4c Modified Absorption Isotherm Model for Aqueous Electrolytes

William ONeal Rains

A large body of experimental evidence supports the relationship between water activity and molality for concentrated electrolytes as embodied by the Stokes-Robinson and Ally-Braunstein modifications of the Brunauer-Emmett-Teller (BET) adsorption isotherm (here after referred to as the BET Model). The BET Model is based on the concept that ions in concentrated solutions exist in varying degrees of hydration, that is some ions have a complete monolayer while others have an incomplete "shell" of H2O; this model has been the subject of renewed interest in recent years due to its simplicity and robustness. This PhD work applies the BET Model to thermodynamic predictions for a number of concentrated electrolyte solutions. The electrolytes chosen are various nitrate salts and nitric acid. The research has applications in a number of applications, including atmospheric aqueous thermodynamics, oxidation of organics in concentrated nitric acid solutions and also in health-related studies. Publications coming from the current research are presented below.

W. O. Rains and R. M. Counce, "Liquidus Curves of LiNO3 (aq) Calculated from the Modified Adsorption Isotherm Model for Aqueous Electrolytes," (in preparation)

W. O. Rains and R. M. Counce, "Liquidus Curves of NH3NO3 (aq) Calculated from the Modified Adsorption Isotherm Model for Aqueous Electrolytes," (in preparation)

W. O. Rains and R. M. Counce, "Liquidus Curves of AgNO3 (aq) Calculated from the Modified Adsorption Isotherm Model for Aqueous Electrolytes," Monatsheft fur Chemie, 134, 1541-1544 (2003)

W. O. Rains, B. B. Spencer and R. M. Counce, "Extension of the BET Model Solution Model to Highly Nonideal Systems," Paper presented at 11th Symposium on Separation Science and Technology for Energy Applications, Gatlinberg, TN (1999).

W. O. Rains, R. M. Counce and B. B. Spencer, "Analysis of the Variability in the BET Solution Model for the Nitric Acid – Water System," Industrial Engineering Chemistry Research, 39(1), 236-239 (2000)

W. O. Rains, R. M. Counce and B. B. Spencer, "Application of the Brunauer-Emmett-Teller to the Water-Nitric Acid System for Determination of Mean Ionic Activity Coefficients," Chem. Engr. Comm., 171, 169-180 (1999), original paper given at 10th Symposium on Separation Science and Technology for Energy Applications, Gatlinburg, TN (1997)