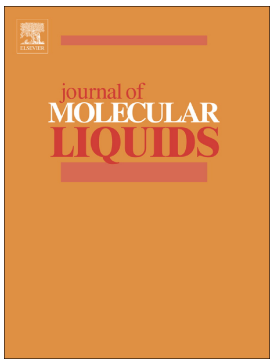

A quantum chemical investigation of the influence of solvent polarity on the structural, electronic, spectroscopic properties and hyperpolarizability in Molybdenum Silylidyne complex CpMo(CO)2(Si-Ph)

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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 $CpMo(CO)_2(\equiv Si\text{-}Ph)$

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Abstract:

In this study, quantum chemical calculations using MPW1PW91 method was applied to analyze of solvent effect on the structural, ^{13}C and ^{29}Si NMR chemical shifts, vibrational analysis, thermochemical parameters and first hyperpolarizability for $CpMo(CO)_2(\equiv Si\text{-}Ph)$ 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 (υ(CO), $\delta(^{13}C)$ and $\delta(^{29}Si)$) with the Kirkwood–Bauer–Magat equation (KBM) and improved form of this equation were explored.

Keywords: Silylidyne complex, Solvent effect, ^{13}C and ^{29}Si 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