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Selective Permeability of Uranyl Peroxide Nanocages to Different Alkali Ions: Influences from Surface Pores and Hydration Shells[1]
YUNYI GAO, Univ of Akron, JENNIFER SZYMANOWSKI, PETER BURNS, University of Notre Dame, TIANBO LIU, Univ of Akron — The precise guidance to different ions across the biological channels is essential for many biological processes. An artificial nanopore system will facilitate the study of ion transport mechanism through nanosized channels and offer new views for designing nanodevices. Here we reveal that a 2.5-nm-size, fullerene-shaped molecular cluster $Li_{48+m}K_{12}(OH)_m[UO_2(O_2)(OH)]_{60-}(H_2O)_n$ (m≈20 and n≈310) (**U_{60}**) shows selective permeability to different alkali ions. The sub-nanometer pores on the water-ligand-rich surface of **U_{60}** are able to block Rb^+ and Cs^+ ions from passing through, while allow Na^+ and K^+ ions, which possess larger hydrated sizes, to enter the interior space of **U_{60}**. An interestingly high entropy gain during the binding process between **U_{60}** and alkali ions suggest that the hydration shells of Na^+/K^+ and **U_{60}** are damaged during the interaction. The ion selectivity of **U_{60}** is greatly influenced by both the morphologies of surface nanopores and the dynamics of the hydration shells.

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