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## Key indicators

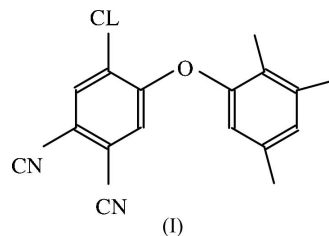
Single-crystal X-ray study  
 $T = 150$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.042  
 $wR$  factor = 0.116  
Data-to-parameter ratio = 17.9For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

## 4-Chloro-3-(2,3,5-trimethylphenoxy)phthalonitrile

The asymmetric unit of the title compound,  $\text{C}_{17}\text{H}_{13}\text{ClN}_2\text{O}$ , contains two independent molecules with no significant difference in their structures. The molecules are non-planar. The dihedral angle between the two benzene rings is  $79.20$  ( $8$ )° in one molecule and  $79.54$  ( $8$ )° in the other.

## Comment

The title compound, (I), is a starting material in the synthesis of symmetrically and unsymmetrically octasubstituted phthalocyanines (McKeown, 1998). Phthalocyanines are traditionally used as dyes and pigments (Moser &amp; Thomas, 1983). For many years, phthalocyanines have attracted continued interest in various research fields, e.g. chemical sensors, electrochromism, batteries, applications in colours, catalysis, photodynamic therapy, semiconductive materials, liquid crystals and non-linear optics (Leznoff &amp; Lever, 1989–1996).

The asymmetric unit contains two independent molecules with no significant difference in their structures (denoted *A* and *B*; Fig. 1). The average  $\text{N}\equiv\text{C}$  bond distance in the cyano groups is short enough to indicate their triple-bond character. The  $\text{C}7-\text{O}1$  bond distance is  $1.353$  ( $3$ ) Å in molecule *A* and  $1.346$  ( $3$ ) Å in molecule *B*, similar to that reported in 4-(1-naphthoxy)phthalonitrile (Karadayı *et al.*, 2003).The  $\text{C}1-\text{C}6$  and  $\text{C}7-\text{C}12$  rings are not coplanar; the dihedral angle between rings  $\text{C}1\text{A}-\text{C}6\text{A}$  and  $\text{C}7\text{A}-\text{C}12\text{A}$  is  $79.20$  ( $8$ )°, and that between rings  $\text{C}1\text{B}-\text{C}6\text{B}$  and  $\text{C}7\text{B}-\text{C}12\text{B}$  is  $79.54$  ( $8$ )°. The bond angles of  $\text{C}10-\text{C}16-\text{N}1$  and  $\text{C}11-\text{C}17-\text{N}2$  are close to  $180^\circ$  in molecules *A* and *B*. There are no hydrogen bonds or  $\pi-\pi$  stacking interactions between molecules.

## Experimental

2,3,5-Trimethylphenol (2.07 g, 15.20 mmol) and 4,5-dichloro-1,2-dicyanobenzene (1.00 g, 5.08 mmol) were stirred at room temperature in dry dimethylformamide (50 ml) under  $\text{N}_2$ . Dry fine-powdered potassium carbonate (2.10 g, 15.22 mmol) was added in portions ( $12 \times 1$  mmol) every 10 min. The mixture was stirred for a further 48 h

Received 12 January 2005

Accepted 28 January 2005

Online 26 February 2005

and poured into ice–water (200 g). The product was filtered off and washed with (10% w/w) NaOH solution and water until the filtrate was neutral. Recrystallization from ethanol gave the pure product (yield 1.00 g, 66.40%). Single crystals were obtained from ethanol at room temperature *via* slow evaporation (m.p. 413 K). Elemental analysis calculated for  $C_{17}H_{13}ClN_2O$ : C 68.81, H 4.42, N 9.44%; found: C 68.84 H 4.40 N 9.46%.

#### Crystal data

$C_{17}H_{13}ClN_2O$   
 $M_r = 296.74$   
 Monoclinic,  $Cc$   
 $a = 12.6986$  (8) Å  
 $b = 12.5724$  (6) Å  
 $c = 18.9151$  (10) Å  
 $\beta = 95.635$  (4)°  
 $V = 3005.2$  (3) Å<sup>3</sup>  
 $Z = 8$

$D_x = 1.312$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 15 817 reflections  
 $\theta = 2.2$ – $27.9$ °  
 $\mu = 0.25$  mm<sup>-1</sup>  
 $T = 150$  K  
 Prism, colourless  
 $0.45 \times 0.33 \times 0.24$  mm

#### Data collection

Stoe IPDS-2 diffractometer  
 $\omega$  scans  
 Absorption correction: by integration (*X-RED32*; Stoe & Cie, 2002)  
 $T_{\min} = 0.911$ ,  $T_{\max} = 0.957$   
 13 168 measured reflections

6783 independent reflections  
 5862 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.143$   
 $\theta_{\text{max}} = 27.9$ °  
 $h = -16 \rightarrow 16$   
 $k = -16 \rightarrow 16$   
 $l = -24 \rightarrow 24$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.042$   
 $wR(F^2) = 0.116$   
 $S = 1.05$   
 6783 reflections  
 379 parameters

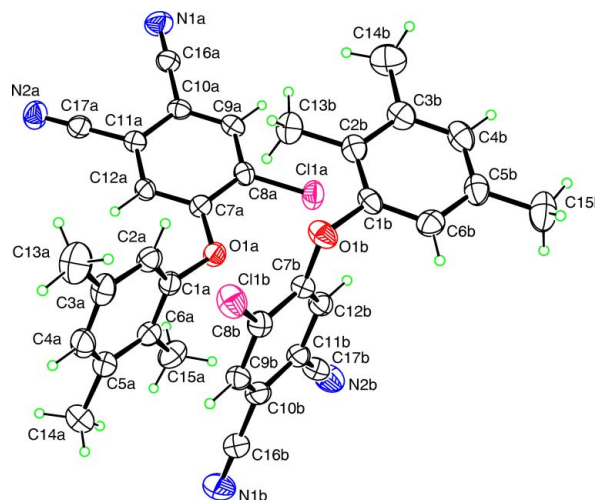
H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0761P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.28$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.25$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

$C7A-O1A$	1.353 (3)	$C7B-O1B$	1.346 (3)
$N1A-C16A-C10A$	179.4 (3)	$N2A-C17A-C11A$	179.2 (3)
$N1B-C16B-C10B$	179.3 (3)	$N2B-C17B-C11B$	179.5 (3)

H atoms were included in calculated positions and refined using a riding model, with aromatic C–H = 0.93 Å and CH<sub>3</sub> C–H = 0.96 Å, and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ . Friedel reflections were merged before the



**Figure 1**

The asymmetric unit of the title compound, showing the atom-numbering scheme and with 50% probability displacement ellipsoids.

final refinement; the Flack (1983) parameter was  $-0.01$  (5).

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).

#### References

- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.  
 Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.  
 Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.  
 Karadayı, N., Akdemir, N., Ađar, E., Gümrukçuođlu, I. E. & Büyükgüngör, O. (2003). *Acta Cryst.* **E59**, o945–o946.  
 Leznoff, C. C. & Lever, A. B. P. (1989–1996). *Phthalocyanines: Properties and Applications*, Vols 1–4. Weinheim & New York: VHC Publishers Inc.  
 McKeown, N. B. (1998). *Phthalocyanine Materials: Synthesis, Structure and Function*. Cambridge University Press.  
 Moser, F. H. & Thomas, A. L. (1983). In *The Phthalocyanines*, Vols. 1 and 2. Boca Raton, Florida: CRC Press.  
 Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.  
 Stoe & Cie (2002). *X-AREA* and *X-RED32*. Stoe & Cie, Darmstadt, Germany.