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2-Amino-3-(4-methoxybenzylideneamino)-butenedinitrile

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In the title compound, $C_{12}H_{10}N_4O$, the structure is stabilized by an extensive network of N—H···N and N—H···O hydrogen bonds, forming columnar stacks down the *c* axis. As a powder, the compound exhibits second-harmonic generation efficiency.

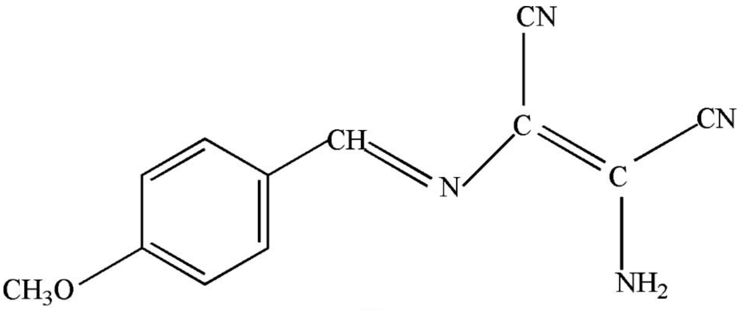
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.048
wR factor = 0.127
Data-to-parameter ratio = 9.0

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

Comment

2-Amino-3-(4-methoxybenzylideneamino)butenedinitrile belongs to a class of compounds that are useful for the synthesis of dyes and pharamceuticals (Begland *et al.*, 1974; Begland & Del, 1975). The donor methoxy group and the nitrile acceptor unit are connected *via* a conjugated system such that the molecule has a pemanent dipole and may display non-linear optical properties. We have an interest in molecules containing the diaminomaleonitrile group (Shi *et al.*, 2006) and report here the structure of the related title compound, (I) (Fig. 1).



(I)

All non-H atoms of the molecule are coplanar, with a maximum deviation of 0.143 (4) Å for atom N3 from the molecular plane. The structure is stabilized by an extensive network of N—H···N and N—H···O hydrogen bonds (Table 1). The planar molecules stack in columns down the *c* axis. As a powder, this material displays second-harmonic generation with an intensity 0.72 times that of urea.

Experimental

4-Methoxybenzaldehyde (4.2 g, 0.0308 mol) and diaminomaleonitrile (3.3 g, 0.0305 mol) were dissolved in ethanol (70 ml) and refluxed for 30 min. The crude product was filtered off, washed with ethanol and dissolved in methanol. Yellow single crystals were obtained on standing at room temperature for two weeks. Analysis found: C 63.36, H 4.25, N 25.15%; calculated for $C_{12}H_{10}N_4O$: C 63.70, H 4.46, N 24.77%. The IR stretching vibrations of the nitrile groups and the C═N bond appeared at 2205 and 1611 cm^{-1}, respectively.

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Crystal data

$C_{12}H_{10}N_4O$
$M_r = 226.24$
Orthorhombic, $Pna2_1$
$a = 11.108$ (2) Å
$b = 25.481$ (5) Å
$c = 4.0203$ (8) Å
$V = 1137.9$ (4) Å^3

$Z = 4$
$D_x = 1.321$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 298$ (2) K
Prism, yellow
0.35 × 0.21 × 0.12 mm

Data collection

Bruker SMART APEX CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.969$, $T_{max} = 0.989$

6445 measured reflections
1403 independent reflections
1361 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 27.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.127$
$S = 1.31$
1403 reflections
156 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0549P)^2 + 0.195P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.011$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.033 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H5B···N2^{i}	0.86	2.17	3.012 (4)	166
N4—H6A···O1^{ii}	0.86	2.46	3.022 (3)	124

Symmetry codes: (i) $x - \frac{1}{2}, -y + \frac{3}{2}, z - 1$; (ii) $-x, -y + 1, z - \frac{1}{2}$.

In the absence of significant anomalous dispersion effects, Freidel pairs were merged. The H atoms were placed in calculated positions and refined as riding, with C—H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for the methyl group, N—H = 0.86 Å and $U_{iso}(H) = 1.2U_{eq}(N)$ for the amino group, and C—H = 0.93° $U_{iso}(H) = 1.2U_{eq}(C)$ for other H atoms.

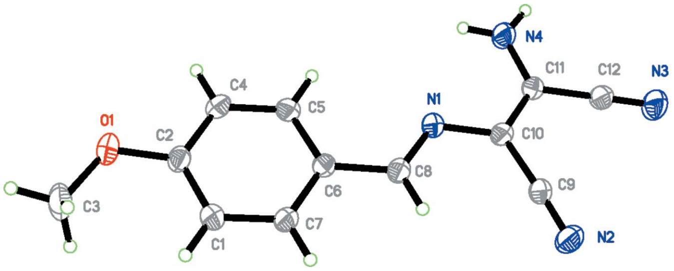

Figure 1
The molecular structure of (I), showing the atom-numbering scheme, with displacement ellipsoids drawn at the 30% probability level.

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

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