

Quantum Chemistry Seminar 7

Helium atom

Exercise 1 (Anila)

Using the results of all the approximate calculations given in lesson 7, calculate the ionization potential of helium (the energy needed to remove an electron from the electronic cloud of the helium atom) and compare the calculated values with a benchmark value (24.6 eV). [Hint: Calculate the ionization potential as a difference between the ground-state energy of He and that of He⁺.]

Exercise 2 (unassigned)

Using the results of all the approximate calculations given in lesson 7, calculate the ground-state energy of ions Li⁺ and Be²⁺ and compare them with benchmark values (-198.1 eV and -371.6 eV).