UV AND IR SPECTROSCOPIC STUDIES OF COLD ALKALI METAL ION-BENZO CROWN ETHER COMPLEXES IN THE GAS PHASE

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We measured UV photodissociation and IR-UV double-resonance spectra of benzo-crown ether complexes with alkali metal ions (Li⁺, Na⁺, K⁺, Rb⁺, and Cs⁺) in a cold, 22-pole ion trap^a. All the complexes show a number of vibronically resolved UV bands in the 36000-38000 cm⁻¹ region. We used the IR-UV spectra in the CH stretching region to distinguish peaks in the UV spectra that belong to different conformers. The use of density functional theory allows us to determine the conformation of the complexes.

^aY. Inokuchi, O. V. Boyarkin, R. Kusaka, T. Haino, T. Ebata and T. R. Rizzo J. Am. Chem. Soc. 133(31), 12256 July 2011.