

Sem 1 (1997/98): Quantum Theory

Q2 : (a) Given a_0 (Bohr's first orbit radius) = 0.5 \AA for H atom.
= $5.0 \times 10^{-11} \text{ m}$

From the formula:

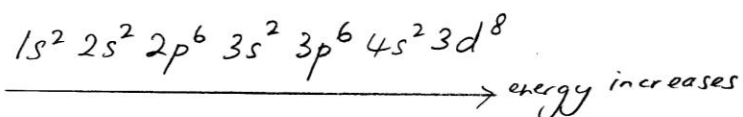
$$a = a_0 \left(\frac{n^2}{Z^2} \right)$$

$\text{Li}^{2+} (Z=3)$:

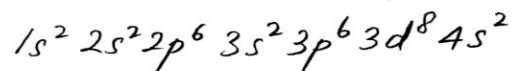
$$\begin{aligned} \text{1st Bohr's first orbit radius} &= a_0 \left(\frac{1^2}{3^2} \right) \\ \text{for } \text{Li}^{2+} & \\ (n=1, Z=3) & \\ &= \left(\frac{0.5}{9} \right) \text{ \AA} \\ &= 0.06 \text{ \AA} // \end{aligned}$$

$$\begin{aligned} \text{2nd Bohr's orbit radius} &= a_0 \left(\frac{2^2}{3^2} \right) \\ (n=2, Z=3) & \\ &= \left(\frac{0.5 \times 4}{9} \right) \text{ \AA} \\ &= 0.22 \text{ \AA} // \end{aligned}$$

(b) $Z=28$ for Ni ($28e^-$)



Due to $3d^8$ has higher penetrating effect compared to $4s^2$ orbital, the stable configuration for Ni will be:



$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} (4s^0)$ ← $4s$ must be filled first (lower energy) compared to $3d$.

Sem 1 (1997/98) : Quantum Theory & Electronic Configuration

Q2(c) (i) $n=6$ $l=5$ $m_l = +5, +4, +3, +2, +1, 0, -1, -2, -3, -4, -5$

$(6, 5, +5, +\frac{1}{2})$	$(6, 5, -5, +\frac{1}{2})$	$(6, 5, 0, +\frac{1}{2})$
$(6, 5, +5, -\frac{1}{2})$	$(6, 5, -5, -\frac{1}{2})$	$(6, 5, 0, -\frac{1}{2})$
$(6, 5, +4, +\frac{1}{2})$	$(6, 5, -4, +\frac{1}{2})$	
$(6, 5, +4, -\frac{1}{2})$	$(6, 5, -4, -\frac{1}{2})$	
$(6, 5, +3, +\frac{1}{2})$	$(6, 5, -3, +\frac{1}{2})$	
$(6, 5, +3, -\frac{1}{2})$	$(6, 5, -3, -\frac{1}{2})$	
$(6, 5, +2, +\frac{1}{2})$	$(6, 5, -2, +\frac{1}{2})$	
$(6, 5, +2, -\frac{1}{2})$	$(6, 5, -2, -\frac{1}{2})$	
$(6, 5, +1, +\frac{1}{2})$	$(6, 5, -1, +\frac{1}{2})$	
$(6, 5, +1, -\frac{1}{2})$	$(6, 5, -1, -\frac{1}{2})$	

11 orbitals
(22 electrons)
each orbital has $2e^-$

(ii) $n=7$, $l=6$; $m_l = +6$

$(7, 6, +6, +\frac{1}{2})$
 $(7, 6, +6, -\frac{1}{2})$ } 2 electrons.

(d) Ti ($Z=22$) Fe ($Z=26$)
V ($Z=23$) Cu ($Z=29$)

Signature

Ti: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^2 4s^2$

Ti⁴⁺: $1s^2 2s^2 2p^6 3s^2$ $(3p^6)$

↑↓	↑↓	↑↓
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 $3p^6$

V: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^3 4s^2$

V³⁺: $1s^2 2s^2 2p^6 3s^2 3p^6$ $(3d^3)$

↑	↑			
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 $3d^3$

Fe: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2$

Fe³⁺: $1s^2 2s^2 2p^6 3s^2 3p^6$ $(3d^5)$

↑	↑	↑	↑	↑
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 $3d^5$ 5 unpaired electrons

Cu: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1$

Cu²⁺: $1s^2 2s^2 2p^6 3s^2 3p^6$ $3d^9$

↑↓	↑↓	↑↓	↑↓	↑
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 $3d^9$

Fe³⁺ ions will be strongly attracted towards the magnetic field because it has the highest number of unpaired electrons ($5e^-$)