（様式４）

二国間交流事業 共同研究報告書

令和 6 年 4 月 10 日

独立行政法人日本学術振興会理事長 殿

［日本側代表者所属機関・部局］
北海道大学・低温科学研究所
［職・氏名］
外国人客員研究員・W.M.C.Sameera
［課題番号］
JPJSBP 120229901

1. 事 業 名 相手国: スウェーデン (振興会対応機関: OP)との共同研究

2. 研究課題名

（和文） 星間塵表面におけるラジカルの振る舞いに関する研究:理論計算と実験によるアプローチ

（英文） Predicting radical behaviors on interstellar dust surface: a collaborative theoretical and experimental approach

3. 共同研究実施期間 2022 年 4 月 1 日 ～ 2024 年 3 月 31 日 (2 年 0 ヶ月)

【延長前】 年 月 日 ～ 年 月 日 (年 ヶ月)

4. 相手国側代表者(所属機関名・職名・氏名【全て英文】)

University of Gothenburg・Professor・Nyman Gunnar

5. 委託費総額(返還額を除く)

本事業により執行した委託費総額		3,900,000 円
内訳	1年度目執行経費	1,900,000 円
	2年度目執行経費	2,000,000 円
	3年度目執行経費	－ 円

6. 共同研究実施期間を通じた参加者数(代表者を含む)

日本側参加者等	8 名
相手国側参加者等	12 名

＊ 参加者リスト(様式 B1(1))に表示される合計数を転記してください(途中で不参加となった方も含め、全ての期間で参加した通算の参加者数となります)。

7. 派遣・受入実績

	派遣		受入
	相手国	第三国	
1 年度目	5		( )
2 年度目	4		( )
3 年度目			( )

＊ 派遣・受入実績(様式 B1(3))に表示される合計数を転記してください。

派遣:委託費を使用した日本側参加者等の相手国及び相手国以外への渡航実績(延べ人数)。

受入：相手国側参加者等の来日実績（延べ人数）。カッコ内は委託費で滞在費等を負担した内数。

8. 研究交流の概要・成果等

(1)研究交流概要（全期間を通じた研究交流の目的・実施状況）

The fundamental building blocks of molecules, leading to the chemical evolution in the Universe, can be formed on cosmic ice dust grains in the interstellar medium. To gain quantitative insights into the chemical evolution in the interstellar medium, it is essential to know the mechanisms of the chemical reactions on ice grains at very low temperatures (e.g., 10 K). As the chemical reactions occur at low temperatures, computing rate constants accounting for quantum tunneling is essential.

The objective of the research exchange with Sweden was to develop computational methods to calculate rate constants of the chemical reactions accounting for quantum tunneling. The Swedish team members are very important, as they are the experts in the quantum effects of chemical reaction dynamics. The Japanese team has expertise in computing potential energy surfaces and performing laboratory experiments.

During 2022 and 2023, Japanese team members visited Sweden twice to present and discuss research progress and outcomes. Both Swedish and Japanese teams actively participated in research discussions and presentations.

(2)学術的価値（本研究交流により得られた新たな知見や概念の展開等、学術的成果）

For the rate constant calculations, our objective was to use three methods, in particular the Wigner method, Harmonic quantum transition state theory, and Eckart potential to compute rate constants accounting for quantum tunneling. Rate constants of several reactions on ice were computed and compared with the available experimental results;

PH3 + H, SO2 + H, NH3 + OH, CH3OH + OH (radical), CO + OH (radical).

Computed potential energy surfaces of the above reactions on ice indicated relatively high reaction barriers, which are difficult to pass thermally at low temperatures (e.g., 10 K). In general, we found that the computed rate constates accounting for quantum tunneling from the Wigner method and Harmonic quantum transition state theory are very small and not realistic. On the other hand, the Eckart potential gave reasonable rate constants, indicating that the above reactions can occur at low temperatures.

3)相手国との交流（両国の研究者が協力して学術交流することによって得られた成果）

The Swedish team focused on theoretical studies of the chemical processes in the interstellar medium, while the Japanese team worked on experimental studies. Thus, two symposiums were organized at the University of Gothenburg in Sweden (one in 2020 and another in 2023) to exchange research outcomes from the ongoing research activities and set up new collaborative research projects. Research outcomes from this project have been published and also presented at several national and international conferences.

(4)社会的貢献（社会の基盤となる文化の継承と発展、社会生活の質の改善、現代的諸問題の克服と解決に資する等の社会的貢献はどのようにあったか）

In 2022, three junior and three senior members of the Japanese team visited Sweden to present their research at the Symposium. In 2023, two senior and three junior members visited Sweden and discussed their research outcomes at the symposium. Each member gave presentations followed by active discussions. Thus, both

Japanese and Swedish team members gave their input to achieve the goals of the projects. Symposium dinners were great occasions to establish good relationships with both teams.

(5)若手研究者養成への貢献(若手研究者養成への取組、成果)

The two symposiums were great occasions, especially for young members of both Swedish and Japanese teams for scientific discussions. The Japanese young team members met Swedish researchers, and their research initiatives, through this project, will initiate new potential research collaborations. Now Japanese young team members are in the position to initiate independent research collaborations with the Swedish team members, which will be beneficial for the future research of young team members

(6)将来発展可能性(本事業を実施したことにより、今後どの様な発展の可能性が認められるか)

This project established computational methods to compute rate constants accounting for quantum tunneling, in particular employing the Wigner method, Harmonic quantum transition state theory, and Eckart potential. Computed rate constants give some insights into the possibility of achieving the reaction under experimental conditions. Thus, the outcomes of the present project will be beneficial for future combined experimental and theoretical studies between Japanese and Swedish team members.

(7)その他(上記(2)～(6)以外に得られた成果があれば記載してください)

例:大学間協定の締結、他事業への展開、受賞など