


## Supplementary information

### **Polymorphism and physical properties of pure and lead-doped monoclinic Sm<sub>2</sub>MoO<sub>6</sub> oxymolybdates**

Ekaterina I. Orlova<sup>a,b\*</sup>, Leon K. Kostanyan<sup>c</sup>, Maria P. Trukhacheva<sup>a,b</sup>, Timofei A. Sorokin<sup>a</sup>, Egor D. Baldin<sup>d</sup>,  Elena P. Kharitonova<sup>a,b</sup>, Nikolay V. Lyskov<sup>e,f</sup>, Vasiliy O. Yapaskurt<sup>g</sup>, Olga A. Alekseeva<sup>a</sup>, Valentina I. Voronkova<sup>b</sup>

<sup>a</sup> *Shubnikov Institute of Crystallography, Kurchatov Complex of Crystallography and Photonics, National Research Centre "Kurchatov Institute," Leninskii Prospekt 59, Moscow, 119333, Russian Federation.*

<sup>b</sup> *Lomonosov Moscow State University, Faculty of Physics, GSP-1, Leninskie Gory, Moscow, 119991, Russian Federation*

<sup>c</sup> *Lomonosov Moscow State University, Department of Chemistry, GSP-1, Leninskie Gory, Moscow, 119991, Russian Federation*

<sup>d</sup> *N.N. Semenov Federal Research Center For Chemical Physics RAS, Kosygina 4, Moscow, 119991, Russian Federation*

<sup>e</sup> *Federal Research Center for Problems of Chemical Physics and Medical Chemistry of the Russian Academy of Sciences, Acad. Semenov av. 1, Chernogolovka, 142432, Russian Federation*

<sup>f</sup> *National Research University "Higher School of Economics", Miasnitskaya Str. 20, Moscow, 101000, Russian Federation*

<sup>g</sup> *Lomonosov Moscow State University, Department of Geology, GSP-1, Leninskie Gory, Moscow, 119991, Russian Federation*

Correspondence:

Ekaterina Orlova, M.V. Lomonosov

Moscow State University, Leninskie gory

1/2, 119991, Moscow, Russia.

E-mail: agapova@polly.phys.msu.ru

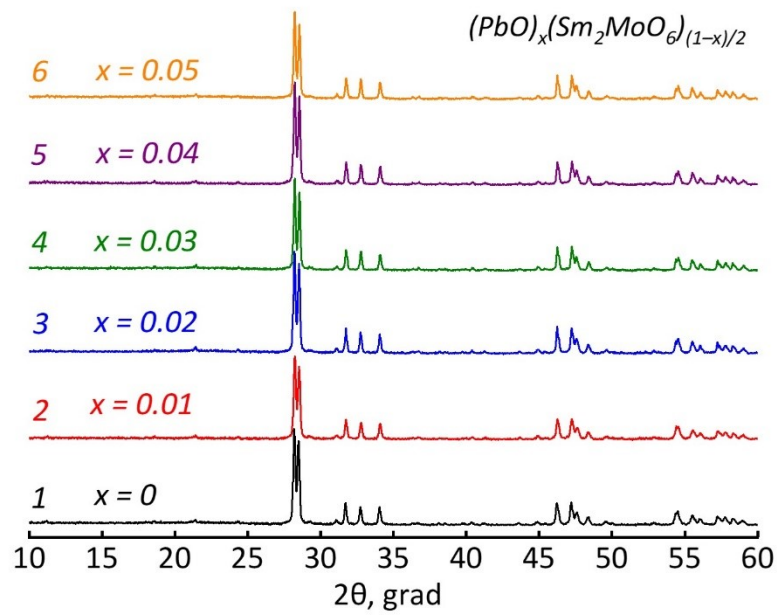


Figure S1. Powder XRD patterns of  $(\text{PbO})_x(\text{Sm}_2\text{MoO}_6)_{(1-x)/2}$  ( $x = 0; 0.01; 0.02; 0.03; 0.04; 0.05$ ) polycrystalline samples.

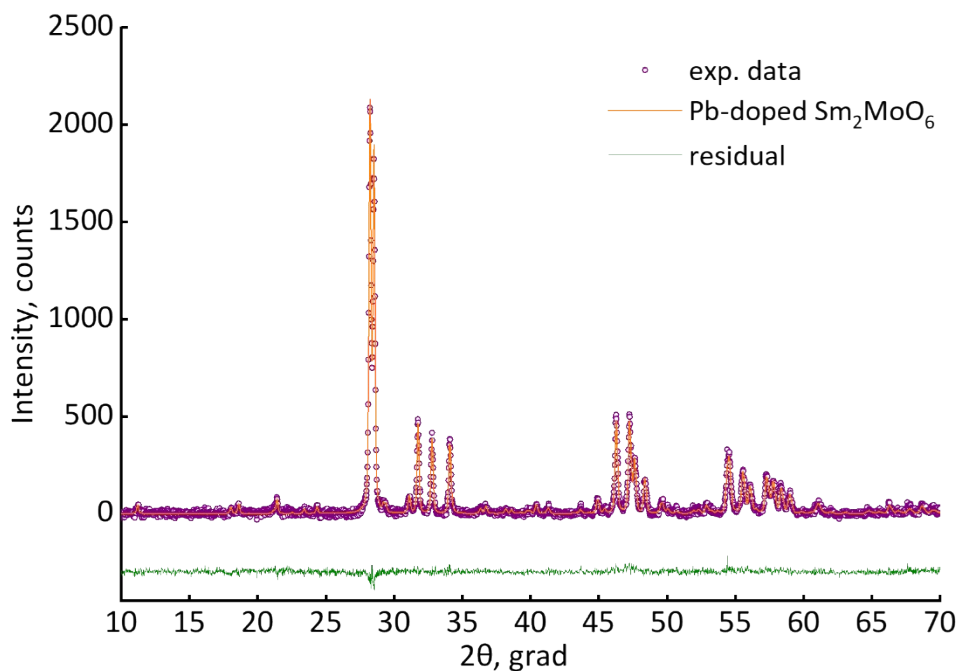


Figure S2. Rietveld refinement of XRD data results for the  $(\text{PbO})_x(\text{Sm}_2\text{MoO}_6)_{(1-x)/2}$  ( $x = 0.01$ ) sample.

Table S1. Unit cell parameters for  $(\text{PbO})_x(\text{Sm}_2\text{MoO}_6)_{(1-x)/2}$  ( $x = 0, 0.01, 0.02, 0.03, 0.04, 0.05, 0.10, 0.125, 0.15, 0.20, 0.30$ ) polycrystalline samples.

Nominal composition $(\text{PbO})_x(\text{Sm}_2\text{MoO}_6)_{(1-x)/2}, x$	a, Å	b, Å	c, Å	v, Å <sup>3</sup>	$\beta$ , °	R <sub>wp</sub> , %
0	16.635(2)	11.278(14)	5.467(7)	974.27	108.34(2)	6.64
0.01	16.635(17)	11.277(11)	5.467(6)	971.64	108.34(2)	6.78
0.02	16.631(8)	11.276(6)	5.469(3)	972.36	108.30(2)	7.18
0.03	16.634(17)	11.279(11)	5.471(5)	970.87	108.27(19)	9.88
0.04	16.635(17)	11.279(11)	5.470(6)	970.95	108.29(18)	9.26
0.05	16.633(16)	11.278(11)	5.471(5)	971.37	108.27(2)	9.97
0.10	16.631(17)	11.273(11)	5.470(6)	970.52	108.280(2)	7.18
0.125	16.627(13)	11.269(9)	5.469(4)	973.30	108.27(2)	6.82
0.15	16.636(2)	11.271(15)	5.472(7)	971.02	108.30(3)	7.13