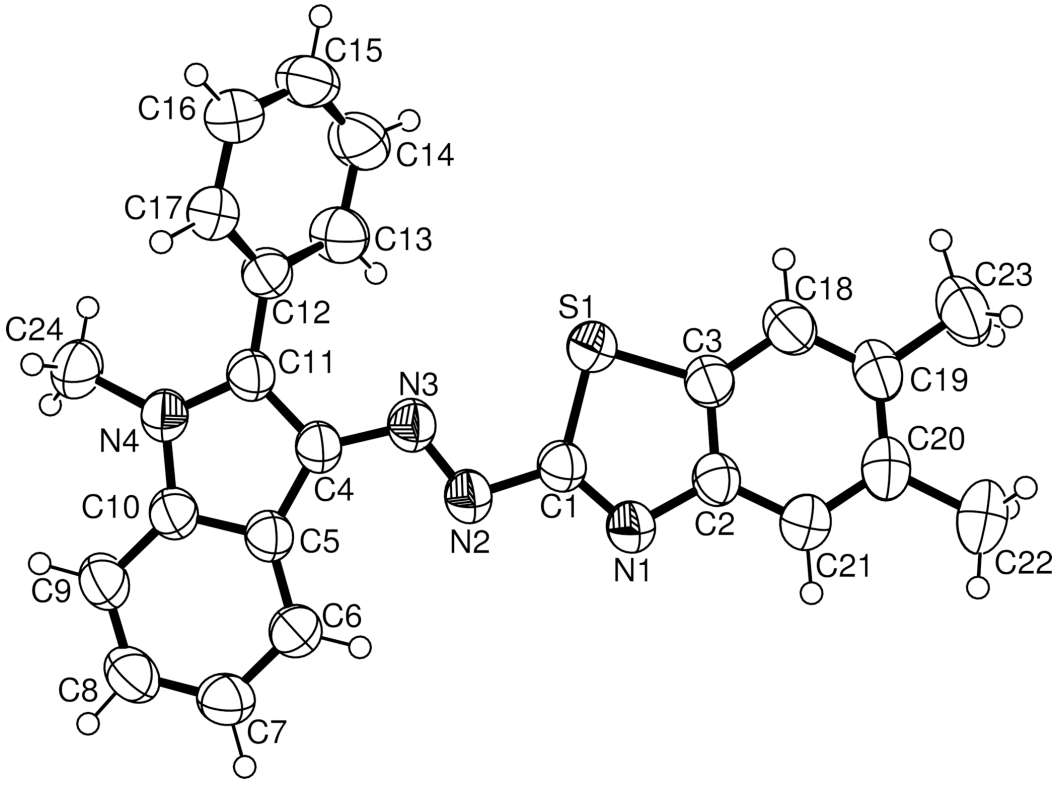
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Fig. 2