VIBRATIONAL SPECTRA AND ASSIGNMENTS OF FUNDAMENTALS OF 1,1-DIFLUOROCYCLOPROPANE AND ITS d_2 AND d_4 ISOTOPOMERS

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Infrared and Raman spectra of 1,1-difluorocyclopropane (DFCP) and its $2,2-d_2$ and d_4 isotopomers have been recorded. Included are gas-phase Raman spectra obtained with an FT instrument and a simplified sample arrangement. A full vibrational assignment has been proposed for the three isotopomers, and normal coordinate calculations have been done in preparation for determining an equilibrium structure for this ring system. A microwave investigation provides the needed rotational constants for a full set of isotopomers of DFCP.^{*a*}

^aA. T. Perretta, V. W. Laurie, J. Chem. Phys. 62, 2469 (1975).