Clustering of sulfamic acid : ESI MS and theoretical study.

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Streszczenie

Sulfamic acid has wide application in industry and has been suggested to act as an effective nucleation agent for the formation of aerosols and cloud particles. From the point of view of the role that sulfamic acid may play in aerosol formation, the study of its homoaggregation is important. Gas phase clustering study was performed for sulfamic acid H3N·SO3, (ASA), from water and methanol-water solutions, by help of a TOF-Q spectrometer equipped with electrospray ionization source, in the negative-ion mode. The structure and stability of the (H3N·SO3)n and [(H3N·SO3)n-H](-) (n = 1-6) were studied using DFT/B3LYP/aug-cc-pVDZ method. The ESI MS study evidenced that both singly and doubly charged clusters are formed when the acids are electrosprayed from water solutions; they may be described as [(H3N·SO3)n-zH](z-) where z = 1 or 2. The largest identified clusters are built of 20 monomers. The theoretical studies showed that formation of higher order (ASA)n aggregates in the gas phase is energetically profitable. In contrast with the gas phase, aqueous solution does not favor the formation of (ASA)n aggregates. The study led to the conclusion that the ASA clusters are formed in the gas phase under the experimental conditions of the mass spectrometer. A hypothetical mechanism concerning the formation of the doubly negatively charged anionic aggregates is discussed. The obtained data suggest that small (NH3·SO3)n aggregates may also contribute to formation of aerosols in heavily polluted atmospheres with relatively large NH3 concentration.

Słowa kluczowe

mass spectra, quantum chemistry calculations, Aggregation, intermolecular interaction, sulfamic acid

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