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Clustering of simple aminosulfonic acids-electrospray ionization mass spectrometric study.

Autorzy

Karolina Haupa

Zbigniew Szewczuk

Zofia Mielke

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Rationale: Aminosulfonic acids are structurally related to amino acids as bifunctional compounds. Some of them like taurine and homotaurine play important roles in biology. Although there is a vast literature devoted to the electrospray ionization mass spectrometric (ESI-MS) study of amino acid aggregation, no such study has been performed so far for aminosulfonic acids.

Methods: A gas-phase clustering study was performed for aminomethanesulfonic acid (AMS), taurine (Tau), homotaurine (HT), and cysteic acid (CA) from water and methanol/water solutions, using a Bruker TOF-Q spectrometer equipped with an ESI source, in the negative-ion mode. For selected anionic clusters the tandem mass (MS/MS) spectra were recorded and the breakdown curves were obtained. The cluster formation abilities (ACS parameter) of the studied molecules were calculated.

Results: Both singly and doubly charged clusters were formed when the acids were electrosprayed from water solutions; they may be described as [(H3N-R-SO3)n-zH](z-), where z = 1 or 2. The largest identified clusters are built of 20, 22, 20 and 4 monomers of AMS, Tau, HT and CA, respectively. The doubly negatively charged clusters were observed for n ≥9, 12, 14 in the case of AMS, Tau and HT. AMS pentamers and Tau, HT tetramers and hexamers show higher stabilities than the other clusters.

Conclusions: The results indicate that aminosulfonic acids form large stable clusters, similarly to aminocarboxylic acids. The cluster formation ability decreases with an increase in CH2 chain length within the series of the studied compounds. The large singly and doubly charged aggregates are formed under the conditions of the experiment, possibly in the droplets. Taurine dissolved in water seems to be a good calibrant for electrospray instruments in negative ion mode.

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