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Key indicators

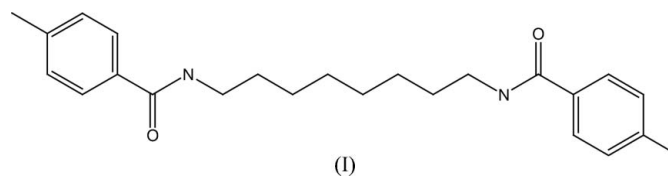
Single-crystal X-ray study
 $T = 100$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.054
 wR factor = 0.166
Data-to-parameter ratio = 14.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.*N,N'*-Octamethylenebis(4-methylbenzamide)

In the title structure, $\text{C}_{24}\text{H}_{32}\text{N}_2\text{O}_2$, the molecule lies on a crystallographic inversion centre at the mid-point of the central C—C bond. The planar $\text{OCN}-(\text{CH}_2)_n-\text{NCO}$ segment is in an all-*trans* configuration. The NH group of the amide group is involved in a single hydrogen bond to the O atom of a symmetry-related molecule to form one-dimensional ribbons parallel to the *b* direction.

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Comment

In organic crystal engineering, the directional hydrogen-bond interaction is widely used to design constructor molecules incorporating sites that can engage reliable directional interaction in order to build up predictable supramolecular architecture with potential application as functional materials (Simard *et al.*, 1991; Leininger *et al.*, 2000 and Holliday & Mirkin, 2001). In addition, it has been observed that chemically symmetrical molecules containing a central aliphatic segment with an even number of methylene groups often have a crystallographic centre of symmetry at the mid-point of the central CH_2-CH_2 bond and the molecules preferentially adopt the fully extended conformation (Awaleh *et al.*, 2005*a,b,c*; Hou *et al.*, 2005). In our continuing effort to study the structure of the organic polymer as well as the metal-organic supramolecular architecture, the title compound, (I), has been synthesized and its structure is reported here.



The molecular structure of (I) is shown in Fig. 1. The molecule has a centre of symmetry at the mid-point of the central C—C bond, namely $\text{C}1-\text{C}1^i$ [symmetry code: (i) $2 - x, 1 - y, 2 - z$]. The values of the torsion angles in the planar sequence $[\text{OCN}-(\text{CH}_2)_8-\text{NCO}]$ indicate an all *trans* arrangement and that the molecules are in a fully extended conformation (Table 1). The dihedral angle between the benzene ring and the $[\text{OCN}-(\text{CH}_2)_8-\text{NCO}]$ sequence is 26.4 (1°). The bond distances and angles in (I) (Table 1) fall in the normal range (Allen *et al.*, 1987). In the crystal structure, the NH group of the amide group is involved in a weak hydrogen-bond interaction with the O atom of a symmetry-related molecule (Table 2) to form one-dimensional ribbons parallel to the *b* direction (Fig. 2). There are no significant $\pi-\pi$ stacking interactions.

Experimental

The title compound was synthesized according to the Pineault (1982) method. The compound was recrystallized from diethyl ether, yielding colourless crystals suitable for X-ray analysis. Yield 93%. Analysis found: C 75.71, H 8.66, N 7.36%; calculated for $C_{12}H_{16}NO$: C 75.75, H 8.48, N 7.36%.

Crystal data

$C_{24}H_{32}N_2O_2$	$Z = 2$
$M_r = 380.52$	$D_x = 1.219 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Cu $K\alpha$ radiation
$a = 7.1190 (2) \text{ \AA}$	$\mu = 0.60 \text{ mm}^{-1}$
$b = 5.1609 (2) \text{ \AA}$	$T = 100 (2) \text{ K}$
$c = 28.4022 (10) \text{ \AA}$	Block, colourless
$\beta = 96.679 (2)^\circ$	$0.19 \times 0.14 \times 0.10 \text{ mm}$
$V = 1036.43 (6) \text{ \AA}^3$	

Data collection

Bruker SMART 6000 diffractometer	14187 measured reflections
ω scans	1885 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1340 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.901$, $T_{\max} = 0.943$	$R_{\text{int}} = 0.079$
	$\theta_{\max} = 68.8^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0755P)^2 + 0.2277P]$
$R[F^2 > 2\sigma(F^2)] = 0.054$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.166$	$(\Delta/\sigma)_{\max} = 0.001$
$S = 1.03$	$\Delta\rho_{\max} = 0.23 \text{ e \AA}^{-3}$
1885 reflections	$\Delta\rho_{\min} = -0.26 \text{ e \AA}^{-3}$
128 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (\AA , $^\circ$).

O1—C5	1.246 (3)	N1—C4	1.458 (3)
N1—C5	1.341 (3)		
C5—N1—C4	120.37 (17)	O1—C5—C6	120.65 (18)
O1—C5—N1	121.88 (19)		
C1 ⁱ —C1—C2—C3	178.1 (2)	C2—C3—C4—N1	179.17 (17)
C1—C2—C3—C4	-177.17 (18)	C4—N1—C5—C6	174.55 (17)
C5—N1—C4—C3	161.85 (19)		

Symmetry code: (i) $-x + 2, -y + 1, -z + 2$.

Table 2

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 ⁱⁱ ...O1 ⁱⁱ	0.88	2.17	3.027 (2)	164

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

H atoms were positioned geometrically ($C-H = 0.95-0.99 \text{ \AA}$ and $N-H = 0.88 \text{ \AA}$) and were included in the riding-model approximation; their displacement parameters were set to 1.5 times those of the equivalent isotropic displacement parameters of the parent site for methyl H atoms and 1.2 times for others. A final verification of possible voids was performed using the VOID routine of the PLATON program (Spek, 2003).

Data collection: SMART (Bruker, 2003); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics:

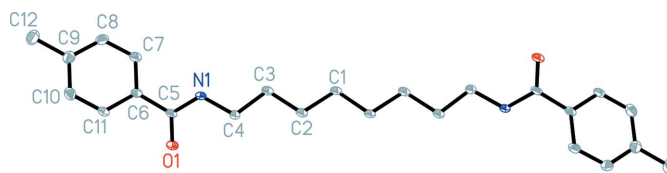


Figure 1

Molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted. The unlabelled part of the molecule is related by the symmetry transformation $(2 - x, 1 - y, 2 - z)$.

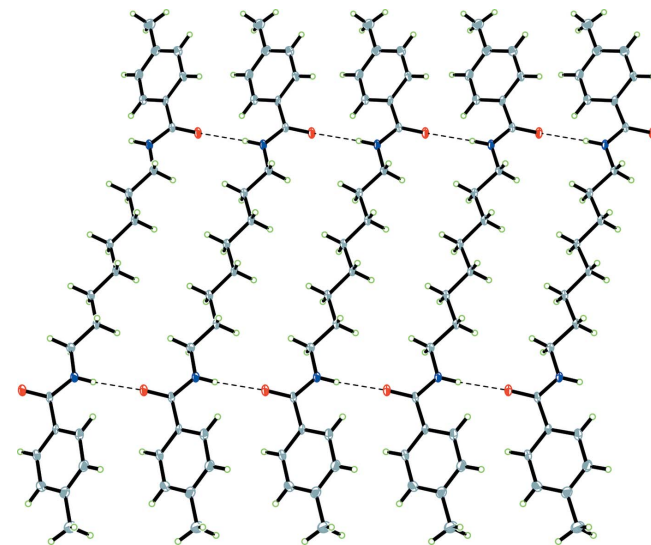


Figure 2

Part of the crystal structure of (I), showing a hydrogen-bonded (dashed lines) ribbon running along the b axis.

SHELXTL (Bruker, 1997); software used to prepare material for publication: UDMX (Maris, 2004).

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