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pyROX: Rapid Opacity X-sections

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Software

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Summary

In recent years, significant advances have been made in exoplanet and brown dwarf observations. By using state-of-the-art models, astronomers can determine properties of their atmospheres, such as temperatures, the presence of clouds, or the chemical abundances of molecules and atoms. Accurate and up-to-date opacities are crucial to avoid inconclusive or biased results, but it can be challenging to compute opacity cross-sections from the line lists provided by various online databases.

We introduce pyROX, an easy-to-use Python package to calculate molecular and atomic cross-sections. Since pyROX works on CPUs, it can compute a small line list on a regular workstation, but it is also easily parallelised on a cluster for larger line lists. In addition to line opacities, pyROX also supports calculations of collision-induced absorption. Tutorials are provided in the online documentation which explain the configuration parameters and different functionalities of pyROX.

Statement of need

The advent of a new generation of telescopes and instruments has led to a dramatically increased quality in observations of exoplanets and brown dwarfs. Such sub-stellar objects are now observed over a wide wavelength range (1-20 µm) with JWST spectra (e.g. August et al., 2023; Carter et al., 2024; Matthews et al., 2025; Miles et al., 2023), for instance, which was previously difficult to access. Developments in ground-based instrumentation allow astronomers to measure young exoplanet companions at closer separations to their host stars (e.g. Landman et al., 2024; Xuan, Mérand, et al., 2024) and at high spectral resolutions (e.g. Nortmann et al., 2025; Xuan, Hsu, et al., 2024). At the same time, progress has also been made in atmospheric modelling using software for radiative transfer, chemistry, circulation models, etc. (e.g. Mollière et al., 2019; Stock et al., 2018; Wardenier et al., 2021). Recently, these observations and software are coupled with sampling algorithms to characterise the atmospheres of the sub-stellar objects (e.g. Barrado et al., 2023; Brogi & Line, 2019; Gibson et al., 2020; Line et al., 2015).

Opacity cross-sections play a key role in accurately modelling sub-stellar atmospheres. Opacity governs the dominant energy transport mechanism (i.e. radiation or convection) which affects the thermal structure of the atmosphere (Marley et al., 2021). Furthermore, high-resolution studies require well-determined frequencies for the transition lines. Inaccuracies in line-list data can result in biased abundance constraints (e.g. Brogi & Line, 2019; de Regt et al., 2024) or ambiguous (non)-detections of certain molecules (e.g. de Regt et al., 2022; Merritt et al., 2020; Serindag et al., 2021). It is therefore important that the most up-to-date and complete opacity data are used. However, it can be difficult to efficiently calculate opacity cross-sections from line lists that sometimes consist of billions of transitions.

To help resolve this challenge, we present pyROX, a user-friendly Python package to calculate molecular and atomic cross-sections for applications in models of sub-stellar atmospheres. pyROX supports line opacity calculations from the ExoMol (Tennyson et al., 2024), HITRAN (Gordon et al., 2022), HITEMP (Rothman et al., 2010), and Kurucz[1] databases. Collision-Induced Absorption (CIA) coefficients can also be calculated from the HITRAN and Borysow[2] databases.

State of the field

Existing open source codes, such as Cthulhu (Agrawal & MacDonald, 2024), ExoCross (Yurchenko et al., 2018; J. Zhang et al., 2024) and HELIOS-K (Grimm et al., 2021; Grimm & Heng, 2015), can calculate cross-sections at comparable performances to pyROX. However, ExoCross is written in Fortran and HELIOS-K utilises GPU-acceleration which can limit their use to experts with the appropriate hardware. pyROX is a Python code that runs only on CPUs which should make it accessible for the opacity needs of most astronomers. Notably, pyROX supports cross-section calculations on any user-provided wavelength or wavenumber grid. This enables the user to fix the spectral resolution ($\mathcal{R} = \lambda/\Delta\lambda$) which cannot be achieved with equal wavelength- or wavenumber-spacing.

Software design

We aim to provide an easy-to-use, comprehensive, and efficient tool to calculate cross-sections for atmospheric gases. These objectives are reflected in the main workflow of pyROX:

- **Download and read files**: The necessary input files (line lists, partition functions, broadening coefficients or CIA files) can be downloaded with a simple command. When reading the relevant parameters, pyROX automatically handles the different data structures of the supported databases (ExoMol, HITRAN/HITEMP, Kurucz, Borysow).
- **Compute line-strengths and -widths**: For line-opacity calculations, pyROX calculates the strength and broadening-widths for each line transition at the user-provided pressure and temperature. Support is offered for various pressure-broadening descriptions. At this point, pyROX can speed up the line-profile computation by selecting only the main line-strength contributors.
- **Compute line profiles**: Next, pyROX computes the Voigt profiles as the real part of the Faddeeva function (Eq. 12 of Gandhi et al., 2020). Although faster approximations exist (Schreier, 2018), we currently support only the more accurate `scipy.special.wofz` implementation[3].
- **Combine and save**: The line profiles are summed into wavelength-dependent cross-sections for each temperature-pressure point. These cross-sections are saved into an efficient HDF5 output file. For CIA calculations, pyROX restructures the coefficients read from the input files into a wavelength- and temperature-dependent grid and also saves these data to an HDF5 file. pyROX offers built-in support for converting its output into the high-resolution opacities used by petitRADTRANS (Mollière et al., 2019). In future releases, we plan to add conversions for other radiative transfer codes popular in the exoplanet and brown dwarf communities.

Documentation for pyROX is available at https://py-rox.readthedocs.io/en/latest/ and includes examples to run the code. The detailed tutorials allow new users to get up to speed with the available options and functionalities. We also welcome suggestions for new features, which can be done by opening an issue on GitHub. If you want to contribute to pyROX, please read the documented guidelines.

[1] http://kurucz.harvard.edu/
[2] https://www.astro.ku.dk/~aborysow/programs/index.html
[3] https://docs.scipy.org/doc/scipy/reference/generated/scipy.special.wofz.html

Research impact statement

Recent publications from our team have employed pyR0X-computed cross-sections (e.g. de Regt et al., 2025; D. González Picos et al., 2025; Darío González Picos et al., 2025; L. Siebenaler et al., 2025; Louis Siebenaler & Miguel, 2025) and this reach is currently expanding to other research groups as well (e.g van Sluijs et al., 2025; Y. Zhang et al., 2026).

AI usage disclosure

Generative AI tools (GPT-4o) were used in the writing of docstrings and code re-factoring. All AI-generated additions or changes were reviewed and edited by the authors to verify that the intended functionality was maintained. No AI tools were used in the writing of this paper and online documentation.

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