Crystal structure of 1-benzyl-1,2,3-triazole, C₉H₉N₃

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Fig. 1. Projection of the molecule on the best plane.

Source of material: synthesized (see ref. 1).

The bond distances and angles do not show any large deviations. The ORTEP plot of the molecule is shown in Fig. 1. The packing of the molecules down *b* shown in Fig. 2.

C₉H₉N₃, monoclinic, *P*12₁1 (No. 4), *a* = 5.545(6) Å, *b* = 7.777(2) Å, *c* = 9.850(4) Å, β = 96.36(5)°, *V* = 422.2 Å³, *Z* = 2, *R*(*F*) = 0.043, *R*_w(*F*²) = 0.130.

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Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
N(1)	2a	0.4984(5)	0.9531(5)	0.6213(3)	0.052(1)	0.090(2)	0.091(2)	0.002(2)	0.015(1)	0.001(2)
N(2)	2a	0.5675(5)	1.1113(5)	0.6537(3)	0.052(1)	0.086(2)	0.096(2)	-0.007(2)	0.008(1)	0.013(2)
C(3)	2a	0.3761(5)	1.1974(5)	0.6932(4)	0.061(2)	0.066(2)	0.091(2)	-0.001(2)	-0.000(1)	0.013(2)
C(4)	2a	0.1814(5)	1.0904(5)	0.6850(3)	0.048(2)	0.066(2)	0.078(2)	0.009(1)	0.003(1)	0.007(2)
N(5)	2a	0.2627(4)	0.9409(4)	0.6398(2)	0.045(1)	0.074(2)	0.062(1)	-0.001(1)	0.0053(9)	0.003(1)
C(6)	2a	0.1339(6)	0.7792(5)	0.6150(3)	0.064(2)	0.076(2)	0.068(2)	-0.006(2)	0.002(1)	-0.012(2)
C(7)	2a	0.1302(5)	0.6706(4)	0.7402(3)	0.053(1)	0.057(2)	0.067(2)	0.001(1)	0.006(1)	-0.013(1)
C(8)	2a	-0.0631(6)	0.5598(5)	0.7522(4)	0.056(2)	0.077(2)	0.094(2)	-0.009(2)	0.006(2)	-0.008(2)
C(9)	2a	-0.0682(6)	0.4545(6)	0.8635(4)	0.066(2)	0.075(2)	0.114(3)	-0.009(2)	0.020(2)	0.007(2)
C(10)	2a	0.1206(6)	0.4584(6)	0.9675(4)	0.084(2)	0.071(2)	0.092(2)	0.004(2)	0.015(2)	0.012(2)
C(11)	2a	0.3133(6)	0.5666(5)	0.9579(4)	0.079(2)	0.071(2)	0.076(2)	0.006(2)	-0.004(2)	-0.002(2)
C(12)	2a	0.3201(5)	0.6711(4)	0.8455(3)	0.060(2)	0.062(2)	0.075(2)	-0.006(2)	0.001(1)	-0.007(2)

Fig. 2. Packing of the molecules down *b*.

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

Crystal:	white, rectangular, size 0.20 x 0.25 x 0.35 mm
Wavelength:	Mo K _α radiation (0.71069 Å)
μ:	0.80 cm ⁻¹
Diffractometer:	Rigaku AFC7S
Scan mode:	ω/2θ
<i>T</i> _{measurement} :	293 K
2θ _{max} :	50°
<i>N</i> (<i>hkl</i>) _{unique} :	805
Criterion for <i>I</i> ₀ :	<i>I</i> ₀ > 2 σ(<i>I</i> ₀)
<i>N</i> (<i>param</i>) _{refined} :	110
Programs:	SHELXS-86, SHELXL-93

References

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