CH/π Interactions between Chelate and Phenyl Rings in Acetylacetonato Complexes

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By coordinating to metal atom with acetylacetonato ligand makes planar chelate ring, with delocalized bonds. Hence, coordinated acetylacetonato ligand could be involved in CH/ π interactions with phenyl ring in two ways, as hydrogen atom donor, or as hydrogen atom aceptor. In first case hydrogen atoms of acetylacetonato ligand could make MLACπ interactions with phenyl ring. Acetylacetonato ligand has negative charge, but by coordinating to metal cation partial positive charge is transferred from the metal cation to the ligand. If enough positive charge is transferred hydrogen atoms of acetylacetonato ligand will get enough positive charge to be involved in MLACπ interactions. In second type of interactions phenyl ring and chelate ring change roles; phenyl ring is hydrogen atom donor whereas chelate ring with delocalised π-system is hydrogen atom acceptor.

Here we report on CH/π interactions between acetylacetonato chelate rings and phenyl rings in acetylacetonato complexes. The results were obtained by searching and analyzing crystal structures in Cambridge Structural Database (CSD) and by quantum chemical calculations. Dependence of CH/π interactions on delocalization in chelate rings that is connected with type of metal in the ring was studied. To the best of our knowledge this is the first time that influence of metal in a chelate ring on CH/π interactions in metal complexes was studied.

Keywords: CH/π interactions, DFT, chelates