Concentration-dependent sedimentation and diffusion coefficient in analytical ultracentrifugation experiments

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Experimental data of analytical ultracentrifugation (AUC) experiments is defined by sedimentation and diffusion transport of molecules in solution. While the sedimentation properties define the position of the measured sedimentation boundaries, information on the diffusion is included in the broadening. Both effects are then analysed with well-established finite element solutions of Lamm's equation The results from this multidimensional analysis provide e.g. molecular mass or size distributions or information on core-shell structures [1,2]. Moreover, it is known that the properties of macromolecules and particles in AUC experiments are influenced by concentration-dependent sedimentation and diffusion coefficients, which are described by two interaction terms k_s and BM. While the Gralen coefficient k_s represents hydrodynamic interactions, the second virial coefficient B is a thermodynamic quantity and is used to correct for non-ideal diffusional properties throughout AUC experiments [3]. Here, we show that by analyzing these parameters via AUC, information of the global interaction of particles in solution can be retrieved. Hence, the second virial coefficient was determined for a lysozyme model system as a function of the pH of the solution from AUC experiments Figure 1 (left) presents the retrieved values for BM from the AUC measurements as black bars. It can be concluded that the interaction term BM is a measure for stability and the tendency of the system to aggregate as it follows the trend of the zeta-potential representing charge-charge interactions. Theoretical considerations from DLVO theory show that with increasing pH of the solution, the contribution from an electrostatic potential decreases and thus predict a decreasing interaction term with increasing pH, as can be seen in Figure 1 (right). This approach paves the way for a direct correlation between global interaction potentials in solution and parameters obtained from AUC experiments.
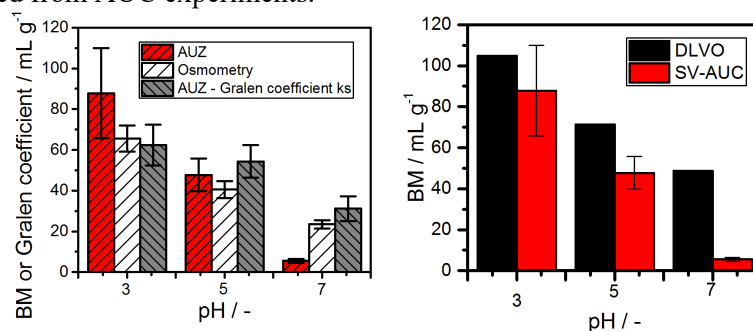

Figure 1: Left: Second virial coefficient from SV AUC experiments (grey bars), osmometric measurements (red bars) alongside the Gralen-coefficients (Grey bars). Right: Second virial coefficient from DLVO theory (black bars) alongside the values from SV-AUC experiments (red bars).

References

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