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(2-Cyanomethoxy-6-methoxyphenoxy)acetonitrile

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.002 Å
R factor = 0.043
wR factor = 0.113
Data-to-parameter ratio = 16.6

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

In the crystal structure of the title compound, $C_{11}H_{10}N_2O_3$, intramolecular C—H···O interactions and intermolecular C—H···N interactions help to stabilize the structure.

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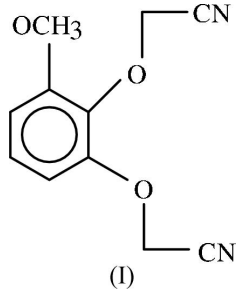
Comment

The chemistry of nitriles is quite interesting, due to their application in heterocyclic syntheses. Nitriles are close relatives of hydrazones, iminoesters and thioamides. They are key compounds for the preparation of various bioactive organic compounds having triazole, imidazole or thidiazole groups (Klingele & Brooker, 2004; Íkizler & Sancak, 1992; Kang *et al.*, 2004; Ram & Nath, 1994). 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 (Brewis *et al.*, 2003). Some derivatives of 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). Phosphinoalkyl nitriles have been used as catalytic coupling reagents of CO_2 and 1,3-butadiene (Pitter & Dinjus, 1997). In a previous paper, we reported the synthesis and crystal structure analysis of an acetonitrile derivative bearing a phenoxy group (Ustabaş *et al.*, 2004). Against this background, we report here the synthesis and crystal structure analysis of the title compound, 2-cyanomethoxy-6-methoxy-phenoxy)-acetonitrile, (I).



(I)

Compound (I) is composed of a benzene ring substituted by two O—CH_2—CN groups at atoms C1 and C2 and an O–CH_3 group (Fig. 1). The CH_2—C≡N groups are both essentially

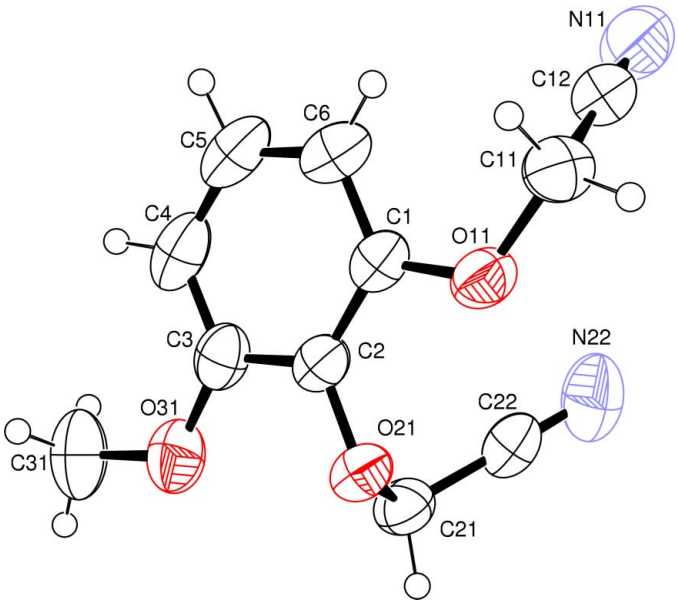


Figure 1
A view of the title compound, with the atom-numbering scheme and 50% probability displacement ellipsoids.

linear, with N22≡C22—C21 and N11≡C12—C11 angles of 179.2 (2) and 179.04 (19)°, respectively. The C22≡N22 and C12≡N11 bond distances are 1.186 (2) Å, similar to values reported in the literature (Çoruh *et al.*, 2003). The C31—O31 bond length of 1.413 (2) Å is in good agrement with values in the literature (Acevedo-Arauz *et al.*, 1992).

There are intramolecular C—H···O interactions and intermolecular C—H···N interactions in the structure of (I). The crystal structure is stabilized by weak intermolecular C11—H11*A*···N22^{i} and C21—H21*A*···O31 hydrogen bonds (symmetry code as in Table 2).

Experimental

A mixture of 3-methoxycatechol (1.40 g, 0.01 mol) dissolved in acetone (400 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 chloroform–carbon tetrachloride (1:2) to give (I) (yield 1.787 g, 82.01%; m.p. 345–346 K).

Crystal data

$C_{11}H_{10}N_2O_3$
M_r = 218.21
Monoclinic, $C2/c$
a = 27.871 (2) Å
b = 4.6083 (3) Å
c = 17.3806 (15) Å
β = 90.949 (7)°
V = 2232.0 (3) Å^3
Z = 8
D_x = 1.299 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 13819 reflections
θ = 2.1–27.1°
μ = 0.10 mm^{-1}
T = 296 K
Prism, colourless
0.47 × 0.30 × 0.13 mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.996, T_{max} = 0.999
16223 measured reflections
2402 independent reflections
1520 reflections with $I > 2\sigma(I)$
R_{int} = 0.057
θ_{max} = 29.0°
$h = -35 \rightarrow 35$
$k = -5 \rightarrow 5$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.113
S = 0.92
2402 reflections
145 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0691P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O31—C31	1.413 (2)	C12—N11	1.186 (2)
C22—N22	1.186 (2)		
N22—C22—C21	179.2 (2)	N11—C12—C11	179.04 (19)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C21—H21*A*···O31	0.97	2.28	2.842 (2)	116
C11—H11*A*···N22^{i}	0.97	2.55	3.302 (3)	135

Symmetry code: (i) $x, y+1, z$.

All H atoms were positioned geometrically and refined using a riding model, with C—H distances in the range 0.93–0.97 Å and with U_{iso}(H) equal to 1.2 or 1.5U_{eq} of the carrier atom.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* for Windows (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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