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2′-(4-Dimethylaminobenzylidene)pyrazine-2-carbohydrazide

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The title compound, $C_{14}H_{15}N_5O$, was synthesized by the reaction of pyrazine-2-carboxylic acid hydrazide with 4-dimethylaminobenzaldehyde in methanol. In the crystal structure, there are intermolecular C—H···O and C—H···N hydrogen bonds. Weak π–π interactions link the molecules into a three-dimensional network.

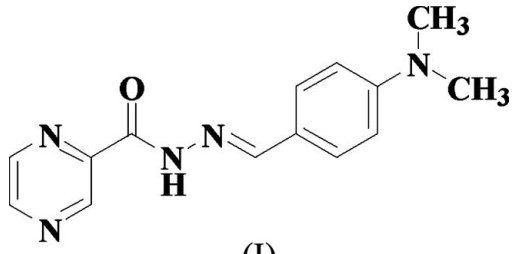
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.046
wR factor = 0.133
Data-to-parameter ratio = 12.6

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

Comment

Hydrazonecarbonyl compounds have received considerable attention for a long time due to their pharmacological activity (Parashar *et al.*, 1988) and their photochromic properties (Hadjoudis *et al.*, 1987). The type of pyrazine derivative reported here has wide application in the treatment of tuberculosis and also exhibits fungicidal activity (Edwards *et al.*, 1975; Kushner *et al.*, 1952). A series of similar pyrazinylcarboxylic acid–hydrazone complexes has been reported previously (Gardner *et al.*, 1956). Here, we report the structure of the title compound, (I).



(I)

Excluding methyl H atoms, the molecule is almost planar, with a dihedral angle of 8.32 (3)° between the pyrazine and benzene rings. The molecules are held together by intermolecular C—H···N and C—H···O hydrogen bonds (Fig. 2 and Table 1)

The molecules are stacked in an antiparallel fashion, with a pyrazine-to-benzene ring centroid–centroid separation of 3.676 Å and a pyrazine-to-pyrazine ring separation of 4.013 Å, indicating the presence of face-to-face π–π stacking interactions (Fig. 3).

Experimental

A mixture of pyrazine-2-carboxylic acid hydrazide (0.01 mol, 1.38 g) and 4-dimethylaminobenzaldehyde (0.01 mol, 1.49 g) in methanol was refluxed for 2 h. The solid material obtained on cooling was filtered, washed with ethanol–diethyl ether (1:1), dried and crystallized from methanol (yield 88%, m.p. 526–528 K). The compound (1.0 mmol, 0.268 g) was dissolved in methanol (30 ml) and left to stand at room temperature for one week, after which yellow block-

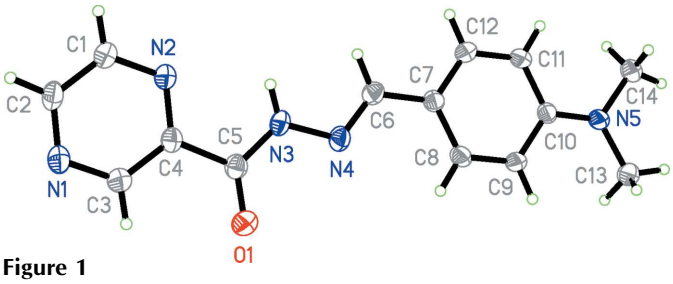


Figure 1
The structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

shaped single crystals formed; these were collected and washed with diethyl ether for X-ray diffraction analysis.

Crystal data

$C_{14}H_{15}N_5O$
M_r = 269.31
Triclinic, $P\overline{1}$
a = 6.049 (2) Å
b = 10.142 (4) Å
c = 11.047 (4) Å
α = 92.547 (6)°
β = 96.063 (6)°
γ = 101.286 (6)°
V = 659.4 (4) Å^3
Z = 2
D_x = 1.356 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
Block, yellow
0.22 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan *SADABS* (Sheldrick, 1996)
T_{min} = 0.980, T_{max} = 0.986
3389 measured reflections
2318 independent reflections
1457 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.133
S = 1.00
2318 reflections
184 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0693P)^2 + 0.0644P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.014 (5)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O1^{i}	0.93	2.44 (1)	3.300 (11)	155 (1)
C2—H2···N1^{ii}	0.93	2.67 (1)	3.486 (6)	148 (1)

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

All H atoms were initially located in a difference Fourier map. The H atoms were then constrained to an ideal geometry, with N—H = 0.86 Å, C(CH$_3$)—H = 0.96 Å, C(phenyl)—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; 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*.

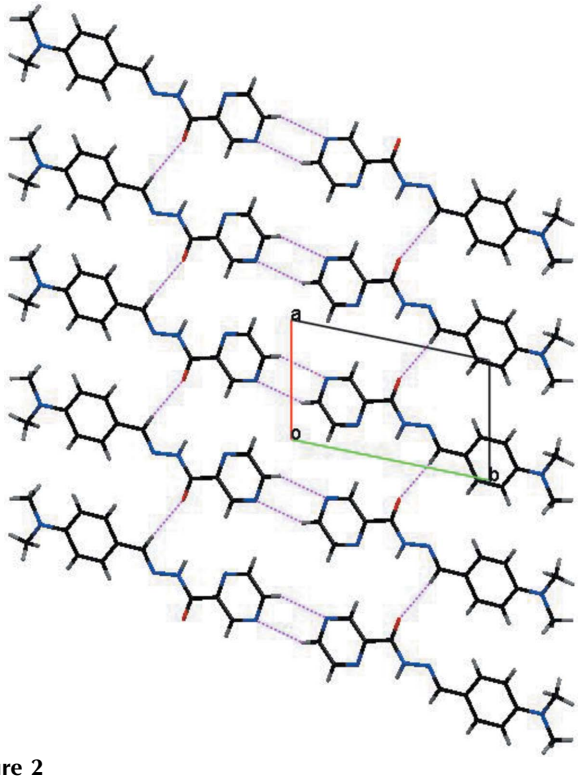


Figure 2
Intermolecular hydrogen bonds (dashed lines).

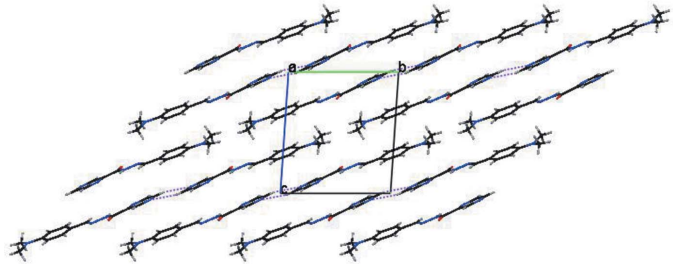


Figure 3
The packing of the title compound, viewed down the *a* axis.

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