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4-(3-Pyridyloxy)phthalonitrile

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Key indicators

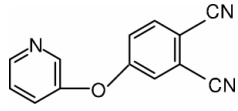
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.040
wR factor = 0.045
Data-to-parameter ratio = 14.0

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

The title compound, $C_{13}H_7N_3O$, contains a phthalonitrile ring and a pyridine ring which are not coplanar, but form a dihedral angle of 85.77 (13)°.

Comment

Phthalocyanines are of enormous technological importance for the manufacture of blue and green pigments. Other areas of current interest include applications in catalysis, chemical sensors, electrochromism, batteries, photodynamic therapy, semiconductive materials, liquid crystals and modified supports for gas–solid chromatography (Leznoff & Lever, 1989–1996). Tetrasubstituted phthalocyanines are generally obtained from mono-substituted phthalonitriles such as 4-(3-pyridyloxy)phthalonitrile (McKeown, 1998), (I), the structure of which is reported here.



(I)

The molecule is non-planar, the dihedral angle between the two six-membered rings being 85.77 (13)°. Bond distances and angles are unexceptional.

Experimental

3-Pyridinol (0.60 g, 6.31 mmol) and 4-nitrophthalonitrile (1.00 g, 5.78 mmol) were dissolved in dry dimethyl sulfoxide (40 ml) with stirring under N_2. Dry fine-powdered potassium carbonate (1.0 g, 7.24 mmol) was added in portions (10 × 1 mmol) every 10 min. The reaction mixture was stirred for 48 h at room temperature and poured into ice–water (150 g). The product was filtered off and washed with (10% *w*/*w*) NaOH solution and water until the filtrate was neutral. Recrystallization from ethanol solution gave a white product (yield 0.73 g, 57.03%). Single crystals were obtained from an absolute ethanol solution of the compound *via* slow evaporation at room temperature (m.p. 384 K).

Crystal data

$C_{13}H_7N_3O$
M_r = 221.22
Monoclinic, $P2_1/c$
a = 4.8686 (5) Å
b = 22.688 (3) Å
c = 10.0658 (11) Å
β = 98.223 (8)°
V = 1100.4 (2) Å^3
Z = 4
D_x = 1.335 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4814 reflections
θ = 1.8–24.1°
μ = 0.09 mm^{-1}
T = 293 K
Rod, colourless
0.33 × 0.17 × 0.08 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: by integration (*X-RED*32; Stoe & Cie, 2002)
T_{min} = 0.982, T_{max} = 0.993
14299 measured reflections
1982 independent reflections
826 reflections with $I > 2\sigma(I)$
R_{int} = 0.090
θ_{max} = 25.2°
$h = -5 \rightarrow 5$
$k = -27 \rightarrow 27$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.045
S = 0.99
1982 reflections
142 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0028P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—O1	1.371 (2)	N1—C9	1.323 (3)
C7—O1	1.404 (3)	N2—C12	1.130 (2)
N1—C8	1.337 (3)	N3—C13	1.131 (2)
N2—C12—C4	179.1 (3)	C8—N1—C9	115.4 (3)
N3—C13—C5	179.2 (3)	C1—O1—C7	117.85 (17)

H atoms were included in the riding-model approximation, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(parent C 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: *WinGX* (Farrugia, 1999).

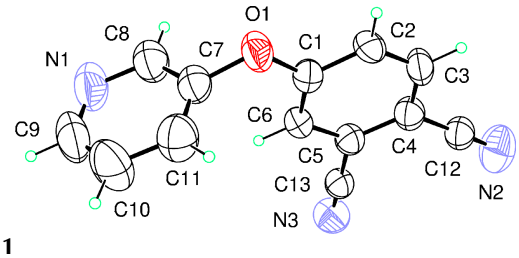


Figure 1
ORTEP-3 (Farrugia, 1997) view of the title compound, showing the atom-numbering scheme and 50% probability displacement ellipsoids.

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