

**P012** Investigation of solvent effect on properties and activities of amino acids: glycine, alanine, leucine, serine, lysine, asparagine, histidine and phenyl alanine

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Abstract: Amino Acids can be defined separately by the unique characteristic rendered to each amino acid molecule as a result of the varying reactive abilities of their side chains. Structural analysis is performed using ab initio calculations in GAUSSIAN 98 program. The behaviour of every atom as well as that of molecular fragments COOH, CH<sub>2</sub>, NH<sub>2</sub> show that atoms in molecules (AIM) and Natural Population Analyses (NPA) charges exhibit not only a good conformational independence but also provide a meaningful picture of the electron charge distribution in this system. In this paper relative energies, dipole moments, rotational constants, vibration frequencies, charges of important atoms in structure of amino acids, NMR chemical shielding (symmetric & asymmetric:  $\Delta\sigma$ ,  $\eta$ ) and hydrogen bonded have been studied by systematic abinitio calculations in three levels of theory: Hartree-Fock(HF), DFT (B3LYP) and MP2. Nine amino acids consist of: alanine, asparagine, glycine, cysteine, methionine, serine, proline, threonine and valine. They were studied in gaseous phase and in two aprotic solvents and different basis sets: 6-31g, 6-311g, 3-21g and 6-311++g were tested and compared to determine which basis set is the most efficient to model these particular amino acids. A series of gauge independent atomic orbital (GIAO) magnetic shielding calculations also have been done in solution and gaseous phase.