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Hydration Structures and Thermodynamic Properties of Cationized Biologically Relevant Molecules, $M^+(Indole)(H_2O)_n$ (M = Na, K; n = 3-6) HAOCHEN KE, JAMES LISY, Univ of Illinois - Urbana — The balance between various noncovalent interactions plays a key role in determining the hydration structures and thermodynamic properties of biologically relevant molecules in biological mediums. Such properties of biologically relevant molecules are closely related to their often unique biological functionalities. The indole moiety is a basic functional group of many important neurotransmitters and hormones and has been used as tractable model for more complex biomolecules. The cationized indole water cluster is a perfect system for the quantitative and systematic study of the competition and cooperation of noncovalent interactions, as electrostatic interactions can be adjusted by introducing different monovalent cations and hydrogen bonding interactions can be adjusted by varying the level of hydration. IRPD spectra with isotopic (H/D) analysis helped unravel the overlapping N-H and O-H stretching modes, a major challenge of earlier studies. Thermodynamic analysis using relative Gibbs free energies, for energy ordering, together with spectral analysis provided unambiguous assignment of spectral features and structural configurations. A systematic hydration model with an in-depth account of noncovalent interactions is presented.

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