View metadata, citation and similar papers at core.ac.uk

brought to you by CORE

provided by Kazan Federal University Digital Repository

ChemPhysChem 2015 vol.16 N13, pages 2890-2898

Estimation of Lattice Enthalpies of Ionic Liquids Supported by Hirshfeld Analysis

Preiss U., Zaitsau D., Beichel W., Himmel D., Higelin A., Merz K., Caesar N., Verevkin S.

Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

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.

http://dx.doi.org/10.1002/cphc.201500249

Keywords

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