Supporting Information

Electronic structure of β-$RbSm(MoO_4)_2$ and chemical bonding in molybdates

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Structural cif file

Table 1S. Fractional atomic coordinates and isotropic displacement parameters (Å^2) of β-$RbSm(MoO_4)_2$

	x	*y*	*z*	B_{iso}
Rb	0.5	0.2721 (3)	0.25	1.2 (3)
Sm	0	0.00564 (19)	0.25	2.0 (2)
Mo	0.5163 (9)	0.09785 (14)	0.9848 (4)	1.0 (2)
O1	0.703 (4)	0.0909 (16)	0.141 (3)	1.5 (4)
O2	0.726 (4)	0.0879 (14)	0.823 (3)	1.5 (4)
O3	0.304 (4)	0.0248 (11)	0.025 (4)	1.5 (4)
O4	0.413 (4)	0.1770 (11)	0.976 (2)	1.5 (4)

Table 2S. Main bond lengths (Å) of β-$RbSm(MoO_4)_2$

Rb—O2^{i}	3.06 (3)	Sm—O3^{vi}	2.76 (3)
Rb—O4^{ii}	2.88 (2)	Mo—O1^{vii}	1.58 (2)
Rb—O4^{iii}	2.95 (2)	Mo—O2	1.70 (2)
Sm—O1^{iv}	2.38 (3)	Mo—O3^{vii}	1.79 (2)
Sm—O2^{v}	2.34 (2)	Mo—O4	1.59 (2)
Sm—O3	2.41 (3)		

Symmetry codes: (i) -*x*+3/2, -*y*+1/2, *z*-1/2; (ii) *x*, *y*, *z*-1; (iii) -*x*+1/2, -*y*+1/2, *z*-1/2; (iv) *x*-1, *y*, *z*; (v) -*x*+1, -*y*, -*z*+1; (vi) -*x*, -*y*, -*z*; (vii) *x*, *y*, *z*+1.

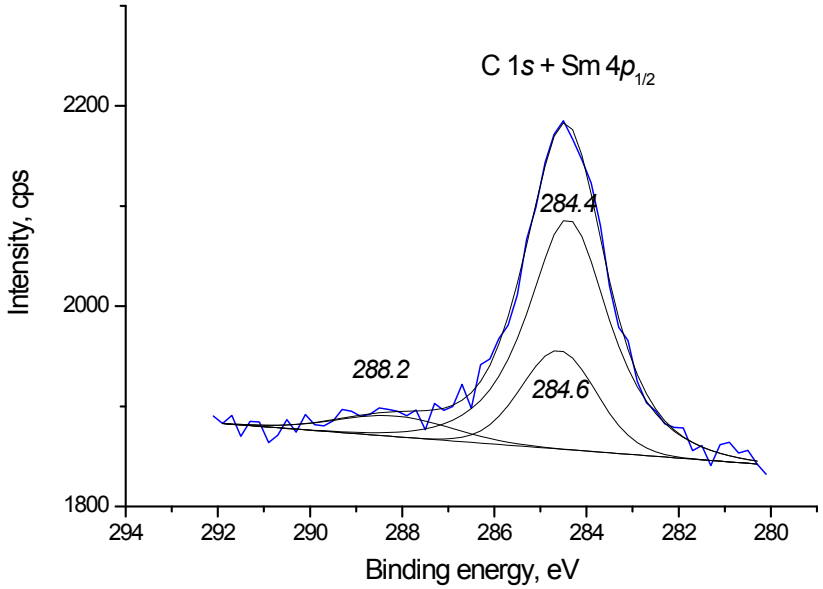

Fig. 1S. Superposition of C 1s and Sm $4p_{1/2}$ lines.

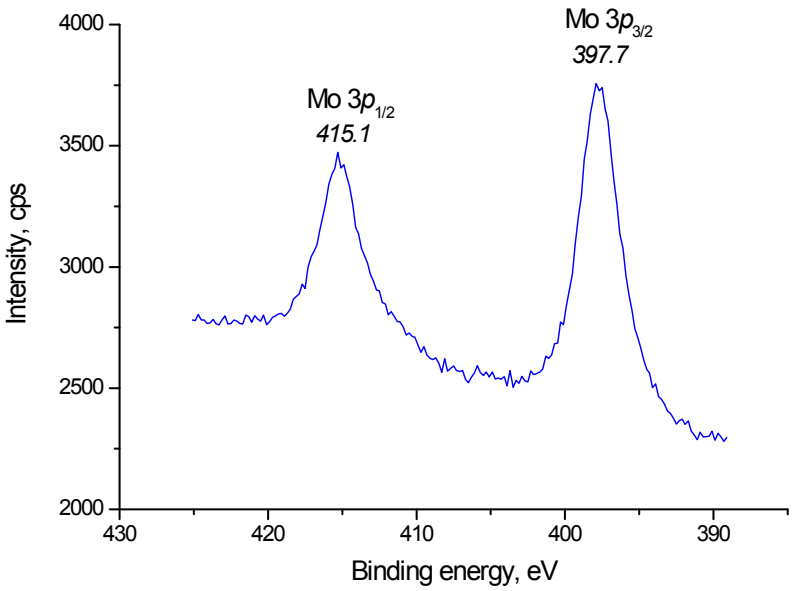

Fig. 2S. Detailed spectrum of Mo 3p doublet.

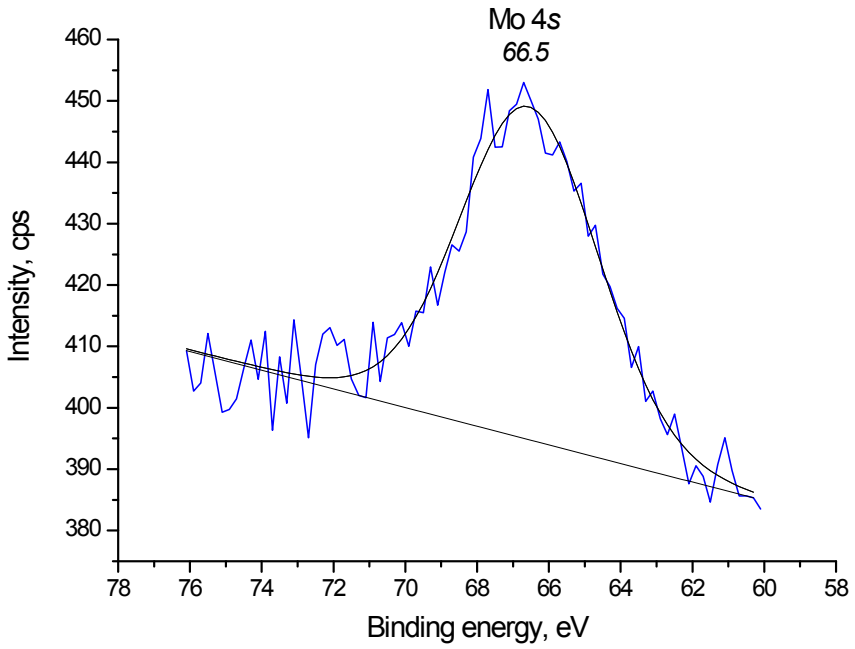

Fig. 3S. Detailed spectrum of Mo 4s core level.

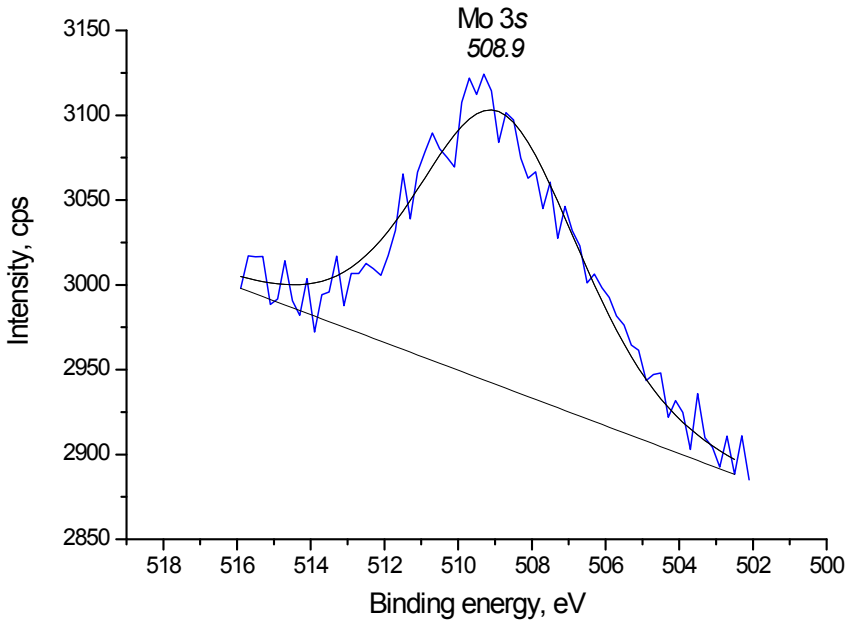

Fig. 4S. Detailed spectrum of Mo 3s core level.

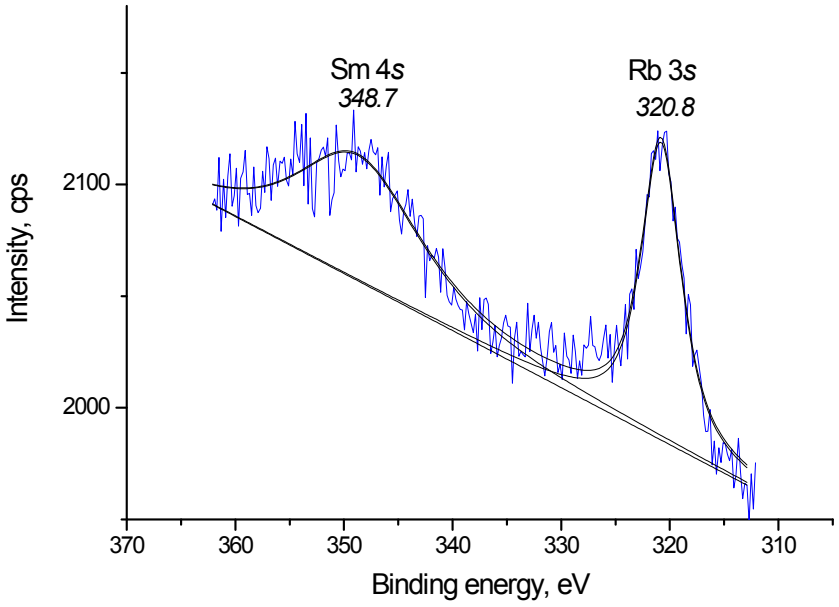

Fig. 5S. Detailed spectrum of Rb 3s and Sm 4s core levels.

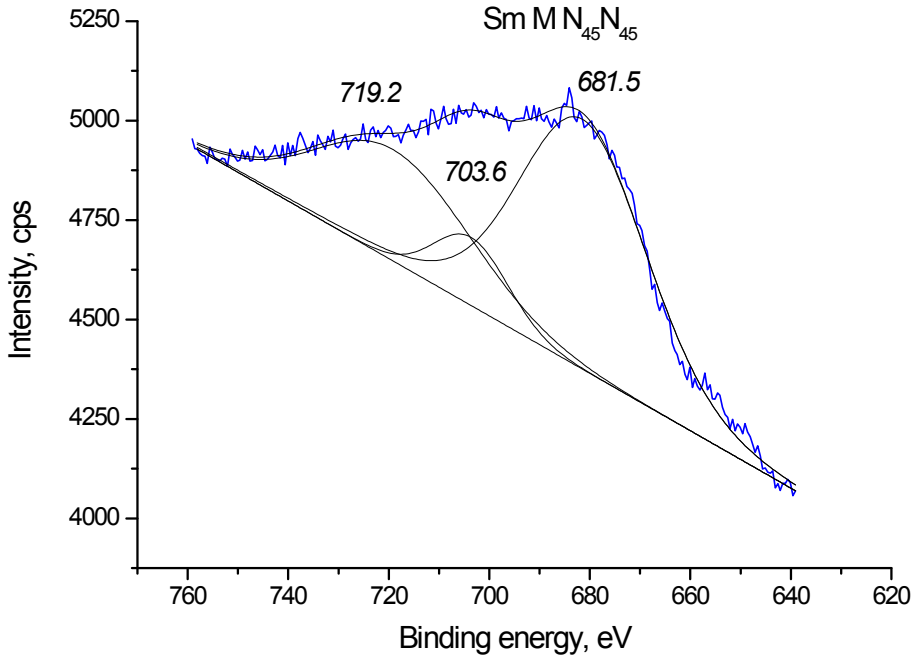
Sm M N45N45
719.2
681.5
703.6
Intensity, cps
5250
5000
4750
4500
4250
4000
760
740
720
700
680
660
640
620
Binding energy, eV

Fig. 6S.

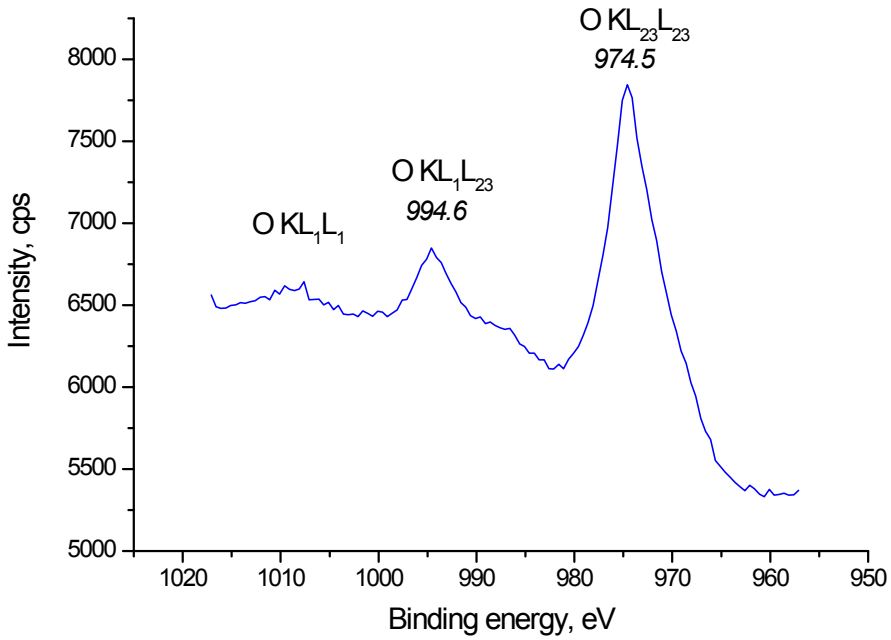
O KL23L23
974.5
O KL1L23
994.6
O KL1L1
Intensity, cps
8000
7500
7000
6500
6000
5500
5000
1020
1010
1000
990
980
970
960
950
Binding energy, eV

Fig. 7S.

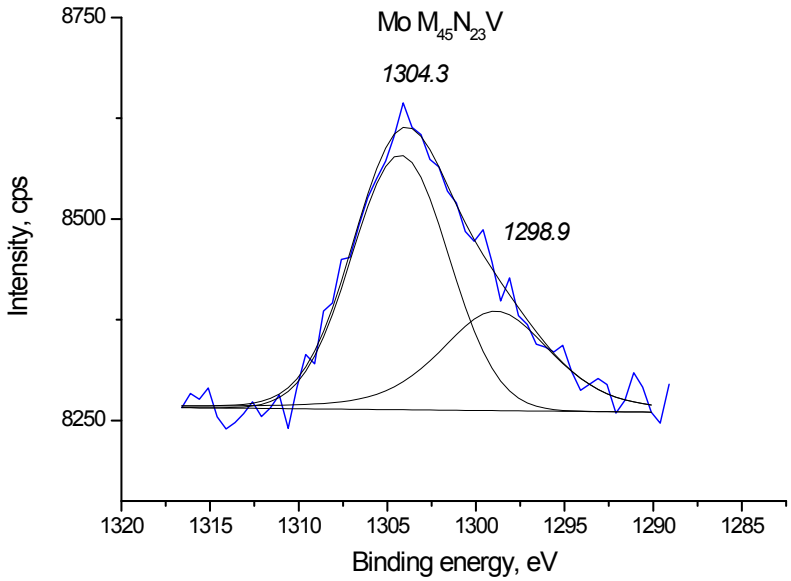
Mo M45N23V
1304.3
1298.9
Intensity, cps
8750
8500
8250
1320
1315
1310
1305
1300
1295
1290
1285
Binding energy, eV

Fig. 8S.

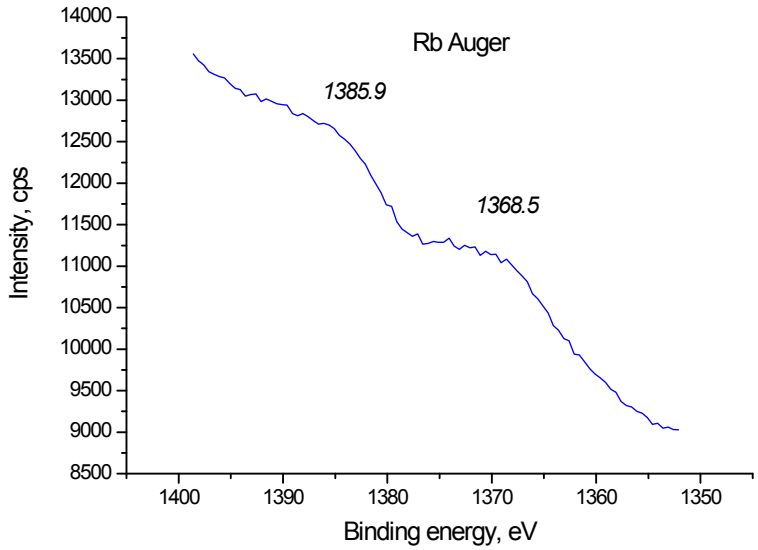
Rb Auger
1385.9
1368.5
Intensity, cps
Binding energy, eV
14000
13500
13000
12500
12000
11500
11000
10500
10000
9500
9000
8500
1400
1390
1380
1370
1360
1350

Fig. 9S.