Liang-Quan Sheng*

Crystal structure of 2-(4-(4*H*-1,2,4-triazol-4-yl)phenyl)acetic acid, C₁₀H₉N₃O₄

<https://doi.org/10.1515/ncrs-2018-0145>

Received May 20, 2018; accepted July 19, 2018; available online July 31, 2018

Abstract

C₁₀H₉N₃O₄, orthorhombic, *P*2₁2₁2₁ (no. 19), *a* = 4.3976(6) Å, *b* = 10.8753(14) Å, *c* = 19.678(3) Å, *V* = 941.1(2) Å³, *Z* = 4, *R*_{gt}(*F*) = 0.0415, *wR*_{ref}(*F*²) = 0.1075, *T* = 296(2) K.

CCDC no.: 1856737

The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of materials

All reagents and solvents were used as obtained commercially without further purification. A solution of *N,N*-dimethyl formamide azine (1.42 g, 10 mmol) in benzene (15 mL) was added slowly to a solution containing 2-(4-aminophenyl)acetic acid (1.51 g, 10 mmol) in 5 mL absolute benzene under heating and stirring. The mixture was refluxed for 1.5 h, then cooled to room temperature, and the colourless solid product obtained was filtered and washed three times with ethanol. Colorless crystals of the title compound suitable for X-ray structural determination were obtained by slow evaporation of an ethanol solution in air after 2 weeks.

Experimental details

Coordinates of hydrogen atoms were refined without any constraints or restraints. Their *U*_{iso} values were set to 1.2*U*_{eq} of

Table 1: Data collection and handling.

Crystal:	Needle, colorless
Size:	0.29 × 0.20 × 0.19 mm
Wavelength:	Mo <i>K</i> α radiation (0.71073 Å)
μ:	0.10 mm ^{−1}
Diffractometer, scan mode:	Bruker SMART, φ and ω-scans
θ _{max} , completeness:	27.5°, >98%
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} , <i>R</i> _{int} :	4647, 2085, 0.019
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ(<i>I</i> _{obs}), 1805
<i>N</i> (<i>param</i>) _{refined} :	137
Programs:	Bruker programs [1], SHELX [2]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} ^{*/} / <i>U</i> _{eq}
C1	0.2276(7)	1.0820(2)	0.90277(12)	0.0397(6)
H1	0.267291	1.165992	0.903731	0.048*
C2	0.0353(6)	1.0358(2)	0.85355(12)	0.0389(6)
H2	−0.055460	1.088230	0.822210	0.047*
C3	−0.0210(5)	0.9108(2)	0.85129(11)	0.0300(5)
C4	0.1112(6)	0.8335(2)	0.89834(12)	0.0374(6)
H4	0.072820	0.749486	0.897004	0.045*
C5	0.3008(6)	0.8819(2)	0.94741(12)	0.0378(6)
H5	0.389361	0.829461	0.979080	0.045*
C6	0.3623(5)	1.0069(2)	0.95057(11)	0.0335(5)
C7	0.5688(6)	1.0587(2)	1.00496(12)	0.0408(6)
H7A	0.756288	1.011771	1.006271	0.049*
H7B	0.619375	1.143224	0.993988	0.049*
C8	0.4174(6)	1.0540(2)	1.07379(12)	0.0373(6)
C9	−0.3402(7)	0.9171(3)	0.74552(14)	0.0521(8)
H9	−0.303864	0.998521	0.733678	0.062*
C10	−0.3375(7)	0.7459(2)	0.79669(14)	0.0471(7)
H10	−0.297610	0.684206	0.828178	0.057*
N1	−0.5129(6)	0.8431(2)	0.71143(11)	0.0518(6)
N2	−0.5114(6)	0.7319(2)	0.74443(11)	0.0491(6)
N3	−0.2196(4)	0.86103(17)	0.80043(9)	0.0325(5)
O1	0.2792(6)	1.15451(18)	1.09051(10)	0.0610(6)
H1A	0.221367	1.149714	1.130039	0.092*
O2	0.4278(8)	0.96670(19)	1.10946(11)	0.0884(10)

the parent atoms except the *U*_{iso} values were set to 1.5*U*_{eq} of the parent oxygen atom. The absolute structure was established by refinement of the Flack parameter (0.1(8) from 609 selected quotients) using Parsons' method [3]. The classical refinement of the Flack parameter gave a similar result (−0.012(23)) [2].

*Corresponding author: Liang-Quan Sheng, College of Chemistry and Chemical Engineering, Fuyang Normal University, Fuyang, Anhui 236041, P.R. China, e-mail: shenglq@fync.edu.cn

Comment

The metal-organic frameworks (MOFs) have attracted much interest in the field of crystal engineering because of their potential application [4, 5]. The most important factor to design and construction of MOFs is the judicious selection of organic ligands [6–10]. Significantly, the ligand containing the carboxy group and triazolyl group is well employed in building MOFs [11, 12]. In this paper, we report the 4-(1,2,4-triazol-4-yl)phenylacetic acid.

The molecular structure of the title compound is shown in the figure. The dihedral angle between the triazole and benzene rings is 10.13(9)°. The C6–C7–C8 angle is 110.82(17)°. In the crystal structure, O–H···N hydrogen bond connects molecules to a chain along *c*. Some non-classical the C–H···O, hydrogen bonds exist in the crystal structure.

Acknowledgements: We gratefully acknowledge support by the Natural Science Foundation of Anhui Provincial Education Commission (No. KH2016B123).

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