Evaluation of the influence of thermodynamic data on the prediction of propane and propene ignition delay times

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The influence of thermodynamic data on prediction of auto ignition chemistry for hydrocarbons such as propane and propene has been investigated. Thermodynamic data with high sensitivity on simulation results have been evaluated thoroughly.

It was found that for example a small change in the enthalpy of formation of propene has high impact on calculated ignition delay times for different propene and propane / oxygen mixtures.

On the other hand, thermochemical data of allyl has a lower sensitivity on the prediction of ignition delay times of propene and propane than thermochemical data of propene, but its positive influence on the prediction of this technical relevant property is still important.
Recently, a value of 168.6 kJ mol^{-1} ± 1.8 kJ mol^{-1}, obtained with the HEAT (High-accuracy Extrapolated Ab initio Thermochemistry) protocol, was recommended for allyl (C_3H_5) for the enthalpy of formation at 298 K [1].

The improvement of the prediction of a detailed reaction mechanism through using accurate thermochemical data, such as the Active Thermochemical Tables Results [2], the IUPAC critical evaluation of thermochemical properties of some free radicals [3] and own quantum chemical calculations with the benchmarked G3B3 composite method is shown.

[1] Daniel P. Tabor, Michael E. Harding, Takatoshi Ichino, and John F. Stanton, High-Accuracy Extrapolated Ab Initio Thermochemistry of the Vinyl, Allyl, and Vinoxy Radicals, *J. Phys. Chem. A*, 116: 7668−7676, 2012.
[2] Active Thermochemical Tables Results available at http://atct.anl.gov/
[3] Branko Ruscic, James E. Boggs, Alexander Burcat, Attila G. Császár, Jean Demaison, Rudolf Janoschek, Jan M. L. Martin, Melita L. Morton, Michel J. Rossi, John F. Stanton, Péter G. Szalay, Phillip R. Westmoreland, Friedhelm Zabel, *J. Phys. Chem. Ref. Data* 34: 573-656 (2005).