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# 2-Amino-4,5-dimethoxybenzonitrile

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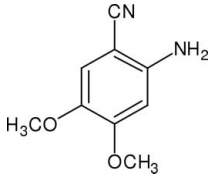
Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.036; $wR$ factor = 0.097; data-to-parameter ratio = 14.6.

The geometric parameters of the title compound, $C_9H_{10}N_2O_2$, which crystallizes with two molecules in the asymmetric unit, are in the usual ranges. The molecules are essentially planar (r.m.s. deviations for all non-H atoms are 0.084 and 0.110 Å for the two molecules in the asymmetric unit). The crystal packing is stabilized by N—H···O hydrogen bonds.

## Related literature

For related literature, see: Brewis *et al.* (2003); Britton *et al.* (2004); İkizler & Sancak (1992, 1995, 1998); Jin *et al.* (1994); Sancak (2005); Urbina *et al.* (2001); Ustabaş *et al.* (2004).




## Experimental

### Crystal data

$C_9H_{10}N_2O_2$
$M_r$ = 178.19
Monoclinic, $P2_1/c$
$a$ = 13.2649 (9) Å
$b$ = 17.0653 (9) Å
$c$ = 7.9635 (5) Å
$\beta$ = 96.769 (5)°
$V$ = 1790.13 (19) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 173 (2) K
0.33 × 0.29 × 0.24 mm

### Data collection

STOE IPDS II two-circle-diffractometer
Absorption correction: none
23314 measured reflections
3722 independent reflections
3163 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.038

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.097
$S$ = 1.02
3722 reflections
255 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.15 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1$A$···O2$A^{i}$ | 0.907 (17) | 2.336 (17) | 3.2296 (14) | 168.1 (14) |
| N1—H1$B$···O2$A$ | 0.916 (16) | 2.540 (16) | 3.3954 (13) | 155.7 (13) |
| N1—H1$B$···O1$A$ | 0.916 (16) | 2.597 (15) | 3.1979 (13) | 123.7 (12) |
| N1$A$—H1$C$···N2$A^{ii}$ | 0.876 (18) | 2.738 (18) | 3.4217 (17) | 135.9 (14) |
| N1$A$—H1$D$···O1$^{iii}$ | 0.894 (17) | 2.257 (17) | 3.0036 (13) | 140.9 (14) |
| N1$A$—H1$D$···O2$^{iii}$ | 0.894 (17) | 2.514 (17) | 3.2971 (13) | 146.7 (14) |

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

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

ANM thanks SeQuent Scientific Ltd, Mangalore for the sample.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2463).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, o4553 [ **doi:10.1107/S1600536807054827** ]

# 2-Amino-4,5-dimethoxybenzonitrile

**B. K. Sarojini, B. Narayana, A. N. Mayekar, H. S. Yathirajan and M. Bolte**

## Comment

Nitriles are close relatives of azoles and hydrazones and are parent compounds for the preparation of various functional organic materials having triazole, imidazole or thidiazole moieties (İkizler & Sancak, 1992; 1995; 1998). The synthesis of new azoles has been a very active area of research and an important aspect is the incorporation of functional units such as, cyanomethyl group in ravuconazol (Urbina *et al.*, 2001). Nitrile derivatives have many industrial applications. For example, phthalonitriles have been used as starting materials for phthalocyanines (Jin *et al.*, 1994), which are important components for dyes, pigments, gas sensors, optical limiters and liquid crystals. They are also used in medicine as singlet oxygen photosensitizers for photodynamic therapy (Brewis *et al.*, 2003). Some related crystal structures, *viz*., (2-cyanomethoxy-6-methoxyphenoxy)acetonitrile (Sancak, 2005), *p*-decylphenyl isocyanide and *p*-decylbenzonitrile: isomorphous isonitrile/nitrile isomers (Britton *et al.*, 2004) and 2-[2-(cyanomethoxy)phenoxy]acetonitrile (Ustabaş *et al.*, 2004) have been reported. A new nitrile derivative was obtained from the industry as a gift sample and its structure is reported.

Geometric parameters of the title compound, which crystallizes with two molecules in the asymmetric unit, are in the usual ranges. The molecules are essentially planar (r.m.s. deviation for all non-H atoms 0.084Å and 0.110Å for the two molecules in the asymmetric unit). The crystal packing is stabilized by N—H···O hydrogen bonds.

## Experimental

2-Amino-4,5-dimethoxybenzonitrile was obtained as a gift sample from SeQuent Scientific Limited, Mangalore and was recrystallized from methanol by slow evaporation technique [m.p: 369–374 K]).

## Refinement

All H atoms were found in a difference map, but those bonded to C were geometrically positioned and refined with fixed individual displacement parameters [$U_{iso}$(H) = 1.2 or 1.5$U_{eq}$(C)] using a riding model with C—H = 0.95 or 0.98 Å. The H atoms of the amino group was freely refined.

## Figures

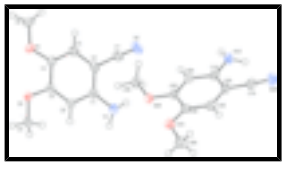


Fig. 1. Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level.

## 2-Amino-4,5-dimethoxybenzonitrile

*Crystal data*

| | |
|---|---|
| $C_9H_{10}N_2O_2$ | $F_{000}$ = 752 |
| $M_r$ = 178.19 | $D_x$ = 1.322 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 21499 reflections |
| $a$ = 13.2649 (9) Å | θ = 3.6–26.8º |
| $b$ = 17.0653 (9) Å | μ = 0.10 mm$^{-1}$ |
| $c$ = 7.9635 (5) Å | $T$ = 173 (2) K |
| β = 96.769 (5)º | Block, colourless |
| $V$ = 1790.13 (19) Å$^3$ | 0.33 × 0.29 × 0.24 mm |
| $Z$ = 8 | |

*Data collection*

| | |
|---|---|
| STOE IPDS II two-circle-diffractometer | 3163 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{int}$ = 0.038 |
| Monochromator: graphite | $\theta_{max}$ = 26.7º |
| $T$ = 173(2) K | $\theta_{min}$ = 3.5º |
| ω scans | $h$ = −16→16 |
| Absorption correction: none | $k$ = −21→21 |
| 23314 measured reflections | $l$ = −10→9 |
| 3722 independent reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.036 | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2)$ = 0.097 | $w = 1/[\sigma^2(F_o^2) + (0.060P)^2 + 0.2526P]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.02 | $(\Delta/\sigma)_{max} < 0.001$ |
| 3722 reflections | $\Delta\rho_{max}$ = 0.15 e Å$^{-3}$ |
| 255 parameters | $\Delta\rho_{min}$ = −0.21 e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*Special details*

**Experimental**. ;

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on $F^2$, conventional *R*-factors *R* are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.07571 (6) | 0.74641 (5) | 0.29441 (12) | 0.0305 (2) |
| O2 | 0.06985 (6) | 0.59747 (5) | 0.23025 (10) | 0.02477 (19) |
| N1 | 0.38490 (8) | 0.54952 (7) | 0.58981 (14) | 0.0286 (2) |
| H1A | 0.3905 (12) | 0.5060 (10) | 0.526 (2) | 0.038 (4)* |
| H1B | 0.4457 (12) | 0.5714 (9) | 0.632 (2) | 0.034 (4)* |
| N2 | 0.46025 (9) | 0.73153 (8) | 0.77100 (17) | 0.0435 (3) |
| C1 | 0.31110 (8) | 0.60122 (7) | 0.51816 (14) | 0.0211 (2) |
| C2 | 0.31248 (8) | 0.68144 (7) | 0.55662 (15) | 0.0233 (2) |
| C3 | 0.23499 (8) | 0.73219 (7) | 0.48324 (15) | 0.0251 (2) |
| H3 | 0.2378 | 0.7865 | 0.5099 | 0.030* |
| C4 | 0.15563 (8) | 0.70339 (6) | 0.37346 (14) | 0.0225 (2) |
| C5 | 0.15205 (8) | 0.62171 (7) | 0.33777 (14) | 0.0204 (2) |
| C6 | 0.22811 (8) | 0.57221 (6) | 0.40866 (14) | 0.0214 (2) |
| H6 | 0.2244 | 0.5178 | 0.3832 | 0.026* |
| C7 | 0.39404 (9) | 0.71128 (7) | 0.67434 (16) | 0.0286 (3) |
| C8 | 0.08316 (10) | 0.83018 (7) | 0.30592 (17) | 0.0319 (3) |
| H8A | 0.0823 | 0.8464 | 0.4238 | 0.048* |
| H8B | 0.0256 | 0.8540 | 0.2358 | 0.048* |
| H8C | 0.1467 | 0.8474 | 0.2660 | 0.048* |
| C9 | 0.05401 (9) | 0.51431 (7) | 0.21645 (17) | 0.0286 (3) |
| H9A | 0.1075 | 0.4908 | 0.1579 | 0.043* |
| H9B | −0.0123 | 0.5039 | 0.1523 | 0.043* |
| H9C | 0.0560 | 0.4915 | 0.3298 | 0.043* |
| O1A | 0.58742 (6) | 0.49611 (5) | 0.81914 (11) | 0.0304 (2) |
| O2A | 0.63026 (6) | 0.61035 (5) | 0.62874 (10) | 0.0270 (2) |
| N1A | 0.88591 (8) | 0.71281 (6) | 1.06092 (15) | 0.0286 (2) |
| H1C | 0.9030 (12) | 0.7465 (10) | 0.986 (2) | 0.038 (4)* |
| H1D | 0.9361 (12) | 0.6981 (10) | 1.139 (2) | 0.038 (4)* |
| N2A | 0.87001 (9) | 0.59744 (7) | 1.42142 (14) | 0.0371 (3) |
| C1A | 0.81333 (8) | 0.65744 (6) | 1.00388 (14) | 0.0220 (2) |
| C2A | 0.78575 (8) | 0.59755 (7) | 1.11092 (14) | 0.0226 (2) |
| C3A | 0.71054 (8) | 0.54145 (7) | 1.05269 (15) | 0.0246 (2) |
| H3A | 0.6942 | 0.5004 | 1.1254 | 0.030* |
| C4A | 0.66133 (8) | 0.54648 (6) | 0.89099 (15) | 0.0229 (2) |
| C5A | 0.68523 (8) | 0.60922 (6) | 0.78508 (14) | 0.0217 (2) |

| | | | | |
|---|---|---|---|---|
| C6A | 0.76065 (8) | 0.66260 (6) | 0.83953 (14) | 0.0224 (2) |
| H6A | 0.7771 | 0.7031 | 0.7656 | 0.027* |
| C7A | 0.83205 (9) | 0.59568 (7) | 1.28329 (15) | 0.0266 (3) |
| C8A | 0.57605 (10) | 0.42399 (8) | 0.9070 (2) | 0.0380 (3) |
| H8A1 | 0.6417 | 0.3971 | 0.9254 | 0.057* |
| H8A2 | 0.5267 | 0.3906 | 0.8393 | 0.057* |
| H8A3 | 0.5520 | 0.4350 | 1.0163 | 0.057* |
| C9A | 0.64180 (10) | 0.67832 (8) | 0.52425 (16) | 0.0313 (3) |
| H9A1 | 0.6245 | 0.7257 | 0.5844 | 0.047* |
| H9A2 | 0.5964 | 0.6736 | 0.4183 | 0.047* |
| H9A3 | 0.7122 | 0.6818 | 0.4992 | 0.047* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0276 (4) | 0.0193 (4) | 0.0418 (5) | 0.0027 (3) | −0.0070 (4) | 0.0019 (3) |
| O2 | 0.0227 (4) | 0.0215 (4) | 0.0277 (4) | 0.0003 (3) | −0.0073 (3) | 0.0001 (3) |
| N1 | 0.0231 (5) | 0.0303 (5) | 0.0301 (6) | 0.0035 (4) | −0.0061 (4) | −0.0019 (4) |
| N2 | 0.0316 (6) | 0.0483 (7) | 0.0477 (7) | −0.0039 (5) | −0.0069 (5) | −0.0177 (6) |
| C1 | 0.0193 (5) | 0.0258 (5) | 0.0183 (5) | 0.0003 (4) | 0.0018 (4) | 0.0006 (4) |
| C2 | 0.0196 (5) | 0.0272 (6) | 0.0228 (6) | −0.0038 (4) | 0.0013 (4) | −0.0024 (4) |
| C3 | 0.0250 (5) | 0.0204 (5) | 0.0299 (6) | −0.0035 (4) | 0.0037 (5) | −0.0021 (4) |
| C4 | 0.0214 (5) | 0.0212 (5) | 0.0246 (6) | 0.0011 (4) | 0.0012 (4) | 0.0026 (4) |
| C5 | 0.0192 (5) | 0.0232 (5) | 0.0182 (5) | −0.0015 (4) | 0.0000 (4) | −0.0001 (4) |
| C6 | 0.0222 (5) | 0.0200 (5) | 0.0214 (5) | 0.0007 (4) | 0.0004 (4) | −0.0014 (4) |
| C7 | 0.0244 (5) | 0.0293 (6) | 0.0318 (7) | −0.0009 (5) | 0.0019 (5) | −0.0062 (5) |
| C8 | 0.0365 (6) | 0.0188 (6) | 0.0400 (7) | 0.0044 (5) | 0.0036 (5) | −0.0002 (5) |
| C9 | 0.0282 (6) | 0.0218 (6) | 0.0328 (6) | 0.0001 (4) | −0.0094 (5) | −0.0058 (5) |
| O1A | 0.0284 (4) | 0.0273 (4) | 0.0339 (5) | −0.0062 (3) | −0.0030 (4) | 0.0005 (4) |
| O2A | 0.0282 (4) | 0.0269 (4) | 0.0238 (4) | 0.0015 (3) | −0.0061 (3) | 0.0025 (3) |
| N1A | 0.0261 (5) | 0.0265 (5) | 0.0313 (6) | −0.0031 (4) | −0.0052 (4) | 0.0020 (4) |
| N2A | 0.0396 (6) | 0.0458 (7) | 0.0245 (6) | 0.0030 (5) | −0.0018 (5) | 0.0021 (5) |
| C1A | 0.0192 (5) | 0.0210 (5) | 0.0254 (6) | 0.0041 (4) | 0.0009 (4) | −0.0014 (4) |
| C2A | 0.0213 (5) | 0.0257 (6) | 0.0203 (5) | 0.0047 (4) | 0.0003 (4) | −0.0002 (4) |
| C3A | 0.0252 (5) | 0.0241 (5) | 0.0248 (6) | 0.0015 (4) | 0.0041 (4) | 0.0037 (4) |
| C4A | 0.0198 (5) | 0.0217 (5) | 0.0269 (6) | 0.0004 (4) | 0.0014 (4) | −0.0019 (4) |
| C5A | 0.0208 (5) | 0.0230 (5) | 0.0207 (5) | 0.0061 (4) | −0.0001 (4) | −0.0010 (4) |
| C6A | 0.0226 (5) | 0.0208 (5) | 0.0235 (6) | 0.0029 (4) | 0.0015 (4) | 0.0028 (4) |
| C7A | 0.0258 (5) | 0.0293 (6) | 0.0249 (6) | 0.0037 (4) | 0.0035 (5) | 0.0016 (5) |
| C8A | 0.0356 (7) | 0.0248 (6) | 0.0523 (9) | −0.0058 (5) | −0.0001 (6) | 0.0031 (6) |
| C9A | 0.0339 (6) | 0.0328 (6) | 0.0254 (6) | 0.0046 (5) | −0.0041 (5) | 0.0079 (5) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C4 | 1.3790 (13) | O1A—C4A | 1.3767 (14) |
| O1—C8 | 1.4353 (14) | O1A—C8A | 1.4323 (16) |
| O2—C5 | 1.3686 (13) | O2A—C5A | 1.3668 (13) |
| O2—C9 | 1.4369 (14) | O2A—C9A | 1.4461 (15) |
| N1—C1 | 1.3895 (15) | N1A—C1A | 1.3867 (15) |

| | | | |
|---|---|---|---|
| N1—H1A | 0.907 (17) | N1A—H1C | 0.876 (18) |
| N1—H1B | 0.916 (16) | N1A—H1D | 0.894 (17) |
| N2—C7 | 1.1506 (17) | N2A—C7A | 1.1549 (16) |
| C1—C2 | 1.4023 (16) | C1A—C2A | 1.4067 (16) |
| C1—C6 | 1.4110 (15) | C1A—C6A | 1.4118 (15) |
| C2—C3 | 1.4165 (16) | C2A—C3A | 1.4205 (16) |
| C2—C7 | 1.4387 (16) | C2A—C7A | 1.4365 (16) |
| C3—C4 | 1.3774 (16) | C3A—C4A | 1.3761 (16) |
| C3—H3 | 0.9500 | C3A—H3A | 0.9500 |
| C4—C5 | 1.4222 (16) | C4A—C5A | 1.4217 (16) |
| C5—C6 | 1.3841 (15) | C5A—C6A | 1.3844 (16) |
| C6—H6 | 0.9500 | C6A—H6A | 0.9500 |
| C8—H8A | 0.9800 | C8A—H8A1 | 0.9800 |
| C8—H8B | 0.9800 | C8A—H8A2 | 0.9800 |
| C8—H8C | 0.9800 | C8A—H8A3 | 0.9800 |
| C9—H9A | 0.9800 | C9A—H9A1 | 0.9800 |
| C9—H9B | 0.9800 | C9A—H9A2 | 0.9800 |
| C9—H9C | 0.9800 | C9A—H9A3 | 0.9800 |
| C4—O1—C8 | 117.24 (9) | C4A—O1A—C8A | 116.39 (10) |
| C5—O2—C9 | 116.42 (8) | C5A—O2A—C9A | 117.02 (9) |
| C1—N1—H1A | 113.0 (10) | C1A—N1A—H1C | 116.8 (10) |
| C1—N1—H1B | 116.0 (10) | C1A—N1A—H1D | 118.0 (11) |
| H1A—N1—H1B | 114.4 (14) | H1C—N1A—H1D | 115.3 (14) |
| N1—C1—C2 | 122.66 (10) | N1A—C1A—C2A | 121.11 (10) |
| N1—C1—C6 | 119.44 (10) | N1A—C1A—C6A | 120.65 (10) |
| C2—C1—C6 | 117.82 (10) | C2A—C1A—C6A | 118.13 (10) |
| C1—C2—C3 | 121.10 (10) | C1A—C2A—C3A | 120.98 (10) |
| C1—C2—C7 | 118.51 (10) | C1A—C2A—C7A | 118.86 (10) |
| C3—C2—C7 | 120.38 (10) | C3A—C2A—C7A | 120.11 (10) |
| C4—C3—C2 | 120.45 (10) | C4A—C3A—C2A | 120.06 (10) |
| C4—C3—H3 | 119.8 | C4A—C3A—H3A | 120.0 |
| C2—C3—H3 | 119.8 | C2A—C3A—H3A | 120.0 |
| C3—C4—O1 | 126.07 (10) | C3A—C4A—O1A | 125.87 (10) |
| C3—C4—C5 | 118.79 (10) | C3A—C4A—C5A | 119.20 (10) |
| O1—C4—C5 | 115.14 (9) | O1A—C4A—C5A | 114.92 (10) |
| O2—C5—C6 | 124.01 (10) | O2A—C5A—C6A | 124.35 (10) |
| O2—C5—C4 | 115.25 (9) | O2A—C5A—C4A | 114.76 (10) |
| C6—C5—C4 | 120.74 (10) | C6A—C5A—C4A | 120.87 (10) |
| C5—C6—C1 | 121.06 (10) | C5A—C6A—C1A | 120.65 (10) |
| C5—C6—H6 | 119.5 | C5A—C6A—H6A | 119.7 |
| C1—C6—H6 | 119.5 | C1A—C6A—H6A | 119.7 |
| N2—C7—C2 | 176.72 (14) | N2A—C7A—C2A | 177.18 (13) |
| O1—C8—H8A | 109.5 | O1A—C8A—H8A1 | 109.5 |
| O1—C8—H8B | 109.5 | O1A—C8A—H8A2 | 109.5 |
| H8A—C8—H8B | 109.5 | H8A1—C8A—H8A2 | 109.5 |
| O1—C8—H8C | 109.5 | O1A—C8A—H8A3 | 109.5 |
| H8A—C8—H8C | 109.5 | H8A1—C8A—H8A3 | 109.5 |
| H8B—C8—H8C | 109.5 | H8A2—C8A—H8A3 | 109.5 |
| O2—C9—H9A | 109.5 | O2A—C9A—H9A1 | 109.5 |

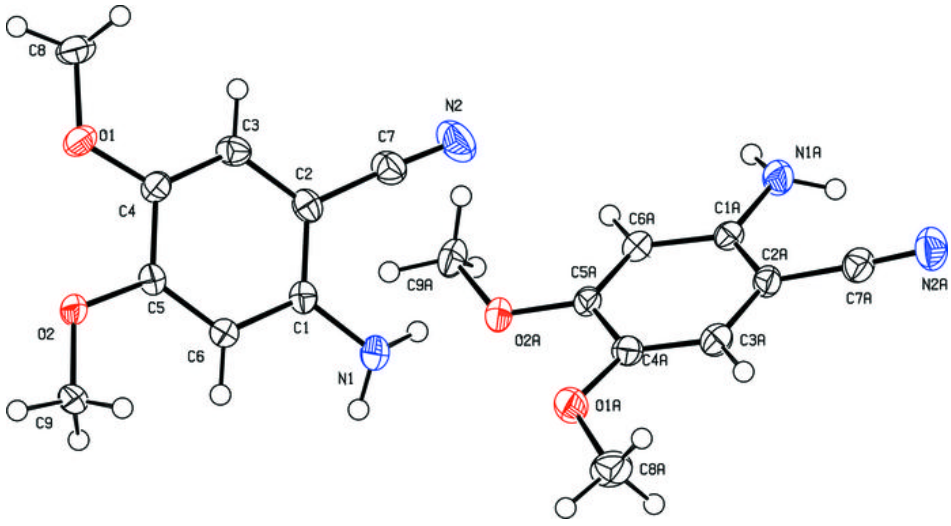
| | | | |
|---|---|---|---|
| O2—C9—H9B | 109.5 | O2A—C9A—H9A2 | 109.5 |
| H9A—C9—H9B | 109.5 | H9A1—C9A—H9A2 | 109.5 |
| O2—C9—H9C | 109.5 | O2A—C9A—H9A3 | 109.5 |
| H9A—C9—H9C | 109.5 | H9A1—C9A—H9A3 | 109.5 |
| H9B—C9—H9C | 109.5 | H9A2—C9A—H9A3 | 109.5 |
| N1—C1—C2—C3 | −178.93 (11) | N1A—C1A—C2A—C3A | 179.28 (10) |
| C6—C1—C2—C3 | −2.21 (16) | C6A—C1A—C2A—C3A | 3.07 (16) |
| N1—C1—C2—C7 | 0.37 (17) | N1A—C1A—C2A—C7A | 1.77 (16) |
| C6—C1—C2—C7 | 177.09 (10) | C6A—C1A—C2A—C7A | −174.44 (10) |
| C1—C2—C3—C4 | 0.76 (17) | C1A—C2A—C3A—C4A | −1.89 (16) |
| C7—C2—C3—C4 | −178.52 (11) | C7A—C2A—C3A—C4A | 175.59 (10) |
| C2—C3—C4—O1 | 179.78 (11) | C2A—C3A—C4A—O1A | 179.91 (10) |
| C2—C3—C4—C5 | 1.13 (17) | C2A—C3A—C4A—C5A | −1.31 (16) |
| C8—O1—C4—C3 | 10.31 (17) | C8A—O1A—C4A—C3A | −13.65 (17) |
| C8—O1—C4—C5 | −171.00 (10) | C8A—O1A—C4A—C5A | 167.52 (10) |
| C9—O2—C5—C6 | 11.52 (16) | C9A—O2A—C5A—C6A | −9.50 (15) |
| C9—O2—C5—C4 | −168.80 (10) | C9A—O2A—C5A—C4A | 172.09 (10) |
| C3—C4—C5—O2 | 178.75 (10) | C3A—C4A—C5A—O2A | −178.21 (10) |
| O1—C4—C5—O2 | −0.04 (14) | O1A—C4A—C5A—O2A | 0.71 (14) |
| C3—C4—C5—C6 | −1.55 (16) | C3A—C4A—C5A—C6A | 3.32 (16) |
| O1—C4—C5—C6 | 179.66 (10) | O1A—C4A—C5A—C6A | −177.76 (10) |
| O2—C5—C6—C1 | 179.73 (10) | O2A—C5A—C6A—C1A | 179.57 (10) |
| C4—C5—C6—C1 | 0.06 (17) | C4A—C5A—C6A—C1A | −2.12 (16) |
| N1—C1—C6—C5 | 178.63 (10) | N1A—C1A—C6A—C5A | −177.29 (10) |
| C2—C1—C6—C5 | 1.79 (16) | C2A—C1A—C6A—C5A | −1.06 (16) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1A···O2A$^{i}$ | 0.907 (17) | 2.336 (17) | 3.2296 (14) | 168.1 (14) |
| N1—H1B···O2A | 0.916 (16) | 2.540 (16) | 3.3954 (13) | 155.7 (13) |
| N1—H1B···O1A | 0.916 (16) | 2.597 (15) | 3.1979 (13) | 123.7 (12) |
| N1A—H1C···N2A$^{ii}$ | 0.876 (18) | 2.738 (18) | 3.4217 (17) | 135.9 (14) |
| N1A—H1D···O1$^{iii}$ | 0.894 (17) | 2.257 (17) | 3.0036 (13) | 140.9 (14) |
| N1A—H1D···O2$^{iii}$ | 0.894 (17) | 2.514 (17) | 3.2971 (13) | 146.7 (14) |

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*, −*y*+3/2, *z*−1/2; (iii) *x*+1, *y*, *z*+1.

**Fig. 1**


C8
O1
C3
C7
N2
C2
C4
C5
C1
C6
O2
C9
N1
C9A
O2A
C5A
C6A
C1A
N1A
C2A
C7A
N2A
C3A
C4A
O1A
C8A