

## Bis[4-(4-nitrophenoxy)phenyl] ketone

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## Key indicators

Single-crystal X-ray study

$T = 173\text{ K}$

Mean  $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$

$R$  factor = 0.040

$wR$  factor = 0.105

Data-to-parameter ratio = 12.7

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

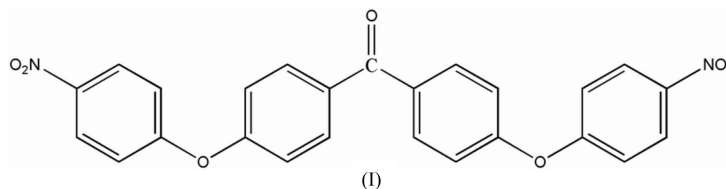
The asymmetric unit of the title compound,  $\text{C}_{25}\text{H}_{16}\text{N}_2\text{O}_7$ , contains two half-molecules both of which are located on twofold rotation axes.

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## Comment

Wholly aromatic polyimides are well accepted as high performance polymers and they are also high temperature resistant materials (Hergenrother *et al.*, 2002). They exhibit a favorable balance of physical and chemical properties and show excellent thermal, mechanical and electrical properties; they are widely used in microelectronics and aerospace engineering (Eastmond & Paprotny, 1999). However, the technological and industrial application of rigid polyimides are limited by processing difficulties due to their high melting points or glass transition temperature and lack of solubility in most organic solvents (Hsio *et al.*, 1997). Strong interaction between polyimide chains and their rigid structures are the main reason for these behaviors. Many efforts have been made in the design and synthesis of new dianhydrides (Eastmond & Paprotny, 1999) and diamines (Yang & Chen, 1993). Incorporation of flexible units, such as  $-\text{NHCO}-$ ,  $-\text{O}-$  (Barikani & Mehdipour-Ataei, 2000),  $-\text{CO}-$  and  $-\text{SO}_2-$ , is one of the most important approaches in overcoming these processing problems (Liaw & Liaw, 2001). The title compound, (I), has been used as a precursor in the synthesis of soluble and flexible polyimides, to overcome the processing difficulties.



The asymmetric unit of (I) contains two half-molecules which are both located on twofold rotation axes. Geometric parameters are unexceptional, differing only in the dihedral angle between the two central benzene rings, which is  $52.76(5)^\circ$  in the first molecule and  $62.97(5)^\circ$  in the second. The dihedral angle between the central benzene ring (C11–C16) and benzene ring C21–C26 of the nitrophenyl ring in the first molecule is  $60.24(5)^\circ$ . The corresponding dihedral angle in the second molecule is  $61.70(5)^\circ$ . The crystal packing is stabilized by intermolecular  $\text{C}-\text{H}\cdots\text{O}$  interactions (Table 2), forming a three-dimensional network (Fig. 2). A  $\pi-\pi$  interaction between the C21–C26 and (C21–C26)<sup>iv</sup> benzene rings [symmetry code: (iv)  $1 - x, 2 - y, 1 - z$ ], the distance between the centroids being  $3.756\text{ \AA}$ .

## Experimental

A mixture of 4,4'-dihydroxybenzophenone (2.0 g, 9.34 mmol), anhydrous potassium carbonate (2.55 g, 18.68 mmol) and 4-fluoronitrobenzene (2.63 g, 18.68 mmol) in a two-necked round-bottomed flask containing 60 ml dimethylacetamide was treated at 373 K for 20 h under a nitrogen atmosphere. After cooling to room temperature, the reaction mixture was poured into 700 ml distilled water, forming a yellow solid which was washed thoroughly with water and separated by filtration. The crude product was recrystallized from dichloromethane to give 3.70 g of (I) in 87% yield (m.p. 423 K).

## Crystal data

$C_{25}H_{16}N_2O_7$	$Z = 4$
$M_r = 456.40$	$D_x = 1.441 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 11.535 (2) \text{ \AA}$	$\mu = 0.11 \text{ mm}^{-1}$
$b = 11.396 (2) \text{ \AA}$	$T = 173 (2) \text{ K}$
$c = 16.724 (3) \text{ \AA}$	Block, light brown
$\beta = 106.90 (3)^\circ$	$0.31 \times 0.26 \times 0.13 \text{ mm}$
$V = 2103.6 (7) \text{ \AA}^3$	

## Data collection

Stoe IPDS-II two-circle diffractometer	3950 independent reflections
$\omega$ scans	3204 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{\text{int}} = 0.055$
17222 measured reflections	$\theta_{\text{max}} = 25.7^\circ$

## Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0618P)^2 + 0.2443P]$
$R[F^2 > 2\sigma(F^2)] = 0.040$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.105$	$(\Delta\sigma)_{\text{max}} < 0.001$
$S = 1.03$	$\Delta\rho_{\text{max}} = 0.24 \text{ e \AA}^{-3}$
3950 reflections	$\Delta\rho_{\text{min}} = -0.25 \text{ e \AA}^{-3}$
310 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	Extinction coefficient: 0.0118 (17)

Table 1

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C12A-H12A\cdots O4^i$	0.95	2.55	3.453 (2)	160
$C15-H15\cdots O1A$	0.95	2.38	3.2340 (19)	149
$C23A-H23A\cdots O3^{ii}$	0.95	2.55	3.283 (2)	135
$C26A-H26A\cdots O1^{iii}$	0.95	2.39	3.1678 (19)	138

Symmetry codes: (i)  $x + \frac{1}{2}, -y + 1, z + \frac{1}{2}$ ; (ii)  $-x, -y + 1, -z + 1$ ; (iii)  $x - 1, y, z$ .

H atoms were located in a difference map and refined using a riding model, with  $C-H = 0.95$  and  $0.99 \text{ \AA}$  for aromatic and methylene H atoms, respectively.  $U_{\text{iso}}(\text{H})$  values were set at  $1.2U_{\text{eq}}(\text{C})$ .

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); 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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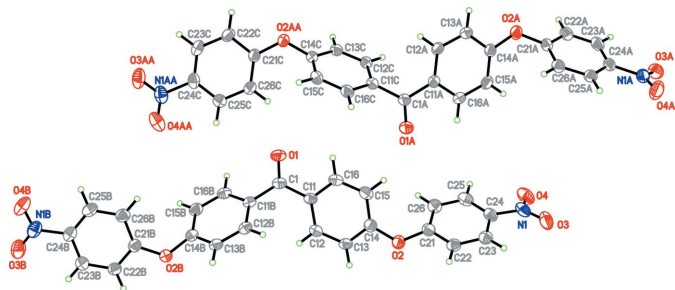


Figure 1

The structure of (I). Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (B)  $-x + \frac{3}{2}, y, -z + \frac{3}{2}$ ; (C)  $-x + \frac{3}{2}, y, -z + \frac{3}{2}$ .]

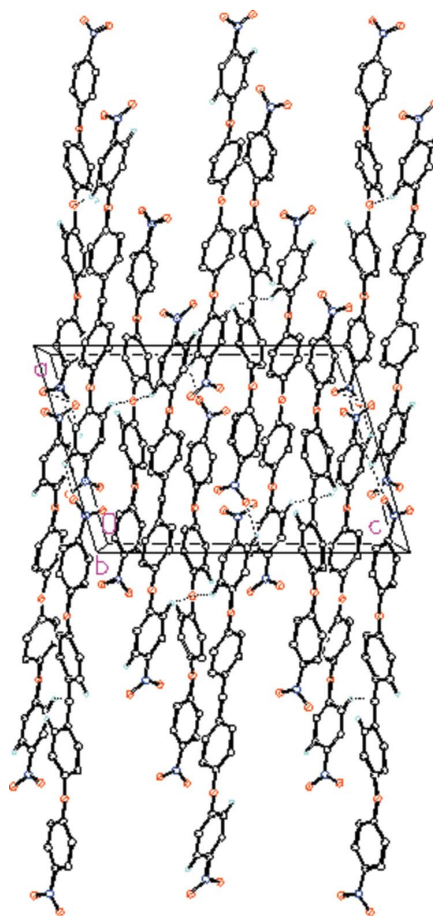


Figure 2

The crystal packing, viewed along  $[010]$ . Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

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