Crystal structure of *catena*-poly[(dimethyl(2-hydroxyethyl)ammonium)-{sodium- μ -[aquatris(dimethyl(2-hydroxyethyl)ammonium)-sodiumheptamolybdate(VI)- O' , O'' , O''' : O'''' , O''''' , O'''''']}diwater], $\{(\text{C}_4\text{H}_{12}\text{NO})[(\text{C}_4\text{H}_{12}\text{NO})_3(\text{H}_2\text{O})\text{Na}_2\text{Mo}_7\text{O}_{24}] \cdot 2\text{H}_2\text{O}\}_n$

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Table 1. Data collection and handling.

Crystal:	colourless, irregular, size $0.2 \times 0.2 \times 0.3$ mm
Wavelength:	Mo K_{α} radiation (0.71073 Å)
μ :	20.99 cm^{-1}
Diffraction, scan mode:	Nicolet P3F, ω
$2\theta_{\text{max}}$:	50°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	4148, 4148
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3420
$N(\text{param})_{\text{refined}}$:	525
Programs:	SHELXS-97 [2], SHELXL-97 [3], SHELXTL/PC [4]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{iso}
H(25A)	4a	-0.1577	0.3638	0.8422	0.059
H(11A)	4a	-0.2070	0.3437	0.9490	0.067
H(11B)	4a	-0.3042	0.3718	0.9239	0.067
H(12A)	4a	-0.2526	0.5079	0.9049	0.197
H(12B)	4a	-0.2285	0.4827	0.9878	0.197
H(11C)	4a	-0.1117	0.4742	0.8717	0.052
C(13)	4a	-0.101(3)	0.571(2)	0.931(2)	0.17(2)
H(13B)	4a	-0.0380	0.5785	0.9193	0.248
H(13C)	4a	-0.1116	0.5860	0.9821	0.248
H(13D)	4a	-0.1365	0.6041	0.8980	0.248
C(14)	4a	-0.0515(9)	0.4534(8)	0.9667(9)	0.22(2)
H(14B)	4a	0.0058	0.4700	0.9468	0.324
H(14C)	4a	-0.0555	0.3945	0.9664	0.324
H(14D)	4a	-0.0576	0.4731	1.0174	0.324
H(26A)	4a	-0.2917	0.5968	0.6844	0.121
H(21A)	4a	-0.1296	0.6276	0.7277	0.090
H(21B)	4a	-0.2025	0.6948	0.7464	0.090
H(22B)	4a	-0.1948	0.6296	0.5973	0.089
H(22C)	4a	-0.2375	0.7143	0.6210	0.089
H(21C)	4a	-0.0577	0.6787	0.6162	0.067
H(23B)	4a	-0.0151	0.8058	0.6549	0.129
H(23C)	4a	-0.0672	0.7605	0.7195	0.129
H(23D)	4a	-0.1163	0.8271	0.6706	0.129
H(24B)	4a	-0.0450	0.7799	0.5281	0.106
H(24C)	4a	-0.1494	0.7926	0.5334	0.106
H(24D)	4a	-0.1105	0.7099	0.5020	0.106
H(27A)	4a	-0.1036	0.3257	0.7166	0.081
H(31A)	4a	-0.2286	0.2449	0.6508	0.052
H(31B)	4a	-0.1575	0.2149	0.7100	0.052
H(32A)	4a	-0.0504	0.2006	0.6223	0.049
H(32B)	4a	-0.1364	0.1582	0.5897	0.049
H(31C)	4a	-0.0619	0.3016	0.5428	0.048
H(33A)	4a	-0.0127	0.1856	0.4865	0.092
H(33B)	4a	-0.0568	0.2464	0.4288	0.092

Abstract

$\text{C}_{16}\text{H}_{54}\text{Mo}_7\text{N}_4\text{Na}_2\text{O}_{31}$, orthorhombic, $P2_12_12_1$ (No. 19), $a = 14.857(3)$ Å, $b = 16.266(3)$ Å, $c = 17.769(3)$ Å, $V = 4294.1$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.049$, $wR_{\text{ref}}(F^2) = 0.121$, $T = 293$ K.

Source of material

The compound was obtained with the reaction of 2-dimethylaminoethanol, ammoniumheptamolybdate tetrahydrate and sodium hydroxide in methanol solution in an open vessel during several weeks.

Discussion

Each molybdenum atom is surrounded by six oxygen atoms [1] as well as the bridging sodium atom, which joins heptamolybdate groups as a linear polymer chain along the c -axis direction. The other sodium atom with three dimethyl(2-hydroxyethyl)ammonium ligands and one water molecule fulfills its coordination sphere with two oxygen atoms from the heptamolybdate group. The nitrogen atoms of the coordinated ammonium cations make hydrogen bonds, as donors, with suitable oxygen atoms of the molybdate group.

The free ammonium cation is hydrogen bonded using its nitrogen atom as a donor. All water molecules are also H-bonded. The overall hydrogen bonding network is therefore three-dimensional.

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Table 2. Continued.

Atom	Site	x	y	z	U_{iso}
H(33C)	4a	-0.1112	0.1703	0.4582	0.092
H(34A)	4a	-0.2105	0.3335	0.5499	0.070
H(34B)	4a	-0.2304	0.2593	0.4961	0.070
H(34C)	4a	-0.1757	0.3352	0.4667	0.070
H(28A)	4a	0.0828	0.8563	0.1952	0.085
H(41A)	4a	0.1273	0.7439	0.2787	0.069
H(41B)	4a	0.1245	0.7071	0.1975	0.069
H(42A)	4a	-0.0069	0.6762	0.2334	0.079
H(42B)	4a	-0.0274	0.7613	0.1961	0.079
H(41C)	4a	-0.0180	0.7307	0.3490	0.062
H(43A)	4a	-0.1655	0.7702	0.3481	0.147

Table 2. Continued.

Atom	Site	x	y	z	U_{iso}
H(43B)	4a	-0.1470	0.6961	0.2939	0.147
H(43C)	4a	-0.1562	0.7853	0.2613	0.147
H(44A)	4a	-0.0365	0.8599	0.3802	0.200
H(44B)	4a	-0.0272	0.8839	0.2952	0.200
H(44C)	4a	0.0552	0.8465	0.3383	0.200
H(11)	4a	-0.6481	0.5042	0.4805	0.103
H(12)	4a	-0.7099	0.4775	0.5271	0.103
H(21)	4a	-0.5301	0.4571	0.6737	0.097
H(22)	4a	-0.5712	0.4786	0.6118	0.097
H(31)	4a	-0.3122	0.4118	0.5953	0.110
H(32)	4a	-0.3967	0.4179	0.6240	0.110

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mo(1)	4a	-0.01376(7)	0.50160(6)	0.53857(6)	0.0265(5)	0.0145(5)	0.0253(5)	0.0005(4)	-0.0003(4)	-0.0003(4)
Mo(2)	4a	0.02689(7)	0.48653(7)	0.72588(6)	0.0368(6)	0.0232(6)	0.0247(6)	-0.0026(5)	0.0048(5)	0.0004(5)
Mo(3)	4a	0.00104(7)	0.51864(7)	0.34969(6)	0.0359(6)	0.0222(6)	0.0242(6)	0.0001(5)	-0.0051(5)	-0.0004(5)
Mo(4)	4a	0.13363(8)	0.36278(6)	0.61601(6)	0.0331(6)	0.0178(5)	0.0294(6)	0.0035(5)	-0.0014(5)	0.0018(5)
Mo(5)	4a	0.12487(8)	0.38219(7)	0.43137(6)	0.0322(6)	0.0181(5)	0.0269(6)	0.0038(5)	0.0001(5)	-0.0034(5)
Mo(6)	4a	0.14035(8)	0.61915(7)	0.63343(6)	0.0359(6)	0.0188(5)	0.0265(6)	-0.0058(5)	0.0006(5)	-0.0019(5)
Mo(7)	4a	0.12605(8)	0.63767(6)	0.45059(6)	0.0350(6)	0.0172(5)	0.0251(5)	-0.0022(5)	-0.0004(5)	0.0020(5)
Na(1)	4a	0.2626(4)	0.4791(4)	0.7799(3)	0.050(3)	0.034(3)	0.044(4)	0.000(3)	-0.005(3)	-0.002(3)
Na(2)	4a	-0.2292(6)	0.4456(4)	0.7165(4)	0.090(5)	0.034(3)	0.069(5)	0.005(4)	-0.024(5)	0.000(3)
O(1)	4a	0.0995(5)	0.4917(5)	0.6217(5)	0.024(4)	0.021(5)	0.031(5)	-0.001(4)	-0.007(4)	0.002(4)
O(2)	4a	0.0894(6)	0.5100(6)	0.4470(5)	0.037(5)	0.027(5)	0.027(5)	0.009(4)	0.003(4)	0.003(5)
O(3)	4a	0.0233(7)	0.3894(6)	0.5287(5)	0.043(6)	0.028(5)	0.018(5)	-0.007(4)	0.008(4)	0.001(4)
O(4)	4a	0.0283(7)	0.6113(6)	0.5467(5)	0.036(5)	0.026(5)	0.031(5)	0.007(4)	-0.003(4)	0.001(4)
O(5)	4a	-0.0813(6)	0.4974(6)	0.6175(5)	0.038(5)	0.025(5)	0.034(5)	0.005(5)	0.006(4)	0.004(5)
O(6)	4a	-0.0881(6)	0.5091(5)	0.4626(5)	0.038(5)	0.023(5)	0.036(5)	-0.001(4)	-0.014(4)	0.004(5)
O(7)	4a	0.0321(6)	0.3767(5)	0.6876(5)	0.038(5)	0.016(4)	0.039(6)	-0.003(4)	0.009(4)	0.009(4)
O(8)	4a	0.0381(7)	0.6011(6)	0.7026(5)	0.039(5)	0.029(5)	0.024(5)	-0.006(4)	0.003(4)	-0.009(4)
O(9)	4a	-0.0772(6)	0.4831(6)	0.7713(5)	0.041(5)	0.043(6)	0.030(5)	-0.012(5)	0.005(4)	-0.014(5)
O(10)	4a	0.1067(6)	0.4797(7)	0.7952(5)	0.050(6)	0.045(6)	0.025(5)	-0.017(5)	-0.010(4)	0.004(5)
O(11)	4a	0.0153(7)	0.4028(6)	0.3696(5)	0.040(6)	0.026(5)	0.034(6)	-0.007(4)	-0.001(4)	-0.011(4)
O(12)	4a	0.0129(6)	0.6292(5)	0.3871(5)	0.042(6)	0.021(5)	0.026(5)	0.010(4)	0.005(4)	0.005(4)
O(13)	4a	-0.1021(6)	0.5230(6)	0.3072(6)	0.036(5)	0.034(5)	0.043(6)	0.008(5)	-0.020(4)	-0.008(5)
O(14)	4a	0.0773(7)	0.5261(6)	0.2771(6)	0.052(6)	0.031(5)	0.031(5)	0.006(5)	0.005(5)	0.006(5)
O(15)	4a	0.1954(7)	0.3865(5)	0.5223(5)	0.041(6)	0.019(5)	0.036(6)	0.005(4)	0.002(4)	0.002(4)
O(16)	4a	0.2217(7)	0.3721(7)	0.6766(5)	0.049(6)	0.040(6)	0.033(6)	0.001(5)	-0.020(5)	-0.001(5)
O(17)	4a	0.1168(8)	0.2593(6)	0.6038(6)	0.052(6)	0.019(5)	0.050(7)	-0.005(5)	0.001(6)	0.006(5)
O(18)	4a	0.1162(6)	0.2780(5)	0.4234(6)	0.034(5)	0.016(4)	0.044(6)	0.004(4)	0.001(5)	-0.004(4)
O(19)	4a	0.2072(7)	0.4100(6)	0.3689(5)	0.045(6)	0.033(5)	0.028(5)	-0.003(5)	0.005(4)	0.009(4)
O(20)	4a	0.1976(6)	0.6139(5)	0.5371(5)	0.030(5)	0.019(4)	0.032(5)	-0.009(4)	0.000(4)	0.003(4)
O(21)	4a	0.2292(7)	0.5923(6)	0.6901(6)	0.046(6)	0.032(6)	0.040(6)	-0.009(5)	-0.003(5)	0.004(5)
O(22)	4a	0.1300(7)	0.7238(5)	0.6407(5)	0.057(6)	0.014(4)	0.040(6)	-0.006(5)	-0.002(6)	-0.002(4)
O(23)	4a	0.1119(8)	0.7413(5)	0.4607(6)	0.061(7)	0.013(5)	0.053(7)	0.000(5)	-0.006(6)	0.007(5)
O(24)	4a	0.2068(7)	0.6270(6)	0.3825(6)	0.049(6)	0.031(6)	0.037(6)	-0.001(5)	0.012(5)	-0.003(5)
O(25)	4a	-0.2146(7)	0.3717(7)	0.8384(7)	0.035(5)	0.039(6)	0.074(8)	0.003(5)	0.021(6)	0.009(6)
C(11)	4a	-0.240(1)	0.381(1)	0.917(1)	0.06(1)	0.05(1)	0.06(1)	-0.010(9)	0.020(9)	-0.01(1)
C(12)	4a	-0.216(2)	0.472(2)	0.935(2)	0.15(3)	0.24(4)	0.10(2)	-0.10(3)	0.08(2)	-0.09(3)
N(11)	4a	-0.1231(8)	0.4876(8)	0.9205(7)	0.051(7)	0.041(7)	0.039(7)	-0.006(7)	-0.001(6)	-0.004(6)
O(26)	4a	-0.2539(9)	0.5871(8)	0.7209(9)	0.08(1)	0.056(8)	0.11(1)	0.029(7)	0.03(1)	0.023(9)
C(21)	4a	-0.188(1)	0.649(1)	0.714(1)	0.06(1)	0.05(1)	0.12(2)	0.013(9)	0.03(1)	0.01(1)
C(22)	4a	-0.188(1)	0.677(1)	0.630(1)	0.06(1)	0.04(1)	0.12(2)	-0.001(9)	-0.02(1)	-0.02(1)
N(21)	4a	-0.101(1)	0.7183(9)	0.6153(9)	0.050(8)	0.044(8)	0.07(1)	0.017(7)	-0.012(8)	-0.015(8)
C(23)	4a	-0.072(2)	0.784(1)	0.670(1)	0.09(2)	0.04(1)	0.13(2)	0.00(1)	-0.04(2)	-0.02(1)
C(24)	4a	-0.1015(7)	0.7533(6)	0.5378(6)	0.06(1)	0.07(1)	0.08(2)	-0.01(1)	0.02(1)	0.02(1)
O(27)	4a	-0.1424(7)	0.3300(6)	0.6804(6)	0.050(6)	0.042(6)	0.071(8)	-0.021(6)	-0.005(6)	-0.016(6)
C(31)	4a	-0.166(1)	0.2474(9)	0.6647(9)	0.054(9)	0.025(8)	0.05(1)	-0.016(7)	-0.013(8)	-0.004(7)
C(32)	4a	-0.111(1)	0.2109(9)	0.6031(8)	0.06(1)	0.029(8)	0.033(8)	-0.009(7)	0.002(7)	0.003(6)
N(31)	4a	-0.1026(9)	0.2610(7)	0.5336(7)	0.044(8)	0.025(6)	0.051(8)	-0.011(6)	0.011(6)	-0.011(6)
C(33)	4a	-0.068(1)	0.212(1)	0.472(1)	0.07(1)	0.05(1)	0.06(1)	-0.00(1)	0.03(1)	-0.00(1)
C(34)	4a	-0.187(1)	0.301(1)	0.510(1)	0.054(9)	0.037(9)	0.05(1)	-0.011(7)	-0.001(8)	0.007(8)

Table 3. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(28)	4a	0.1268(9)	0.8264(7)	0.1997(8)	0.072(8)	0.053(8)	0.09(1)	-0.005(7)	-0.016(8)	0.013(7)
C(41)	4a	0.100(1)	0.750(1)	0.229(1)	0.07(1)	0.05(1)	0.05(1)	0.011(9)	-0.01(1)	0.020(9)
C(42)	4a	0.004(2)	0.735(1)	0.238(1)	0.10(2)	0.04(1)	0.05(1)	0.01(1)	-0.01(1)	-0.006(9)
N(41)	4a	-0.037(1)	0.7657(7)	0.3122(8)	0.067(9)	0.023(6)	0.064(9)	0.003(6)	-0.009(8)	0.016(7)
C(43)	4a	-0.135(2)	0.753(2)	0.303(2)	0.07(2)	0.08(2)	0.14(3)	0.01(1)	-0.02(2)	-0.01(2)
C(44)	4a	-0.0091(7)	0.8454(7)	0.3331(7)	0.22(4)	0.05(1)	0.13(2)	0.00(2)	-0.08(3)	-0.02(2)
O(1W)	4a	-0.6577(7)	0.4992(7)	0.5276(7)	0.042(6)	0.066(9)	0.10(1)	-0.010(6)	-0.011(6)	0.004(8)
O(2W)	4a	-0.5215(9)	0.4578(8)	0.6261(6)	0.074(8)	0.077(9)	0.042(7)	0.008(7)	0.010(6)	-0.010(6)
O(3W)	4a	-0.3470(9)	0.3944(9)	0.6306(7)	0.058(7)	0.09(1)	0.08(1)	-0.003(7)	0.000(7)	0.005(8)

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