Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diphenylcarbonohydrazide–phenylsemicarbazide (1/1)

Chun-Xia Wei, Jian-Xin Chen,* Zhong-Shui Li, Ting-Yan Lan and Yuan-Biao Huang

College of Chemistry and Materials Science, Fujian Normal University, Fuzhou, Fujian 350007, People's Republic of China

Correspondence e-mail: jxchen_1964@163.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.054
wR factor = 0.105
Data-to-parameter ratio = 17.2

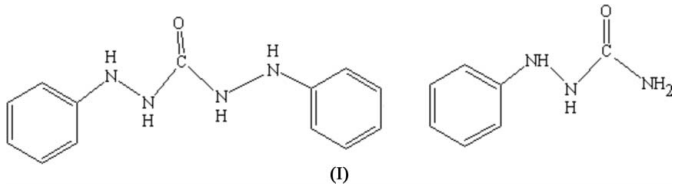
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 28 March 2006
Accepted 30 March 2006
Online 5 April 2006

In the title compound, $C_{13}H_{14}N_4O\cdot C_7H_9N_3O$, a phenylcarbonohydrazide molecule cocrystallizes with a phenylsemicarbazide molecule. In the crystal structure, extensive hydrogen-bonding and π–π stacking interactions stabilize the structure.

Comment

Diphenylcarbonohydrazide, an artificial electron-donor material, has various applications (Verma & Singh, 1995; Melis *et al.*, 1992; Prasad *et al.*, 1991; Sundari & Raghavendra, 1990; Mishra *et al.*, 1993), especially in the fields of biophysics, microbiology and analytical chemistry (El-Kabbany *et al.*, 1997). The structure of diphenylcarbonohydrazide ($C_{13}H_{14}N_4O$) has been determined previously (De Ranter *et al.*, 1979). A number of diphenylcarbonohydrazide derivatives have also been prepared (Jian *et al.*, 2003; Martynova *et al.*, 1985; Wang *et al.*, 2001; Hamuro *et al.*, 1999).



(I)

We present here the structure of the title compound, a cocrystal with a 1-phenylsemicarbazide, molecule 1, and a diphenylcarbonohydrazide, molecule 2 (Fig. 1 and Table 1). In molecule 2, ring 2 (C8–C13) is approximately parallel to ring 3 (C15–C20), with a dihedral angle of 12.64 (13)°. Ring 1, from molecule 1, makes dihedral angles of 49.53 (6) and 59.83 (6)°, respectively, with rings 2 and 3.

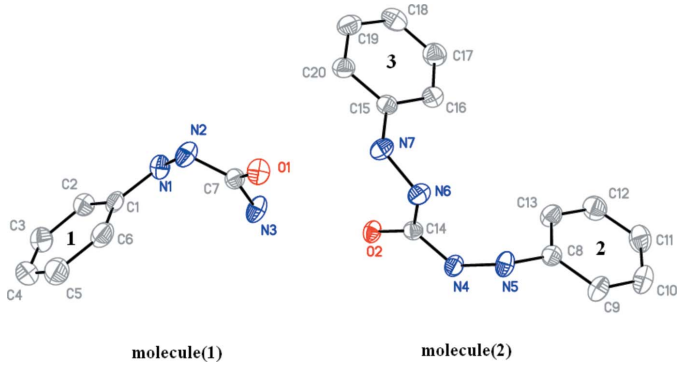


Figure 1
The asymmetric unit of (I), showing the atom-labeling scheme. Displacement ellipsoids are shown at the 50% probability level. All H atoms have been omitted for clarity.

In the crystal structure, molecules form a network structure through intermolecular N—H···O hydrogen bonds (Fig. 2 and Table 2). Moreover, there are offset face-to-face π–π stacking interactions in the crystal structure, with centroid-centroid distances of 3.584–3.700 Å (Fig. 2). These interactions increase the stability of the structure.

Experimental

A mixture of $(PhNHNH)_2C{=}O$ (diphenylcarbonohydrazide, 0.0605 g, 0.25 mmol), $(PhNHNH)(NH_2)C{=}O$ (phenylsemicarbazide, 0.0378 g, 0.25 mmol), $Co(OAc)_2$ (0.0443 g, 0.25 mmol) and water (12 ml) was sealed in a 23 ml Teflon-lined stainless steel autoclave to approximately 60% of capacity. The resulting mixture was heated at a rate of *ca* 100 K h^{-1} to 413 K and held at this temperature for 5 d. Subsequently, the autoclave was cooled at a rate of *ca* 3 K h^{-1} to room temperature. The resulting colorless plates were filtered off, washed with water and dried at ambient temperature.

Crystal data

$C_{13}H_{14}N_4O{\cdot}C_7H_9N_3O$
M_r = 393.45
Monoclinic, $P2_1/n$
a = 14.0097 (9) Å
b = 5.8841 (3) Å
c = 24.3124 (19) Å
β = 94.273 (3)°
V = 1998.6 (2) Å^3
Z = 4
D_x = 1.308 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
Plate, colorless
0.32 × 0.17 × 0.07 mm

Data collection

Rigaku Weissenberg IP diffractometer
ω scans
Absorption correction: multi-scan (*TEXSAN*; Molecular Structure Corporation, 1998)
T_{min} = 0.836, T_{max} = 0.994
18299 measured reflections
4516 independent reflections
1815 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.105
S = 0.97
4516 reflections
262 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0229P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.248 (3)	N4—N5	1.406 (3)
O2—C14	1.257 (3)	N5—C8	1.421 (3)
N1—N2	1.391 (3)	N6—C14	1.345 (3)
N1—C1	1.419 (3)	N6—N7	1.398 (3)
N2—C7	1.351 (3)	N7—C15	1.408 (3)
N3—C7	1.341 (3)	C1—C6	1.372 (4)
N4—C14	1.337 (3)	C15—C20	1.397 (3)
N2—N1—C1	116.9 (2)	O1—C7—N2	121.2 (2)
C7—N2—N1	121.67 (19)	N3—C7—N2	116.7 (2)
C14—N4—N5	121.88 (19)	C13—C8—C9	118.9 (2)
N4—N5—C8	116.27 (19)	C13—C8—N5	121.6 (2)
C14—N6—N7	122.8 (2)	C9—C8—N5	119.6 (2)
N6—N7—C15	117.85 (18)	O2—C14—N4	120.5 (2)
C6—C1—C2	120.0 (3)	O2—C14—N6	122.7 (2)
C6—C1—N1	122.3 (3)	N4—C14—N6	116.8 (2)
C2—C1—N1	117.7 (2)	C16—C15—C20	119.2 (3)
O1—C7—N3	122.1 (2)	C20—C15—N7	117.8 (2)

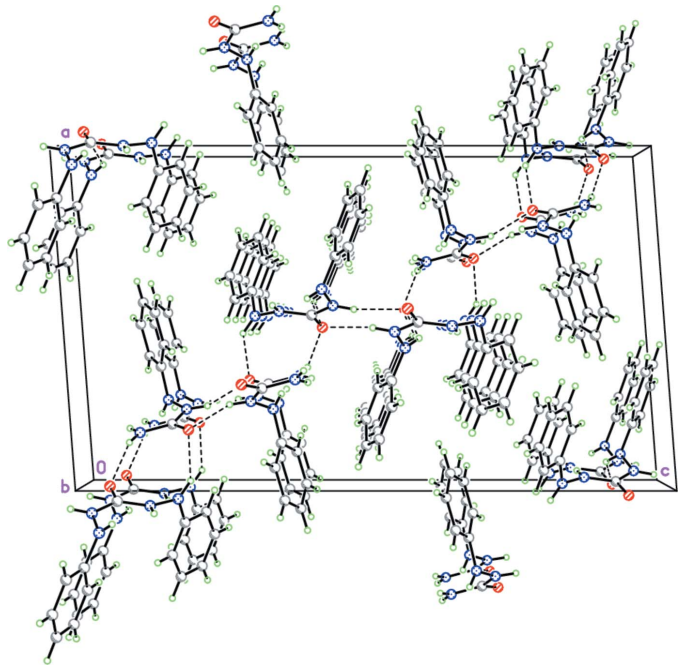


Figure 2
Packing diagram of (I), showing the π–π stacking along the b axis. Hydrogen bonds are drawn as dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3B···O2	0.86	2.15	2.952 (2)	154
N7—H7A···O1	0.86	2.35	2.973 (3)	129
N1—H1A···O1^{i}	0.86	2.61	3.098 (3)	117
N2—H2B···O1^{ii}	0.86	2.11	2.899 (2)	153
N4—H4B···O2^{iii}	0.86	2.10	2.946 (2)	168
N5—H5B···O2^{iv}	0.86	2.48	3.079 (3)	128

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

All H atoms were positioned geometrically and allowed to ride on their parent C or N atoms, with aromatic C—H = 0.93 Å and N—H = 0.86 Å, and U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *TEXSAN* (Molecular Structure Corporation, 1998); cell refinement: *TEXSAN*; data reduction: *TEXSAN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1993); software used to prepare material for publication: *SHELXL97*.

We are grateful for financial support from the Natural Science Foundation of Fujian Province, People's Republic of China (E0310016) and the Education Commission Foundation of Fujian Province, People's Republic of China (JB05309).

References

De Ranter, C. J., Blaton, N. M. & Peeters, O. M. (1979). *Acta Cryst.* B**35**, 1295–1297.
El-Kabbany, F., Taha, S., Mansey, F. M. & Shehap, A. (1997). *Infrared Phys. Technol.* **38**, 169–175.
Hamuro, Y., Marshall, W. J. & Scialdone, M. A. (1999). *J. Comb. Chem.* **1**, 163–172.

Jian, F. F., Xiao, H. L. & Wang, Y. (2003). *Jiegou Huaxue* (*Chin. J. Struct. Chem.*), **22**, 55–59. (In Chinese.)
Martynova, T. K., Neverov, V. A., Byushkin, V. N., Shafranskii, V. N. & Mal'kova, T. A. (1985). *Koord. Khim.* (*Coord. Chem.*), **11**, 132–135. (In Russian.)
Melis, A., Nemson, J. A. & Hanison, M. A. (1992). *Biochim. Biophys. Acta*, **1100**, 312–320.
Mishra, U., Kashyap, A. K. & Pande, J. (1993). *Environ. Technol.* **14**, 373–378.
Molecular Structure Corporation (1998). *TEXSAN*. Version 1.9. MSC, The Woodlands, Texas, USA.
Prasad, S. M., Singh, J. B., Rai, L. C. & Kumar, H. D. (1991). *FEMS Microbiol. Lett. Fed. Eur. Microbiol. Soc.* **82**, 95–100.
Sheldrick, G. M. (1993). *SHELXTL/PC*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sundari, D. S. & Raghavendra, A. S. (1990). *Photosynth. Res.* **23**, 95–99.
Verma, K. & Singh, D. P. (1995). *Curr. Microbiol.* **30**, 373–379.
Wang, Y., Jian, F.-F., Yang, X.-J., Lu, L.-D., Wang, X., Fun, H.-K., Chantrapromma, S. & Razak, I. A. (2001). *Acta Cryst.* E**57**, o312–o314.