Han-Lin Zhao, Jin-Ke Jiang, Yu-Tong Chu, Gang-Mei Li, Xi-Xi Li and Xin Jin*

Crystal structure of poly[diammine-bis(μ_4 -4-hydroxypyridine-3-sulfonato- $\kappa^5 N:O$, $O':O'':O''$)(μ_2 -pyrazinyl- $\kappa^2 N:N'$)tetrasilver(I)], $C_7H_8Ag_2N_3O_4S$

<https://doi.org/10.1515/ncrs-2020-0537>

Received October 17, 2020; accepted November 29, 2020;
published online December 9, 2020

Abstract

$C_7H_8Ag_2N_3O_4S$, triclinic, $P\bar{1}$ (no. 2), $a = 7.3758(3)$ Å, $b = 8.7361(4)$ Å, $c = 9.2906(4)$ Å, $\alpha = 112.877(4)^\circ$, $\beta = 90.054(4)^\circ$, $\gamma = 102.568(4)^\circ$, $V = 535.90(4)$ Å³, $Z = 2$, $R_{gt}(F) = 0.0235$, $wR_{ref}(F^2) = 0.0600$, $T = 293(2)$ K.

CCDC no: 2036006

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

*Corresponding author: Xin Jin, College of Biology and Pharmaceutical Engineering, Jilin Agricultural Science and Technology University, Jilin, 132101, Province Jilin, P.R. China, E-mail: jinxinc@126.com. <https://orcid.org/0000-0002-4436-9729>
Han-Lin Zhao, Yu-Tong Chu, Gang-Mei Li and Xi-Xi Li, College of Biology and Pharmaceutical Engineering, Jilin Agricultural Science and Technology University, Jilin, 132101, Province Jilin, P.R. China
Jin-Ke Jiang, State Key Laboratory of Crystal Materials, Shandong University, Jinan, 250100, Shandong, P.R. China

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.13 × 0.11 × 0.04 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	3.85 mm ⁻¹
Diffractometer, scan mode:	XtaLAB Pro, ω
θ_{max} , completeness:	29.7°, 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	8872, 2695, 0.030
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 2260
$N(param)_{refined}$:	155
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3], WinGX/ORTEP [4], Diamond [5]

Source of material

The Ag_2CO_3 (0.138 g, 0.5 mmol) and 4-hydroxypyridine-3-sulfonic acid (0.088 g, 0.5 mmol) were added to 15 mL $H_2O/EtOH$ (1:2, v/v). Ammonia water was added dropwise to the solution to make it clear and after 5 min, the pyrazine (0.010 g, 1 mmol) also was added. The reaction mixture was stirred for about 30 min in the air. Colorless crystal could be obtained after several weeks.

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$).

Atom	X	Y	Z	U_{iso}^*/U_{eq}
C1	0.2194 (4)	0.4187 (3)	0.3758 (3)	0.0254 (5)
H1	0.264188	0.456009	0.480280	0.030*
C2	0.2511 (4)	0.2662 (3)	0.2701 (3)	0.0212 (5)
C3	0.1897 (4)	0.2048 (3)	0.1070 (3)	0.0220 (5)
C4	0.0816 (4)	0.3060 (3)	0.0730 (3)	0.0249 (5)
H4	0.026056	0.269344	-0.028346	0.030*
C5	0.0575 (4)	0.4554 (3)	0.1858 (3)	0.0277 (6)
H5	-0.010949	0.518109	0.156554	0.033*
C6	0.4810 (4)	-0.3674 (3)	0.1289 (3)	0.0240 (5)
H6	0.469433	-0.276960	0.220765	0.029*
C7	0.4342 (4)	-0.5087 (3)	-0.1382 (3)	0.0262 (5)
H7	0.389562	-0.518549	-0.235817	0.031*
Ag1	0.13936 (3)	0.76905 (3)	0.50352 (3)	0.03312 (8)
Ag2	0.33162 (4)	-0.14823 (3)	-0.01735 (3)	0.04248 (9)
N1	0.1272 (3)	0.5168 (3)	0.3364 (3)	0.0280 (5)
N2	0.4157 (3)	-0.3752 (3)	-0.0089 (3)	0.0234 (4)
N3	0.1344 (4)	1.0212 (3)	0.6615 (3)	0.0307 (5)
H3A	0.163851	1.034211	0.754794	0.046*
H3B	0.023312	1.033832	0.662323	0.046*
H3C	0.207193	1.105651	0.648564	0.046*
O1	0.3915 (3)	0.2411 (3)	0.5126 (2)	0.0360 (5)
O2	0.5642 (3)	0.1831 (4)	0.2850 (3)	0.0440 (6)
O3	0.2788 (3)	-0.0208 (3)	0.2821 (3)	0.0377 (5)
O4	0.2271 (3)	0.0758 (2)	-0.0033 (2)	0.0298 (4)
S1	0.38147 (10)	0.15875 (9)	0.34321 (7)	0.02478 (14)

Experimental details

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

Comment

As is depicted in the left picture, the silver atoms have different coordinating environments. The Ag1 is three-coordinated by one oxygen atom, coming from the sulfonate group of the 4-hydroxypyridine-3-sulfonato (dpdS) ligand, and two nitrogen atoms, from another dpdS ligand and one NH_3 molecule (see the left part of the Figure). The Ag2 is four-coordinated by three oxygen atoms (O3, O4, O2D) and a nitrogen atom (N2). The O3 and O4 atoms, belonging to the same ligand form a chelate coordination to Ag2, the N2 and O2D atoms come from pyrazine

and dpdS ligands respectively. At the same time, O2 is shared by two silver(I) atoms (Ag2D, Ag1A). The bond distances of Ag-N and Ag-O range from 2.127(2) to 2.232(3) $\text{\AA}$, 2.135(3) to 2.526(3) $\text{\AA}$. The distance of Ag...Ag is 3.087 $\text{\AA}$. These coordinations lead to a 2D coordination polymer (see the right part of the figure) which is well known for related structures [6–9] (symmetry codes: A = 1 - x, 1 - y, 1 - z; B = x, 2 + y, 1 + z; C = x, 1 + y, 1 + z; D = 1 - x, - y, - z; E = 1 - x, - 1 - y, - z).

Acknowledgements: The authors would like to express their thanks to the responsible editor for the discussion and help to refine the title crystal structure.

Author contribution: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Research funding: Youth Foundation of Jilin Agricultural Science and Technology University (no. 20190394).

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

References

1. Corporation R. *CrysAlis^{PRO}*; Yarnton: Oxfordshire, England, 2015.
2. Sheldrick G. M. SHELXT-Integrated space-group and crystal-structure determination. *Acta Crystallogr.* 2015, *A71*, 3–8.
3. Sheldrick G. M. Crystal structure refinement with SHELXL. *Acta Crystallogr.* 2015, *C71*, 3–8.
4. Farrugia L. J. WinGX and ORTEP for Windows: An update. *J. Appl. Crystallogr.* 2012, *45*, 849–854.
5. Brandenburg K. DIAMOND. Visual Crystal Structure Information System. Ver. 3.2; Crystal Impact: Bonn, Germany, 2012.
6. Wu H., Dong X.-W., Liu H.-Y., Ma J.-F., Liu Y.-Y., Liu Y.-Y., Yang J. Construction of a series of inorganic–organic hybrid coordination polymers based on hexamethylenetetramine and sulfonate ligands. *Inorg. Chim. Acta.* 2011, *373*, 19–26.
7. Zhang X.-L., Tang G.-M., Wang Y.-T. Tunable luminescent behaviors of Ag-containing metal coordination polymers with *N*-heterocyclic and sulfonate group. *Polyhedron* 2018, *147*, 26–35.
8. Li J.-W., Jiang J.-K., Jiang H. Crystal structure of poly[aqua(μ_2 -2-amino-1,4-benzenedisulfonato- κ^2O : O')bis(μ_2 -pyrazin- $\kappa^2N:N'$) silver(I)], $C_{14}H_{16}Ag_2N_5O_8S_2$. *Z. Kristallogr. NCS* 2019, *234*, 1193–1194.
9. Jiang J.-K., Li X.-X., Jiang H., Dong X.-W. Crystal structure of poly [aqua (μ_2 -2-amino-1,4-benzenedisulfonato- κ^3N, O : O')-(μ_4 -hexamethylenetetramino- κ^4N : N' : N'' : N''')disilver(I)] monohydrate, $C_{12}H_{21}Ag_2N_5O_8S_2$. *Z. Kristallogr. NCS* 2019, *234*, 1251–1252.