

# Chemical Bonding

**Examination 22-10-20**

**Online**

**Canvas assignment**

**13.00 – 16.00 (16.45 for students with additional  
time)**

Write clearly and place your name and student number on each page with answers to the examination problems.

The examination consists of 6 problems.

**Allowed: The textbook, notes, solutions to problems and homework, presentations for the lectures, the periodic table, a (graphical) calculator, Excel for calculations BiNaS.**

$$1 \text{ J} = 1 \text{ kg m}^2 \text{ s}^{-2}$$

$$1 \text{ eV} = 1.60217662 \times 10^{-19} \text{ J}$$

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### Problem 1 (Photoelectric effect) (15 pt)

Irradiation of a metal with photons can lead to the emission of electrons. The kinetic energy of these electrons is given by:

$$E_{kin}(\text{electron}) = \frac{1}{2} m v^2 = h \nu - \phi$$

$m_e$ : mass of the electron,  $v$ : velocity of the electron,  $h$ : Planck constant;  $\nu$  = frequency of the light and  $\phi$  is the work function of the metal.

a) (3 pt) The work functions of Be, Mg and Ca are:

$$\text{Be: } 4.98 \text{ eV} \quad \text{Mg: } 3.66 \text{ eV} \quad \text{Ca: } 2.87 \text{ eV}$$

Discuss the trend these work functions.

b) (3 pt) The work functions of Pd, Ag and Cd are:

$$\text{Pd: } 5.22 \text{ eV} \quad \text{Ag: } 4.26 \text{ eV} \quad \text{Cd: } 4.08 \text{ eV}$$

Discuss the trend these work functions.

c) (3 pt) i) Calculate the minimum frequency,  $\nu_0$ , of the light that can eject electrons from Ag, ii) calculate the maximal wavelength,  $\lambda$ , of the photons that can eject electrons from Ag.

d) (3 pt) i) Calculate the kinetic energy of the electrons ejected from Ag when irradiated with photons with a wavelength of 200 nm, ii) Calculate the wavelength,  $\lambda_e$ , of the electrons ejected from Ag when irradiated with photons with a wavelength of 200 nm.

e) (3 pt) Irradiation of Ag with photons with a total energy of 100  $\mu\text{J}$  with a wavelength of 200 nm lead to emission of electrons. Calculate the maximum number of electrons that can be ejected from the Ag.

### Problem 2 (Particle in a box) (15 pt)

The energy,  $E_n$ , of an electron in a one-dimensional box is given by:

$$E_n = \frac{n^2 h^2}{8m_e L^2}$$

$n = 1, 2, 3, \dots$   $h$ : Planck's constant;  $m_e$ : mass of the electron;  $L$ : length of the box

**a)** (3 pt) Consider a one-dimensional box with a length  $L = 200$  pm. Calculate the difference in energy,  $\Delta E$ , between the energy levels with: **i)**  $n_2 = 2$  and  $n_1 = 1$  and **ii)**  $n_3 = 3$  and  $n_2 = 2$ . Discuss the results with the help of a drawing.

The energy,  $E_n$ , of an electron in a two-dimensional box with lengths,  $L_x$  and  $L_y$ , is given by:

$$E_{n_x n_y} = \frac{h^2}{8m_e} \left[ \frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} \right]$$

$n_1 = 1, 2, 3, \dots$   $n_2 = 1, 2, 3, \dots$

**b)** (6 pt) Consider a two-dimensional box with length of  $L_x = 200$  pm and  $L_y = 200$  pm. Calculate the difference in energy,  $\Delta E$ , between the energy levels:

**i)**  $n_x = 1, n_y = 2$  and  $n_x = 1, n_y = 1$

**ii)**  $n_x = 1, n_y = 3$  and  $n_x = 1, n_y = 2$  of  $n_x = 2, n_y = 1$

The energy,  $E_n$ , of an electron in a three-dimensional box with the lengths  $L_x$ ,  $L_y$  and  $L_z$  is given by:

$$E_{n_x, n_y, n_z} = \frac{h^2}{8m_e} \left[ \frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right]$$

**c)** (6 pt) Consider a three-dimensional box with sides of  $L_x = 200$  pm,  $L_y = 200$  pm and  $L_z = 100$  pm. Calculate **i)** the difference in energy,  $\Delta E$ , between the second energy level and the first energy level and **ii)** the difference in energy,  $\Delta E$ , between the third and the second energy level of the three-dimensional box.

### Problem 3 (Wave functions) (15 pt)

The wavefunctions for the 1s and 2s levels for the hydrogen atom are:

1s

$$\psi(r, \theta, \phi) = 2 \left( \frac{1}{a_0} \right)^{3/2} e^{-r/a_0} \frac{1}{2\pi^{1/2}}$$

2s

$$\psi(r, \theta, \phi) = \frac{1}{8^{1/2}} \left( \frac{1}{a_0} \right)^{3/2} \left( 2 - \frac{1r}{a_0} \right) e^{-r/2a_0} \frac{1}{2\pi^{1/2}}$$

- a) (4 pt) Give the equations for the probability density,  $\psi^2$ , of the 1s and 2s levels for the hydrogen atom.
- b) (3 pt) i) Draw for the 1s level of the hydrogen atom the probability density a function of  $r$ ; ii) Draw for the 2s level of the hydrogen atom the probability density a function of  $r$ .
- c) (4 pt) Calculate for the 1s level: i) the ratio between the probability densities at  $r = a_0$  and at  $r = 0$  and ii) the ratio between the probability densities at  $r = 4a_0$  and at  $r = 0$ .
- d) (4 pt) Calculate for the 2s level: i) the ratio between the probability densities at  $r = a_0$  and at  $r = 0$  and ii) the ratio between the probability densities at  $r = 4a_0$  and at  $r = 0$ .

### Problem 4 (Quantum numbers and electron configuration) (15 pt)

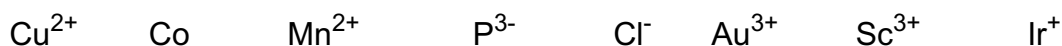
a) (4 pt) The electron configuration of elements is given by four quantum numbers ( $n$ ,  $l$ ,  $m_l$  and  $m_s$ ). Which of the following combinations of quantum numbers are allowed and which ones are not? Explain briefly the answers.

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|--|--|
| 1. $n = 3, l = 2, m_l = 1, m_s = 1/2$  | 5. $n = 1, l = 2, m_l = 1, m_s = 1/2$    |
| 2. $n = 5, l = 1, m_l = 0, m_s = -1/2$ | 6. $n = 2, l = 0, m_l = 1, m_s = -1/2$   |
| 3. $n = 2, l = 1, m_l = 2, m_s = 1/2$  | 7. $n = 6, l = 2, m_l = -2, m_s = 1/2$   |
| 4. $n = 2, l = -1, m_l = 0, m_s = 0$   | 8. $n = 2, l = -2, m_l = -2, m_s = -1/2$ |

b) (3 pt) Draw a figure with the relative energies of all levels with  $n = 1, 2$  and  $3$  of the hydrogen atom. Add the electron to the figure so that the ground state of the hydrogen atom is represented.

c) (4 pt) Draw in different figures all energy levels with  $n = 1, 2, 3$  and  $4$  (not the  $4d$  and  $4f$  levels) of i) the N atom, ii) the P atom, and iii) the As atom. Add the electrons to the individual figures so that the ground state of N, P and As is represented, respectively.

d) (4 pt) Which of the following atoms and ions have the same the electron configuration and which ones have a different electron configuration.



### Problem 5 (MO theory) (20 pt)

a) (5 pt) Draw the MO diagrams of: **i)**  $\text{H}_2^{2+}$ , **ii)** NaH, **iii)** HCl, **iv)**  $\text{ClO}^\bullet$  and **v)** ClF. Place the electron(s) in the MO diagrams such the ground state is represented of **i)**  $\text{H}_2^{2+}$ , **ii)** NaH, **iii)** HCl, **iv)**  $\text{ClO}^\bullet$  and **v)** ClF.

B.O. =  $\frac{1}{2}(N - N^*)$ , N = number of electrons in bonding MO's and  $N^*$  number of electrons in anti-bonding MO's).

b) (3 pt) Give the bond order of: **i)**  $\text{H}_2^{2+}$ , **ii)** NaH, **iii)** HCl, **iv)**  $\text{ClO}^\bullet$  and **v)** ClF.

c) (5 pt) Draw the MO diagrams of: **i)**  $\text{O}_2$ , **ii)** SO and **iii)**  $\text{S}_2$ . Place the electron(s) in the MO diagrams such the ground state is represented of **i)**  $\text{O}_2$ , **ii)** SO and **iii)**  $\text{S}_2$ .

d) (3 pt) Give the bond order of: **i)**  $\text{O}_2$ , **ii)** S and **iii)**  $\text{S}_2$

e) (4 pt) Explain briefly the following experimental facts:

	$\text{O}_2$	SO	$\text{S}_2$
Bond length	121 pm	148 pm	189 pm
Bond strength	498 $\text{kJ mol}^{-1}$	unknown	265 $\text{kJ mol}^{-1}$

### Problem 6 (Valence Bond Theory and MO theory) (20 pt)

a) (3 pt) Draw the Lewis structure of the  $\text{NH}_2^\bullet$  radical.

b) (3 pt) Give the geometry of the  $\text{NH}_2^\bullet$  radical.

c) (3 pt) Give the hybridisation of the N atom in the  $\text{NH}_2^\bullet$  radical.

d) (7 pt) **i)** Draw with the help to the figure below a simple MO diagram of the  $\text{NH}_2^\bullet$  radical, **ii)** indicate in the MO diagram the bonding, non-bonding and anti-bonding molecular orbitals.

e) (4 pt) How many unpaired electrons are in the following species: **i)**  $\text{NH}_2^\bullet$ , **ii)**  $\text{NH}_2^-$  and **iii)**  $\text{NH}_2^+$ .

