



Fig. S1. (a) Asymmetric unit contents of kristiansenite according Ferraris et al. (2001) with the atom numbering scheme. (b) Packing of the ions in the structure of kristiansenite according Ferraris et al. (2001) viewed along [010] and (c) along [100]. Lattice directions a, b, and c are marked by red, green and blue lines, respectively. Transformation matrix of kozłowskiite structure to kristiansenite according Ferraris et al. (2001):

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/4 \\ 0 & 0 & 1 & -1/4 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

