



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>)



SDI Review Form 1.6

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		
Minor REVISION comments	<p>The manuscript presents interesting results and I recommend it for publication after some minor revision, as follows below:</p> <p>In the abstract the authors explained that they used different computational basis set for calculate chemical properties and spectra. Please, in the abstract inform which method was the best.</p> <p>I recommend that the authors compare their results with those previously published in the follow paper: Medetalibeyoğlu H, Yüksek H. Gaussian calculations of novel 3-(methyl/ethyl/n-propyl)-4-[3-ethoxy-4-(4-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1H-1,2,4-triazol-5-ones Bulg. Chem. Com. 2017; 49(1),78–89.</p> <p>Is there not a range in the melting point showed in the line 76?</p> <p>Please, clarify in the manuscript if it is a novel compound or not.</p> <p>If there is a crystallographic data of the compound 3 previously published in the literature, compare the theoretical bond angles and bond lengths with the experimental data.</p> <p>In the UV-Vis results (Figure 3), please provide the experimental UV-Vis spectra.</p> <p>In the Figure 4, the HOMO representation comes first than LUMO representation. Please, represent the results in the Figure 4, as graphical with the y axis.</p> <p>Insert a discussion on the results presented in the Table 10 and Table 11.</p> <p>The language in this manuscript must be improved greatly with help of native speakers.</p>	
Optional/General comments		

Reviewer Details:

Name:	Otávio Augusto Chaves
Department, University & Country	Department of Chemistry, Universidade Federal Rural do Rio de Janeiro, Brazil