

1,4-Bis(3,4-dicyanophenoxy)-2-butyne

Yavuz Köysal,^a Aysen Ağar,^b
Nesuhi Akdemir^b and Şamil
Işık^{a*}

^aDepartment of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, Kurupelit, 55139 Samsun, Turkey, and ^bDepartment of Chemistry, Faculty of Arts and Sciences, Ondokuz Mayıs University, Kurupelit, 55139 Samsun, Turkey

Correspondence e-mail: yavuzk@omu.edu.tr

Key indicators

Single-crystal X-ray study

$T = 293$ K

Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å

R factor = 0.038

wR factor = 0.091

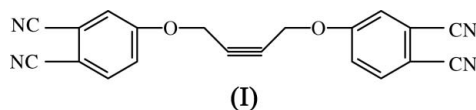
Data-to-parameter ratio = 13.9

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, $\text{C}_{20}\text{H}_{10}\text{N}_4\text{O}_2$, the molecule is arranged around a twofold axis passing through the mid-point of the $\text{C}\equiv\text{C}$ triple bond. The dicyanophenoxy group is planar. The molecule is stabilized by intermolecular $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonding.

Comment

The title compound, (I), is a precursor in the synthesis of polymeric phthalocyanines and high-performance aromatic polymers (McKeown, 1998; Takekoshi, 1987). Phthalocyanine derivatives displaying photophysical properties, electron-transfer ability and oxido-reduction capabilities have been studied for application in electrophotography, optical date-recording systems, electronic devices, photovoltaic cells, fuel cells and electrochromic displays (McKeown, 1998). Polymeric phthalocyanines have been described for use as dyes and industrial high-technology materials and are also of additional interest because of their high thermostability (Leznoff & Lever, 1989–1996). Against this background, we present here the structure of the title compound, (I).



In the molecule of (I), a twofold axis passes through the mid-point of the $\text{C}\equiv\text{C}$ triple bond (Fig. 1). The $\text{C}\equiv\text{N}$ triple-bond distances in the cyano groups are in good agreement with our previous report (Işık & Köysal, 2006). Atom O1 and the CN groups are coplanar with atoms C1–C6, the largest deviation from this plane being 0.065 (2) Å for O1.

There are weak $\text{C}-\text{H}\cdots\text{N}$ hydrogen-bonding interactions present in the crystal structure of (I), which link the molecules into a discrete chain of dimers (Table 1, Fig. 2).

Experimental

2-Butyne-1,4-diol (0.30 g, 3.49 mmol) and 4-nitrophthalonitrile (1.16 g, 6.70 mmol) were dissolved in dry dimethylformamide (40 ml) with stirring under N_2 . Dry fine-powdered potassium carbonate (2.5 g, 18.12 mmol) was added in portions (10×1 mmol) every 10 min. The reaction mixture was stirred for 48 h at 313 K and then poured into ice-water (250 g). The product was filtered off and washed with water and ethanol to give a white product (yield 0.60 g, 53.12%). Single crystals of (I) were obtained from a solution in dry dimethylformamide at room temperature *via* slow evaporation (m.p. 455–458 K).

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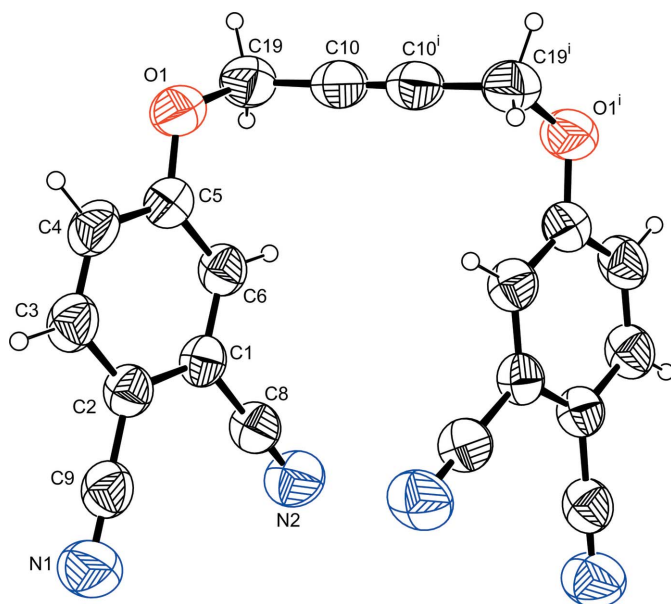


Figure 1
A view of compound (I), with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii. [Symmetry code: (i) $-x, y, -z + \frac{1}{2}$]

Crystal data

$C_{20}H_{10}N_4O_2$
 $M_r = 338.33$
 Monoclinic, $C2/c$
 $a = 22.023 (7) \text{ \AA}$
 $b = 9.570 (2) \text{ \AA}$
 $c = 8.339 (2) \text{ \AA}$
 $\beta = 108.30 (2)^\circ$
 $V = 1668.6 (8) \text{ \AA}^3$

$Z = 4$
 $D_x = 1.347 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 $\mu = 0.09 \text{ mm}^{-1}$
 $T = 293 (2) \text{ K}$
 Prism, colourless
 $0.75 \times 0.21 \times 0.06 \text{ mm}$

Data collection

Stoe IPDS-2 diffractometer
 φ scans
 Absorption correction: integration
 ($X\text{-RED32}$; Stoe & Cie, 2002)
 $T_{\min} = 0.960, T_{\max} = 0.994$

7313 measured reflections
 1641 independent reflections
 1042 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.058$
 $\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.091$
 $S = 0.99$
 1641 reflections
 118 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.044P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.10 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.14 \text{ e \AA}^{-3}$

Table 1
Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$C6-H6 \cdots N2^i$	0.93	2.48	3.369 (2)	159

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

H atoms were positioned geometrically and refined using a riding model, with $C-H = 0.93 \text{ \AA}$ (C_{aromatic}) and 0.97 \AA (CH_2) and with $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$.

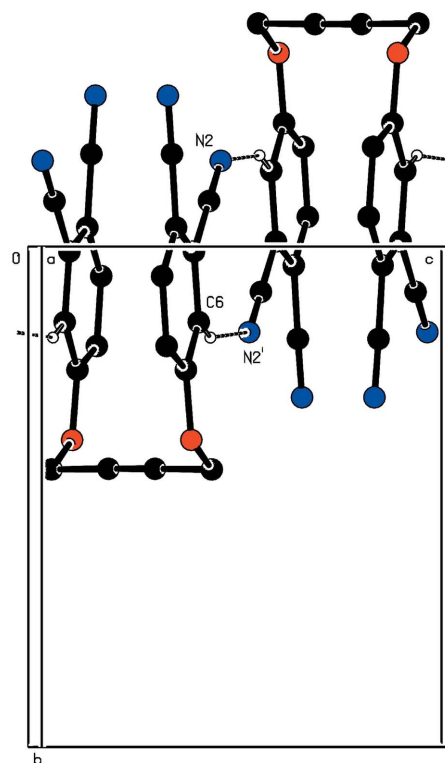


Figure 2
Part of the packing, showing the formation of a chain of dimers via $C-H \cdots N$ hydrogen bonds (dashed lines). H atoms not involved in the hydrogen bonds have been omitted for clarity. [Symmetry code: (i) $1 - x, 1 - y, -z$.]

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: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

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