A model study of the intermolecular interactions of amino acids in aqueous solution: the glycine-water system. Foerner, Wolfgang; Otto, Peter; Bernhardt, Julius; Ladik, Janos J

Abstract

Calcns. of the glycine zwitterion surrounded by H2O were performed using the mutually consistent field (MCF) method and perturbation theor. expressions. Two different models for the hydration shell were chosen: the glycine.6H2O and glycine.12H2O complexes, representing the most probable first and second solvation shell, resp. The electrostatic approach was used to study the part of the potential energy surface which is detd. by varying lengths of H bonds between glycine and water in glycine.12H2O.