IR Spectroscopy of Allyl Radicals in Helium Nanodroplets

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Superfluid helium nanodroplets have been demonstrated to be an effective tool for cooling species, forming clusters of controlled size, and studying these clusters with IR-spectroscopy and mass spectrometry. Due to the strong cooling effect, also reactive species such as radicals can be investigated using this method. Because of their high reactivity the knowledge of these systems and their interactions is still in its infancy, although their importance is unquestionably related to their common presence in real life.

The allyl radical (CH_2CHCH_2) is the simplest π-conjugated hydrocarbon radical having an open-shell electronic structure due to its unpaired electron [1]. It has been firmly established that the allyl radical has C_{2v} symmetry with a $2A_2$ ground electronic state [2].

Like all other C3-hydrocarbon units the Allyl radicals are believed to be precursors in the formation of soot and polynuclear aromatic hydrocarbons, because two C3 units can combine to form an aromatic unit, like phenyl-radicals [3]. Furthermore the allyl radical is also a key intermediate in tropospheric chemistry.

[1] K. Tonokura and M. Koshi, J. Phys. Chem. A, 2000, 104, 8456-8461.
[2] J.Han et. al., J. Chem. Phys., 2002, 116, No. 15.
[3] T. Schultz and I. Fischer, J. Chem. Phys., 1998, 109, No. 14.