HIGH ACCURACY MOLECULAR STRUCTURES

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Molecular structures determine spectroscopic parameters that allow molecular identification and reveal qualitative information about bonding and energetics. Over the years, a number of distinct operational definitions of molecular structure (bond lengths and bond angles) have emerged and some confusion often exists when theoreticians and experimentalists debate "a bond length". Here I briefly review the practical value of accurate molecular structures and survey existing experimental and theoretical methods for determining them. I place particular emphasis on the Kraitchman r_s substitution structure, the computationally obtained r_e structure and the semi-experimental r_e^{SE} structure. Ultimately, the most satisfactory method for determining very high-accuracy structures today is a mixed experimental-theoretical approach that uses data from microwave spectroscopy and quantum-chemical calculations. After discussing that, I talk in detail about a different approach to obtaining Kraitchman substitution structures that we have recently employed.