Ze-Sen Jin, Xiao-jing Liu, Zhuang-Yu Li, E. Liu, Fang-fang Jian* and Tongling Liang

Crystal structure of (*E*)-(2-((1*H*-pyrrol-2-yl)methylene)hydrazineyl)(amino)methaniminium nitrate monohydrate, C₆H₁₂N₆O₄

Table 1: Data collection and handling.

Crystal:	Colourless prism
Size:	0.25 × 0.07 × 0.06 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.13 mm ⁻¹
Diffractometer, scan mode:	XtaLAB AFC10 (RCD3), ω
$\theta_{\max}$, completeness:	31.1°, >99% (2 θ = 50°)
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	11027, 2662, 0.025
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2219
$N(\text{param})_{\text{refined}}$:	148
Programs:	CAD-4 [1, 2], Olex2 [3]

$V = 1019.87(7) \text{ \AA}^3$, $Z = 4$, $R_{\text{gt}}(F) = 0.0349$, $wR_{\text{ref}}(F^2) = 0.1018$, $T = 170 \text{ K}$.

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The asymmetric unit of the title crystal 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

Pyrrole-2-formaldehyde (0.95 g, 0.01 mol) was dissolved in 15 ml ethanol at room temperature, and added to asymmetric unit of the title crystal nitrate (1.37 g, 0.01 mol) solution containing 10 ml water and 8 ml ethanol. The mixture was heated and stirred for 8 h, and cooled to room temperature. Then the precipitate was removed, and the filtrate was left standing to precipitate colorless crystals.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

As organic reagents and ligands, Schiff bases have important applications in medicine [4], analytical chemistry [5] and

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Abstract

C₆H₁₂N₆O₄, monoclinic, $P2_1/n$ (no. 14), $a = 7.3652(3) \text{ \AA}$, $b = 16.8683(7) \text{ \AA}$, $c = 8.3779(3) \text{ \AA}$, $\beta = 101.525(4)^\circ$,

***Corresponding author: Fang-fang Jian**, School of Chemical Engineering and Pharmaceuticals, Henan University of Science and Technology, Luoyang Hekeda Recycling Energy Co.Ltd., Luoyang, Henan 471003, P. R. China, E-mail: Fangfjian@126.com

Ze-Sen Jin, Xiao-jing Liu and Zhuang-Yu Li, School of Chemical Engineering and Pharmaceuticals, Henan University of Science and Technology, Luoyang, Henan 471003, P. R. China. <https://orcid.org/0000-0003-2287-4166> (Z.-S. Jin). <https://orcid.org/0000-0002-5358-3479> (X.-j. Liu). <https://orcid.org/0000-0003-4445-1455> (Z.-Y. Li)

E. Liu, School of Chemical Engineering and Pharmaceuticals, Henan University of Science and Technology, Luoyang Hekeda Recycling Energy Co.Ltd., Luoyang, Henan 471003, P. R. China

Tongling Liang, Institute of Chemistry, Chinese Academy of Sciences, Zhongguancun, Beijing 100190, P. R. China

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

Atom	x	y	z	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
O1	0.78340 (11)	0.66144 (5)	1.09532 (10)	0.0252 (2)
O2	1.07563 (11)	0.65417 (5)	1.20516 (10)	0.0273 (2)
O3	0.91897 (12)	0.54751 (5)	1.13061 (10)	0.0285 (2)
O4	0.65052 (12)	0.46042 (6)	0.90657 (11)	0.0313 (2)
H4C	0.720967	0.487709	0.978859	0.047*
H4D	0.724196	0.432718	0.863333	0.047*
N1	0.07810 (12)	0.40868 (5)	0.31197 (11)	0.0203 (2)
H1	0.062920	0.457186	0.280488	0.024*
N2	0.29044 (12)	0.51121 (5)	0.55228 (10)	0.0188 (2)
N3	0.39788 (13)	0.55282 (5)	0.67928 (11)	0.0198 (2)
H3	0.455364	0.528767	0.765136	0.024*
N4	0.32418 (13)	0.66711 (6)	0.53082 (11)	0.0222 (2)
H4A	0.332319	0.717722	0.522132	0.027*
H4B	0.260355	0.639987	0.452284	0.027*
N5	0.50839 (13)	0.67247 (6)	0.78646 (11)	0.0233 (2)
H5A	0.516906	0.723101	0.778288	0.028*
H5B	0.563835	0.648735	0.873470	0.028*
N6	0.92539 (12)	0.62103 (5)	1.14381 (10)	0.0191 (2)
C1	0.00062 (16)	0.34485 (7)	0.22632 (13)	0.0231 (2)
H1A	−0.077721	0.346307	0.124469	0.028*
C2	0.05694 (15)	0.27776 (7)	0.31478 (14)	0.0243 (2)
H2	0.024593	0.225850	0.284167	0.029*
C3	0.17275 (15)	0.30231 (7)	0.46042 (14)	0.0224 (2)
H3A	0.231089	0.269500	0.544370	0.027*
C4	0.18436 (14)	0.38386 (6)	0.45650 (12)	0.0183 (2)
C5	0.28866 (14)	0.43608 (7)	0.57477 (12)	0.0189 (2)
H5	0.357100	0.414954	0.670682	0.023*
C6	0.40972 (14)	0.63101 (7)	0.66485 (12)	0.0179 (2)

catalysis [6]. In the field of medicine, Schiff bases have anti-bacterial, bactericidal, antitumor and antiviral biological activities; in the field of catalysis, the cobalt and nickel complexes of Schiff bases have been used as catalysts. At the same time, Schiff base compounds also have unique applications in the fields of corrosion [7] and photochromism [8]. According to the previous studies [9, 10], we synthesized the title compound.

The crystal structure of the title compound is shown in the figure. The bond length and angle are in the normal range [11, 12]. The bond length of C5–N2 is 1.2817 Å, which means C=N double bond.

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