INFRARED SPECTRA, OUT-OF-PLANE RING MODES, AND POTENTIAL ENERGY SURFACE FOR PHTHALAN. A CASE OF STRONG VIBRATIONAL COUPLING

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The far- and mid-infrared spectra of phthalan have been recorded and the ring-puckering and ring-flapping (butterfly) vibrations, which have fundamental frequencies of 31 and 216 cm^{-1} respectively have been examined in detail. These two vibrations are strongly coupled and result in complex spectra with numerous sum, difference and hot bands series. Since a one-dimensional potential energy function for the ring-puckering vibration cannot adequately account for the spectra, previous analysis of the far-infrared and dispersed fluorescence spectra were not accurate. We have utilized a two-dimensional potential energy surface along with calculated kinetic energy expansions to attain a very nice agreement between observed and calculated transition frequencies. This bicyclic ring molecule is found to be nearly planar with a small barrier to planarity (around 50 cm^{-1}), due to the ring puckering.