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Computational and Mathematical Approaches to Clusters, Fullerenes and Proteomes

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Abstract: We propose to consider several exciting applications of computational and mathematical approaches to cluster with special emphasis on combinatorics, graph theory based algorithms to a number of scientific disciplines, particularly in fullerene chemistry and computational biology. We shall demonstrate that enumerative combinatorics and algorithms find numerous applications to enumeration of structures and three dimensional fullerene cages and their nuclear spin statistics and spectroscopy. We propose to consider cross fertilization of graph theory with chemistry and biology which seems to provide a fertile ground for interdisciplinary research in bioinformatics, predictive toxicology, molecular and drug design. Examples of applications from each of these fields will be provided and would include DNA algorithm and graph theoretical characterization of proteomics and genomics.

Keywords: Combinatorics of fullerenes, spectroscopy fullerenes, proteomics, graph theory

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1. Introduction

Computational and mathematical techniques have made substantial impact in all branches of science, particularly in chemistry and biology in recent years. With the advent of supercomputers and very powerful desktop workstations, it is becoming increasingly feasible to carry out sophisticated computations concerning electronic structure, spectroscopy and dynamics of many large molecules and chemical systems. It is also noteworthy that these computers have made it possible to solve some of the complex and demanding algorithms and applications concerning combinatorics and graph theory which could not be done otherwise. In fact some unsolved mathematical problems in the field of graph theory and combinatorics could be addressed with such powerful computers. We show here that a combination of graph theory, combinatorics and computational algorithms result in exciting solutions to a number of problems concerning fullerene cages, their spectroscopy, nuclear spin statistics and so on.

Applications of quantum chemistry, combinatorics and graph theory to biological systems and predictive toxicology are emerging in recent years. We show that the application of graph theory combined with complex algebra can provide powerful tools for the characterization of proteome patterns and response of proteomes induced by externally applied chemicals. Graph theory which is basically algebra of connectivity can provide powerful tools and algorithms for complex patterns such as the proteome of a living cell. Typically the proteome is characterized by a two-d gel electrophoresis technique which involves separation of a complex set of proteins in the proteome into individual

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proteins on the basis of their mass and charge. Graph theory provides a powerful method to characterize the proteome in terms of mass and charge and relative abundances.

We have applied mathematical techniques to main-group molecular structures such as water clusters, clusters of TATB, etc. We have also carried out methods developments for these species. We provide here only a brief of summary of highlights. Doped fullerene cages are of recent interest as novel materials for faster devices, lasers and high-energy materials. Doping fullerenes with Group 13 and 15 elements have received particular attention. We have considered the vibrational and rovibrionic spectra of $C_{60}N_{12}$ cages and the group theoretical analysis of the nuclear spin statistics of these cages as $^{14}N$ nuclei are spin-1 particles. A recent experimental work indicated the possibility of 3 stable isomers of $C_{60}H_{36}$ shown on Fig. 1.

![Fig 1 Three Isomers of $C_{60}H_{36}$](image)

We obtained the computed ESR spectra of these isomers to contrast them as shown in Fig 2 for 2 of the isomers.

![Fig 3 ESR Spectra of Isomer of $C_{60}H_{36}$](image)

Relativistic double group spinor representations were developed for non-rigid molecules containing very heavy atoms. The representations facilitate spinor wavefunctions for non-rigid molecules containing very heavy atoms. Moreover the rovibrionic levels of such species would be split by both torsional tunneling and spin-orbit coupling. Thus it is necessary to have such a formalism. We have developed these techniques for the first time. Several group theoretical developments have also been carried for the development of group theory of water pentamer.

We have combined mathematical and computational quantum chemical computations to predict biological phenomena. In particular we have been focusing our efforts in two areas, one concerns with toxicity prediction and the other deals with the characterization of proteome and its response to applied chemicals. The toxicity of chemicals that have received considerable attention in the field of environmental chemistry. Both halocarbons and dioxins are known to be harsh pollutants of the environment and it is important to understand the mechanisms of their toxicity and which ones are most harmful. Thus our quantum chemical computations of the main group species had environment and
atmospheric chemistry as their central theme and thus we focused our work on halocarbons, polychlorinated dibenzo-p-dioxins, and dibenzofuran. In the case of halocarbons we considered 55 species with known toxicity and we used quantum chemical and other statistical methods to predict and correlate the toxicity of these species using electron attachment as the key mechanism governing hepatotoxicity of these species.

In collaboration with Basak and coworkers, We have developed a complex graph matrix representation to characterize proteomics maps obtained from 2d-gel electrophoresis. In this method each bubble in a 2d-gel proteomics map is represented by a complex number with components being charge and mass. Then a graph with complex weights is constructed by connecting the vertices in the relative order of abundance. This yields adjacency matrices and distance matrices of the proteomics graph with complex weights. We have computed the spectra, eigenvectors and other properties of complex graphs and the Euclidian/graph distance obtained from the complex graphs. The leading eigenvalues, eigenvectors and likewise the smallest eigenvalues and eigenvectors and the entire graph spectral patterns of the complex matrices derived from them yield novel weighted biodescriptors that characterize proteomics maps with information of charge and masses of proteins. We have also applied these eigenvector and eigenvalue maps to contrast the normal cells and cells exposed to four peroxisome proliferators, namely, clofibrate, DEHP, PFDA and PFOA.

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References


