Chem231B: Quiz #3

February 11, 2020

1. -20 eV; singlet
2. -12 eV; degeneracy of 1
3. -2 eV
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. $\hat{H} = \sum_i^3 -\frac{1}{2}\nabla_i^2 - \sum_i^3 \frac{3}{|r_i - R|} + \sum_i^3 \sum_{j \neq i}^3 \frac{1}{2|r_i - r_j|}$
6. $J = \{2, 1, 0\}$, $M = \{-2, -1, 0, 1, 2\}$
7. ???
8. $E_{\mathrm{IP}} = |E_N^{\mathrm{He}} - E_{N-1}^{\mathrm{He}}| = |-79.0 + 54.4| = 24.6$ eV
9. 1.2% Error
10. From lowest to highest in energy: ${}^4S$, ${}^2P$, ${}^2D$