N,N,N′N′-Tetraphenyl-2,2′-(o-phenylenedioxy)-diacetamide

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In the title compound, $C_{34}H_{28}N_2O_4$, the molecule lies on a crystallographic twofold axis. In the crystal structure, the molecules are linked by C—H···O hydrogen bonds into double chains along the c axis. These chains are interlinked via C—H···π interactions.
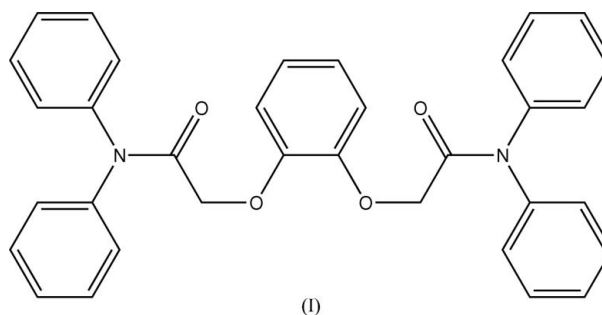
Comment

In our ongoing study of amide-type polyethers, we have synthesized the title compound, (I). Here, we report its crystal structure.

(I)

The asymmetric unit of (I) contains one half-molecule, the other half being related by a crystallographic twofold axis (Fig. 1). Bond lengths in (I) (Table 1) are within normal ranges (Allen *et al.*, 1987). The sum of the angles around atom N1 is 359.9°, implying a planar configuration. The dihedral angle between the two benzene rings attached to atom N1 is
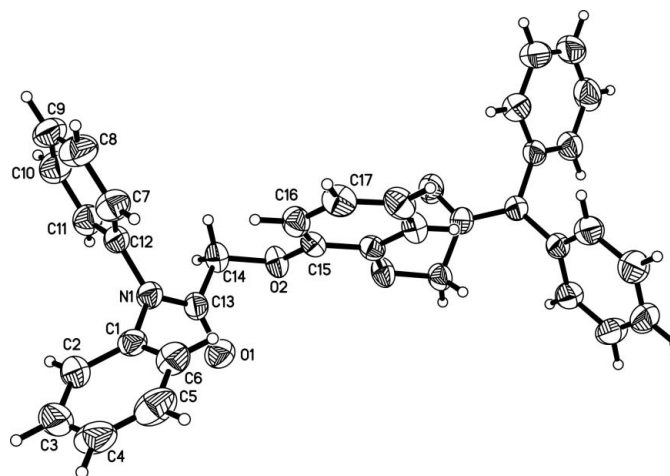
Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. Unlabelled atoms are related to labelled atoms by the symmetry operator $(-x, y, \frac{1}{2} - z)$.

83.91 (5)°, while these two rings (C1–C6 and C7–C12) make angles of 62.68 (5) and 54.89 (6)°, respectively, with the central benzene ring.

In the crystal structure, molecules of (I) are linked into double chains along the c axis (Fig. 2) via C11—H11A···O1^i hydrogen bonds (symmetry code as in Table 2). The packing is further stabilized by C—H···π interactions involving the C1—C6 benzene ring (centroid Cg1).

Experimental

Compound (I) was prepared according to the literature method of Wen *et al.* (2005). Yellow single crystals suitable for an X-ray diffraction study were obtained by slow evaporation of a petroleum ether–ethyl acetate solution (1:3 *v/v*) over a period of 8 d.

Crystal data

$C_{34}H_{28}N_2O_4$	$D_x = 1.290$ Mg m^{-3}
$M_r = 528.58$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 2861
$a = 16.0863\ (10)$ Å	reflections
$b = 11.0050\ (7)$ Å	$\theta = 2.4$–26.0°
$c = 16.5816\ (11)$ Å	$\mu = 0.09$ mm^{-1}
$\beta = 111.981\ (1)°$	$T = 293\ (2)$ K
$V = 2722.1\ (3)$ Å^3	Plate, yellow
$Z = 4$	$0.32 \times 0.19 \times 0.08$ mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	2674 independent reflections
	2284 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.016$
Absorption correction: multi-scan	$\theta_{max} = 26.0°$
(*SADABS*; Sheldrick, 1996)	$h = -19 \rightarrow 19$
$T_{min} = 0.973$, $T_{max} = 0.993$	$k = -13 \rightarrow 10$
7490 measured reflections	$l = -20 \rightarrow 20$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0486P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.042$	$+ 1.2205P]$
$wR(F^2) = 0.106$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
2674 reflections	$\Delta\rho_{max} = 0.15$ e Å^{-3}
181 parameters	$\Delta\rho_{min} = -0.19$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

O1—C13	1.2157 (16)	N1—C13	1.3635 (17)
O2—C15	1.3740 (15)	N1—C12	1.4404 (17)
O2—C14	1.4228 (16)		
C13—N1—C12	124.88 (11)	C12—N1—C1	116.82 (10)
C13—N1—C1	118.21 (11)		
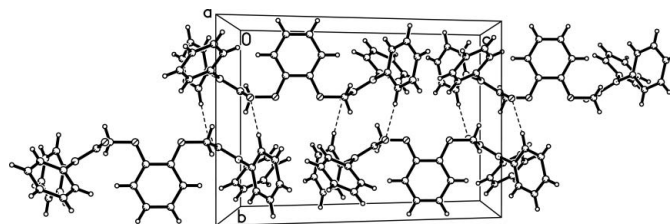
Figure 2
The crystal packing of (I), showing a hydrogen-bonded (dashed lines) double chain.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11A···O1^i	0.93	2.41	3.308 (2)	162
C17—H17A···Cg1^{ii}	0.93	2.70	3.563 (2)	154

Symmetry codes: (i) $-x, -y + 2, -z + 1$; (ii) $-x, -y + 1, -z + 1$. Cg1 is the centroid of ring C1–C6.

All H atoms were positioned geometrically and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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