

## **A Python Interface to ChemApp**

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ChemApp is an extremely useful and powerful tool for doing sophisticated thermochemical calculations and investigations, and for creating process models. The equilibrium calculation results can provide important insight into the behaviour of chemically reactive systems. When programming with ChemApp, there are a number of challenges, though. The API is compact, with a small number of functions, and short function names. This can make it difficult to understand, difficult to remember, and hard to master. ChemApp programs can also be quite bulky, with even relatively simple tasks requiring several lines of code.

Python is an open-source interpreted programming language. It is becoming increasingly popular in science and engineering. It is simple, easy to learn, and uses compact but clear code. A myriad of useful packages are available in Python, which cover numerical methods, linear algebra, chemistry, and many other important areas. The collection of packages is growing all the time. Python has been dubbed the "perfect glue language".

We have developed a package that contains two Python interfaces to ChemApp, the traditional 'tq' interface, as well as a more friendly one. The friendly interface gives the user the best of both worlds. It is possible to have the power of ChemApp, and the simplicity, speed of development, and clarity of Python. The package is presented and demonstrated.