




# h3ppy: An open-source Python package for modelling and fitting $\text{H}_3^+$ spectra

Henrik Melin <sup>1</sup>

<sup>1</sup> Department of Mathematics, Physics, and Electrical Engineering, Northumbria University, Newcastle upon Tyne, UK

DOI: [10.21105/joss.07536](https://doi.org/10.21105/joss.07536)

## Software

- [Review](#) 
- [Repository](#) 
- [Archive](#) 

Editor: [Dan Foreman-Mackey](#) 

## Reviewers:

- [@tedjohnson12](#)
- [@VincentKofman](#)

Submitted: 21 August 2024

Published: 16 March 2025

## License

Authors of papers retain copyright and release the work under a Creative Commons Attribution 4.0 International License ([CC BY 4.0](#)).

## Summary

h3ppy is an open-source Python package for modelling and fitting the near-infrared spectrum of the tri-hydrogen cation  $\text{H}_3^+$ . This molecular ion is a main component of the charged particle ionospheres of the giant planets (Jupiter, Saturn, Uranus, and Neptune), and observations of these systems span over 30 years ([Miller et al., 2020](#)), using facilities such as ground-based telescopes (e.g. Keck, Very Large Telescope, NASA Infrared Telescope Facility), orbital spacecraft (e.g. Cassini and Juno), and space-based observatories (e.g., James Webb Space Telescope). By fitting the  $\text{H}_3^+$  spectra, physical properties can be determined: 1) the temperature of the upper atmosphere and 2) the column integrated density of  $\text{H}_3^+$  ions. The spatial and temporal distribution of these parameters reveal the processes and dynamics that govern the upper atmospheres of the giant planets, and in particular, how this region couples to both the lower atmosphere below and to the magnetic field beyond. h3ppy provides the tools required to both model the  $\text{H}_3^+$  spectrum and perform these spectral retrievals.

## Statement of need

h3ppy seeks to simplify the process of analysing  $\text{H}_3^+$  spectra by providing a standardised tool for the planetary science community. It is written in Python and installation is accessible via `pip`, which makes installing the package and maintaining it very straightforward. First-time users can generate a spectrum with only a few lines of code, whilst at the same time, the code provides more advanced control of the modelling and fitting process. Whilst other  $\text{H}_3^+$  fitting codes exist in the literature (e.g., [Dinelli et al., 2017](#); [Uno et al., 2014](#)), none are open-source.

For a given temperature and  $\text{H}_3^+$  column density, the code calculates the radiance of each individual  $\text{H}_3^+$  transition, then distributes these in wavelength space by giving them Gaussian line shapes, the width of which is (principally) governed by the spectral resolving power of the spectrograph. The sum of all the individual Gaussian lines then make up the model spectrum. By making use of NumPy array features (NumPy is the only dependency, [Harris et al., 2020](#)), there are significant computational gains, making the code very fast. The fitting procedure uses a hard-coded least-squares approach using partial derivatives of the spectral function, invoking Cramer's Rule ([Bevington & Robinson, 2003](#)). h3ppy implements the  $\text{H}_3^+$  line list of Neale et al. ([1996](#)) and the partition function of Miller et al. ([2010](#)).

By making a h3ppy child class, the core functionality can also be used for other molecular species, and an example on how to use h3ppy to model and fit quadrupole molecular hydrogen spectra ( $\text{H}_2$ ) is provided.

The h3ppy code has already been used in published scientific studies, characterising the ionosphere of Uranus ([Thomas et al., 2023](#)) and Jupiter ([Melin et al., 2024](#)).

## Acknowledgements

HM was supported by a STFC James Webb Fellowship (ST/W001527/2) at Northumbria University, UK.

## References

- Bevington, P. R., & Robinson, D. K. (2003). *Data reduction and error analysis for the physical sciences*. McGraw-Hill.
- Dinelli, B. M., Fabiano, F., Adriani, A., Altieri, F., Moriconi, M. L., Mura, A., Sindoni, G., Filacchione, G., Tosi, F., Migliorini, A., Grassi, D., Piccioni, G., Noschese, R., Cicchetti, A., Bolton, S. J., Connerney, J. E. P., Atreya, S. K., Bagenal, F., Gladstone, G. R., ... Olivieri, A. (2017). Preliminary JIRAM results from Juno polar observations: 1. Methodology and analysis applied to the Jovian northern polar region. *Geophysical Research Letters*, 44(10), 4625–4632. <https://doi.org/10.1002/2017GL072929>
- Harris, C. R., Millman, K. J., Walt, S. J. van der, Gommers, R., Virtanen, P., Cournapeau, D., Wieser, E., Taylor, J., Berg, S., Smith, N. J., Kern, R., Picus, M., Hoyer, S., Kerkwijk, M. H. van, Brett, M., Haldane, A., Río, J. F. del, Wiebe, M., Peterson, P., ... Oliphant, T. E. (2020). Array programming with NumPy. *Nature*, 585(7825), 357–362. <https://doi.org/10.1038/s41586-020-2649-2>
- Melin, H., O'Donoghue, J., Moore, L., Stallard, T. S., Fletcher, L. N., Roman, M. T., Harkett, J., King, O. R. T., Thomas, E. M., Wang, R., Tiranti, P. I., Knowles, K. L., de Pater, I., Fouchet, T., Fry, P. H., Wong, M. H., Holler, B. J., Hueso, R., James, M. K., ... Showalter, M. R. (2024). Ionospheric irregularities at Jupiter observed by JWST. *Nature Astronomy*. <https://doi.org/10.1038/s41550-024-02305-9>
- Miller, S., Stallard, T., Melin, H., & Tennyson, J. (2010).  $\text{H}_3^+$  cooling in planetary atmospheres. *Faraday Discussions*, 147, 283–+. <https://doi.org/10.1039/c004152c>
- Miller, S., Tennyson, J., Geballe, T. R., & Stallard, T. (2020). Thirty years of  $\text{H}_3^+$  astronomy. *Reviews of Modern Physics*, 92(3), 035003. <https://doi.org/10.1103/RevModPhys.92.035003>
- Neale, L., Miller, S., & Tennyson, J. (1996). Spectroscopic properties of the  $\text{H}_3^+$  molecule: A new calculated line list. *The Astrophysical Journal*, 464, 516–+. <https://doi.org/10.1086/177341>
- Thomas, E. M., Melin, H., Stallard, T. S., Chowdhury, M. N., Wang, R., Knowles, K., & Miller, S. (2023). Detection of the infrared aurora at Uranus with Keck-NIRSPEC. *Nature Astronomy*. <https://doi.org/10.1038/s41550-023-02096-5>
- Uno, T., Kasaba, Y., Tao, C., Sakanoi, T., Kagitani, M., Fujisawa, S., Kita, H., & Badman, S. V. (2014). Vertical emissivity profiles of Jupiter's northern  $\text{H}_3^+$  and  $\text{H}_2$  infrared auroras observed by Subaru/IRCS. *Journal of Geophysical Research (Space Physics)*, 119(12), 10, 219–210, 241. <https://doi.org/10.1002/2014JA020454>