



SDI Review Form 1.6

Journal Name:	Asian Journal of Chemical Sciences
Manuscript Number:	Ms_AJOCS_40462
Title of the Manuscript:	Comparison of 6-311G(d) and 3-21G(DFT/HF) Methods of 3-Methyl-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1H-1,2,4-triazol-5-one
Type of the Article	Original Research Article

General guideline for Peer Review process:

This journal's peer review policy states that **NO** manuscript should be rejected only on the basis of '**lack of Novelty**', provided the manuscript is scientifically robust and technically sound. To know the complete guideline for Peer Review process, reviewers are requested to visit this link:

(<http://www.sciencedomain.org/page.php?id=sdi-general-editorial-policy#Peer-Review-Guideline>)

PART 1: Review Comments

	Reviewer's comment	Author's comment (if agreed with reviewer, correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)
Compulsory REVISION comments	There are some thpo errors such as After the vibrational frequencies and their relative intensities had calculated with the aid 88 of B3LYP/6-311G(d), HF/6-311G(d) and B3LYP/3-21G, HF/3-21G basis sets, Have the excitation energies, oscillator strengths (f) and absorption wavelengths (λ) of UV–Vis electronabsorption spectroscopy of the title molecule been calculated in ethanol solvent by using B3LYP/HF methods with 6-311G(d) and 3-21G basis sets ? Futhermore, What do you mean with the following sentences “the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) have been simulated for this compound have been determined” The Autjur only put the Table but no comment, To calculate with 3-21G is not need. . Presentation of the manuscript is poor The manuscript needs major language editing	B3LYP/6-311G(d), HF/6-311G(d) and B3LYP/3-21G, HF/3-21G basis sets were compared with experimental data. I selected the best method and results. Also I added the necessary comments in discussion section. I changed the manuscripit
Minor REVISION comments		
Optional/General comments		