

Possible use of group 4 metallocene methyl cations as potential neutralizers for FOX-7

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The possible use of group 4 metallocene cations as neutralizers for some energetic molecules has been assessed using quantum chemical calculations. In particular, titanocene, zirconocene, and hafnocene methyl cations were tested as neutralizers for FOX-7, an energetic molecule that has been synthesized in 1998. Quantum chemical calculations allowed to geometrically optimize these systems and find 3D maps of the molecular electrostatic potential and the dual descriptor. Dual descriptor is a local reactivity descriptor coming from conceptual density functional theory, which reveals regions on a molecule that are more susceptible to undergo nucleophilic and electrophilic attacks of covalent nature. This local reactivity descriptor helped to orientate the FOX-7 with respect to the spatial orientation of the respective metallocene methyl cation (MMC) to favor the interplay between these two species, thus revealing that one of the nitro groups of FOX-7 is able to form a chemical bond with the transition metal atom in the MMC. The procedure exposed in this article highlights the fact that a complete exploration of the hypersurface of potential energy was not necessary to perform because the dual descriptor has revealed unambiguously the nucleophilic and electrophilic zones on each molecular system thus allowing to select the best geometry that favors the intermolecular interplay inasmuch as, according to dual descriptor, the MMC+FOX-7 reaction progresses through the formation of a covalent bond between the metal atom of the MMC and the oxygen atom of FOX-7. © 2014 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim.

Conceptual density functional theory

Dual descriptor

FOX-7

Group 4 metallocene cations

Humanitarian demining

Local reactivity descriptors

Neutralizer of explosives

Atoms

Molecular oxygen

Molecules

Organometallics

Positive ions

Potential energy

Quantum chemistry

Synthesis (chemical)

Transition metals

Conceptual density functional theory

Descriptors

FOX-7

Group 4

Humanitarian demining

Local reactivity descriptors

Density functional theory