## High-Pressure Synthesis of *A*-site Ordered Perovskite PbMn<sub>3</sub>(CrMn<sub>3</sub>)O<sub>12</sub> with Long-range Antiferromagnetic Ordering and Spin Glass Transition

Man Xue<sup>a</sup>, Xiaohui Yan<sup>a</sup>, Deyang Xu<sup>a</sup>, Bin Zheng<sup>a</sup>, Wenbin Guo<sup>a\*</sup>, Xiaojun Kuang<sup>a,b</sup>, Xiuyun Lei<sup>a\*</sup>, Congling Yin<sup>a\*</sup>

a. MOE Key Laboratory of New Processing Technology for Nonferrous Metal and Materials, Guangxi Key Laboratory of Optical and Electronic Materials and Devices, Collaborative Innovation Center for Exploration of Nonferrous Metal Deposits and Efficient Utilization of Resources, College of Materials Science and Engineering, Guilin University of Technology, Guilin 541004, P. R. China b. Guangxi Key Laboratory of Electrochemical and Magnetochemical Functional Materials, College of Chemistry and Bioengineering, Guilin University of Technology,

Guilin 541004, P. R. China

E-mail: <u>guo0281@163.com</u> (W. G.), <u>xiuyun.lei@glut.edu.cn</u> (X. L), and <u>congling.yin@glut.edu.cn</u> (C.Y.)



**Figure S1**. Experimental (open circles), calculated (green line), and difference (blue line) laboratory XRPD patterns of PbMn<sub>3</sub>CrMn<sub>3</sub>O<sub>12</sub> at 295 K. The bars show reflection positions for PbMn<sub>3</sub>CrMn<sub>3</sub>O<sub>12</sub>. Arrows mark the reflections of Mn<sub>2</sub>O<sub>3</sub> impurity.



Figure S2. Schema of the cis ligand-metal-ligand angles  $\varphi_i$ , which is the parameter to calculate the angle distortion following the formula  $\sum_{i=1}^{12} |\varphi_i - 90|$ . The higher value  $\Sigma$  indicates the stronger distortion of polyhedron <sup>1</sup>.



**Figure S3**. Structural overlay of  $Mn/CrO_6$  and  $(Mn/Cr)_2O_{11}$  in  $PbMn_3CrMn_3O_{12}$  (green line) and  $PbMn_3Mn_1Cr_3O_{12}$  (red line) at 300 K.



**Figure S4.** The compared magnetic susceptibilities of  $PbMn_3CrMn_3O_{12}$  and  $Mn_2O_3$ , showing the anomaly around 80 K resulted from the impurity  $Mn_2O_3$ .

Reference

1 R. Ketkaew, Y. Tantirungrotechai, P. Harding, G. Chastanet, P. Guionneau, M. Marchivie, and D. J. Harding. *Dalton Trans.*, 2021, **50**, 1086-1096.