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2-(5-Formyl-2-methoxyphenoxy)acetonitrile

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.130
Data-to-parameter ratio = 13.0

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

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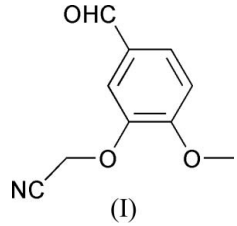
The title compound, $C_{10}H_9NO_3$, crystallizes with two molecules in the asymmetric unit. Intermolecular C—H···O and C—H···(O,O) interactions help to consolidate the crystal packing.

Comment

There has been a steady growth of interest in the synthesis, structure, and reactivity of Schiff bases due to their potential applications in areas such as biological modeling, catalysis, and molecular magnets (Jones *et al.*, 1979; Larson & Pecoraro, 1991). Consequently, a significant effort has been devoted to the synthesis of new Schiff base derivatives (Santos *et al.*, 2001).



(I)

As a part of our interest in the coordination properties of Schiff bases functioning as ligands, we investigated the title compound, (I), used as a precursor in the preparation of Schiff bases.

The asymmetric unit of (I) consists of two independent molecules, which are similar to each other. All the bond lengths and angles are within the normal ranges (Allen *et al.*, 1987). Both of the vanillin groups are essentially planar, with an r.m.s. deviation for fitted atoms of 0.0114 Å for C1–C6/C8/O1/O2 and 0.0153 Å for C11–C16/C18/O4/O5. The dihedral angle between the two vanillin mean planes is 12.77 (8)°.

Various C—H···O and bifurcated C—H···(O,O) intermolecular interactions are found in the crystal structure of (I) (Table 1). These result in one-dimensional chains of molecules propagating along [010] (Fig. 2).

Experimental

An anhydrous acetonitrile solution (50 ml) of 3-hydroxy-4-methoxybenzaldehyde (1.52 g, 10 mmol) was added dropwise to a solution (100 ml) of 2-chloroacetonitrile (0.76 g, 10 mmol) and potassium carbonate (1.38 g, 10 mmol) in acetonitrile over a period of 30 min, and the mixture refluxed for 24 h under a nitrogen atmosphere. The solvent was removed and the resultant mixture poured into ice–water (100 ml). The pale-yellow precipitate was then isolated, recrystallized from acetonitrile, and dried in a vacuum to

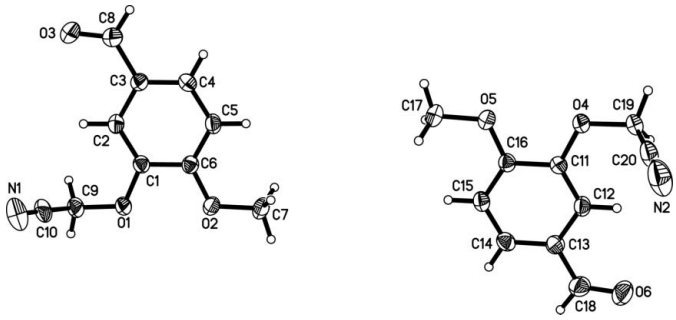


Figure 1
The asymmetric unit of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

give the pure compound in 52% yield. Colorless single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{10}H_9NO_3$	V = 953.9 (4) Å^3
M_r = 191.18	Z = 4
Triclinic, $P\overline{1}$	D_x = 1.331 Mg m^{-3}
a = 8.428 (2) Å	Mo $K\alpha$ radiation
b = 10.138 (3) Å	μ = 0.10 mm^{-1}
c = 12.629 (3) Å	T = 294 (2) K
α = 69.136 (4)°	Block, colorless
β = 84.967 (4)°	0.26 × 0.24 × 0.14 mm
γ = 71.163 (4)°	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	4846 measured reflections
ω scans	3322 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	2166 reflections with $I > 2\sigma(I)$
T_{min} = 0.958, T_{max} = 0.986	R_{int} = 0.019
	θ_{max} = 25.0°

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0578P)^2 + 0.1537P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.045	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.130	$\Delta\rho_{max}$ = 0.15 e Å^{-3}
S = 1.04	$\Delta\rho_{min}$ = −0.21 e Å^{-3}
3322 reflections	
255 parameters	
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
C19—H19A···O2^{i}	0.97	2.39	3.330 (2)	162
C19—H19A···O1^{i}	0.97	2.52	3.168 (3)	125
C9—H9A···O5^{ii}	0.97	2.46	3.410 (2)	168
C9—H9A···O4^{ii}	0.97	2.49	3.206 (3)	131
C19—H19B···O3^{iii}	0.97	2.48	2.985 (3)	112
C9—H9B···O6^{iv}	0.97	2.49	3.036 (3)	116

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

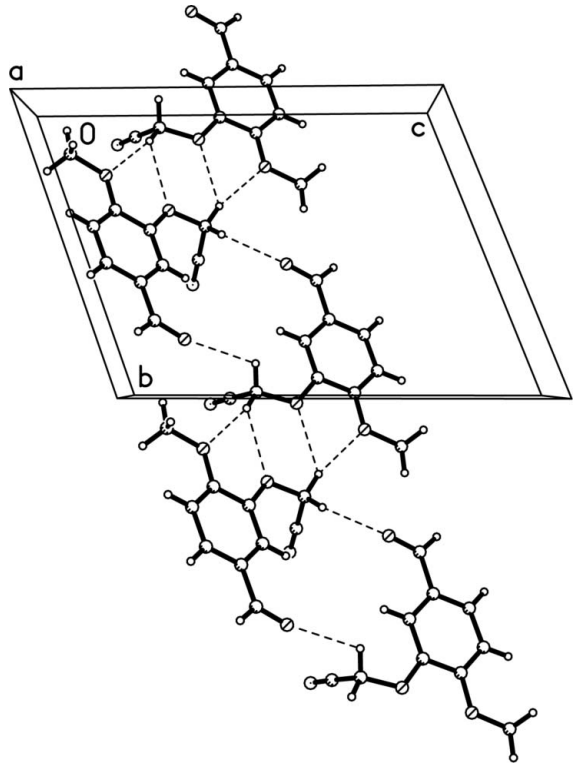


Figure 2
Packing diagram for (I), with C—H···O interactions drawn as dashed lines.

H atoms were included in calculated positions (C—H = 0.93–0.97 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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