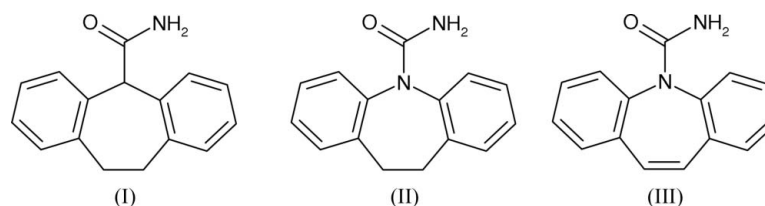
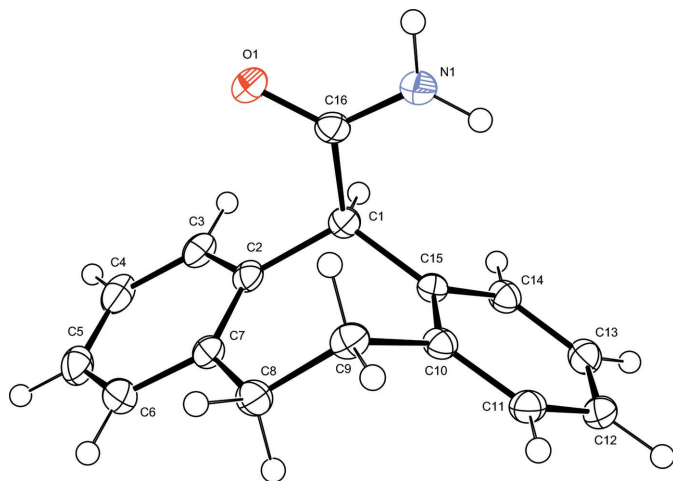


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alastair.florence@strath.ac.uk**Key indicators**Single-crystal X-ray study  
 $T = 150$  K  
Mean  $\sigma(C-C) = 0.002$  Å  
 $R$  factor = 0.035  
 $wR$  factor = 0.086  
Data-to-parameter ratio = 10.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**A low-temperature redetermination of cyheptamide**In the title compound [systematic name: 10,11-dihydro-5*H*-dibenz[*a,d*]cycloheptene-5-carboxamide],  $C_{16}H_{15}NO$ ,  $N-H \cdots O$  and  $N-H \cdots \pi$  interactions combine to create a catemeric motif that is also observed in crystal structures of the closely related compound dihydrocarbamazepine.Received 1 November 2006  
Accepted 20 November 2006**Comment**Cyheptamide, (I), is an analogue of dihydrocarbamazepine, (II), the latter being a recognized impurity (Cyr *et al.*, 1987) in the widely used antiepileptic drug carbamazepine, (III). The crystal structure of (I) was first reported by Codding *et al.* (1984) and the structure reported here (Fig. 1) is a low-temperature redetermination. This work forms part of a wider investigation that couples automated parallel crystallization (Florence, Johnston, Fernandes *et al.*, 2006) with crystal-structure prediction methodology to investigate the basic science underlying the solid-state diversity of (III) and its analogues (Florence, Johnston, Price *et al.*, 2006).

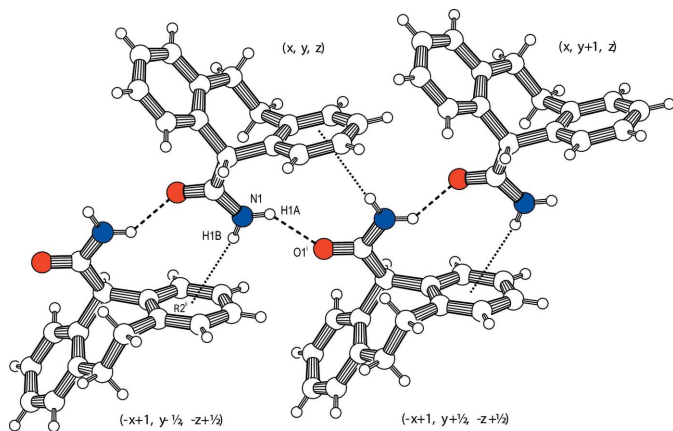
The intermolecular interactions in (I) combine to create the catemeric motif shown in Fig. 2, with the geometric parameters listed in Table 1. Infinite [010] chains of molecules are linked by an  $N1 \cdots O1^i$  [symmetry code: (i)  $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$ ] hydrogen bond, supplemented by an  $N-H \cdots \pi$  interaction,  $N1 \cdots Cg2^{ii}$  [symmetry code: (ii)  $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$ ], where  $Cg2$  is the centroid of ring  $R2$  (atoms C10–C15). The robustness of this motif is reflected in the fact that it is observed in all three polymorphic forms of (II) (monoclinic: Bandoli *et al.*, 1992; orthorhombic: Harrison *et al.*, 2006; triclinic: Leech *et al.*, 2006) and in a predicted crystal structure of (III) that is isostructural with the orthorhombic form of (II) (Florence, Leech *et al.*, 2006). It is notable also that the crystal structure of (I) is essentially isostructural with the monoclinic form of (II) [ $P2_1/c$ ;  $a = 5.433$  (3) Å,  $b = 9.129$  (2) Å,  $c = 24.196$  (5) Å,  $\beta = 96.47$  (3)°,  $V = 1192.4$  (8) Å<sup>3</sup> at  $T = 150$  K; Leech, 2006].

**Experimental**

A single-crystal of the title compound was selected from the sample as supplied (Sigma–Aldrich Co.) without recrystallization.



**Figure 1**  
The molecular structure of (I), showing the atom-numbering scheme and 50% probability displacement ellipsoids.



**Figure 2**  
The catemeric motif of (I). Hydrogen bonds are indicated by dashed lines.

#### Crystal data

$C_{16}H_{15}NO$   
 $M_r = 237.29$   
 Monoclinic,  $P2_1/c$   
 $a = 5.6035$  (7) Å  
 $b = 9.1716$  (11) Å  
 $c = 23.579$  (3) Å  
 $\beta = 96.752$  (12)°  
 $V = 1203.4$  (3) Å<sup>3</sup>

$Z = 4$   
 $D_x = 1.310$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 0.08$  mm<sup>-1</sup>  
 $T = 150$  (2) K  
 Block, colourless  
 $0.26 \times 0.17 \times 0.16$  mm

#### Data collection

Oxford Diffraction Gemini diffractometer  
 $\omega$  and  $\varphi$  scans  
 Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)  
 $T_{\min} = 0.956$ ,  $T_{\max} = 0.983$

11433 measured reflections  
 2407 independent reflections  
 1928 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.029$   
 $\theta_{\text{max}} = 26.4^\circ$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.035$   
 $wR(F^2) = 0.086$   
 $S = 1.04$   
 2407 reflections  
 223 parameters  
 All H-atom parameters refined

$$w = 1/[\sigma^2(F_o^2) + (0.0353P)^2 + 0.4305P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.18 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.16 \text{ e \AA}^{-3}$

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1A\cdots O1^i$	0.91 (2)	2.13 (2)	2.842 (2)	135 (1)
$N1-H1B\cdots Cg2^{ii}$	0.93 (2)	2.78 (2)	3.676 (1)	162 (1)

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

All H atoms were located in a Fourier difference map and the atomic coordinates and  $U_{\text{iso}}$  parameters were refined freely.  $X-H$  distances refined to  $N1-H1A = 0.90$  (2) Å,  $N1-H1B = 0.93$  (2) Å,  $C1-H1 = 1.03$  (2) and  $0.96$  (2)– $1.01$  (2) Å for aromatic H atoms and  $0.98$  (2)– $1.00$  (2) Å for the  $CH_2$  H atoms.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Version 011105; Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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