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Estimation of Lattice Enthalpies of Ionic Liquids Supported by Hirshfeld Analysis

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Abstract

© 2015 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim. New measurements of vaporization enthalpies for 15 1:1 ionic liquids are performed by using a quartz-crystal microbalance. Collection and analysis of 33 available crystal structures of organic salts, which comprise 13 different cations and 12 anions, is performed. Their dissociation lattice enthalpies are calculated by a combination of experimental and quantum chemical quantities and are divided into the relaxation and Coulomb components to give an insight into elusive short-range interaction enthalpies. An empirical equation is developed, based on interaction-specific Hirshfeld surfaces and solvation enthalpies, which enables the estimation of the lattice enthalpy by using only the crystal-structure data. A compound view: A combination of newly collected experimental and computational data delivers the lattice enthalpies of ionic compounds. By using Hirshfeld surfaces and COSMO solvation enthalpies (see figure), a simple equation for the estimation of lattice enthalpies that requires only lattice data can be established. This paves the way to understand short-range interactions in the solid state.

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Keywords

ionic liquids, phase transitions, quantum chemistry, structure-activity relationships, thermodynamics