

عنوان مقاله:

A COMPARATIVE STUDY OF THE DONOR-ACCEPTOR PROPERTIES IN ANALOGOUS ORGANOMETALLIC $Al_4 \dots X$ ($X=CO$, CS , and CSe) ASSISTED BY NBO ANALYSIS

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خلاصه مقاله:

Charge transfer between a metal and its ligand is fundamental for the structure and reactivity of a metal complex as it directly dictates the distribution of electron density within the complex. In this work, the nature and extent of the orbital interaction between Al_4 and CO , CS or CSe can be judged by comparing the forms and occupancies of the NBOs in the isolated fragments with those in the complexes. The NBO result demonstrates that the most significant changes in the occupancy of $Al_4 \dots X$ ($X=CO$, CS , and CSe) are related to disembedding of the carbon lone pair [1]. The π^* orbital on CO receives electrons from the π orbital on Al , thus an increase of in occupancy of the CO π^* NBO's with an associated depletion of the Al_4 total π symmetry. In this paper we reported the results of charge transfer analysis with associated thermodynamic properties for $Al_4 \dots CO$, $Al_4 \dots CS$, and $Al_4 \dots CSe$ complexes that obtained by HF/3-21G level calculation.

کلمات کلیدی:

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