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Crystal structure of 2-amino-3-phenacyl-4,5-dimethyloxazolium bromide, $[C_3NO]^+(NH_2)(CH_3)_2[(CH_2CO)C_6H_5]Br^-$

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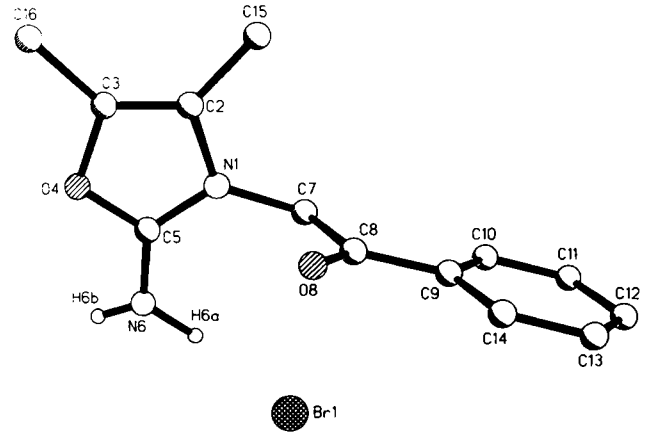

Source of material: The title compound was synthesized by reaction of 2-amino-4,5-dimethyloxazole with phenacylbromide (see ref. 1).

$C_{13}H_{15}BrN_2O_2$, monoclinic, $P2_1/n$ (No. 14), a =8.881(1) Å, b =12.204(1) Å, c =13.480(1) Å, β =106.19(1)°, V =1403.1 Å^3, Z =4, $R(F)$ =0.042, $R_w(F)$ =0.039.

Table 1. Parameters used for the X-ray data collection

Crystal:	colorless prism, size 0.45 x 0.55 x 0.6 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	29.30 cm^{-1}
Diffractometer:	Siemens P4
Scan mode:	ω
$T_{measurement}$:	293 K
$2\theta_{max}$:	55°
N(hkl)$_{unique}$:	3213
Criterion for F_o:	$F_o > 3\ \sigma(F_o)$
N($param$)$_{refined}$:	171
Program:	SHELXTL-plus

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

Atom	Site	x	y	z	U_{iso}
H(6A)	4e	0.018(5)	–0.432(3)	0.611(3)	0.13(2)
H(6B)	4e	–0.162(4)	–0.434(3)	0.535(3)	0.08(1)
H(7A)	4e	0.1213(4)	–0.3169(3)	0.7395(3)	0.08
H(7B)	4e	0.0985(4)	–0.2174(3)	0.8074(3)	0.08
H(10)	4e	0.3586(4)	–0.2571(3)	0.8740(3)	0.08
H(11)	4e	0.6102(5)	–0.2655(3)	0.9894(3)	0.08
H(12)	4e	0.6607(5)	–0.3827(3)	1.1318(3)	0.08
H(13)	4e	0.4569(5)	–0.4871(3)	1.1622(3)	0.08
H(14)	4e	0.2028(4)	–0.4780(3)	1.0486(3)	0.08
H(15A)	4e	–0.2703(5)	–0.1138(3)	0.8541(3)	0.08
H(15B)	4e	–0.1032(5)	–0.0958(3)	0.8393(3)	0.08
H(15C)	4e	–0.1318(5)	–0.1914(3)	0.9096(3)	0.08
H(16A)	4e	–0.5213(4)	–0.1537(3)	0.7199(4)	0.08
H(16B)	4e	–0.5824(4)	–0.2660(3)	0.6675(4)	0.08
H(16C)	4e	–0.5430(4)	–0.1702(3)	0.6014(4)	0.08

Table 3. Final 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)	4e	0.26032(5)	–0.49330(3)	0.64404(3)	0.0621(3)	0.0733(3)	0.0632(3)	0.0165(2)	0.0006(2)	–0.0133(2)
N(1)	4e	–0.1014(3)	–0.2874(2)	0.7308(2)	0.046(2)	0.049(2)	0.048(2)	–0.001(1)	0.013(1)	0.003(1)
C(2)	4e	–0.2170(4)	–0.2237(3)	0.7580(3)	0.056(2)	0.050(2)	0.064(2)	0.003(2)	0.028(2)	0.002(2)
C(3)	4e	–0.3504(4)	–0.2452(3)	0.6900(3)	0.053(2)	0.058(2)	0.073(3)	0.004(2)	0.026(2)	0.006(2)
O(4)	4e	–0.3230(3)	–0.3224(2)	0.6183(2)	0.044(1)	0.064(2)	0.064(2)	–0.003(1)	0.011(1)	0.003(1)
C(5)	4e	–0.1718(4)	–0.3454(3)	0.6479(3)	0.048(2)	0.048(2)	0.049(2)	–0.002(2)	0.011(2)	0.010(2)
N(6)	4e	–0.1107(4)	–0.4176(3)	0.5983(3)	0.056(2)	0.062(2)	0.053(2)	–0.002(2)	0.012(2)	–0.008(2)
C(7)	4e	0.0641(4)	–0.2903(3)	0.7854(3)	0.049(2)	0.051(2)	0.047(2)	–0.002(2)	0.015(2)	0.001(2)
C(8)	4e	0.0963(4)	–0.3643(3)	0.8791(3)	0.054(2)	0.051(2)	0.057(2)	–0.004(2)	0.015(2)	0.008(2)
O(8)	4e	–0.0093(3)	–0.4182(3)	0.8928(3)	0.061(2)	0.118(3)	0.106(2)	–0.027(2)	0.005(2)	0.059(2)
C(9)	4e	0.2577(4)	–0.3669(3)	0.9501(3)	0.053(2)	0.047(2)	0.047(2)	0.003(2)	0.013(2)	–0.003(2)

Table 3. (Continued)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(10)	4*e*	0.3783(4)	–0.3044(3)	0.9332(3)	0.055(2)	0.060(2)	0.065(3)	–0.001(2)	0.019(2)	0.003(2)
C(11)	4*e*	0.5274(5)	–0.3097(3)	1.0012(3)	0.057(3)	0.072(3)	0.078(3)	–0.002(2)	0.018(2)	–0.013(2)
C(12)	4*e*	0.5570(5)	–0.3780(3)	1.0854(3)	0.060(3)	0.077(3)	0.060(3)	0.007(2)	0.005(2)	–0.023(2)
C(13)	4*e*	0.4363(5)	–0.4399(3)	1.1029(3)	0.079(3)	0.067(2)	0.043(2)	0.019(2)	0.011(2)	–0.006(2)
C(14)	4*e*	0.2859(4)	–0.4350(3)	1.0358(3)	0.062(2)	0.059(2)	0.049(2)	0.007(2)	0.017(2)	–0.000(2)
C(15)	4*e*	–0.1771(5)	–0.1497(3)	0.8481(3)	0.083(3)	0.075(3)	0.091(3)	0.006(2)	0.038(3)	–0.009(3)
C(16)	4*e*	–0.5135(4)	–0.2052(3)	0.6678(4)	0.057(3)	0.085(3)	0.106(4)	0.008(2)	0.028(3)	0.012(3)

References

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