

Problem 1

- (a) How many different sets of quantum numbers (n, l, m_l, m_s) are possible for an electron in the $4f$ level of an atom? Explain your answer.
- (b) Suppose that an atom has four electrons in the $4f$ level. What is the maximum possible value for the total m_s of the four electrons?
- (c) What is the maximum possible total m_l of four $4f$ electrons?
- (d) Suppose an atom instead has ten electrons in the $4f$ level. What is the maximum possible value for the total m_s of the ten $4f$ electrons?
- (e) What is the maximum possible total m_l of the ten $4f$ electrons?

- a.) The n value is set. For $n=4$, 4 values of l are possible. For each value of l , $l*2+1$ values of m_l are possible. And for all those, we multiply by two for the two possible values of spin. Thinking only of l and m_l , There are 16 possible combinations of l and m_l . We can multiply this by two for spin and get a total of 32.

l	m_l	total
0	0	1
1	-1, 0, 1	3
2	-2, -1, 0, 1, 2	5
3	-3, -2, -1, 0, 1, 2, 3	7

- b.) If all the electrons are $+1/2$, the total will be 2.
- c.) The highest m_l is 3, which two electrons can have. $3 + 3 + 2 + 2 = 10$.
- d.) After 7 electrons fill the available $+$ spin spots, they will have to be negative. So the total is the same, 2.
- e.) We'll have to fill all the $l=3$ m_l s before hitting the higher ones a second time for a higher value. So 7 go 1 each, then 3 give 3,2,1 for a total of 6.

Problem 2

- (a) What is the electronic configuration of Fe ($Z=26$)? (b) In its ground state, what is the maximum possible total m_s of its electrons? (c) When the electrons have their maximum possible total m_s , what is the maximum total m_l ? (d) Suppose one of the d electrons is excited to the next highest level. What is the maximum possible total m_s , and when m_s has its maximum total what is the maximum total m_l ?

- a.) $[Ar]4s^23d^6$
- b.) All the full groups will have a total of zero. There must be one pair of electrons in the $3d$ layer, so there will be 4 unpaired ones. If they're all positive, that gives $+2$.
- c.) If the $+2$ l is the full one, we get $+2$.
- d.) We get the maximum total m_s if the paired electron is the one that's excited, adding 1 for $+3$. In this situation all the $3d$ electrons are unpaired which means the total m_l for them is zero. To get the highest possible m_l the excited electron must be in the $4s^1 +2$.

Problem 3

The ground state of singly ionized lithium ($Z = 3$) is $1s^2$. Use the electron screening model to predict the energies of the $1s^1 2p^1$ and $1s^1 3d^1$ excited states for singly ionized lithium? Compare your predictions with the measured energies (13.4 eV and 6.0 eV, respectively).

$1s^1 2p^1$:

The excited electron is screened by the one remaining 1s electron.

$$Z_{eff} = 3 - 1 = 2$$

$$E_n = (-13.6) \frac{Z_{eff}^2}{n^2}$$

$$E_n = (-13.6) \frac{2^2}{2^2} = -13.6 \text{ eV}$$

There is pretty good agreement with the measured value, implying there is some penetration of the 2p electron into the 1s layer.

$1s^1 3d^1$:

$$E_n = (-13.6) \frac{2^2}{3^2} = -6.0 \text{ eV}$$

There is exact agreement here, implying that there is no penetration of the excited electron into the screened layer.

Problem 4

The molecular vibrational energy of CO is 0.2691 eV, when the constituents of the molecule are the most abundant isotopes of carbon ($m = 12.00$ u) and oxygen ($m = 16.00$ u). (a) What would be the vibrational energy if the oxygen were replaced by the less abundant isotope with mass 18.00 u? (b) What would be the vibrational energy if the carbon in the original CO were instead replaced with radioactive carbon (used in radiocarbon dating) with mass 14.00 u?