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Crystal structure of poly[aqua(5-dimethylamino)naphthalene-1-sulfonato- $\kappa^2N:O$](μ_2 -4,4'-bipyridyl - $\kappa^2N:N'$)silver(I)], $C_{44}H_{44}Ag_2N_6O_8S_2$

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Abstract

$C_{44}H_{44}Ag_2N_6O_8S_2$, triclinic, $P\bar{1}$ (no. 2), $a = 11.3967(5)$ Å, $b = 12.6953(6)$ Å, $c = 14.9539(7)$ Å, $\alpha = 80.903(4)^\circ$, $\beta = 89.801(4)^\circ$, $\gamma = 83.911(4)^\circ$, $V = 2124.14(17)$ Å³, $Z = 2$, $R_{gt}(F) = 0.0421$, $wR_{ref}(F^2) = 0.1130$, $T = 293(2)$ K.

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Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.19 × 0.16 × 0.11 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.08 mm ^{−1}
Diffractometer, scan mode:	XtaLAB Pro, ω -scans
θ_{max} , completeness:	29.8°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	38875, 10654, 0.037
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 7535
$N(param)_{refined}$:	569
Programs:	CrysAlis ^{PRO} [1], WinGX and ORTEP [2], SHELX [3]

Source of materials

A mixture of $AgNO_3$ (0.170 g, 1 mmol) and 5-bimethylamino-1-naphthalene sulfonic acid (0.2513 g, 1 mmol) in 15 mL DMF/ acetonitrile (1:2, v/v) reacted for 30 minutes. The methyl alcohol containing 4,4'-bipyridine (0.078 g, 0.5 mmol) was put into the system. The solution was kept in the dark room at room temperature and the crystals were gained.

Experimental details

Data were collected by CrysAlis^{PRO} 1.171.39.7e [1], the structure was solved by SHELXT with WinGX [2], and refined by SHELXL [3]. Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

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

Atom	x	y	z	U_{iso}^*/U_{eq}
Ag1	0.79002(2)	1.04026(2)	0.62128(2)	0.05605(10)
Ag2	0.83622(2)	0.24623(3)	0.72862(2)	0.06733(11)
S1	0.79547(6)	0.37138(6)	0.48145(6)	0.04434(18)
S2	0.79625(9)	0.89625(9)	0.87051(7)	0.0661(3)
N6	0.60047(18)	1.0426(2)	0.61480(18)	0.0390(5)
O1	0.7607(2)	0.2754(2)	0.53653(17)	0.0598(6)
N4	0.02536(19)	0.2518(2)	0.73251(19)	0.0476(6)
O2	0.7155(2)	0.46660(19)	0.48845(18)	0.0571(6)
N5	−0.02132(18)	1.03880(19)	0.60896(19)	0.0404(6)
O3	0.9171(2)	0.3874(2)	0.49641(18)	0.0621(7)
O2W	0.8385(3)	0.6256(2)	0.5555(2)	0.0680(7)
H2A	0.907203	0.604681	0.538680	0.102*
H2B	0.794063	0.584179	0.535974	0.102*
N3	0.6461(2)	0.2536(2)	0.7411(2)	0.0489(7)
C27	0.3551(2)	1.0372(2)	0.60702(19)	0.0326(5)
C30	0.2252(2)	1.0365(2)	0.60504(19)	0.0328(5)
C40	0.2693(2)	0.2622(2)	0.7463(2)	0.0371(6)
O1W	0.8122(4)	0.8046(3)	0.6482(3)	0.0921(10)
H1A	0.800632	0.797409	0.704920	0.138*
H1B	0.782242	0.752279	0.631418	0.138*
C25	0.5316(2)	1.1200(2)	0.5649(2)	0.0447(7)
H30	0.566365	1.176819	0.532179	0.054*
O6	0.7117(3)	0.9213(3)	0.9378(2)	0.0901(10)
O5	0.7650(3)	0.8095(3)	0.8248(2)	0.0909(10)
O4	0.8226(3)	0.9903(3)	0.8091(2)	0.0854(9)
C37	0.3997(2)	0.2625(2)	0.7491(2)	0.0375(6)
N2	1.1705(3)	0.5878(2)	1.1514(2)	0.0552(7)
C41	0.1993(2)	0.3325(3)	0.6826(2)	0.0490(8)
H39	0.232927	0.384698	0.643013	0.059*
C31	0.1515(2)	1.1192(2)	0.5578(2)	0.0439(7)
H28	0.183228	1.176505	0.523084	0.053*
C6	0.6773(2)	0.3403(2)	0.3246(2)	0.0389(6)
C2	0.8912(3)	0.3319(2)	0.3222(2)	0.0447(7)
H9	0.962181	0.336434	0.351112	0.054*
C1	0.7870(2)	0.3477(2)	0.3666(2)	0.0399(6)
C26	0.4103(2)	1.1207(3)	0.5590(2)	0.0471(8)
H29	0.365772	1.177101	0.522919	0.056*
C18	0.9419(3)	0.7467(3)	0.9907(2)	0.0424(7)
C28	0.4284(2)	0.9561(2)	0.6579(2)	0.0482(8)
H32	0.396471	0.897427	0.690383	0.058*
C16	1.1351(3)	0.7907(3)	1.0359(2)	0.0442(7)
H24	1.203230	0.773500	1.071564	0.053*
C3	0.8913(3)	0.3091(2)	0.2335(2)	0.0455(7)
H8	0.962674	0.298488	0.204126	0.055*
C17	1.0493(3)	0.7165(2)	1.0415(2)	0.0396(6)
C8	0.4649(3)	0.3460(3)	0.3218(3)	0.0536(8)
H11	0.392777	0.356639	0.350047	0.064*
C44	0.0922(3)	0.1875(3)	0.7955(3)	0.0539(9)
H33	0.055723	0.137862	0.835634	0.065*
C29	0.5485(2)	0.9615(3)	0.6607(3)	0.0522(8)
H31	0.595459	0.906204	0.696216	0.063*
C32	0.0307(2)	1.1177(3)	0.5616(2)	0.0468(7)
H27	−0.016784	1.175093	0.529242	0.056*
C38	0.4721(2)	0.1829(3)	0.8021(2)	0.0489(8)
H35	0.439296	0.130638	0.842140	0.059*
C5	0.6788(2)	0.3169(2)	0.2343(2)	0.0431(7)
C4	0.7885(3)	0.3022(3)	0.1896(2)	0.0464(7)
H7	0.789939	0.287974	0.130491	0.056*
C13	0.9302(3)	0.8468(3)	0.9322(2)	0.0457(7)

Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
C43	0.2119(3)	0.1894(3)	0.8052(3)	0.0519(8)
H34	0.253967	0.142385	0.850873	0.062*
C39	0.5930(2)	0.1807(3)	0.7958(2)	0.0518(8)
H36	0.639753	0.125595	0.831657	0.062*
C15	1.1195(3)	0.8856(3)	0.9799(3)	0.0540(8)
H23	1.176733	0.933054	0.977220	0.065*
C14	1.0174(3)	0.9128(3)	0.9259(3)	0.0548(8)
H22	1.009154	0.976696	0.885315	0.066*
C36	0.4554(3)	0.3400(3)	0.6935(3)	0.0533(8)
H38	0.410544	0.396744	0.657951	0.064*
C42	0.0793(2)	0.3249(3)	0.6783(2)	0.0539(9)
H40	0.034017	0.373142	0.635380	0.065*
N1	0.5778(3)	0.2789(3)	0.1002(2)	0.0673(9)
C9	0.4666(3)	0.3218(3)	0.2340(3)	0.0561(9)
H12	0.395756	0.315859	0.205489	0.067*
C7	0.5661(3)	0.3546(3)	0.3676(2)	0.0473(7)
H10	0.562513	0.369723	0.426508	0.057*
C22	1.0633(3)	0.6159(3)	1.1010(2)	0.0484(7)
C19	0.8508(3)	0.6780(3)	1.0052(3)	0.0595(9)
H21	0.780038	0.696622	0.972934	0.071*
C21	0.9712(4)	0.5552(3)	1.1120(3)	0.0641(10)
H19	0.979535	0.491034	1.152292	0.077*
C35	0.5773(3)	0.3331(3)	0.6911(3)	0.0565(9)
H37	0.612764	0.385698	0.653251	0.068*
C33	0.1704(3)	0.9538(3)	0.6530(3)	0.0675(12)
H26	0.215816	0.894667	0.684924	0.081*
C10	0.5707(3)	0.3067(3)	0.1889(2)	0.0521(8)
C34	0.0484(3)	0.9578(3)	0.6541(3)	0.0684(12)
H25	0.014117	0.901308	0.687856	0.082*
C20	0.8655(4)	0.5863(4)	1.0651(3)	0.0719(11)
H20	0.803981	0.543355	1.075001	0.086*
C24	1.1679(4)	0.5010(4)	1.2285(3)	0.0786(13)
H18	1.103494	0.518011	1.267112	0.118*
H16	1.240820	0.492862	1.262135	0.118*
H17	1.157810	0.435227	1.206843	0.118*
C23	1.2755(4)	0.5656(4)	1.0976(3)	0.0690(10)
H14	1.277095	0.494844	1.082199	0.104*
H15	1.345064	0.570003	1.132261	0.104*
H13	1.273064	0.617307	1.043207	0.104*
C11	0.4805(4)	0.3255(6)	0.0396(3)	0.107(2)
H2	0.410393	0.293208	0.059132	0.161*
H3	0.498915	0.312746	−0.020759	0.161*
H1	0.467707	0.401343	0.040137	0.161*
C12	0.5961(5)	0.1627(5)	0.1003(4)	0.0922(16)
H6	0.661990	0.132095	0.139041	0.138*
H5	0.611723	0.149176	0.039749	0.138*
H4	0.526522	0.130952	0.121972	0.138*

Comment

As is depicted in the left part of figure, the silver(I) atoms have different coordinating environments. The Ag1 is four-coordinated by two nitrogen atoms from two 4,4'-bipyridine (bpy), two oxygen atoms from water molecule and 5-bimethylamino-1-naphthalene sulfonic acid (bttS) separately. The Ag2 is also four-coordinated by three nitrogen atoms and one oxygen atom. And two nitrogen atoms from

bpy ligands, one nitrogen atom from bttS ligand. The one oxygen atom from bttS ligand. The bond lengths and angles are similar to other coordinated polymers [4–7]. After calculating, there is not $\pi \cdots \pi$ interaction. Lastly, the existence of weak intramolecular interaction such as $CH \cdots O$ make it become a three-dimensional structure (*cf.* right part of the figure). (symmetry codes: $A = 2 - x, 1 - y, 2 - z$; $B = 1 + x, y, z$).

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