Sem 1 (1997/98): Quantum Theory

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

From the formula:

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

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

1st Bohr's first orbit radius for Li^{2+} $(n = 1,\ Z = 3)$

$$= a_0\left(\frac{1^2}{3^2}\right) = \left(\frac{0.5}{9}\right)\text{Å} = 0.06\,\text{Å}$$

2nd Bohr's orbit radius $(n = 2,\ Z = 3)$

$$= a_0\left(\frac{2^2}{3^2}\right) = \left(\frac{0.5 \times 4}{9}\right)\text{Å} = 0.22\,\text{Å}$$

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

$1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,4s^2\,3d^8$

⟶ energy increases

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

$1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,3d^8\,4s^2$

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

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

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

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

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)

Ti : $1s^2 2s^2 2p^6 3s^2 3p^6 3d^2 4s^2$
Ti^{4+} : $1s^2 2s^2 2p^6 3s^2 (3p^6)$ [↑↓|↑↓|↑↓] $3p^6$

V : $1s^2 2s^2 2p^6 3s^2 3p^6 3d^3 4s^2$
V^{3+} : $1s^2 2s^2 2p^6 3s^2 3p^6 (3d^2)$ [↑|↑| | |] $3d^2$

Fe : $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2$
Fe^{3+} : $1s^2 2s^2 2p^6 3s^2 3p^6 (3d^5)$ [↑|↑|↑|↑|↑] $3d^5$ ← 5 unpaired electron

Cu : $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1$
Cu^{2+} : $1s^2 2s^2 2p^6 3s^2 3p^6 3d^9$ [↑↓|↑↓|↑↓|↑↓|↑] $3d^9$

Fe^{3+} ions will be strongly attracted towards the magnetic field. because it has the highest number of unpaired electrons (5 e⁻)

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