

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

SACHIE SAKURAI, NIKLAS MEINANDER, JAAN LAANE, *Department of Chemistry, Texas A&M University, College Station, TX 77843*; TIM KLOTS, *BDM Oklahoma, Bartlesville, OK 74001*.

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.