HEAVY ATOM LARGE AMPLITUDE MOTION IN RG-CYCLOPROPANE COMPLEXES

WOLFGANG JÄGER and YUNJIE XU, *Department of Chemistry, University of Alberta, Edmonton, AB, Canada, T6G 2G2*.

Rotation-tunneling spectra of the van der Waals complex Ne-cyclopropane, and pure rotational spectra of Ar-cyclopropane and Kr-cyclopropane, were measured with a Fourier transform microwave spectrometer in the frequency range from 4 to 19 GHz. The observed transitions are all of a-type and are in accord with those of prolate symmetric top molecules where the rare gas atom is positioned on the C_3 axis of the cyclopropane subunit above its symmetry plane. Effective separations between the center-of-mass of cyclopropane and the rare gas atoms were obtained from the ground state rotational constants. Transitions of two isomers were observed for complexes that contain monodeuterated cyclopropane. In the case of the parent Ne-cyclopropane complex, and its ^{22}Ne- and mono ^{13}C-isotopomers, all transitions appeared as doublets. This is attributed to a tunneling internal rotation motion of the cyclopropane unit within the complex.