

## Accepted Manuscript

A quantum chemical investigation of the influence of solvent polarity on the structural, electronic, spectroscopic properties and hyperpolarizability in Molybdenum Silylidyne complex  $\text{CpMo}(\text{CO})_2(\text{Si-Ph})$



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PII: S0167-7322(18)30324-6  
DOI: doi:[10.1016/j.molliq.2018.05.068](https://doi.org/10.1016/j.molliq.2018.05.068)  
Reference: MOLLIQ 9123  
To appear in: *Journal of Molecular Liquids*  
Received date: 21 January 2018  
Accepted date: 16 May 2018

Please cite this article as: Hadis Ghobadi, Reza Ghiasi, Saeid Jamehbozorgi , A quantum chemical investigation of the influence of solvent polarity on the structural, electronic, spectroscopic properties and hyperpolarizability in Molybdenum Silylidyne complex  $\text{CpMo}(\text{CO})_2(\text{Si-Ph})$ . The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Molliq(2017), doi:[10.1016/j.molliq.2018.05.068](https://doi.org/10.1016/j.molliq.2018.05.068)

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

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**Abstract:**

In this study, quantum chemical calculations using MPW1PW91 method was applied to analyze of solvent effect on the structural,  $^{13}\text{C}$  and  $^{29}\text{Si}$  NMR chemical shifts, vibrational analysis, thermochemical parameters and first hyperpolarizability for  $\text{CpMo}(\text{CO})_2(\equiv\text{Si-Ph})$  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 ( $\epsilon$ ) and refractive index ( $n_D$ ) of the liquid medium were explored. Correlations of the calculated spectral parameters ( $\nu(\text{CO})$ ,  $\delta(^{13}\text{C})$  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,  $^{13}\text{C}$  and  $^{29}\text{Si}$  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 these 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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