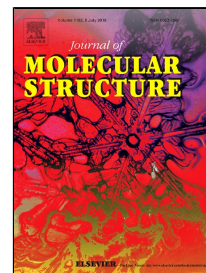


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Synthesis, structural, vibrational, electronic, thermal and Fukui analysis of diethyl (hydroxy(4-methoxyphenyl) methyl) phosphonate



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1 **Synthesis, structural, vibrational, electronic, thermal and Fukui analysis of**
2 **diethyl (hydroxy(4-methoxyphenyl) methyl) phosphonate**

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9 **Abstract**

10 In this paper diethyl (hydroxy(4-methoxyphenyl) methyl) phosphonate has been synthesized
11 and characterized by FTIR, FT-Raman UV-Vis. The structural geometrical parameters,
12 vibrational, electronic, HOMO-LUMO, Fukui analysis, and the thermodynamic properties of the
13 molecule were performed on the basis of DFT calculations at B3LYP/6-311G(d,p) basis set
14 using Gaussian 09 package. Thermogravimetric (TG) analysis was also carried out to study
15 thermal stability of compound. The HOMO-LUMO study to find the band gap of compound has
16 been extended to calculate ionization potential, electron affinity, global hardness, electron
17 chemical potential and global electrophilicity to study the chemical behavior of compound. A
18 good agreement between observed and calculated wavenumbers has been obtained. The
19 correlations between the statistical thermodynamics and temperature show that increase in
20 temperature increases heat capacities, entropies and enthalpies.

21 **Keywords:** FTIR, FT-RAMAN, UV-Vis, TGA, HOMO-LUMO, Fukui Functions

22 **1. Introduction**

23 Organophosphonates are versatile substrates that constitute core unit of several natural
24 products [1] and bioactive compounds [2]. Due to the diverse applications of phosphonates in
25 industrial, medicinal and agricultural purposes, their synthesis has been a focus of interest for
26 organic and medicinal chemists [3].

27 In particular, α - hydroxyphosphonates represents an elite class of organic compounds due to their
28 broad range of pharmacological properties such as antifungal [4], antiviral [5], anticancer [6],
29 rennin inhibitory [7], HIV protease [8]. These medicinally privileged scaffolds are also applied

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