Competition between direct exchange interaction and superexchange interaction in layered compounds $LiCrSe_2$, $LiCrTe_2$, and $NaCrTe_2$ with a triangular lattice

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Table S_1. Atomic positions and isotropic displacement parameters for $LiCrSe_2$, $LiCrTe_2$, and $NaCrTe_2$ at room temperature obtained from Rietveld analysis with preferred-orientation parameters. Errors are obtained from the standard deviation of the Rietveld refinement using the RIETAN-FP program. Space group, lattice parameters, reliability factors (R-factors) are also shown in the table.

$LiCrSe_2$					
Space group			$P\bar{3}m1$		
Lattice parameters (Å)			a=3.6544(1), c=6.2911(1)		
atom	site	x	y	z	$U_{\rm iso}$
Li	$1b$	0	0	0.5	0.02
Cr	$1a$	0	0	0	0.0168(6)
Se	$2d$	1/3	2/3	0.2253(1)	0.0168(6)
R-factors: $R_{\rm P}$=9.59%, $R_{\rm wp}$=13.33%, S=1.68					
Constraint on isotropic atomic displacement: $U_{\rm iso}$(Li) = 0.02, $U_{\rm iso}$(Cr) = $U_{\rm iso}$(Se).					

$LiCrTe_2$					
Space group			$P\bar{3}m1$		
Lattice parameters (Å)			a=3.9596(4), c=6.6990(3)		
atom	site	x	y	z	$U_{\rm iso}$
Li	$1b$	0	0	0.5	0.02
Cr	$1a$	0	0	0	0.0146(8)
Te	$2d$	1/3	2/3	0.2275(2)	0.0146(8)
R-factors: $R_{\rm P}$=8.59%, $R_{\rm wp}$=12.32%, S=1.22					
Constraint on isotropic atomic displacement: $U_{\rm iso}$(Li) = 0.02, $U_{\rm iso}$(Cr) = $U_{\rm iso}$(Te).					

$NaCrTe_2$					
Space group			$P\bar{3}m1$		
Lattice parameters (Å)			a=4.0193(2), c=7.3954(3)		
atom	site	x	y	z	$U_{\rm iso}$
Na	$1b$	0	0	0.5	0.02
Cr	$1a$	0	0	0	0.0155(8)
Te	$2d$	1/3	2/3	0.2018(2)	0.0155(8)
R-factors: $R_{\rm P}$=6.98%, $R_{\rm wp}$=8.95%, S=0.818					
Constraint on isotropic atomic displacement: $U_{\rm iso}$(Na) = 0.02, $U_{\rm iso}$(Cr) = $U_{\rm iso}$(Te).					

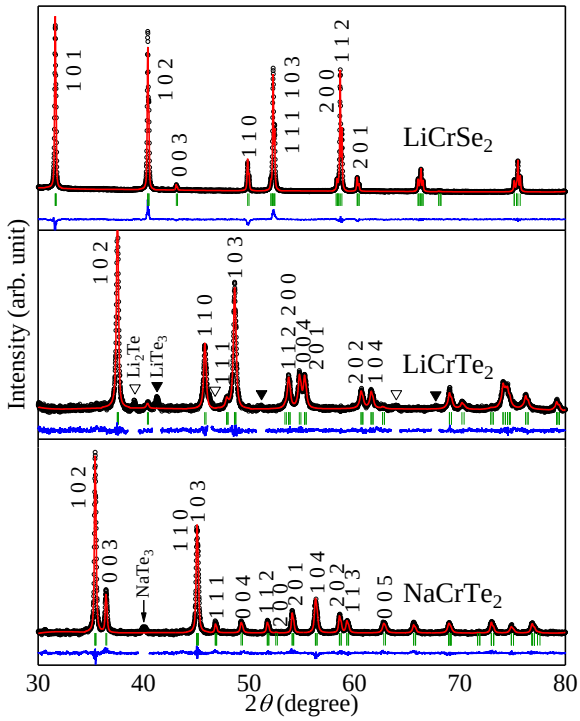

Figure S_1. Rietveld fits to the XRD patterns at room temperature obtained for $LiCrSe_2$, $LiCrTe_2$, and $NaCrTe_2$. Black circles (○), red lines, and blue lines indicate the experimental data, calculated patterns, and deviation between the experimental and calculated intensities, respectively. The short vertical green lines below the profiles indicate the position of the peaks of all possible Bragg reflections. The peaks from impurity phases are indicated by markers (▽: Li_2Te, ▼: $LiTe_3$, ↓: $NaTe_3$).