STUDY OF ALKALI METAL ION−HYDROCARBON CLUSTERS: INFRARED SPECTROSCOPY OF $Li^+(CH_4)_n$ (n=1-7) CLUSTERS

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Previous work from our group[a] has revealed a surprisingly strong interaction between an alkali metal ion, Li^+, and the aliphatic hydrocarbon, cyclohexane. This study is directed to obtain a better understanding of the interaction of hydrocarbons with alkali metal ions by starting with the simplest of all hydrocarbons, methane. Using a combination of mass spectrometry and infrared spectroscopy, the C−H stretches of methane were studied in the 2800-3100 cm^{-1} region for $Li^+(CH_4)_n$ (n=1-7) clusters. The methane ν_1 C−H symmetric stretch at 2914 cm^{-1} is ordinarily IR inactive (Raman active), however, our studies show an intense band slightly lower in frequency for all cluster sizes. For cluster sizes n=5-7, we were able to detect the onset of occupation in the second shell by the appearance of new bands shifted to slightly higher frequency for the symmetric stretch region and in the region of the triply degenerate IR-active ν_3 C−H stretch (3020 cm^{-1}). *Ab initio* calculations using the Gaussian 03 suite of programs were performed to assist in characterizing the experimental results.

[a] G. N. Patwari and J. M. Lisy *J. Phys. Chem. A* **111**, 7585 (2007).