

Electronic structure of molecules containing very heavy & superheavy elements

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Relativistic computations that include both relativistic and electron correlation effects such as complete active space multi-configuration interaction (CAS-MCSCF) followed by multi-reference configuration interaction (MRSDCI) computations that included up to 50 million configurations of molecules containing very heavy and superheavy elements reveal surprising trends compared to their lighter analogs in the periodic table. We shall discuss these unusual features and trends concerning structure and properties of these very heavy to superheavy molecules. We have computed not only the ground electronic states, but also several excited electronic states. It is shown that Jahn-Teller distortion is quenched by spin-orbit coupling in these very heavy species. We have carried out relativistic computations for the electronic states of the newly discovered superheavy elements and yet to be discovered elements such as 113 (eka-thallium) 114 (eka-lead) and 114+. Many unusual periodic trends in the energy separations of the electronic states of the elements 114, 113, 114+, (113)H, 114H, etc., and unusual features in electronic state compositions are found due to relativistic effects. The potential energy surfaces of (114)H₂ exhibit unusual trends compared to PbH₂ due to relativity and break-down of singlet and triplet features of the electronic states due to spin-orbit coupling. Unusual features have been computed for the Lawrencium and Nobelium compounds. All of these species will be considered with emphasis on unusual periodic trends.