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5-Methoxysalicylaldehyde 3-methoxybenzoylhydrazone

Hapipah M. Ali, Subramaniam Puvaneswary, Wan Jefri Basirun and Seik Weng Ng*

Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.124
Data-to-parameter ratio = 12.1

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

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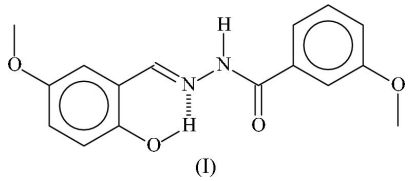
The molecules of the title compound, $C_{16}H_{16}N_2O_4$, are linked by hydrogen bonds into a zigzag chain running along the *c* axis of the monoclinic cell.

Comment

The report on 3-methoxysalicylaldehyde 4-methoxybenzoylhydrazone monohydrate noted that the planar conformations of the Schiff bases that are derived from the condensation of salicylaldehydes with benzoylhydrazines are a result of hydrogen bonds originating from solvent molecules that contribute to stabilizing the structure (Huo *et al.*, 2004). The parent salicylaldehyde benzoylhydrazone is not flat (Lyubchova *et al.*, 1995), and neither is the title compound, 5-methoxysalicylaldehyde 3-methoxybenzoylhydrazone (Fig. 1).



(I)

The aromatic ring having the hydroxy substituent is twisted by 20.0 (1)° with respect to the planar —N═N—C(═O)– fragment, whereas the other aromatic ring is twisted by 31.1 (1)°. The crystal structure features a long *b* axis; adjacent molecules interact *via* hydrogen bonds to form a zigzag chain along the *c* axis (Fig. 2).

Experimental

5-Methoxysalicyldehyde (0.30 g, 1.97 mmol) and 3-methoxybenzoylhydrazide (0.33 g, 1.97 mmol) were heated in ethanol. The title

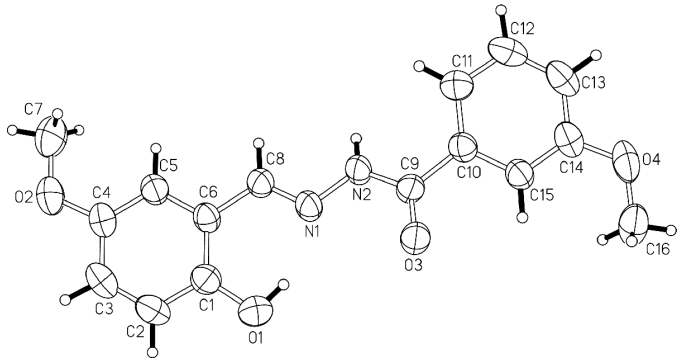


Figure 1
ORTEPII plot (Johnson, 1976) of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii.

compound separated from the cool solution as yellow prism-shaped crystals.

Crystal data

$C_{16}H_{16}N_2O_4$	D_x = 1.360 Mg m^{-3}
M_r = 300.31	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 3157 reflections
a = 6.4024 (4) Å	θ = 2.6–27.1°
b = 31.441 (2) Å	μ = 0.10 mm^{-1}
c = 7.3660 (5) Å	T = 295 (2) K
β = 98.330 (1)°	Prism, yellow
V = 1467.1 (2) Å^3	0.48 × 0.32 × 0.21 mm
Z = 4	

Data collection

Bruker SMART area-detector diffractometer	2285 reflections with $I > 2\sigma(I)$
	R_{int} = 0.016
φ and ω scans	θ_{max} = 27.1°
Absorption correction: none	$h = -8 \rightarrow 6$
7971 measured reflections	$k = -25 \rightarrow 40$
3190 independent reflections	$l = -8 \rightarrow 9$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0681P)^2 + 0.1473P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.041	
$wR(F^2)$ = 0.124	
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.001
3190 reflections	$\Delta\rho_{max}$ = 0.16 e Å^{-3}
263 parameters	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
All H-atom parameters refined	

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1o···N1	0.86 (1)	1.84 (1)	2.626 (2)	151 (2)
N2—H2n···O3^{i}	0.86 (1)	2.04 (1)	2.869 (2)	164 (2)

Symmetry code: (i) $x - \frac{1}{2}, \frac{1}{2} - y, z - \frac{1}{2}$.

The carbon-bound H atoms were refined with a distance restraint of 0.95 (1) Å and the nitrogen- and oxygen-bound H atoms with a distance restraint of 0.85 (1) Å.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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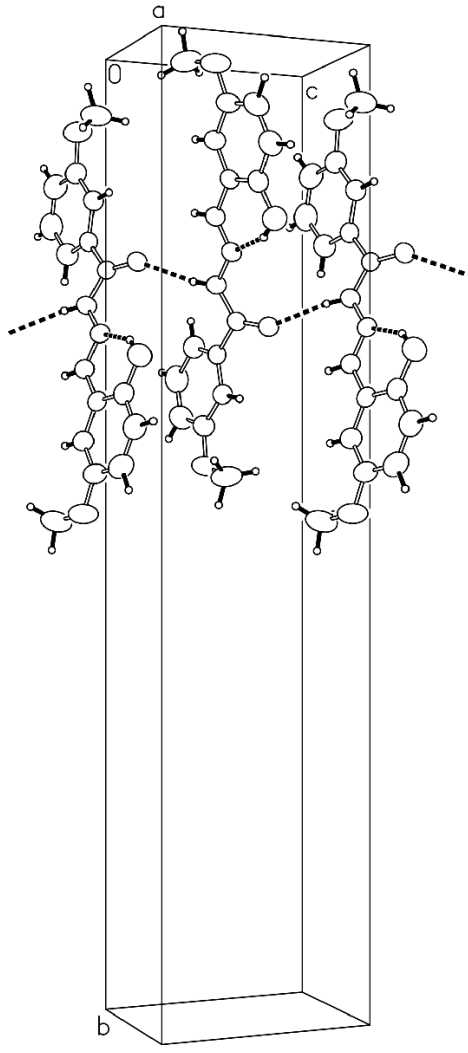

Figure 2
ORTEPII (Johnson, 1976) plot of the hydrogen-bonded chain (dashed lines) in (I).

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