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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