JTHERGAS

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JTHERGAS: Thermodynamic estimation from 2D graphical representations of molecules

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Abstract
JTHERGAS is a versatile calculator (implemented in JAVA) to estimate thermodynamic information from two-dimensional graphical representations of molecules and radicals involving covalent bonds based on the Benson additivity method. The versatility of JTHERGAS stems from its inherent philosophy that all the fundamental data used in the calculation should be visible, to see exactly where the final values came from, and modifiable, to account for new data that can appear in the literature. 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. The thermodynamical data for radicals is calculated by taking the difference due to the lost of a hydrogen radical taking into account changes in symmetry, spin, rotations, vibrations and steric hindrances. The software is public domain and is based on standard libraries such as Chemistry Development Kit (CDK) and Chemical Markup Language (CML).