Thesis of PhD dissertation

1. I performed small angle neutron scattering studies on the aqueous solutions of 1,2- and α,ω-diols containing n = 3 to 7 carbon atoms in the alkyl chain in a wide concentration and temperature range. From the experimental results I have determined the Ornstein-Zernike correlation lengths; from the shape of the scattering curves I have found that diols with n = 5 - 7 are forming aggregates in their solutions.

2. On the scattering curves of the aqueous solutions of 1,2-diols of high concentration ($x_{diol} > 0.10$), in contrast with those of α,ω-diol solutions, a diffraction peak appears, indicating the development of a higher order in the solutions. I have determined the repeating distances in the function of concentration and temperature. I have found that this distance is decreasing with concentration; this can be interpreted as the decrease of the thickness of the water-rich domains between the diol domains. The position of the peak is temperature independent; its maximum is decreasing with increasing temperature indicating the gradual breaking up of the aggregates.

3. From the forward scattering intensities I calculated the Kirkwood-Buff integrals. I have found that the attractive diol-diol interaction is stronger in the solutions of 1,2-diols in heavy water than in the solutions of α,ω-diols with the same hydrocarbon chain length. In the low concentration range ($x_{diol} < 0.10$) the attractive diol-diol interaction is increasing with the length of the hydrocarbon chain and with increasing temperature (a feature characteristic of hydrophobic interactions).

4. From the small angle neutron scattering curves of heavy water solutions of dimethylethyleneurea (DMEU) and dimethylpropyleneurea (DMPU) I have determined the radii of gyration of the scattering particles. I have arrived at the conclusion that, in the concentration range studied (0.005 – 0.5 mole fraction), pairs of solute molecules are formed in both solutions. The DMEU-DMEU molecule pairs are more stable than the DMPU-DMPU molecule pairs.

5. From the experimental forward scattering intensities I have determined the second osmotic virial coefficients in the solutions of dimethylethyleneurea and dimethylpropyleneurea in

heavy water. I have found that, in contrast to the previous results on tetramethylurea, the values of the virial coefficients are temperature independent suggesting the non-hydrophobic character of the solute-solute interactions.

6. The values of the molal volume second virial coefficients, calculated from the density data on the solutions of DMEU and DMPU in water, show that the DMPU molecule has a more pronounced structure making effect on water than the DMEU molecule.