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Crystal structure of 2-(5-(pyridin-3-yl)-4-(pyridin-4-yl)-4H-1,2,4-triazol-3-yl)pyridine, C₁₇H₁₂N₆

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.28 × 0.22 × 0.20 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.09 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
$\theta_{\max}$, completeness:	27.3°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	8438, 3172, 0.027
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2081
$N(\text{param})_{\text{refined}}$:	208
Programs:	Bruker [1], Olex2 [2], SHELX [3, 4]

<https://doi.org/10.1515/ncrs-2020-0223>

Received May 7, 2020; accepted May 28, 2020; available online July 8, 2020

Abstract

C₁₇H₁₂N₆, monoclinic, $P2_1/n$ (no. 14), $a = 5.8617(14)$ Å, $b = 15.845(4)$ Å, $c = 15.326(4)$ Å, $\beta = 92.650(5)^\circ$, $V = 1422.0(6)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0449$, $wR_{\text{ref}}(F^2) = 0.1132$, $T = 296(2)$ K.

CCDC no.: 2006279

The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

All starting materials were used as received. A mixture of 2-(5-(pyridin-3-yl)-4-(pyridin-4-yl)-4H-1,2,4-triazol-3-yl)pyridine (0.300 g, 1 mmol) was added to 30 mL THF and stirred for 15 min under room temperature, then filtered. One night later,

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.6869(3)	0.18375(10)	0.64504(11)	0.0402(4)
C2	0.8608(3)	0.15050(10)	0.58826(12)	0.0411(4)
C3	1.0435(3)	0.10567(11)	0.62556(13)	0.0486(4)
H3	1.055098	0.096400	0.685516	0.058*
C4	1.2069(3)	0.07522(12)	0.57262(13)	0.0547(5)
H4	1.330716	0.044788	0.596178	0.066*
C5	1.1857(3)	0.09008(12)	0.48528(15)	0.0606(5)
H5	1.296304	0.070839	0.448515	0.073*
C6	0.9993(4)	0.13378(13)	0.45191(14)	0.0618(5)
H6	0.985343	0.142715	0.391922	0.074*
C7	0.4221(3)	0.25962(10)	0.70225(11)	0.0397(4)
C8	0.2531(3)	0.32541(11)	0.71940(10)	0.0402(4)
C9	0.2797(3)	0.40879(11)	0.69625(11)	0.0445(4)
H9	0.407345	0.426029	0.667090	0.053*
C10	0.1145(3)	0.46604(12)	0.71698(12)	0.0526(5)
H10	0.129643	0.522686	0.702474	0.063*
C11	−0.0728(3)	0.43868(13)	0.75929(13)	0.0563(5)
H11	−0.184716	0.477897	0.771824	0.068*
C12	0.0613(3)	0.30276(12)	0.76390(12)	0.0494(5)
H12	0.045600	0.246790	0.780894	0.059*
C13	0.5516(3)	0.31017(9)	0.55640(10)	0.0348(4)
C14	0.3629(3)	0.31396(11)	0.49954(11)	0.0432(4)
H14	0.234639	0.280970	0.508129	0.052*
C15	0.3705(3)	0.36842(12)	0.42931(12)	0.0516(5)
H15	0.243724	0.370706	0.390574	0.062*
C16	0.7243(3)	0.41275(12)	0.47062(13)	0.0584(5)
H16	0.849753	0.446973	0.461287	0.070*
C17	0.7354(3)	0.36066(11)	0.54244(12)	0.0463(4)
H17	0.864011	0.359794	0.580335	0.056*

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Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
N1	0.5533(2)	0.25411(8)	0.63046(8)	0.0368(3)
N2	0.6390(2)	0.14924(9)	0.71981(10)	0.0491(4)
N3	0.4711(3)	0.19719(9)	0.75618(10)	0.0490(4)
N4	0.8348(3)	0.16448(10)	0.50231(11)	0.0580(4)
N5	−0.1031(3)	0.35806(11)	0.78359(11)	0.0622(5)
N6	0.5470(3)	0.41764(10)	0.41361(10)	0.0586(4)

many colorless block crystals appeared in the solution, yield 53% (based on the raw title compound).

Experimental details

The structure was solved by direct methods with the SHELXS-2018 program. All H-atoms from C atoms were positioned with idealized geometry and refined using a riding model with C—H = 0.930 Å with $U_{iso}(H) = 1.2U_{eq}(C)$.

Comment

To the best of our knowledge, the title compound, 2-(5-(pyridin-3-yl)-4-(pyridin-4-yl)-4H-1,2,4-triazol-3-yl)pyridine, has been used as N-containing ligand to construct transition-metal coordination compounds, with metal ions such as Cu(I), Co(II), Ni(II), Zn(II) Ag(I) and Cd(II) [5–13]. However, the single crystal structure of it has not been reported. We herein report the crystal structure of the title compound.

As shown in the figure, the title compound crystallizes with one molecule in the asymmetric unit. There are four rings in the title compound, including three pyridine rings and one 1,2,4-triazole ring. Any two rings of the four rings are not co-planar. All of the bond lengths of the title compound are comparable with those in its complexes [5–13].

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