Original Article

Int. J. New Chemistry, Vol. 1, No. 2, Summer 2014, 87-98

ISSN: 2383-188X

International Journal of New Chemistry

Theoretical insight of substituent effect in *para* substituted $Fe(CO)_4$–pyridine complexes

R. Ghiasi[1,*], M. Daghighi Asl[2], S. Azmayesh[2], P. Makkipour[1]

[1] *Department of chemistry, Basic science faculty, East Tehran Branch, Islamic Azad University*

[2] *Department of chemistry, Basic science faculty, Central Tehran Branch, Islamic Azad University, Tehran, Iran*

Received: 5 July 2014; Accepted: 25 August 2014

Abstract:

Systematic studies on the substituent effect in para substituted Fe(CO)4–pyridine complexes have been studied on the basis of DFT quantum-chemical calculations. The following substituents were taken into consideration: NO2, CN, CHO, F, H, CH3, and OH. Additionally, the Fe–N and Fe–C bonds were characterized on the basis of Atoms in Molecules topological analysis of electron density. It has been found that the substituents in position 4 of the pyridine ring influence the Fe–N bond of Fe(CO)4–pyridine complex in a systematic manner, as a result of with, the pyridine moiety has a diversified ability of participating in the interaction with the Fe atom of Fe(CO)4 moiety. It has also been found, that the electron withdrawing substituents additionally stabilize the Fe–N bond, whereas the electron donating ones weaken it. The substituent effect mainly affects the component of the Fe–N bond.

Keywords: complexes, Fe–N bond, DFT, $Fe(CO)_4$–pyridine

(*) Corresponding Author: e-mail: rezaghiasi1353@yahoo.com, rghyasi@qdiau.ac.ir