Practice Modern Physics II, W2018, Set 1

Question 1 Energy Level Diagram of Boron ion B^{2+} For neutral B, Z = 5.

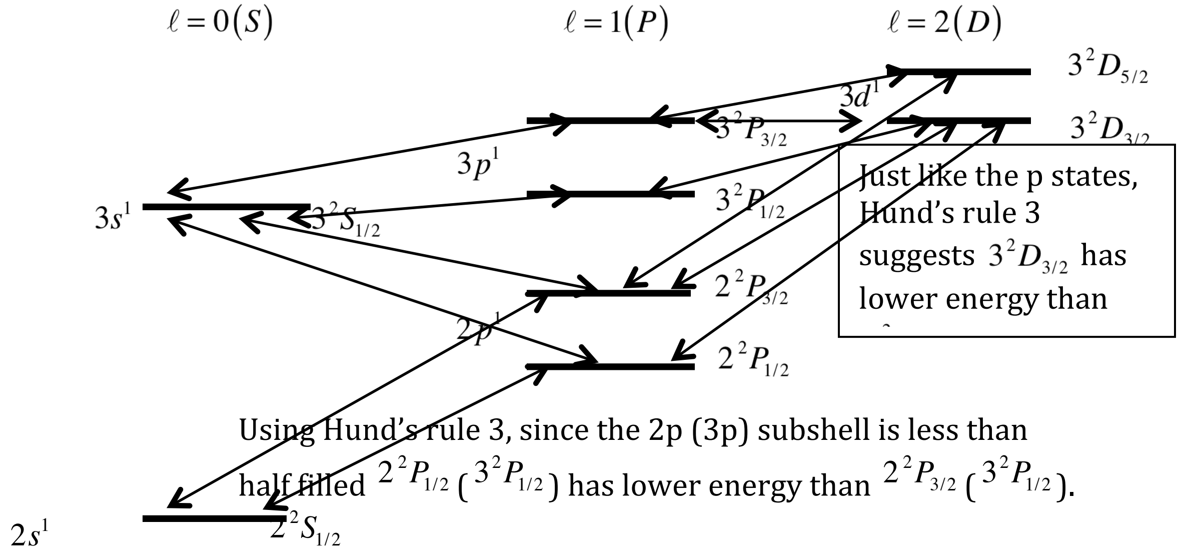
(A) Draw the fine-structure diagram of B^{2+} that includes all n = 3 states. Label the states in **spectroscopic notation.**(B) Using the selection rules of equation 8.8 draw all the allowed transitions of B^{2+} . Such diagrams are called **Grotian diagrams**.

The ground state B^{2+} has three electrons, electronic configuration is $1s^2 2s^1$. As shown in class, only the electron in the unfilled subshell $2s^1$ contributes to the angular momentum of the atom. We show in class that $S = s_1 = 1/2, L = \ell_1 = 0, J = L + S = S = 1/2$, with term symbol $2^2S_{1/2}$.

The first excited states electronic configuration is $1s^2 2p^1$. There is a single electron in the unfilled $2p^1\left(\ell_1 = 1\right)$ subshell. So $S = 1/2$ and $L = 1$. The possible values of $J = L + 1/2, L - 1/2$ gives **two states** $J = 3/2, 1/2$. The states are: 1) $S = 1/2, L = 1, J = 1/2$ giving $2^2P_{1/2}$; 2) $S = 1/2, L = 1, J = 3/2$ giving $2^2P_{3/2}$

The next excited state electronic configuration is $1s^2 3s^1$. It should be clear that that $S = s_1 = 1/2, L = \ell_1 = 0, J = L + S = S = 1/2$, with term symbol $3^2S_{1/2}$.The next excited states electronic configuration is $1s^2 3p^1$. The $3p^1$ electron gives $S = 1/2$ and $L = 1$. The possible values of $J = L + 1/2, L - 1/2$ gives **two states** $J = 3/2, 1/2$. The states are: 1) $S = 1/2, L = 1, J = 1/2$ giving $3^2P_{1/2}$; 2) $S = 1/2, L = 1, J = 3/2$ giving $3^2P_{3/2}$.

The final excited states for the n = 3 shell has electronic configuration is $1s^2 3d^1$. The $3d^1\left(\ell_1 = 2\right)$ electron gives $S = 1/2$ and $L = \ell_1 = 2$. The possible values of $J = L + 1/2, L - 1/2$ gives $J = 5/2, 3/2$. The states are: 1) S =1/2, L =2, J = 3/2 giving $3^2D_{3/2}$; 2) $S = 1/2, L = 2, J = 5/2$ giving $3^2D_{5/2}$.The schematic energy diagram is below:



Just like the p states, Hund's rule 3 suggests $3^2D_{3/2}$ has lower energy than

Using Hund's rule 3, since the 2p (3p) subshell is less than half filled $2^2P_{1/2}$ ($3^2P_{1/2}$) has lower energy than $2^2P_{3/2}$ ($3^2P_{1/2}$).

In the diagram, a thick line indicates a state of B^{2+}, with the term symbol, n^2L_J, on the right of the line. The electronic configurations are on the left of the lines. The double-arrow lines that connect two states indicate allowed transitions that obey the transition rules of equation 8.8.

Question 2 Atomic Physics (Fine Structure and Zeeman Effects)

Excited states of atoms, fine-structure, and Zeeman effects. The ground-state configuration of **SODIUM** (Z = 11) is $1s^2 2s^2 2p^6 3s^1$, **in term symbol** is $3^2S_{1/2}$.

A) Write is the **first excited state electronic configuration of Sodium**. Find **the spectroscopic notation** (term symbol) of the **two states** associated with this excited state. **Hint**: find all the total orbital Angular Momentum (L) and total spin (S), and all the **possible** total angular momentum (J). **Also see equation sheet for energy order**!!

The electronic configuration of the first excited state is $1s^2 2s^2 2p^6 3p^1$.

For this configuration, only the $3p^1$ electron contribute to the angular momentum, and hence $S = 1/2$, $L = 1$. The **total angular momentum** is $J = L + S, \ldots |L - S|$.

There are **two states:**

i) $J = L + S = 3/2$ with $S = 1/2$ and $L = 1$. The term symbol is $3^2P_{3/2}$.

ii) $J = |L - S| = 1/2$ with $S = 1/2$ and $L = 1$. The term symbol is $3^2P_{1/2}$.

B) Write the **second excited state electronic configuration of SODIUM**. Find **the spectroscopic notation** (term symbol) of the **one state** associated with this excited state. Briefly explain why there is **only one state. Look at the energy order list in back!**

The electronic configuration of the second excited state is $1s^2 2s^2 2p^6 4s^1$. For this configuration, only the $4s^1$ electron contribute to the angular momentum, and hence $S = 1/2$, $L = 0$. There is only value of **total angular momentum** is $J = S = 1/2$. For $J = 1/2, S = 1/2$ and $L = 0$. The term symbol is $4^2S_{1/2}$.

C) The first excited state of **LITHIUM** (Z = 3) has electronic configuration $1s^2 2p^1$, and is split into two states (doublet) $2^2P_{1/2}$ and $2^2P_{3/2}$. It is estimated that the **internal magnetic field** for this state is $B_{\text{int}} = 0.36T$. Find the **fine-structure** energy difference between the $2^2P_{1/2}$ and $2^2P_{3/2}$ states.

Fine-structure splitting is

$$\Delta V_{fs} = 2\mu_B B_{\text{int}} = 2\left(5.788 \times 10^{-5} eV/T\right)\left(0.36T\right) = 4.17 \times 10^{-5} eV$$

D) Suppose the **LITHIUM** atom is placed in an external magnetic field of magnitude $B = 0.5T$. How many energy levels do the $2^2P_{3/2}$ have? Draw a schematic diagram to illustrate these energy levels. Find the energy spacing between adjacent energy levels. **HINT:** This is the Zeeman Effects! Lande factor is relevant!

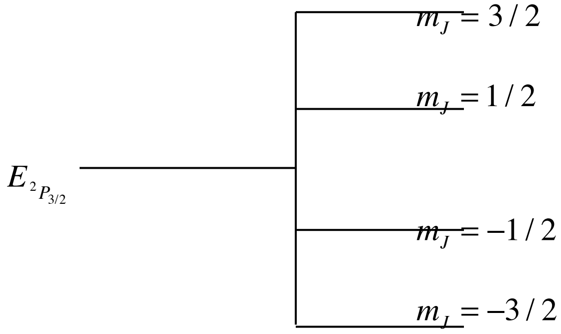
The **Zeeman energy** of these levels are given by $V_z = \mu_B B_{ext} g m_J$. For $2^2P_{3/2}$, $J = 3/2$ and $m_J = -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}$ giving four distinct energy levels.

The energy separation between **adjacent levels** (for example $m_j = 3/2$ and $m_j = 1/2$, or $m_j = 0$ and $m_j = -1/2$) is simply, $\Delta V_z = \mu_B B_{ext} g \Delta m_j = \mu_B B_{ext} g$, where $\Delta m_j = 1$ for adjacent levels. For ${}^2P_{3/2}$ state $J = \frac{3}{2}$, L = 1, and S = ½

$$g = 1 + \frac{1.5(1.5+1) + 0.5(0.5+1) - 1(1+1)}{2(1.5)(1.5+1)} = 1.33$$

For $B_{ext} = 0.50T$, we use $\mu_B = 5.788 \times 10^{-5} eV/T$ and g = 1.33 to obtain for the energy difference between adjacent Zeeman ${}^2P_{3/2}$ levels,

$$\Delta V_z = \mu_B g B_{ext} = 5.788 \times 10^{-5} eV/T(0.5T)(1.33) = 3.84 \times 10^{-5} eV$$



Question 3 Molecular Spectroscopy: It is known that the hydrogen molecule H_2 has a vibration absorption (emission) frequency of $\nu_0 = 1.32 \times 10^{14} Hz$.

A) Model the H_2 molecule as two H atoms connected by a spring. Based on the data given calculate the spring constant k. Use m_H = 1u.

Reduced mass $\mu = \frac{m_H m_H}{m_H + m_H} = \frac{1}{2} m_H = 8.33 \times 10^{-28} kg.$

$$\omega = \sqrt{\frac{k}{\mu}} \rightarrow \nu = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}} \rightarrow k = 4\pi^2 \nu^2 \mu = 4\pi^2 \left(1.32 \times 10^{14} s^{-1}\right)^2 \left(8.33 \times 10^{-28} kg\right) = 573 \frac{N}{m}$$

B) Now consider a deuterium molecule D_2, where D is a heavy hydrogen with nucleus of one proton and one neutron with a mass m_D = 2amu. Use the data of part A to calculate the vibration frequency of this molecule.

$$\mu = \frac{m_D m_D}{m_D + m_D} = \frac{1}{2} m_D = 1.67 \times 10^{-27} kg.$$

$$\nu = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}} = \frac{1}{2\pi}\sqrt{\frac{573 N/m}{1.67 \times 10^{-27} kg}} = 9.3 \times 10^{13} Hz$$

C) Are H2 and D2 **infrared active**? Briefly explain your answer.

No. Only vibration modes that induce a change in the dipole moment of the molecule are infrared active. Since homonuclear diatomic molecules such as H2 and D2 do not even have dipole moments, they cannot be infrared active.

Question 4 Vibrational Energy Level of oxygen molecule O_2

A) Assume that the O_2 molecule behaves like a harmonic oscillator with a force constant of 210 N/m. Find the energy (in eV) of its **ground** (n = 0) and **first excited** (n = 1) vibrational states. For ^{16}O, $m_0 = 16\ \text{u}$, where $1\ \text{u} = 1.66\times10^{-27}\,kg$.

For ^{16}O, $m_0 = 1\ 6\text{u}$, where $1\ \text{u} = 1.66\times10^{-27}\,kg$.

First $m_O = 1\ 6\text{u}\times\left(1.66\times10^{-27}\,kg/u\right) = 2.66\times10^{-26}\,kg$

Reduced mass $\mu = \dfrac{m_O m_O}{m_O + m_O} = \dfrac{m_O}{2} = \dfrac{\left(2.66\times10^{-26}\,kg\right)}{2} = 1.33\times10^{-26}\,kg$

The fundamental vibrational frequency is $\omega = \sqrt{\dfrac{k}{\mu}}$, where k = 210 N/m

$$\omega = \sqrt{\frac{210\,N/m}{1.33\times10^{-26}\,kg}} = 1.26\times10^{14}\,Hz\ ,\ E_{\text{vibr}} = (n+1/2)\hbar\omega,\ \text{n} = 0,1,2...$$

Ground state v = 0, $E_0 = \dfrac{\hbar\omega}{2} = \dfrac{\left(1.055\times10^{-34}\,J\bullet s\right)\left(1.26\times10^{14}\,Hz\right)}{2} = 6.63\times10^{-21}\,J$

In eV, $\Delta E_0 = 6.63\times10^{-21}\,J\times\left(\dfrac{1}{1.6\times10^{-19}}\dfrac{eV}{J}\right) = 0.0415eV$ (**0.5 point**)

First excited state v = 1,

$$E_1 = \frac{3h\nu_0}{2} = \frac{3\left(1.055\times10^{-34}\,J\bullet s\right)\left(1.26\times10^{13}\,Hz\right)}{2} = 1.99\times10^{-20}\,J\ \ (\textbf{0.5 point})$$

In eV, $\Delta E_1 = 1.99\times10^{-21}\,J\times\left(\dfrac{1}{1.6\times10^{-19}}\dfrac{eV}{J}\right) = 0.124eV$ (**0.5 point**)

B) Find the vibration quantum number that approximately corresponds to its 1.5-eV dissociation energy. **Hint:** see dissociation equation on the equation sheet.

$E_{\text{vibr}} = (n+1/2)\hbar\omega - U_0$, where U_0 is the dissociation energy.

The dissociation energy is found when $E_{vibr} = 0$, which gives

$$0 = (n+1/2)\hbar\omega - U_0 \Rightarrow \text{n} = \frac{U_0}{\hbar\omega} - \frac{1}{2}$$

Using $U_0 = 1.5eV$, $\omega = 1.26\times10^{14}\,Hz$, and $h = 4.136\times10^{-5}\,eV\bullet s$. The vibrational quantum number that approximately corresponds to its 1.5-eV dissociation energy is $\text{v} = \dfrac{U_0}{\hbar\omega} - \dfrac{1}{2} = \dfrac{1.5eV}{\left(6.582\times10^{-16}\,eV\bullet s\right)\left(1.26\times10^{14}\,Hz\right)} - \dfrac{1}{2} = 17.6$

After rounding off v = 18.

C) Is O_2 **infrared active**? Briefly explain your answer.

For a vibrational mode to be active, the vibration must change the dipole moment. Since O_2 is a homonulcear diatomic molecule, it possesses no dipole moment, and its one stretch vibration mode does not change the dipole. Hence it is **infrared inactive**.

Question 5 Microwave Spectroscopy: The rotational transition from the $\ell = 2$ to the $\ell = 1$ state in CO is accompanied by the emission of a $9.55 \times 10^{-4}\,eV$ photon

A) Use this information to find the rotational inertia of the CO molecule.

Use $E_\ell = \ell(\ell+1)\dfrac{\hbar^2}{2I}$, and the transition. For the $\ell \to \ell - 1$ transition, the change of energy is $\Delta E = E_\ell - E_{\ell-1} = \dfrac{\hbar^2 \ell}{I}$, which equals the photon energy is

$\Delta E = 9.55 \times 10^{-4}\,eV \times 1.6 \times 10^{-19}\,J \bullet eV^{-1} = 1.53 \times 10^{-22}\,J == \dfrac{\hbar^2 \ell}{I} \to I = \dfrac{\hbar^2 \ell}{\Delta E}$. Use

$h = 6.626 \times 10^{-34}\,J \bullet s$ or $\hbar = \dfrac{h}{2\pi} = 1.054 \times 10^{-34}\,J \bullet s$, and $\ell = 2$,

$I = \dfrac{\hbar^2 \ell}{\Delta E} = 1.46 \times 10^{-46}\,kg \bullet m^2$.

B) What is the bond length between the C and O atoms. Data: Mass of carbon $m_C = 12\text{u}$; Mass of oxygen $m_O = 16\text{u}$; $1\ \text{u} = 1.66 \times 10^{-27}\,kg$.

Mass of carbon $m_C = 1\ 2\text{u} \times \left(1.66 \times 10^{-27}\,kg/u\right) = 1.99 \times 10^{-26}\,kg$

Mass of oxygen $m_O = 1\ 6\text{u} \times \left(1.66 \times 10^{-27}\,kg/u\right) = 2.66 \times 10^{-26}\,kg$

Reduced Mass $\mu = \dfrac{m_C m_O}{m_C + m_O} = \dfrac{\left(1.99 \times 10^{-26}\,kg\right)\left(2.66 \times 10^{-26}\,kg\right)}{1.99 \times 10^{-26}\,kg + 2.66 \times 10^{-26}\,kg} = 1.14 \times 10^{-26}\,kg$

$I = \mu R^2 \to R = \sqrt{I/\mu} = \sqrt{1.46 \times 10^{-46}\,kg \bullet m^2 / 1.14 \times 10^{-26}\,kg} = 1.13 \times 10^{-10}\,m$