

Supporting information for

**The impact of A-site cation on the crystal structure and magnetism of the new double perovskites  $A\text{LaCoTeO}_6$  ( $A = \text{Na}$  and  $\text{K}$ )**

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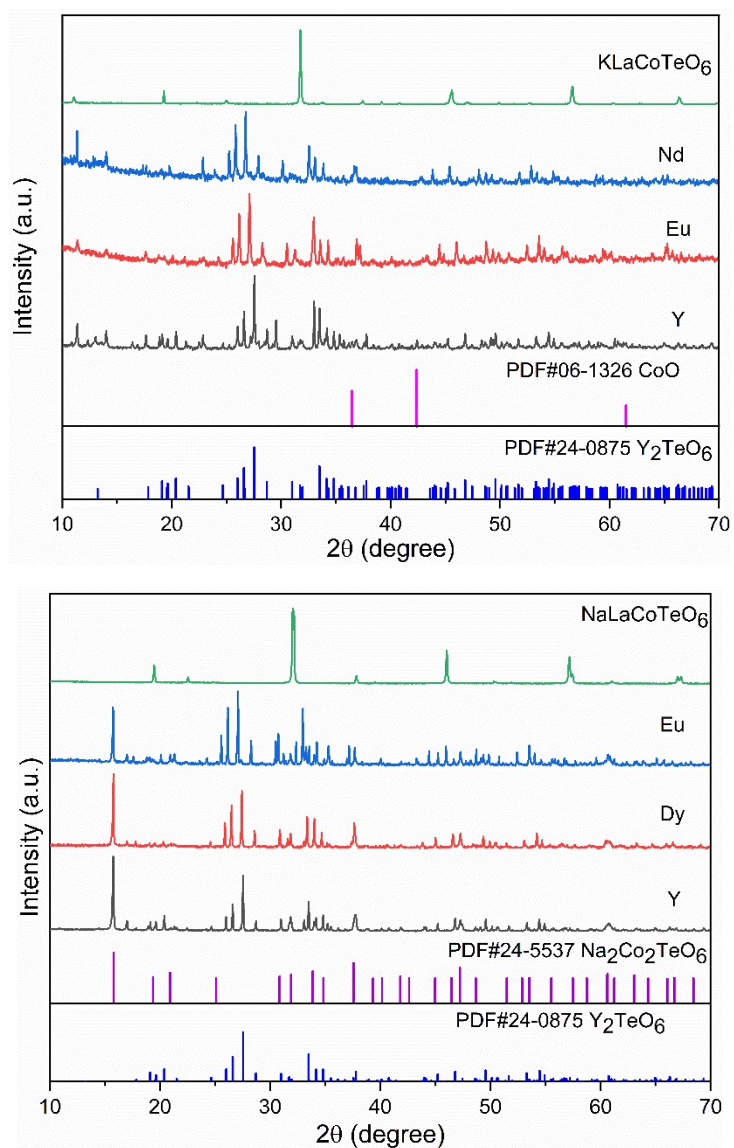
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**Table S1** Crystallographic Data for  $ALaCoTeO_6$  (A = K and Na) from Rietveld Refinement against PXRD and ND Data.

formula	parameters		
	KLaCoTeO <sub>6</sub>	NaLaCoTeO <sub>6</sub>	
temperature (K)	298	298	
source	Cu K <sub>α1</sub>	Cu K <sub>α1</sub>	neutron
wavelength (Å)	1.5406	1.5406	1.622
Space group (no.)	<i>P4/nmm</i> (no. 129)	<i>I</i> -1 (no. 1)	
<i>d</i> -spacing range (Å)	0.89–9.0	0.82–8.8	0.82–10.0
<i>a</i> (Å)	5.62355(2)	5.5864(7)	
<i>b</i> (Å)	5.62355(2)	7.8751(9)	
<i>c</i> (Å)	7.98442(5)	5.5676(1)	
$\alpha$ (°)	90	90.345(5)	
$\beta$ (°)	90	89.934(3)	
$\gamma$ (°)	90	90.0403(9)	
cell volume (Å <sup>3</sup> )	252.502(3)	244.85(1)	
<i>Z</i>	2	2	
<i>R</i> <sub>wp</sub> (%)	2.10	1.78	4.30
<i>R</i> <sub>p</sub> (%)	1.56	1.37	3.39
<i>R</i> <sub>exp</sub> (%)	1.50	1.05	2.91
$\chi^2$	1.40	1.69	1.48

**Table S2.** The Co–O and Te–O bond distances in KLaCoTeO<sub>6</sub> and NaLaCoTeO<sub>6</sub>.

KLaCoTeO <sub>6</sub>		NaLaCoTeO <sub>6</sub>	
Co–O3 × 2	1.93(2)	Co–O1	1.96(1)
Co–O2 × 2	2.087(8)	Co–O3 × 4	2.068(3)
Co–O1 × 2	2.13(2)	Co–O2	2.18(1)
<Co–O>	2.05(2)	<Co–O>	2.069(5)
Te–O1 × 2	1.84(1)	Te–O2	1.91(1)
Te–O2 × 2	1.912(9)	Te–O1	1.94(1)
Te–O3 × 2	2.08(2)	Te–O3 × 4	1.939(4)
<Te–O>	1.94(1)	<Te–O>	1.934(6)



**Fig. S1** XRPD patterns for the compositions of  $\text{KLnCoTeO}_6$  (Ln = La, Nd, Eu, Y) and  $\text{NaLnCoTeO}_6$  (Ln = La, Eu, Dy, Y).

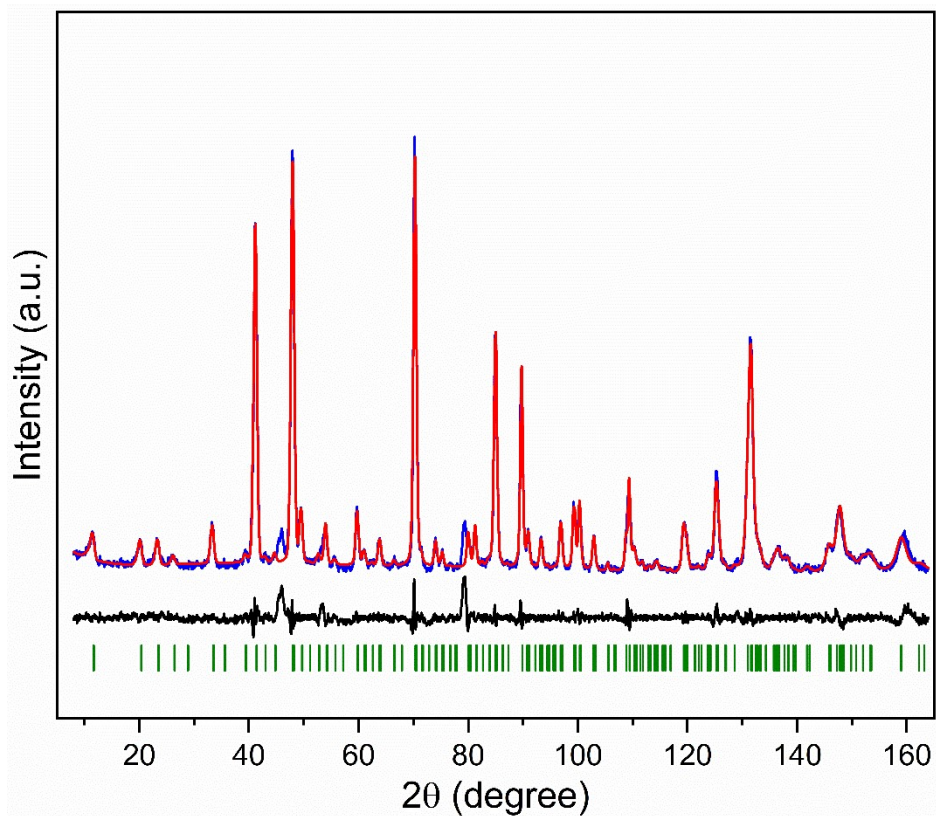


Fig. S2 Le-Bail fitting to the NPD data of KLaCoTeO<sub>6</sub> using the space group *P4/nmm*.

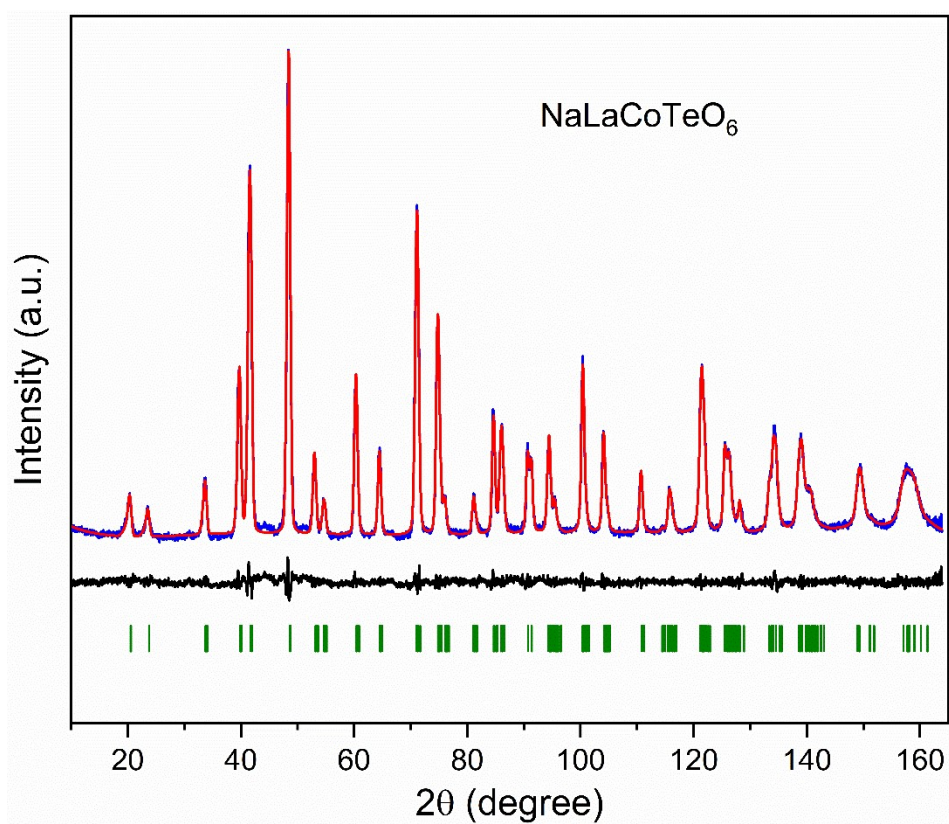
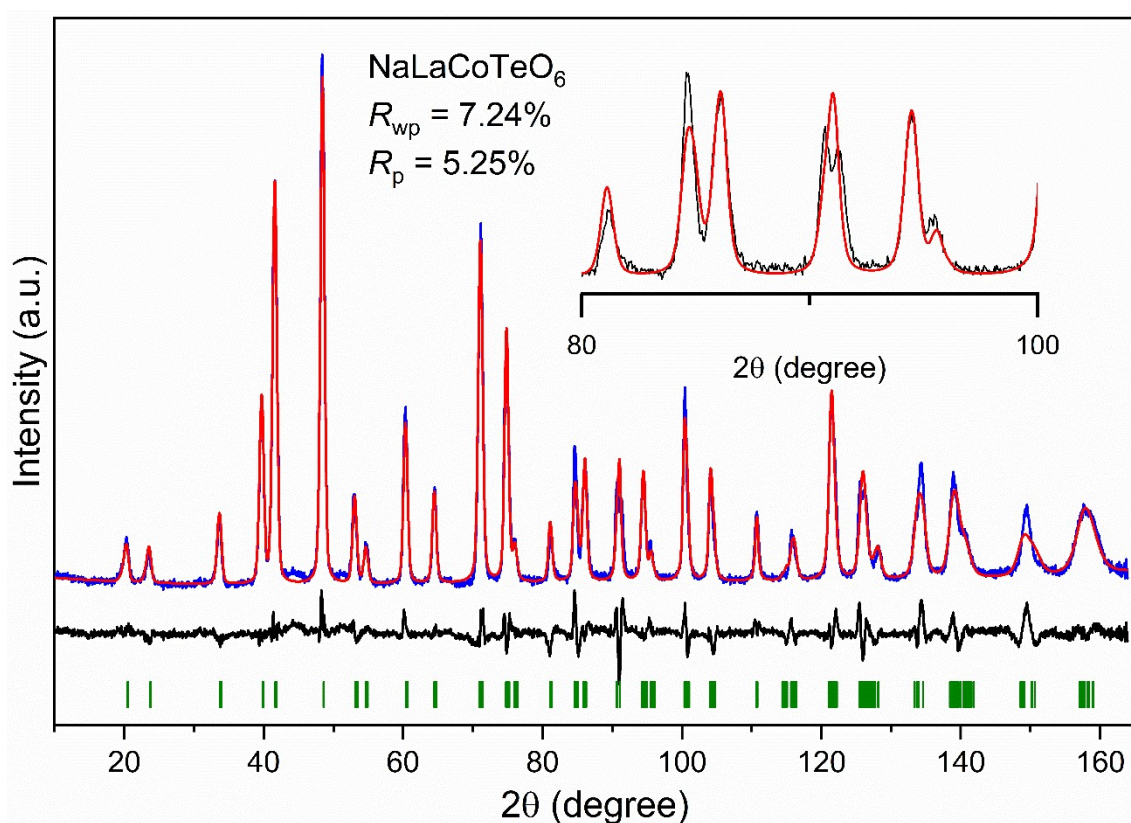
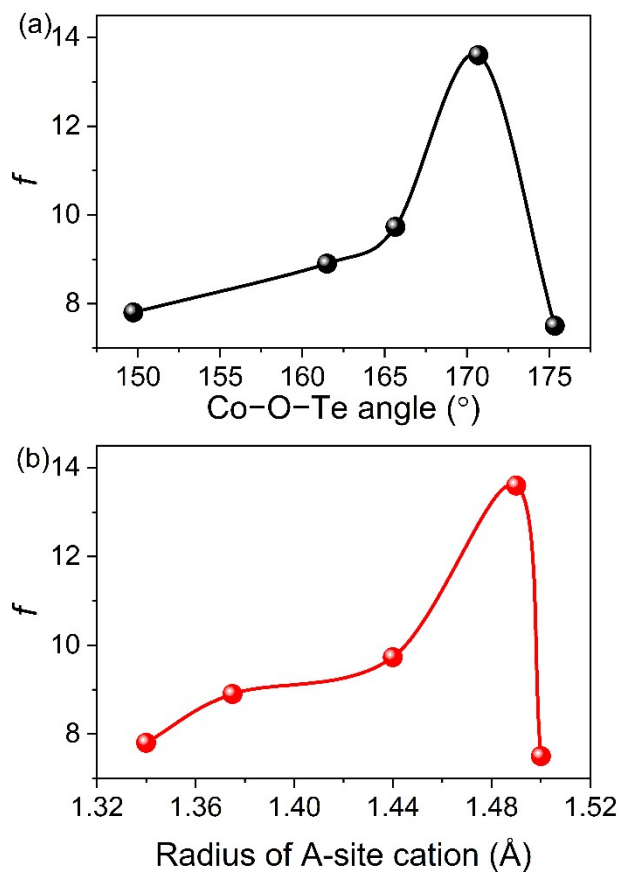


Fig. S3 Le-Bail fitting to the NPD data of NaLaCoTeO<sub>6</sub> using the space group *I2/m*.



**Fig. S4** Rietveld refinement plots of NPD data for NaLaCoTeO<sub>6</sub>. The blue, red, and black solid lines indicate the observed, calculated, and difference curves, respectively. The expected Bragg positions are presented as green bars at the bottom of the pattern.



**Fig. S5** Plots of the frustration factor as a function of average Co-O-Te bond angle (a) and radius of A-site cation radius (b).