IRMPD SPECTROSCOPY OF $Fe(H_2)_{1,2}^+$ AND OVERTONE STUDY OF $Ar_{1,2}FeH^+$ AND THEIR DEUTERATED SPECIES: LOOKING FOR IRON HYDRADES IN THE INTERSTELLAR MEDIUM

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Apart of being the most abundant metal in earth and the well-known leading role in the field of organic prosthetic group of proteins, iron potentially represents a crucial element for understanding interstellar processes, the evolution of interstellar dust and interstellar medium (ISM) composition. Despite the presumable gas-phase presence of iron in the ISM due to its very high abundance in the galaxy, its difficult detection in the interstellar gas-phase to date may be due to depletion of iron hidden in interstellar dust. Nevertheless, although ISM observations show iron to be severely depleted, it is highly expected to find iron-containing gas-phase molecular species in the ISM. This idea is reinforced by detection of FeCN in the ISM[a] or observed evidence of FeO presence in interstellar molecular clouds.[b] Gas-phase iron dihydrogen clusters and their deuterium substitutes were formed and stored in a cooled cell (ca. 80K) of a 4.7 T Fourier-Transform Ion Cyclotron Resonance instrument. Infrared photodissociation spectra were recorded in the H–H and D–D stretch region of 2230–4000 cm–1, supported by quantum chemical calculations. The spectral signature of the infrared photon absorption was reflected in the dissociation of intact H_2 or D_2 molecule. Additionally, to provide spectroscopic data on FeH^+ and complete previous analysis of Ar_2FeH^+,[c] we investigated overtone bands of Ar_2FeH^+ and $ArFeH^+$ in the 2300–4000 cm–1 region. We observed that while $ArFeH^+$ exhibits only a Fe–H overtone vibration in this region other plausible electronic transitions appear for Ar_2FeH^+, correlated with the ^5D state of the iron atom. Ion FT-IR spectroscopy combined with mass spectrometry represent a proven high-resolution tool to determine the molecular composition and structural behavior. Furthermore, overtone bands recognition may be used as a valuable strategy to obtain unambiguous identification of polyatomic aggregates fingerprints and further understanding of ISM composition and reactivity.

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[b] C.M. Walmsley, R. Bachiller, G.P. Des Forêts and P. Schilke, Astrophys. J., 2002, 566(2), L109-L112
[c] S. Jin, J. Heller, C. van der Linde, M. Ončák and M.K. Beyer, J Phys Chem Lett, 2022, 13(25), 5867