

Stability structures of acetonitrile ionic clusters for astrochemical implications

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Abstract: Acetonitrile, CH₃CN, was first detected on the Sgr A and Sgr B molecular clouds, and since then had been detected in a lot of galactic sources, as Titan's atmosphere, comets, molecular clouds, protoplanetary disks and proto-stars.¹ Its relevance as an important astrophysical molecule is due to its high dipole moment (3.9 Debye), what makes it possible to estimative the temperature and density of molecular clouds by means of its emission lines due to rotational transitions.

Inside molecular clouds, at about 10K, the formation of acetonitrile ice on dust grains, forming ice mantles, is expected. Such mantles are exposed to different forms of radiation, as UV, X-rays, cosmic rays, stellar winds and charged particles.² These agents unleash several chemical reactions on the ice surface and desorption of molecules to gas-phase, being a good explanation for the molecular abundance on molecular clouds. The objective of this work is to study ionic clusters of acetonitrile with hydrogen, CH_xCN (x= 4 to 8), which has already been detected experimentally by the TOF-MS technique.³ The structures of these clusters were determined at Density Functional Theory (DFT), with M06 functional and cc-pVTZ basis. The relative energies and vibration frequencies of the cluster were calculated and correlated with the intensity of the TOF-MS spectrum obtained in such conditions as to mimic the astrophysical environment.

Key-words: acetonitrile, astrochemistry, stability structures

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