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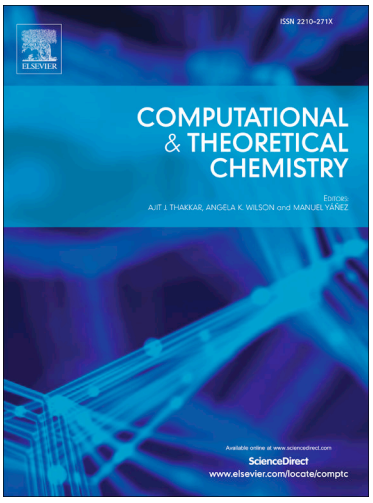

Density functional reactivity theory characterizing the reactivity of frustrated Lewis pairs

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Density functional reactivity theory characterizing the reactivity of frustrated Lewis pairs

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Abstract

Previously, theoretical studies for 2,6-lutidine/BR_3 (R = F, Me, C_6F_5) (J. Phys. Chem. A2010) and $PR_3/B(C_6F_5)_3$ (R = Me, Ph, tBu, C_6F_5) (Chem. Phys. Lett.2012) pairs have been carried out by us to fully understand the reactivity differences between classical Lewis adducts and frustrated Lewis pairs (FLPs). Fukui function, as a conceptual DFT-based reactivity descriptor, was calculated and shown to explain well the observed reactivity of these Lewis pairs. The initially promising results encouraged us to focus on the reactivity for a huge number of published FLPs by using other conceptual DFT-based reactivity descriptors. In this work, various descriptors were used to understand the intermolecular and intramolecular Lewis centers' reactivities of FLPs. The calculated results shown that, although there are a few exceptions, the adducts and "frustrated complex" of nonreactive pairs and reactive pairs are characterized by the opposite reactivity descriptors. The reactivity of Lewis pairs evaluated by reactivity descriptors also achieves some thermodynamic support from the Gibbs free energies of H_2 activation.

Keywords: FLPs, chemical reactivity, Conceptual DFT, reactivity descriptors

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