

Evaluating the Quality of Excess Properties Predictions

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The aim of this work is the proper quantification of the success of a model or theory in predicting excess or excess-like properties in binary mixtures. Ideally, the goodness of these predictions should be evaluated in such a way that: i) the evaluations made for different systems or properties can be compared with each other, and ii) the reliability of the evaluations does not depend on the shape or on the symmetry of the curves. It came as a surprise that, after conducting an exhaustive review of the literature, we were not able to find any method to measure the deviation between experimental and estimated values fulfilling both conditions. We will expound and critically discuss the various options found and we will finish with the proposal of a more suitable alternative. An immediate application of the recommended expression is its use as an objective function in deviation minimization techniques designed to fit experimental data to theoretical equations and not involving derivation.