THE INFRARED SPECTRA OF IONS DERIVED FROM ALLENE AND PROPYNE AND TRAPPED IN SOLID NEON

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When a Ne:allene or a Ne:propyne sample was codeposited at approximately 5 K with a sample of pure neon that had been excited in a microwave discharge to provide a 16.6-16.85 eV energy source, prominent new infrared absorptions which can be assigned to the allene and propyne cations and to the allenyl anion resulted. Comparison of the product spectra observed in experiments on the various isotopically substituted precursor molecules with the vibrational fundamental patterns obtained from density functional and ab initio calculations is crucial to the positive identification of these three products. These results may be contrasted with those of the corresponding gas-phase studies, in which cyc-$C_3H_3^+$ predominates in this excitation energy range. In the present experiments, collisions with the excess of neon atoms in the sampling region rapidly remove excess energy from the initially formed allene and propyne cations, inhibiting the loss of an H atom from those two species.