Quantum Computing for Quantum Chemistry - Exercises

EUMEN Team - Quantinuum

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1 Lecture 1 – Solutions

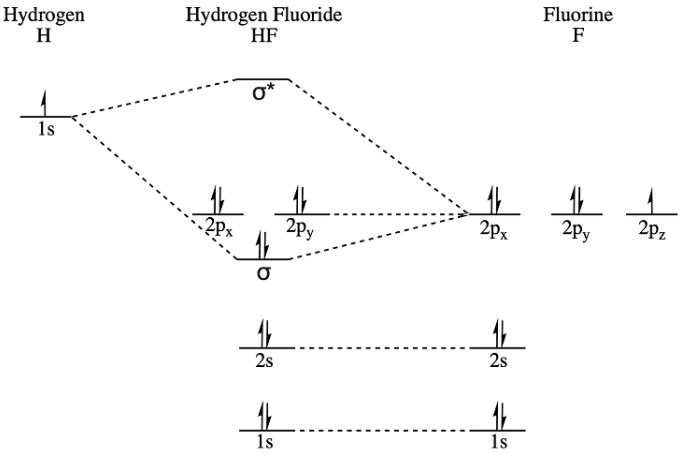
1(a) i $1s^2\ 2s^2\ 2p^6$

ii $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p_x^2\ 3p_y^2\ 3p_z^1$

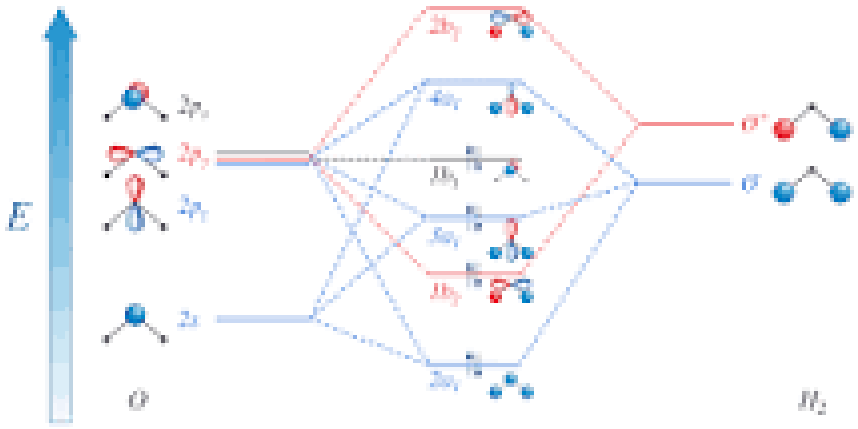
iii $1s^2\ 2s^2\ 2p_x^1\ 2p_y^1$

iv $1s^2\ 2s^2\ 2p_x^2\ 2p_y^1\ 2p_z^1$

v $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p_x^2\ 4p_y^2\ 4p_z^2$



1(b) i



ii

2. (a) Substitute $m = 1$, $Z = 1$ into expression for E, differentiate w/respect to ξ, solve for ξ.

$$E = \frac{\xi^2}{2} - \xi \tag{1}$$

$$\frac{\partial E}{\partial \xi} = \xi - 1 = 0 \tag{2}$$

$$\xi = 1 \tag{3}$$

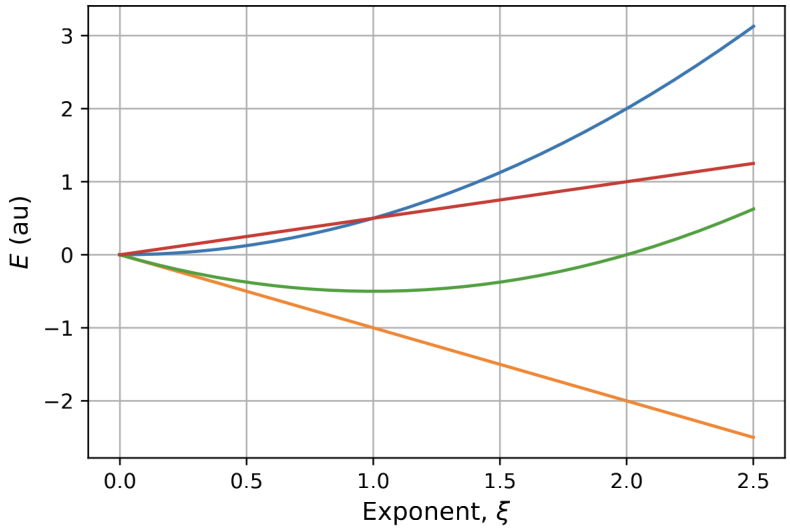


Figure 1: The kinetic (blue), potential (orange) and total (green) energies of the H atom as a function of orbital exponent. The red line is $-V/2$ where V is the potential energy.

(b)

(c) Intersect is at 1.0, matches exponent. Only nonzero intersect obtained at minimum and when virial theorem satisfied. Virial theorem only satisfied at energetic minimum.

(d) Starting from asymptotic separation, no change until about 7.75 bohr. When atomic orbitals start to overlap potential energy goes **up**, not down, contrary to what most undergraduate textbooks say. Kinetic energy goes down. Inspection of plot from part (b/c) shows that kinetic energy goes down when wavefunction more diffuse, electron can occupy more space without tunneling. Kinetic energy therefore responsible for driving bond formation. Once within close proximity, orbital contracts, less space for electron to occupy, kinetic energy goes up. Electron "closer" to nucleus, potential energy goes down. Potential energy takes over driving bond formation once it has already been initiated.