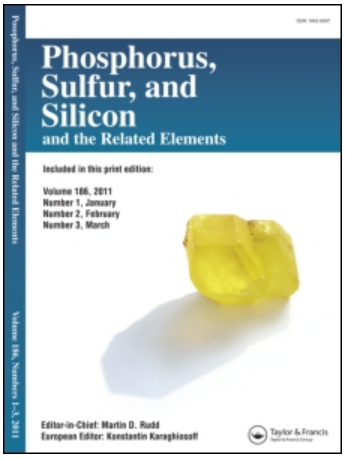

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Simulation of 1-Aminopropanephosphonic Acids with Consideration of Aqueous Solutions

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SIMULATION OF 1-AMINOPROPANEPHOSPHONIC ACIDS WITH CONSIDERATION OF AQUEOUS SOLUTIONS

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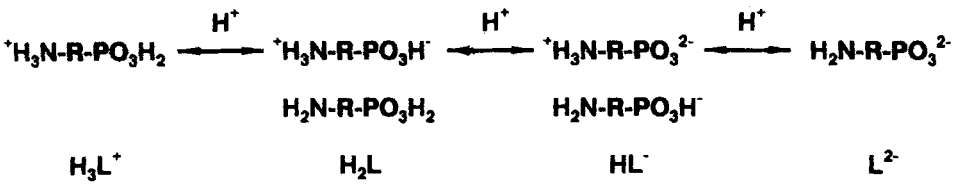
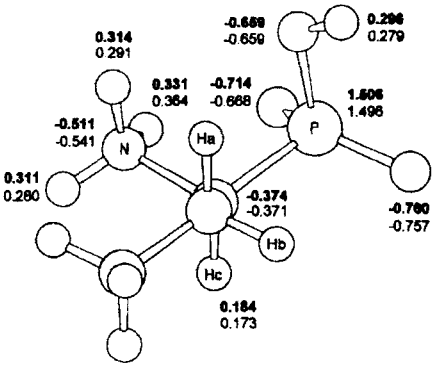
While solid state structures of aminophosphonic acids are well characterised by X-Ray methods only few informations are available concerning the solution state structures. We have attempted to simulate the structures of acids and corresponding cations and anions in aqueous solutions. It proved to be difficult to describe correctly the electrostatic interactions of solute and solvent by theoretical methods.

As a model system we used the 1-aminopropanephosphonic acid, well-known from basic research in the London group of. The protonation equilibrium of $CH_3CH_2CH(NH_2)PO_3H_2$ is described by the following scheme:



The structures of ionic species in aqueous solutions may help to interprete biological activities. The atomic partial charge contribution is important to discriminate between the micro-dissociation species of LH_2 and LH^-.

Results from ab-initio calculations with 3-21G** and 6-31+G** basis sets confirm the protonation sequence.



As example the molecular structure and the calculated atomic partial charges for the zwitter ionic form of the LH_2 species with GAUSSIAN 92 (3-21G**) for the gasphase (normal font) and in a polar medium (bold font) using the SCRF method with ε=78.36 for H_2O are given in the figure.