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1,4-Bis(4-nitrophenoxy)benzene

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.107
Data-to-parameter ratio = 15.4

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, $C_{18}H_{12}N_2O_6$, crystallizes with two half-molecules in the asymmetric unit. All molecules lie on a centre of inversion. The dihedral angles between the central and terminal benzene rings are 74.75 (4) and 85.25 (5)° for the two molecules in the asymmetric unit.

Comment

Aromatic polyimides are considered to be one of the most important classes of high performance polymers because they have excellent thermal, mechanical and electrical properties (Choi *et al.*, 2001), as well as outstanding chemical resistance (Sroog, 1991). However, their applications are often limited because of their poor solubility and high processing temperature, partially due to strong interchain interactions (Butt *et al.*, 2005). To overcome these limitations, many efforts have been made to improve the processability of the polyimides while maintaining their excellent properties (Chung & Kim, 2000). Different structural modifications of the polymer backbone have been studied to reduce the chain interactions, such as the introduction of flexible links (O, S, CO, SO, CH_2, *etc*.) to the main chain (Eastmond et al., 1996), which disrupt the conjugation and increases the chain flexibility, and the addition of bulky substituents which hinder the chain packing but do not affect the glass transition temperature (Rozhanskii *et al.*, 2000 or 2005). The title compound, (I), is the result of an attempt to prepare soluble and processable polyimides.

(I)

Compound (I) crystallizes with two half-molecules in the asymmetric unit. All molecules lie on a centre of inversion. The dihedral angles between the central and terminal benzene rings are 74.75 (4) and 85.25 (5)° for the two molecules in the asymmetric unit

Experimental

A mixture of 2 g (0.018 mol) hydroquinone, 5.0 g (0.036 mol) anhydrous K_2CO_3 and 3.81 ml (0.036 mol) 4-fluoronitrobenzne in a two-necked round-bottomed flask containing 70 ml dimethyl acetamide (DMAc) was heated at 373 K for 20 h under a nitrogen atmosphere. The colour of the solution changed from yellow to dark brown as the reaction proceeded. After cooling to room temperature, the reaction mixture was poured into 800 ml of water. The resulting yellow solid was washed thoroughly with water and then separated by filtration.

The crude product was recrystallized from ethanol (yield 87%, m.p. 511 K).

Crystal data

$C_{18}H_{12}N_2O_6$
M_r = 352.30
Triclinic, $P\overline{1}$
a = 7.2861 (6) Å
b = 10.1381 (9) Å
c = 12.0838 (11) Å
α = 91.973 (7)°
β = 106.497 (7)°
γ = 110.152 (6)°
V = 794.74 (12) Å^3
Z = 2
D_x = 1.472 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 173 (2) K
Needle, colourless
0.38 × 0.11 × 0.10 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: none
18200 measured reflections
3644 independent reflections
3064 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 27.6°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.107
S = 1.03
3644 reflections
236 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0545P)^2 + 0.2087P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.021 (4)

H atoms were found in a difference map, but were positioned geometrically and allowed to ride on their parent C atoms at a distance of 0.95 Å, and with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*.

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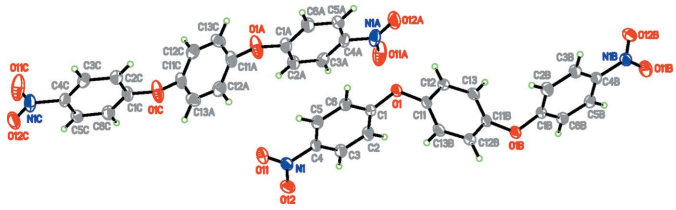

Figure 1
The structure of the two independent molecules of the title compound, (I). Displacement ellipsoids are drawn at the 50% probability level. Atoms with suffix B are related to atoms with no suffix by $-x+2, -y+1, -z+1$. Atoms with suffix C are related to atoms with suffix A by $-x, -y+2, -z$.

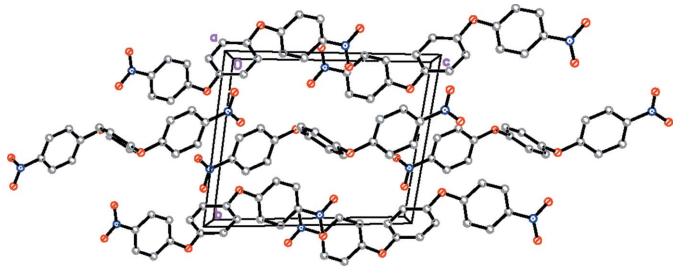

Figure 2
Packing diagram of (I), viewed along the a axis. H atoms have been omitted.

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