VIBRATIONAL ANALYSIS AND VALENCE FORCE FIELD FOR NITROTOLUENES, DIMETHYLANILINES AND SOME SUBSTITUTED METHYLBENZENES

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The Fourier transform infrared (FTIR) and Raman spectra of 2-amino-4-nitro-toluene; 2-amino-5-nitrotoluene; 2,4-dimethylaniline; 2,5-dimethylaniline; 2,6-dimethylaniline; 1,2,4-trimethylbenzene; 1,3,5-trimethylbenzene and pentamethyl-benzene have been recorded in the range 4000-400 cm^{-1} and 4000-30 cm^{-1}, respectively. A normal coordinate analysis was carried out for both in-plane and out-of-plane vibrations of these molecules using an 81-parameter modified valence force field. The force constants were refined using 251 frequencies of eight molecules in the Overlay least-square technique. The reliability of force constants was tested by making zero-order calculations for both in-plane and out-of plane vibrations for five related molecules. The potential energy distribution (PED) and eigen vectors calculated in the process were used to make unambiguous vibrational assignment of all the fundamentals.