

Notes on the SUPCRT & CPRONS CODES

1. SUPCRT calculates the standard state properties of reactions containing one or more species from the primary data file SPRONS.
2. After any edits to the primary data file (SPRONS), the code CPRONS is used to make the secondary file (DPRONS), which is needed to run SUPCRT.
3. SUPCRT needs the file DPRONS, and a PT file (e.g. Psat), as well as a reaction file containing one or more reactions containing one or more species (e.g. Calcite.in).
4. Both the PT file and the reaction file can be supplied by you (as in the example given) or built for you by SUPCRT, with the option of saving them for repeated use.