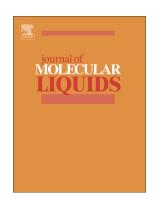
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A quantum chemical investigation of the influence of solvent polarity on the structural, electronic, spectroscopic properties and hyperpolarizability in Molybdenum Silylidyne complex CpMo(CO)2(Si-Ph)



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A quantum chemical investigation of the influence of solvent polarity on the structural, electronic, spectroscopic properties and hyperpolarizability in Molybdenum Silylidyne complex CpMo(CO)₂(≡Si-Ph)

Hadis Ghobadi¹, Reza Ghiasi^{2,*}, Saeid Jamehbozorgi³

¹ Department of chemistry, faculty of science, Arak branch, Islamic Azad University, Arak, Iran

² Department of Chemistry, Faculty of science, East Tehran Branch, Islamic Azad University, Tehran, IRAN.

³ Department of chemistry, faculty of science, Hamedan Branch, Islamic Azad University, Hamedan, Iran

Correspond: E-mail to: rezaghiasi1353@yahoo.com

Abstract:

In this study, quantum chemical calculations using MPW1PW91 method was applied to analyze of solvent effect on the structural, ¹³C and ²⁹Si NMR chemical shifts, vibrational analysis, thermochemical parameters and first hyperpolarizability for CpMo(CO)₂(=Si-Ph) complex. The solvent effects were examined by the self-consistent reaction field theory (SCRF) based on Polarizable Continuum Model (PCM). The correlations between these parameters and solvent polarity functions, involve both the dielectric constant (ε) and refractive index (n_D) of the liquid medium were explored. Correlations of the calculated spectral parameters ($\nu(CO)$, $\delta(^{13}C)$ and $\delta(^{29}\text{Si})$) with the Kirkwood–Bauer–Magat equation (KBM) and improved form of this equation were explored.

Keywords: Silylidyne complex, Solvent effect, ¹³C and ²⁹Si NMR chemical shifts, Kirkwood– Bauer–Magat equation (KBM), Hyperpolarizability.

Introduction:

The chemistry of alkylidyne complexes is a rigorously investigated subject within organometallic science by the discovery of the first transition metal carbyne complex in 1973 [1]. The synthesis, structure, reactivity and properties of theses complexes stimulated many studies in the organometallics area [2-6]. They are contributed in numerous catalytic transformations [7-11]. In comparison, there are silicon analogues of the alkylidyne complexes [12], a series of compounds featuring metal-germanium, metal-tin, or metal-lead triple bonds have been obtained by reacting

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