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2-Amino-4,5-dimethoxybenzonitrile

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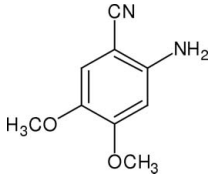
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.097; data-to-parameter ratio = 14.6.

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
β = 96.769 (5)°
V = 1790.13 (19) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 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—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) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (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).

References

Brewis, M., Helliwell, M. & McKeown, N. B. (2003). *Tetrahedron*, **59**, 3863–3872.
Britton, D., Sowa, J. R. & Mann, K. R. (2004). *Acta Cryst.* C**60**, o418–o420.
İkizler, A. A. & Sancak, K. (1992). *Monatsh. Chem.* **123**, 257–263.
İkizler, A. A. & Sancak, K. (1995). *Collect. Czech. Chem. Commun.* **60**, 903–909.
İkizler, A. A. & Sancak, K. (1998). *Rev. Roum. Chim.* **43**, 133–138.
Jin, Z., Nolan, K., McArthur, C. R., Lever, A. B. P. & Leznoff, C. C. (1994). *J. Organomet. Chem.* **468**, 205–212.
Sancak, K. (2005). *Acta Cryst.* E**61**, o2015–o2017.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stoe & Cie (2001). *X-AREA*. Stoe & Cie, Darmstadt, Germany.
Urbina, J. A., Payares, G., Sonja, A. R. L. & Pomanha, J. (2001). *Int. J. Antimicrob. Agents*, **21**, 27–38.
Ustabaş, R., Çoruh, U., Sancak, K., Er, M., Ünver, Y. & Yavuz, M. (2004). *Acta Cryst.* E**60**, o968–o970.

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supplementary materials

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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 1.5U_{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

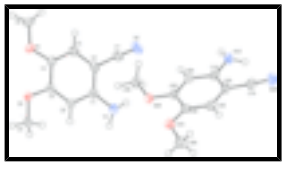


Fig. 1. Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level.

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 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	θ_{max} = 26.7º
T = 173(2) K	θ_{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	$w = 1/[\sigma^2(F_o^2) + (0.060P)^2 + 0.2526P]$ 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

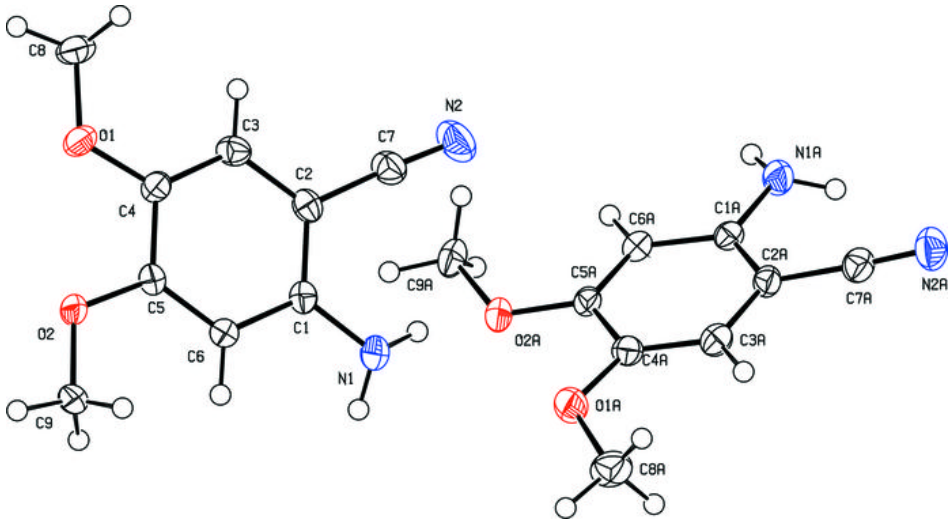
O2—C9—H9B	109.5	O2A—C9A—H9A2	109.5
H9A—C9—H9B	109.5	H9A1—C9A—H9A2	109.5
O2—C9—H9C	109.5	O2A—C9A—H9A3	109.5
H9A—C9—H9C	109.5	H9A1—C9A—H9A3	109.5
H9B—C9—H9C	109.5	H9A2—C9A—H9A3	109.5
N1—C1—C2—C3	−178.93 (11)	N1A—C1A—C2A—C3A	179.28 (10)
C6—C1—C2—C3	−2.21 (16)	C6A—C1A—C2A—C3A	3.07 (16)
N1—C1—C2—C7	0.37 (17)	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