Ion-pair extraction by using cage-functionalized hosts: Strategy for selective extraction of NaOH from wastes

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Non-competitive extraction of Na^+X^- has been performed by using nitrogen-containing cage-annulated macrocycles. Interestingly, plots of the logarithm of Na^+ distribution *vs.* the reciprocal of thermochemical anion radii for extraction of Na^+X^- into $PhNO_2$ reveals that these hosts display markedly enhanced avidity toward selective NaOH extraction. In a related study, the X-ray crystal structure of a K^+ complexed bis-cage-annulated (20-crown-6) has been obtained. Therein, we note that the picrate anion is intimately involved in stabilization of the host-guest complex. Importantly, this effect has not been taken into account in previous calculations. Indeed, the computational results obtained from previous attempts to model complexation of cage-functionalized crown ethers and cryptands with alkali metal cations are not able to account for observations based upon the results of alkali metal picrate solution extraction experiments. In the present study, the Basis Set Superposition Error (BSSE)-corrected interaction energy has been estimated at the B3LYP level of theory in an attempt to quantify the stabilization energy contribution from picrate.