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# 1-Methyl-2-phenyl-3-(1,3,4-thiadiazol-2-yldiazenyl)-1*H*-indole

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**Key indicators**

Single-crystal X-ray study
$T$ = 294 K
Mean $\sigma$(C–C) = 0.003 Å
$R$ factor = 0.053
$wR$ factor = 0.146
Data-to-parameter ratio = 17.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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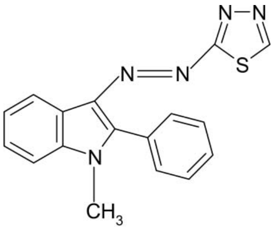
In the molecule of the title compound, $C_{17}H_{13}N_5S$, all of the rings are individually planar. The thiadiazole and phenyl rings form dihedral angles of 7.67 (4) and 49.77 (5)°, respectively, with the indole ring system.

## Comment

Heterocycles containing the 1,3-thiazole ring system exhibit a wide spectrum of biological activities, including acting as antiviral and antifungal agents, and this 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). Thiadiazole and its derivatives are also used for biological activities such as antiviral, antibacterial, antifungal and anti-tubercular. Indole and its derivatives form a class of toxic recalcitrant *N*-heterocyclic compounds that are considered as pollutants (Florin *et al.*, 1980). Azo dyes have wide applicability as optical materials and their structures have also attracted considerable attention (Biswas & Umapathy, 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*a*,*b*,*c*; Seferoğlu *et al.*, 2006). This study was undertaken in order to ascertain the crystal structure of (I).



(I)

The molecular structure of the title compound, (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 all of the rings are planar. In the indole ring system there is a dihedral angle of 4.26 (7)° between rings *A* (C4–C9) and *B* (N1/C3/C4/C9/C10). In the closely related compounds 3-(4-chlorophenyldiazenyl)-1-methyl-2-phenyl-1*H*-indole, (II) (Seferoğlu *et al.*, 2006*a*), *N*-{4-[(2-phenyl-1*H*-indol-3-yl)diazenyl]phenyl}acetamide, (III) (Seferoğlu *et al.*, 2006*b*), ethyl[2-(2-phenyl-1*H*-indol-3-yldiazenyl)-1,3-thiazol-4-yl]acetate, (IV) (Seferoğlu *et al.*, 2006*c*), and ethyl 2-{2-[(1-methyl-2-phenyl-1*H*-indol-3-yl)diazenyl]thiazol-4-yl}acetate, (V) (Seferoğlu *et al.*, 2006), the observed *A*/*B* dihedral angles are 1.56 (11) and 0.77 (12)°

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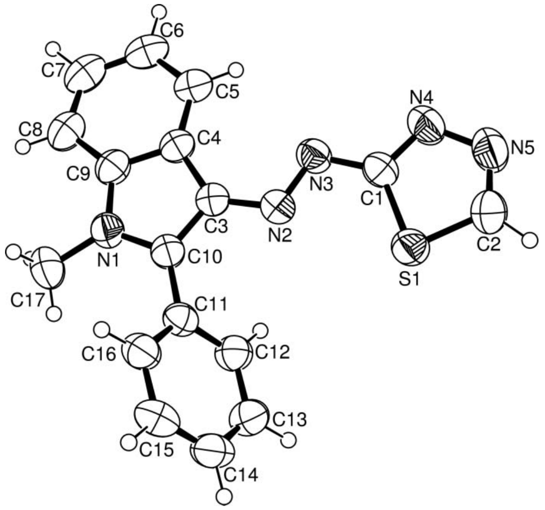

**Figure 1**
The molecular structure of (I) with 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

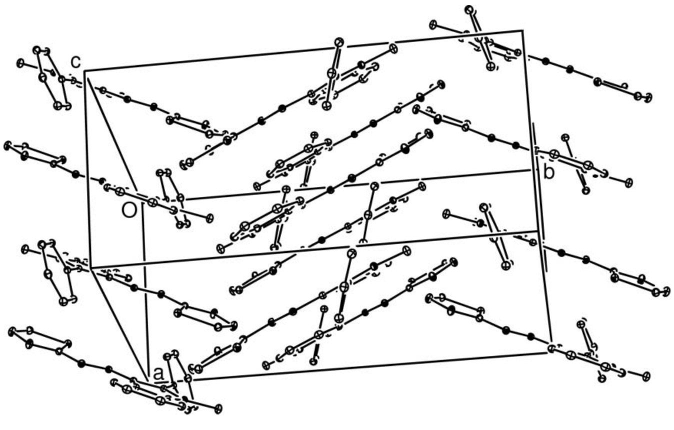

**Figure 2**
A packing diagram of (I). H atoms have been omitted for clarity.

in (II), 1.63 (14)° in (III), 0.99 (10)° in (IV) and 0.59 (7)° in (V). The orientations of the rings *C* (C11—C16) and *D* (S1/N4/N5/C1/C2) with respect to the indole ring system may be described by the dihedral angles of 49.77 (5) and 7.67 (4)°, respectively.

Dipole–dipole and van der Waals interactions are effective in the molecular packing.

## Experimental

For the preparation of (I), 2-aminothiadiazole (202 mg, 2 mmol) was dissolved in a hot glacial acetic acid–propionic acid mixture (2:1, 6 ml). The solution was cooled rapidly in an ice–salt bath and then added dropwise with stirring to a cold solution of nitrosylsulfuric acid (80%, 3 ml) over a period of 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 4–5 by the addition of a saturated sodium carbonate solution (30 ml). The mixture was stirred for a further 1 d. The resulting solid was filtered off, washed with cold water and crystallized from ethanol (yield 500 mg, 79%).

*Crystal data*

$C_{17}H_{13}N_5S$
$M_r = 319.38$
Monoclinic, $P2_1/n$
$a = 8.0288$ (2) Å
$b = 17.3757$ (3) Å
$c = 11.1899$ (3) Å
$\beta = 104.4222$ (14)°
$V = 1511.86$ (6) Å$^3$
$Z = 4$
$D_x = 1.403$ Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu = 0.22$ mm$^{-1}$
$T = 294$ (2) K
Block, orange
0.30 × 0.20 × 0.15 mm

*Data collection*

Rigaku R-AXIS RAPID-S diffractometer
$\omega$ scans
Absorption correction: multi-scan (Blessing, 1995)
$T_{\min} = 0.937$, $T_{\max} = 0.958$
44017 measured reflections
4636 independent reflections
3243 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.058$
$\theta_{\max} = 30.7°$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.146$
$S = 1.05$
4636 reflections
261 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0634P)^2 + 0.1946P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.22$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.32$ e Å$^{-3}$
Extinction correction: *SHELXL97*
Extinction coefficient: 0.072 (4)

H atoms were located in a difference synthesis and refined isotropically [C—H = 0.94 (2)–1.03 (3) Å and $U_{\rm iso}$(H) = 0.055 (5)–0.122 (10) Å$^2$].

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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