MEST - Assignment 5

Due date: 12/05/2022
(For each solution, show your work through a set of important steps.)

1. For the hydrogen atom, plot the radial wavefunction for (i) the exact $1s$ AO, and (ii) approximate AO using CGTOs. (3 pts)

2. For the $HMn(CO)_5$ molecule, enumerate the total number of CGTOs that constitute the 6-31G and STO-3G basis sets. Try to answer this without and with the help of the basis-set website (https://www.basissetexchange.org/). How many spatial MOs will be occupied and how many will be empty? (3 pts)

3. For NH_3 molecule, the five lowest-energy spatial MOs in terms of AOs are:

$$\psi_1 = 0.99339\phi_{N_{1s}} + 0.03182\phi_{N_{2s}} - 0.00440\phi_{N_{2p_z}} - 0.00658(\phi_{H1_{1s}} + \phi_{H2_{1s}} + \phi_{H3_{1s}})$$

$$\psi_2 = -0.22026\phi_{N_{1s}} + 0.73925\phi_{N_{2s}} - 0.12153\phi_{N_{2p_z}} + 0.16182(\phi_{H1_{1s}} + \phi_{H2_{1s}} + \phi_{H3_{1s}})$$

$$\psi_3 = 0.58945\phi_{N_{2p_x}} + 0.42798(\phi_{H2_{1s}} - \phi_{H3_{1s}})$$

$$\psi_4 = 0.58945\phi_{N_{2p_y}} + 0.49419\phi_{H1_{1s}} - 0.24710(\phi_{H2_{1s}} + \phi_{H3_{1s}})$$

$$\psi_1 = -0.08049\phi_{N_{1s}} + 0.40462\phi_{N_{2s}} + 0.91261\phi_{N_{2p_z}} - 0.11245(\phi_{H1_{1s}} + \phi_{H2_{1s}} + \phi_{H3_{1s}})$$

   For this configuration, calculate the individual AO electronic population, Gross electronic population on each atom, and the net charges. All AOs are normalized while the overlap integrals are given by:

$$\langle\phi_{N_{1s}}|\phi_{N_{2s}}\rangle = 0.235038, \langle\phi_{N_{2p_y}}|\phi_{H1_{1s}}\rangle = 0.411956$$

$$\langle\phi_{N_{1s}}|\phi_{H1_{1s}}\rangle = \langle\phi_{N_{1s}}|\phi_{H2_{1s}}\rangle = \langle\phi_{N_{1s}}|\phi_{H3_{1s}}\rangle = 0.0573208$$

$$\langle\phi_{N_{2s}}|\phi_{H1_{1s}}\rangle = \langle\phi_{N_{2s}}|\phi_{H2_{1s}}\rangle = \langle\phi_{N_{2s}}|\phi_{H3_{1s}}\rangle = 0.489927$$

$$\langle\phi_{N_{2p_z}}|\phi_{H1_{1s}}\rangle = \langle\phi_{N_{2p_z}}|\phi_{H2_{1s}}\rangle = \langle\phi_{N_{2p_z}}|\phi_{H3_{1s}}\rangle = -0.145649$$

$$\langle\phi_{H_{1s}}|\phi_{H2_{1s}}\rangle = \langle\phi_{H1_{1s}}|\phi_{H3_{1s}}\rangle = \langle\phi_{H2_{1s}}|\phi_{H3_{1s}}\rangle = 0.201445$$

$$\langle\phi_{N_{2p_y}}|\phi_{H2_{1s}}\rangle = \langle\phi_{N_{2p_y}}|\phi_{H3_{1s}}\rangle = -0.205978$$

$$\langle\phi_{N_{2p_x}}|\phi_{H2_{1s}}\rangle = -\langle\phi_{N_{2p_x}}|\phi_{H3_{1s}}\rangle = 0.356765$$

   (5 pts)

4. The $U(R)$ curve for a repulsive electronic-state of a diatomic molecule can be approximated by the function $ae^{-bR} - c$, where a,b, and c are positive constants with $a > c$. (Note:This function omits the Van der Waals minimum and fails to go to infinity at R = 0.) Sketch U, $\langle T_{el}\rangle$, and $\langle V\rangle$ as functions of R for this function.($V = V_{el} + V_{nn}$). (4 pts)