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The heavy element FPD composite method: Applications to atomic and molecular actinide species

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The Feller-Peterson-Dixon (FPD) composite thermochemistry method, modified for heavy element calculations, is based on complete basis set (CBS) extrapolations at the scalar relativistic CCSD(T) level of theory using all-electron correlation consistent Gaussian basis sets. In addition to the usual contributions of outer-core electron correlation and zero-point vibrational corrections, spin-orbit coupling effects, both molecular and atomic, are accurately recovered using predominately 4-component all-electron methods. As in calculations involving light elements, electron correlation beyond CCSD(T) is also considered when computationally feasible. Recent work using this approach that will be highlighted will include atomic and molecular ionization energies, including high ionization energies of several lanthanide and actinide atoms, electron affinities of early actinide atoms, as well as current efforts to interpret recent anion photodetachment spectra of various thorium- and uranium-containing anions.