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学 位 論 文 内 容 の 要 旨

博士の専攻分野の名称　博士（総合化学）氏名　Mohammad Ali

学 位 論 文 題 名

Study on Atom-to-Atom Mapping Using Ising Computing
（イジング計算を用いた原子間マッピングの研究）

Chemical reactions are fundamental transformations of chemical structures, and understanding the correspondence between atoms in reactants and products has been a long-standing question in chemistry. This correspondence, referred to as atom-to-atom mapping (AAM), establishes relationships between the atoms of reactants and products, providing insight into the mechanistic pathways of chemical reactions. Currently, automatic AAM tools play a pivotal role in various chemo-informatics tasks, such as reaction prediction, pathway elucidation, and metabolic engineering. Despite the availability of automatic AAM tools, achieving accurate automatic AAM for complex or unknown reactions within a reasonable computation time remains a significant challenge because of the combinatorial nature of the problem and the difficulty in applying appropriate reaction rules.

To address these challenges, a rule-free AAM algorithm is proposed to enumerate all possible atom-to-atom correspondences that minimize the number of bond cleavages and formations during a reaction. The problem of minimizing bond changes is an NP-hard combinatorial optimization problem, which is inherently computationally intensive. To reduce the computational burden associated with this optimization problem (i.e., minimizing bond changes) and to find all possible optimal solutions, an Ising computing-based enumeration algorithm is developed. Ising computing is a computing paradigm that has gained significant attention for its efficiency in solving hard combinatorial optimization problems.

The results demonstrate that the Ising computing-based enumeration algorithm outperforms conventional combinatorial optimization algorithms in terms of computation times, making it feasible to solve the AAM problem without reaction rules in an acceptable time. Furthermore, the proposed AAM algorithm successfully found the correct AAM solution for all problems in a benchmark dataset. In contrast, conventional AAM algorithms based on chemical heuristics failed for several problems. Specifically, these algorithms either failed to find the optimal solution in terms of bond changes or identified only one optimal solution, which was incorrect when multiple optimal solutions exist. These results emphasize the importance of enumerating all optimal correspondences that minimize bond changes, which is effectively achieved by our Ising-computing framework.

Overall, this research highlights the critical importance of enumerating all optimal atom-to-atom correspondences to capture the full spectrum of possibilities in chemical transformations. By eliminating dependence on reaction rules and leveraging the computational advantages of Ising computing, the proposed approach sets a new standard for AAM, offering a versatile and efficient solution for this longstanding challenge in chemo-informatics. This study not only advances the state of the art in AAM methodologies but also illustrates the transformative potential of computational paradigms like Ising computing in solving intricate problems at the intersection of chemistry and computational science.

My thesis is organized into five chapters, outlined as follows:

Chapter 1: General Introduction

This chapter introduces the importance of atom-to-atom mapping (AAM) in chemical reactions. It presents the background and motivation behind the research, defines the scope and objectives of the study, and outlines the key contributions made through this work. The chapter concludes with an overview of the thesis structure.

Chapter 2: Theoretical background

This chapter provides a comprehensive review of conventional approaches to AAM, including manual methods and a variety of automated algorithms. Their strengths and limitations are discussed in detail. It also explains how AAM problems can be reformulated using graph-theoretical approaches and highlights the computational challenges associated with such formulations, particularly in solving maximum clique problems.

Chapter 3: Proposed Enumeration Algorithm for Combinatorial Optimization Problems using Ising Computing

This chapter presents our proposed enumeration algorithm designed to solve combinatorial optimization problems using Ising computing. The algorithm's design and operational principles are discussed in detail.

Chapter 4: Applications of the Proposed Enumeration Algorithm to AAM Problems

This chapter presents and discusses the details of our proposed AAM algorithm with the results of our proposed AAM algorithm. It includes a comparative analysis of computational time for maximum clique enumeration and an evaluation of the chemical accuracy of the AAM solutions. In addition, the performance of our algorithm is compared with some traditional AAM methods.

Chapter 5: General Conclusions

The final chapter summarizes the key findings of this research, highlighting both the strengths and limitations of the proposed method. It also outlines potential directions for future work.