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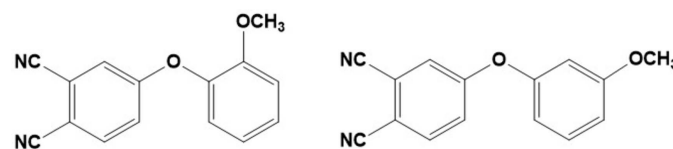
Crystal structures of 4-(2/3-methoxyphenoxy)- phthalonitrile

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The syntheses and crystal structures are reported of 4-phenoxy-substituted phthalonitriles with methoxy groups in the *ortho*- and *meta*-positions of the terminal benzene rings, respectively, namely, 4-(2-methoxyphenoxy)phthalonitrile and 4-(3-methoxyphenoxy)phthalonitrile, both C₁₅H₁₀N₂O₂. The <https://journals.iucr.org/e/issues/2023/03/00/molecular-structure> was determined using the single-crystal X-ray diffraction method. It is shown that short contacts play a more decisive role in the molecular packing compared to van der Waals interactions.

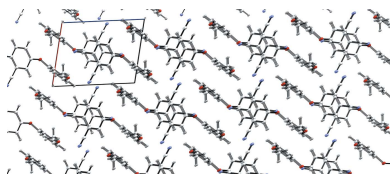
1. Chemical context

Phthalonitriles are a class of organic compounds with high thermal and oxidative stability (Laskowski *et al.*, 2016). That destruction only takes place at high temperatures facilitates using these molecules as building blocks for polymer composite materials with a high degree of cross-linking (Wang *et al.*, 2019). In addition, phthalonitriles are among the most promising precursors for the preparation of phthalocyanine complexes of various structures based on building blocks derived from them.

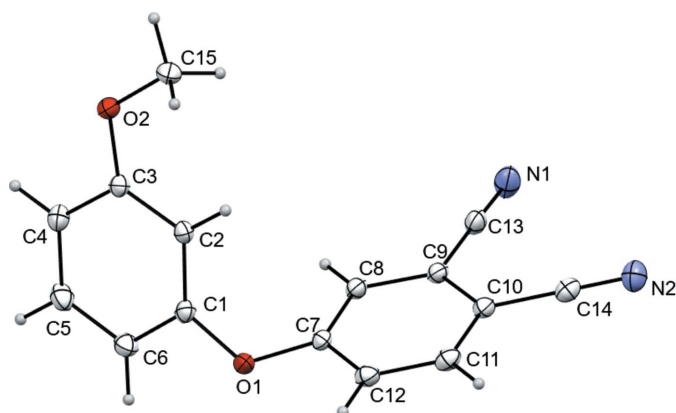


Phthalocyanines, as a result of their structural features and the possibility of introducing almost any functional moieties to their periphery, have found wide application in areas of societal and industrial importance such as catalysis, optics, medicine, light industry, etc. (Botnar *et al.*, 2020, 2021). Substituted phthalocyanines, which attract the most attention, however, are obtained from phthalonitriles with various fragments in the 3 and 4 positions.

Thus, it is of general interest to obtain functionally substituted nitriles and to study their properties. Here, we report the crystal structures of methoxyphenoxyphthalonitriles with the methoxy group in the *meta*- and *ortho*-substitution, respectively, which have been prepared for the synthesis of the corresponding substituted phthalocyanines. X-ray diffraction data for the *ortho*-isomer are already described in the literature (Agar *et al.*, 2007). However, no discussion is provided of



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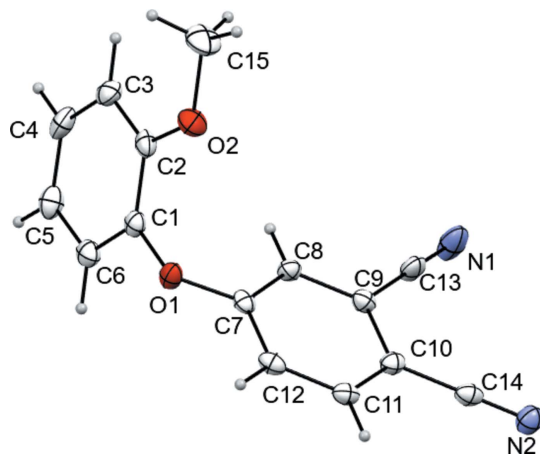

Figure 1

The molecular structure of *o*-4-(3-methoxy phenoxy)phthalonitrile, showing the atom labeling. Displacement ellipsoids are drawn at the 50% probability level.

the influence of the structure of the substituted nitrile on the crystal-packing stabilization. The presence of oxygen atoms in the composition of the molecules leads to the formation of interesting intermolecular interactions, which are discussed in this communication.

2. Structural commentary

Both substituted nitriles crystallize as solvent-free crystals; the structures are illustrated in Figs. 1 and 2. The phthalonitrile (*A*, C7–C12 atoms) and phenoxy (*B*, C1–C6 atoms) rings are oriented at dihedral angles of 66.61 (5) and 83.84 (11)° in the cases of *meta*- and *ortho*-substitution, respectively. For both nitriles, the C13, C14, N1, N2 and O1 atoms are practically coplanar to the *A* ring with a maximum deviation of 12° in the case of the C13N1 fragment. The O1, O2, and C15 atoms and the *B* rings are essentially coplanar. The plane of the methoxy group (C15/O2) and its *B*-ring pivot atom (C3 or C2) is at an angle to the *B*-ring plane of only 2.21 (6)° (*meta*) or 1.43 (15)°


Figure 2

The molecular structure of *m*-4-(2-methoxy phenoxy)phthalonitrile, showing the atom labeling. Displacement ellipsoids are drawn at the 50% probability level.

Table 1

Hydrogen-bond geometry (Å, °) for *o*-C₁₅H₁₀N₂O₂.

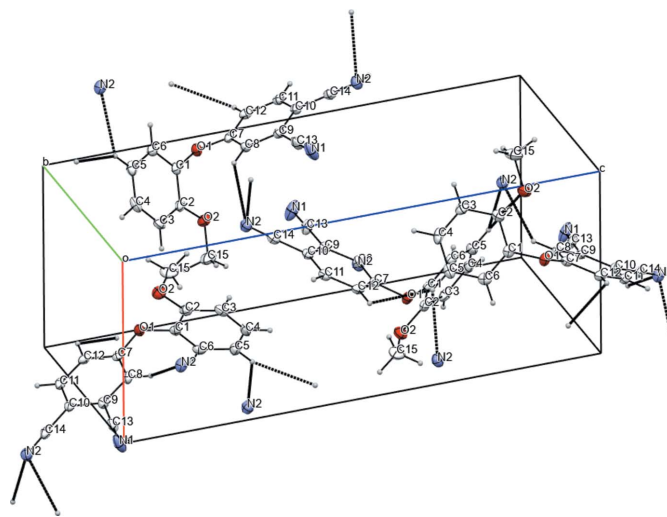
<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C3–H3A···O2 ⁱ	0.95	2.95	3.629 (3)	129
C5–H5A···N2 ⁱⁱ	0.95	2.66	3.394 (3)	134
C5–H5A···N1 ⁱⁱⁱ	0.95	2.90	3.557 (3)	128
C5–H5A···O1 ^{iv}	0.95	2.96	3.453 (3)	113
C8–H8A···N2 ^v	0.95	2.69	3.469 (3)	140
C11–H11A···O2 ^{vi}	0.95	2.82	3.735 (3)	161
C11–H11A···O1 ^{vi}	0.95	2.75	3.546 (3)	142
C12–H12A···N1 ^{vii}	0.95	2.44	3.199 (3)	137

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

(*ortho*). The torsion angles (C15–O2–C3–C2 for *meta* and C15–O2–C2–C1 for *ortho*) are 1.32 (15) and -179.1 (2)°, respectively.

3. Supramolecular features

In 4-(2-methoxyphenoxy)phthalonitrile, stabilization of the intermolecular packing is realized mainly through the formation of hydrogen bonds between the donor C8–H8A group of the *A* ring with the cyano group (C14≡N2) acceptor attached to the *A* ring of an adjacent molecule (C8–H8A···N2; symmetry operator: $x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$; Fig. 3, Table 1). The formation of a weaker but bifurcated intermolecular hydrogen-bonding interaction C11–H11···O1/O2($-\frac{1}{2} + x, \frac{1}{2} - y, 1 - z$) is also found in this structure, which additionally supports the packing. In the case of 4-(3-methoxyphenoxy)phthalonitrile, because of the favorable spatial arrangement of two *A* rings of neighboring molecules, stabilization occurs largely through respective π – π interactions. The planes of the *A* rings of two neighboring molecules are parallel to each other, but offset (angle between the ring normal and the


Figure 3

The molecular structure of the *o*-4-(2-methoxyphenoxy) phthalonitrile dimer, linked by C–H···N hydrogen bonds. Displacement ellipsoids are drawn at the 50% probability level.

Table 2
Hydrogen-bond geometry (Å, °) for *m*-C₁₅H₁₀N₂O₂.

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C2–H2A···N2 ⁱ	0.95	2.64	3.5839 (13)	175
C8–H8A···O2 ⁱⁱ	0.95	2.47	3.3447 (11)	153
C11–H11A···N1 ⁱⁱⁱ	0.95	2.62	3.2718 (13)	126
C12–H12A···N1 ⁱⁱⁱ	0.95	2.74	3.3325 (13)	121
C12–H12A···O2 ^{iv}	0.95	2.67	3.5343 (12)	151

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

centroid vector is 22.6° with a slippage of 1.41 Å). The distance between the centers of the *A* rings is 3.6632 (6) Å (centroid–centroid distance). These geometric characteristics imply the presence of a significant intermolecular π – π attraction (Janiak, 2000). The hydrogen atom of the aromatic C11–H11 moiety of one and the O1 oxygen atom of the adjacent molecule may be engaged in additional bidirectional contacts

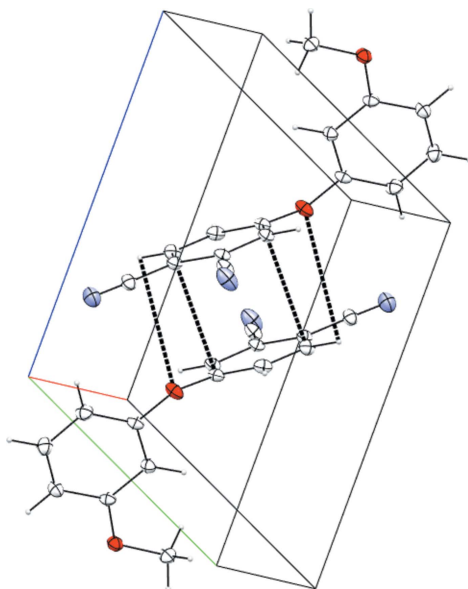


Figure 4
The molecular structure of *m*-4-(3-methoxy phenoxy)phthalonitrile dimer, linked by π – π -interactions and supporting weak H···O contacts. Displacement ellipsoids are drawn at the 50% probability level.

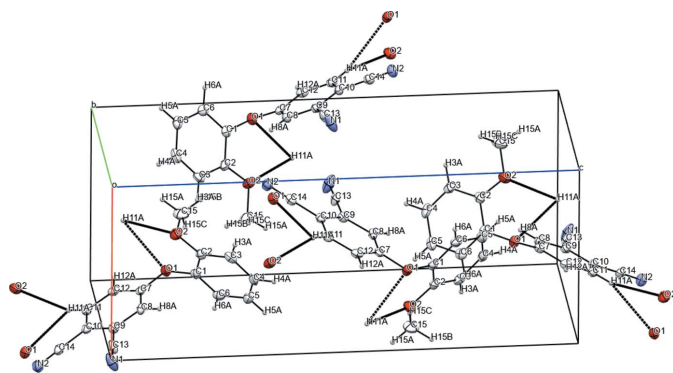


Figure 5
Representation of bifurcated O···H···O hydrogen bond exhibited by the *m*-4-(2-methoxyphenoxy)phthalonitrile dimer. Displacement ellipsoids are drawn at the 50% probability level.

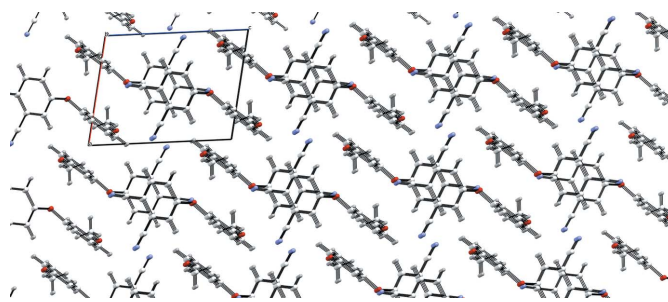


Figure 6
A view along the *b* axis of the crystal packing of *o*-4-(3-methoxyphenoxy)phthalonitrile. Intermolecular hydrogen bonds have been removed for clarity.

(Fig. 4), which support the π – π interaction as well as its slippage. In both cases, a number of weaker hydrogen-bonding contacts are observed, comprising additional contributions to the stabilization of the crystal structures. Thus, the packing of the *ortho*-isomer exhibits in total eight intermolecular hydrogen-bonding interactions, while for the *meta*-isomer, in addition to the π – π interaction, five hydrogen bonds are observed (Tables 1, 2, Fig. 5). The resulting crystal packings for the title 4-(2/3-methoxyphenoxy)phthalonitriles are shown in Figs. 6 and 7.

4. Database survey

A survey of the CSD (Groom *et al.*, 2016) using ConQuest version 2022 3.0 (Bruno *et al.*, 2002) for closely related 4-(phenoxy)phthalonitriles with ether-functionalized substituents on the phenoxy moiety in the *ortho*- and *meta*-positions results in only two and one hits, respectively. The *ortho*-isomers are a phthalonitrile dimer bridged by the *o*-phenoxy moiety (refcode: NAGJEN; Köç *et al.*, 2016), and the same molecule as the one reported here (refcode: JEVNII; Açar & Ocak İskeleli, 2007). The *meta*-isomer is also a phthalonitrile dimer now bridged by the *m*-phenoxy moiety (refcode: HAMVIB; Devci *et al.*, 2004). Notably, with regard to the phthalonitrile dimers, π – π -stacking is observed for the *meta*-isomer but not for the *ortho*-isomer; the same observation was made for the two title compounds.

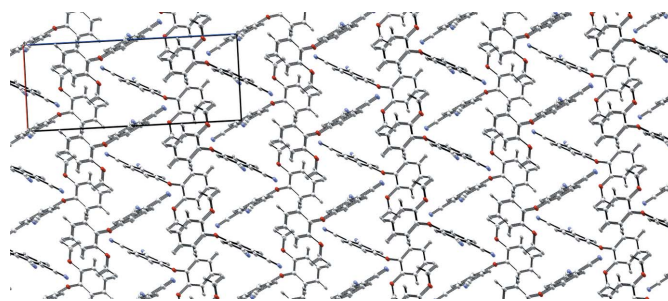


Figure 7
A view along the *b* axis of the crystal packing of *m*-4-(2-methoxyphenoxy)phthalonitrile. Intermolecular hydrogen bonds have been removed for clarity.

Table 3
Experimental details.

	<i>o</i> -C ₁₅ H ₁₀ N ₂ O ₂	<i>m</i> -C ₁₅ H ₁₀ N ₂ O ₂
Crystal data		
M_r	250.25	250.25
Crystal system, space group	Orthorhombic, $P2_12_12_1$	Triclinic, $P\bar{1}$
Temperature (K)	100	100
a, b, c (Å)	7.7329 (3), 8.2536 (3), 19.2301 (7)	8.0609 (3), 8.4672 (4), 9.9999 (4)
α, β, γ (°)	90, 90, 90	104.638 (1), 95.078 (1), 110.570 (1)
V (Å ³)	1227.35 (8)	606.31 (4)
Z	4	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm ⁻¹)	0.09	0.09
Crystal size (mm)	0.24 × 0.24 × 0.07	0.45 × 0.30 × 0.27
Data collection		
Diffractometer	Bruker D8 Quest (CMOS)	Bruker D8 Quest (CMOS)
Absorption correction	Multi-scan (SADABS; Krause <i>et al.</i> , 2015)	Multi-scan (SADABS; Krause <i>et al.</i> , 2015)
T_{\min}, T_{\max}	0.903, 0.971	0.903, 0.971
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19395, 3035, 2616	10029, 3395, 3040
R_{int}	0.046	0.017
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.667	0.694
Refinement		
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.045, 0.095, 1.09	0.039, 0.105, 1.06
No. of reflections	3035	3395
No. of parameters	173	173
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.21, -0.32	0.37, -0.27
Absolute structure	Flack x determined using 931 quotients [[I^+)-(I^-)]/[$(I^+)+(I^-)$] (Parsons <i>et al.</i> , 2013)	-

Computer programs: APEX3 and SAINT (Bruker, 2003), SHELXT2014/5 (Sheldrick, 2015a), SHELXL2018/3 (Sheldrick, 2015b), SHELXTL (Sheldrick, 2008), and Mercury (Macrae *et al.*, 2020).

5. Synthesis and crystallization

Materials and physical methods: All reagents were purchased from Sigma–Aldrich. Reaction progress was monitored by thin-layer chromatography (TLC) on silica-gel plates.

Synthesis of substituted phthalonitriles: 4-nitrophthalonitrile and 2/3-methoxyphenol in a 1:1 molar ratio were placed in a flask and dissolved in DMF. Further, after complete dissolution of the reagents, 1 mol of potassium carbonate and 1/3 portion of water (in relation to DMF) were added to the mixture. The reaction mass was stirred at 353–363 K for 2.5 h, after which it was cooled to 278 K and poured into a threefold excess (by volume) of 15% aqueous NaCl solution. The precipitate was filtered off, recrystallized from 50% aqueous 2-propanol solution and then dried at 343 K. As a result, light crystals of 4-(2-methoxyphenoxy) phthalonitrile (75%) and 4-(3-methoxyphenoxy) phthalonitrile (89%) were obtained, respectively. Crystals were obtained by slow evaporation of solvent from a saturated solution of phthalonitriles in chloroform.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All hydrogen atoms were placed in calculated positions and were refined using a riding model [$U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$] for CH₃ groups and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for other groups).

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supporting information

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Crystal structures of 4-(2/3-methoxyphenoxy)phthalonitrile

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Computing details

For both structures, data collection: *APEX3* (Bruker, 2003); cell refinement: *SAINTE* (Bruker, 2003); data reduction: *SAINTE* (Bruker, 2003); program(s) used to solve structure: *SHELXT2014/5* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *Mercury* (Macrae *et al.*, 2020).

4-(2-Methoxyphenoxy)benzene-1,2-dicarbonitrile (o-C₁₅H₁₀N₂O₂)

Crystal data

C₁₅H₁₀N₂O₂

$M_r = 250.25$

Orthorhombic, $P2_12_12_1$

$a = 7.7329$ (3) Å

$b = 8.2536$ (3) Å

$c = 19.2301$ (7) Å

$V = 1227.35$ (8) Å³

$Z = 4$

$F(000) = 520$

$D_x = 1.354$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9781 reflections

$\theta = 2.7\text{--}30.1^\circ$

$\mu = 0.09$ mm⁻¹

$T = 100$ K

Prism, colorless

$0.24 \times 0.24 \times 0.07$ mm

Data collection

Bruker D8 Quest (CMOS)
diffractometer

Radiation source: microfocus tube

ω scans

Absorption correction: multi-scan
(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.903$, $T_{\max} = 0.971$

19395 measured reflections

3035 independent reflections

2616 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.046$

$\theta_{\max} = 28.3^\circ$, $\theta_{\min} = 2.1^\circ$

$h = -10 \rightarrow 10$

$k = -11 \rightarrow 11$

$l = -25 \rightarrow 25$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.045$

$wR(F^2) = 0.095$

$S = 1.09$

3035 reflections

173 parameters

0 restraints

Primary atom site location: dual

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0385P)^2 + 0.3865P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.21$ e Å⁻³

$\Delta\rho_{\min} = -0.32$ e Å⁻³

Absolute structure: Flack x determined using

931 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.6870 (2)	0.31404 (19)	0.64727 (8)	0.0195 (4)
O2	0.9772 (2)	0.4854 (2)	0.66084 (9)	0.0268 (4)
N1	0.4498 (4)	0.9100 (3)	0.50573 (12)	0.0377 (6)
N2	0.3018 (3)	0.6112 (3)	0.36049 (11)	0.0244 (5)
C1	0.7085 (3)	0.4120 (3)	0.70640 (12)	0.0172 (5)
C2	0.8609 (3)	0.5003 (3)	0.71355 (12)	0.0193 (5)
C3	0.8807 (3)	0.5958 (3)	0.77286 (13)	0.0235 (5)
H3A	0.982511	0.658542	0.779084	0.028*
C4	0.7515 (3)	0.5990 (3)	0.82256 (12)	0.0249 (6)
H4A	0.765466	0.665266	0.862552	0.030*
C5	0.6029 (3)	0.5081 (3)	0.81540 (12)	0.0242 (5)
H5A	0.516618	0.509974	0.850546	0.029*
C6	0.5809 (3)	0.4138 (3)	0.75631 (12)	0.0210 (5)
H6A	0.478840	0.351196	0.750360	0.025*
C7	0.6104 (3)	0.3826 (3)	0.59041 (11)	0.0160 (5)
C8	0.5802 (3)	0.5471 (3)	0.58379 (11)	0.0166 (5)
H8A	0.611760	0.619803	0.619924	0.020*
C9	0.5027 (3)	0.6041 (3)	0.52311 (11)	0.0174 (5)
C10	0.4544 (3)	0.4968 (3)	0.46957 (11)	0.0170 (5)
C11	0.4861 (3)	0.3315 (3)	0.47775 (12)	0.0178 (5)
H11A	0.454353	0.257754	0.442035	0.021*
C12	0.5635 (3)	0.2752 (3)	0.53775 (12)	0.0180 (5)
H12A	0.584819	0.162514	0.543185	0.022*
C13	0.4736 (3)	0.7744 (3)	0.51398 (12)	0.0235 (5)
C14	0.3705 (3)	0.5595 (3)	0.40833 (12)	0.0187 (5)
C15	1.1358 (3)	0.5737 (4)	0.66790 (16)	0.0365 (7)
H15A	1.209911	0.552231	0.627585	0.055*
H15B	1.195310	0.539339	0.710413	0.055*
H15C	1.110784	0.689945	0.670515	0.055*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0259 (9)	0.0151 (8)	0.0175 (8)	0.0017 (7)	-0.0029 (7)	-0.0003 (6)
O2	0.0213 (8)	0.0321 (10)	0.0270 (9)	-0.0034 (8)	0.0053 (8)	0.0023 (8)
N1	0.0639 (18)	0.0183 (11)	0.0310 (12)	0.0001 (11)	-0.0236 (13)	-0.0027 (10)
N2	0.0281 (11)	0.0235 (11)	0.0216 (11)	0.0009 (10)	-0.0029 (10)	-0.0021 (9)
C1	0.0213 (11)	0.0130 (10)	0.0172 (11)	0.0032 (10)	-0.0023 (10)	0.0017 (9)
C2	0.0193 (11)	0.0204 (11)	0.0183 (11)	0.0025 (10)	0.0003 (9)	0.0067 (10)

C3	0.0216 (12)	0.0234 (13)	0.0255 (12)	-0.0002 (11)	-0.0092 (11)	0.0033 (10)
C4	0.0317 (14)	0.0266 (13)	0.0165 (12)	0.0070 (12)	-0.0083 (10)	-0.0031 (10)
C5	0.0267 (13)	0.0280 (13)	0.0177 (11)	0.0067 (12)	0.0025 (10)	0.0004 (10)
C6	0.0197 (11)	0.0193 (12)	0.0241 (12)	0.0019 (10)	-0.0016 (10)	0.0053 (10)
C7	0.0137 (10)	0.0174 (11)	0.0168 (10)	-0.0005 (9)	0.0038 (9)	0.0016 (9)
C8	0.0192 (11)	0.0162 (11)	0.0144 (10)	-0.0032 (9)	0.0003 (9)	-0.0029 (9)
C9	0.0183 (11)	0.0150 (11)	0.0187 (11)	-0.0016 (9)	0.0010 (10)	-0.0004 (9)
C10	0.0162 (10)	0.0183 (11)	0.0164 (10)	-0.0011 (10)	0.0009 (9)	-0.0026 (9)
C11	0.0162 (11)	0.0183 (11)	0.0191 (11)	-0.0029 (9)	0.0020 (9)	-0.0042 (9)
C12	0.0175 (11)	0.0123 (11)	0.0243 (12)	0.0000 (9)	0.0028 (10)	-0.0015 (9)
C13	0.0320 (14)	0.0208 (13)	0.0175 (11)	-0.0029 (11)	-0.0098 (11)	-0.0038 (10)
C14	0.0196 (11)	0.0167 (11)	0.0199 (12)	-0.0030 (9)	0.0021 (10)	-0.0054 (9)
C15	0.0195 (12)	0.0447 (17)	0.0451 (17)	-0.0050 (13)	0.0056 (12)	0.0081 (14)

Geometric parameters (Å, °)

O1—C7	1.366 (3)	C6—H6A	0.9500
O1—C1	1.405 (3)	C7—C8	1.384 (3)
O2—C2	1.360 (3)	C7—C12	1.394 (3)
O2—C15	1.434 (3)	C8—C9	1.394 (3)
N1—C13	1.145 (3)	C8—H8A	0.9500
N2—C14	1.145 (3)	C9—C10	1.408 (3)
C1—C6	1.377 (3)	C9—C13	1.434 (3)
C1—C2	1.393 (3)	C10—C11	1.395 (3)
C2—C3	1.395 (3)	C10—C14	1.441 (3)
C3—C4	1.382 (4)	C11—C12	1.381 (3)
C3—H3A	0.9500	C11—H11A	0.9500
C4—C5	1.379 (4)	C12—H12A	0.9500
C4—H4A	0.9500	C15—H15A	0.9800
C5—C6	1.388 (3)	C15—H15B	0.9800
C5—H5A	0.9500	C15—H15C	0.9800
C7—O1—C1	117.45 (17)	C7—C8—C9	118.8 (2)
C2—O2—C15	116.7 (2)	C7—C8—H8A	120.6
C6—C1—C2	122.1 (2)	C9—C8—H8A	120.6
C6—C1—O1	119.1 (2)	C8—C9—C10	120.9 (2)
C2—C1—O1	118.8 (2)	C8—C9—C13	120.1 (2)
O2—C2—C1	116.0 (2)	C10—C9—C13	119.0 (2)
O2—C2—C3	126.0 (2)	C11—C10—C9	119.1 (2)
C1—C2—C3	118.0 (2)	C11—C10—C14	121.5 (2)
C4—C3—C2	119.8 (2)	C9—C10—C14	119.4 (2)
C4—C3—H3A	120.1	C12—C11—C10	120.0 (2)
C2—C3—H3A	120.1	C12—C11—H11A	120.0
C5—C4—C3	121.5 (2)	C10—C11—H11A	120.0
C5—C4—H4A	119.2	C11—C12—C7	120.4 (2)
C3—C4—H4A	119.2	C11—C12—H12A	119.8
C4—C5—C6	119.3 (2)	C7—C12—H12A	119.8
C4—C5—H5A	120.4	N1—C13—C9	179.0 (3)

C6—C5—H5A	120.4	N2—C14—C10	178.6 (2)
C1—C6—C5	119.3 (2)	O2—C15—H15A	109.5
C1—C6—H6A	120.4	O2—C15—H15B	109.5
C5—C6—H6A	120.4	H15A—C15—H15B	109.5
O1—C7—C8	123.6 (2)	O2—C15—H15C	109.5
O1—C7—C12	115.53 (19)	H15A—C15—H15C	109.5
C8—C7—C12	120.9 (2)	H15B—C15—H15C	109.5

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C3—H3 <i>A</i> ...O2 ⁱ	0.95	2.95	3.629 (3)	129
C5—H5 <i>A</i> ...N2 ⁱⁱ	0.95	2.66	3.394 (3)	134
C5—H5 <i>A</i> ...N1 ⁱⁱⁱ	0.95	2.90	3.557 (3)	128
C5—H5 <i>A</i> ...O1 ^{iv}	0.95	2.96	3.453 (3)	113
C8—H8 <i>A</i> ...N2 ^v	0.95	2.69	3.469 (3)	140
C11—H11 <i>A</i> ...O2 ^{vi}	0.95	2.82	3.735 (3)	161
C11—H11 <i>A</i> ...O1 ^{vi}	0.95	2.75	3.546 (3)	142
C12—H12 <i>A</i> ...N1 ^{vii}	0.95	2.44	3.199 (3)	137

Symmetry codes: (i) $-x+2, y+1/2, -z+3/2$; (ii) $-x+1/2, -y+1, z+1/2$; (iii) $-x+1, y-1/2, -z+3/2$; (iv) $-x+1, y+1/2, -z+3/2$; (v) $x+1/2, -y+3/2, -z+1$; (vi) $x-1/2, -y+1/2, -z+1$; (vii) $x, y-1, z$.

4-(3-Methoxyphenoxy)benzene-1,2-dicarbonitrile (m-C₁₅H₁₀N₂O₂)

Crystal data

C₁₅H₁₀N₂O₂ $M_r = 250.25$ Triclinic, $P\bar{1}$ $a = 8.0609$ (3) Å $b = 8.4672$ (4) Å $c = 9.9999$ (4) Å $\alpha = 104.638$ (1)° $\beta = 95.078$ (1)° $\gamma = 110.570$ (1)° $V = 606.31$ (4) Å³ $Z = 2$ $F(000) = 260$ $D_x = 1.371$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9781 reflections

 $\theta = 2.7\text{--}30.1^\circ$ $\mu = 0.09$ mm⁻¹ $T = 100$ K

Prism, colorless

0.45 × 0.30 × 0.27 mm

Data collection

Bruker D8 Quest (CMOS)

diffractometer

Radiation source: microfocus tube

 ω scansAbsorption correction: multi-scan
(SADABS; Krause *et al.*, 2015) $T_{\min} = 0.903$, $T_{\max} = 0.971$

10029 measured reflections

3395 independent reflections

3040 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.017$ $\theta_{\max} = 29.6^\circ$, $\theta_{\min} = 2.2^\circ$ $h = -11 \rightarrow 11$ $k = -11 \rightarrow 11$ $l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.039$ $wR(F^2) = 0.105$ $S = 1.06$

3395 reflections

173 parameters

0 restraints

Primary atom site location: dual

Secondary atom site location: difference Fourier map
 Hydrogen site location: inferred from neighbouring sites
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0528P)^2 + 0.2143P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.37 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.27 \text{ e } \text{\AA}^{-3}$

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.56496 (10)	0.59440 (10)	0.80203 (7)	0.01795 (16)
O2	0.87906 (10)	0.47550 (9)	1.17760 (7)	0.01716 (16)
N1	0.95411 (13)	0.23336 (15)	0.44743 (10)	0.0277 (2)
N2	0.46049 (13)	-0.06002 (13)	0.21559 (10)	0.0253 (2)
C1	0.69339 (13)	0.64698 (13)	0.92463 (10)	0.01494 (18)
C2	0.72490 (12)	0.52173 (12)	0.97939 (9)	0.01389 (18)
H2A	0.668855	0.398795	0.929816	0.017*
C3	0.84135 (13)	0.58336 (12)	1.10919 (9)	0.01423 (18)
C4	0.92411 (14)	0.76450 (13)	1.18106 (10)	0.01779 (19)
H4A	1.004512	0.805311	1.269112	0.021*
C5	0.88827 (14)	0.88403 (13)	1.12324 (11)	0.0203 (2)
H5A	0.943632	1.007075	1.172592	0.024*
C6	0.77200 (14)	0.82629 (13)	0.99356 (10)	0.0186 (2)
H6A	0.747571	0.908341	0.953705	0.022*
C7	0.55405 (13)	0.45928 (12)	0.68822 (9)	0.01418 (18)
C8	0.70450 (12)	0.42664 (12)	0.65164 (9)	0.01438 (18)
H8A	0.820847	0.493469	0.709832	0.017*
C9	0.67994 (12)	0.29370 (12)	0.52775 (9)	0.01387 (18)
C10	0.50752 (12)	0.19245 (12)	0.44232 (9)	0.01434 (18)
C11	0.35970 (13)	0.22881 (13)	0.48119 (10)	0.01664 (19)
H11A	0.242865	0.161880	0.423787	0.020*
C12	0.38297 (13)	0.36220 (13)	0.60321 (10)	0.01613 (19)
H12A	0.282369	0.387620	0.629065	0.019*
C13	0.83370 (13)	0.26098 (14)	0.48459 (10)	0.0185 (2)
C14	0.48277 (13)	0.05290 (13)	0.31588 (10)	0.01762 (19)
C15	0.79525 (14)	0.28892 (13)	1.10841 (11)	0.0189 (2)
H15A	0.829282	0.225820	1.168675	0.028*
H15B	0.835383	0.260815	1.018882	0.028*
H15C	0.663676	0.252294	1.090253	0.028*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0233 (4)	0.0224 (4)	0.0123 (3)	0.0155 (3)	0.0020 (3)	0.0032 (3)

O2	0.0211 (3)	0.0165 (3)	0.0143 (3)	0.0086 (3)	0.0001 (3)	0.0046 (3)
N1	0.0205 (4)	0.0418 (6)	0.0197 (4)	0.0167 (4)	0.0019 (3)	0.0014 (4)
N2	0.0272 (5)	0.0235 (5)	0.0203 (4)	0.0083 (4)	0.0016 (4)	0.0019 (3)
C1	0.0167 (4)	0.0193 (4)	0.0115 (4)	0.0094 (3)	0.0045 (3)	0.0051 (3)
C2	0.0156 (4)	0.0145 (4)	0.0126 (4)	0.0073 (3)	0.0041 (3)	0.0034 (3)
C3	0.0163 (4)	0.0164 (4)	0.0124 (4)	0.0081 (3)	0.0049 (3)	0.0052 (3)
C4	0.0195 (4)	0.0176 (5)	0.0135 (4)	0.0060 (4)	0.0021 (3)	0.0022 (3)
C5	0.0246 (5)	0.0141 (4)	0.0198 (5)	0.0064 (4)	0.0047 (4)	0.0027 (4)
C6	0.0240 (5)	0.0170 (4)	0.0184 (4)	0.0105 (4)	0.0063 (4)	0.0068 (4)
C7	0.0187 (4)	0.0165 (4)	0.0110 (4)	0.0097 (3)	0.0042 (3)	0.0059 (3)
C8	0.0139 (4)	0.0178 (4)	0.0123 (4)	0.0070 (3)	0.0019 (3)	0.0050 (3)
C9	0.0136 (4)	0.0179 (4)	0.0122 (4)	0.0078 (3)	0.0025 (3)	0.0056 (3)
C10	0.0148 (4)	0.0164 (4)	0.0126 (4)	0.0063 (3)	0.0022 (3)	0.0055 (3)
C11	0.0126 (4)	0.0212 (5)	0.0167 (4)	0.0060 (3)	0.0022 (3)	0.0076 (4)
C12	0.0150 (4)	0.0222 (5)	0.0160 (4)	0.0100 (4)	0.0055 (3)	0.0090 (3)
C13	0.0170 (4)	0.0247 (5)	0.0127 (4)	0.0096 (4)	0.0003 (3)	0.0026 (3)
C14	0.0159 (4)	0.0196 (5)	0.0166 (4)	0.0060 (3)	0.0012 (3)	0.0062 (4)
C15	0.0244 (5)	0.0160 (4)	0.0181 (4)	0.0099 (4)	0.0029 (4)	0.0058 (3)

Geometric parameters (Å, °)

O1—C7	1.3658 (11)	C6—H6A	0.9500
O1—C1	1.3959 (11)	C7—C12	1.3939 (14)
O2—C3	1.3669 (11)	C7—C8	1.3942 (13)
O2—C15	1.4303 (12)	C8—C9	1.3914 (12)
N1—C13	1.1464 (14)	C8—H8A	0.9500
N2—C14	1.1468 (14)	C9—C10	1.4067 (13)
C1—C6	1.3782 (14)	C9—C13	1.4404 (13)
C1—C2	1.3954 (13)	C10—C11	1.3946 (13)
C2—C3	1.3915 (13)	C10—C14	1.4384 (13)
C2—H2A	0.9500	C11—C12	1.3834 (13)
C3—C4	1.3975 (13)	C11—H11A	0.9500
C4—C5	1.3835 (14)	C12—H12A	0.9500
C4—H4A	0.9500	C15—H15A	0.9800
C5—C6	1.3934 (15)	C15—H15B	0.9800
C5—H5A	0.9500	C15—H15C	0.9800
C7—O1—C1	120.56 (7)	C9—C8—C7	118.33 (8)
C3—O2—C15	117.05 (7)	C9—C8—H8A	120.8
C6—C1—C2	122.83 (9)	C7—C8—H8A	120.8
C6—C1—O1	116.08 (8)	C8—C9—C10	121.08 (8)
C2—C1—O1	120.80 (8)	C8—C9—C13	119.63 (8)
C3—C2—C1	117.62 (8)	C10—C9—C13	119.28 (8)
C3—C2—H2A	121.2	C11—C10—C9	119.29 (8)
C1—C2—H2A	121.2	C11—C10—C14	119.99 (8)
O2—C3—C2	123.86 (8)	C9—C10—C14	120.72 (8)
O2—C3—C4	115.26 (8)	C12—C11—C10	120.09 (9)
C2—C3—C4	120.85 (9)	C12—C11—H11A	120.0

C5—C4—C3	119.61 (9)	C10—C11—H11A	120.0
C5—C4—H4A	120.2	C11—C12—C7	119.99 (9)
C3—C4—H4A	120.2	C11—C12—H12A	120.0
C4—C5—C6	120.85 (9)	C7—C12—H12A	120.0
C4—C5—H5A	119.6	N1—C13—C9	178.59 (10)
C6—C5—H5A	119.6	N2—C14—C10	178.88 (11)
C1—C6—C5	118.24 (9)	O2—C15—H15A	109.5
C1—C6—H6A	120.9	O2—C15—H15B	109.5
C5—C6—H6A	120.9	H15A—C15—H15B	109.5
O1—C7—C12	115.57 (8)	O2—C15—H15C	109.5
O1—C7—C8	123.07 (8)	H15A—C15—H15C	109.5
C12—C7—C8	121.20 (9)	H15B—C15—H15C	109.5

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2A \cdots N2 ⁱ	0.95	2.64	3.5839 (13)	175
C8—H8A \cdots O2 ⁱⁱ	0.95	2.47	3.3447 (11)	153
C11—H11A \cdots N1 ⁱⁱⁱ	0.95	2.62	3.2718 (13)	126
C12—H12A \cdots N1 ⁱⁱⁱ	0.95	2.74	3.3325 (13)	121
C12—H12A \cdots O2 ^{iv}	0.95	2.67	3.5343 (12)	151

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