INFRARED SPECTROSCOPIC AND THEORETICAL STUDY OF THE HC_nO^+(N=5-12) CATIONS

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Carbon chains and derivatives are highly active species, which are widely existed as reactive intermediates in many chemical processes including atmospheric chemistry, hydrocarbon combustion, as well as interstellar chemistry. The carbon chain cations, HC_nO^+ (n = 5-12) are produced via pulsed laser vaporization of a graphite target in supersonic expansions containing carbon monoxide and hydrogen. The infrared spectra are measured via mass-selected infrared photodissociation spectroscopy of the CO "tagged" [HC_nO·CO] cation complexes in the 1600-3500 cm^{-1}region. The geometries and electronic ground states of these cation complexes are determined by their infrared spectra in conjunction with theoretical calculations. All the HC_nO^+ (n = 5-12) core cations are characterized to be linear carbon chain derivatives terminated by hydrogen and oxygen. The HC_nO^+ cations with odd n have closed-shell singlet ground states with polyyne-like structures, while those with even n have triplet ground states with allene-like structures.