



EXTENDED SYMMETRIC POISSON-BOLTZMANN THEORY

By ARUP MUKHERJEE

LAP Lambert Acad. Publ. Aug 2010, 2010. Taschenbuch. Book Condition: Neu. 220x150x5 mm. This item is printed on demand - Print on Demand Neuware - To study the structural and thermodynamic properties of electrolyte solutions the Symmetric Poisson-Boltzmann theory has been extended up to six components and the resulting coupled equations for the mean electrostatic potentials have been solved numerically using a quasi-linearization iterative procedure. The exclusion volume term approximated by PY hard sphere RDF has been calculated using Perram's method along with Verlet and Weis corrections. The RDFs have been computed for four-component systems comprising a single electrolyte with two other neutral components for various cases. Excellent agreement has been found for each case when compared with MC data. The theory predicts the experimental trends when applied to measure the second virial coefficient in a colloidal system of silicotungstate, in a solution of HCl, LiCl or NaCl. The extended theory and the numerical solution techniques can be utilized to study the structural and thermodynamic properties of multicomponent electrolytes which are of great interest because of their frequent presence in industrial processes and in branches of sciences like colloid and surface science, polymer science, biophysics and chemistry. 80 pp. Englisch.

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