Data reduction: *HKL Package*. Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *SHELXTL* (Sheldrick, 1997). Software used to prepare material for publication: *SHELXTL*.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: GS1018). Services for accessing these data are described at the back of the journal.

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N,*N'*-Bis(2-methoxyethyl)pyromellitimide†

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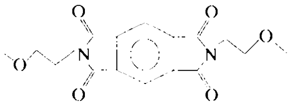
Abstract

The structure of the title compound, $C_{16}H_{16}N_2O_6$, is organized in layers perpendicular to the *b* axis. The central part of the molecule is planar; the lateral chains are also planar and are almost perpendicular (79°) to the ring plane.

Comment

We recently undertook the study of the structure of a family of copolymers in which aromatic moieties and oxyethylene segments alternate in the main chain (Djurado *et al.*, 1997). These systems are used as electrodes in electrochemical or electrochromic devices because of their electroactive properties (Michot *et al.*, 1995).

In this framework, the title compound, PMT, can be considered as the elementary chemical unit constituting these polymers. Its structure was solved in order to obtain details about the stacking mode of the aromatic units. This knowledge could give us a reliable starting point for modelling the structure of semi-crystalline phases of copolymers which can only be studied by X-ray powder diffraction. In the molecule of PMT, the lateral chains can rotate around the N10—C15 and N20—C25 bonds. The planes through these chains make two angles of 79° [79.47 (6) and 79.17 (6)°] with the plane through the benzenoid ring of the aromatic unit. We observed neither disorder nor abnormally high displacement parameters for the ends of the chains. The molecule was found to be almost perfectly centrosymmetrical (*BUNYIP*; Hester & Hall, 1995), but the additional inversion centre is not a crystallographic one and does not lead to another space group.



PMT

The structure of PMT can be described as a regular stacking of layers perpendicular to the *b* axis, in which π overlapping between the aromatic parts is not at a maximum.

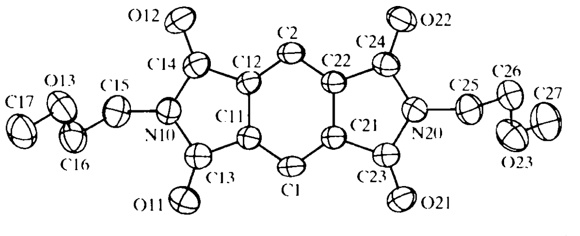


Fig. 1. The molecular structure of PMT showing the atom numbering, with displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted for clarity.

Experimental

PMT was synthesized by M. Armand. Crystals were obtained by evaporation of a solution of acetonitrile at 277 K. The same

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† Alternative name: 2,6-bis(3-oxabutyl)-2,3,6,7-tetrahydro-1*H*,5*H*-pyrrolo[3,4-*f*]isoindole-1,3,5,7-tetrone.

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kind of crystals are obtained from a solution of dimethylformamide. It should be noted that another phase, obtained from water at room temperature, may be due to the presence of water and hydrogen bonding in the crystal.

Crystal data

$C_{16}H_{16}N_2O_6$
$M_r = 332.3$
Monoclinic
$P2_1/c$
$a = 7.8620\,(8)$ Å
$b = 19.526\,(2)$ Å
$c = 10.469\,(1)$ Å
$\beta = 105.15\,(1)°$
$V = 1551.3\,(3)$ Å^3
$Z = 4$
$D_x = 1.423$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 20 reflections
$\theta = 10–12°$
$\mu = 0.11$ mm^{-1}
$T = 293$ K
Parallelepiped
$0.4 \times 0.3 \times 0.3$ mm
Translucent pale white

Data collection

Nonius CAD-4 diffractometer
ω scans
Absorption correction: none
4965 measured reflections
4504 independent reflections
2981 reflections with $I_{net} > 2\sigma(I_{net})$

$R_{int} = 0.012$
$\theta_{max} = 29.96°$
$h = 0 \rightarrow 11$
$k = 0 \rightarrow 27$
$l = -14 \rightarrow 14$
2 standard reflections every 100 reflections intensity decay: 0.5%

Refinement

Refinement on F
$R = 0.044$
$wR = 0.036$
$S = 1.526$
2967 reflections
282 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F) + 0.1F]$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.279$ e Å^{-3}
$\Delta\rho_{min} = -0.167$ e Å^{-3}
Extinction correction: Zachariasen (1963)
Extinction coefficient: 0.26 (2)
Scattering factors from *International Tables for X-ray Crystallography* (Vol. IV)

Table 1. *Selected bond lengths (Å)*

C14—N10	1.382 (2)	N20—C23	1.390 (2)
C14—O12	1.204 (2)	N20—C25	1.460 (3)
O22—C24	1.204 (2)	N10—C15	1.462 (3)
C13—N10	1.389 (2)	O23—C26	1.396 (3)
C13—O11	1.205 (2)	O23—C27	1.421 (3)
O21—C23	1.205 (2)	O13—C16	1.403 (3)
N20—C24	1.390 (2)	O13—C17	1.411 (3)

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989). Cell refinement: *CAD*-4 *Software*. Data reduction: *Xtal*3.2 *SORTRF* and *ADDREF* (Hall *et al.*, 1992). Program(s) used to solve structure: *Xtal*3.2 *GENTAN*. Program(s) used to refine structure: *Xtal*3.2 *CRYLSQ*. Molecular graphics: *Xtal*3.2 *ORTEP*. Software used to prepare material for publication: *Xtal*3.2 *BONDLA* and *CIFIO*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1219). Services for accessing these data are described at the back of the journal.

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Bond-length alternation in rigidized merocyanines

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Abstract

The two merocyanines 7-(4-dimethylaminophenyl)-2,3,4,4a,5,6,10,10a-octahydroanthracen-2-one [$C_{22}H_{25}NO$, (2)] and [2,3,4,4a,5,6,10,10a-octahydro-7-(5-piperidino-2-thienyl)-2-anthrylidene]methanedicarbonitrile [$C_{26}H_{27}N_3S$, (4)] show somewhat shortened single bonds [1.434 (4)–1.452 (4) Å in (2) and 1.421 (4)–1.425 (4) Å in (4)] and elongated double bonds [1.345 (4)–1.358 (4) Å in (2) and 1.355 (4)–1.365 (4) Å in (4)] compared to standard bond lengths in polyenes. A comparison of the merocyanines reveals that (4) exhibits a slightly smaller bond length alternation within the rigidized hexatriene moiety than (2), probably because of an increased ground-state polarization.

Comment

Photorefractive materials have a high potential for optical information processing and storage (Kippelen *et*