

Active Thermochemical Tables

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Active Thermochemical Tables (ATcT) have been hailed in the peer-reviewed literature as the most significant improvement in thermodynamics in decades. As opposed to traditional sequential thermochemistry (A begets B, B begets C, ...), ATcT obtain accurate, robust, and internally consistent thermochemical quantities by taking advantage of the Thermochemical Network (TN) approach. The TN contains all available thermochemical interdependencies between the targeted chemical species, such as reaction enthalpies, reaction Gibbs energies, constants of equilibria, adiabatic ionization energies and electron affinities, etc., irrespective of whether they were determined experimentally (actual measurements) or accurately computed (virtual measurements). The determinations that are included in the TN act as a set of qualified constraints that must be satisfied simultaneously by the resulting enthalpies of formation, once the ATcT statistical analysis identifies and corrects the determinations that are inconsistent with the prevailing knowledge content of the TN (i.e. determinations that possess ‘optimistic’ uncertainties). The end result is the extraction of the best possible thermochemistry, based on using optimally all of the currently available knowledge, and characterized by significantly enhanced accuracy and robustness compared to conventional tabulations of thermochemical values.

The ATcT website, ATcT.anl.gov, presently attracts a quarter of a million *different* visitors each year. The most recent publicly available version (ver. 1.124) of ATcT results provides enthalpies of formation for nearly 2800 thermochemically distinct chemical species, while the latest developmental version exceeds 3000 species, interlinked in the TN by >30,000 thermochemically-relevant determinations. ATcT is currently under consideration as a candidate for accession to the distinguished set of U.S. Department of Energy Office of Science Public Reusable Research (DOE SC PuRe) Datasets.

Recent developments and future plans with respect to ATcT will be briefly outlined.

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