

Enhancement of the Curie temperature along the perovskite series $\text{RCu}_3\text{Mn}_4\text{O}_{12}$ driven by chemical pressure of R^{3+} cations (R= rare earths)

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Supporting Information (SI)

Figure Captions (SI)

Fig. SI-1. XRD pattern for $\text{LuCu}_3\text{Mn}_4\text{O}_{12}$ indexed in a cubic unit cell with $a = 7.2409(1) \text{ \AA}$.

Fig. SI-2. Observed (circles), calculated (full line), and difference (bottom) NPD Rietveld profiles for R=Nd, Y, Er, Lu at room temperature, $\lambda=1.594 \text{ \AA}$. The second series of Bragg reflections corresponds to the magnetic structure.

Fig. SI-3. Rietveld fit of the Synchrotron XRD data for R=Sm, Eu, Gd samples, $\lambda=0.8255 \text{ \AA}$.

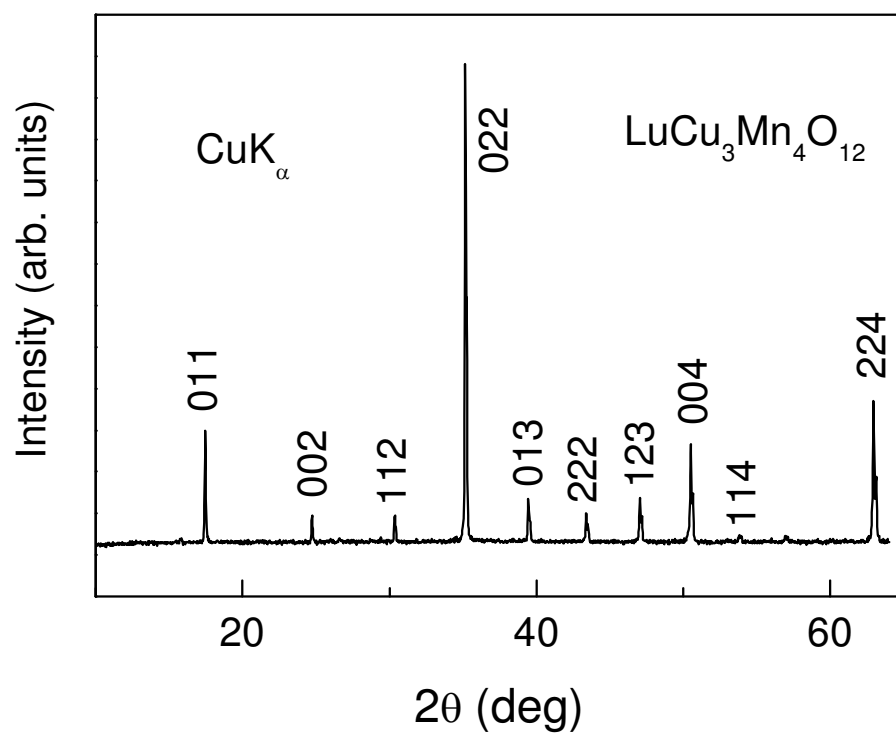


Figure SI-1

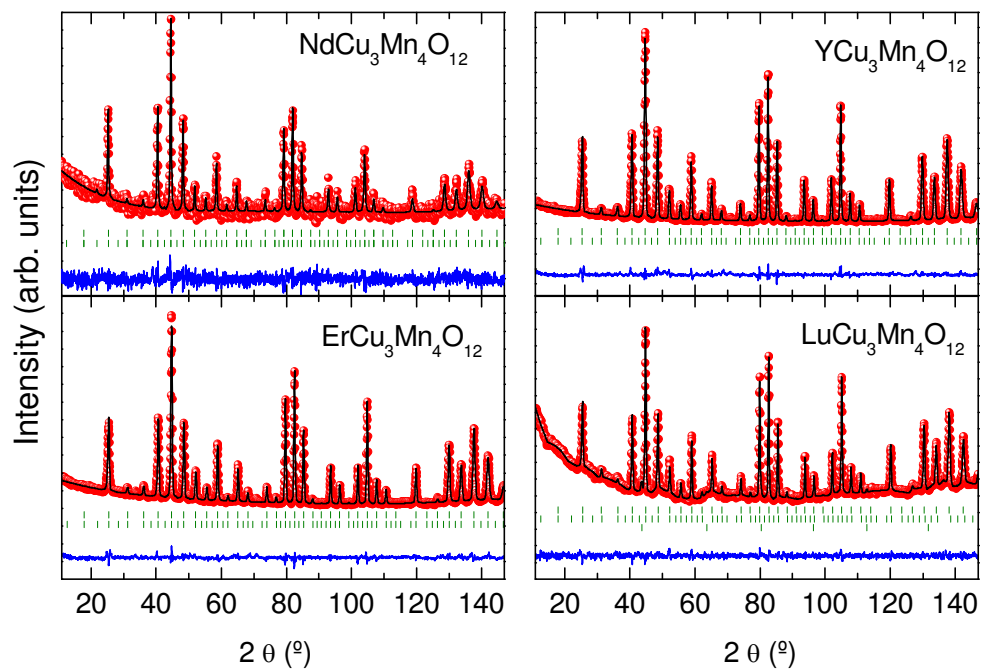


Figure SI-2

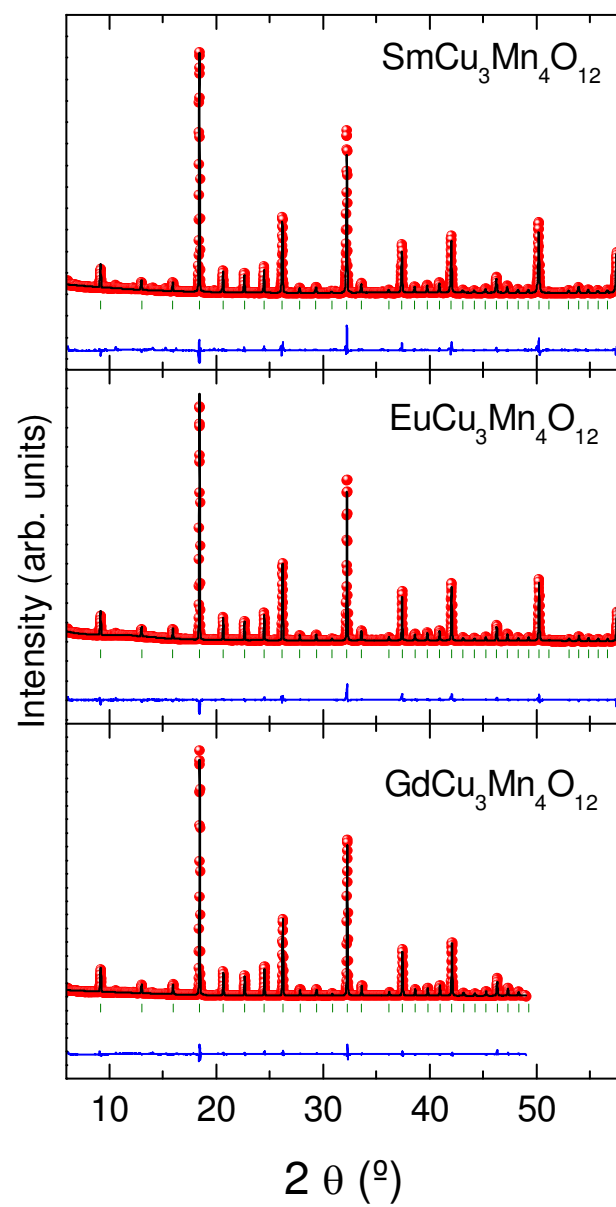


Figure SI-3

Table SI-1. Main bond distances (Å) and selected angles (°) for $\text{RCu}_3\text{Mn}_4\text{O}_{12}$ determined from NPD and synchrotron XRD data at 295K.

R		Nd	Sm	Eu	Gd	Y	Er	Lu
<i>RO₁₂ polyhedra</i>								
R-	O (x12)	2.566(5)	2.576(6)	2.568(4)	2.555(4)	2.5254(8)	2.5268(9)	2.500(1)
<i>CuO₁₂ polyhedra</i>								
Cu-	O (x4)	2.740(3)	2.725(3)	2.728(3)	2.737(2)	2.7511(5)	2.7457(6)	2.7603(7)
Cu-	O (x4)	1.956(5)	1.952(7)	1.955(5)	1.954(4)	1.9537(10)	1.9544(12)	1.9439(13)
Cu-	O (x4)	3.205(4)	3.201(5)	3.196(4)	3.194(3)	3.1837(7)	3.1786(8)	3.1766(10)
O-Cu-O*		84.7(5)	85.5(5)	85.2(4)	84.5(3)	83.19(7)	83.40(8)	82.10(9)
O-Cu-O*		95.3(4)	94.5(5)	94.8(4)	95.5(3)	96.81(8)	96.60(9)	97.90(10)
<i>MnO₆ octahedra</i>								
Mn-	O (x6)	1.9295(9)	1.927(6)	1.9248(17)	1.9238(14)	1.9190(7)	1.9170(8)	1.9149(10)
O-Mn-O		89.4(2)	89.9(3)	89.6(2)	89.2(2)	88.21(5)	88.33(5)	87.49(6)
O-Mn-O		90.6(2)	90.1(3)	90.4(2)	90.8(2)	91.79(6)	91.67(7)	92.51(8)
Cu-O-Mn		108.75(16)	108.82(19)	108.69(16)	108.65(13)	108.45(3)	108.40(4)	108.47(4)
Mn-O-Mn		141.80(7)	141.86(9)	142.02(7)	141.93(6)	141.92(1)	142.072(16)	141.483(19)

*for Cu-O short distances, within CuO₄ square units.

Table SI-2. Curie temperature for the $\text{RCu}_3\text{Mn}_4\text{O}_{12}$ series.

R	La	Ce	Th	Pr	Nd	Sm	Eu	Gd	Tb	Dy	Y	Ho	Er	Tm	Yb	Lu
T _C (K)	360	397	370	376	386	393	394	394	396	396	401	404	405	406	400	398
<i>Ref.</i>	<i>20</i>	<i>27</i>	<i>28</i>	<i>22</i>	*	*	*	*	<i>21</i>	<i>22</i>	*	<i>22</i>	*	<i>22</i>	<i>22</i>	*

* *This work*

