JTHERGAS

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JTHERGAS (a JAVA implementation of THERGAS) estimates thermodynamic information from two dimensional graphical representations of molecules and radicals based on the Benson additivity method. The main use of this method is within automatic combustion mechanism generation systems where fast estimation of a large number and variety of chemical species is needed. The implementation strategy is based on meta-atom definitions and substructure analysis allowing a highly extensible database without modification of the core algorithms. Several interfaces for the database and the calculations are provided from terminal line commands, to graphical interfaces to web-services. The first order estimation of thermodynamics is based summing up the contributions of each heavy atom bonding description. Second order corrections due to steric hindrance and ring strain are made. Automatic estimate of contributions due to internal, external and optical symmetries are also made. Radicals are calculated by taking the difference due to the lost of hydrogen radicals taking into account changes in symmetry, spin, rotations, vibrations and steric hindrances. The software is public domain.

The project is still under development, but a development version is visible on the following link.
- Login as 'Guest' (just press the guest button).
- Click through the 'Thermodynamic Queries(upper left hand box) and again 'Thermodynamic Queries' (again upper left hand box)
- This brings you to the menu for entering a Nancy Linear Form (similar toSMILES) to calculate the thermodynamic quantities.The following is an example of 2-methylpropane (ch3/ch(ch3)/ch3):

- Benson Rules
- 3 methyl groups
- The tertiary carbon (carbon 2 of 2-methylpropane)
- Symmetry Corrections
- Internal Symmetry: 4 CR3 rotors: 81 (39)
- Eternal Symmetry CR3 connected to a linear group (single atoms are linear).

Some examples of Nancy Linear Form: ch3/ch2/ch2/ch3 butane ch3/ch(oh)/ch2/ch3 sec-butyl alcohol o(#1)/ch2/ch2/ch2/ch2/1 tetrahydrofuran c(#1)h2/ch2/ch2/ch2/1 cyclobutane ch3/ch2/o/o/ch2/ch3 ethyl peroxide c(#1)h2/ch//ch/ch//ch/1 cyclopentadienech3(.)
methyl radical
ch2(.)/ch2/ch2/ch2/ch3 1-pentyl radical
ch3/ch2/ch2/ch(.)/ch3 2-pentyl radical
ch3/ch2/ch(/o/o(.))/ch2/ch3 3-peroxybutyl radical

The JTHERGAS system is built on a very flexible structure: