

DFT MODELLING OF SOLID STATE MOLECULAR STRUCTURES OF PHOSPHONIC DERIVATIVES OF AMINO ACIDS

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SUBJECT OF OUR STUDIES

Substituted alkanephosphonic acids constitute a class of analogs of natural amino acids in which the peptide bond is formed between the carboxylic group of an amino acid and the amino one of the phosphonic moiety. They have been found to act as antibacterial agents, neuroactive compounds, anticancer drugs and pesticides. In this work we present results obtained for the phosphonic derivatives of glycine and proline (fig. 1).

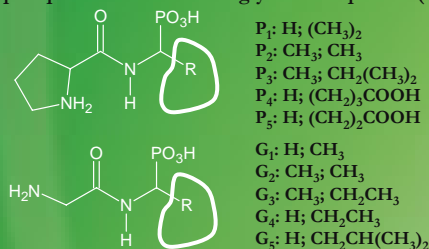


Fig. 1. Compounds presented here.

AIM

Our studies focus on evaluation of an appropriate theoretical model of the title compounds for which calculations of IR and Raman spectra would give proper description of experimental data. As models for calculations, we took into consideration various rotamers predicted from calculations of potential energy structures with respect to selected dihedral angles, structures with various deprotonation patterns and models with intra- as well as intermolecular H-bonding. Crystallographic data [1] of the analogous compounds (glycine, phenylalanine and leucine derivatives) reveal that these type of molecules exist as zwitterions surrounding by water molecules and forming complex H-bonding with the neighbouring phosphonic moieties (fig. 2). To mimic such an environment, we calculated vibrational spectra by using PCM model ($\epsilon=78.4$) for the zwitterions. As shown below, this approach yielded the best simulation of the experimental spectra. All the calculations were performed by using Gaussian 03 and Gamess packages [2,3].

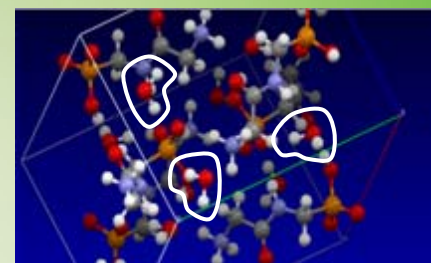


Fig. 2. Crystallographic structure of glycyl-aminomethylphosphonic acid monohydrate [1].

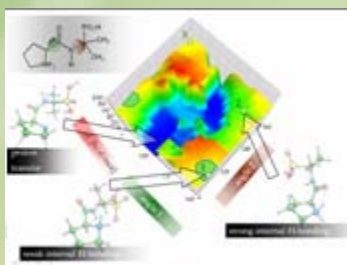


Fig. 3. Exemplary PES analysis for P2 (AM1).

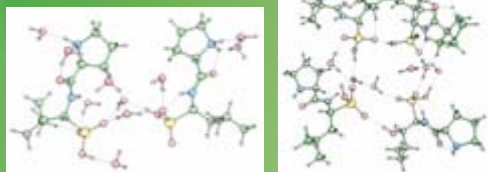


Fig. 4. Dimer (left) and tetramer (right) models for P2.

Fig. 5. Comparison of calculated and experimental vibrational spectra for P₂.

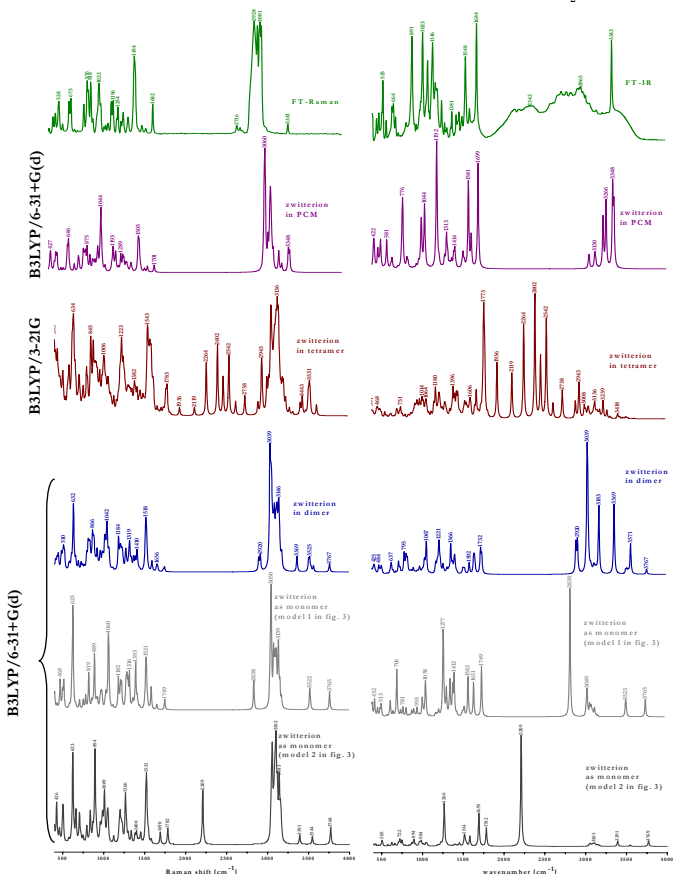


Fig. 6. Comparison of calculated and experimental vibrational spectra for G₂.

