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Supporting information for article:

Low-temperature phase transition and magnetic properties of K3YbSi2O7

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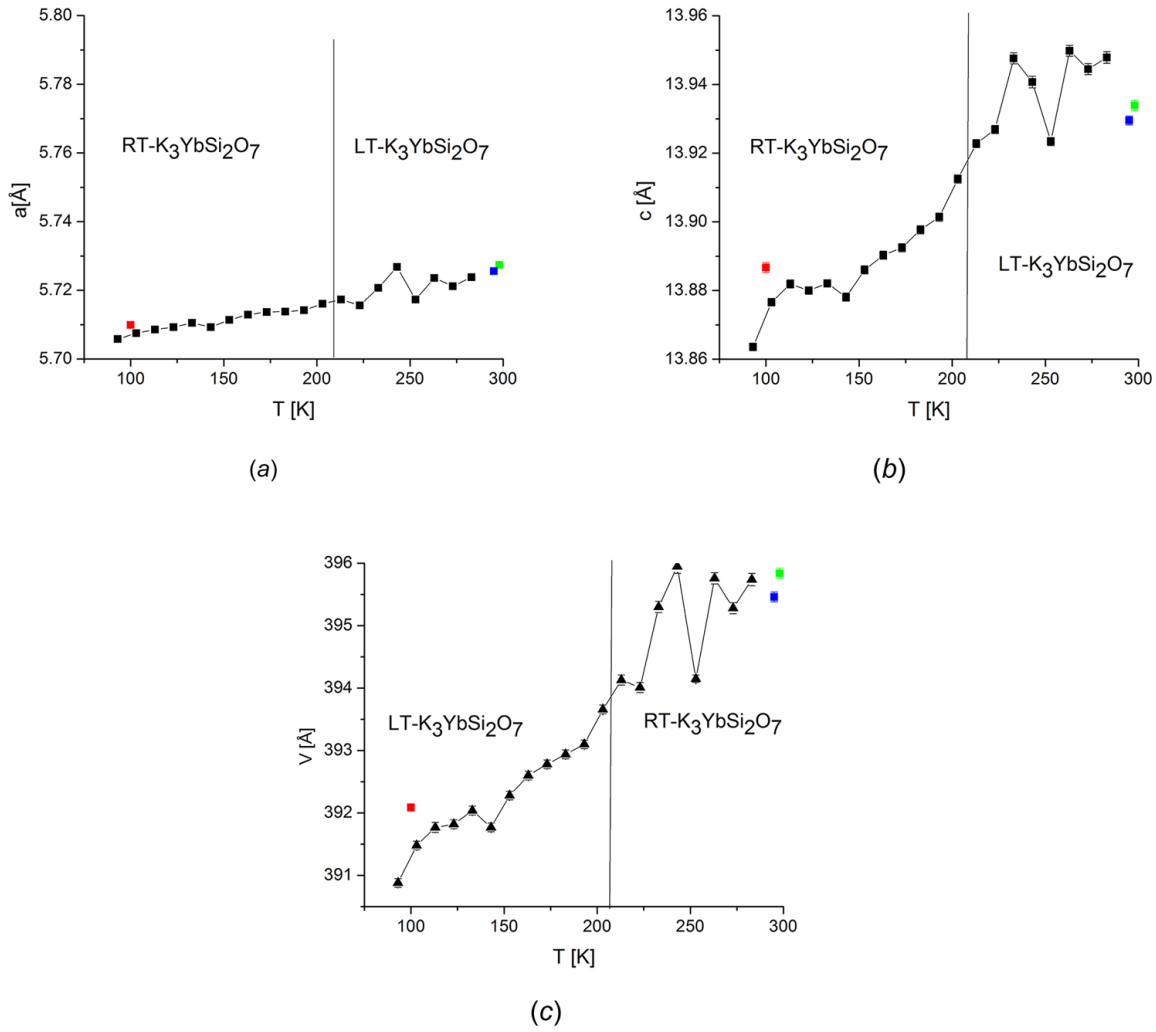

Figure S1 Changes in the unit cell (hexagonal for both β-$K_3YbSi_2O_7$ and β'-$K_3YbSi_2O_7$) parameters *a*, *c* and *V* as a function of temperature. A rather smooth change (*a*) of *a* in the whole temperature range and an abrupt change (*b*) of *c* and *V* (*c*) near 200 K associated with phase transition from β-$K_3YbSi_2O_7$ to β'-$K_3YbSi_2O_7$ is observed. The red and green symbols correspond to crystal 1, while blue and black symbols correspond to crystal 2.

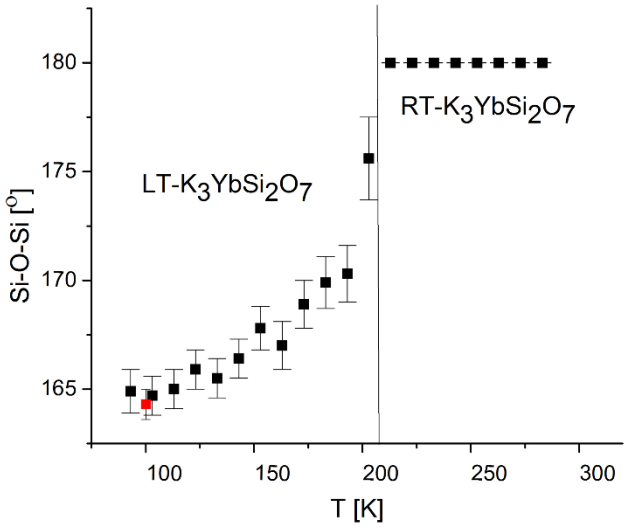

Figure S2 The bridging oxygen angle Si–O–Si as a function of temperature in the β-$K_3YbSi_2O_7$ and β'-$K_3YbSi_2O_7$ polymorphs. The 180° angle is dictated by the space group symmetry of *P*6$_3$/*mmc*. Data marked with red and black symbols correspond to crystal 1 and crystal 2, respectively.

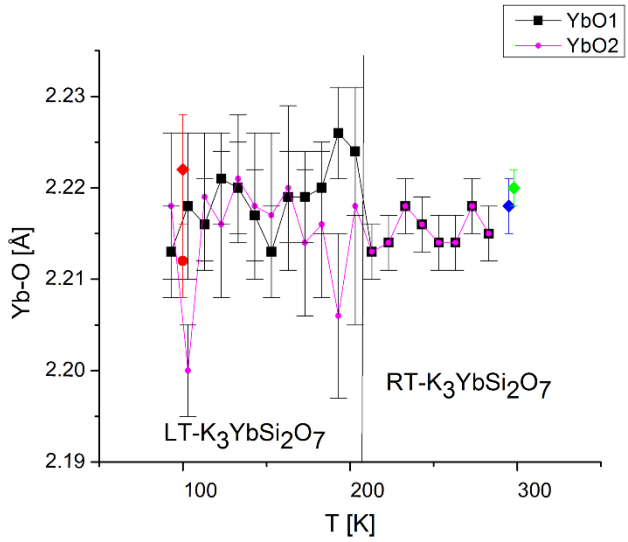

Figure S3 The variation of Yb–O distances as a function of temperature in β-$K_3YbSi_2O_7$ and β'-$K_3YbSi_2O_7$ polymorphs. The Yb–O1 and Yb–O2 distances in orthorhombic β'-$K_3YbSi_2O_7$ are the same between 93 and 203 K within estimated standard deviations. The equality of six Yb–O bonds in hexagonal β-$K_3YbSi_2O_7$ is dictated by the space group symmetry of *P*6$_3$/*mmc*. The red and green symbols correspond to crystal 1, while blue, magenta and black symbols correspond to crystal 2.

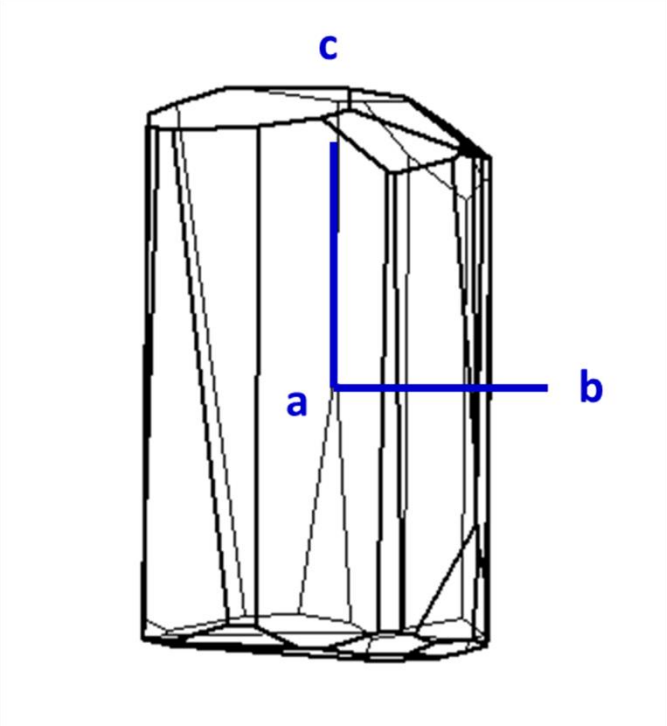

Figure S4 Schematic representation of $K_3YbSi_2O_7$ crystal with crystallographic axes.