IR SPECTROSCOPY OF $[Ag{\cdot}(CO_2)_n]^-$ CLUSTERS: IMPLICATIONS FOR REDUCTIVE ACTIVATION OF CO_2

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Reduction of CO_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_2 molecule, which could be a significant step towards CO_2 recycling. However there is still much uncertainty in the role of solvent effects on these chemical processes. We present infrared spectra of $[Ag{\cdot}(CO_2)_n]^-$ ($n = 2 - 11$) 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_2 in the presence of a Ag anion. The structures of the $[Ag{\cdot}(CO_2)_n]^-$ clusters are discussed in the framework of density functional theory. We compare and contrast the findings of $[Ag{\cdot}(CO_2)_n]^-$ to those recently published on $[Au{\cdot}(CO_2)_n]^-$ [1].

1. B.J. Knurr and J.M. Weber, J. Amer. Chem. Soc., 134 (2012) 18804-18808.