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Crystal structure of 1-acetyl-2-phenylcarbamoylmethylsemicarbazide, $CH_2N_2H(COCH_3)(CONH_2)(CONHC_6H_5)$

K. Peters*[I], E.-M. Peters[I], A. Hetzheim[II] and P. Köckritz[II]

[I] Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70506 Stuttgart, Germany
[II] Ernst-Moritz-Arndt-Universität Greifswald, Institut für Chemie und Biochemie, Soldmannstraße 16, D-17487 Greifswald, Germany

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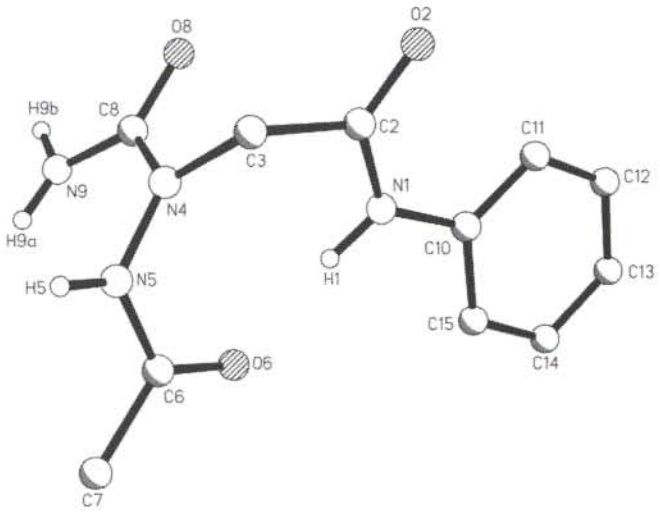

Abstract

$C_{11}H_{14}N_4O_3$, triclinic, $P\bar{1}$ (No. 2), $a = 5.5864(3)$ Å, $b = 7.4116(3)$ Å, $c = 15.319(1)$ Å, $\alpha = 102.035(5)°$, $\beta = 90.115(5)°$, $\gamma = 107.825(5)°$, $V = 589.1$ Å^3, $Z = 2$, $R_{gt(F)} = 0.050$, $wR(F) = 0.051$, $T = 293$ K.

Source of material

The title compound was synthesized by reaction of 2-amino-5-methyl-3-phenacyl-1,3,4-oxadiazolium bromide with hydroxyl ammonium chloride [1].

Table 1. Data collection and handling.

Crystal:	colourless plate, 0.55 × 0.6 × 0.2 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	1.10 cm^{-1}
Diffractometer, scan mode:	Siemens P4, ω
$2\theta_{max}$:	55°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	3506, 2692
Criterion for F_{obs}, $N(hkl)_{gt}$:	$F_{obs} > 3\,\sigma(F_{obs})$, 2505
$N(param)_{refined}$:	189
Program:	SHELXTL-plus [2]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1)	2*i*	–0.050(4)	0.489(3)	0.260(1)	0.057(5)
H(3A)	2*i*	–0.1471(3)	0.5169(2)	0.05126(9)	0.043(4)
H(3B)	2*i*	–0.2936(3)	0.5801(2)	0.13319(9)	0.043(4)
H(5)	2*i*	–0.654(3)	0.227(2)	0.125(1)	0.045(5)
H(7A)	2*i*	–0.8939(3)	0.1310(2)	0.2275(1)	0.110(9)
H(7B)	2*i*	–0.7992(3)	0.2552(2)	0.3243(1)	0.099(8)
H(7C)	2*i*	–0.7783(3)	0.0451(2)	0.2962(1)	0.092(7)
H(9A)	2*i*	–0.422(3)	–0.050(2)	0.097(1)	0.047(5)
H(9B)	2*i*	–0.191(3)	–0.083(2)	0.052(1)	0.049(5)
H(11)	2*i*	0.5676(3)	0.8147(2)	0.2503(1)	0.059(5)
H(12)	2*i*	0.8704(4)	0.9328(3)	0.3719(1)	0.065(6)
H(13)	2*i*	0.7728(4)	0.8585(3)	0.5105(1)	0.080(7)
H(14)	2*i*	0.3639(4)	0.6693(3)	0.5301(1)	0.091(7)
H(15)	2*i*	0.0583(3)	0.5501(2)	0.4103(1)	0.046(5)

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(1)	2*i*	0.0901(3)	0.5866(2)	0.24921(8)	0.0344(7)	0.0424(7)	0.0352(6)	0.0004(6)	0.0017(5)	0.0137(5)
C(2)	2*i*	0.0764(3)	0.6254(2)	0.16753(9)	0.0373(8)	0.0333(7)	0.0354(7)	0.0077(6)	0.0077(6)	0.0098(5)
O(2)	2*i*	0.2389(2)	0.7456(2)	0.13829(8)	0.0532(8)	0.0547(7)	0.0484(6)	0.0093(6)	0.0042(6)	0.0241(5)
C(3)	2*i*	0.1736(3)	0.5142(2)	0.11294(9)	0.0366(8)	0.0360(7)	0.0333(7)	0.0113(6)	0.0055(6)	0.0116(5)
N(4)	2*i*	0.2811(2)	0.3111(2)	0.11907(7)	0.0262(6)	0.0356(6)	0.0319(5)	0.0078(5)	0.0079(5)	0.0090(4)
N(5)	2*i*	0.5098(2)	0.2487(2)	0.15631(7)	0.0234(6)	0.0467(7)	0.0304(6)	0.0089(5)	0.0061(5)	0.0111(5)
C(6)	2*i*	0.5135(3)	0.2418(2)	0.24474(9)	0.0323(8)	0.0362(7)	0.0333(7)	0.0091(6)	0.0066(6)	0.0117(5)
O(6)	2*i*	0.3203(2)	0.2923(2)	0.29294(7)	0.0375(6)	0.0654(7)	0.0374(6)	0.0010(5)	0.0012(5)	0.0218(5)
C(7)	2*i*	0.7689(3)	0.1611(2)	0.2760(1)	0.0367(8)	0.0504(9)	0.0436(8)	0.0114(7)	0.0154(7)	0.0169(7)
C(8)	2*i*	0.1604(3)	0.1805(2)	0.08321(8)	0.0271(7)	0.0384(7)	0.0234(6)	0.0083(6)	0.0013(5)	0.0080(5)
O(8)	2*i*	0.0512(2)	0.2426(1)	0.05545(6)	0.0278(5)	0.0430(5)	0.0344(5)	0.0101(4)	0.0076(4)	0.0109(4)
N(9)	2*i*	0.2746(3)	0.0077(2)	0.08150(9)	0.0367(8)	0.0360(7)	0.0461(7)	0.0092(6)	0.0121(6)	0.0085(5)

* Correspondence author
(e-mail: karpet@vsibm1.mpi-stuttgart.mpg.de)

Table 3. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(10)	2*i*	0.2852(3)	0.6700(2)	0.31843(9)	0.0354(8)	0.0323(6)	0.0354(7)	0.0073(6)	0.0035(6)	0.0063(5)
C(11)	2*i*	0.5248(3)	0.7839(2)	0.3073(1)	0.0392(9)	0.0493(9)	0.0406(8)	0.0042(7)	0.0077(7)	0.0113(6)
C(12)	2*i*	0.7036(4)	0.8533(3)	0.3795(1)	0.038(1)	0.075(1)	0.055(1)	0.0062(9)	0.0007(8)	0.0160(9)
C(13)	2*i*	0.6464(4)	0.8108(3)	0.4615(1)	0.050(1)	0.077(1)	0.046(1)	0.004(1)	0.0095(9)	0.0129(9)
C(14)	2*i*	0.4058(4)	0.6983(3)	0.4727(1)	0.055(1)	0.070(1)	0.0381(8)	0.0065(9)	0.0005(8)	0.0164(8)
C(15)	2*i*	0.2253(3)	0.6282(2)	0.4021(1)	0.0398(9)	0.0502(9)	0.0397(8)	0.0026(7)	0.0049(7)	0.0140(7)

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References

1. Köckritz, P.; Hetzheim A.; Radeglia, R.: Eine neuartige Umlagerung von 2-Amino-3-phenacyl-1,3,4-oxadiazoliumhalogeniden mit Hydroxylamin. J. prakt. Chem. **338** (1996) 436-440.
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