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## Investigation of Calix-crown (CBC & CC6) for selective cesium separation from nitric acid medium: Theoretical and experimental evidences

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Two macro-cyclic compounds viz. calix-benzo-crown (CBC) and calix-crown-6 (CC6) has been synthesized indigenously at large scale for selective separation of cesium from simulated high level liquid waste solution. The solvent extraction studies of Cs(I) ion and some typical metals ions like, Na(I), K(I), La(III), Y(III), Rb(I), Mo(VI), Zr(IV), Sr(II), Ba(II), Ru(III), and Pd(II) with both the ligands in nitric acid medium has been carried out. It was found that the both the ligands exhibited a strong extraction ability and selectivity for Cesium (I) over all the metal ions. In order to explain the high cesium selectivity over sodium ions by theoretically, the three different models has been selected. The structure of Cs & Na metal hydrates and their complexes with CBC and CC6 were optimized at hybrid B3LYP level using SVP basis set in TURBOMOLE 7.0 Package. The gas phase binding energy and free energy indicates the selectivity order:  $\text{Na}^+ > \text{Cs}^+$  whereas after suitable hydration of metal and nitrate the order becomes reverse as obtained in the solvent extraction results. In addition to this the DCs value for CBC was found to be higher than CC6. The same trend has been validated in terms of binding energy and free energy of complexation by using same level of theory in gas phase as well as solution phase.

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## Tracer-scale chemistry of volatile oxygen-bearing compounds formed by U, Pu and Cm

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Tracer-scale chemistry has some distinguishing characteristics which differ it from common (macro) chemistry. For example, the common redox reaction  $2\text{Pu(IV)} + \text{U(IV)} \rightarrow 2\text{Pu(III)} + \text{U(VI)}$  does not occur in extremely diluted solutions as collisions between microcomponents are practically excluded. Considerable differences in the chemical behavior micro- and macroquantities of some actinides in the gas phase had also been observed. The initial sample contained a tracer quantity of the actinide under study that was adsorbed on the surface of quartz powder. The experiments were carried out using open quartz thermochromatographic columns (I.D. = 3 mm); oxygen served as a reagent and helium was a carrier gas; the flow rate of the gas mixture was  $20 \text{ cm}^3 \text{ min}^{-1}$ ; the initial sample was heated in a gas stream at  $700\text{-}750^\circ\text{C}$ ; the final part of the thermal-gradient section was cooled to  $-165^\circ\text{C}$ ; the temperature gradient was  $-18^\circ\text{C cm}^{-1}$ ; the duration of each experiment was 30 min. It was found that uranium formed volatile dioxide and trioxide that were adsorbed at  $450 \pm 25$  and  $250 \pm 25^\circ\text{C}$ . Two plutonium radioisotopes  $^{238,239}\text{Pu}$  were used in similar experiments. Contrary to the previous results, plutonium formed three oxides. The centers of their deposition zones were registered at  $450 \pm 30^\circ\text{C}(\text{PuO}_2)$ ,  $250 \pm 30^\circ\text{C}(\text{PuO}_3)$  and at  $-105 \pm 25^\circ\text{C}(\text{PuO}_4)$ . In similar conditions, Cm formed also three oxides:  $\text{CmO}_2$ ,  $\text{CmO}_3$  and  $\text{CmO}_4$ . They were adsorbed at  $550 \pm 25$ ,  $390 \pm 25$  and  $-80 \pm 50^\circ\text{C}$  respectively. The values of adsorption enthalpy for these oxides on quartz and their chemical yields were determined.

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