

物理化学セミナー・日本分光学会中国四国支部 広島地区講演会

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“Exploring potential energy landscapes of cluster ions using mass-selected infrared laser spectroscopy. Applications to solutions and biological systems”

日時：2019年5月27日（月）14：50～16：05

場所：広島大学大学院理学研究科 E211 講義室

Infrared laser spectroscopy coupled with cryogenic ion trap mass spectrometry can probe conformational differences of small cluster ions as reflected in their vibrational spectra. When combined with computational methods, the structural differences can be revealed. Two examples will be presented.

- 1) The structures of sodium and potassium ions complexed to AcYHNMe, a termini-protected peptide sequence to model the GYG portion of the selectivity filter of a K⁺ channel, have been determined. Three conformations have been identified for both ions: two conformations have the ion bound to the two C=O groups; a third conformation has, in addition, a cation- π interaction with the aromatic ring of tyrosine, i.e. tridentate binding. The relative contributions of the three conformers are approximately the same for K⁺AcYHNMe, while the tridentate conformer is preferred for Na⁺AcYHNMe.
- 2) The structure of Cs⁺(H₂O)₃ has been characterized as a function of temperature and messenger tag (Ar and D₂). The tagging process and the temperature dependence indicate the well depths and barriers between different structural conformers.

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