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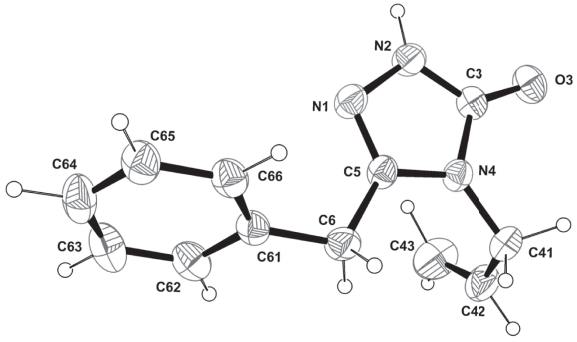
The crystal structure of 4-allyl-5-benzyl-2, 4-dihydro-3*H*-1,2,4-triazol-3-one, $C_{12}H_{13}N_3O$



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Abstract

$C_{12}H_{13}N_3O$, monoclinic, $P2_1/c$ (no. 14), $a = 11.0784(3)$ Å, $b = 14.4910(4)$ Å, $c = 7.1565(2)$ Å, $\beta = 97.668(2)°$, $V = 1138.61(5)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0432$, $wR_{ref}(F^2) = 0.1328$, $T = 296$ K.

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The crystal structure is shown in the figure, Tables 1–3 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title compound was prepared according to the published procedure [7]. Crystals suitable for X-ray structure analysis were grown by slow evaporation of an ethanol solution.

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Table 1: Data collection and handling.

Crystal:	Colourless, prism, size 0.09×0.21×0.33 mm
Wavelength:	Cu K_α radiation (1.54178 Å)
μ:	6.71 cm^{-1}
Diffractometer, scan mode:	Bruker APEX-II CCD, φ and ω scans
$2\theta_{max}$:	133.15°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	16366, 2009
$N(param)_{refined}$:	185
Programs:	Bruker data collection and reduction software [8], SHELX [9], WinGX and ORTEP [10]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	Site	*x*	*y*	*z*	U_{iso}
H(2)	4*e*	0.060(2)	0.311(2)	0.832(4)	0.086
H(6A)	4*e*	0.311(2)	0.551(2)	0.591(4)	0.086
H(6B)	4*e*	0.189(3)	0.611(2)	0.593(4)	0.086
H(41A)	4*e*	0.153(2)	0.509(2)	0.293(3)	0.086
H(41B)	4*e*	0.082(3)	0.415(2)	0.226(4)	0.086
H(42)	4*e*	0.286(3)	0.415(2)	0.143(5)	0.110
H(43A)	4*e*	0.406(4)	0.318(3)	0.344(5)	0.147
H(43B)	4*e*	0.310(3)	0.324(3)	0.518(6)	0.147
H(62)	4*e*	0.468(3)	0.566(2)	0.846(4)	0.096
H(63)	4*e*	0.540(3)	0.624(2)	1.150(4)	0.118
H(64)	4*e*	0.405(3)	0.693(2)	1.336(4)	0.112
H(65)	4*e*	0.191(3)	0.707(2)	1.220(4)	0.097
H(66)	4*e*	0.121(3)	0.645(2)	0.913(3)	0.083

Experimental details

All hydrogen atoms were identified in difference Fourier syntheses and their positions were refinement freely with $U_{iso}(H) = 1.5U_{eq}(C)$].

Discussion

1,2,4-Triazoles and their derivatives possess a wide range of biological activities, including analgesic [1], antibacterial [2], fungicidal [3], antinflammatory [4], antiviral [5] and anti-cancer [6] properties. The title compound was synthesized as potential antibacterial agent [7]. Its crystal structure determinations was undertaken in order to confirm the

Table 3: Atomic displacement parameters (Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(3)	4*e*	0.0173(1)	0.2903(1)	0.4565(2)	0.067(1)	0.0526(9)	0.070(1)	−0.0081(7)	0.0033(8)	−0.0193(7)
N(1)	4*e*	0.1463(2)	0.4344(1)	0.8158(2)	0.080(1)	0.046(1)	0.044(1)	−0.0110(9)	0.0071(9)	−0.0029(7)
N(2)	4*e*	0.0803(2)	0.3572(1)	0.7477(2)	0.078(1)	0.046(1)	0.049(1)	−0.0136(9)	0.0109(9)	−0.0031(8)
N(4)	4*e*	0.1284(2)	0.4275(1)	0.5051(2)	0.055(1)	0.0438(9)	0.0409(9)	−0.0005(8)	0.0039(7)	−0.0014(7)
C(3)	4*e*	0.0697(2)	0.3500(1)	0.5599(3)	0.051(1)	0.040(1)	0.054(1)	0.0035(9)	0.0073(9)	−0.0065(9)
C(5)	4*e*	0.1735(2)	0.4750(1)	0.6659(3)	0.058(1)	0.039(1)	0.042(1)	−0.0004(9)	0.0027(9)	−0.0023(8)
C(6)	4*e*	0.2424(2)	0.5632(2)	0.6623(3)	0.073(2)	0.045(1)	0.054(1)	−0.009(1)	0.009(1)	0.0021(9)
C(41)	4*e*	0.1529(2)	0.4433(2)	0.3135(3)	0.068(2)	0.064(2)	0.041(1)	0.003(1)	0.004(1)	0.005(1)
C(42)	4*e*	0.2686(2)	0.4011(2)	0.2739(4)	0.071(2)	0.100(2)	0.050(1)	0.007(1)	0.015(1)	0.001(1)
C(43)	4*e*	0.3364(3)	0.3453(3)	0.3823(5)	0.083(2)	0.118(3)	0.098(2)	0.037(2)	0.028(2)	0.018(2)
C(61)	4*e*	0.2884(2)	0.5994(1)	0.8558(3)	0.059(1)	0.034(1)	0.055(1)	−0.0047(9)	0.002(1)	0.0018(9)
C(62)	4*e*	0.4109(2)	0.5941(2)	0.9253(4)	0.061(2)	0.045(1)	0.083(2)	0.001(1)	0.004(1)	−0.001(1)
C(63)	4*e*	0.4530(3)	0.6288(2)	1.1020(4)	0.070(2)	0.056(2)	0.101(2)	0.001(1)	−0.023(2)	−0.005(1)
C(64)	4*e*	0.3734(3)	0.6695(2)	1.2102(4)	0.100(2)	0.048(1)	0.068(2)	−0.007(1)	−0.018(2)	−0.007(1)
C(65)	4*e*	0.2519(3)	0.6756(2)	1.1410(3)	0.082(2)	0.045(1)	0.066(2)	−0.004(1)	0.004(1)	−0.008(1)
C(66)	4*e*	0.2103(2)	0.6406(1)	0.9654(3)	0.059(1)	0.042(1)	0.063(1)	−0.002(1)	0.002(1)	−0.002(1)

synthesis pathway and identification its tautomeric form in the solid state.

In the crystalline state, the molecule exists in N2-amino/O3-keto tautomeric form, as evidenced by the C3–O3 bond length of 1.233(2) Å typical for the carbonyl group and the position of the H atom in the vicinity of N2 atom of pyrazole ring in the difference electron-density map.

The triazole and benzene rings are planar to within 0.010(2) and 0.003(2) Å, respectively. The benzyl substituent adopts a *cis-gauche* conformation with respect to the triazole ring with the torsion angles N1–C5–C6–C61 of 4.7(3)° and C5–C6–C61–C62 of 106.6(2)°. The allyl substituent is situated almost perpendicular to the plane of the triazole ring as shown by the torsion angles C3–N4–C41–C42 and N4–C41–C42–C43 of −86.7(3) and 9.0(5)°, respectively.

In the crystal structure the molecules related by *c* glide planes are connected into molecular chains parallel to *c* direction *via* medium strong intermolecular hydrogen bonding: N2–H2$\cdots$O3^{i}, where N2–H2 = 0.95(3) Å, H2$\cdots$O3 = 1.81(3) Å, N2$\cdots$O3 = 2.751(2) Å, N2–H2$\cdots$O3 = 170(3)° and $(i) = x$, $1/2-y$, $1/2+z$.

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