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Methyl 3-(4-methylbenzylidene)dithiocarbazate

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Crystals of the title compound, $C_{10}H_{12}N_2S_2$, were obtained from a condensation reaction of methyl dithiocarbazate and 4-methylbenzaldehyde. The essentially planar molecule exhibits an *E* configuration. Weak intermolecular N—H···S hydrogen bonds link the molecules into centrosymmetric dimers.

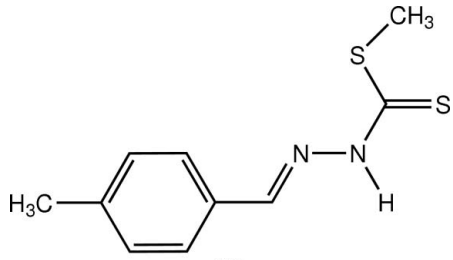
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
R factor = 0.036
wR factor = 0.105
Data-to-parameter ratio = 19.8

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

Comment

Hydrazine and its derivatives have attracted our attention because of their biological applications (Okabe *et al.*, 1993; Hu *et al.*, 2001). As part of ongoing research into new anti-cancer compounds, the title compound, (I), has been prepared in our laboratory and its structure is presented here.



(I)

The molecule of (I) exhibits an *E* configuration. The molecular skeleton is essentially planar (Fig. 1), with the maximum deviation from the mean plane being 0.0442 (15) Å for atom C7. The N2—C9 bond distance (Table 1) is much shorter than the typical value for a C—N single bond (Orpen

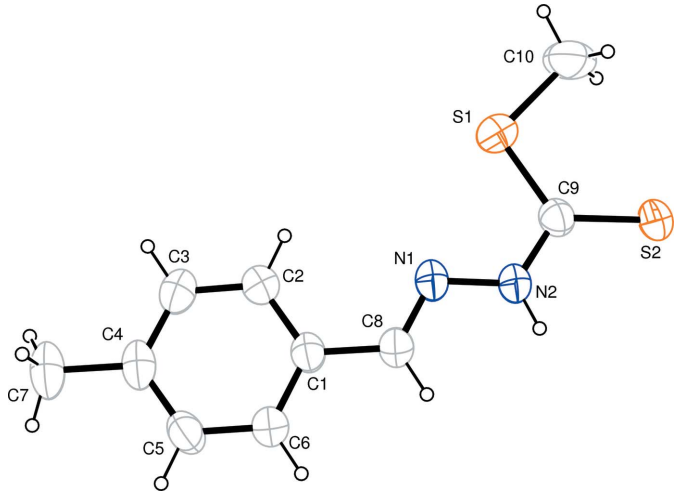


Figure 1
The molecular structure of (I), with 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

et al., 1992), suggesting electron delocalization in the molecule of (I).

Weak intermolecular N—H···S hydrogen bonds (Table 2) link the molecules into centrosymmetric dimers. The crystal packing (Fig. 2) is further stabilized by van der Waals forces.

Experimental

Methyl dithiocarbazate was synthesized in the manner reported previously by Hu *et al.* (2001). Methyl dithiocarbazate (1.24 g, 10 mmol) and 4-methylbenzaldehyde (1.20 g, 10 mmol) were dissolved in ethanol (10 ml) and refluxed for 4 h. Fine colourless crystals appeared on cooling. These were separated and washed with cold water three times. Single crystals of (I) were obtained by recrystallization from absolute ethanol.

Crystal data

$C_{10}H_{12}N_2S_2$
M_r = 224.33
Monoclinic, $P2_1/n$
a = 4.604 (2) Å
b = 11.049 (4) Å
c = 22.3554 (18) Å
β = 96.57 (2)°
V = 1129.7 (6) Å^3
Z = 4
D_x = 1.319 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.43 mm^{-1}
T = 295 (2) K
Block, colourless
0.28 × 0.24 × 0.22 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: none
9833 measured reflections
2557 independent reflections
1939 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.105
S = 1.09
2557 reflections
129 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0633P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected bond lengths (Å).

S1—C9	1.7441 (16)	N1—C8	1.273 (2)
S1—C10	1.7950 (19)	N1—N2	1.3783 (17)
S2—C9	1.6572 (15)	N2—C9	1.3352 (19)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···S2^{i}	0.86	2.59	3.432 (2)	166

Symmetry code: (i) $-x, -y+1, -z+1$.

Methyl H atoms were placed in calculated positions, with C—H = 0.96 Å, and their torsion angles were refined to fit the electron density. They were treated as riding, with U_{iso}(H) = 1.5U_{eq}(C). Other H atoms were placed in calculated positions, with C—H = 0.93 and N—H = 0.86 Å, and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C,N).

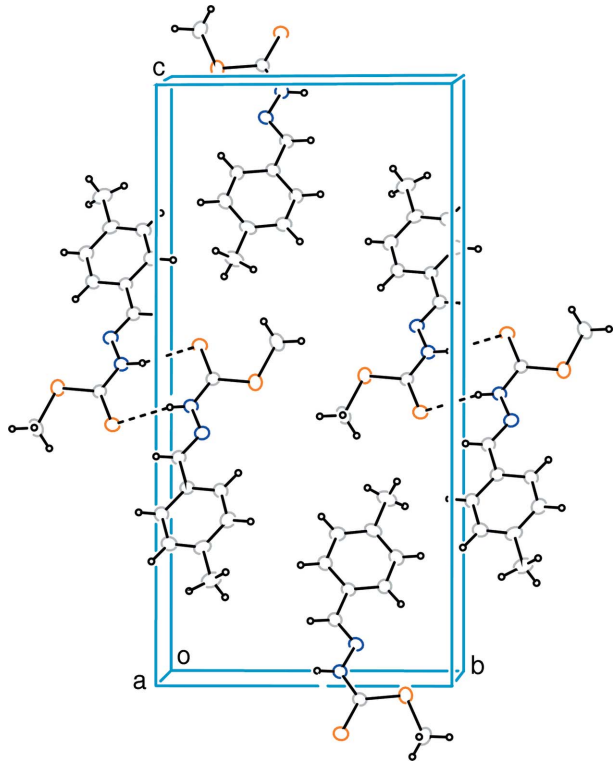


Figure 2
The crystal packing of (I), viewed approximately down the *a* axis, showing the hydrogen-bonded (dashed lines) dimers.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); 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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