

Electronic Supplementary Information for
Coordination and Thermophysical Properties of Select Trivalent Lanthanides in LiCl-KCl

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Supplemental Data Items

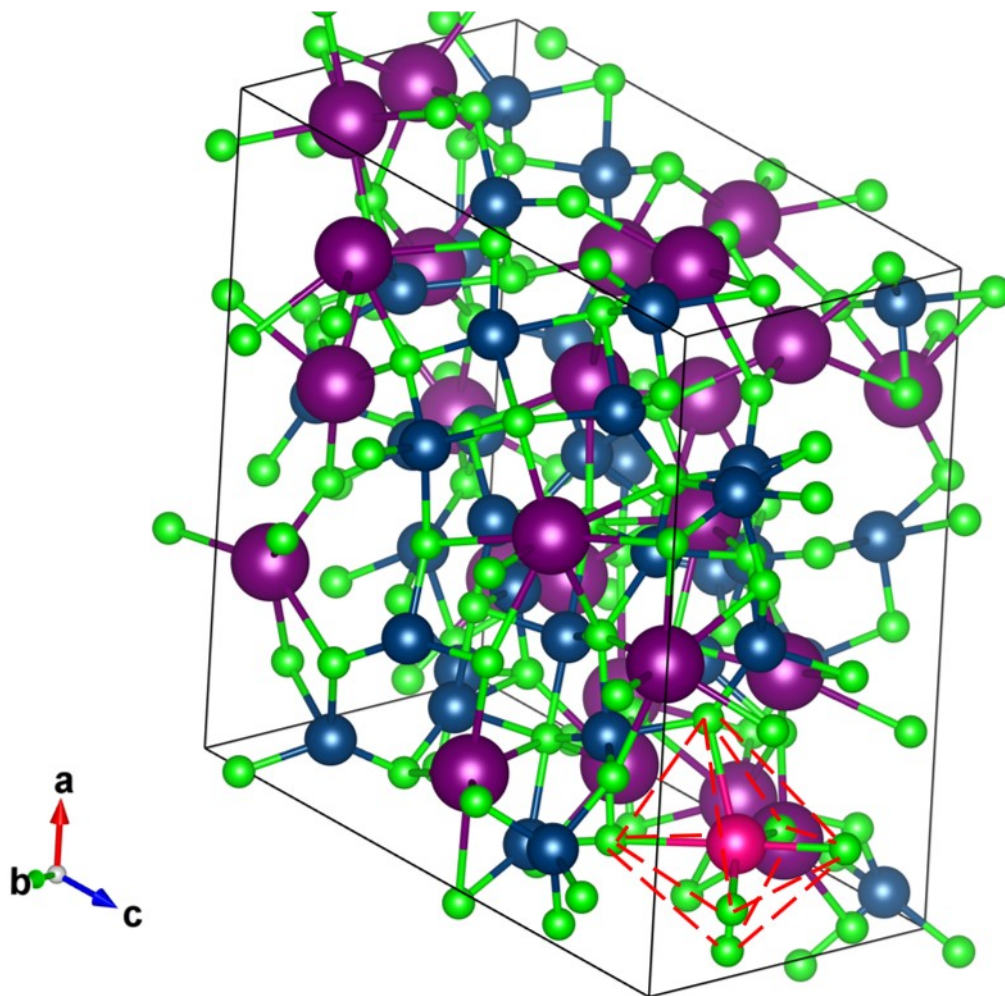


Fig. S1 - QM-MD-obtained preferred coordination of trivalent Ce in magenta. Li, Cl and K atoms are shown in dark blue, green and purple, respectively. The octahedral CeCl_6^{3-} structure is shown with dashed red lines to indicate the geometry of the chlorocomplex. Significant distortion from an ideal octahedral structure is noted in the chlorocomplex for low wt.% (single Ce) systems.

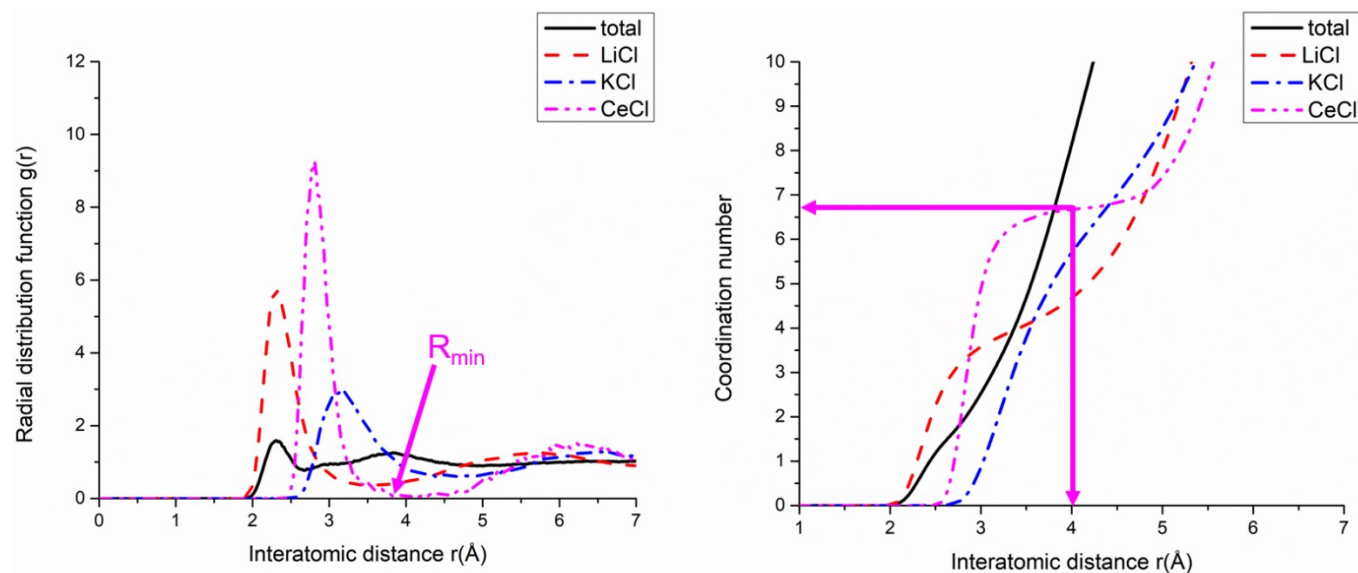


Fig. S2 - Radial distribution function $g(r)$ (left) and coordination number (right) for Ce^{3+} (CeCl_6^{3-}) (19.4 wt. %) in LiCl-KCl eutectic composition at 500°C . LiCl, KCl, and CeCl are represented by dashed red, blue and magenta lines, respectively, while the average total values of RDF and CN are represented by a black line. R_{\min} and CN are indicated with magenta arrows for clarity. The CN for CeCl is found to be decreased with respect to the low wt. % case shown in Fig. 3, with corresponding increases in the CN for LiCl and KCl.

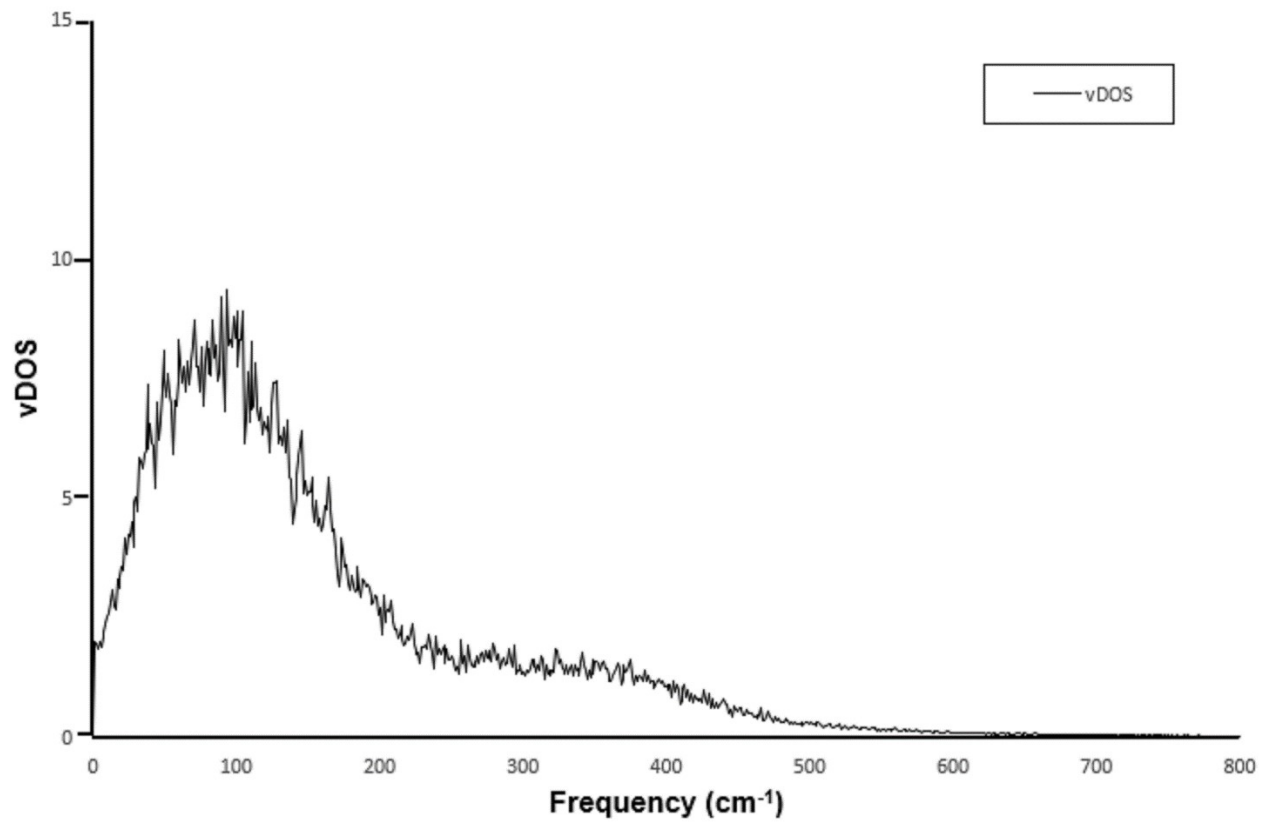


Fig. S3 - Vibrational DOS (black) of LiCl-KCl eutectic at 500°C.

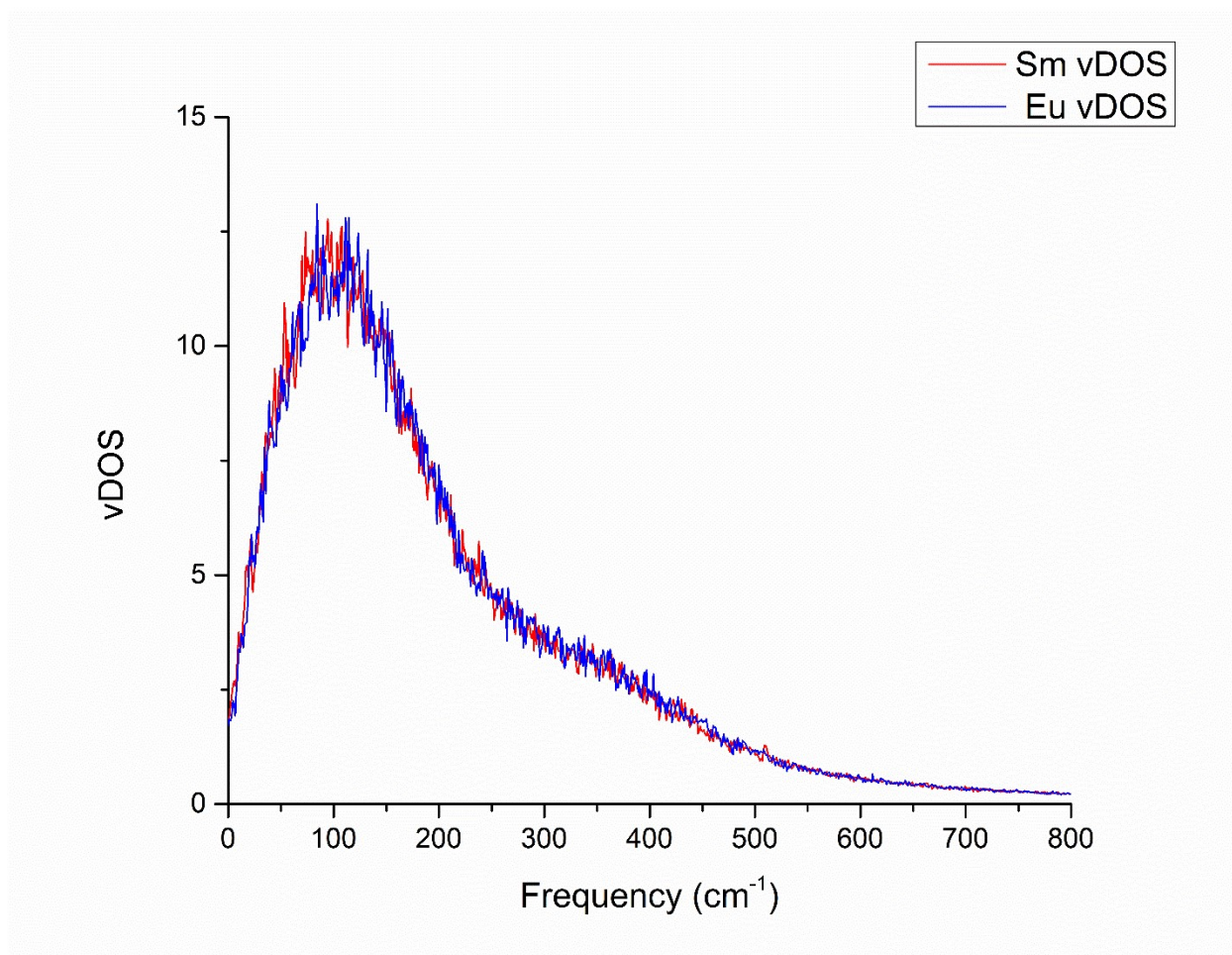


Fig. S4 – Vibrational DOS of Sm^{3+} (red) and Eu^{3+} (blue) in LiCl-KCl eutectic composition, overlaid. Primary difference is noted in the main response region ($\sim 50\text{-}150\text{ cm}^{-1}$) with general similarity across the rest of the vDOS.