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Small Angle Neutron Scattering Studies of the Counterion Effects on the Molecular Conformation and Structure of Charged G4 PAMAM Dendrimers in Aqueous Solutions WEI-REN CHEN, SNS, ORNL, LIONEL PORCAR, YUN LIU, PAUL BUTLER, NCNR NIST — The structural properties of generation 4 (G4) poly(amidoamine) starburst dendrimers (PAMAM) with an ethylenediamine (EDA) central core in D_2O solutions have been studied by small angle neutron scattering (SANS). Upon the addition of DCl, SANS patterns show pronounced inter-particle correlation peaks due to the strong repulsion introduced by the protonation of the amino groups of the dendrimers. By solving the Ornstein-Zernike integral equation (OZ) with hypernetted chain closure (HNC), the dendrimer-dendrimer structure factor S(Q) is determined and used to fit the experimental data. Quantitative information such as the effective charge per dendrimer and its conformational change at different pH values is obtained. The results show clear evidence that significant counterion association occurs, strongly mediating the inter-dendrimer interaction. The influence of interplay between counterions and molecular protonation of dendrimers imposes a strong effect on the dendrimer conformation and effective interaction.

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