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## Key indicators

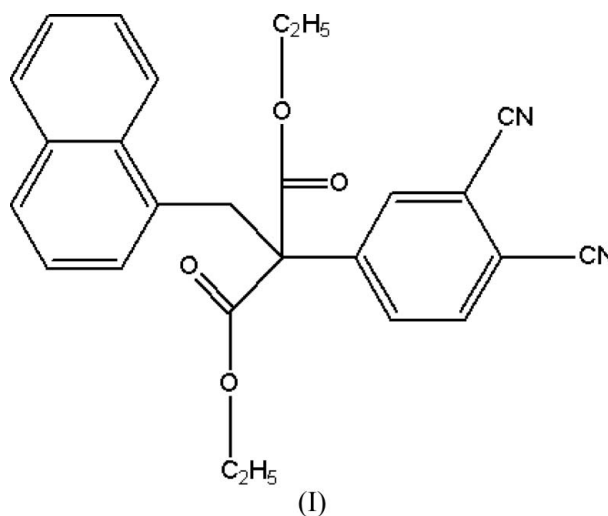
Single-crystal X-ray study  
 $T = 273$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
 $R$  factor = 0.053  
 $wR$  factor = 0.118  
Data-to-parameter ratio = 11.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## Diethyl 2-(3,4-dicyanophenyl)-2-[(2-naphthyl)-methyl]malonate

The asymmetric unit of the title compound,  $\text{C}_{26}\text{H}_{22}\text{N}_2\text{O}_4$ , contains two crystallographically independent molecules. The crystal structure is stabilized by intra- and intermolecular  $\text{C}-\text{H}\cdots\text{O}$  interactions.Received 28 October 2005  
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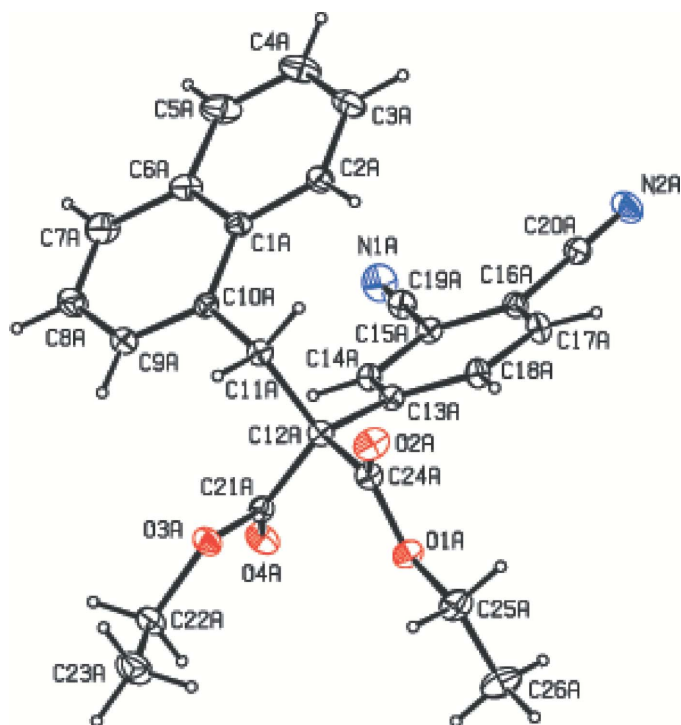
## Comment

Phthalonitriles are desirable precursors for the synthesis of phthalocyanines displaying unusual chemical, coordination or physical properties. In addition to their well known high thermal and chemical stabilities, phthalocyanines have recently become noted for their special optical and electrical properties, such as electrical conductivity, photovoltaic effects and electrochromism. Also, their use as efficient photosensitizers in obtaining singlet oxygen is becoming especially important in the photodynamic therapy (PDT) of tumours (Leznoff &amp; Lever, 1989–1996).

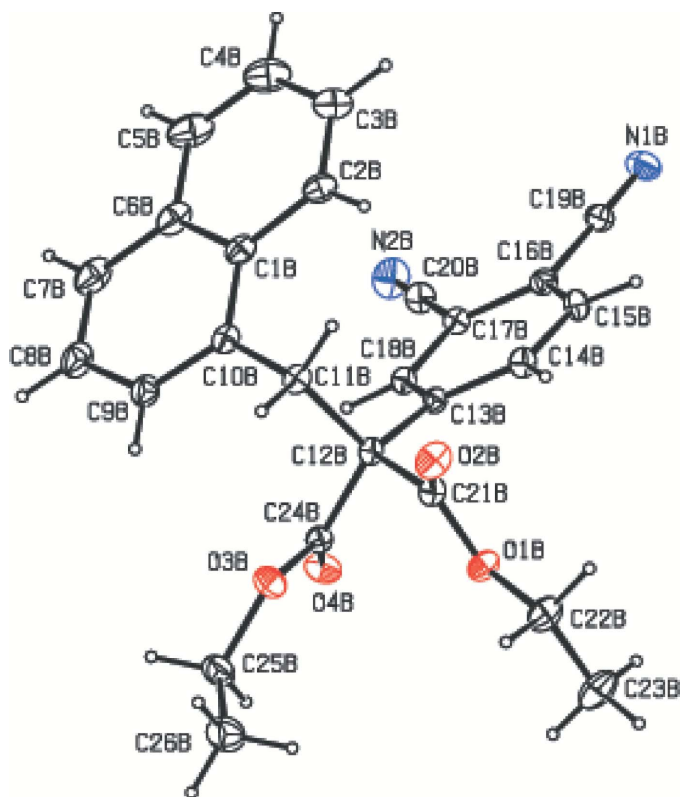


*ORTEP3* (Farrugia, 1997) plots of the independent molecules *A* and *B* in the asymmetric unit of the title compound, (I), showing the atom-labelling schemes, are presented in Figs. 1 and 2, respectively. In both molecules, all the geometrical parameters agree well with literature values (Allen *et al.*, 1987). The naphthalene ring systems of both molecules are essentially planar, the maximum deviations being 0.038 (3) Å for atom C10*A* of molecule *A* and 0.032 (3) Å for atom C10*B* of molecule *B*. The dihedral angle between the naphthalene plane and the benzene ring of the phthalonitrile group is 26.65 (13)° in molecule *A* and 27.63 (13)° in molecule *B*.

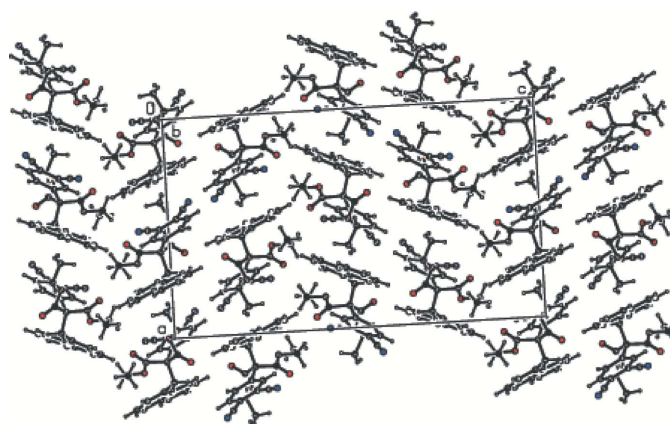
The crystal packing, viewed down the *b* axis, is shown in Fig. 3. The structure of (I) is stabilized by  $\text{C}-\text{H}\cdots\text{O}$  interactions (Table 1).



**Figure 1**  
One of the two independent molecules of (I), showing the labelling of the non-H atoms. Displacement ellipsoids are shown at the 10% probability level.



**Figure 2**  
The other of the two independent molecules of (I), showing the labelling of the non-H atoms. Displacement ellipsoids are shown at the 10% probability level.



**Figure 3**  
View, down the *b* axis, of the molecular packing of (I).

### Experimental

The title compound was obtained through the displacement reaction of 4-nitrophthalonitrile with diethyl malonate and then in a further reaction with 1-(chloromethyl)naphthalene (Şener *et al.*, 2005). Single crystals were obtained by slow evaporation of a solution in absolute ethanol at room temperature.

#### Crystal data

$C_{26}H_{22}N_2O_4$   
 $M_r = 426.46$   
 Orthorhombic,  $Pna2_1$   
 $a = 15.3760$  (3) Å  
 $b = 11.5504$  (2) Å  
 $c = 26.0798$  (5) Å  
 $V = 4631.75$  (15) Å<sup>3</sup>  
 $Z = 8$   
 $D_x = 1.223$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation  
 Cell parameters from 6578 reflections  
 $\theta = 2.2$ – $30.0^\circ$   
 $\mu = 0.08$  mm<sup>-1</sup>  
 $T = 273$  (2) K  
 Needle, colorless  
 $0.68 \times 0.24 \times 0.19$  mm

#### Data collection

Siemens SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{min} = 0.946$ ,  $T_{max} = 0.984$   
 54546 measured reflections

6881 independent reflections  
 3609 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.059$   
 $\theta_{max} = 30.1^\circ$   
 $h = -21 \rightarrow 21$   
 $k = -15 \rightarrow 16$   
 $l = -36 \rightarrow 29$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.053$   
 $wR(F^2) = 0.118$   
 $S = 1.01$   
 6881 reflections  
 577 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0512P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} < 0.001$   
 $\Delta\rho_{max} = 0.10$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.13$  e Å<sup>-3</sup>

**Table 1**  
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>
C2A–H2AA···O2B <sup>i</sup>	0.93	2.60	3.399 (4)	145
C7B–H7BA···O4A	0.93	2.59	3.369 (6)	141
C14A–H14A···O4A	0.93	2.43	2.908 (4)	112
C18B–H18B···O4B	0.93	2.43	2.903 (3)	111
C25B–H25C···O4B	0.97	2.38	2.723 (4)	100

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

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 (aromatic), 0.96 (methyl) and 0.97 Å (methylene);  $U_{\text{iso}}(\text{H}) = 1.2$  (1.5 for methyl) times  $U_{\text{eq}}(\text{carrier atom})$ . In the absence of significant anomalous dispersion effects, the Friedel pairs were averaged.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINTE* (Siemens, 1996); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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