IR SPECTROSCOPY OF $Au^-\cdot(CO_2)_n$ CLUSTERS: STRONG CLUSTER SIZE DEPENDENCE OF METAL-LIGAND INTERACTION

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Gold is a widely used catalyst in many reactions. For example, negatively charged gold clusters have been shown to catalyze the oxidation of CO to CO_2 [1], although the precise role of negative charge has not been understood. A previous study from our laboratory has shown that the binary complex $[AuCO_2]^-$ has the CO_2 ligand covalently bound to the gold, leading to significant charge transfer onto the CO_2 unit and concomitant decrease of the OCO bond angle and weakening of the CO bonds [2]. The structure of this aurylformate anion is reminiscent of structural motifs assumed to play a role in a recent approach towards production of solar fuels using reductive activation of CO_2 [3].

We report infrared spectra of $Au^-\cdot(CO_2)_n$ clusters highlighting solvation mediated changes in the infrared signatures of the ligands. These results are discussed in the framework of quantum chemistry calculations.

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