# Vibrational Analysis of Trimethylphenyl Ammonium Chloride

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An FT-IR spectrum of trimethylphenyl ammonium chloride (TMPAC) has been recorded in the region 4000 – 400 $cm^{-1}$. The optimized geometry and vibrational spectrum TMPAC in the ground state have been calculated by using ab initio Hartree-Fock (HF) calculations and the density functional method B3LYP with the 6-31G (d) basis set. The obtained vibrational frequencies and optimized geometric parameters (bond lengths and bond angles) were in very good agreement with the experimental data. The comparison of the observed and calculated results for the vibrational frequencies of TMPAC exhibited that the scaled B3LYP method is superior compared to the scaled HF method. Furthermore the calculated infrared and Raman intensities are also reported.

*Key words:* Trimethylphenyl Ammonium Chloride; Wavenumbers; IR Spectra; Raman Spectra; HF; DFT.