

ION INDUCED REACTIONS IN IMS STUDIED BY DFT

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Abstract. Sulfur containing hydrocarbons are being studied both experimentally and theoretically. Electron and ion induced processes are of main interest, represented by ionization reactions, electron attachment, as well as charge transfer reactions. In industry, the sulfur containing compounds (thiophenes) in crude oil are among the most abundant constituents, in some cases as high as 10% (Hua et al. 2004). On the other hand, sulfur is the tenth most abundant element in the universe and is known to play a significant role in biological systems, investigation of sulfur containing astrochemical molecules is therefore of high interest (Mifsud et al. 2021). Either sulfur containing hydrocarbons considered as industrial contaminant or highly important astrochemical molecules, among all possible chemicals five- or six-member rings containing sulfur atom are of interest as well. In this work Atmospheric Pressure Chemical Ionization of thiophen, its methyl-, dimethyl- and benzo- derivatives are studied with Ion Mobility Spectrometry (IMS) combined with Mass Spectrometry (Michalczuk et al. 2020). Quantum chemistry is used to model the thermochemical properties, ionization energies, electron affinities, bond energies in ions, proton affinities and reactions leading to formation of clusters of the studied analytes with reactant ions in IMS, produced with corona discharge source in ambient air.

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