INFRARED SPECTRUM OF THE CYCLOBUTYL RADICAL IN He DROPLETS

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Gas phase cyclobutyl radical (C_4H_7) is produced via pyrolysis of cyclobutyl methyl nitrite ($C_4H_7(CH_2)ONO$). The nascent radicals are promptly solvated in liquid He droplets, allowing for the acquisition of the infrared spectrum in the CH stretching region. Anharmonic frequencies are predicted by VPT2+K simulations based upon a CCSD(T)/ANO0 force field. Several resonance polyads emerge in the 2800-3000 cm^{-1}region as a result of anharmonic coupling between the CH stretching fundamentals and CH_2 bend overtones and combinations. Evidence of rotational fine structure is observed for two bands. The vibrationally averaged cyclobutyl radical geometry and the C_4H_7 potential energy surface will be discussed. In agreement with the findings by Schultz[1] and coworkers, 1,3-butadiene is formed from cyclobutyl ring opening and H atom loss, given a sufficiently high pyrolysis temperature. However, signatures of 1-methylallyl and allylcarbinyl radicals, proposed[1] as intermediates along the above mentioned reaction path, are yet to be seen.

1. Schultz, J.C., Houle, F.A., Beauchamp, J.L. J. Am. Chem. Soc. 1984, 106, 7336-7347.