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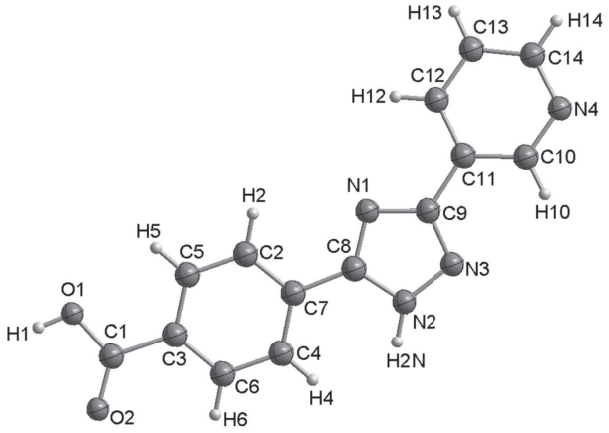
Crystal structure of 4-(3-(pyridin-3-yl)-1H-1,2, 4-triazol-5-yl)benzoic acid, $C_{14}H_{10}N_4O_2$



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Abstract

$C_{14}H_{10}O_2N_4$, monoclinic, $P2_1/c$, $a = 11.750(18)$ Å, $b = 8.194(13)$ Å, $c = 12.91(2)$ Å, $\beta = 102.306(19)°$, $V = 1214(3)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0505$, $wR_{ref}(F^2) = 0.1098$, $T = 296(2)$ 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

A mixture of $Cd(OAc)_2{\cdot}2H_2O$ (0.1 mmol, 238 mg), THF (10 mL), 4-(3-(pyridin-3-yl)-1H-1,2,4-triazol-5-yl)benzoic acid (0.3 mmol, 266 mg) was dissolved in 8 mL H_2O. Then the solution was heated in a 23 mL Teflon-lined autoclave under autogenous pressure at 403 K for five days. After cooling to room temperature colourless block crystals formed. The colourless crystals suitable for X-ray diffraction analysis were collected.

Table 1: Data collection and handling.

Crystal:	Colourless, block, size 0.18×0.22×0.31 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	1.02 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω scans
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	8428, 2257
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1385
$N(param)_{refined}$:	182
Programs:	SHELX [7]

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

Atom	Site	x	y	z	U_{iso}
H(2N)	4e	0.7572	0.5459	−0.2112	0.046
H(1)	4e	0.2780	0.0296	0.0355	0.071
H(2)	4e	0.6739	0.3886	0.0943	0.046
H(4)	4e	0.5908	0.3968	−0.2233	0.052
H(5)	4e	0.5130	0.2325	0.0969	0.046
H(6)	4e	0.4291	0.2386	−0.2204	0.051
H(10)	4e	1.0818	0.8165	−0.0549	0.045
H(12)	4e	0.9387	0.7264	0.1943	0.049
H(13)	4e	1.0848	0.8832	0.2973	0.056
H(14)	4e	1.2231	1.0002	0.2206	0.055

Results and discussion

Over the past few decades, supramolecular chemistry depending upon hydrogen bonding and intermolecular weak interactions have been a field of rapid growth due to potential application such as catalysis, magnetism, semiconductor, nonlinear optical materials, biological activity [1–6]. Benzimidazole and its derivatives, which are one kind of important building modules of N-containing heterocyclic ring compounds, may provide supramolecular recognition sites for N–H···O, C–H···O, C–H···π and π–π interactions to construct supramolecular architectures.

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

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(1)	4*e*	0.8217(2)	0.5696(3)	0.0261(2)	0.039(1)	0.037(2)	0.030(1)	−0.005(1)	0.008(1)	0.000(1)
N(2)	4*e*	0.7896(2)	0.5682(3)	−0.1466(2)	0.044(2)	0.042(2)	0.031(1)	−0.008(1)	0.008(1)	−0.003(1)
N(3)	4*e*	0.8851(2)	0.6638(3)	−0.1165(2)	0.043(2)	0.043(2)	0.033(1)	−0.012(1)	0.009(1)	−0.001(1)
N(4)	4*e*	1.1655(2)	0.9188(3)	0.0758(2)	0.041(1)	0.039(2)	0.039(1)	−0.006(1)	0.012(1)	−0.002(1)
O(1)	4*e*	0.3344(2)	0.0896(3)	0.0379(1)	0.051(1)	0.057(2)	0.035(1)	−0.020(1)	0.013(1)	−0.001(1)
O(2)	4*e*	0.2886(2)	0.0532(3)	−0.1367(2)	0.056(1)	0.062(2)	0.034(1)	−0.021(1)	0.004(1)	−0.004(1)
C(1)	4*e*	0.3506(3)	0.1131(3)	−0.0577(2)	0.043(2)	0.035(2)	0.033(2)	−0.003(1)	0.008(1)	−0.000(1)
C(2)	4*e*	0.6248(2)	0.3588(4)	0.0307(2)	0.039(2)	0.046(2)	0.027(1)	−0.008(2)	0.004(1)	0.001(1)
C(3)	4*e*	0.4541(2)	0.2174(3)	−0.0608(2)	0.038(2)	0.034(2)	0.032(1)	−0.002(1)	0.009(1)	−0.000(1)
C(4)	4*e*	0.5754(3)	0.3637(4)	−0.1588(2)	0.051(2)	0.051(2)	0.028(2)	−0.017(2)	0.012(1)	−0.002(1)
C(5)	4*e*	0.5285(2)	0.2648(4)	0.0322(2)	0.044(2)	0.043(2)	0.028(1)	−0.005(2)	0.009(1)	0.004(1)
C(6)	4*e*	0.4785(3)	0.2686(4)	−0.1569(2)	0.050(2)	0.049(2)	0.029(1)	−0.016(2)	0.006(1)	−0.004(1)
C(7)	4*e*	0.6501(2)	0.4101(3)	−0.0643(2)	0.038(2)	0.032(2)	0.033(1)	−0.002(1)	0.008(1)	0.000(1)
C(8)	4*e*	0.7527(2)	0.5131(3)	−0.0614(2)	0.038(2)	0.033(2)	0.030(1)	0.001(1)	0.009(1)	0.002(1)
C(9)	4*e*	0.9009(2)	0.6609(3)	−0.0117(2)	0.038(2)	0.031(2)	0.031(2)	−0.000(1)	0.011(1)	0.001(1)
C(10)	4*e*	1.0818(2)	0.8292(4)	0.0167(2)	0.044(2)	0.037(2)	0.033(2)	−0.004(2)	0.012(1)	−0.002(1)
C(11)	4*e*	0.9940(2)	0.7532(3)	0.0568(2)	0.036(2)	0.031(2)	0.034(1)	−0.003(1)	0.009(1)	0.001(1)
C(12)	4*e*	0.9956(3)	0.7745(4)	0.1641(2)	0.047(2)	0.042(2)	0.036(2)	−0.009(2)	0.013(1)	−0.001(1)
C(13)	4*e*	1.0824(3)	0.8678(4)	0.2255(2)	0.059(2)	0.049(2)	0.033(2)	−0.015(2)	0.014(2)	−0.003(1)
C(14)	4*e*	1.1649(3)	0.9374(4)	0.1789(2)	0.052(2)	0.045(2)	0.040(2)	−0.010(2)	0.007(2)	−0.001(2)

The crystal structure determined by X-ray diffraction reveals that the asymmetric unit is composited of one moieties. The carboxyl group is coplanar with the benzene ring. But the dihedral angle between benzene ring and pyridine is ∼4°. The bond connecting the triazolyl ring and pyridine ring is a single bond, which can rotate, and this is confirmed by the bond length of 1.462(4) Å, while in triazolyl ring, bond length of C8–N1, C8–N2, C9–N1, C9–N3, N2–N3 are found to be 1.326(4), 1.343(4), 1.363(4), 1.325(4), 1.356(3) Å, respectively. Some are listed as follows: N(2)—H(2N)—O(2)#1, [O···N = 2.756(5) Å, N–H···O = 162.5°]; O(1)—H(1)···N(4)#2, [O···N = 2.559(4) Å, N–H···O = 160.7°]. Symmetry codes: #1 $-x+1$, $y+1/2$, $-z-1/2$; #2 $x-1$, $y-1$, z. Hydrogen bonds between all moieties form a three-dimensional framework.

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