Glycine and sodium glycinate in water: Molecular dynamics simulations and experiment

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In recent years, aqueous solutions of amino acid salts have attracted attention as promising carbon dioxide absorbents, in addition to the fundamental role in processes of life played by amino acids in general. To understand physicochemical properties of amino acids and their salts in solutions, computer simulations, particularly molecular dynamics (MD), are quite helpful when their results are matched to the experimental data. One problem here is adjusting the model potential parameters, typically within the framework of an existing force field, to reproduce the behavior of the system as observed in experiment. While the simplest amino acid, glycine, was extensively studied by MD before, this is not the case for its anionic salts.

In the present work, we performed MD simulations of glycine (Gly) and sodium glycinate (NaGly) aqueous solutions, using the OPLS-AA force field for short-range interactions, testing two water models (SPC/E and TIP4P/2005), different atomic charge sets for the glycine zwitterion and the glycinate anion, and different model potentials for Na^+. The MD results were compared with our measurements of diffusion in those solutions by the PGSE NMR method and with experimental data on densities and transport characteristics from other authors.

We have found that in MD, to obtain a reasonable agreement with the experiment, one should assume relatively low charges on N and H in amino groups. MD using the TIP4P/2005 water model (that predicts the diffusion coefficient and viscosity of pure H_2O better than SPC/E), the Joung – Cheatham potential for Na^+, and CNDO atomic charges for glycine and glycinate gives a quite satisfactory agreement with the experimental data for both Gly and NaGly solutions.

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