INFRARED PHOTODISSOCIATION SPECTROSCOPY OF SILICON-CARBONYL CATIONS: EVIDENCE FOR ASSYMETRIC CARBONYL COORDINATION.

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Cationic silicon carbonyl clusters, consisting of up to twenty carbonyl ligands, are produced via laser vaporization with a pulsed nozzle source and cooled in a supersonic beam. The cations and their argon tagged analogues are mass selected in a reflectron time-of-flight mass spectrometer and studied with infrared laser photodissociation spectroscopy near the free molecular CO vibration (2143 cm^1). Silicon carbonyl complexes having more than two ligands fragment by loss of CO, whereas the argon tagged complexes fragment by loss of argon. All clusters have resonances near the free molecular CO stretch that provide distinctive patterns from which information on their structure and bonding can be obtained. The number of infrared-active bands, their frequency positions and relative intensities, indicate that species larger than n=2 consist of an asymmetrically coordinated $Si(CO)_2^+$ core with additional CO ligands attached via van der Waals interactions. Density functional theory computations are carried out in support of the experimental spectra.