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1,2-Dibenzoylhydrazine

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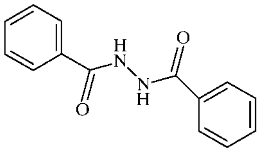
In the crystal structure of the title compound, $C_{14}H_{12}N_2O_2$, the molecule lies about a twofold axis; two carbonyl groups and the H atoms of the N—N bond are in a *trans* orientation with respect to each other. In the crystal, each molecule is linked to the other and *vice versa* by intermolecular N—H···O hydrogen bonds between the amide hydrogen and the O atoms of neighbouring molecules to form two ten-membered rings, each of which has the graph-set motif $C4R_2^2(10)$. This extends as a polymeric chain along the *c* axis.

Comment

Both *S*-methyldithiocarbazate and *S*-benzylcarbazate can be prepared by the addition of chloromethane or benzyl chloride to a mixture of hydrazine and carbon disulfide, respectively (Lanfredi *et al.*, 1977; Mattes & Weber, 1980; Ali & Tarafder, 1977). However, under the same conditions, 1,2-dibenzoyl hydrazine, (I), was obtained instead of *S*-benzoyldithiocarbazate when benzoyl chloride was added to the reaction mixture.



(I)

The dihedral angle of 24.0 (1)° between the phenyl ring and the N1—C7=O1 group shows that the molecule is not planar. The asymmetric unit contains half the molecule and the other half is related by a crystallographic twofold axis passing through the N1—N1^{i} bond [symmetry code: (i) $-x, y, \frac{1}{2} - z$]. The symmetry-related group adopts an anticlinal orientation with respect to the N—N bond, the torsion angle C7—N1—N1^{i}—C7^{i} being 104.3 (2)°. The two carbonyl groups and the H atoms of the N—N bond are in a *trans* orientation with respect to each other.

The bond lengths and angles are comparable with those of *N*,*N*′-bis(picolinoyl)hydrazine (Shao *et al.*, 1999), except for C=O which is slightly longer and the N—C—C angle [114.7 (1)°] which is 2° larger, possibly due to the greater twist along the N—N^{i} bond [torsion angle C—N—N^{i}—C^{i} in Shao *et al.* (1999) is −70.9 (2)°].

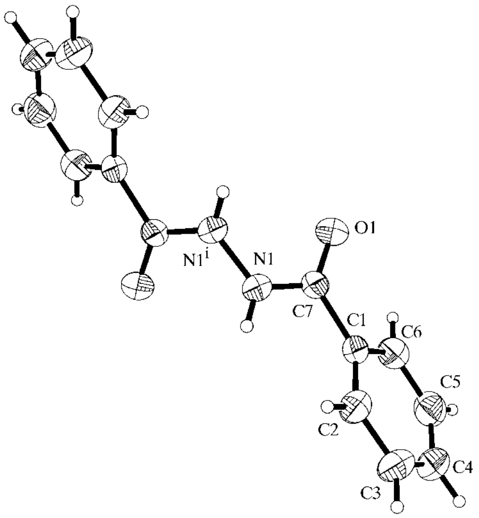


Figure 1
The structure of the title compound showing 50% probability displacement ellipsoids and the atom-numbering scheme [symmetry code: (i) $-x, y, \frac{1}{2} - z$].

In the crystal, each molecule is linked to another and *vice versa* by intermolecular N—H···O hydrogen bonds between the amide H atom and the O atoms of neighbouring molecules to form two ten-membered rings, each of which has the graph-set motif $C4R_2^2(10)$ (Bernstein *et al.*, 1995). This extends as a polymeric chain along the *c* axis.

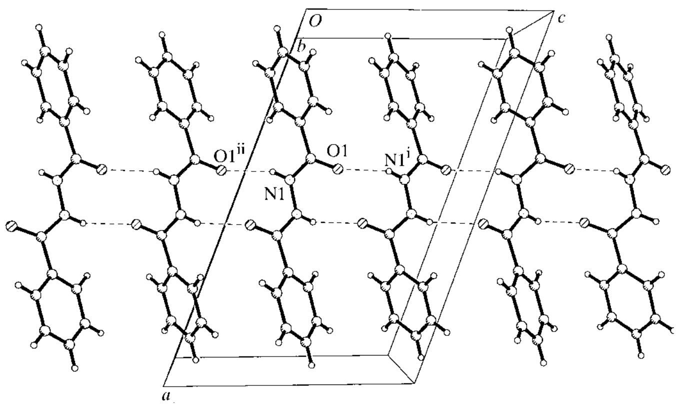


Figure 2
The polymeric chain of the packing of the title compound along the *c* axis.

Experimental

The title compound was prepared by adding benzoyl chloride to a mixture of hydrazine, potassium hydroxide and carbon disulfide in 20% aqueous ethanol at 273 K. The precipitate was washed with water and dried. The crystal used for analysis was obtained by recrystallization from ethanol.

Crystal data

$C_{14}H_{12}N_2O_2$
$M_r = 240.26$
Monoclinic, $C2/c$
$a = 14.5439$ (2) Å
$b = 9.7314$ (3) Å
$c = 9.0181$ (3) Å
$\beta = 110.938$ (1)°
$V = 1192.07$ (6) Å^3
$Z = 4$

$D_x = 1.339$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2038 reflections
$\theta = 3.00$–28.29°
$\mu = 0.092$ mm^{-1}
$T = 293$ (2) K
Block, light yellow
0.32 × 0.30 × 0.28 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
4148 measured reflections
1471 independent reflections
965 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.054$
$\theta_{\rm max} = 28.30$°
$h = -19 \rightarrow 14$
$k = -12 \rightarrow 12$
$l = -10 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.164$
$S = 0.959$
1471 reflections
83 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0975P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.30$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.28$ e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 1997)
Extinction coefficient: 0.021 (5)

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.229 (2)	N1—N1$^{\rm i}$	1.385 (3)
N1—C7	1.354 (2)		
C7—N1—N1$^{\rm i}$	118.6 (1)	O1—C7—C1	122.0 (2)
O1—C7—N1	121.3 (2)	N1—C7—C1	116.7 (1)

Symmetry code: (i) $-x, y, \frac{1}{2} - z$.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1$^{\rm i}$	0.86	2.13	2.924 (2)	154

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

Data collection was as as described in Shanmuga Sundara Raj *et al.* (1999).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT*; data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PARST* (Nardelli, 1995).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: NA1474). Services for accessing these data are described at the back of the journal.

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