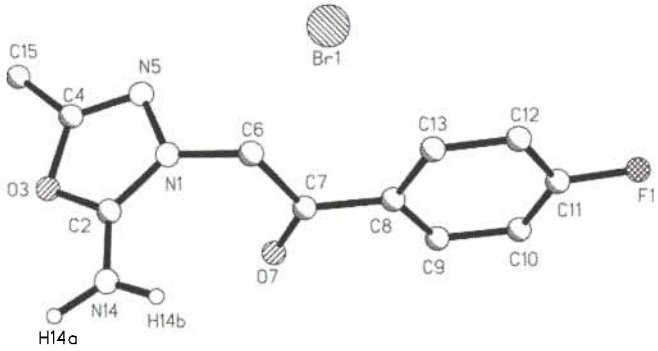
Crystal structure of 2-amino-3-(4-fluorophenacyl)-5-methyl-1,3,4-oxadiazolium bromide, $[C_2N_2O]^+[NH_2][CH_3][(CH_2CO)C_6H_4F]Br^-$

K. Peters*,[I], E.-M. Peters[I], A. Hetzheim[II] and T. Irrgang[II]

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

Received December 13, 1999, CCDC-No. 1267/365



Abstract

$C_{11}H_{11}BrFN_3O_2$, triclinic, $P\bar{1}$ (No. 2), a = 5.114(1) Å, b = 9.930(1) Å, c = 12.966(2) Å, α = 89.62(1)°, β = 82.48(1)°, γ = 88.57(1)°, V = 652.6 Å^3, Z = 2, $R_{gt}(F)$ = 0.037, $wR(F)$ = 0.037, T = 273 K.

Source of material

The title compound was synthesized by 1h refluxing of equimolecular amounts of 2-amino-5-methyl-1,3,4-oxadiazole with 4-fluorophenacylbromide in ethanol; mp 546 K (decomp.) [1].

Table 1. Data collection and handling.

Crystal:	colourless prism, size 0.35 × 0.45 × 0.65 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	31.60 cm^{-1}
Diffractometer, scan mode:	Bruker AXS P4, ω
$2\theta_{max}$:	55°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	3990, 3002
Criterion for F_{obs}, $N(hkl)_{gt}$.	$F_{obs} > 3\,\sigma(F_{obs})$, 2765
$N(param)_{refined}$:	165
Program:	SHELXTL-plus [2]

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

Atom	Site	x	y	z	U_{iso}
H(6A)	2*i*	0.2164(6)	0.4750(3)	0.7577(2)	0.08
H(6B)	2*i*	0.3903(6)	0.5439(3)	0.8323(2)	0.08
H(9)	2*i*	0.8476(7)	0.5925(4)	0.5116(2)	0.08
H(10)	2*i*	0.7459(9)	0.7695(4)	0.3991(3)	0.08
H(12)	2*i*	0.0851(8)	0.8628(4)	0.5954(3)	0.08
H(13)	2*i*	0.1905(7)	0.6918(3)	0.7094(3)	0.08
H(14A)	2*i*	0.8906	0.3515	0.9785	0.11(2)
H(14B)	2*i*	0.7798	0.4798	0.9129	0.07(1)
H(15A)	2*i*	0.2161(9)	−0.0207(4)	0.8086(4)	0.08
H(15B)	2*i*	0.3045(9)	−0.0319(4)	0.9197(4)	0.08
H(15C)	2*i*	0.5097(9)	−0.0592(4)	0.8208(4)	0.08

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}
Br(1)	2*i*	−0.16306(7)	0.71394(3)	0.90166(2)	0.0563(2)	0.0453(2)	0.0538(2)	0.0035(1)	−0.0076(1)	0.0037(1)
N(1)	2*i*	0.4451(5)	0.3458(3)	0.8240(2)	0.046(1)	0.039(1)	0.045(1)	0.000(1)	−0.008(1)	0.008(1)
C(2)	2*i*	0.6268(6)	0.3118(3)	0.8832(2)	0.047(2)	0.042(2)	0.041(1)	0.004(1)	−0.000(1)	0.006(1)
O(3)	2*i*	0.6220(4)	0.1794(2)	0.8969(2)	0.059(1)	0.040(1)	0.050(1)	0.005(1)	−0.010(1)	0.0076(9)
C(4)	2*i*	0.4229(7)	0.1359(4)	0.8444(2)	0.065(2)	0.043(2)	0.052(2)	0.001(2)	−0.012(2)	0.002(1)
N(5)	2*i*	0.3142(5)	0.2322(3)	0.7981(2)	0.060(2)	0.042(1)	0.050(1)	−0.004(1)	−0.012(1)	0.005(1)
C(6)	2*i*	0.3882(6)	0.4761(3)	0.7799(2)	0.048(2)	0.039(2)	0.045(2)	0.003(1)	−0.006(1)	0.009(1)
C(7)	2*i*	0.5910(6)	0.5102(3)	0.6868(2)	0.043(2)	0.042(2)	0.044(1)	−0.004(1)	−0.007(1)	0.003(1)
O(7)	2*i*	0.7949(4)	0.4446(3)	0.6708(2)	0.052(1)	0.059(1)	0.060(1)	0.010(1)	0.002(1)	0.010(1)
C(8)	2*i*	0.5262(6)	0.6240(3)	0.6205(2)	0.050(2)	0.039(2)	0.041(1)	−0.007(1)	−0.010(1)	0.003(1)
C(9)	2*i*	0.6914(7)	0.6476(4)	0.5290(2)	0.064(2)	0.049(2)	0.046(2)	−0.009(2)	−0.007(1)	0.005(1)
C(10)	2*i*	0.6311(9)	0.7513(4)	0.4621(3)	0.095(3)	0.059(2)	0.042(2)	−0.019(2)	−0.010(2)	0.009(2)
C(11)	2*i*	0.4090(9)	0.8251(4)	0.4880(3)	0.100(3)	0.041(2)	0.059(2)	−0.012(2)	−0.032(2)	0.013(2)
C(12)	2*i*	0.2406(8)	0.8069(4)	0.5789(3)	0.075(2)	0.044(2)	0.076(2)	0.004(2)	−0.019(2)	0.008(2)
C(13)	2*i*	0.3029(7)	0.7059(3)	0.6451(3)	0.061(2)	0.045(2)	0.056(2)	−0.002(2)	−0.006(2)	0.007(1)
N(14)	2*i*	0.7863(5)	0.3858(3)	0.9255(2)	0.051(2)	0.048(2)	0.062(2)	−0.005(1)	−0.018(1)	0.009(1)
C(15)	2*i*	0.3578(9)	−0.0061(4)	0.8488(4)	0.110(3)	0.044(2)	0.098(3)	−0.003(2)	−0.031(3)	0.010(2)
F(1)	2*i*	0.3446(6)	0.9215(3)	0.4210(2)	0.151(2)	0.063(2)	0.085(2)	−0.002(2)	−0.039(2)	0.035(1)

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

References

1. Hetzheim, A.: Unpublished results.
2. Sheldrick, G. M.: Program Package SHELXTL-Plus. Release 4.1, Siemens Analytical X-Ray Instruments Inc., Madison (WI 53719), USA 1990.