

Thermochemical and Spectroscopy Properties Across the Periodic Table

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In the rational analysis and design of molecular species, energetic data is often the most critical information needed. One longstanding challenge is in achieving accurate energetics (i.e., enthalpies of formation, ionization energies) for molecules species across the periodic table, and for molecules of increasing size. Challenges that can be encountered include limited experimental gauges for calculations, computational (i.e., computer memory, disk space, and CPU time) limitations, and increasing atomic and molecular complexity beyond the first rows of the periodic table. Strategies for addressing these challenges and predicting quantitatively accurate energies and spectroscopic properties will be discussed. The importance of the choice of thermochemical pathway, effective gauges and insight into computational approaches, particularly for transition metal species and heavy element species will be discussed, as will ground state and excited state species.