

Thermodynamic Property Screening of Ionic Liquids Using COSMO-RS

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Our quantum chemically based thermodynamic property prediction method COSMO-RS was originally developed and solely parameterized on neutral compounds. Nevertheless, it turned out to be applicable to ionic liquids with no adjustment. We consider this as a remarkable proof the predictive power of the COSMO-RS methodology. By the fact, that the (moderately) time-demanding quantum chemical calculations can be done for anions and cations separately, the prediction and screening of the thermodynamic properties can be performed extremely fast by combining anions and cations from our database of COSMO files of ionic liquid anions and cations. Missing ions can easily be added.

Meanwhile a number of research groups have reported successful application of COSMO-RS to ionic liquid. An overview of these applications will be given together with a few recent results from our own research.