

# Experimental Determination and Bond Energy Decomposition Analysis of Metal-Olefin Bonding Interactions: Towards a Quantitative Metal-Olefin Bonding Model

David L. Cedeño, Department of Chemistry, Illinois State University

Metal-olefin bonding is currently described using the Dewar-Chatt-Duncanson model, which is a qualitative depiction based on frontier molecular orbital interactions. Transition metal-olefin bond strengths depends on the balance of attractive (electrostatic and covalent) and repulsive (steric) interactions between the olefin and the metal complex counterpart. However, the bonding interaction involves conformational changes (reorganization) in these entities, which could be energetically expensive, thus largely influencing the strength of the metal-alkene bond. Our research involves experimental determinations and computational modeling (DFT level) and analysis of the bonding interaction in order to account for the extent of electronic, steric and reorganizational effects in metal-olefin bond strengths.

