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Crystal structure of poly[(5-bimethylamino-1-naphthalenesulfonato- κO)-(μ_3 -hexamethylenetetramino- $\kappa^3 N:N':N''$)silver(I)] dihydrate, $C_{36}H_{52}Ag_2N_{10}O_8S_2$

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Abstract

$C_{36}H_{52}Ag_2N_{10}O_8S_2$, orthorhombic, $Pna2_1$ (no. 33), $a = 11.7911(16)$ Å, $b = 31.310(5)$ Å, $c = 10.6883(11)$ Å, $V = 3945.9(9)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0353$, $wR_{ref}(F^2) = 0.0784$, $T = 293(2)$ 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.

Experimental details

Data of a single crystal were collected via CrysAlis^{PRO} at 293 K [1], structure was solved by SHELXT [2] within WinGX [3], refined by SHELXL [4] and the graphics were finished using Diamond [5].

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.24 × 0.20 × 0.17 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.16 mm ^{−1}
Diffractometer, scan mode:	XtaLAB Pro, ω
θ_{max} , completeness:	25.0°, 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	18516, 6557, 0.039
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 5756
$N(param)_{refined}$:	533
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 4], WinGX/ORTEP [3], Diamond [5]

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

Atom	x	y	z	U_{iso}^*/U_{eq}
C1	0.8936(7)	0.4023(2)	0.0835(8)	0.0415(19)
C2	0.8990(6)	0.4128(2)	0.2067(11)	0.0465(17)
H38	0.8457(40)	0.4017(85)	0.2621(10)	0.056*
C3	0.9831(9)	0.4399(3)	0.2508(8)	0.058(2)
H37	0.9868(86)	0.4459(76)	0.3358(82)	0.070*
C4	1.0592(8)	0.4575(3)	0.1725(7)	0.050(2)
H39	1.1168(04)	0.4746(31)	0.2043(36)	0.060*
C5	1.0526(7)	0.4502(2)	0.0426(7)	0.0393(17)
C6	0.9702(7)	0.4210(2)	−0.0026(7)	0.0354(17)
C7	0.9696(7)	0.4119(3)	−0.1325(8)	0.0443(19)
H42	0.9138(67)	0.3943(10)	−0.1660(44)	0.053*
C8	1.0498(8)	0.4289(3)	−0.2076(8)	0.051(2)
H41	1.0512(21)	0.4210(78)	−0.2915(39)	0.062*

Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
C9	1.1310(8)	0.4577(3)	−0.1633(8)	0.047(2)
H40	1.185798	0.468418	−0.217418	0.056*
C10	1.1301(7)	0.4702(3)	−0.0417(7)	0.0421(18)
C11	1.1556(9)	0.5395(3)	0.0584(10)	0.063(3)
H43	1.207404	0.551422	0.118141	0.094*
H44	1.085629	0.532378	0.099338	0.094*
H45	1.141293	0.559914	−0.006658	0.094*
C12	1.3028(8)	0.5111(4)	−0.0746(11)	0.071(3)
H46	1.354808	0.528794	−0.028804	0.107*
H47	1.277862	0.526045	−0.148145	0.107*
H48	1.340031	0.485131	−0.098709	0.107*
C13	0.3356(6)	0.4125(2)	0.5543(7)	0.0355(16)
C14	0.2435(7)	0.4306(3)	0.4986(7)	0.045(2)
H25	0.190922	0.413560	0.457188	0.054*
C15	0.2279(7)	0.4749(3)	0.5036(8)	0.046(2)
H26	0.164019	0.487371	0.467816	0.055*
C16	0.3071(7)	0.4996(3)	0.5614(8)	0.043(2)
H27	0.295899	0.528957	0.565273	0.052*
C17	0.4054(6)	0.4821(2)	0.6155(7)	0.0354(17)
C18	0.4193(7)	0.4372(2)	0.6165(7)	0.0362(17)
C19	0.5138(7)	0.4203(3)	0.6798(7)	0.045(2)
H28	0.526294	0.390931	0.678218	0.054*
C20	0.5867(7)	0.4456(3)	0.7427(8)	0.053(2)
H29	0.645907	0.433435	0.787839	0.064*
C21	0.5739(8)	0.4897(3)	0.7407(7)	0.052(2)
H30	0.625553	0.506725	0.783460	0.062*
C22	0.4878(7)	0.5082(3)	0.6776(7)	0.0417(19)
C23	0.5012(9)	0.5709(3)	0.5515(9)	0.062(3)
H31	0.465039	0.554803	0.486237	0.093*
H32	0.581974	0.569934	0.540153	0.093*
H33	0.475911	0.599999	0.548201	0.093*
C24	0.5280(12)	0.5769(4)	0.7693(9)	0.080(4)
H34	0.504867	0.566309	0.849631	0.120*
H35	0.507474	0.606444	0.761987	0.120*
H36	0.608703	0.573987	0.760832	0.120*
C25	0.4003(8)	0.1671(3)	0.4466(8)	0.0372(19)
H3	0.327391	0.161023	0.408570	0.045*
H4	0.456171	0.148599	0.407727	0.045*
C26	0.5401(6)	0.2209(2)	0.4833(5)	0.0262(14)
H7	0.559923	0.250701	0.470690	0.031*
H8	0.598628	0.203617	0.444756	0.031*
C27	0.3429(6)	0.2386(2)	0.4824(6)	0.0278(15)
H11	0.270158	0.232898	0.443339	0.033*
H12	0.360556	0.268518	0.469921	0.033*
C28	0.5038(6)	0.1668(2)	0.6351(7)	0.0350(17)
H5	0.561294	0.148535	0.598192	0.042*
H6	0.499867	0.160291	0.723728	0.042*
C29	0.3078(6)	0.1841(2)	0.6337(7)	0.0380(17)
H1	0.301868	0.177479	0.722126	0.046*
H2	0.235133	0.177915	0.595032	0.046*
C30	0.4473(5)	0.2383(2)	0.6726(6)	0.0260(15)
H9	0.466120	0.268136	0.660039	0.031*
H10	0.444066	0.233154	0.762039	0.031*
C31	0.2515(8)	0.3406(2)	0.9520(8)	0.0325(17)
H13	0.322858	0.348404	0.913132	0.039*
H14	0.192332	0.358291	0.916141	0.039*
C32	0.3193(6)	0.2697(2)	0.9818(6)	0.0263(14)

Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
H17	0.306279	0.239662	0.965005	0.032*
H18	0.390800	0.277663	0.943303	0.032*
C33	0.2151(5)	0.2654(2)	1.1742(6)	0.0280(15)
H23	0.199399	0.235403	1.159200	0.034*
H24	0.218624	0.269715	1.263977	0.034*
C34	0.1511(6)	0.3364(2)	1.1435(6)	0.0310(15)
H21	0.091452	0.354331	1.109545	0.037*
H22	0.155158	0.341669	1.232861	0.037*
C35	0.3479(6)	0.3222(2)	1.1403(6)	0.0317(16)
H15	0.352379	0.327438	1.229589	0.038*
H16	0.419943	0.330136	1.103266	0.038*
C36	0.1182(6)	0.2841(2)	0.9859(6)	0.0262(14)
H19	0.057998	0.301234	0.949773	0.031*
H20	0.100949	0.254293	0.969724	0.031*
Ag1	0.21235(4)	0.27894(2)	0.71427(6)	0.03515(13)
Ag2	−0.04739(4)	0.27043(2)	1.21066(6)	0.05288(19)
N1	1.2047(6)	0.5011(2)	0.0043(7)	0.0514(18)
N2	0.4723(7)	0.5526(2)	0.6719(6)	0.0508(19)
N3	0.3945(5)	0.1575(2)	0.5775(6)	0.0376(15)
N4	0.4309(5)	0.21218(19)	0.4216(5)	0.0279(12)
N5	0.5370(5)	0.21191(18)	0.6186(5)	0.0249(12)
N6	0.3346(5)	0.22975(18)	0.6179(5)	0.0272(12)
N7	0.2267(5)	0.29519(18)	0.9258(5)	0.0257(12)
N8	0.2581(5)	0.34818(18)	1.0866(5)	0.0329(14)
N9	0.1220(5)	0.29132(18)	1.1221(5)	0.0271(12)
N10	0.3266(4)	0.27648(18)	1.1181(5)	0.0241(12)
O1	0.8779(6)	0.3269(2)	0.0005(11)	0.092(3)
O2	0.7288(5)	0.3744(2)	−0.0579(7)	0.0673(18)
O1W	0.5611(8)	0.3159(2)	−0.1566(9)	0.085(2)
H1A	0.514823	0.334154	−0.186478	0.128*
H1B	0.604771	0.330523	−0.109906	0.128*
O3	0.7408(7)	0.3478(3)	0.1495(7)	0.091(3)
O2W	0.5953(7)	0.3075(2)	0.3213(8)	0.074(2)
H2A	0.644400	0.326127	0.300748	0.111*
H2B	0.535562	0.321851	0.336104	0.111*
O4	0.4576(6)	0.34722(19)	0.4915(6)	0.0614(18)
O5	0.2535(7)	0.3422(2)	0.4683(8)	0.065(2)
O6	0.3418(6)	0.34098(18)	0.6726(5)	0.0630(19)
S1	0.80208(17)	0.35937(6)	0.0399(2)	0.0470(5)
S2	0.34806(19)	0.35643(6)	0.5454(2)	0.0445(5)

Experimental detail

Hydrogen atoms of the organic ligands are positioned using a riding model [4]. The coordinates of the hydrogen atoms of the water molecules are refined freely. U_{iso} parameters of all hydrogen atoms are constrained depending of the attached parent atoms.

Comment

As is depicted in the left part of the figure, the Ag1 is four-coordinated by three nitrogen atoms and one oxygen atom. And three nitrogen atoms come from three hexamethylenetetramine ligands, one oxygen atom comes

from 5-bimethylamino-1-naphthalenesulfonate. The bond distances of Ag—O and Ag—N are in the normal ranges. Additionally, there are two free water molecules. Most importantly, the weak interaction $CH \cdots O$ also plays an important role in forming a 3D structure [6–8] (*cf.* right part of the figure). (symmetry codes: $A = -1/2 + x, 1/2 - y, z$).

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