

On the principle of spin potential equalization.

D. Guerra^{1,4}, A. Cedillo², P. Fuentealba³, **A. Aizman**⁴ and R. Contreras⁵.

¹ Departamento de Ciencias Química, Facultad de Ecología y Recursos Naturales, Universidad Andrés Bello, Av. república 275, Santiago Chile, ² Departamento de Química, Universidad Autónoma Metropolitana-Iztapalapa, San Rafael Atlixco 186, Iztapalapa, DF 09340, México, ³ Departamento de Física, Facultad de Ciencias, Universidad de Chile, Casilla 653-Santiago, Chile, ⁴ Universidad Técnica Federico Santa María, Casilla 110-V Valparaíso, Chile, ⁵ Departamento de Química, Facultad de Ciencias, Universidad de Chile, Casilla 653-Santiago, Chile

Abstract.

In analogy with Sanderson's electronegativity equalization principle, it is possible to postulate a principle of spin potential equalization in the E [N α , N β] representation of the spin polarized density functional theory. The principle provides simple expressions to evaluate the energy changes ΔE between two interacting molecules A and B together with the electron transfer $\Delta N\alpha$ and $\Delta N\beta$. The model is illustrated for a series of addition reactions of electrophilic, nucleophilic and ambiphilic carbenes to alkenes in their singlet and triplet multiplicities. The results are in a consistent qualitative agreement with the experimental reactivity established for these systems.