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, which describe how strongly atmospheric gases absorb radiation, are therefore crucial to avoid inconclusive or biased results. Due to continuous expansion of the line lists that tabulate the quantum transitions, however, it has become challenging to compute the wavelength-dependent cross sections of the diverse array of molecules and atoms.

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 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; Niraula et al., 2022, 2023) or ambiguous (non)-detections of certain molecular gases (e.g. de Regt et al., 2022; Merritt et al., 2020; Serindag et al., 2021; Simonnin et al., 2025). 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 databases. Collision-induced absorption (CIA) coefficients can also be calculated from the HITRAN and Borysow 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 performance 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 and hardware of most astronomers. In contrast to `Cthulhu`, 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 spacing in wavelength or wavenumber. Unlike the aforementioned codes, pyROX can also account for collision-induced absorption, which is a considerable source of opacity in sub-stellar atmospheres (Freedman et al., 2014).

Software design

We aim to provide an easy-to-use and comprehensive tool to calculate cross sections for atmospheric gases. Although more efficient languages exist, we chose to develop pyROX in Python to keep it readily accessible to the astronomy community. The main workflow of pyROX is as follows:

- **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, namely (1) transition-specific broadening from the ExoMol data, (2) parameterised broadening based on the rotational quantum numbers, or (3) constant coefficients. 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. On a single CPU, this computes 10000 lines in about 3 seconds, using $\Delta\nu = 0.01\ \mathrm{cm}^{-1}$ and a wing-cutoff of $100\ \mathrm{cm}^{-1}$.
- **Combine cross sections**: The line profiles are summed into wavelength-dependent cross sections for each temperature-pressure point. Multiple temperature-pressure points can be calculated simultaneously through the use of the joblib package, enabling straightforward CPU parallelisation for larger line lists.
- **Format and save**: The cross-section table is 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.

pyR0X 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.

The documentation for pyR0X includes examples to run the code and 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 pyR0X, please read the documented guidelines.

Research impact statement

Recent publications from our team have employed pyR0X-computed cross sections (e.g. de Regt et al., 2025; González Picos, de Regt, et al., 2025; González Picos, Snellen, et al., 2025; Siebenaler et al., 2025; Siebenaler & Miguel, 2026), 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 refactoring. 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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