INFRARED AND RAMAN SPECTRA, NORMAL COORDINATE ANALYSIS AND TRANFERABILITY OF FORCE CONSTANTS OF SOME MONONITRO SUBSTITUTED MOLECULES

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The Raman and Fourier transform infrared (FTIR) spectra of p-, m- and o- nitrobenzamides, p-, m- and o- nitrobenzaldehydes and p-, m- and o- nitrotoluenes were measured. Raman polarization measurements were made wherever possible. A normal coordinate analysis was carried out for both in-plane and out-of plane vibrations of these molecules using 111-parameter modified valence force field. An overlay least-squares technique was employed to refine the force constants using 316 frequencies of nine molecules. The reliability of these force constants was tested by making a zero-order calculation for both in-plane and out-of plane vibrations of p-, m- and o- methyl benzaldehydes; 3,5,-dichloro-p-anisamide, 3,5,-dibromo-p-anisamide and 3,5-dibromo-4-hydroxy benzamide; 4-chloro-3-nitrotoluene, 2-bromo-4-nitrotoluene and 2-bromo-5-nitrotoluene. Unambiguous vibrational assignments of all the fundamentals were made by using the potential energy distributions and eigen vectors.