# Estimation of New Modified UNIFAC (NIST) Interaction Parameters

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The group contribution method is in important position of industrial usage such as selection of selective solvents, separation through distillation and process simulations. Design and optimization of these applications requires quantitative understanding of phase equilibrium and excess properties in multicomponent mixtures. The modified UNIFAC model achieved number of model parameters to increase the prediction capability of the phase equilibrium. In this study, the existing NIST-modified UNIFAC model has been extended and revised to produce more accurate interaction parameters. Also, improved SLE group interaction parameters with recent publications experimental data points are given. Furthermore, for the increased demand of the phase equilibrium data of amine and silicone in industry, the missing group interaction parameters for amine and silicon derivatives with the help of quantum mechanics-based calculation (COSMO-COnductor-like Screening MOdel) has been estimated.