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Single crystal X-ray diffraction and Raman characterization of ternary Ce(IV) and Pu(IV) peroxo-carbonate compounds comprised of rare dimeric molecular units

The environmental fate and transport of transuranium elements and the search for alternative f-element separation methods require a better understanding of the speciation of transuranics under oxidizing alkaline conditions, especially in the presence of ubiquitous ligands such as peroxide and carbonate. From our exploration of the Ce and Pu peroxo-carbonate systems several new structures containing the known $[(\text{CO}_3)_3\text{M}(\text{O}_2)_2\text{Ce}(\text{CO}_3)_3]_8$ ($\text{M} = \text{Ce(IV)}$ or Pu(IV)) dimer were found. A simplified synthetic procedure was used to prepare crystalline products of several novel compounds, namely $[\text{NH}_4]_8[(\text{CO}_3)_3\text{Ce}(\text{O}_2)_2\text{Ce}(\text{CO}_3)_3] \cdot 6\text{H}_2\text{O}$, $[\text{C}(\text{NH}_2)_3]_8[(\text{CO}_3)_3\text{Ce}(\text{O}_2)_2\text{Ce}(\text{CO}_3)_3] \cdot 4\text{H}_2\text{O}$, $\text{Na}_8[(\text{CO}_3)_3\text{Ce}(\text{O}_2)_2\text{Ce}(\text{CO}_3)_3] \cdot 12\text{H}_2\text{O}$ and $\text{K}_8[(\text{CO}_3)_3\text{Pu}(\text{O}_2)_2\text{Ce}(\text{CO}_3)_3] \cdot 12\text{H}_2\text{O}$. Structural characterization of the aforementioned compounds was performed using single crystal x-ray diffraction. It was observed that the crystal packing of the $[(\text{CO}_3)_3\text{M}(\text{O}_2)_2\text{Ce}(\text{CO}_3)_3]_8$ dimeric unit varied significantly depending on the cation incorporated into the structure (e.g., Na^+ , K^+ , NH_4^+ , and $\text{C}(\text{NH}_2)_3^+$). Additional characterization of the f-element compounds was performed on single crystals using a high-resolution microscope-based Raman spectrometer.

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