INFRARED SPECTROSCOPY OF CARBOCATIONS UPON ELECTRON IONIZATION OF ETHYLENE IN HELIUM NANODROPLETS

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The electron impact ionization of helium droplets doped with ethylene molecules and clusters yields diverse $C_XH_Y{}^+$ cations embedded in the droplets. The ionization primarily produces $C_2H_2{}^+$, $C_2H_3{}^+$, $C_2H_4{}^+$, and $CH_2{}^+$, whereas larger carbocations are produced upon the reactions of the primary ions with ethylene molecules. The vibrational excitation of the cations leads to the release of bare cations and cations with a few helium atoms attached. The laser excitation spectra of the embedded cations show well resolved vibrational bands with a few wavenumber widths—an order of magnitude less than those previously obtained in solid matrices or molecular beams by tagging techniques. Comparison with the previous studies of free and tagged $CH_2{}^+$, $CH_3{}^+$, $C_2H_2{}^+$, $C_2H_3{}^+$, and $C_2H_4{}^+$ cations shows that the helium matrix typically introduces a shift in the vibrational frequencies of less than about 20 cm-1, enabling direct comparisons with the results of quantum chemical calculations for structure determination. This work demonstrates a facile technique for the production and spectroscopic study of diverse carbocations, which act as important intermediates in gas and condensed phases.

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