SRI KRISHNA DUTT ACADEMY

(Recognized by NCTE and Affiliated to University of Lucknow)

Criterion 3

Research, Innovations and Extension

3.3 Research Publications and Awards

3.3.2 Number of books and chapters in edited volumes/books published and papers published in national/ international conference proceedings per teacher during last five years

APPENDIX-I

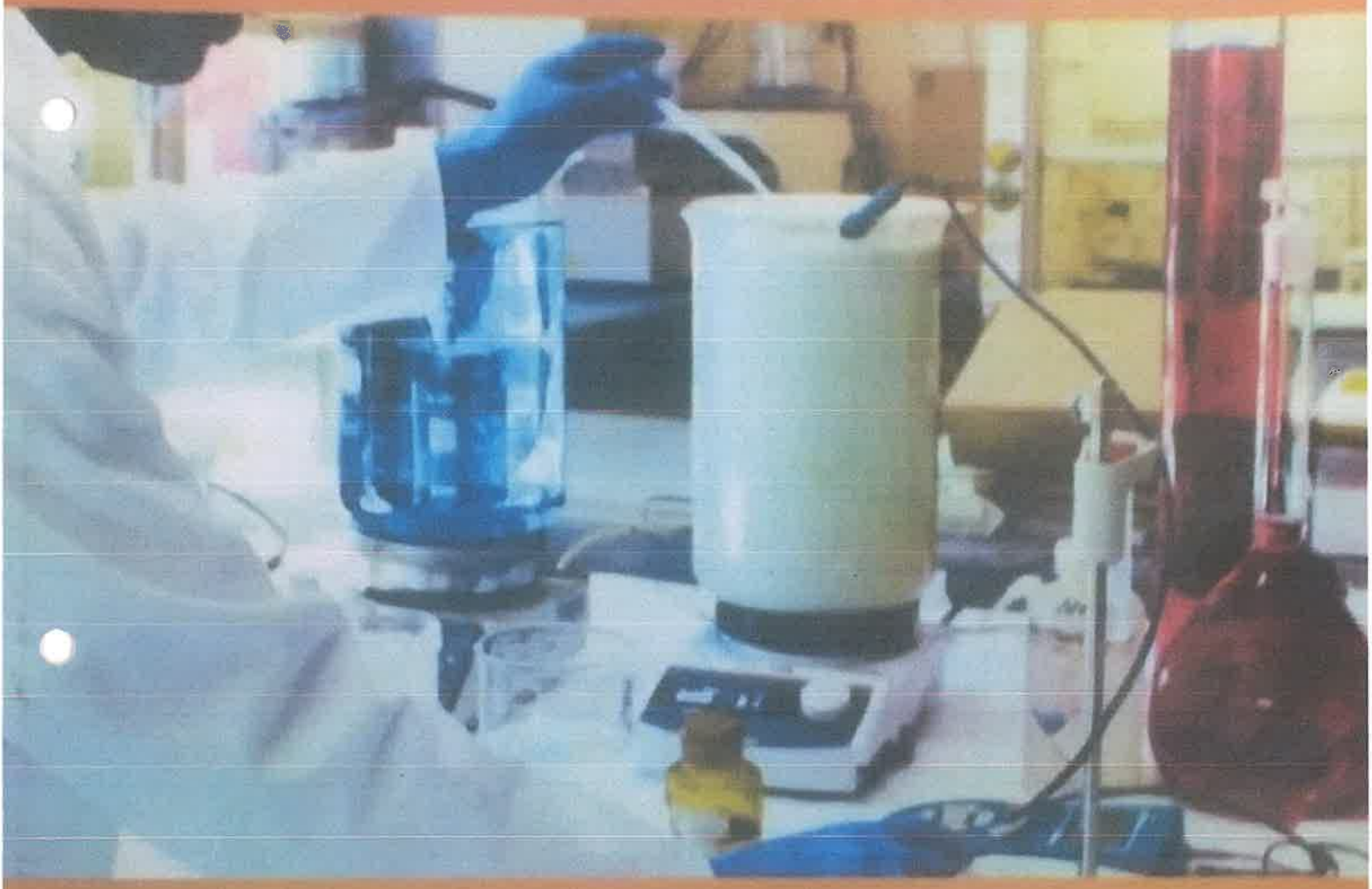
3.3.2 Number of books and chapters in edited volumes/books published and papers published in national/international conference proceeding per teacher during last five year

S.No	Name of the Teacher	Title of the book/chapters published	Title of the paper	Title of the proceeding of the conference	Name of the conference	National/ Internatio nal	Year of Publicati on	ISBN number of the proceeding	Affiliating institute at the time of publication	Name of the publisher
1	Dr. Madhu Gupta	Applied Research Development	Comparative Quantum Chemical Approach for the study of some pharmaceutical Drugs and their oscidation products	NA	NA	National	2021	978-93-91248-49-9	Lucknow University	MKES Publications

Principal
SRI KRISHNA DUTT ACADEMY
2D/HS-1, Vrindavan Yojna
Raibareilly Road, Lucknow

Principal

Applied Research Development in Physical & Chemical Sciences and Engineering



Edited by:
Prof. R. K. Shukla | Dr. Bhuvan Bhasker Srivastava | Dr. Susheel Kumar Singh

MKSES PUBLICATIONS
LUCKNOW, INDIA

Contents

Chapter-18

Comparative Quantum-Chemical Approach for the Study of Some Pharmaceutical Drugs and their oxidation products

[1]Amrita Srivastava, [1]Madhu Gupta*[1,3] and [2]Sheila Srivastava
[1]Department of Chemistry, University of Lucknow, Lucknow-226007, Uttar Pradesh, India
[2]Chemical Laboratories, Feroze Gandhi College, Raebareli-229001, Uttar Pradesh, India
[3]Department of Education in Science & Mathematics, Regional Institute Education, Bhopal (M.P.)
*e-mail: guptamadhu30@rediffmail.com, madhugupt30@gmail.com

Abstract:

Density Functional Theory (DFT) is progressively becoming vital for the study of pharmaceutical drugs and also to find out the applications of substrates. Since past few years DFT has appeared as a Quantum Mechanical (QM) method which is satisfactorily meticulous as well as competent to be employed in pharmaceutical studies. Biologically important molecular systems can be exactly described using DFT at a lesser computational cost than other methods making it a highly utilized technique. Current manuscript presents prospective applications of DFT in kinetic and mechanistic study of a chemical reaction along with its utilization for calculation of thermodynamic parameters and some enhanced applications of both reactants and products. To begin with, the basis of DFT is discussed. Next, accuracy of DFT for the analysis of this kinetic is discussed followed by applications of DFT for molecular modelling in drug chemistry.

Keywords –Quantum Mechanical (QM), DFT, Computational, Kinetic, Thermodynamic.

Introduction

The field of medicinal chemistry and drug designing is most growing area now a days and has a lot of scope for future research. If we applied quantum approach to this study then it becomes quite informative for application purpose also by using several methods [1-7]. Among several methods, Density Functional Theory (DFT) has excellent level of accuracy with least time requirement comparatively and cost effective also. The basic phenomenon of DFT is that, electron density determines the ground state energy and other molecular properties [8-9]. This ground state energy term consists of three terms which are kinetic energy, potential energy and exchange correlation energy of the system. The first and second term can be calculated easily and third term is calculated using different approximations, i.e. generalized gradient approximations (GGA), local-density approximations (LDA) and hybrid functionals, are used for the exchange correlation functional. B3LYP is a hybrid functional

Criteria 3.3.2. :	**Number of books and chapters in edited volumes/books published and papers published in national/ international conference proceedings per teacher during last five years**
DVV Finding	Please submit the cover page, table of contents, and the first page of the chosen publication, along with a web link for books. In case if documents are in regional language please provide translated copy in English. Google drive links are not accepted.
Response/ Clarification	1- the cover page, table of contents, and the first page of the chosen publication.(Appendix-I)

2024

Cr-3 Coordinator

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Principal
SRI KRISHNA DUTT ACADEMY
2D/HS-1, Vrindavan Yojna
Raibareilly Road, Lucknow

Principal