

Active Thermochemical Tables as a U.S. DOE Office of Science Public Reusable Data Resource

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Active Thermochemical Tables (ATcT) have been recently promoted to the status of U.S. DOE Office of Science Public Reusable (DOE SC PuRe) Data Resource. The ATcT website, ATcT.anl.gov, presently attracts a quarter of a million *different* visitors each year. The most recent publicly available version (ver. 1.130) of ATcT results provides enthalpies of formation for more than 3000 thermochemically distinct chemical species.

As opposed to the traditional sequential approach to thermochemistry (A begets B, B begets C, etc.), ATcT is based on a distinctly different paradigm that enables the derivation of accurate and reliable thermodynamic properties for a broad range of chemical species by constructing, analyzing, and solving a Thermochemical Network (TN). The TN contains the full breadth of available thermochemical interdependencies between the targeted chemical species, such as reaction enthalpies or free energies, constants of equilibria, adiabatic ionization energies and electron affinities, etc., and effectively represents a set of qualified constraints that must be simultaneously satisfied by the resulting enthalpies of formation. The statistical analysis of the TN identifies constraints that may be - because of the finite accuracies of measurements - inconsistent with the prevailing knowledge content of the TN. The end result is the extraction of the best possible thermochemistry, based on using optimally all of the currently available knowledge. Moreover, ATcT offer a number of additional features that are not available (nor even possible) in the traditional approach. With ATcT, new knowledge can be painlessly added and propagated through all affected thermochemical values. Furthermore, one of the features of the TN approach is that it provides an explicit and quantitative account of intricate correlations between the thermochemistry of the included species, which are normally concealed in sequentially constructed thermochemical tabulations. ATcT also allow hypothesis testing and evaluation, as well as discovery of weak links in the TN, which provide pointers to new determinations that can efficiently improve the underlying body of knowledge.

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