OXALATE FORMATION IN TITANIUM–CARBON DIOXIDE ANIONIC CLUSTERS STUDIED BY INFRARED PHOTODISSOCIATION SPECTROSCOPY

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Carbon-carbon bond formation during carbon dioxide fixation would enable bulk synthesis of hydrocarbon chains, generally through formation of an oxalate intermediate. In this talk, we demonstrate the formation of $[\mathrm{Ti}(\mathrm{CO_2})_y]^-$ (y = $4 - 6$) gas phase clusters with an oxalate ligand bearing significant (> 1 e^-) negative charge. Gas phase anionic clusters were generated using laser ablation of a titanium metal target in the presence of a CO_2 expansion, and the infrared photodissociation spectra were measured from $950 - 2400$ cm^{-1}, revealing vibrations characteristic of the oxalate anion. The molecular structure of these clusters was identified by comparing the experimental vibrational spectra with density functional theory calculations.