INFRARED AND RAMAN SPECTRA AND PSEUDOROTATION OF 1,3-DITHIOLANE AND TETRAHYDROTHIOPHENE

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The vibrational spectra of 1,3-dithiolane and tetrahydrothiophene have been recorded and analyzed with a focus on the low-frequency ring-bending and ring-twisting vibrations. For 1,3 dithiolane, the bending series occurs in the 35 to 60 (cm^{-1}) region of the far-infrared spectrum while for tetrahydrothiophene bands were observed between 40 and 115 (cm^{-1}). These bands can be interpreted utilizing potential energy surfaces for the out-of-plane vibrations. The mid-infrared and Raman spectra were utilized to assign the other vibrations of these molecules and to compare the experimental frequencies to predicted values from the MM3 molecular mechanics program.