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***N,N'*-Diphenylperylene-3,4:9,10-bis(dicarboximide)**

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N,N'-Diphenylperylene-3,4:9,10-bis(dicarboximide)

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Key indicators

Single-crystal X-ray study

$T = 93\text{ K}$

Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$

R factor = 0.055

wR factor = 0.146

Data-to-parameter ratio = 11.0

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

The title compound, $\text{C}_{36}\text{H}_{18}\text{N}_2\text{O}_4$, has one half-molecule in the asymmetric unit with the other half generated by a crystallographic inversion centre. The perylene-imide skeleton is entirely planar, but the terminal benzene rings are twisted in the same directions by $55.55(8)^\circ$. The molecules are stacked along the b axis.

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Comment

Perylene compounds are industrially important pigments that exhibit a variety of shades in the solid state from red *via* maroon to black, depending on the substituents (Herbst & Hunger, 1993). Besides their application as colorants, they are also found useful as materials for electrophotographic photoreceptors (Borsenberger *et al.*, 1984), photovoltaic elements (Gregg, 1996), optical disks (Mizuguchi, 1998), and hydrogen-gas sensors (Sato *et al.*, 2006). The title compound, (I) or PPI, has recently also attracted attention as a material for organic field-effect transistors (FETs) (Horowitz *et al.*, 1996), where the molecular arrangement plays a determinant role for the carrier mobility. We report here the structure of (I) and compare it with PPI-analogues (used for hydrogen-gas sensors) which include pyridyl rings instead of the benzene rings, *viz.* the *ortho*-pyridyl (OPP) (Mizuguchi *et al.*, 2005a), *meta*-pyridyl (MPP) (Mizuguchi *et al.*, 2005b) and *para*-pyridyl (PPP) derivatives (Hino *et al.*, 2005).

In the title compound, (I) (Fig. 1), the molecule has C_i symmetry. The perylene-imide skeleton is entirely planar, as indicated by the mean deviation of $0.037\text{ \AA}$ from the least-squares plane defined by all non-H atoms which constitute the skeleton. However, the terminal benzene rings are twisted in the same directions by $55.55(8)^\circ$. The molecules are stacked along the b axis (Fig. 2). The molecular conformation and arrangement are quite similar to those of MPP. OPP and PPP have different molecular packing arrangements since the molecules stack in parallel, along the short axis, with tilt angles of about 52.5 and 31.5° , respectively.

Experimental

PPI was synthesized by the reaction of perylenetetracarboxylic dianhydride with aniline in the presence of diethanolamine at 450 K for 2 h according to the literature procedure of Spietschka & Troester (1986). The product was then purified three times by sublimation at 750 K, using a two-zone furnace (Mizuguchi, 1981). Single crystals of PPI were grown from the vapour phase in a closed system based upon a two-zone furnace. After 48 h, a number of block-shaped single crystals were obtained.

Crystal data

$C_{36}H_{18}N_2O_4$
 $M_r = 542.52$
 Monoclinic, $P2_1/c$
 $a = 16.805(2) \text{ \AA}$
 $b = 3.8795(5) \text{ \AA}$
 $c = 18.381(2) \text{ \AA}$
 $\beta = 98.953(9)^\circ$
 $V = 1183.8(2) \text{ \AA}^3$

$Z = 2$
 $D_x = 1.522 \text{ Mg m}^{-3}$
 Cu $K\alpha$ radiation
 $\mu = 0.81 \text{ mm}^{-1}$
 $T = 93 \text{ K}$
 Block, red
 $0.20 \times 0.05 \times 0.04 \text{ mm}$

Data collection

Rigaku R-AXIS RAPID
 diffractometer
 ω scans
 Absorption correction: multi-scan
 (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.960$, $T_{\max} = 0.968$

8862 measured reflections
 2107 independent reflections
 1316 reflections with $F^2 > 2\sigma(F^2)$
 $R_{\text{int}} = 0.057$
 $\theta_{\max} = 68.2^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.055$
 $wR(F^2) = 0.146$
 $S = 0.89$
 2107 reflections
 191 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0948P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.33 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.24 \text{ e \AA}^{-3}$

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent C atoms, with $C-H = 0.95 \text{ \AA}$ and $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2005); program(s) used to solve structure: *SHELXS97*; program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-III* (Burnett & Johnson, 1996); software used to prepare material for publication: *CrystalStructure*.

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Figure 1

A view of the molecular structure of (I), showing 50% probability displacement ellipsoids. The unlabelled atoms are related to the labelled atoms by the symmetry operation $(1 - x, 1 - y, 1 - z)$.

Figure 2

The packing arrangement in (I). For clarity reasons, only some molecules are shown and the H atoms have been omitted.

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