

Problem 1

| | Z | $^2P_{1/2}$ (eV) | $^2P_{3/2}$ (eV) | ΔE (eV) | ζ (eV) |
|-------------------|---|------------------|------------------|-----------------|--------------|
| H I | 1 | 10.1988057 | 10.1988511 | 4.54E-05 | 4.53058E-05 |
| He ⁺ | 2 | 40.813029 | 40.8137552 | 0.0007262 | 0.000724892 |
| Li ⁺⁺ | 3 | 91.8393488 | 91.843026 | 0.0036772 | 0.003669766 |
| Be ⁺⁺⁺ | 4 | 163.284606 | 163.296231 | 0.011625 | 0.011598274 |
| B ⁺⁺⁺⁺ | 5 | 255.159221 | 255.187609 | 0.028388 | 0.028316098 |

Problem 2

| | Z | singlet | triplet | ΔE (eV) |
|------------------|---|------------|------------|-----------------|
| He | 2 | 20.6157736 | 19.8196134 | 0.7961602 |
| Li ⁺ | 3 | 60.92268 | 59.020812 | 1.901868 |
| Be ⁺⁺ | 4 | 121.651 | 118.591 | 3.06 |
| B ⁺⁺⁺ | 5 | 202.8034 | 198.5663 | 4.2371 |

| | $R_{\text{OH}} (a_0)$ | θ |
|--------------|-----------------------|-------------|
| Experimental | 0.958 | 104.5 |
| Gaussian | 0.96666657 | 107.6799801 |

The bond distance yields and error of 1%; the angle, 3%.

Orbital Energies for the ground state configuration:

| | $1a_1^2$ | $2a_1^2$ | $1b_1^2$ | $3a_1^2$ | $1b_1^2$ |
|--------|-------------|-------------|-------------|-------------|--------------|
| E (HF) | -20.42413 | -1.32207 | -0.69196 | -0.52709 | -0.4764 |
| E (eV) | -555.769092 | -35.9753705 | -18.8291977 | -14.3428548 | -12.96350912 |

| Sym Species | No | Exp. Freq (A) | Gaussian (A) |
|-------------|----|---------------|--------------|
| a_1 | 1 | 3657 | 3812 |
| a_1 | 2 | 1595 | 1799 |
| b_1 | 3 | 3756 | 3945 |