Supplementary Material (ESI) for Journal of Materials Chemistry

Supporting Information for "High Temperature orbital order melting in the $KCrF_3$ Perovskite"

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Table S1. Refined parameters and selected bond distances for $KCrF_3$ as obtained by Rietveld refinement of the synchrotron X-ray powder diffraction data at 298 K in the space group *I4/mcm* with unit cell parameters, a = 6.05377(1) Å and c = 8.02356(1) Å (agreement factors: R_{wp} = 4.83%, R_{exp} = 3.42%).

Atom	*n*	*x*	*y*	*z*	Position	B_{iso} (Å^2)
K	1	0	0	1/4	*4a*	1.49(2)
Cr	1	0	1/2	0	*4d*	0.66(1)
F(1)	1	0	1/2	1/4	*4b*	1.94(4)
F(2)	1	0.2301(2)	0.7301(2)	0	*8h*	2.12(3)
Selected Distances						
Cr-F(1)	2.00589(1)					
Cr-F(2)	1.970(2)					
Cr-F(2)	2.311(2)					

Table S2. Refined parameters and selected bond distances for $KCrF_3$ as obtained by Rietveld refinement of the synchrotron X-ray powder diffraction data at 973 K in the space group *Pm-3m* with unit cell parameters, a = 4.231800(3) Å (agreement factors: R_{wp} =4.98 %, R_{exp} = 3.12%).

Atom	*n*	*x*	*y*	*z*	Position	B_{iso} (Å^2)
K	1	1/2	1/2	1/2	*1b*	5.1(4)
Cr	1	0	0	0	*1a*	2.71(2)
F(1)	1	1/2	0	0	*3d*	6.04(8)
Selected Distances						
Cr-F(1)	2.115900(2)					