INFRARED STUDIES OF METAL CATION-DIHYDROGEN COMPLEXES

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Interactions between molecular hydrogen and metal cations play a key role in several contexts, including in the storage of molecular hydrogen in zeolites, metal-organic frameworks, and doped carbon nano structures, in which dihydrogen is typically attached to oxidised metal atoms. Arguably, the clearest view of the interaction between dihydrogen and a metal cation is obtained by probing M^+-H_2 complexes in the gas phase, free from the complicating influences of solvents or substrates. To this end, we have used infrared spectroscopy to examine a series of M^+-H_2 complexes, including complexes containing alkali metals (Li^+-H_2, Li^+-D_2, Na^+-H_2, Na^+-D_2), alkaline earth metals (Mg^+-H_2, Mg^+-D_2), main group metals and metalloids (B^+-H_2, B^+-D_2, Al^+-H_2), and transition metals (Cr^+-D_2, Mn^+-H_2, Zn^+-D_2 and Ag^+-H_2). These species have been characterized through their infrared absorptions in the H-H or D-D stretch regions (3700-4150 cm^{-1} and 2500-3000 cm^{-1} ranges, respectively) by monitoring metal cation photo-fragments as the infrared wavelength is scanned. The spectra, which typically display full resolution of rotational structure, can be used to develop and test intermolecular potential energy surfaces, and systematically explore the way in which the size and electronic structure of the metal cation influences the properties of the intermolecular $M^+ \cdots H_2$ bond.