

Multivariate Analysis for Chemistry-Property Relationships in Molten Salts

Changwon Suh^a, Slobodan Gadzuric^{b,c}, Marcelle Gaune-Escard^b, and Krishna Rajan^a

^a Combinatorial Sciences and Materials Informatics Collaboratory (CoSMIC),
NSF International Materials Institute, Department of Materials Science and Engineering,
Iowa State University, Ames, IA 50011, USA

^b Ecole Polytechnique, IUSTI CNRS 6595, Technopôle de Château-Gombert,
5 rue Enrico Fermi, 13453 Marseille cedex 13, France

^c Faculty of Science, Department of Chemistry, University of Novi Sad, Trg. D. Obradovica 3,
21000 Novi Sad, Serbia

Reprint requests to Prof. K. R.; Fax: 515-294-5444; E-mail: krajan@iastate.edu

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We systematically analyze the molten salt database of Janz to gain a better understanding of the relationship between molten salts and their properties. Due to the multivariate nature of the database, the intercorrelations amongst the molten salts and their properties are often hidden and defining them is challenging. Using principal component analysis (PCA), a data dimensionality reduction technique, we have effectively identified chemistry-property relationships. From the various patterns in the PCA maps, it has been demonstrated that information extracted with PCA not only contains chemistry-property relationships of molten salts, but also allows us to understand bonding characteristics and mechanisms of transport and melting, which are difficult to otherwise detect.

Key words: Molten Salts; Multivariate Analysis; Data Mining; Principal Component Analysis (PCA).