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Title: Energy Decomposition Analysis of Metal-Ligand Bonding in Transition Metal Complexess with Carbenes and Ylides Ligands: Significance of Electrostatic Interactions in Bond Analysis ‡

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This work describes a pedagogical approach to understanding chemical bonding by emphasizing the significance of electrostatic interactions in Metal-Ligand Bonding, particularly in Transition Metal Complexes with Carbenes and Ylides Ligands. Energy Decomposition Analysis (EDA) is a powerful method for quantitatively interpreting chemical bonds in terms of three major components. The instantaneous interaction energy ΔEint between two fragments M and L in a molecule M←L is partitioned into three terms: (1) the electrostatic interaction ΔE_{elstat} between the fragments, (2) the repulsive exchange, Pauli interaction ΔE_{Pauli} between electrons of the two fragments with the same spin, and (3) the orbital (covalent) interaction ΔE_{orb}, which arises from orbital relaxation and orbital mixing between the fragments. The latter term can be further decomposed into contributions from orbitals with different symmetries, enabling the distinction between σ, π, and δ bonding The results demonstrate that the EDA terms can be interpreted in a chemically meaningful way, thus establishing a connection between quantum chemical calculations and heuristic bonding models of traditional chemistry. The nature of the L→M bond in the complexes was analyzed using NBO, AIM, EDA, and ETS-NOCV methods.The findings confirm that the electrostatic interaction term, ΔEelstat, becomes notably higher and contributes significantly to the orbital interactions in the studied complexes.

Keywords: EDA, Transition Metal Complexes, Ylide, Carbene

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