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"A database of small molecule thermochemistry for combustion"

In this poster we will present high-accuracy ab initio thermochemistry
for over 200 small hydrocarbons that are important in combustion.  The
poster will compare our results with the standard thermochemistry
databases, including ATcT, NIST, Baulch, and PrIMe.  Using ATcT as a
benchmark, we have developed a Bond Additivity Correction (BAC) for the
QCI electronic structure method.  Application of the BAC lowers the
uncertainty in the enthalpy of formation at 298 K to 0.9 kcal/mol at the
3-sigma level.  We also present an uncertainty analysis for the
partition function, computing the uncertainty in the entropy at 298 K
and the heat capacity as a function of temperature.  Finally, the
resulting thermochemistry are available in NASA polynomials, already
formatted for use with CHEMKIN or other standard software packages.  We
believe that this new database will be extremely valuable for the
combustion community, and the Flame Chemistry Workshop is the perfect
place to get the word out.

Thank you very much.

Kind regards,
Franklin