



A non-covalent dimer formation of quaternary ammonium cation with unusual charge neutralization in electrospray-ionization mass spectrometry.

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Streszczenie

Specific and nonspecific non-covalent molecular association of biomolecules is characteristic for electrospray-ionization mass spectrometry analysis of biomolecules. Understanding the interaction between two associated molecules is of significance not only from the biological point of view but also gas phase analysis by mass spectrometry. Here we reported a formation of noncovalent dimer of quaternary ammonium denatonium cation with +1 charge detected in the positive ion mode electrospray ionization mass spectrometry analysis of denatonium benzoate. Hydrogen deuterium exchange of amide and carbon-bonded hydrogens revealed that charge neutralization of one denatonium cation is the consequence of amide hydrogen dissociation. DFT (Density Functional Theory) calculations proved high thermodynamic stable of formed dimer stabilized by the short and strong N..H-N hydrogen bond. The signal intensity of the peak characterizing non-covalent dimer is low intensity and does not depend on the sample concentration. Additionally, dimer observation was found to be instrument-dependent. The current investigation is the first experimental and theoretical study on the quaternary ammonium ions dimer. Thus the present study has great significance for understanding the structures of the biomolecules as well as materials.

Słowa kluczowe

non-covalent dimers, gas phase, quaternary ammonium cation, charge neutralization, ESI-MS, hydrogen-deuterium exchange, computational analysis, DFT

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