FURTHER REFINEMENTS OF THE BOND DISSOCIATION ENERGY IN WATER AND HYDROXYL RADICAL USING THE ACTIVE THERMOCHEMICAL TABLE APPROACH

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The bond dissociation energies of water and hydroxyl radical, D_0(H-OH) and D_0(OH), were recently revised by thermochemically significant amounts (approx. 2 kJ/mol)[a]. Using the thermochemical network approach (a.k.a. Active Thermochemical Table approach), we have now addressed a much smaller remaining inconsistency (approx. 20 cm^{-1}) between some of the competing measurements. The recently developed Active Table tool, via statistical analysis of the supplied thermochemical network (which contains all available measurements, including those that appeared after the revision) helps identify measurements that have "optimistic" error bars, i.e. indicates which of the experimental values that are included in the network are highly unlikely. In addition, the Active Table approach allows convincing tests of alternate hypotheses via "what if" scenarios. The resulting thermochemical values fully validate the recently revised values, and further fortify them by providing significantly lower uncertainties. 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] B. Ruscic, A. F. Wagner, L. B. Harding, R. L. Asher, D. Feller, D. A. Dixon, K. A. Peterson, Y. Song, X. Qian, C.-Y. Ng, J. Liu, W. Chen, and D. W. Schwenke *J. Phys. Chem. A* **106**, 2727 (2002)