

NIST Computational Chemistry Comparison and Benchmark Database

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The Computational Chemistry Comparison and Benchmark Database (CCCBDB) is a collection of experimental and calculated ab initio thermochemical, vibrational, geometric and electrostatic data for 700 molecules and a web site of over 400 pages to display and compare the experimental and computed properties. The database contains results from over 110 000 calculations and is growing in both the number of calculations and the number of molecules. The addition of new molecules is guided by user requests. Previously the molecules contained atoms through Chlorine, but we are expanding with the addition of molecules that contain Bromine, Titanium, Copper, or Zinc, more aromatic species, and hydrogen-bonded systems. We will review the experimental and calculated geometry data present and discuss which calculations perform poorly. The CCCBDB is online at: <http://srdata.nist.gov/cccbdb>