Crystal structure of ethyl 2-(5-methyl-4*H*-1,2,4-triazol-3-yl)acetate, $C_7H_{11}N_3O_2$

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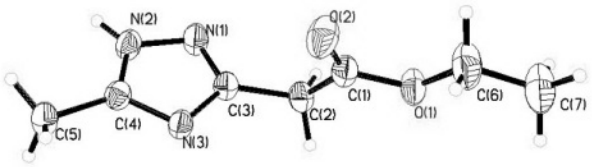
Received February 19, 2012, accepted July 19, 2012, available online November 09, 2012, CCDC no. 1267/3832



Abstract

$C_7H_{11}N_3O_2$, triclinic, $P\bar{1}$ (no. 2), a = 5.0843(3) Å, b = 7.8399(5) Å, c = 12.361(1) Å, α = 107.030(2)°, β = 95.273(1)°, γ = 103.183(1)°, V = 452.0 Å^3, Z = 2, $R_{gt}(F)$ = 0.0672, $wR_{ref}(F^2)$ = 0.1895, T = 298 K.

Table 1. Data collection and handling.

Crystal:	colourless columns, size 0.08×0.12×0.48 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.93 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω
$2\theta_{max}$:	50°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	2288, 1568
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1029
$N(param)_{refined}$:	111
Programs:	SHELX [4]

Source of material

1,2-(5-methyl-4*H*-1,2,4-triazol-3-yl) acetic acid (0.1mol, 14.1 g) was dissolved in enthanol (30 ml) with a reflux condenser. A catalytic amount of concentrated sulfuric acid was added at room temperature and the mixture was refluxed for another 2 hours. After the mixture was cooled in the ice bath, colouress column crystals were precipitated, filtered, washed with water for three times.

Experimental details

All H atoms were positioned geometrically (C–H = 0.96 Å for the aromatic H atoms and C–H = 0.97 Å for the aliphatic H atoms) and were refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) and U_{iso}(H) = 1.2U_{eq}(N).

Discussion

There has been much research interest in triazole due to its biological activities [1, 2]. In this work, we report the crystal structure of the title compound, 2-(5-methyl-4*H*-1,2,4-triazol-3-yl)acetate (Fig. 1). In this compound all bond lengths are within normal ranges [2].

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

Atom	Site	x	y	z	U_{iso}
H(2)	2*i*	–0.2035	0.6975	0.6440	0.066
H(2A)	2*i*	0.3252	0.5560	0.8993	0.064
H(2B)	2*i*	0.6027	0.6479	0.8682	0.064
H(5A)	2*i*	–0.0033	0.7559	0.4723	0.095
H(5B)	2*i*	0.2986	0.7424	0.4673	0.095
H(5C)	2*i*	0.2431	0.9239	0.5448	0.095
H(6A)	2*i*	0.7871	0.1499	0.7553	0.111
H(6B)	2*i*	0.5245	0.0516	0.7939	0.111
H(7A)	2*i*	1.0283	0.2258	0.9380	0.154
H(7B)	2*i*	0.9132	0.0106	0.8820	0.154
H(7C)	2*i*	0.7667	0.1209	0.9735	0.154

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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*	0.0145(5)	0.6209(3)	0.7542(2)	0.056(2)	0.076(2)	0.060(1)	0.029(1)	0.016(1)	0.035(1)
N(2)	2*i*	–0.0465(5)	0.6825(3)	0.6647(2)	0.047(1)	0.069(2)	0.061(1)	0.026(1)	0.009(1)	0.029(1)
N(3)	2*i*	0.3815(4)	0.6783(3)	0.6675(2)	0.047(1)	0.054(1)	0.049(1)	0.020(1)	0.007(1)	0.022(1)
O(1)	2*i*	0.6251(4)	0.3272(2)	0.8616(2)	0.084(2)	0.059(1)	0.056(1)	0.029(1)	–0.004(1)	0.0225(9)
O(2)	2*i*	0.3792(5)	0.2688(3)	0.6889(2)	0.102(2)	0.072(2)	0.060(1)	0.036(1)	–0.017(1)	0.005(1)
C(4)	2*i*	0.4711(6)	0.3703(4)	0.7852(2)	0.056(2)	0.062(2)	0.052(2)	0.020(1)	0.006(1)	0.024(1)
C(3)	2*i*	0.4261(6)	0.5581(4)	0.8365(2)	0.061(2)	0.059(2)	0.047(1)	0.022(1)	0.011(1)	0.024(1)
C(2)	2*i*	0.2727(6)	0.6192(3)	0.7523(2)	0.049(2)	0.052(2)	0.044(1)	0.019(1)	0.010(1)	0.019(1)
C(1)	2*i*	0.1720(6)	0.7161(3)	0.6141(2)	0.050(2)	0.047(2)	0.050(1)	0.019(1)	0.005(1)	0.014(1)
C(5)	2*i*	0.1781(6)	0.7913(4)	0.5158(2)	0.070(2)	0.066(2)	0.061(2)	0.020(2)	0.002(1)	0.032(1)
C(6)	2*i*	0.692(1)	0.1518(5)	0.8199(3)	0.130(4)	0.069(2)	0.081(2)	0.050(2)	–0.009(2)	0.019(2)
C(7)	2*i*	0.865(1)	0.1250(6)	0.9112(3)	0.138(4)	0.092(3)	0.092(3)	0.059(3)	–0.001(2)	0.034(2)

Acknowledgments. This project was funded by the Priority Academic Program Development of Jiangsu Higher Education Institutions, China.

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