AIM and ELF analysis of the H-, Me-, and F-substituted Fe^{III}-TAML complexes.

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Rok wydania

2011

Czasopismo

Chemical Physics Letters

Numer woluminu

507

Strony

29-36

DOI

10.1016/j.cplett.2011.03.044

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Structure, bonding, and proton affinities of the H-, Me-, and F-substituted [Fe^{III}–TAML] complexes and their protonated counterparts were investigated with the topological analysis of the electron density (AIM) and electron localization function (ELF) at the B3LYP/6-31 + G** level. Two protonation sites were found on each of the terminal oxygen atoms. The AIM analysis revealed existence of some weak interactions in the studied molecules. Changes induced by substitution of the tail Me groups by highly electronegative fluorine atoms are rather small (except for C25 atom) and do not fully explain experimentally observed high H^+-tolerance of [Fe^{III}–$TAML_{RF}$] molecule.

Adres publiczny

https://doi.org/10.1016/j.cplett.2011.03.044

Strona internetowa wydawcy

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