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Excalibur: An Open Source Molecular and Atomic Cross Section Computation Code for Substellar Atmospheres

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Summary

Atmospheric studies of exoplanets and brown dwarfs are a cutting-edge and rapidly-evolving area of astrophysics research. Powerful new telescopes, such as the James Webb Space Telescope (JWST) and the upcoming Extremely Large Telescopes (ELTs), are able to capture in detail spectra of planets and brown dwarfs and thereby probe their chemical composition and physical properties. Calculating models of exoplanet or brown dwarf spectra requires knowledge of the wavelength-dependent absorption of light (cross sections) by the molecules and atoms in the atmosphere. Without accurate cross sections, one cannot reliably measure the chemical composition of substellar atmospheres.

Cross sections are typically pre-computed on a grid of pressures and temperatures from large databases of quantum mechanical transitions (line lists), such as ExoMol (Tennyson et al., 2020), HITRAN (Gordon et al., 2022), HITEMP (Rothman et al., 2010), and VALD (Pakhomov et al., 2017). However, the process of calculating cross sections from line lists is often computationally demanding and has required complex and specialized tools. We aim here to lower the access barrier for users to learn how to calculate molecular and atomic cross sections.

`Excalibur` is a fully Python package that rapidly calculates cross sections from atomic and molecular line lists. `Excalibur` includes modules to automatically download molecular line lists from online databases and compute cross sections on a user-specified temperature, pressure, and wavenumber grid. `Excalibur` requires only CPUs and can run on a user's laptop (for smaller line lists) or on a large cluster in parallel (for billions of lines). `Excalibur` includes in-depth Jupyter tutorials in the online documentation. Finally, `Excalibur` is intended not only for research purposes, but as an educational tool to demystify the process of making cross sections for atmospheric models.

Computing Molecular and Atomic Cross Sections with `Excalibur`

The purpose of the `Excalibur` package is schematically represented in Figure 1. Here we walk through this flowchart, highlighting major use cases of `Excalibur` and the package's role in the broader process of modelling exoplanetary and brown dwarf atmospheres.

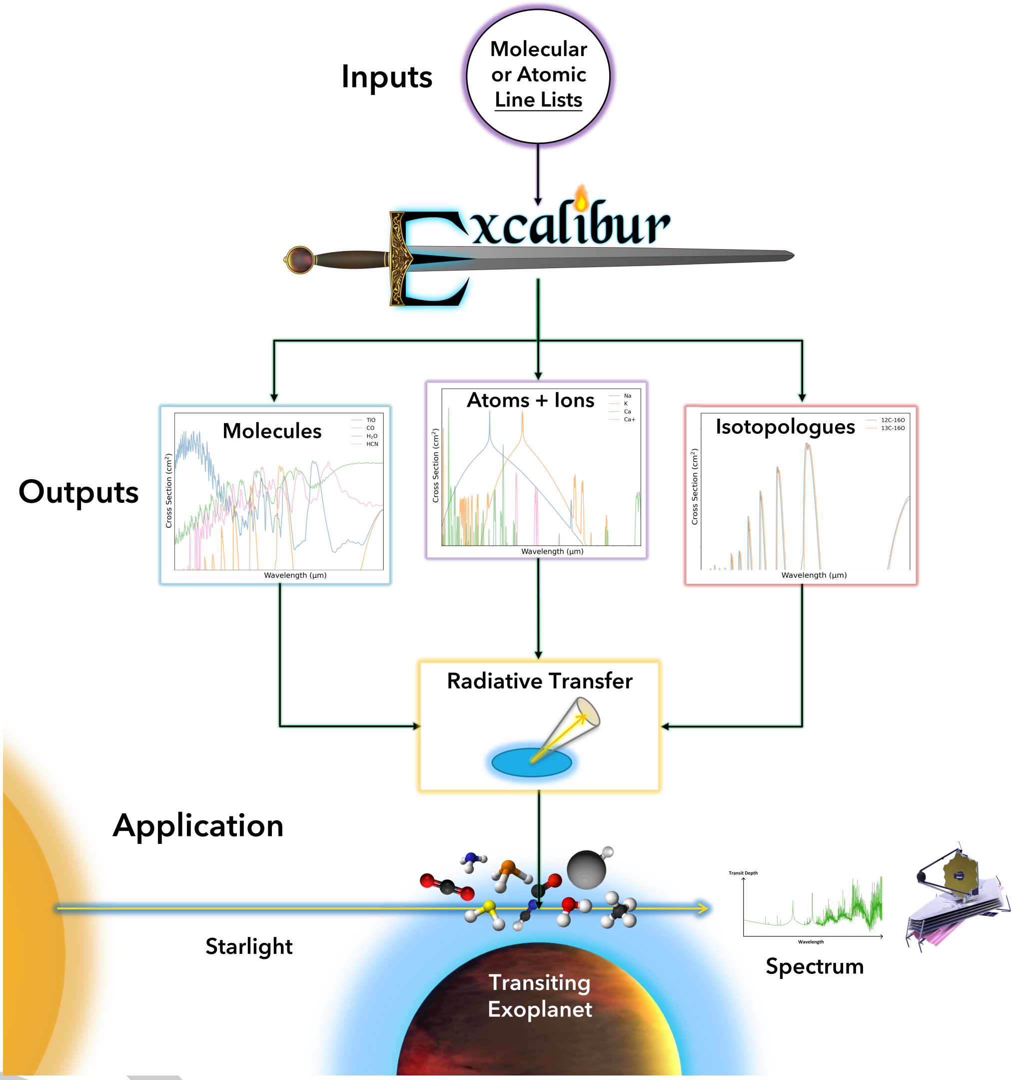

Figure 1: The role and applications of the `Excalibur` Python package. `Excalibur` can download molecular and atomic line lists and calculate the corresponding absorption cross sections as a function of temperature, pressure, and wavenumber. Cross sections made by `Excalibur` can be used in radiative transfer codes to calculate model spectra of exoplanet and brown dwarf atmospheres.

The first use of `Excalibur` is to download existing molecular line lists from online databases. `Excalibur`'s `summon` function can automatically download lines lists from ExoMol and HITRAN/HITEMP (for the latter a user must make an account on https://hitran.org/) and reformat the line lists into space-efficient HDF5 files. Ancillary input files required to calculate cross sections, such as partition functions and pressure broadening files, are also downloaded automatically. Alternatively, the user may manually download a line list from their respective websites and point `Excalibur` to the directory hosting the files. VALD line lists must be downloaded manually by a user with an account on http://vald.astro.uu.se/ (given the terms of use for VALD3), but we provide instructions on how to do this in the `Excalibur` documentation. `Excalibur` currently supports ExoMol, HITRAN, HITEMP, and VALD line lists, though we welcome user requests for additional line list databases support. Once a line list has been downloaded, the user can move onto the next major use case of `Excalibur`, computing cross sections.

The foremost feature of `Excalibur` is its ability to straightforwardly compute atomic and molecular cross sections at high speeds (typically > 100,000 lines per second on one CPU). `Excalibur` is widely accessible, as it does not require GPUs, can run on a standard laptop, and as a fully Python code it is easy for beginners to install and use. To compute a cross section, a user simply calls `Excalibur`'s `compute_cross_section` function, specifying the location of the line list, the temperature and pressure, and the wavenumber range. More advanced users can specify custom settings via optional arguments (e.g. Voigt wing cutoffs, intensity cutoffs, or a user-provided pressure broadening file). The documentation and function doc strings explain the various arguments users can provide to `compute_cross_section`. The computed cross section is output by default as a .txt file in the `output` folder on the user's machine, but `Excalibur` also offers utility functions to combine multiple cross sections (e.g. a grid of temperature and pressures for one or more chemical species) into a HDF5 cross section database.

Figure 1 illustrates three example applications of `Excalibur`: (i) molecular cross section calculations for common opacity sources in hot giant exoplanets; (ii) atomic and ionic cross sections, including sub-Voigt wings for the Na and K resonance doublets; and (iii) cross sections for different isotopologues of the same molecule.

The cross section database HDF5 files produced by `Excalibur` can be readily plugged into the user's favourite exoplanet or brown dwarf modeling or retrieval code. The lower part of Figure 1 illustrates one such application, namely the calculation of exoplanet transmission spectra. In this case, `Excalibur`'s cross sections would be used to calculate the slant optical depth for a ray passing through a transiting exoplanet atmosphere and hence the overall planet's transmission spectrum seen by a distant observer.

Statement of Need

JWST has recently significantly expanded the number of exoplanet and brown dwarfs with high-quality spectra spanning a wide wavelength range. These higher fidelity spectra are motivating detailed intercomparisons of exoplanet and brown dwarf modeling codes, which often require opacity database updates to the latest state-of-the-art molecular line lists. Furthermore, the accurate interpretation of ground-based high spectral resolution exoplanet datasets critically relies on up-to-date opacity data. However, the process of calculating molecular and atomic cross sections is a non-trivial task that is typically outside the speciality of many exoplanet and brown dwarf researchers.

We have built `Excalibur` to provide a user-friendly tool for beginners to learn how to work with the most commonly used line list databases and to readily calculate molecular and atomic cross sections. There are other open source codes that can calculate cross sections, such as HELIOS-K (Grimm et al., 2021; Grimm & Heng, 2015) and ExoCross (Yurchenko et al., 2018), that offer impressive computational performance and are excellent tools for experts to calculate cross sections. However, HELIOS-K requires Nvidia GPUs to run while ExoCross is built in Fortran, which can pose an accessibility issues for beginner's. We offer `Excalibur`, a fully Python code designed to run on CPUs, as a user-friendly entry point into the world of cross sections for substellar atmospheres.

Future Developments

`Excalibur` v1.0 supports line lists from the commonly used ExoMol, HITRAN, HITEMP, and VALD databases, but support for other databases (e.g. Kurucz) can be added in the future. `Excalibur` currently uses Voigt profiles by default (with the exception of the strong Na and K resonance features), but more complex line profiles (e.g. Speed-dependent Voigt) are under consideration for future releases. Suggestions for additional features are more than welcome.

Documentation

Documentation for Excalibur, with step-by-step tutorials illustrating research applications, is available at https://excalibur-xsec.readthedocs.io/en/latest/.

Similar Tools

HELIOS-K (Grimm et al., 2021; Grimm & Heng, 2015), ExoCross (Yurchenko et al., 2018), RADIS (Pannier & Laux, 2019)

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