IR SPECTROSCOPY OF [Ag·(CO\textsubscript{2})\textsubscript{n}]\textsuperscript{−} CLUSTERS: IMPLICATIONS FOR REDUCTIVE ACTIVATION OF CO\textsubscript{2}

BENJAMIN J. KNURR and J. MATHIAS WEBER, JILA and Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO 80309.

Reduction of CO\textsubscript{2} is an essential step in its chemical conversion from a greenhouse gas to useable fuel stocks, but is energetically unfavorable. Association with anions has been shown to facilitate partial charge transfer to a target CO\textsubscript{2} molecule, which could be a significant step towards CO\textsubscript{2} recycling. However there is still much uncertainty in the role of solvent effects on these chemical processes. We present infrared spectra of [Ag·(CO\textsubscript{2})\textsubscript{n}]\textsuperscript{−} (n = 2 – 11) to elucidate the nature of the charge carrier in the cluster, the effects of solvation on the charge distribution and the amount of reductive activation of CO\textsubscript{2} in the presence of a Ag anion. The structures of the [Ag·(CO\textsubscript{2})\textsubscript{n}]\textsuperscript{−} clusters are discussed in the framework of density functional theory. We compare and contrast the findings of [Ag·(CO\textsubscript{2})\textsubscript{n}]\textsuperscript{−} to those recently published on [Au·(CO\textsubscript{2})\textsubscript{n}]\textsuperscript{−} [1].