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4-(4-Allyl-2-methoxyphenoxy)benzene-1,2-dicarbonitrile

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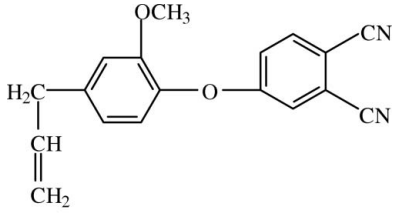
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.035; wR factor = 0.099; data-to-parameter ratio = 8.6.

In the title compound, $C_{18}H_{14}N_2O_2$, the dihedral angle between the two benzene rings is 88.6 (1)°. The allyl group is disordered over two orientations, with refined occupancies of 0.695 (6) and 0.305 (6). The methoxy group is coplanar with the attached benzene ring. C—H···N intermolecular hydrogen bonds link the molecules into a $C(6)$ chain along the a axis. The chain structure is further strengthened by C—H···π interactions.

Related literature

For general background, see: Agar *et al.* (1999); Leznoff & Lever (1996); McKeown (1998); Wöhrle (2001).



Experimental

Crystal data

$C_{18}H_{14}N_2O_2$
M_r = 290.31
Orthorhombic, $Pna2_1$
a = 14.7784 (13) Å
b = 11.9726 (9) Å
c = 8.6133 (6) Å
V = 1524.0 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 K
0.78 × 0.40 × 0.17 mm

Data collection

Stoe IPDSII diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.969, T_{max} = 0.989
14749 measured reflections
1930 independent reflections
1317 reflections with $I > 2\sigma(I)$
R_{int} = 0.074

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.099
S = 0.91
1930 reflections
225 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.08 e Å^{-3}
$\Delta\rho_{min}$ = −0.10 e Å^{-3}

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

$Cg1$ is the centroid of the C1–C6 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···N2^{i}	0.93 (3)	2.61 (3)	3.510 (3)	166 (2)
C16—H16A···$Cg1^{i}$	0.97	2.88	3.808 (4)	160

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z$.

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: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2458).

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supplementary materials

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4-(4-Allyl-2-methoxyphenoxy)benzene-1,2-dicarbonitrile

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Comment

Phthalonitriles have been used as starting materials for phthalocyanines (Leznoff & Lever, 1996), 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) (McKeown, 1998). Some phthalocyanines have been used in the petroleum industry as catalysts, for the oxidation of sulfur compounds in the gasoline fraction. Applications as photoconductors in the xerographic double layers of laser printers and copying machines, and as active materials in writable data-storage disks, are also known (Wöhrle, 2001). The synthetic details of the title compound was published elsewhere (Agar *et al.*, 1999). We report here the crystal structure of the title compound.

The benzene rings are essentially planar [the atoms having the largest deviations in the two benzene rings are C4 (0.009 (2) Å) and C12 (0.017 (2) Å)] and they form a dihedral angle of 88.6 (1)° (Fig. 1). The methoxy group is coplanar with the attached ring, with the C13—C14—O2—C15 torsion angle being 0.6 (4)°.

The crystal packing is stabilized by C—H···N intermolecular hydrogen bonds and C—H···π interactions (Table 1). The C—H···N hydrogen bonds link the molecules into a C(6) chain along the *a* axis (Fig. 2). The chain is further strengthened by C16—H16A···π interactions involving the C1—C6 benzene ring (centroid *Cg*1).

Experimental

The title compound was prepared using the method reported previously by Agar *et al.* (1999).

Refinement

Atoms C17 and C18 of the allyl group are disordered over two sites, with refined occupancies of 0.695 (6) and 0.305 (6). The corresponding C—C distances involving the disordered atoms were restrained to be the same. The H atoms of the benzene rings were located in a difference map and refined freely, with U_{iso}(H) = 1.2U_{eq}(C). All other H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C). 1315 Friedel pairs were merged before the final refinement.

Figures

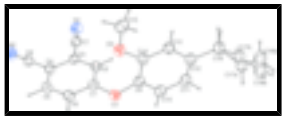

Fig. 1. The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level. Both disorder components are shown.

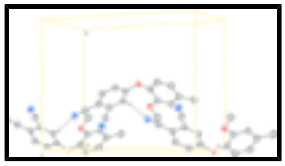

Fig. 2. A packing diagram for (I), showing a C—H···N hydrogen-bonded (dashed lines) chain. H atoms not involved in hydrogen bonding have been omitted for clarity.

4-(4-Allyl-2-methoxyphenoxy)benzene-1,2-dicarbonitrile

Crystal data

$C_{18}H_{14}N_2O_2$	F_{000} = 608
M_r = 290.31	D_x = 1.265 Mg m^{-3}
Orthorhombic, *Pna*2$_1$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P 2c -2n	Cell parameters from 11502 reflections
a = 14.7784 (13) Å	θ = 1.7–27.8º
b = 11.9726 (9) Å	μ = 0.08 mm^{-1}
c = 8.6133 (6) Å	*T* = 296 K
V = 1524.0 (2) Å^3	Prism, colourless
Z = 4	0.78 × 0.40 × 0.17 mm

Data collection

Stoe IPDSII diffractometer	1930 independent reflections
Radiation source: fine-focus sealed tube	1317 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.074
Detector resolution: 6.67 pixels mm^{-1}	θ_{max} = 28.0º
T = 296 K	θ_{min} = 2.2º
ω scans	*h* = −19→19
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	*k* = −15→15
T_{min} = 0.969, T_{max} = 0.989	*l* = −10→11
14749 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.035	$w = 1/[\sigma^2(F_o^2) + (0.0656P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.099	$(\Delta/\sigma)_{max}$ = 0.001
S = 0.91	$\Delta\rho_{max}$ = 0.08 e Å^{-3}
1930 reflections	$\Delta\rho_{min}$ = −0.10 e Å^{-3}
225 parameters	Extinction correction: none
3 restraints	

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Special details

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}	Occ. (<1)
O1	0.49053 (11)	0.51155 (13)	0.3686 (2)	0.0736 (5)	
O2	0.53129 (11)	0.33713 (16)	0.1909 (2)	0.0828 (5)	
N1	0.36210 (17)	0.1802 (2)	0.8284 (4)	0.1042 (9)	
N2	0.12638 (15)	0.2620 (2)	0.6747 (4)	0.0956 (7)	
C1	0.41981 (14)	0.45549 (17)	0.4342 (3)	0.0608 (5)	
C2	0.42998 (15)	0.37518 (17)	0.5476 (3)	0.0617 (5)	
H2	0.4858 (17)	0.352 (2)	0.584 (3)	0.074*	
C3	0.35322 (14)	0.32673 (17)	0.6111 (3)	0.0613 (5)	
C4	0.26687 (14)	0.35687 (18)	0.5590 (3)	0.0642 (5)	
C5	0.25886 (15)	0.4388 (2)	0.4455 (3)	0.0708 (6)	
H5	0.1964 (18)	0.462 (2)	0.410 (3)	0.085*	
C6	0.33423 (16)	0.4874 (2)	0.3835 (3)	0.0682 (6)	
H6	0.3309 (15)	0.543 (2)	0.302 (4)	0.082*	
C7	0.36038 (15)	0.2447 (2)	0.7318 (3)	0.0740 (6)	
C8	0.18843 (16)	0.3044 (2)	0.6234 (3)	0.0730 (6)	
C9	0.57803 (13)	0.46782 (19)	0.3737 (3)	0.0642 (5)	
C10	0.64291 (18)	0.5200 (2)	0.4616 (4)	0.0764 (6)	
H10	0.6209 (17)	0.576 (2)	0.528 (4)	0.092*	
C11	0.73302 (17)	0.4895 (2)	0.4442 (4)	0.0790 (7)	
H11	0.7764 (19)	0.531 (2)	0.516 (4)	0.095*	
C12	0.75807 (15)	0.4089 (2)	0.3391 (3)	0.0732 (6)	
C13	0.69107 (16)	0.3541 (2)	0.2541 (3)	0.0710 (6)	
H13	0.7080 (17)	0.296 (2)	0.174 (4)	0.085*	
C14	0.60094 (15)	0.38315 (18)	0.2714 (3)	0.0669 (6)	
C15	0.5531 (2)	0.2518 (2)	0.0813 (4)	0.0978 (9)	
H15A	0.5949	0.2806	0.0061	0.147*	
H15B	0.4989	0.2276	0.0297	0.147*	
H15C	0.5801	0.1896	0.1344	0.147*	
C16	0.85578 (17)	0.3797 (3)	0.3059 (4)	0.0944 (9)	
H16A	0.8696	0.3101	0.3583	0.113*	0.695 (6)

H16C	0.8618	0.3665	0.1953	0.113*	0.695 (6)
H16D	0.8699	0.4052	0.2030	0.113*	0.305 (6)
H16B	0.8615	0.2999	0.3060	0.113*	0.305 (6)
C17A	0.9235 (3)	0.4622 (4)	0.3515 (7)	0.0994 (15)	0.695 (6)
H17A	0.9160	0.5350	0.3159	0.119*	0.695 (6)
C18A	0.9929 (3)	0.4418 (6)	0.4376 (8)	0.124 (2)	0.695 (6)
H18A	1.0026	0.3700	0.4754	0.148*	0.695 (6)
H18B	1.0333	0.4987	0.4618	0.148*	0.695 (6)
C17B	0.9235 (6)	0.4196 (9)	0.4153 (14)	0.0994 (15)	0.305 (6)
H17B	0.9228	0.3906	0.5155	0.119*	0.305 (6)
C18B	0.9847 (10)	0.4930 (13)	0.382 (3)	0.124 (2)	0.305 (6)
H18C	0.9872	0.5235	0.2825	0.148*	0.305 (6)
H18D	1.0263	0.5152	0.4567	0.148*	0.305 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0676 (8)	0.0717 (9)	0.0815 (12)	0.0061 (7)	0.0087 (8)	0.0191 (9)
O2	0.0739 (9)	0.0871 (11)	0.0874 (13)	−0.0033 (8)	−0.0090 (9)	−0.0118 (10)
N1	0.1000 (16)	0.1026 (17)	0.110 (2)	−0.0132 (13)	−0.0126 (14)	0.0421 (17)
N2	0.0752 (13)	0.1035 (16)	0.108 (2)	−0.0108 (12)	0.0071 (13)	−0.0001 (15)
C1	0.0660 (12)	0.0597 (11)	0.0568 (13)	0.0000 (9)	0.0044 (9)	−0.0005 (10)
C2	0.0622 (11)	0.0620 (11)	0.0607 (14)	0.0009 (9)	−0.0053 (10)	−0.0006 (10)
C3	0.0697 (12)	0.0576 (11)	0.0567 (13)	−0.0039 (9)	−0.0022 (9)	−0.0003 (10)
C4	0.0609 (11)	0.0682 (12)	0.0636 (14)	−0.0013 (9)	0.0013 (10)	−0.0050 (11)
C5	0.0656 (13)	0.0756 (13)	0.0711 (16)	0.0084 (10)	−0.0023 (11)	0.0017 (13)
C6	0.0718 (13)	0.0713 (14)	0.0616 (15)	0.0088 (10)	−0.0010 (11)	0.0061 (12)
C7	0.0703 (13)	0.0751 (13)	0.0766 (17)	−0.0089 (10)	−0.0071 (12)	0.0100 (13)
C8	0.0634 (12)	0.0784 (13)	0.0772 (17)	−0.0002 (11)	0.0007 (11)	−0.0007 (13)
C9	0.0631 (12)	0.0650 (12)	0.0646 (14)	−0.0006 (9)	0.0042 (10)	0.0100 (11)
C10	0.0858 (16)	0.0753 (14)	0.0680 (17)	−0.0058 (12)	0.0048 (13)	0.0063 (13)
C11	0.0739 (14)	0.0878 (15)	0.0753 (17)	−0.0131 (12)	−0.0074 (13)	0.0062 (14)
C12	0.0677 (12)	0.0778 (13)	0.0743 (18)	−0.0015 (11)	−0.0009 (11)	0.0156 (13)
C13	0.0700 (14)	0.0703 (13)	0.0727 (16)	0.0021 (11)	0.0026 (12)	0.0040 (13)
C14	0.0651 (11)	0.0704 (13)	0.0652 (14)	−0.0038 (10)	−0.0036 (10)	0.0089 (11)
C15	0.101 (2)	0.0907 (17)	0.102 (2)	−0.0066 (14)	−0.0140 (17)	−0.0210 (17)
C16	0.0680 (14)	0.104 (2)	0.111 (3)	−0.0034 (13)	−0.0023 (14)	0.0154 (19)
C17A	0.0668 (18)	0.090 (3)	0.141 (5)	0.000 (2)	−0.001 (2)	0.035 (3)
C18A	0.085 (2)	0.135 (6)	0.151 (7)	−0.016 (3)	−0.031 (3)	0.022 (4)
C17B	0.0668 (18)	0.090 (3)	0.141 (5)	0.000 (2)	−0.001 (2)	0.035 (3)
C18B	0.085 (2)	0.135 (6)	0.151 (7)	−0.016 (3)	−0.031 (3)	0.022 (4)

Geometric parameters (Å, °)

O1—C1	1.364 (3)	C11—H11	1.02 (3)
O1—C9	1.396 (3)	C12—C13	1.395 (4)
O2—C14	1.358 (3)	C12—C16	1.513 (4)
O2—C15	1.428 (3)	C13—C14	1.385 (3)
N1—C7	1.136 (3)	C13—H13	1.02 (3)

N2—C8	1.137 (3)	C15—H15A	0.96
C1—C2	1.379 (3)	C15—H15B	0.96
C1—C6	1.391 (3)	C15—H15C	0.96
C2—C3	1.386 (3)	C16—C17B	1.456 (9)
C2—H2	0.93 (3)	C16—C17A	1.460 (5)
C3—C4	1.400 (3)	C16—H16A	0.97
C3—C7	1.434 (4)	C16—H16C	0.97
C4—C5	1.390 (3)	C16—H16D	0.96
C4—C8	1.431 (3)	C16—H16B	0.96
C5—C6	1.366 (4)	C17A—C18A	1.289 (6)
C5—H5	1.01 (3)	C17A—H17A	0.93
C6—H6	0.97 (3)	C18A—H18A	0.93
C9—C10	1.372 (4)	C18A—H18B	0.93
C9—C14	1.385 (4)	C17B—C18B	1.294 (9)
C10—C11	1.389 (4)	C17B—H17B	0.93
C10—H10	0.94 (3)	C18B—H18C	0.93
C11—C12	1.374 (4)	C18B—H18D	0.93
C1—O1—C9	120.80 (16)	O2—C14—C13	124.9 (2)
C14—O2—C15	117.20 (19)	O2—C14—C9	115.89 (19)
O1—C1—C2	123.6 (2)	C13—C14—C9	119.2 (2)
O1—C1—C6	115.6 (2)	O2—C15—H15A	109.5
C2—C1—C6	120.8 (2)	O2—C15—H15B	109.5
C1—C2—C3	118.8 (2)	H15A—C15—H15B	109.5
C1—C2—H2	123.2 (16)	O2—C15—H15C	109.5
C3—C2—H2	118.0 (16)	H15A—C15—H15C	109.5
C2—C3—C4	120.8 (2)	H15B—C15—H15C	109.5
C2—C3—C7	120.8 (2)	C17B—C16—C12	117.3 (6)
C4—C3—C7	118.4 (2)	C17A—C16—C12	116.6 (3)
C5—C4—C3	119.0 (2)	C17A—C16—H16A	108.1
C5—C4—C8	120.9 (2)	C12—C16—H16A	108.1
C3—C4—C8	120.1 (2)	C17B—C16—H16C	128.8
C6—C5—C4	120.4 (2)	C17A—C16—H16C	108.1
C6—C5—H5	120.3 (15)	C12—C16—H16C	108.1
C4—C5—H5	119.2 (15)	H16A—C16—H16C	107.3
C5—C6—C1	120.1 (2)	C17B—C16—H16D	110.1
C5—C6—H6	122.4 (14)	C12—C16—H16D	108.0
C1—C6—H6	117.5 (14)	H16A—C16—H16D	131.0
N1—C7—C3	177.0 (3)	C17B—C16—H16B	105.4
N2—C8—C4	179.6 (3)	C17A—C16—H16B	127.8
C10—C9—C14	120.9 (2)	C12—C16—H16B	108.3
C10—C9—O1	119.6 (2)	H16D—C16—H16B	107.3
C14—C9—O1	118.8 (2)	C18A—C17A—C16	124.9 (5)
C9—C10—C11	119.4 (3)	C18A—C17A—H17A	117.6
C9—C10—H10	114.7 (17)	C16—C17A—H17A	117.6
C11—C10—H10	125.8 (16)	C17A—C18A—H18A	120.0
C12—C11—C10	120.9 (3)	C17A—C18A—H18B	120.0
C12—C11—H11	125.0 (17)	H18A—C18A—H18B	120.0
C10—C11—H11	114.0 (17)	C18B—C17B—C16	123.9 (13)
C11—C12—C13	119.0 (2)	C18B—C17B—H17B	118.0

C11—C12—C16	122.9 (2)	C16—C17B—H17B	118.0
C13—C12—C16	118.0 (3)	C17B—C18B—H18C	120.0
C14—C13—C12	120.5 (2)	C17B—C18B—H18D	120.0
C14—C13—H13	118.9 (15)	H18C—C18B—H18D	120.0
C12—C13—H13	120.4 (15)		
C9—O1—C1—C2	21.1 (3)	C10—C11—C12—C13	−2.8 (4)
C9—O1—C1—C6	−161.3 (2)	C10—C11—C12—C16	174.6 (3)
O1—C1—C2—C3	177.3 (2)	C11—C12—C13—C14	2.3 (4)
C6—C1—C2—C3	−0.2 (3)	C16—C12—C13—C14	−175.3 (2)
C1—C2—C3—C4	1.3 (3)	C15—O2—C14—C13	0.6 (4)
C1—C2—C3—C7	−178.6 (2)	C15—O2—C14—C9	178.3 (2)
C2—C3—C4—C5	−1.9 (3)	C12—C13—C14—O2	178.0 (2)
C7—C3—C4—C5	178.0 (2)	C12—C13—C14—C9	0.3 (3)
C2—C3—C4—C8	178.7 (2)	C10—C9—C14—O2	179.7 (2)
C7—C3—C4—C8	−1.4 (3)	O1—C9—C14—O2	−10.3 (3)
C3—C4—C5—C6	1.4 (3)	C10—C9—C14—C13	−2.4 (4)
C8—C4—C5—C6	−179.2 (2)	O1—C9—C14—C13	167.6 (2)
C4—C5—C6—C1	−0.3 (4)	C11—C12—C16—C17B	14.8 (6)
O1—C1—C6—C5	−178.0 (2)	C13—C12—C16—C17B	−167.7 (5)
C2—C1—C6—C5	−0.3 (4)	C11—C12—C16—C17A	−18.7 (5)
C1—O1—C9—C10	−111.8 (2)	C13—C12—C16—C17A	158.7 (3)
C1—O1—C9—C14	78.0 (3)	C17B—C16—C17A—C18A	27.7 (11)
C14—C9—C10—C11	1.9 (4)	C12—C16—C17A—C18A	126.7 (6)
O1—C9—C10—C11	−168.0 (2)	C17A—C16—C17B—C18B	−17.3 (12)
C9—C10—C11—C12	0.8 (4)	C12—C16—C17B—C18B	−113.7 (14)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···N2^{i}	0.93 (3)	2.61 (3)	3.510 (3)	166 (2)
C16—H16A···Cg1^{i}	0.97	2.88	3.808 (4)	160

Symmetry codes: (i) *x*+1/2, −*y*+1/2, *z*.

Fig. 1

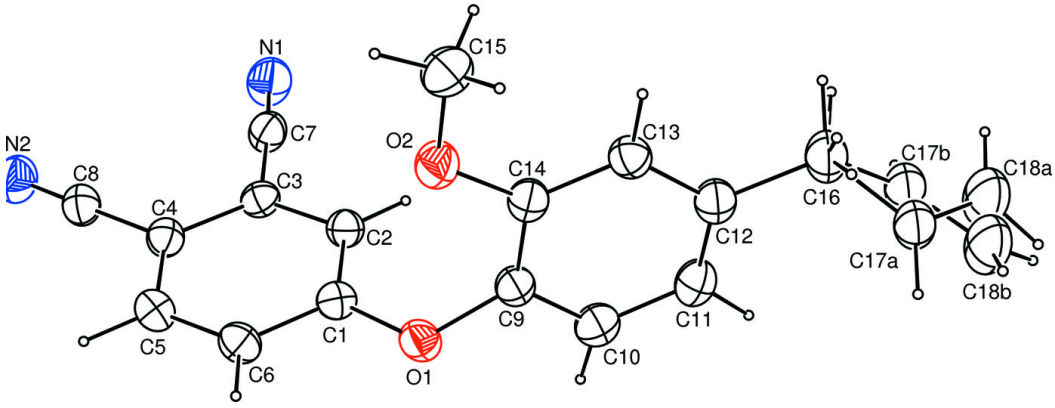
N1
C15
N2
C7
O2
C13
C8
C3
C14
C17b
C18a
C4
C16
C2
C12
C17a
C18b
C5
C1
C9
C11
C6
O1
C10

Fig. 2