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Molecular Signature of Atmospheric Organic Aerosols

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Aerosols are microscopic solid particles and/or liquid droplets suspended in air or gas. Aerosols can be natural (fog, forest exudates, for example) or artificial produced by anthropogenic activities. The study of aerosol particles has become quite relevant in recent years as they are found to influence, directly or indirectly, the climate, both at local and global scale. Atmospheric aerosols play a crucial role in the earth-atmosphere system affecting the natural cycles of rain and drought, precipitation and cloud formation, intensity of storms among others, which, as a consequence, may alter the nature of the local ecosystem and human health conditions. Depending on the size, they may also put influence on the radiative balance of the earth's atmosphere. Aerosol particles may scatter the solar radiation efficiently altering the atmospheric visibility, while others can absorb solar radiation readily to warm the atmosphere. In the Amazon region the aerosol particles play an important role as they act as cloud condensation nuclei (CCN) controlling the process of formation and lifetime of clouds and, thereby, influencing the local hydrological cycle. Understanding how these particles are formed and alter the atmospheric characteristics is of paramount importance for sustainable development [1,2].

In this work we study the interaction of methanesulfinic acid (CH_3SO_2H) and methanesulfonic acid (CH_3SO_3H) with atmospheric nucleation precursors such as H_2SO_4/NH_3 to see if they participate in the formation of aerosols. Analysis of the hydrogen bond for each structure and the structural, thermodynamics and spectroscopic properties were made. In addition, optical and electrical properties of the clusters were considered to analyze the atmospheric implications of each system. In order to obtain these properties we use Density Functional Theory (DFT) in Gaussian 03 [3] program.

Key-words: Aerosol, Methanesulfinic Acid, Methanesulfonic Acid.
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