Chem231B: Quiz #3

February 12, 2020

1. -20 eV; singlet
2. -12 eV; degeneracy of 4
3. ???
4. $\Psi^{\mathrm{HF}} = \frac{1}{\sqrt{2}}(\phi_1(x_1)\alpha(x_1)\phi_2(x_2)\beta(x_2) - \phi_2(x_1)\beta(x_1)\phi_1(x_2)\alpha(x_2))$
   spatial orbitals $\phi_1(x)$ and $\phi_2(x)$ with spin α and β for electrons x_1 and x_2
5. $\hat{H} = \sum_i^3 -\frac{1}{2}\nabla_i^2 - \sum_i^3 \frac{3}{|r_i|} + \sum_i^3 \sum_{j\neq i}^3 \frac{1}{2|r_i - r_j|}$
6. $J = 1$, $M = \{-1, 0, 1\}$, a total of $2J + 1 = 3$ states
7. ???
8. $E_{\mathrm{IP}} = |E_N^{\mathrm{He}} - E_{N-1}^{\mathrm{He}}| = |-77.9 + 54.4| = 23.5$ eV
9. 5.6% Error
10. From lowest to highest in energy: ^4S, ^2D, ^2P