N,N'-Diphenylperylene-3,4:9,10-bis(dicarboximide)
Kazuyuki Sato and Jin Mizuguchi
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Department of Applied Physics, Graduate School of Engineering, Yokohama National University, Tokiwadai 79-5, Hodogaya-ku, Yokohama 240-8501, Japan

Correspondence e-mail: mizu-j@ynu.ac.jp

Key indicators
Single-crystal X-ray study
T = 93 K
Mean σ(C–C) = 0.003 Å
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.

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The title compound, C_{36}H_{18}N_{2}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)^°. The molecules are stacked along the b axis.

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 Å 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)^°. 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, but 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

\[ \text{C}_{36}\text{H}_{18}\text{N}_2\text{O}_4 \]

\[ M_r = 542.52 \]

Monoclinic, \( P2_1/c \)

\[ \alpha = 16.805 \ (2) \ \text{Å} \]

\[ \beta = 98.953 \ (9) \]

\[ V = 1183.8 \ (2) \ \text{Å}^3 \]

Data collection

Rigaku R-AXIS RAPID

diffractometer

Absorption correction: multi-scan


8862 measured reflections

2107 independent reflections

1316 reflections with \( F^2 > 2\sigma(F^2) \)

\[ R_{	ext{e}} = 0.057 \]

\[ \theta_{	ext{max}} = 68.2^\circ \]

Refinement

Refinement on \( F^2 \)

\[ \text{H-atom parameters constrained} \]

\[ w = 1/[(\sigma(F)^2 + 0.0964P)^2] \]

Where \( P = (\text{F}^2 + 2F^2)/3 \)

\[ (\Delta/\sigma)_{\text{max}} < 0.001 \]

\[ \Delta \rho_{\text{max}} = 0.33 \ \text{e Å}^{-3} \]

\[ \Delta \rho_{\text{min}} = -0.24 \ \text{e Å}^{-3} \]

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

Data collection: \textit{PROCESS-AUTO} (Rigaku, 1998); cell refinement: \textit{PROCESS-AUTO}; data reduction: \textit{CrystalStructure} (Rigaku/MSC, 2005); program(s) used to solve structure: \textit{SHELXS97}; program(s) used to refine structure: \textit{SHELXL97}; molecular graphics: \textit{ORTEPIII} (Burnett & Johnson, 1996); software used to prepare material for publication: \textit{CrystalStructure}.

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References


