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easyCHEM: A Python package for calculating chemical equilibrium abundances in exoplanet atmospheres

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Summary

For modeling the spectra of exoplanets one must know their atmospheric composition. This is necessary because the abundance of molecules, atoms, ions and condensates is needed to construct the total cross-section for the interaction between electro-magnetic radiation and matter. In addition, when solving for the temperature structure of an atmosphere the so-called adiabatic temperature gradient must be known, which prescribes the pressure-temperature dependence in convectively unstable regions[1]. Depending on the planetary properties, the composition and adiabatic gradients may be well described by equilibrium chemistry, which means that chemical reactions occur faster than any other processes in the atmosphere, such as mixing. What is more, the equilibrium assumption often serves as a useful starting point for non-equilibrium calculations. Efficient and easy-to-use codes for determining equilibrium abundances are therefore needed.

Statement of need

easyCHEM is a Python package for calculating chemical equilibrium abundances (including condensation) and adiabatic gradients by minimization of the so-called Gibbs free energy. easyCHEM implements the equations presented in Gordon & McBride (1994) (which details the theory behind NASA's CEA equilibrium code) from scratch in modern Fortran, and wraps them in Python to provide an easy-to-use package to the community. For efficient matrix inversion, required for the Gibbs minimization, easyCHEM incorporates the optimized `dgesv` routine of the LAPACK library. Users can interact with easyCHEM's `ExoAtmos` class to calculate atmospheric compositions with just a few lines of code. Users have full control over the atmospheric elemental composition and chemical reactant selection.

The CEA code itself is written in a fixed-form FORTRAN77 style and interacted with the user via input files. In Mollière et al. (2017) we introduced easyCHEM as a from-scratch implementation using the Gordon & McBride (1994) equations and modern Fortran, without the need for input files for run specification. easyCHEM was benchmarked with CEA, leading to identical results. It was also successfully benchmarked with other equilibrium chemistry codes in Baudino et al. (2017). easyCHEM calculations have been used in many publications, such as Nasedkin et al. (2024) and de Regt et al. (2024), to name a few recent ones. Here we report on the Python-wrapped version and make all of its source code public, to further increase its usefulness and accessibility.

We note that other open-source Python packages for computing chemical equilibrium abundances exist, such as TEA (Blecic et al., 2016) or FastChem (Kitzmann et al., 2024).

[1]The corresponding convective region is called "troposphere" on Earth.

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