Chemistry Central Journal

ChemistryCentral

Poster presentation

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Chemoinformatics of ionic liquids and solids

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from 4th German Conference on Chemoinformatics
Goslar, Germany. 9–11 November 2008

Published: 5 June 2009

Chemistry Central Journal 2009, **3**(Suppl 1):P36 doi:10.1186/1752-153X-3-S1-P36

This abstract is available from: http://www.journal.chemistrycentral.com/content/3/S1/P36

Ionic liquids and solids are salts composed of cations and anions. The chemical constitution and structure of the ions determine whether an ionic compound is liquid or solid at a given temperature. Today, room-temperature ionic liquids (RTILs) receive rapidly growing attention as sustainable reaction media, catalysts and components in electrochemical devices and advanced materials. Novel design and modeling of ionic compounds, therefore, have a need for versatile, ion-based data representation and search strategies. However, the knowledge of the relation between a chemical compound and its constituent ions is in most cases not an integral part of database design. Herein, we review open-source web services for accessing information on ionic liquids and solids and investigate relationships between physicochemical properties of ionic compounds and properties of their constituent ions.

We demonstrate the ion and salt search abilities of the Ionic Liquids Database (ILThermo) [1] and the Chemical Property Viewer (CPV) [2]. ILThermo provides access to thermodynamic and transport properties of ionic liquids. CPV is a gateway to physicochemical properties of compounds in the ThermoML Archive [3]. CPV differs from ILThermo in that it is not restricted to ionic liquids. CPV additionally supports search via ion classes. We apply the XML Topic Maps (XTM) [4] approach to represent cations, anions and compounds thereof. Synonyms and special identifiers of salts and ions and ion class notations are captured via the XTM <variant> relation. We include short structural notations that are close to those which have been evolved in the ionic liquids literature. Ion class memberships are encoded as XTM <association> relations. Currently, our Ionic Identification XTM (IIXTM) base includes over 1250 inorganic and organic salt files including many ionic liquids and over 700 files with cation and anion data. We discuss the combined use of IIXTM, the ThermoML Archive, and an in-house annotation database to efficiently search information on ionic compounds and to derive structure-property relationships in advancing application-oriented selection of supporting electrolytes and RTIL media.

References

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