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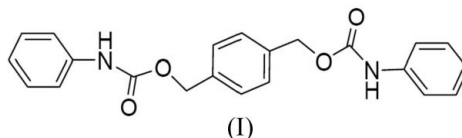
## Key indicators

Single-crystal X-ray study  
 $T = 294$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.040  
 $wR$  factor = 0.117  
Data-to-parameter ratio = 14.6For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.*p*-Phenylenedimethylene bis(*N*-phenylcarbamate)The molecule of the title compound,  $\text{C}_{22}\text{H}_{20}\text{N}_2\text{O}_4$ , is centrosymmetric. Intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds link the molecules, forming a ribbon structure.

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## Comment

As a useful building block for pharmaceuticals (Leffler & Matson, 1948), the title compound, (I), was synthesized by the reaction of phenyl isocyanate and 1,4-phenylenedimethanol in the presence of a trace of triethylamine (Alizadeh *et al.*, 2002). The molecular structure of (I) and the atom-numbering scheme are shown in Fig. 1.The molecule of (I) is centrosymmetric. The two terminal phenyl rings are thus parallel, and they are almost perpendicular to the central ring, with dihedral angles of  $84.47$  ( $2$ )°. The bond length of  $\text{N1}-\text{C7}$  (Table 1) is longer than that ( $1.32$  Å) for a peptide linkage (Taira *et al.*, 1988).  $\text{N1}-\text{C6}$  is shorter than a normal  $\text{C}-\text{N}$  single bond, and longer than a normal  $\text{C}=\text{N}$  double bond, probably as a result of electron delocalization, suggesting that the  $\text{C6}-\text{N1}$  bond is conjugated with the benzene ring (Li & Zhou, 2006). $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds (Table 2) link molecules together, forming ribbons along the  $b$  axis (Fig. 2).

## Experimental

A mixture of 1,4-phenylenedimethanol (Alizadeh *et al.*, 2002) ( $14.5$  mmol) and phenyl isocyanate ( $44.12$  mmol) was added to dry dichloromethane ( $35$  ml) with a trace amount of dry triethylamine ( $0.05$  g) (Griffin *et al.*, 1996). The mixture was stirred at room temperature for  $2$  h and then boiled under reflux for  $6$  h (reaction monitored by TLC), and left overnight. The precipitate was filtered off and washed with ethanol three times, giving a colorless solid ( $3.37$  g,  $61.8\%$ ). Single crystals suitable for crystallographic analysis were obtained by slow evaporation of a solution in ethanol (m.p.  $457$ – $461$  K).

## Crystal data

 $\text{C}_{22}\text{H}_{20}\text{N}_2\text{O}_4$   
 $M_r = 376.40$   
Monoclinic,  $P2_1/c$   
 $a = 18.973$  ( $5$ ) Å  
 $b = 5.0236$  ( $14$ ) Å  
 $c = 9.915$  ( $3$ ) Å  
 $\beta = 95.944$  ( $5$ )°  
 $V = 939.9$  ( $5$ ) Å<sup>3</sup> $Z = 2$   
 $D_x = 1.330$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
 $\mu = 0.09$  mm<sup>-1</sup>  
 $T = 294$  ( $2$ ) K  
Block, colorless  
 $0.30 \times 0.26 \times 0.18$  mm

## Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.973$ ,  $T_{\max} = 0.984$

4948 measured reflections  
 1911 independent reflections  
 1210 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.026$   
 $\theta_{\text{max}} = 26.3^\circ$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.040$   
 $wR(F^2) = 0.117$   
 $S = 1.01$   
 1911 reflections  
 131 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0555P)^2 + 0.1435P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.13 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.14 \text{ e } \text{\AA}^{-3}$

Table 1

Selected bond lengths (Å).

N1—C7	1.341 (2)	N1—C6	1.417 (2)
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Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1\cdots O1^i$	0.85 (2)	2.07 (2)	2.906 (2)	166.4 (19)

Symmetry code: (i)  $x, y + 1, z$ .

All C-bound H atoms were positioned geometrically and refined as riding ( $C-H = 0.93-0.97 \text{ \AA}$ ), with  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$ . The H atom of the NH group was refined isotropically.

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1997); software used to prepare material for publication: SHELXTL.

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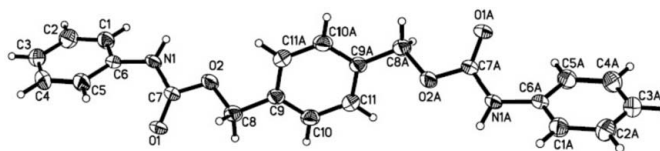


Figure 1

The molecular structure of (I) showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 35% probability level. [Symmetry code: (A)  $-x, 1 - y, -z$ .]

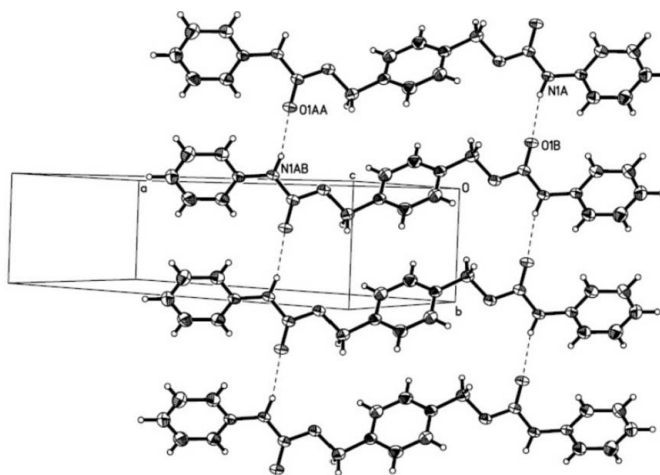


Figure 2

The formation of molecular ribbons through intermolecular  $N-H\cdots O$  hydrogen bonds (dashed lines). [Symmetry codes: (A)  $x, y, z$ ; (B)  $x, 1 + y, z$ ; (AA)  $-x, 1 - y, -z$ ; (AB)  $-x, 2 - y, -z$ .]

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