

LEWIS MOLECULAR ACIDITY OF IONIC LIQUIDS FROM EMPIRICAL ENERGY- DENSITY MODELS

Renato Contreras^[a], Arie Aizman^[b], Ricardo A. Tapia^[c] and Andrea Cerda-Monje^[a]

The comparisons of experimental acidity descriptors against the electronic structure indices provides a novel and interesting approach to rationalize the electronic origin of molecular Lewis acidity in a wide series of 45 RTIL. In this context, the present model of Lewis molecular acidity assesses first order energy-density relationships through the electronic chemical potential. Second order polarization contributions are embodied in a charge capacity index, which is indirectly related to the regional softness at the cation fragments of the RTIL.

Our results stress the reliability of the electronic chemical potential as a descriptor of the intramolecular charge transfer that is naturally associated with the H-bond formation process. Molecular acidity appears as a regional property of molecules. Overall, the present contribution opens an alternative way in the attempt to classify in general terms the HB-acidity using information from the electronic structure of matter.

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- a. Departamento de Química, Laboratorio de Química Teórica
Universidad de Chile, Facultad de Ciencias
Casilla 653, Santiago, Chile.
- b. Departamento de Química
Universidad Técnica Federico Santa María
Casilla 110-V, Valparaíso, Chile.
- c. Departamento de Química Orgánica
Pontificia Universidad Católica de Chile, Facultad de Química
702843, Santiago, Chile.