## INFRARED SPECTROSCOPY OF $M^+(CH_4)_n(H_2O)_{3-4}$ CLUSTERS (M=Li, Na): INDUCING $H_2O \cdots H_2O$ AND $H_2O \cdots CH_4$ HYDROGEN BONDS IN METHANATED CLUSTERS

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Experiments on  $M^+(CH_4)_n(H_2O)_{3-4}$  (M=Li and Na) have been carried out using tandem mass spectrometry and infrared spectroscopy in the O-H stretching region from 3400 cm<sup>-1</sup> to 3800 cm<sup>-1</sup>. We have found, for example, that a single CH<sub>4</sub> can induce hydrogen bonded conformers in the cases of Li<sup>+</sup>(CH<sub>4</sub>)<sub>1</sub>(H<sub>2</sub>O)<sub>3</sub>Ar<sub>0-1</sub>, which are absent in the Li<sup>+</sup>(H<sub>2</sub>O)<sub>3</sub>Ar<sub>0-1</sub> spectra<sup>*a*,*b*</sup>. Furthermore, upon addition of multiple CH<sub>4</sub> ligands, hydrogen bonding is not only maintained, but features associated with H<sub>2</sub>O···CH<sub>4</sub> hydrogen bonds are more intense, indicating the affinity of CH<sub>4</sub> to bind to available O-H sites. Spectra of Li<sup>+</sup>(CH<sub>4</sub>)<sub>1-3</sub>(H<sub>2</sub>O)<sub>4</sub> and Na<sup>+</sup>(CH<sub>4</sub>)<sub>1-3</sub>(H<sub>2</sub>O)<sub>3-4</sub> clusters will also be discussed, all of which exhibit the curious trait of H<sub>2</sub>O···H<sub>2</sub>O and H<sub>2</sub>O···CH<sub>4</sub> hydrogen bonding in the presence of hydrophobic, non-polar CH<sub>4</sub>. To better understand the nature and onset of H<sub>2</sub>O···CH<sub>4</sub> hydrogen bonding, the Li<sup>+</sup>(CH<sub>4</sub>)<sub>n</sub>(H<sub>2</sub>O)<sub>1-2</sub> spectra will be discussed.

<sup>&</sup>lt;sup>a</sup>D.J. Miller and J.M. Lisy J. Am. Chem. Soc. **130**, 15381 (2008).

<sup>&</sup>lt;sup>b</sup>D.J. Miller and J.M. Lisy J. Am. Chem. Soc. **130**, 15393 (2008).