

Review Form 1.6

Journal Name:	Asian Journal of Chemical Sciences
Manuscript Number:	Ms_AJOCS_83962
Title of the Manuscript:	Synthesis spectral charecterization of chalcone: Structural elucidation through single-crystal XRD, Hirshfeld surface analysis, and DFT calculations
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:

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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	<p>The compound has already been prepared by another group virtually by the same method (Reddy, G. Jagath; Reddy, R. Shailaja; Pallavi, K.; Rao, K. Srinivasa, Heterocyclic Communications (2004), 10, (1), 93-96. This reference must be included. The yield of the reaction must be given. The ¹H NMR of the product is not pure (most likely remaining solvent). Thus, it may not necessarily be opportune to show the ¹H NMR. ¹H NMR and IR spectral data should be listed in the usual way. Note should be taken of significant digits (for ¹H NMR: x.xx ppm). If needed, the data can still be discussed. Coupling constants must be given. A rationale for preparing the compound needs to be given. Interestingly, Reddy et al. did not give the spectral data of the compound as they used it in a reaction to their target compound. This may give the authors a rationale to have carried out this research. It must be clarified on which diffractometer the X-ray crystal structure was measured. The crystal packing is not clear. Figure 5 should be revised. Close contacts in the crystal packing should be shown. The crystal packing should be described in the text. There is something missing in the sentence "by full-matrix least-squares procedures to a final R-value of 0.0645 for 0.1794 observed reflections" as the sentence does not make sense. The extinction coefficient is not given for the UV absorption. It is not clear at what concentration the UV spectrum was taken. The absorption looks very broad – why was CCl₄ used. It would be good to take other solvents as well and to look for solvent effects. Most likely, measurements of the compound at lower concentrations would be beneficial.</p>	
Minor REVISION comments	<p>References should be checked carefully (incl. punctuation, bold highlighting, and word spacing)</p>	
Optional/General comments		

PART 2:

	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)
Are there ethical issues in this manuscript?	<i>(If yes, Kindly please write down the ethical issues here in details)</i>	

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