# RATE

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## Rate constant calculation

Rate provides the canonical and semiempirical rate constant over a surface. All the program is written in Fortran 90.

The code is based entirely in the approach to the calculation of rate constants shown in [1].No libraries dependencies are present in this code. Compilation can be done directly with the typical **gfortran -o "name of the executable" rate.90**.

In order to run it, two main inputs must be given to the program and must be present at the executable folder. The first one *modes.dat* must contain in the three first lines the number of vibrational modes of reactants, products and activated complex respectively. The next lines must contain the vibrational modes of R, P and TS.

The second input *parameters.dat* first line, has the limit temperatures in which the rate constant is going to be evaluated. The next line must contain the Electronic+ZPE energy of R,P and TS

## References

[1] Justin T. Fermann and Scott Auerbach. *Modeling proton mobility in acidic zeolite clusters: II. Room temperature tunneling effects from semiclassical rate theory.* The Journal of Chemical Physics, 112, 15:6787-6794, 2000.