# Density Functional Theory and ab initio Hartree-Fock Calculations of Molecular Structure and Vibrational Spectra of Anilinium Nitrate

Davut Avcı, Adil Başoğlu, and Yusuf Atalay

Sakarya Üniversitesi, Fen Edebiyat Fakültesi, Esentepe Kampüsü, Fizik Bölümü, 54140, Adapazarı, Turkey

Reprint requests to Y. A.; Fax: +90 264 295 5950; E-mail: yatalay@sakarya.edu.tr

Z. Naturforsch. **63a,** 712 – 720 (2008); received February 1, 2008

The molecular geometry, vibrational frequencies, infrared intensities, Raman scattering activities and several thermodynamic parameters of anilinium nitrate in the ground state have been calculated by both Hartree-Fock (HF) and three density functional theory (DFT) methods (B3LYP, BLYP and B3PW91) using the 6-31G(d) basis set. The results of the optimized molecular structure are presented and compared with the experimental X-ray structure. The optimized geometric bond lengths are described very well by the HF method while bond angles are reproduced more accurately by the DFT methods. Comparison between the observed fundamental vibrational frequencies of anilinium nitrate and the results of DFT and HF methods indicates that B3LYP is superior to the scaled HF, BLYP and B3PW91 approaches for molecular vibrational problems. The computed vibrational frequencies are used to determine the types of molecular motions associated with each of the experimental bands observed. In addition, calculated results are related to the linear correlation plot of computed data versus experimental geometric parameters and IR data.

*Key words:* Anilinium Nitrate; DFT; HF; IR and Raman Spectra; Structure Elucidation; Vibrational Assignment; Thermodynamic Parameters.