

*N*-Benzoyl-*N,N'*-dicyclohexylurea

Ma. Laura Orea Flores,<sup>a</sup> Alberto Galindo Guzmán,<sup>a</sup> Dino Gnecco Medina<sup>a</sup> and Sylvain Bernès<sup>b\*</sup>

<sup>a</sup>Centro de Química, Instituto de Ciencias, Universidad Autónoma de Puebla, AP 1613, 72000 Puebla, Pue., Mexico, and <sup>b</sup>DEP, Facultad de Ciencias Químicas, UANL, Guerrero y Progreso S/N, Col. Treviño, 64570 Monterrey, NL, Mexico

Correspondence e-mail: sylvain\_bernes@HotMail.com

## Key indicators

Single-crystal X-ray study

*T* = 296 K

Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$

*R* factor = 0.036

*wR* factor = 0.092

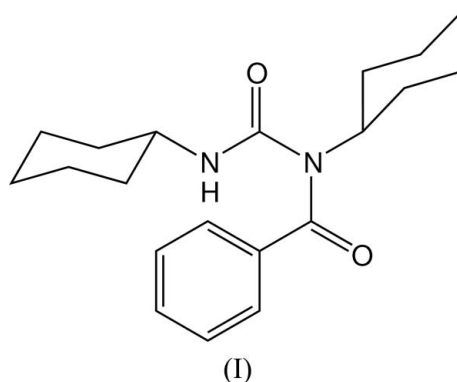
Data-to-parameter ratio = 8.7

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

The title compound,  $\text{C}_{20}\text{H}_{28}\text{N}_2\text{O}_2$ , and *N,N'*-dicyclohexyl-*N*-(2-pyrazinoyl)urea are isostructural. Molecules are linked into chains through (amide) $\text{N}-\text{H}\cdots\text{O}=\text{C}$ (amide) intermolecular hydrogen bonds.

## Comment

The title compound resulted from a condensation reaction of benzoic acid with *N,N'*-dicyclohexylcarbodiimide (DCC) catalysed by 4-(dimethylamino)pyridine (DMAP). The DCC/DMAP system is commonly used as a dehydrating agent for the synthesis of amides and esters starting, for example, from carboxylic acids. However, one should be aware that, as in the present case, DCC may react with the carboxylic acid.

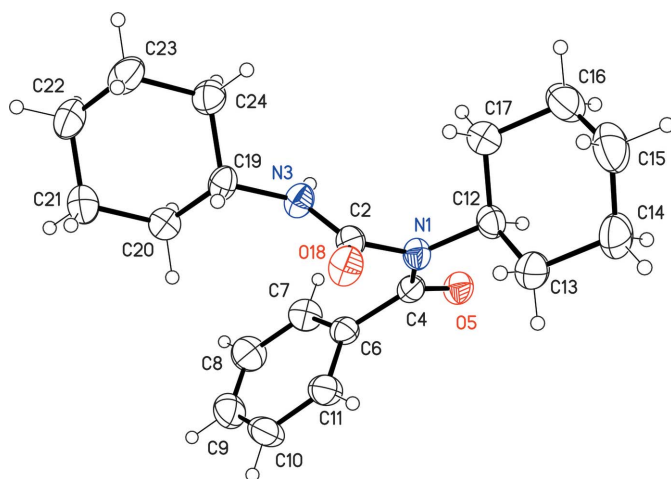


Bond lengths for the amide group in the title compound, (I) (Table 1), are in agreement with the keto tautomer, which is the preferred tautomer for *N*-substituted amides in the solid state (Rodríguez *et al.*, 2005). The unit-cell parameters, symmetry and atomic coordinates indicate that the structure of (I) and that reported for *N,N'*-dicyclohexyl-*N*-(2-pyrazinoyl)urea (Chérioux *et al.*, 2002) are isomorphous and isostructural; the r.m.s. deviation for a least-squares overlay of atomic positions, excluding H atoms, is 0.080 Å. The conformation for the central C(cyclohexyl)-NH-(C=O)-NR-C(cyclohexyl) unit in (I) has also been observed in related compounds (*e.g.* Ball *et al.*, 1990; Salas-Coronado *et al.*, 2001).

The molecules of (I) pack in chains *via*  $\text{N}-\text{H}\cdots\text{O}=\text{C}$  hydrogen bonds, reinforced by  $\text{C}-\text{H}\cdots\text{O}=\text{C}$  contacts (Table 2). No additional  $\text{C}-\text{H}\cdots\text{O}$  weak interactions are observed by substitution of the N atoms in the pyrazinoyl ring by C-H groups in (I). Surprisingly, this supramolecular arrangement is not conserved in a closely related nicotinoyl-containing urea (Gallagher *et al.*, 1999); in that case, the crystal packing is dominated by an (amide) $\text{N}-\text{H}\cdots\text{N}(\text{py})$  hydrogen bond.

Received 2 May 2006

Accepted 9 June 2006.



**Figure 1**  
The structure of (I), with displacement ellipsoids drawn at the 30% probability level for non-H atoms.

## Experimental

Benzoic acid (0.069 g, 0.561 mmol) was dissolved in  $\text{CHCl}_3$  (15 ml) and DCC (0.116 g, 0.561 mmol) and DMAP (0.069 g, 0.562 mmol) were added to this solution. The mixture was stirred at 273 K for 2 h. After removal of the solvent, a yellow solid was isolated, which was washed with  $\text{CH}_2\text{Cl}_2$ , affording (I) as a colourless solid. Single crystals were obtained from  $\text{CH}_2\text{Cl}_2/\text{Et}_2\text{O}$  (1:1).

### Crystal data

$\text{C}_{20}\text{H}_{28}\text{N}_2\text{O}_2$	$Z = 4$
$M_r = 328.44$	$D_x = 1.153 \text{ Mg m}^{-3}$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 9.7060$ (14) Å	$\mu = 0.07 \text{ mm}^{-1}$
$b = 12.0125$ (12) Å	$T = 296$ (1) K
$c = 16.2342$ (13) Å	Needle, colourless
$V = 1892.8$ (4) Å <sup>3</sup>	$0.60 \times 0.28 \times 0.14 \text{ mm}$

### Data collection

Bruker P4 diffractometer	$R_{\text{int}} = 0.020$
$2\theta/\omega$ scans	$\theta_{\text{max}} = 25.0^\circ$
Absorption correction: none	3 standard reflections
3205 measured reflections	every 97 reflections
1922 independent reflections	intensity decay: 1%
1411 reflections with $I > 2\sigma(I)$	

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2 + 0.0188P]$
$R[F^2 > 2\sigma(F^2)] = 0.037$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.092$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.12 \text{ e } \text{Å}^{-3}$
1922 reflections	$\Delta\rho_{\text{min}} = -0.12 \text{ e } \text{Å}^{-3}$
222 parameters	Extinction correction: <i>SHELXTL-Plus</i>
H atoms treated by a mixture of independent and constrained refinement	Extinction coefficient: 0.0077 (11)

**Table 1**  
Selected geometric parameters (Å, °).

N1—C2	1.441 (3)	C2—N3	1.321 (3)
N1—C4	1.372 (3)	N3—C19	1.464 (3)
N1—C12	1.489 (3)	N3—H3	0.85 (3)
C2—O18	1.222 (3)	C4—O5	1.223 (3)
C4—N1—C2	121.40 (19)	C2—N3—C19	123.6 (2)
C2—N1—C12	118.02 (19)	C2—N3—H3	119.3 (19)
C4—N1—C12	120.5 (2)	C19—N3—H3	117.1 (19)
O18—C2—N1	120.9 (2)	O5—C4—N1	122.7 (2)
O18—C2—N3	125.3 (2)	O5—C4—C6	120.7 (2)
N3—C2—N1	113.77 (19)	N1—C4—C6	116.4 (2)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N3—H3}\cdots\text{O18}^i$	0.85 (3)	2.14 (3)	2.990 (3)	174 (3)
$\text{C19—H19A}\cdots\text{O5}^{ii}$	0.98	2.43	3.361 (3)	159

Symmetry codes: (i)  $x - \frac{1}{2}, -y + \frac{3}{2}, -z + 1$ ; (ii)  $x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$ .

The H atom bonded to N3 was found in a difference map and refined freely to obtain an unbiased geometry for the hydrogen-bonding scheme. H atoms bonded to C atoms were placed in idealized positions and refined as riding on their parent atoms. Constrained C—H distances: methine 0.98 Å, methylene 0.97 Å and aromatic 0.93 Å. Isotropic displacement parameters were set to  $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$ . In the absence of significant anomalous scattering effects, 813 Friedel pairs were averaged.

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL-Plus* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL-Plus*; molecular graphics: *SHELXTL-Plus*; software used to prepare material for publication: *SHELXTL-Plus*.

We are grateful to PROMEP (Mexico) for financial support (Project 103.5/03/2549).

## References

- Ball, R. G., Brown, R. S. & Bennet, A. J. (1990). *Acta Cryst.* **C46**, 2491–2493.
- Chérioux, F., Therrien, B., Stoeckli-Evans, H. & Süß-Fink, G. (2002). *Acta Cryst.* **E58**, o27–o29.
- Gallagher, J. F., Kenny, P. T. M. & Sheehy, M. J. (1999). *Acta Cryst.* **C55**, 1607–1610.
- Rodríguez, V., Barba, V., Bernès, S., Quintero, L. & Sartillo-Piscil, F. (2005). *Acta Cryst.* **E61**, o2733–o2735.
- Salas-Coronado, R., Vásquez-Badillo, A., Medina-García, M., García-Colón, J. G., Nöth, H., Contreras, R. & Flores-Parra, A. (2001). *J. Mol. Struct. (Theochem)*, **543**, 259–275.
- Sheldrick, G. M. (1998). *SHELXTL-Plus*. Release 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
- Siemens (1996). *XSCANS*. Version 2.21. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.