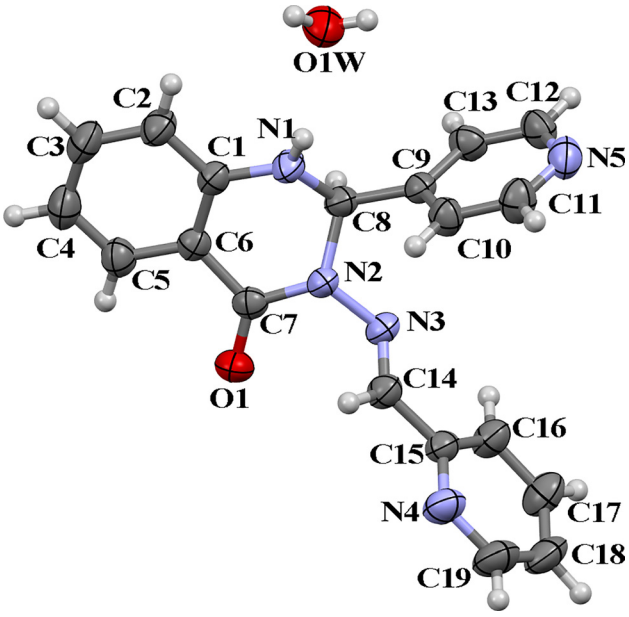
Ying Xiong, Gao Chuan and Ya An*

Crystal structure of (*S*,*E*)-3-((pyridin-2-ylmethylene)amino)-2-(pyridin-4-yl)-2,3-dihydroquinazolin-4(1*H*)-one monohydrate, $C_{19}H_{15}N_5O{\cdot}H_2O$



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Abstract

$C_{19}H_{15}N_5O{\cdot}H_2O$, triclinic, $P\bar{1}$ (no. 2), a = 9.1132(7) Å, b = 9.6788(9) Å, c = 11.0964(10) Å, α = 65.796(3)°, β = 79.406(3)°, γ = 87.484(3)°, V = 876.96(13) Å^3, Z = 2, $R_{gt}(F)$ = 0.0482, $wR_{ref}(F^2)$ = 0.1405, T = 273(2) K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

***Corresponding author: Ya An**, School of Chemistry and Materials, Guizhou Normal University, Guiyang 550025, China,
E-mail: 124251038@qq.com
Ying Xiong and Gao Chuan, School of Chemistry and Materials, Guizhou Normal University, Guiyang 550025, China. https://orcid.org/0000-0002-5790-3396 (Y. Xiong)

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.25 × 0.20 × 0.18 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.09 mm^{-1}
Diffractometer, scan mode:	φ and ω
θ_{max}, completeness:	26.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	24,458, 3432, 0.112
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2419
$N(param)_{refined}$:	238
Programs:	Olex2 [1], Bruker [2], SHELX [3], Diamond [4]

Source of materials

The compound (*E*)-2-amino-*N*′-(pyridin-2-ylmethylene) benzohydrazide (961 mg, 4 mmol), prepared by a literature procedure [5], was mixed with pyridine-4-carboxaldehyde (856 mg, 4 mmol) in anhydrous ethanol. The solution was refluxed for 24 h then cooled to room temperature, and the solvent was removed under reduced pressure. The resulting solid was recrystallized from ethanol to give colourless block crystals.

Experimental details

Using Olex2 [1], the structure was solved using Charge Flipping and refined with the ShelXL [3] refinement. All hydrogen atoms were positioned geometrically, with the d(C–H) = 0.97–0.99 Å, U_{iso}(H) = 1.2 times U_{eq}(C) and U_{iso}(H) = 1.5 times U_{eq}(O).

Comment

Chirality is an important property and commonly used in biological functions and material sciences. Chiral molecules have attracted an extensively attention in chiral separation, asymmetric synthesis and catalysis, as well as supramolecular

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.32478 (18)	0.64318 (19)	0.24995 (17)	0.0386 (4)
C2	0.3878 (2)	0.7156 (2)	0.11393 (19)	0.0504 (5)
H2	0.450911	0.664033	0.071884	0.060*
C3	0.3558 (2)	0.8639 (2)	0.0428 (2)	0.0571 (5)
H3	0.396797	0.911739	−0.048128	0.069*
C4	0.2634 (2)	0.9439 (2)	0.1037 (2)	0.0576 (5)
H4	0.242646	1.044177	0.054031	0.069*
C5	0.2029 (2)	0.8738 (2)	0.2380 (2)	0.0484 (5)
H5	0.140907	0.926888	0.279223	0.058*
C6	0.23388 (18)	0.72302 (19)	0.31321 (17)	0.0377 (4)
C7	0.18394 (18)	0.65543 (19)	0.46031 (17)	0.0377 (4)
C8	0.24144 (19)	0.41366 (19)	0.44163 (16)	0.0391 (4)
H8	0.147844	0.405806	0.412907	0.047*
C9	0.29273 (18)	0.25677 (19)	0.51965 (16)	0.0369 (4)
C10	0.4135 (2)	0.2333 (2)	0.58373 (19)	0.0477 (5)
H10	0.465692	0.314980	0.581435	0.057*
C11	0.4556 (2)	0.0877 (2)	0.6510 (2)	0.0549 (5)
H11	0.536426	0.073662	0.694706	0.066*
C12	0.2732 (2)	−0.0102 (2)	0.5926 (2)	0.0534 (5)
H12	0.225416	−0.093453	0.593029	0.064*
C13	0.2217 (2)	0.1314 (2)	0.52490 (19)	0.0467 (5)
H13	0.139661	0.142269	0.483140	0.056*
C14	0.1969 (2)	0.4627 (2)	0.73978 (18)	0.0440 (4)
H14	0.267266	0.542269	0.707153	0.053*
C15	0.1396 (2)	0.3891 (2)	0.88437 (17)	0.0417 (4)
C16	0.0204 (2)	0.2858 (2)	0.93938 (19)	0.0511 (5)
H16	−0.027741	0.258821	0.884765	0.061*
C17	−0.0262 (2)	0.2232 (3)	1.0772 (2)	0.0632 (6)
H17	−0.106522	0.153574	1.116661	0.076*
C18	0.0473 (3)	0.2647 (3)	1.1552 (2)	0.0641 (6)
H18	0.017725	0.224287	1.248062	0.077*
C19	0.1652 (3)	0.3670 (3)	1.0930 (2)	0.0685 (6)
H19	0.215256	0.393789	1.146542	0.082*
N1	0.35264 (16)	0.49445 (16)	0.32629 (14)	0.0430 (4)
H1	0.432726	0.452399	0.305662	0.052*
N2	0.21921 (15)	0.50455 (15)	0.52281 (13)	0.0377 (4)
N3	0.15302 (16)	0.42044 (16)	0.65838 (14)	0.0420 (4)
N4	0.2130 (2)	0.43078 (19)	0.96007 (16)	0.0574 (5)
N5	0.38718 (19)	−0.03490 (18)	0.65723 (17)	0.0553 (4)
O1	0.12276 (14)	0.72658 (14)	0.52376 (13)	0.0494 (4)
O1W	0.53107 (17)	0.33793 (17)	0.18410 (16)	0.0653 (4)
H1WA	0.607422	0.390006	0.131089	0.098*
H1WB	0.564684	0.252234	0.228477	0.098*

architectures due to their ability to generate an asymmetric environment [5]. X-ray structural determination reveals that the compound is a racemic mixture. The asymmetric unit contains one molecule and one water molecule (see the figure). In the title molecule, one terminal pyridine ring remains almost perpendicular with the central aromatic ring where the dihedral angle is 85.43°, and the dihedral angle between the other pyridine ring and the central aromatic ring is 77.39°. The bond angles and bond lengths are in the normal ranges [5, 6]. The molecules are packed in alternating layers and the lattice water molecules are found to be hydrogen bonded with the pyridine.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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