Ab Initio calculation on muonic atoms and molecules

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Abstract

In this work, we investigated muonic atoms and molecules from a quantum chemist's viewpoint by incorporating muons in the CASSCF model. With the aim of predicting muonic X-ray energies, primitive muonic basis sets were developed for a selection of elements. The basis sets were then used in CASSCF calculations of various atoms and molecules to calculate muonic excited states. We described the influence of nuclear charge distribution in predicting muonic X-ray energies (see Illustration 1). Effects of the electronic wave function on the muonic X-ray energies were also examined. We have computationally demonstrated how the muon can act as a probe for the nuclear charge distribution or electronic wave function by considering lower or higher muonic excited states, respectively.

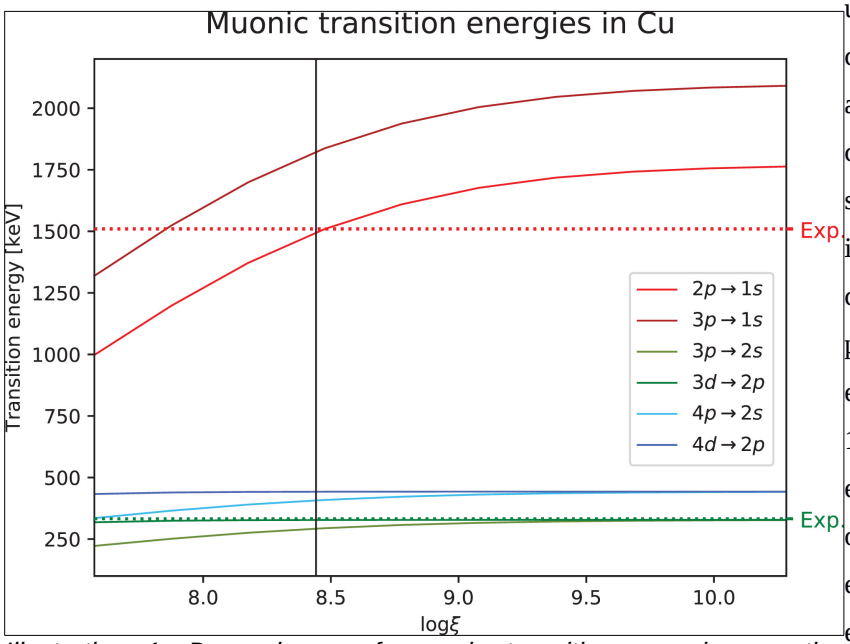

Illustration 1: Dependence of muonic transition energies on the logarithm of the Gaussian nuclear charge distribution.The vertical line denotes the default value, $\xi = 2.767 \cdot 108$, for the Gaussian nuclear charge distribution. For comparison we have depicted the experimental transition energies with dashed horizontal lines.