



國立陽明交通大學

NATIONAL YANG MING CHIAO TUNG UNIVERSITY

出國報告（出國類別：國際會議）

**7th Asian Workshop on Molecular  
Spectroscopy  
Workshop on Interstellar Matter 2023**

**第 7 屆亞洲分子光譜研討會  
2023 年星際物質研討會**

服務機關：應用化學所

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派赴國家：日本 札幌

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## 摘要

此次承教育部高教深耕研究計畫補助前往日本札幌，參與 2023 年 11 月 5 日至 10 日在北海道大學舉辦的「第 7 屆亞洲分子光譜研討會」(7th Asian Workshop on Molecular Spectroscopy) 與「2023 年星際物質研討會」(Workshop on Interstellar Matter 2023)，並發表 1 篇報告，題目為 "Infrared spectra of isomers of protonated and hydrogenated phenanthridine isolated in solid parahydrogen"，主要研究為 phenanthridine 和仲氫在低溫間質中共同沉積，並於沉積時以電子束撞擊靶面上之間質形成質子化與氫化的 phenanthridine。為了區分兩者，將間質放置黑暗中一段時間或是照射紫外光，藉由差異光譜來觀測質子化分子吸收之下降與氫化產物吸收上升。最後，利用理論計算對觀測到的光譜作進一步的指認，並對形成產物的反應機構加以研究分析。另外，也利用此機會和世界各國來此與會的教授、學者們討論有關吸收光譜與理論計算的最新訊息。

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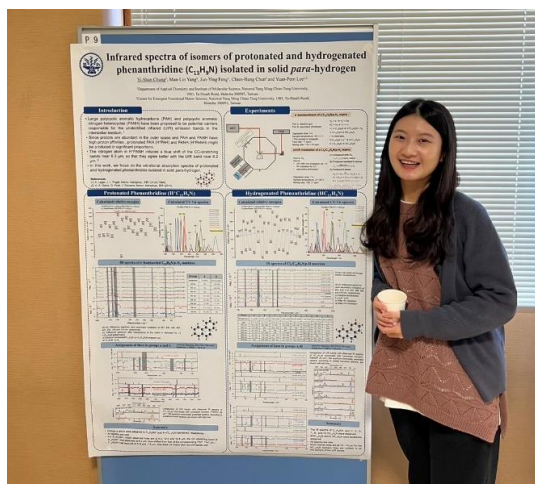
# 本文

## 一、目的

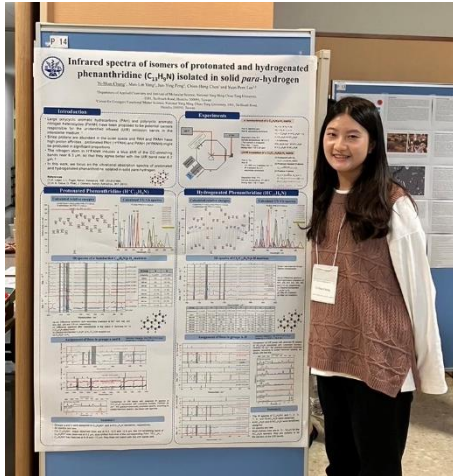
此次前往日本札幌北海道大學分別參與了 7th Asian Workshop on Molecular Spectroscopy 2023 和 Workshop on Interstellar Matter 2023 (ISM2023) 兩場研討會，並將在研討會中針對目前實驗成果進行口頭報告及壁報展示。

## 二、過程

此次兩個研討會為期共五天，於日本北海道大學進行。於 11 月 3 日搭乘長榮班機前往札幌，並於 11 月 6 日 9 點前往會場---北海道大學低溫科學研究所。11 月 6 日至 11 月 7 日期間參與 7th Asian Workshop on Molecular Spectroscopy 2023 (AWMS2023)，此研討會的目的以鼓勵亞洲的年輕學者參與國際研討會為主，並以分子光譜為主題展開。研討會分為口頭報告及壁報展示兩部分，口頭報告每人 25 分鐘，包含演講及問答，兩天總共有 23 位講者輪流發表研究。在 11 月 6 日下午時分別展示我的壁報以及發表口頭報告，並於 11 月 7 日下午再次展示了我的壁報。



主辦單位在此期間順道頒發第 6 屆亞洲分子光譜研討會的 Jon Hougen 獎及 Li-Hing Xu 獎。在會議的最後，Baba 教授主持會議閉幕的演講，並藉由這個機會緬懷已過世的 Jon Hougen 教授，該教授對於分子光譜領域有很大的貢獻，也非常鼓勵年輕學者參與國際研討會，對亞洲學者的照顧不遺餘力，並促成前幾屆亞洲分子光譜研討會的舉辦。



11月8日至11月10日期間一樣在北海道大學參與了另一場國際研討會--- Workshop on Interstellar Matter 2023(ISM2023)。研討會分為口頭報告及壁報展示兩個部分，兩天共有30位講者輪流發表研究。此研討會的講者多數為教授及博士後研究員，主題圍繞在星際物質，討論的內容主要分為觀測、理論及實驗這三個面向，報告時間為20到40分鐘不等。我分別於8日以及9日下午展示

我的壁報，並同時與參與者進行討論，針對有關理論計算以及實驗方法的進一步可能性進行討論。在會議的最後(10日)由 Kobayashi 教授來主持閉幕會議的演講，同時感謝所有與會人士及主辦人員們。研討會結束後，我去參觀了 Watanabe 教授的實驗室並聽教授介紹目前用於研究星際物質的四套低溫系統。

### 三、心得及建議

#### (一) 心得

對於此次能夠出國參加研討會感到非常榮幸，這是我第一次出國參加國際學術研討會。在 AWMS2023 中，與會者主要來自台灣、日本及中國。我的報告題目為 "Infrared spectra of isomers of protonated and hydrogenated phenanthridine isolated in solid para-hydrogen" 透過在仲氫間質中沉積 phenanthridine 並使用二次光解來研究氫化以及質子化的產物，目的是為探討 phenanthridine 是否為外太空未指認的紅光譜 (Ultraviolet bands) 的載體。在壁報展示時，有做理論計算的學者問我為何不用理論計算直接去探討氫原子的轉移，這是我沒有想過的問題，給了我一個新的面向去重新思考並完整我的實驗。雖然此次研討會的參與人數較少，但相對我們有更多的時間能去細細了解他人的報告內容。

在研討會 (AWMS2023) 中，我印象最深刻的研究是來自東京電機大學的 Jun Miyazaki 對於在間質中光解 cyclopentadiene 的研究。說明了此分子以及它的光解產物在不不論是氫氣間質或是仲氫間質中的穩定與活性，和我的研究內容是有部分重疊到的，因此他的實驗條件值得我去做比較。

在此研討會的閉幕時，Baba 教授回顧了此會的歷史及由來，從簡報的歷史照片中，讓我看到許多人在這個領域貢獻了幾十年，許多熟悉的教授出現在 40 年前的研討會照片中，讓人感到十分熱血，對於能參與在其中感到與有榮焉。

在 ISM2023 中，與會人士較多元，相較前一個研討會更多來自歐美的研究者。與會者的報告的內容較前一個研討會來的廣及深，更多著重在理論及觀測。在此研討會中，我壁報展示的題目與前一個研討會一樣，印象深刻的是被人詢問藥品的來源。因在 8 日及 9 日各有兩小時的展示時間，我參觀了許多人的壁報，雖然不是很了解他人的實驗內容，但這個相互介紹並努力去理解的過程很讓人開心。同時，見到了許多以往在論文中掛名的作者，是個特別的經驗。

在研討會 (ISM2023) 中，我印象最深刻的研究是來自荷蘭萊登大學的 Thanja Lamberts 教授的報告。講者主要介紹了水和二氧化碳的冰混合物之光譜及 CN 自由基在此混合物上的反應，在最後探討了此實驗在星際中的影響。

對於我來說，從研討會中學習到的不只是跟學術相關的知識，更多的是理解到自己在口頭報告上的不足以及英語表達上的進步。很多的講者對於自己報告內容的自信以及在表達上的吸引力是我所沒有的，尤其是來自荷蘭萊登大學的 Thanja Lamberts 教授的報告，即使報告內容對我來說是個陌生的領域，但我仍能跟著講者從中理解內容並感到有趣。同時也來自台灣的學者 Yao-Lun Yang 在討論的過程中，更理解到因為大家的研究方向不同，或許實驗的結果不是最重要的，重要的是要如何吸引聽眾並讓他們在聽完後有所啟發。在壁報展示的時候，用英文介紹自己的研究並與參與者相互討論，都進一步訓練我的表達能力也不再那麼害怕與別人交談。這經驗是從來沒有過的，很開心能夠有此體悟，並期許自己能夠更進一步的努力，將來能帶給他人如此的感受。

此外，很開心能在 AWMS2023 中得到 Li-Hing Xu 獎，謝謝李遠鵬教授、馮俊英學姐以及楊曼琳學姐的幫助。

## (二) 建議

希望未來有機會能讓更多學生參與國際的研討會，不僅能擴展研究的方向，還能增加思考的廣度，以增進學者的實驗。

## 四、附錄

### 論文摘要

#### Infrared spectra of isomers of protonated and hydrogenated phenanthridine isolated in solid *para*-hydrogen

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#### Abstract

Large polycyclic aromatic hydrocarbons (PAH) and polycyclic aromatic nitrogen heterocycles (PANH) have been proposed to be potential carriers responsible for the unidentified infrared (UIR) emission bands in the interstellar medium.<sup>1</sup> The nitrogen atom in PANH induces a blue shift of the CC-stretching mode of the PAH, occurring around 6.3  $\mu\text{m}$ . In addition to PANH, several protonated polycyclic aromatic hydrocarbons ( $\text{H}^+\text{PAH}$ ) and the corresponding nitrogen heterocycles ( $\text{H}^+\text{PANH}$ ) also exhibit blue shifts.<sup>2</sup> Therefore, the CC-stretching band of the  $\text{H}^+\text{PANH}$  might agree better with the UIB band at 6.2  $\mu\text{m}$  and  $\text{H}^+\text{PANH}$  might be potential candidates that contribute to the UIR bands.

We report the infrared (IR) spectra of two isomers of protonated phenanthridine ( $\text{H}^+\text{C}_{13}\text{H}_9\text{N}$ ) and seven isomers of mono-hydrogenated phenanthridine ( $\text{HC}_{13}\text{H}_9\text{N}$ ), produced upon electron-bombardment of a mixture of phenanthridine ( $\text{C}_{13}\text{H}_9\text{N}$ ) and *para*-hydrogen (*p*- $\text{H}_2$ ) during matrix deposition at 3.2 K. IR spectra of protonated species  $\text{C}_{13}\text{H}_9\text{NH}^+$  and 4- $\text{H}^+\text{C}_{13}\text{H}_9\text{N}$  were observed. In addition to the hydrogenation on the N atom of  $\text{C}_{13}\text{H}_9\text{N}$  to form  $\text{C}_{13}\text{H}_9\text{NH}$ , mono-hydrogenation at six carbon sites to form 1-, 2-, 3-, 7-, 9-, and 10- $\text{HC}_{13}\text{H}_9\text{N}$ , respectively, were also observed. To confirm the spectral identification of hydrogenated phenanthridine, additional experiments on a  $\text{C}_{13}\text{H}_9\text{N}/\text{Cl}_2/p\text{-H}_2$  matrix were performed; the matrix was irradiated at 365 nm to generate Cl atoms, followed by IR irradiation to generate H atoms via  $\text{Cl} + \text{H}_2 (v=1) \rightarrow \text{HCl} + \text{H}$ . The H atoms thus generated propagated throughout the matrix and reacted with  $\text{C}_{13}\text{H}_9\text{N}$  via quantum tunneling. In these experiments, six hydrogenated phenanthridine species, except the one hydrogenated at the carbon site 3, were clearly observed. Spectral groupings were achieved according to the behaviors of lines upon secondary photolysis at various wavelengths, chosen according to the vertical electronic transitions of various isomers of  $\text{HC}_{13}\text{H}_9\text{N}$  predicted with the TD-B3LYP/6-311++G(d,p) method. The spectral assignments were supported via comparison of the experimental results with the vibrational wavenumbers and IR intensities of possible isomers predicted with the B3LYP/6-311++G(d,p) method. All spectra of  $\text{H}^+\text{C}_{13}\text{H}_9\text{N}$  and  $\text{HC}_{13}\text{H}_9\text{N}$  are new.

For  $\text{H}^+\text{C}_{13}\text{H}_9\text{N}$ , major observed lines are at 2.95, 6.22 and 12.53  $\mu\text{m}$ ; the CC-stretching band of  $\text{C}_{13}\text{H}_9\text{NH}^+$  was observed at 6.22  $\mu\text{m}$ , blue shifted from that of the corresponding PAH, 10- $\text{C}_{14}\text{H}_{11}^+$ . For  $\text{HC}_{13}\text{H}_9\text{N}$ , major lines were observed at 13.43, 13.16, and 13.55  $\mu\text{m}$  for  $\text{C}_{13}\text{H}_9\text{NH}$ , 9- $\text{HC}_{13}\text{H}_9\text{N}$ , and 2- $\text{HC}_{13}\text{H}_9\text{N}$ , respectively. Based on the overall spectral pattern, these protonated and hydrogenated species are unlikely to be the carriers of the UIR bands, characterized by emission bands near 3.3, 6.2, 7.7, 8.6, 11.2, and 12.0  $\mu\text{m}$ .

#### References

- (1) A. Leger, J. L. Puget, *Astron. Astrophys.*, **137**, L5-L8 (1984).
- (2) H. A. Galue, O. Pirali, J. Oomens, *Astron. Astrophys.*, **517** (2010).

#### NOTES



## Infrared spectra of isomers of protonated and hydrogenated phenanthridine isolated in solid *para*-hydrogen

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### References

- [1] A. Leger, J. L. Puget, *Astron. Astrophys.*, **137**, L5-L8 (1984).
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