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h3ppy: An open-source Python package for modelling and fitting H_3^+ spectra

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Software

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Summary

h3ppy is an open source Python package for modelling and fitting the near-infrared spectrum of the tri-hydrogen cation 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 H_3^+ spectra, physical properties can be determined: 1) the temperature of the upper atmosphere and 2) the column integrated density of 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 H_3^+ spectrum and perform these spectral retrievals.

Statement of need

h3ppy seeks to simplify the process of analysing 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 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 H_3^+ column density, the code calculates the radiance of each individual 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), 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 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 (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).

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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

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). 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 $H_3{}^+$ 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 H_3^+ Molecule: A New Calculated Line List. *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 $H_3{}^+$ and 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