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# *N*-Benzoyl-*N*′-phenylurea

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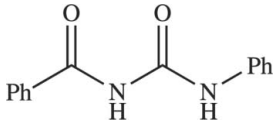
Key indicators: single-crystal X-ray study; $T$ = 150 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.039; $wR$ factor = 0.098; data-to-parameter ratio = 10.5.

In the title compound, $C_{14}H_{12}N_2O_2$, the molecular conformation is determined by a strong intramolecular N—H···O=C hydrogen bond. In the crystal, pairs of molecules are connected by intermolecular N—H···O=C hydrogen bonds, forming centrosymmetric dimers. No specific interactions between dimers could be found.

## Related literature

For related structures, see: Bart *et al.* (1989); Zhong *et al.* (1998); Moon *et al.* (2002), Yamin & Mardi (2003); Chen *et al.* (2004); Su (2005); Yan *et al.* (2007, 2008); Liu *et al.* (2008, 2008*a*,*b*). For graph-set notation, see: Etter (1990). The title compound was obtained as a byproduct during the synthesis of a copper(I) complex with *N*-benzoyl-*N*′-phenylthiourea prepared according to Frank & Smith (1948).




## Experimental

### *Crystal data*

$C_{14}H_{12}N_2O_2$
$M_r$ = 240.26
Monoclinic, $P2_1/c$
$a$ = 15.5641 (8) Å
$b$ = 4.6564 (3) Å
$c$ = 21.1029 (15) Å
$\beta$ = 128.716 (4)°
$V$ = 1193.31 (15) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 150 K
0.54 × 0.10 × 0.09 mm

### *Data collection*

Oxford Diffraction Xcalibur diffractometer with a Sapphire2 (large Be window) detector
Absorption correction: analytical [*CrysAlis PRO* (Oxford Diffraction, 2009); analytical numeric absorption correction using a multi-faceted crystal model based on expressions derived by Clark & Reid (1995)]
$T_{min}$ = 0.971, $T_{max}$ = 0.993
4425 measured reflections
2221 independent reflections
1575 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.022

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.098
$S$ = 0.94
2221 reflections
211 parameters
Only H-atom coordinates refined
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.14 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O2 | 0.93 (2) | 1.85 (2) | 2.634 (2) | 140 (1) |
| N2—H2···O1$^{i}$ | 0.93 (2) | 1.97 (2) | 2.882 (1) | 169 (1) |

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO* program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2175).

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# supporting information

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## *N*-Benzoyl-*N*′-phenylurea

**Andrzej Okuniewski, Jaroslaw Chojnacki and Barbara Becker**

### S1. Comment

*N*-Benzoyl-*N*′-phenylurea halogeno derivatives are used as pesticides. For instance 1-(3,5-dichloro-2,4-difluorophenyl)-3-(2,6-difluorobenzoyl)urea was found to act as chitin synthesis inhibitor (Zhong *et al.*,1998).

*N*-benzoyl-*N*′-phenylurea molecules adopt a conformation that allows formation of N—H···O═C intramolecular hydrogen bonds, denoted as **R**(6) in graph set notation (Etter, 1990). This conformation is commonly noted among all *N*′-monosubstituted or *N*′-unsubstituted *N*-benzoylureas and *N*-benzoylthioureas (see: related structures). Additional N—H···O═C intermolecular $\mathbf{R}^2_2(8)$ hydrogen bonds bind two urea derivative molecules to form a centrosymmetric dimer (Fig. 1), which is also common. Only one known structure does not exhibit such a motif (Moon *et al.*, 2002).

No $\pi$-$\pi$ stacking interactions can be found in this structure (closest ring centroids distance is about 5.60 Å with the dihedral angle between the rings $\alpha$ about 80°).

The dihedral angle N1—C1—N2—C2 describing the twist of two amide subunits of urea derivatives is equal to 3.0 (2)°. This value is in the range known from other studies: from 0.07° (Yan *et al.*, 2007) to 7.45° (Su, 2005).

### S2. Experimental

*N*-benzoyl-*N*′-phenylurea was obtained as a byproduct during the synthesis of a copper(I) complex with *N*-Benzoyl-*N*′-phenylthiourea prepared according to Frank & Smith (1948). Obviously the ligand underwent basic hydrolysis with $CH_3ONa$ in acetone. Colourless single crystals suitable for X-ray diffraction analysis were isolated from the reaction mixture after it was kept at room temperature for a few days. From 5.12 g (0.02 mol) of thiourea derivative 0.87 g of *N*-benzoyl-*N*′-phenylurea was obtained. Yield: 18%.

### S3. Refinement

All hydrogen atoms were found from difference Fourier map and refined without constraints.

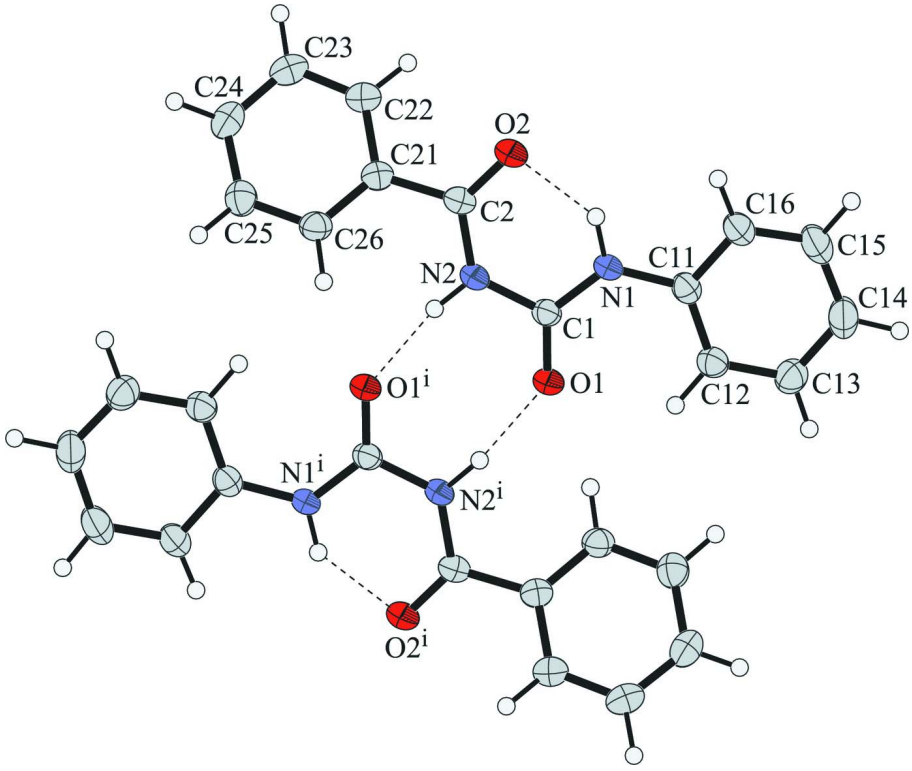


**Figure 1**

Structure of centrosymmetric *N*-benzoyl-*N*′-phenylurea dimer. Ellipsoids are drawn at 50% probability level. Symmetry code: (i) –*x*+1, –*y*+1, –*z*.

### *N*-Benzoyl-*N*′-phenylurea

*Crystal data*

$C_{14}H_{12}N_2O_2$
$M_r = 240.26$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 15.5641\ (8)$ Å
$b = 4.6564\ (3)$ Å
$c = 21.1029\ (15)$ Å
$\beta = 128.716\ (4)°$
$V = 1193.31\ (15)$ Å$^3$
$Z = 4$
$F(000) = 504$
$D_x = 1.337$ Mg m$^{-3}$
Melting point: 482(2) K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2481 reflections
$\theta = 2.5–28.4°$
$\mu = 0.09$ mm$^{-1}$
$T = 150$ K
Needle, colourless
0.54 × 0.10 × 0.09 mm

*Data collection*

Oxford Diffraction Xcalibur diffractometer with a Sapphire2 (large Be window) detector
Radiation source: Mo K$\alpha$ radiation
Graphite monochromator
Detector resolution: 8.1883 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: analytical [*CrysAlis PRO* (Oxford Diffraction, 2009); analytical numeric absorption correction using a multi-faceted crystal model based on expressions derived by Clark & Reid (1995)]
$T_{min} = 0.971$, $T_{max} = 0.993$
4425 measured reflections
2221 independent reflections
1575 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$

$\theta_{max}$ = 25.5°, $\theta_{min}$ = 2.5°
$h$ = −18→9
$k$ = −3→5
$l$ = −21→25

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.098
$S$ = 0.94
2221 reflections
211 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
Only H-atom coordinates refined
$w = 1/[\sigma^2(F_o^2) + (0.0656P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.14 e Å$^{-3}$

*Special details*

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted $R$-factor $wR$ and goodness of fit $S$ are based on $F^2$, conventional $R$-factors $R$ are based on $F$, with $F$ set to zero for negative $F^2$. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating $R$-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. $R$-factors based on $F^2$ are statistically about twice as large as those based on $F$, and $R$- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.58625 (7) | 0.6582 (2) | −0.00745 (6) | 0.0384 (3) |
| O2 | 0.82393 (7) | 0.2951 (2) | 0.21526 (6) | 0.0396 (3) |
| N1 | 0.77093 (9) | 0.6517 (3) | 0.09887 (7) | 0.0295 (3) |
| N2 | 0.64890 (9) | 0.3566 (3) | 0.09771 (7) | 0.0284 (3) |
| C1 | 0.66640 (10) | 0.5660 (3) | 0.05886 (8) | 0.0274 (3) |
| C2 | 0.72519 (10) | 0.2381 (3) | 0.17319 (8) | 0.0282 (3) |
| C11 | 0.81196 (11) | 0.8530 (3) | 0.07373 (9) | 0.0297 (4) |
| C12 | 0.74750 (12) | 0.9966 (3) | −0.00011 (9) | 0.0330 (4) |
| C13 | 0.79673 (13) | 1.1897 (4) | −0.01876 (10) | 0.0393 (4) |
| C14 | 0.90876 (14) | 1.2390 (4) | 0.03479 (11) | 0.0469 (5) |
| C15 | 0.97228 (13) | 1.0949 (4) | 0.10784 (12) | 0.0516 (5) |
| C16 | 0.92476 (12) | 0.9038 (4) | 0.12780 (11) | 0.0411 (4) |
| C21 | 0.68355 (10) | 0.0351 (3) | 0.20329 (8) | 0.0275 (3) |
| C22 | 0.75435 (12) | −0.0253 (3) | 0.28626 (9) | 0.0336 (4) |
| C23 | 0.72257 (13) | −0.2128 (4) | 0.31894 (10) | 0.0389 (4) |
| C24 | 0.61969 (13) | −0.3423 (4) | 0.26921 (10) | 0.0390 (4) |
| C25 | 0.54898 (12) | −0.2851 (3) | 0.18661 (10) | 0.0368 (4) |
| C26 | 0.58046 (11) | −0.0960 (3) | 0.15362 (9) | 0.0316 (4) |
| H1 | 0.8205 (12) | 0.559 (3) | 0.1480 (10) | 0.039 (4)* |
| H13 | 0.7502 (12) | 1.291 (4) | −0.0711 (10) | 0.041 (4)* |
| H12 | 0.6663 (12) | 0.961 (3) | −0.0395 (8) | 0.032 (4)* |
| H2 | 0.5745 (13) | 0.328 (3) | 0.0717 (9) | 0.041 (4)* |
| H23 | 0.7751 (12) | −0.257 (3) | 0.3782 (10) | 0.040 (4)* |

| | | | | |
|---|---|---|---|---|
| H26 | 0.5289 (12) | −0.059 (3) | 0.0951 (9) | 0.032 (4)* |
| H22 | 0.8256 (13) | 0.077 (4) | 0.3210 (9) | 0.044 (4)* |
| H25 | 0.4762 (13) | −0.375 (3) | 0.1504 (9) | 0.043 (4)* |
| H24 | 0.5963 (12) | −0.477 (4) | 0.2916 (9) | 0.043 (4)* |
| H14 | 0.9397 (13) | 1.385 (4) | 0.0187 (10) | 0.056 (5)* |
| H15 | 1.0520 (15) | 1.117 (4) | 0.1465 (10) | 0.060 (5)* |
| H16 | 0.9654 (14) | 0.800 (4) | 0.1778 (11) | 0.055 (5)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0223 (5) | 0.0518 (7) | 0.0288 (6) | −0.0014 (4) | 0.0100 (5) | 0.0106 (5) |
| O2 | 0.0231 (5) | 0.0527 (7) | 0.0304 (6) | −0.0018 (5) | 0.0107 (5) | 0.0068 (5) |
| N1 | 0.0205 (6) | 0.0363 (7) | 0.0235 (6) | −0.0025 (5) | 0.0097 (5) | 0.0026 (6) |
| N2 | 0.0199 (6) | 0.0351 (7) | 0.0239 (6) | −0.0017 (5) | 0.0106 (5) | 0.0007 (6) |
| C1 | 0.0234 (7) | 0.0333 (8) | 0.0226 (7) | −0.0020 (6) | 0.0130 (6) | −0.0018 (7) |
| C2 | 0.0237 (7) | 0.0320 (8) | 0.0243 (7) | 0.0018 (6) | 0.0128 (6) | −0.0015 (7) |
| C11 | 0.0275 (7) | 0.0316 (8) | 0.0297 (8) | −0.0041 (6) | 0.0178 (6) | −0.0048 (7) |
| C12 | 0.0308 (8) | 0.0373 (9) | 0.0289 (8) | −0.0040 (6) | 0.0178 (7) | −0.0030 (7) |
| C13 | 0.0443 (9) | 0.0417 (10) | 0.0360 (9) | −0.0046 (7) | 0.0270 (8) | −0.0006 (8) |
| C14 | 0.0473 (10) | 0.0458 (11) | 0.0562 (11) | −0.0118 (8) | 0.0366 (9) | −0.0009 (9) |
| C15 | 0.0303 (9) | 0.0560 (12) | 0.0579 (12) | −0.0089 (8) | 0.0223 (9) | 0.0049 (10) |
| C16 | 0.0273 (8) | 0.0438 (10) | 0.0413 (10) | −0.0041 (7) | 0.0162 (7) | 0.0051 (9) |
| C21 | 0.0279 (7) | 0.0267 (8) | 0.0276 (7) | 0.0058 (6) | 0.0173 (6) | 0.0011 (7) |
| C22 | 0.0333 (8) | 0.0339 (9) | 0.0286 (8) | 0.0037 (6) | 0.0169 (7) | 0.0011 (7) |
| C23 | 0.0441 (9) | 0.0422 (10) | 0.0296 (8) | 0.0067 (7) | 0.0227 (7) | 0.0047 (8) |
| C24 | 0.0471 (9) | 0.0367 (9) | 0.0444 (9) | 0.0052 (7) | 0.0340 (8) | 0.0080 (8) |
| C25 | 0.0357 (8) | 0.0356 (9) | 0.0425 (9) | 0.0002 (7) | 0.0261 (8) | 0.0015 (8) |
| C26 | 0.0282 (7) | 0.0355 (9) | 0.0286 (8) | 0.0033 (6) | 0.0165 (7) | 0.0026 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C1 | 1.2308 (16) | C14—H14 | 1.007 (19) |
| O2—C2 | 1.2304 (15) | C15—C16 | 1.381 (2) |
| N1—C1 | 1.3419 (16) | C15—H15 | 0.975 (18) |
| N1—C11 | 1.4114 (18) | C16—H16 | 0.956 (19) |
| N1—H1 | 0.926 (16) | C21—C26 | 1.394 (2) |
| N2—C2 | 1.3731 (18) | C21—C22 | 1.3950 (19) |
| N2—C1 | 1.4058 (18) | C22—C23 | 1.382 (2) |
| N2—H2 | 0.930 (15) | C22—H22 | 0.988 (16) |
| C2—C21 | 1.494 (2) | C23—C24 | 1.388 (2) |
| C11—C12 | 1.388 (2) | C23—H23 | 0.998 (16) |
| C11—C16 | 1.3907 (19) | C24—C25 | 1.386 (2) |
| C12—C13 | 1.388 (2) | C24—H24 | 0.983 (17) |
| C12—H12 | 1.001 (14) | C25—C26 | 1.388 (2) |
| C13—C14 | 1.380 (2) | C25—H25 | 0.980 (16) |
| C13—H13 | 0.984 (17) | C26—H26 | 0.979 (15) |
| C14—C15 | 1.378 (3) | | |

| | | | |
|---|---|---|---|
| C1—N1—C11 | 128.07 (12) | C14—C15—C16 | 120.59 (15) |
| C1—N1—H1 | 113.5 (9) | C14—C15—H15 | 122.2 (10) |
| C11—N1—H1 | 118.4 (9) | C16—C15—H15 | 117.2 (11) |
| C2—N2—C1 | 127.79 (11) | C15—C16—C11 | 120.10 (16) |
| C2—N2—H2 | 118.7 (9) | C15—C16—H16 | 123.5 (10) |
| C1—N2—H2 | 112.3 (10) | C11—C16—H16 | 116.4 (10) |
| O1—C1—N1 | 125.41 (14) | C26—C21—C22 | 119.31 (14) |
| O1—C1—N2 | 118.47 (11) | C26—C21—C2 | 123.99 (13) |
| N1—C1—N2 | 116.12 (12) | C22—C21—C2 | 116.69 (13) |
| O2—C2—N2 | 122.27 (13) | C23—C22—C21 | 120.37 (14) |
| O2—C2—C21 | 120.53 (12) | C23—C22—H22 | 121.3 (9) |
| N2—C2—C21 | 117.20 (12) | C21—C22—H22 | 118.3 (9) |
| C12—C11—C16 | 119.63 (14) | C22—C23—C24 | 120.06 (15) |
| C12—C11—N1 | 124.25 (12) | C22—C23—H23 | 119.3 (9) |
| C16—C11—N1 | 116.12 (13) | C24—C23—H23 | 120.7 (9) |
| C11—C12—C13 | 119.38 (14) | C25—C24—C23 | 120.03 (15) |
| C11—C12—H12 | 120.2 (8) | C25—C24—H24 | 119.1 (9) |
| C13—C12—H12 | 120.4 (8) | C23—C24—H24 | 120.9 (9) |
| C14—C13—C12 | 120.96 (16) | C24—C25—C26 | 120.07 (15) |
| C14—C13—H13 | 120.3 (9) | C24—C25—H25 | 121.3 (9) |
| C12—C13—H13 | 118.7 (9) | C26—C25—H25 | 118.6 (9) |
| C15—C14—C13 | 119.33 (16) | C25—C26—C21 | 120.16 (14) |
| C15—C14—H14 | 123.1 (10) | C25—C26—H26 | 118.5 (9) |
| C13—C14—H14 | 117.5 (10) | C21—C26—H26 | 121.4 (9) |
| | | | |
| N1—C1—N2—C2 | 3.0 (2) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O2 | 0.93 (2) | 1.85 (2) | 2.634 (2) | 140 (1) |
| N2—H2···O1$^{i}$ | 0.93 (2) | 1.97 (2) | 2.882 (1) | 169 (1) |

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