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2-[2-(Cyanomethoxy)phenoxy]acetonitrile

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.048
wR factor = 0.107
Data-to-parameter ratio = 20.4

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

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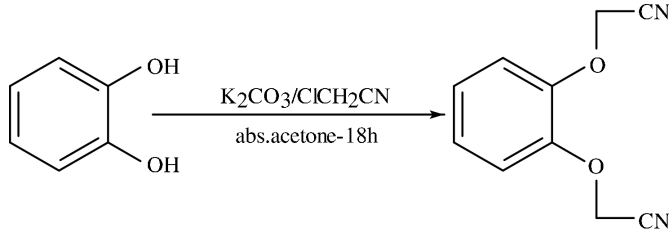
The title compound, $C_{10}H_8N_2O_2$, consisting of a benzene ring with two O—CH_2—CN *ortho* substituents, has approximately C_2 symmetry. The supramolecular structure of the compound is determined by two hydrogen bonds and two π–π stacking interactions.

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 one important aspect has been the incorporation of functional units, such as the cyanomethyl group in ravuconazol (Urbina *et al.*, 2001). Nitrile derivatives have found 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, and which are also used in medicine, as singlet oxygen photosensitisers for photodynamic therapy (PDT; Brewis *et al.*, 2003). Porphyrins are photosensitizers which are currently the subject of active research effort for possible use in PDT, because of their ability to localize in malignant tumours and to generate potent reactive species on excitation (Moan & Berg, 1992; Henderson & Dougherty, 1992; Levy, 1994; Jori, 1996). Some phthalocyanines have been used in the petroleum industry as catalysts, for the oxidation of sulfur compounds in the xerographic double layers of laser printers and copying machines, and as active materials in writable data-storage disks (Dandliker *et al.*, 1995). Against this background, we now report the synthesis and crystal structure analysis of the title compound, 2-[2-(cyanomethoxy)phenoxy]acetonitrile, (II).



(I) (II)

Compound (II) is composed of a benzene ring substituted by two O—CH_2—CN groups at atoms C1 and C6 (Fig. 1). As can be seen in Fig. 1, the molecule has approximately C_2 symmetry, with a twofold axis passing through the mid-points of the C3—C4 and C1—C6 bonds. The CH_2—C≡N moieties

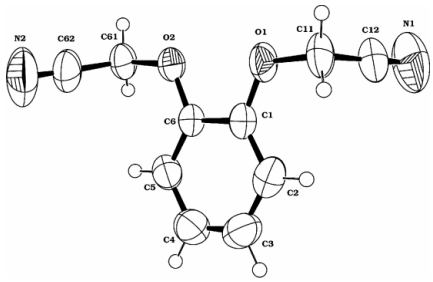


Figure 1
A view of the molecule of (II), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

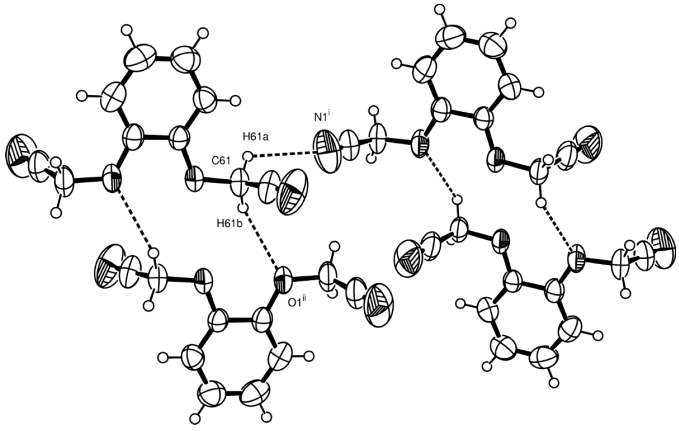


Figure 2
The hydrogen-bonding network (dashed lines) observed in (II).

are each almost linear, with C61—C62≡N2 and C11—C12≡N1 angles of 178.22 (21) and 177.81 (21)°, respectively. The C12≡N1 and C62≡N2 bond distances are 1.115 (3) and 1.120 (3) Å, respectively, similar to values reported in the literature (Çoruh *et al.*, 2002, 2003; Öztürk *et al.*, 1999; Subbiah Pandi *et al.*, 2002). The benzene ring is essentially planar, with a maximum deviation of 0.004 (1) Å for atom C6.

As can be seen from the packing diagram (Fig. 3), the molecules of (II) extend parallel to the *c* axis and are stacked along the *a* axis. In addition to dipole–dipole and van der Waals interactions, the crystal structure of (II) is stabilized by intermolecular C61—H61*A*···N1^{i} and C61—H61*B*···O1^{ii} hydrogen bonds (Fig. 2; symmetry codes as in Table 2) and two π–π stacking interactions. These π–π stacking interactions involve the benzene ring *R*1 at (*x*, *y*, *z*) and the symmetry-related rings *R*2 at ($x-\frac{1}{2}, \frac{1}{2}-y, z$) and *R*3 at ($\frac{1}{2}+x, \frac{1}{2}-y, z$). The distance between the centroids of rings *R*1 and *R*2 is 3.897 (1) Å, and that between the centroids of rings *R*1 and *R*3 is 3.877 (1) Å.

Experimental

A mixture of catechol, (I) (1.01 g, 0.01 mol), dissolved in acetone (300 ml), and powdered potassium carbonate (4.10 g, 0.03 mol) was stirred vigorously while heating at gentle reflux for 30 min. The reaction mixture was then cooled, chloroacetonitrile (1.50 g, 0.02 mol) was added and the mixture was refluxed with stirring for 20 h. After cooling, the reaction mixture was filtered, the filtrate was removed under reduced pressure and the residue was dried over $CaCl_2$. The solid residue was then recrystallized from acetone–carbon tetrachloride (1:1) to give (II) (yield 1.291 g, 74.02%; m.p. 355–356 K). Spectroscopic analysis: IR (KBr, ν, cm^{-1}): 3067 and 2959 (C—H), 2246 (C≡N), 1596 (C=C), 1113 (C—O—C), 744 (phenyl ring); ^{1}H NMR (DMSO-d_6, δ, p.p.m.): 5.18 (*s*, 4H, 2 O—CH_2), 7.10–7.22 (*d*, 4H, CH_{phenyl}); ^{13}C NMR (DMSO-d_6, δ, p.p.m.): 54.51 (2 O—CH_2), 115.31 (2 C≡N), 116.73 (phenyl$_{quaternary}$ C1 and C2), 123.45 (phenyl, C3 and C4), 146.40 (phenyl, C5 and C6).

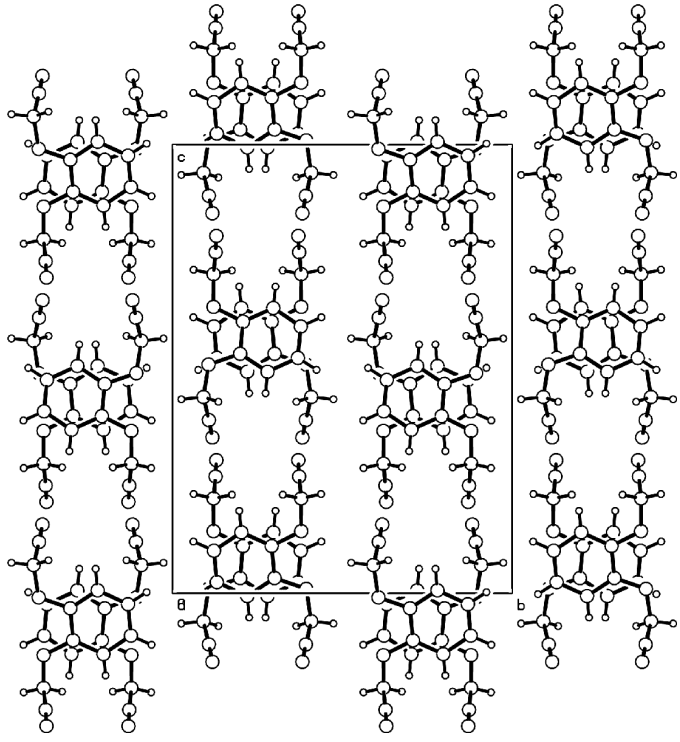


Figure 3
A packing diagram for (II), viewed along the [100] axis of the orthorhombic cell.

Crystal data

$C_{10}H_8N_2O_2$
M_r = 188.18
Orthorhombic, *Pcab*
a = 7.4940 (12) Å
b = 13.9150 (11) Å
c = 18.3770 (13) Å
V = 1916.34 (1) Å^3
Z = 8
D_x = 1.305 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 17 120 reflections
θ = 2–26°
μ = 0.09 mm^{-1}
T = 293 (2) K
Prism, colourless
0.35 × 0.30 × 0.20 mm

Data collection

Stoe IPDS 2 diffractometer
ω scans
Absorption correction: none
17 120 measured reflections
2592 independent reflections
1014 reflections with $I > 2\sigma(I)$
R_{int} = 0.100
θ_{max} = 29.3°
$h = -9 \rightarrow 10$
$k = -19 \rightarrow 19$
$l = -25 \rightarrow 25$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.107
S = 0.73
2592 reflections
127 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.049P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.3785 (18)	N1—C12	1.115 (3)
O1—C11	1.4107 (16)	N2—C62	1.120 (3)
O2—C6	1.3748 (18)	C1—C6	1.3942 (18)
O2—C61	1.4139 (16)	C3—C4	1.365 (3)
C1—O1—C11	118.73 (12)	O2—C6—C5	125.36 (12)
C6—O2—C61	117.98 (11)	O1—C11—C12	110.15 (13)
O1—C1—C2	126.19 (13)	N1—C12—C11	177.8 (2)
O1—C1—C6	113.99 (13)	O2—C61—C62	110.78 (13)
O2—C6—C1	114.31 (13)	N2—C62—C61	178.2 (2)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C61—H61*A*···N1^{i}	0.97	2.61	3.184 (3)	118
C61—H61*B*···O1^{ii}	0.97	2.52	3.2871 (19)	135

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

H atoms were positioned geometrically and refined using a riding model, with an aromatic C—H distance of 0.93 Å and a methylene C—H distance of 0.97 Å. The U_{iso}(H) values were constrained to be $1.2U_{eq}$ of the carrier atom.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED*32 (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97, *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2003).

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