REFINEMENTS OF THE BOND DISSOCIATION ENERGY OF CARBON MONOXIDE AND OF THE ENTHALPY OF FORMATION OF CARBON ATOM IN GAS PHASE USING THE ACTIVE THERMOCHEMICAL TABLES APPROACH

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As opposed to conventional sequential thermochemistry, Active Thermochemical Tables (ATcT), which are being developed at Argonne in conjunction with the Collaboratory for Multi-Scale Chemical Science, are based on a Thermochemical Network (TN) approach. An analisys of the basic TN has indicated that several key thermochemical values need improvement. One of them is the enthalpy of formation of carbon atom in gas phase, equiv. to the vaporization enthalpy of graphite. The quantity is used regularly by ab initio theoretical approaches to convert computed atomization energies to enthalpies of formation. The currently accepted value (716.68 +- 0.45 kJ/mol), recommended by CODATA,[a] is primarily based on D_0(CO) that appears to be somewhat too low. A revised value for the enthalpy of formation of C (g), with a significantly improved uncertainty, has been now obtained by combining state-of-the-art ab initio computations of D_0(CO), a re-analysis of previous spectroscopic data on CO, and other existing thermochemical data via an ATcT treatment of the underlying TN. This work was supported by the U.S. Department of Energy, Division of Chemical Sciences, Geosciences and Biosciences of the Office of Basic Energy Sciences, and by the Mathematical, Information, and Computational Science Division of the Office of Advanced Scientific Computing Research, under Contract No. W-31-109-ENG-38.

[a] J. D. Cox, D. D. Wagman, and V. A. Medvedev, *CODATA Key Values for Thermodynamics*, Hemisphere, New York, 1989