

Equilibrium Molecular Structures : Exploring accuracy of the 4th decimal place

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Molecular structures determine spectroscopic parameters that allow molecular identification and reveal qualitative information about bonding, energetics and other things. Over the years, a number of distinct operational definitions of molecular structure have emerged and likewise there's many approached or techniques to getting an equilibrium structure.

Today, the most satisfactory method for determining very high-accuracy structures is a mixed experimental-theoretical approach that uses ground state rotational constant data from microwave spectroscopy and vibrational corrections obtained from quantum-chemical calculations. Here in we explore the legitimacy and confidence in reporting a bond distance to four decimal places (10^{-4} Å) for semi experimental structures of some small molecules. We also compare energy vs geometry based *ab initio* composite schemes for obtaining equilibrium structures.