Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(Cyanomethoxy)benzonitrile

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Received 9 January 2007
Accepted 15 January 2007

In the title compound, $C_9H_6N_2O$, two independent and almost identical molecules, pseudosymmetrically related by twofold rotation, form the asymmetric unit. The molecules adopt an overall L-shaped structure in which the cyanomethoxy residue is approximately perpendicular to the benzonitrile plane. The molecules assemble into dimers *via* C—H$\cdots$N and C—H$\cdots$O interactions, forming a sheet structure approximately in the (404) plane. Noteworthy π–π interactions result in two distinct types of offset π-stacking arrangements.

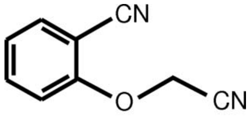
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
R factor = 0.067
wR factor = 0.170
Data-to-parameter ratio = 10.9

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

Comment

The title compound, (I), is an intermediate in the synthesis of various benzofuro[3,2-*d*]pyrimidine derivatives (Sangapure & Agasimundin, 1976). Two independent and almost identical molecules of (I), namely (I*A*) and (I*B*), form the asymmetric unit. In both of the molecules, the cyanomethoxy residue is approximately perpendicular to the benzonitrile plane, giving rise to an overall L-shaped structure (Fig. 1). The planar groups of (I*A*), *viz*. C1*A*—C7*A*/C9*A*/O1*A*/N2*A* and C7*A*/C8*A*/N1*A*, are inclined at 88.6 (7)° and those of (I*B*), *viz*. C1*B*–C7*B*/C9*B*/O1*B*/N2*B* and C7*B*/C8*B*/N1*B*, at 86.7 (10)°. The molecular geometry is largely unexceptional. The bond distances of conjugated pairs, *i.e.* $\cdots$C2*A*–C9*A*≡ and $\cdots$C2*B*–C9*B*≡ are 1.425 (5) and 1.431 (4) Å, respectively, and agree well with the reported average values (Allen *et al.*, 1987). The torsion angles describing the molecular conformation are as follows: C2*A*—C1*A*—O1*A*—C7*A* = 177.4 (3), C1*A*—O1*A*—C7*A*—C8*A* = −76.7 (4), C2*B*—C1*B*—O1*B*—C7*B* = 179.0 (3) and C1*B*—O1*B*—C7*B*—C8*B* = −75.9 (4)°.



(I)

In the crystal structure, two different types of dimers are formed: the first is between molecules (I*B*), related by an inversion center *via* C5*B*—H5*B*$\cdots$N1*B*$^{\rm v}$ interactions and characterized by an $R_2^2(16)$ graph set (Bernstein *et al.*, 1995), while the other, an asymmetric one of $R_2^2(10)$ type between (I*A*) and (I*B*), is formed by C7*A*—H7*A*2$\cdots$N2*B*$^{\rm ii}$ and C7*B*—H7*B*2$\cdots$O1*A*$^{\rm iv}$ interactions. The $R_2^2(16)$ dimers are interconnected by C7*A*—H7*A*1$\cdots$N2*A*$^{\rm i}$ and C7*B*—H7*B*1$\cdots$N2*B*$^{\rm iii}$ hydrogen bonds along the *b* axis, forming an $R_4^3(12)$ motif and giving a sheet structure approximately in the (404) plane (Fig. 2 and Table 1). π–π Interactions between benzene rings result in two distinct types of offset π-stacking arrangements. Aromatic

doi:10.1107/S1600536807001912

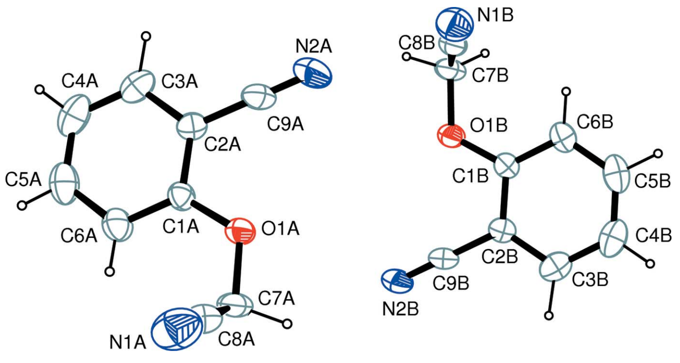


Figure 1
The asymmetric unit, showing the atom-numbering scheme and the relative orientation of molecules (I*A*) and (I*B*). Displacement ellipsoids are drawn at the 30% probability level.

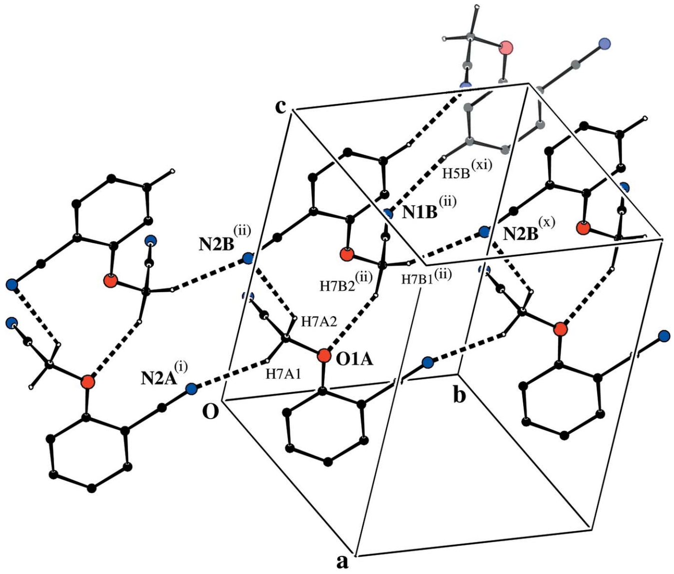


Figure 2
The crystal packing in (I), showing C—H$\cdots$N and C—H$\cdots$O hydrogen bonded molecular dimers and their association into a sheet structure approximately in the (404) plane. Molecules that do not form part of this sheet are shaded in gray. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted. Color key: C black, H white, N blue and O red. [Symmetry codes: (x) $x - 1, 1 + y, z$; (xi) $-x, 2 - y, 1 - z$.]

rings of inversion-related molecules of (I*A*) are stacked along the $[\bar{1}10]$ direction, while those of (I*B*) are arranged along the [100] direction (Fig. 3 and Table 2).

Molecules (I*A*) and (I*B*) are pseudosymmetrically related by twofold rotation with an angle of rotation of 179.1° and direction cosines, [−1, 0.39, −0.12] (Fig. 4). The r.m.s. deviation between (I*A*) and (I*B*) is 0.03 Å for all non-H atoms. The exceptional 'low-symmetry' crystal-packing arrangement with $Z' > 1$ has been observed in only 8% of all reported cases (Steiner, 2000; Aitipamula *et al.*, 2003; Steed, 2003). In the present case, we believe that the differential weak hydrogen-bonding patterns between (I*A*) and (I*B*) (Table 1) give rise to such 'low-symmetry' packing with $Z' = 2$.

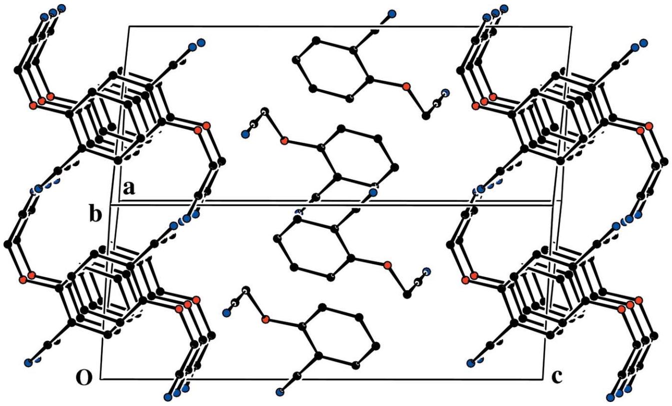


Figure 3
The two distinct types of offset π-stacking interactions of the aromatic rings in molecules (I*A*) and (I*B*). H atoms have been omitted.

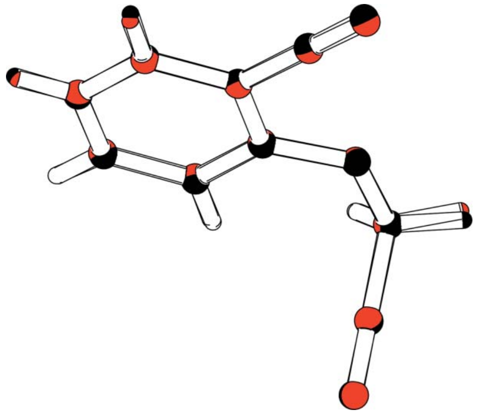


Figure 4
An overlay of the structures of molecules (I*A*) (red) and (I*B*) (black).

Experimental

The synthetic procedure for compound (I) is described in the literature (Sangapure & Agasimundin, 1976). Crystals were grown by slow evaporation of an ethyl acetate–petroleum ether

Crystal data

$C_9H_6N_2O$
$M_r = 158.16$
Triclinic, $P\bar{1}$
$a = 7.4807$ (8) Å
$b = 7.7018$ (8) Å
$c = 15.8021$ (17) Å
$\alpha = 86.934$ (2)°
$\beta = 85.235$ (2)°
$\gamma = 66.910$ (3)°
$V = 834.39$ (15) Å^3
$Z = 4$
$D_x = 1.259$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 295$ (2) K
Needle, colorless
0.28 × 0.14 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{\min} = 0.970$, $T_{\max} = 0.986$
5850 measured reflections
2887 independent reflections
1551 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.037$
$\theta_{\max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.067$
$wR(F^2) = 0.170$
$S = 1.01$
2887 reflections
265 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0772P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7A—H7A1···N2A^{i}	0.98 (3)	2.57 (3)	3.418 (5)	145 (2)
C7A—H7A2···N2B^{ii}	1.06 (3)	2.61 (4)	3.337 (5)	125 (3)
C7B—H7B1···N2B^{iii}	0.98 (3)	2.62 (3)	3.479 (5)	147 (2)
C7B—H7B2···O1A^{iv}	1.07 (5)	2.53 (4)	3.429 (5)	141 (3)
C5B—H5B···N1B^{v}	0.99 (4)	2.58 (3)	3.551 (6)	167 (3)

Symmetry codes: (i) $x, y-1, z$; (ii) $x-1, y, z$; (iii) $x, y+1, z$; (iv) $x+1, y, z$; (v) $-x+1, -y+2, -z+1$.

Table 2
Geometrical parameters of $\pi\cdots\pi$ interactions (Å, °).

	Centroid–centroid distance	Interplanar angle	Perpendicular distance
$Cg1\cdots Cg1^{vi}$	3.888 (2)	0	3.636
$Cg1\cdots Cg1^{vii}$	4.640 (2)	0	3.444
$Cg2\cdots Cg2^{vii}$	3.835 (2)	0	3.512
$Cg2\cdots Cg2^{ix}$	4.111 (2)	0	3.524

*Cg*1 and *Cg*2 are the centroids of rings (C1*A*-C6*A*) and (C1*B*-C6*B*), respectively. Symmetry codes: (vi) $-x, 1-y, -z$; (vii) $1-x, -y, -z$; (viii) $1-x, 1-y, 1-z$; (ix) $2-x, 1-y, 1-z$.

H atoms were located in difference syntheses, and refined isotropically [C—H = 0.92 (3)–1.07 (4) Å and U_{iso}(H) = 0.056 (8)–0.114 (13) Å^2].

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PLATON*.

We express our appreciation for the use of the CCD facility, set up under the IRPHA–DST program at the Indian Institute of Science, Bangalore. RSR acknowledges the Science and Engineering Research Council (DST), Government of India, for providing a Fast-Track Young Scientist grant.

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