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Supporting information for article:

Synthesis, crystal structures and properties of the new compounds K7–*x*Ag1+*x*(*X*O4)4 (*X* = Mo, W)

Tatyana S. Spiridonova, Sergey F. Solodovnikov, Aleksandra A. Savina, Zoya A. Solodovnikova, Sergey Yu. Stefanovich, Bogdan I. Lazoryak, Iliya V. Korolkov and Elena G. Khaikina

S1. Computing details

For $K_{6.69}Ag_{1.31}(MoO_4)_4$, data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004); absorption correction: *SADABS* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2017* (Sheldrick, 2017); molecular graphics: *DIAMOND* (Brandenburg, 2008); software used to prepare material for publication: *SHELXL* (Sheldrick, 2008).

Table S1 The calculated and observed values of XRD data for $K_7Ag(WO_4)_4$

$2\theta_{obs}$ (°)	I/I_0	d_{obs} (Å)	h	k	l	$\Delta 2\theta$
8.173	2	10.81	1	0	0	–0.007
14.175	2	6.243	1	1	0	–0.008
14.421	5	6.137	1	0	1	–0.001
16.374	27	5.409	2	0	0	–0.001
20.269	100	4.378	2	0	1	–0.001
23.864	98	3.726	0	0	2	–0.003
24.67	1	3.606	3	0	0	–0.004
24.818	3	3.585	2	1	1	–0.003
25.257	29	3.523	1	0	2	+0.001
27.859	46	3.200	1	1	2	–0.002
28.563	81	3.123	2	2	0	–0.006
29.075	72	3.069	2	0	2	+0.001
32.144	3	2.7824	3	1	1	–0.013
32.482	17	2.7542	2	1	2	+0.000
33.097	6	2.7044	4	0	0	–0.004
34.586	8	2.5913	3	0	2	–0.001
35.274	7	2.5423	4	0	1	–0.002
36.167	1	2.4816	3	2	0	–0.007
37.104	10	2.4210	1	0	3	–0.002
37.545	29	2.3936	2	2	2	0.000
38.100	0.3	2.3600	4	1	0	–0.015
38.191	3	2.3546	3	2	1	–0.005
38.490	10	2.3370	3	1	2	–0.002
39.905	23	2.2573	2	0	3	–0.003
40.050	1	2.2495	4	1	1	–0.022
41.211	16	2.1887	4	0	2	–0.003
42.545	3	2.1231	2	1	3	+0.001
43.437	1	2.0816	3	3	0	–0.011
43.532	0.2	2.0773	5	0	1	–0.016
43.789	3	2.0657	3	2	2	–0.001
44.268	4	2.0444	4	2	0	–0.004
45.441	10	1.9943	4	1	2	+0.001

45.994	13	1.9716	4	2	1	–0.002
47.476	5	1.9135	3	1	3	0.000
48.381	0.4	1.8798	5	1	1	–0.013
48.622	3	1.8710	5	0	2	–0.004
48.845	5	1.8630	0	0	4	–0.002
49.613	5	1.8359	1	0	4	–0.003
49.800	7	1.8295	4	0	3	–0.002
50.149	4	1.8176	3	3	2	–0.001
50.584	14	1.8030	6	0	0	–0.006
50.902	11	1.7924	4	2	2	–0.001
51.117	22	1.7854	1	1	4	+0.001
51.309	0.5	1.7792	4	3	0	+0.017
51.861	1	1.7615	2	0	4	0.000
52.049	2	1.7556	3	2	3	–0.006
52.876	0.5	1.7301	4	3	1	+0.002
53.117	3	1.7228	5	1	2	–0.005
54.048	6	1.6953	2	1	4	–0.004
54.295	0.5	1.6882	5	2	1	+0.026
55.469	15	1.6552	3	0	4	–0.002
56.337	1	1.6317	5	0	3	+0.004
56.666	7	1.6230	6	0	2	–0.003
57.129	1	1.6110	6	1	1	+0.004
57.353	4	1.6052	4	3	2	+0.003
57.556	9	1.6000	2	2	4	0.000
58.240	3	1.5829	3	1	4	+0.002
58.414	8	1.5786	4	2	3	–0.003
58.722	3	1.5710	5	2	2	+0.003
59.120	10	1.5614	4	4	0	–0.008
59.790	0.5	1.5455	5	3	0	–0.004
60.272	1	1.5343	4	0	4	–0.002
60.448	1	1.5302	5	1	3	–0.013
61.200	0.3	1.5132	7	0	1	–0.007
61.408	1	1.5086	6	1	2	–0.001
61.792	1	1.5001	6	2	0	–0.009
62.261	1	1.4899	3	2	4	–0.004
62.896	6	1.4764	1	0	5	–0.005
63.167	6	1.4707	6	2	1	–0.003
63.561	11	1.4626	4	1	4	+0.001
64.381	0.2	1.4459	4	3	3	–0.013
64.667	5	1.4402	4	4	2	–0.001
64.841	2	1.4367	2	0	5	–0.009
65.300	1	1.4278	5	3	2	+0.007
65.661	0.3	1.4208	5	2	3	–0.011
66.134	1	1.4118	5	0	4	–0.005
66.744	4	1.4003	2	1	5	–0.001
67.213	4	1.3917	6	2	2	–0.002

67.396	4	1.3884	3	3	4	–0.002
67.548	0.3	1.3856	5	4	0	+0.021
68.020	1	1.3771	4	2	4	+0.001
68.175	1	1.3744	6	1	3	+0.001
68.870	0.4	1.3622	5	4	1	+0.017
69.448	1	1.3523	8	0	0	–0.006
69.894	1	1.3447	5	1	4	–0.005
70.098	0.2	1.3413	6	3	1	+0.030
70.329	2	1.3375	7	1	2	–0.002
70.490	4	1.3348	3	1	5	–0.004
70.746	2	1.3306	8	0	1	–0.002
71.886	1	1.3123	7	0	3	–0.001
72.319	1	1.3055	4	0	5	+0.006
72.574	0.3	1.3015	7	2	1	+0.006
72.756	0.5	1.2987	5	4	2	+0.020
72.949	2	1.2958	6	0	4	+0.004
73.556	1	1.2866	4	3	4	+0.004
73.709	3	1.2843	6	2	3	0.000
73.988	1	1.2801	6	3	2	+0.001
74.149	4	1.2777	3	2	5	–0.004
74.580	2	1.2714	8	0	2	+0.012
74.770	6	1.2686	5	2	4	–0.003
76.388	2	1.2458	7	2	2	+0.004
76.635	1	1.2423	0	0	6	+0.021
76.697	3	1.2415	6	4	0	+0.036
77.184	1	1.2349	6	1	4	–0.021
77.725	1	1.2276	5	0	5	+0.014
77.995	3	1.2241	6	4	1	–0.008
78.439	2	1.2182	1	1	6	+0.002
79.040	4	1.2105	2	0	6	–0.007
79.515	1	1.2044	4	2	5	+0.001
79.966	1	1.1988	8	1	2	–0.012
80.120	1	1.1968	4	4	4	+0.005
80.715	1	1.1895	7	0	4	–0.001
80.795	1	1.1885	2	1	6	+0.008
80.835	2	1.1881	8	0	3	+0.025
81.121	0.5	1.1846	5	5	2	+0.011
81.266	1	1.1828	5	1	5	+0.018
81.462	5	1.1805	8	2	0	+0.004
81.715	2	1.1775	6	4	2	+0.004
81.960	1	1.1746	3	0	6	+0.018
82.499	0.2	1.1683	6	2	4	–0.023
83.474	0.3	1.1571	7	3	2	+0.002
83.737	8	1.1541	2	2	6	–0.002
84.323	1	1.1476	3	1	6	–0.004
84.654	1	1.1439	9	0	2	–0.010

84.804	1	1.1423	4	3	5	–0.009
85.402	2	1.1358	7	1	4	–0.005
86.071	2	1.1287	4	0	6	–0.003
86.394	3	1.1253	8	2	2	–0.001
86.768	0.2	1.1214	6	5	1	+0.019
87.869	2	1.1102	6	4	3	0.000
88.298	1	1.1059	6	1	5	–0.010
88.894	2	1.1000	6	3	4	–0.007
88.992	1	1.0991	4	1	6	–0.017
89.445	0.2	1.0947	8	0	4	+0.023
90.457	1	1.0850	6	5	2	+0.004
90.795	0.3	1.0819	10	0	0	–0.003
91.199	1	1.0781	7	2	4	+0.012
91.282	1	1.0774	5	0	6	+0.017
91.631	1	1.0742	7	4	2	–0.008
91.776	2	1.0728	5	3	5	–0.003
92.013	1	1.0707	10	0	1	+0.004
92.486	0.4	1.0665	3	3	6	–0.025
93.030	2	1.0616	4	2	6	+0.013
93.273	1	1.0595	1	0	7	+0.001
93.510	0.4	1.0575	6	2	5	+0.008
93.795	0.2	1.0550	9	2	1	–0.033
94.674	1	1.0475	8	1	4	+0.027
94.771	1	1.0467	5	1	6	+0.018
95.016	2	1.0446	2	0	7	+0.006
95.442	2	1.0411	6	6	0	+0.005
95.701	0.5	1.0390	10	0	2	–0.003
95.849	0.4	1.0377	5	5	4	+0.019
96.483	0.2	1.0326	6	4	4	–0.031
96.620	0.2	1.0315	6	5	3	–0.023
96.785	1	1.0302	2	1	7	–0.012
97.709	3	1.0229	6	0	6	+0.002
98.221	1	1.0189	7	3	4	–0.012
98.771	1	1.0147	5	4	5	+0.007

Table S2 Atomic coordinates and equivalent isotropic displacement parameters for $K_{6.68}Ag_{1.32}(MoO_4)_4$ and $K_7Ag(WO_4)_4$

Atom	***x/a***	***y/b***	***z/c***	U_{eq} (Å^2)
$K_{6.68}Ag_{1.32}(MoO_4)_4$				
Mo(1)	0.33333	0.66667	0.2815(3)	0.01895(17)
Mo(2)	0.33981(4)	0.16990(2)	0.1711(3)	0.01329(9)
K(1)	0	0	0	0.0188(4)
K(2)	0.17108(6)	0.34216(13)	0.1756(4)	0.0251(2)
K(3)*	0.5161(4)	0.4839(4)	0.3916(8)	0.0254(6)
Ag(1)	0.66667	0.33333	0.3296(3)	0.0274(2)
Ag(2)**	0.5074(12)	0.4926(12)	0.428(4)	0.055(8)
O(1)	0.33333	0.66667	0.522(2)	0.079(5)
O(2)	0.4100(2)	0.5900(2)	0.2003(8)	0.0345(11)
O(3)	0.3559(4)	0.2931(4)	0.0376(7)	0.0450(9)
O(4)	0.1885(4)	0.0943(2)	0.2621(7)	0.0339(10)
O(5)	0.4512(4)	0.22559(18)	0.3471(7)	0.0308(9)
$K_7Ag(WO_4)_4$				
W(1)	0.3333	0.6667	0.2858(12)	0.0330(8)
W(2)	0.33899(19)	0.16950(10)	0.1731(12)	0.0272(4)
K(1)	0	0	–0.0049(14)	0.0424(14)
K(2)	0.1702(4)	0.3404(9)	0.1865(2)	0.0424(14)
K(3)	0.5143(4)	0.4857(4)	0.4068(14)	0.0424(14)
Ag(1)	0.6667	0.3333	0.3319(13)	0.0385(15)
O(1)	0.3333	0.6667	0.516(4)	0.070(4)
O(2)	0.4098(1)	0.5902(1)	0.2008(2)	0.070(4)
O(3)	0.3564(11)	0.3036(12)	0.0549(2)	0.070(4)
O(4)	0.1915(17)	0.0958(8)	0.2723(2)	0.020(5)
O(5)	0.4508(1)	0.2254(1)	0.3481(1)	0.059(7)

* Site occupation factor is 0.894(5).

** Site occupation factor is 0.106(5).