Homework 5 Key

2, 4, 6, 10, 14, 16, 18, 20, 24, 32, 34, 54, 56

② Which quantum number combinations are allowed and which are not, $1e^-$ system

A. $N=3, l=2, M=1, M_s=0$
Not allowed, M_s can not $=0$

B. $N=2, l=0, M=0, M_s=-\frac{1}{2}$
Allowed. Shows a 2S electron

C. $N=7, l=2, M=-2, M_s=-\frac{1}{2}$
Allowed. Shows a 7d electron.

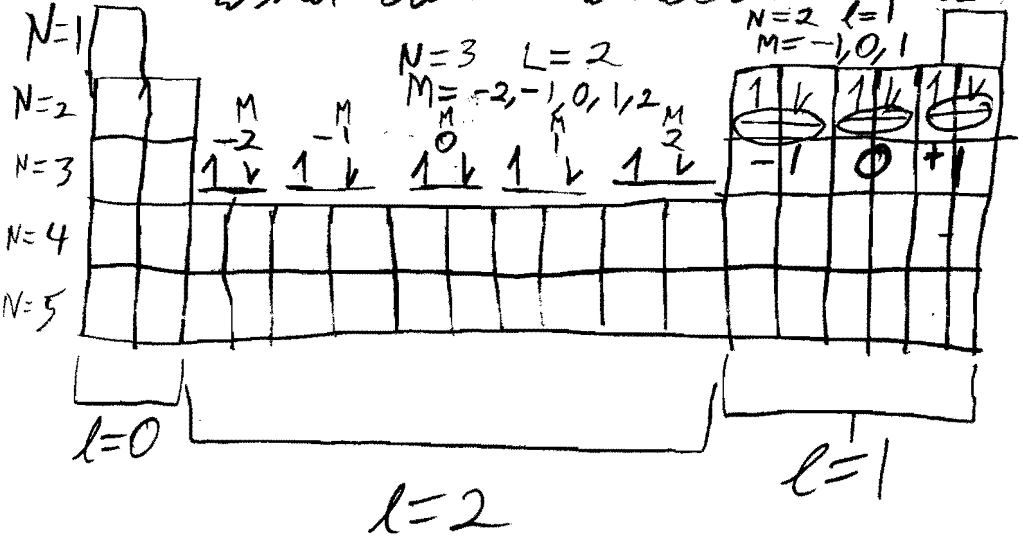
D. $N=3 \quad l=-3, M_s=-\frac{1}{2}$
Not Allowed, l can not be negative.

Selection Rules

$N = 1, 2, 3, 4$
$l = n-1$
$M = +l, \ldots, 0, \ldots -l$
$M_s = \pm \frac{1}{2}$

$M_s = \pm\frac{1}{2}$ or (↑ or ↓)

What do the selection Rules mean?



④ Label the Orbitals

A. $N=3$, $l=2$ 3d

(3rd row, $l=2=d$)

B. $N=7$, $l=4$ 7G

$$M \quad \frac{\quad}{-4}\ \frac{\quad}{-3}\ \frac{\quad}{-2}\ \frac{\quad}{-1}\ \frac{\quad}{0}\ \frac{\quad}{1}\ \frac{\quad}{2}\ \frac{\quad}{3}\ \frac{\quad}{4}$$

$S=0$ $P=1$ $D=2$ $F=3$ $G=4$

$M=1$ spot $M=3$ spots $M=5$ spots $M=7$ spots $G=9$ spots

C. $N=5$, $l=1$ 5P

⑥ # of radial nodes & # of angular nodes.

A. 3d 0 radial & 2 angular

B. 7G 2 radial & 4 angular

C. 5P 3 radial & 1 angular,

Total nodes $= N-1$ total nodes $- l =$ radial nodes

$l=$ angular nodes.

⑩ He^+ = one e^- $Z=2$

Calculate average distance of e^- to the nucleus. in the 2S & 2P orbital

$2Se^- = N=2 \;\; l=0$

$2Pe^- = N=2 \;\; l=1$

$Z=2$

Equation 5.7

$a_0 = 0.529 \times 10^{-10}$ M

0.529 Å

$$\bar{r}_{nl} = \frac{n^2 a_0}{Z}\left\{1 + \tfrac{1}{2}\left(1 - \frac{l(l+1)}{n^2}\right)\right\}$$

$$2Se^- \quad r_{nl} = \frac{2^2 a_0}{2}\left\{1 + \tfrac{1}{2}\left(1 - \frac{0(0+1)}{2^2}\right)\right\} = 3a^\circ = \boxed{1.587 \text{ Å}}$$

$$2Pe^- \quad r_{nl} = \frac{2^2 a_0}{2}\left\{1 + \tfrac{1}{2}\left(1 - \frac{1(1+1)}{2^2}\right)\right\} = 2.5a^\circ = \boxed{1.3225 \text{ Å}}$$

⑭ Calculate the average distance of $1e^-$ from the nucleus. in the Na 3S orbital, the Li 2S and the H 1s orbital.

$$\bar{r}_{nl} = \frac{n^2 a_0}{Z_{eff}}\left\{1 + \tfrac{1}{2}\left(1 - \frac{l(l+1)}{n^2}\right)\right\}$$

$Z_{eff(3s)} = 1.84$

$$\bar{r}_{3s}(Na) = \frac{3^2 a_0}{1.84}\left\{1 + \tfrac{1}{2}\left[1 - \frac{0(0+1)}{3^2}\right]\right\} = 7.34 a_0 = 3.88 \text{ Å}$$

$$\bar{r}_{2s}(Li) = \frac{2^2 a_0}{1.26}\left\{1 + \tfrac{1}{2}\left[1 - \frac{0(0+1)}{2^2}\right]\right\} = 4.76 a_0 = 2.52 \text{ Å}$$

$$\bar{r}_{1s}(H) = \frac{1^2 a_0}{1}\left\{1 + \tfrac{1}{2}\left(1 - \frac{0(0+1)}{1^2}\right)\right\} = 1.50 a_0 = 0.794 \text{ Å}$$

⑯ Ground state e^- Config

A. P: [Ne]$3s^2 3p^3$

B. Tc: [Kr] $4d^5 5s^2$

C. Ho: [Xe] $4f^{11} 6s^2$

⑱ Ground state Config for these ions

Li^-: $1s^2 2s^2$ diamag.
B^+: $1s^2 2S^2$ diamag.
F^-: $1s^2 2S^2 2P^6$ diamag.
Al^{+3}: $1s^2 2S^2 2p^6$ diamag.
S^-: $1s^2 2S^2 2p^6 3s^2 3p^5$ paramag.
Ar^+: $1s^2 2S^2 2p^6 3s^2 3p^5$ paramag.
Br^+: [Ar] $3d^{10} 4s^2 4p^4$ paramag.
Te^-: [Kr] $4d^{10} 5s^2 5p^5$ paramag.

⑳ Identify the atom or ion

A. Os
B. F^-
C. Ag^{+5}

㉔ ① $Z = 3$ $1s^3$
② $Z = 15$ $1s^3 2s^3 3p^9$
③ $Z = 27$ $1s^3 2S^3 3P^9 4S^3 5P^9$

㉜ Larger Radius

A. Sm or Sm^{+3}: Sm

B. Mg or Ca: Ca

C. I^- or Xe: I^-

D. Ge or As: Ge

E. Sr^+ or Rb: Rb

㉞ Predict the larger ion:

A. S^{-2}, Cl^-: S^{-2}

B. Tl^+, Tl^{+3}: Tl^+

C. Ce^{3+}, Dy^{3+}: Ce^{+3}

D. S^-, I^-: I^-

(54) 650nm   K atom   find the other λ

K atom 419×10^3 J/mole ionization

$\Delta E = h\nu \qquad c = \lambda \nu$

$\Delta E = \frac{hc}{\lambda}$

$$\frac{hc}{\lambda_1} + \frac{hc}{\lambda_2} \geq 419 \times 10^3 \text{ J/mol}$$

$$\frac{1}{650\text{nm}} + \frac{1}{\lambda_2} \geq \frac{419 \times 10^3 \text{ J/mol} \cdot (10^{-9} \text{ m/nm})}{(3.0 \times 10^8 \text{ m/s})(6.626 \times 10^{-34} \text{ Js})(6.022 \times 10^{23} \text{ atoms/mol})}$$

$$\frac{1}{\lambda_2} \geq 0.003502 \text{ nm}^{-1} - \frac{1}{650\text{nm}}$$

$$\boxed{\lambda_2 \geq 509 \text{ nm}}$$

(56) Ⓐ Al: $1s^2 2s^2 2p^6 3s^2 3p^1$

Ⓑ: 4S → ground 395 nm

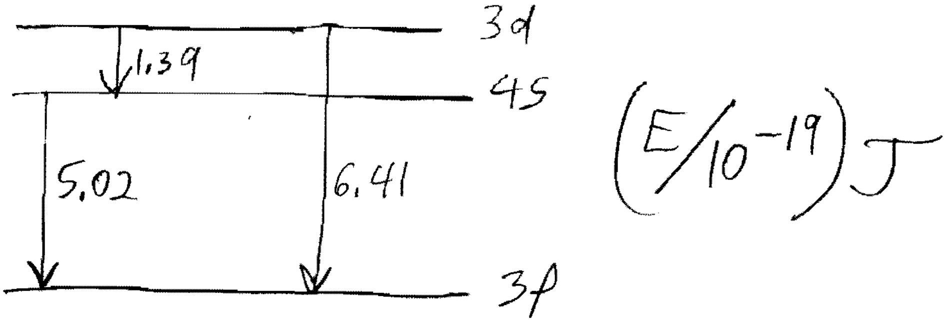
$$\Delta E = \frac{hc}{\lambda} = \frac{(6.626\times10^{-34}\,Js)(2.998\times10^{8}\,M/s)}{(395\times10^{-9}\,M)} =$$

$$\Delta E = 5.02\times10^{-19}\,J$$

Ⓒ 3d → ground 310 nm radiation
Calculate the separation between 3d and 4S

$$\Delta E = \frac{hc}{\lambda} = \frac{(6.626\times10^{-34}\,Js)(2.998\times10^{8}\,M/s)}{(310\times10^{-9}\,M)} =$$

$$\Delta E = 6.41\times10^{-19}\,J$$



Other Problems

① Find the energies for the ring system

$E\Psi = \Psi\hat{H}$ $\quad\quad$ $\hat{H} = -\frac{\hbar^2}{2M}\nabla^2$

$$\hat{H} = -\frac{\hbar^2}{2Mr^2}\frac{\partial^2}{\partial\Phi^2}$$

$\Psi_n(\Phi) = \frac{1}{\sqrt{2\pi}} exp(in\Phi)$ $\quad\quad$ $n = 0, \pm 1, \pm 2$

$$\Psi_n(\Phi)\, d\Phi = \frac{1}{\sqrt{2\pi}}\cdot i\cdot n\cdot exp(in\Phi)$$

$$\Psi_n(\Phi)\frac{\partial^2}{\partial\Phi^2} = \frac{1}{\sqrt{2\pi}}\cdot i^2\cdot n^2\cdot exp(in\Phi) = \nabla^2$$

$$\frac{1}{\sqrt{2\pi}}\cdot\sqrt{-1}\cdot\sqrt{-1}\cdot n^2\, exp(in\Phi)\, d\Phi$$

$$\Psi_n(\Phi)\frac{\partial^2}{\partial\Phi^2} = -\frac{n^2}{\sqrt{2\pi}}\, exp(in\phi)$$

$$E\Psi = \hat{H}\Psi$$

$$E\Psi = \underbrace{-\frac{\hbar^2}{2Mr^2}\frac{\partial^2}{\partial\Phi^2}}_{\hat{H}}\cdot\underbrace{\frac{1}{\sqrt{2\pi}}\, exp(in\Phi)}_{\Psi}$$

$\Psi = \frac{1}{\sqrt{2\pi}} exp(in\Phi)$

$$E\Psi = -\frac{\hbar^2}{2Mr^2}\cdot\frac{1}{\sqrt{2\pi}}\cdot exp(in\phi)\cdot i^2\cdot n^2$$

$$E\Psi = -\frac{\hbar^2}{2Mr^2}\cdot\frac{1}{\sqrt{2\pi}}\cdot exp(in\Phi)\cdot -1\cdot n^2$$

$$E\Psi = \frac{\hbar^2}{2Mr^2}\cdot\frac{1}{\sqrt{2\pi}}\cdot exp(in)\cdot n^2$$

$E = \frac{\hbar^2 n^2}{2Mr^2} \rightarrow$ Let $\frac{\hbar^2}{2Mr^2} = C$ = Constant

$E_0 = 0$ $\quad\quad$ $E_1 = 1C$ $\quad\quad$ $E_2 = 4C$ $\quad\quad$ $E_3 = 9C$

② Probable radius of 1s H-atom wavefunction, and 1s He^+

Find: $r^2[R_{1s}(r)]^2 dr = 0$

$$R_{1s} = 2\left(\frac{z}{a_0}\right)^{3/2} exp\left(-\frac{zr}{a_0}\right)$$

$$R_{1s}^2 = 4\left(\frac{z}{a_0}\right)^3 exp\left(-2\,\frac{zr}{a_0}\right)$$

H^+ $$r^2[R_{1s}(r)]^2 dr = \frac{8re^{\left(-\frac{2r}{a_0}\right)}}{a_0^3} - \frac{8r^2e^{\left(-\frac{2r}{a_0}\right)}}{a_0^4}$$

$$\frac{8r\cancel{e^{\left(-\frac{2r}{a_0}\right)}}}{a_0^3} - \frac{8r^2\cancel{e^{\left(-\frac{2r}{a_0}\right)}}}{a_0^4} \longrightarrow \frac{r}{a_0^3} = \frac{r^2}{a_0^4} \rightarrow \frac{a_0^4}{a_0^3} = \boxed{r = a_0}$$

He^+ $$r^2[R_{1s}(r)]^2 dr = \frac{64re^{\left(-\frac{4r}{a_0}\right)}}{a_0^3} - \frac{128r^2e^{\left(-\frac{4r}{a_0}\right)}}{a_0^4}$$

$$\frac{64r}{a_0^3} = \frac{128r^2}{a_0^4}$$

$$\frac{r}{a_0^3} = \frac{2r^2}{a_0^4} \rightarrow \frac{a_0^4}{2a_0^3} = r$$

$$\boxed{r = \frac{a_0}{2}}$$

③ distance of the radial node of 3p for H

$R_{3p} = 0$

$R_{3p} = \frac{4}{8\sqrt{6}}\left(\frac{1}{a_0}\right)^{3/2}(6\sigma - \sigma^2)\exp\left(-\frac{\sigma}{3}\right)$

A node occurs at $6\sigma - \sigma^2 = 0$

$6\sigma = \sigma^2$

$6 = \sigma$

$\boxed{6a_0}$

④ Integral needed to solve the radius for 90% probability of 2pz of H atom

$$90\% = \int_0^{r=90\%} r^2 R_{nl}^2 \, dr \underbrace{\int_0 Y_{lm}^2}_{4\pi}$$

$$\boxed{0.9 = \int_0^{r=90\%} 4\pi r^2 R^2 \, dr}$$

$$R_{2p} = \frac{1}{2\sqrt{6}} \left(\frac{Z}{a_0}\right)^{3/2} \sigma \exp\left(\frac{-\sigma}{2}\right)$$

$$0.9 = \int_0^{r=90} 4\pi r^2 \left(\frac{1}{2\sqrt{6}} \left(\frac{Z}{a}\right)^{3/2} \sigma \exp\left(-\frac{\sigma}{2}\right)\right)^2 dr$$

⑤ Ne: IE_1

2080.7 KJ/Mol

$$\mathcal{E} = \left|\frac{Z_{eff}}{n^2}\right|^2$$

$$Z_{eff} = \sqrt{n^2(-\mathcal{E}_n \text{ in rydberg})}$$

$IE = -\mathcal{E}_n$ Rydberg = 1312.7136 KJ/Mol

$$\frac{2080.7 \text{ KJ}}{\text{Mol}} \cdot \frac{1 \text{ Rydberg}}{1312.7136 \text{ KJ/Mol}} = 1.585 \text{ Rydberg}$$

Ionization 1 $Z_{eff} = \sqrt{2^2(-(-1.585_R)} = \boxed{2.5}$

Protons 7.5 cancelled

Na^+ 2nd IE is $n=2$

Ionization 2 $Z_{eff} = \sqrt{2^2\left(\frac{-(-4562 \text{ KJ/Mol}) \cdot \text{Rydberg}}{1312.7136 \text{ KJ/Mol}}\right.} = \boxed{3.72}$

7.28 protons Canceled

These numbers say that the shielding is nearly equivalent

Both cancel the same # of protons.