عنوان مقاله:

Is there any correlation between some theoretical and experimental parameters at similar and dissimilar beta-diketone complexes .

محل انتشار:

بیستمین کنگره شیمی ایران (سال: 1397)

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خلاصه مقاله:

The most interesting thing in metal complexes of β-diketones comes up from their applications in science and industry. These compounds are frequently used in preparation of supported catalysts as precursors of heterogeneous catalysts. They have also been extensively applied in medicine as active pharmaceutical ingredients, antiasthmatic and lung disease drugs, and antidiabetic agents [1,2]. Furthermore, these complexes are also used as fuel additives [3]. This study presents our view of any correlation between theoretical and experimental parameters for conventional (metal-ligand) and unconventional (dihydrogen bond) strength of some similar and dissimilar beta-diketone complexes, such as bond length, vibrational frequency, total electronic density (ρBCP), and Laplacian of total electronic density in critical points, by using density functional theory (DFT) and Atoms In Molecules (AIM) calculations. So, the selected compounds classified in three categories. In the first category, the copper(II) acetylacetonate, Cu(acac)2, participates with copper(II) benzoylacetonato, Cu(bzac)2, and copper(II) dibenzoylmethane Cu(dbm)2, by one and two phenyl groups instead of methyl groups in Cu(acac)2, and in the other ones, 5,5-dimethyl hexane-2,4-dionato, Cu(dmhd)2, 2,2,6,6-tetramethyl-3,5-heptanedionato, Cu(tmhd)2 with one and two t-butyl groups have been substituted by methyl groups of Cu(acac)2, respectively. The last class that have been investigated include a molecule with different β substitutions, which are named: 4,4,4-trifluoro-1-phenyl-1,3-butanedione Cu(tfba)2 (with CF3 and phenyl groups) (Fig.1). By investigating the effect of replacing one or two similar substitutions by CH3 in the values of mentioned compounds, a linear correlation has been obtained for the titled similar β-diketone complexes (Fig.2). This conclusion also achieved for Cu(tfba)2 with different groups in beta positions. AIM results indicate that the unconventional hydrogen bonds occur in the β-diketone complexes including phenyl groups, which the strength of unconventional hydrogen bond is very weak and there is a linear correlation between them.

کلمات کلیدی:

لینک ثابت مقاله در پایگاه سیویلیکا: