

Faculty of Science

# Exam

## Chemical Bonding 2021-2022 5252CBPC6Y Premaster Chemistry (Joint-Degree)

Resit

Date: 6 December 2021

Time: 17:00 – 20:00

Number of pages: 8 (including front page)

Number of questions: 6

Maximum number of points to earn: 100

At each question is indicated how many points it is worth.

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### BEFORE YOU START

- Please **wait** until you are instructed to open the booklet.
- Check if your version of the exam is complete.
- Write down **your name, student ID number**, and if applicable the **version number** of the exam **on each sheet** that you hand in. Also **number the pages**.
- Your **mobile phone** has to be switched off and in the coat or bag. Your **coat and bag** must be under your table.
- **Tools allowed:** (graphic) calculator.

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### PRACTICAL MATTERS

- The first 30 minutes and the last 15 minutes you are not allowed to leave the room, not even to visit the toilet.
- You are obliged to identify yourself at the request of the examiner (or his representative) with a proof of your enrolment or a valid ID.
- During the examination it is not permitted to visit the toilet, unless the invigilator gives permission to do so.
- 15 minutes before the end, you will be warned that the time to hand in is approaching.
- If applicable, please fill out the evaluation form at the end of the exam.
- This exam paper may be taken with you afterwards: yes

**Good luck**



### Challenge 1 (Photoelectric effect) (18 points)

By irradiating (“bestralen”) a metal with photons, electrons can be ejected from the metal. The kinetic energy of electrons is given by the formula

$$E_{kin,electron} = \frac{1}{2}m_e v^2 = h\nu - \Phi$$

With  $m_e$ : mass of the electron,  $v$ : speed of the electron,  $h$ : Planck’s constant,  $\nu$ : frequency of the photon and  $\Phi$  the work function of the metal

**a)** (3pt) Explain in your own words what the work function represents and how it is related to the ability to eject electrons from a metal.

**b)** (3pt) The work functions for Li, Na, K are

Li: 2.93 eV      Na: 2,36 eV      K: 2.2 eV

Explain the trend in work functions

**b)** (3pt) The work functions for Pd, Ag, Cd are

Pd: 5.22 eV      Ag: 4.26 eV      Cd: 4.08 eV

Explain the trend in work functions

**d)** (3pt) **i)** Calculate the minimum frequency  $\nu_0$  that is required for the photons to be able to remove electrons from Pd. **ii)** Calculate the maximum wavelength  $\lambda$  of the photons that can remove electrons from Pd.

**e)** (3pt) **i)** Calculate the kinetic energy of the electrons that are ejected through irradiation of Cd with a wavelength of 200 nm. **ii)** Calculate the wavelength  $\lambda_e$  of the electrons that are ejected through irradiation of Cd with a wavelength of 200 nm.

**f)** (3pt) Irradiating Ag with photons with a wavelength of 300 nm and a total energy of 50  $\mu$ J leads to an ejection of electrons. Calculate the maximum number of electrons that can be ejected from Ag.



## Challenge 2 (Heisenberg's uncertainty principle) (14 points)

Heisenberg's famous uncertainty principle tells us that we cannot simultaneously know the position and the momentum of a particle. There is a limit, given by  $\frac{h}{4\pi}$ , that determines to what extent the position and momentum can be determined.

$$\Delta x \Delta p \geq \frac{h}{4\pi}$$

Consider a proton with a speed of 80 km/s.

a) (4pt) If the uncertainty in its momentum is 0.200%, what uncertainty in its location must be tolerated?

Now consider an electron confined in a space of 100 pm (=  $100 \cdot 10^{-12}$  m).

b) (4pt) What is its uncertainty in position and in momentum? Express the uncertainty in momentum in wavelength  $\lambda$  (hint: use/rearrange De Broglie relation  $\lambda = \frac{h}{p}$ . You do *not* have to fill in the electron's mass).

The average distance from the nucleus in hydrogenic atoms are given by the following expression.

$$\langle r \rangle = n^2 \left\{ 1 + \frac{1}{2} \left( 1 - \frac{l(l+1)}{n^2} \right) \right\} \frac{a_0}{Z}$$

with  $n$  = principal quantum number and  $l$  = azimuthal quantum number

c) (2pt) Determine the average distance from the nucleus  $\langle r \rangle$  for an electron in the 1s, 2s, 2p and 3s orbital of an hydrogen atom. Express your answer in units [m] with three significant digits.

Let us assume that the uncertainty in position is 40% of the value for the average distance  $\langle r \rangle$ , meaning that  $\Delta x = 0.40 \langle r \rangle$

d) (4pt) Calculate the uncertainty in momentum for one electron in a 1s, 2s, 2p and 3s orbital of an hydrogen atom. What do you notice by comparing the  $\Delta x$  and  $\Delta p$  values?



### Challenge 3 (Quantum numbers and electron configurations) (14 points)

a) (4 pt) The electron configurations of atoms are given by four quantum numbers ( $n$ ,  $l$ ,  $m_l$  and  $m_s$ ). Show which of the following combinations of quantum numbers are allowed and which are not. Explain your answer if the combination is not allowed!

1.  $n = 4, l = 2, m_l = 1, m_s = \frac{1}{2}$

5.  $n = 3, l = 2, m_l = 1, m_s = \frac{1}{2}$

2.  $n = 5, l = 1, m_l = 2, m_s = -\frac{1}{2}$

6.  $n = 2, l = 0, m_l = 1, m_s = -\frac{1}{2}$

3.  $n = 2, l = 1, m_l = 2, m_s = \frac{1}{2}$

7.  $n = 6, l = 2, m_l = -2, m_s = \frac{1}{2}$

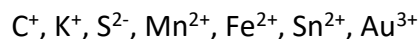
4.  $n = 2, l = -1, m_l = 0, m_s = \frac{1}{2}$

8.  $n = 2, l = 2, m_l = -2, m_s = -1$

b) (3 pt) i) The first three quantum numbers classify atomic orbitals. Explain the meaning of these three quantum numbers. ii) Explain the meaning of the fourth quantum number  $m_s$ .

c) (3 pt) Draw in one figure the relative energy levels for the 1s, 2s, 2p, 3s, 3p and 3d orbitals of the H atom. Assign the electron to the orbital it occupies in the ground state of the hydrogen atom.

d) (4 pt) i) Give the electron configurations of the following ions and ii) the number of unpaired electrons in the following ions:





### Challenge 4 (Wavefunctions and electron configuration) (22 points)

a) (7 pt) The expressions for the wavefunctions of the  $2p_x$ ,  $2p_y$  and  $2p_z$  levels are given below:

$$\mathbf{2p_x} \quad \Psi(r, \theta, \phi) = \frac{1}{2\sqrt{6}} \left( \frac{1}{a_0} \right)^{5/2} r e^{-r/2a_0} \left( \frac{3}{4\pi} \right)^{1/2} \sin\theta \cos\phi$$

$$\mathbf{2p_y} \quad \Psi(r, \theta, \phi) = \frac{1}{2\sqrt{6}} \left( \frac{1}{a_0} \right)^{5/2} r e^{-r/2a_0} \left( \frac{3}{4\pi} \right)^{1/2} \sin\theta \sin\phi$$

$$\mathbf{2p_z} \quad \Psi(r, \theta, \phi) = \frac{1}{2\sqrt{6}} \left( \frac{1}{a_0} \right)^{5/2} r e^{-r/2a_0} \left( \frac{3}{4\pi} \right)^{1/2} \cos\theta$$

The electron distribution in the 2p level is given by the sum of the squares of these wavefunctions:

$$\Psi^2(2p_x) + \Psi^2(2p_y) + \Psi^2(2p_z)$$

Show that the electron distribution in the 2p level of the ground state of the N atom is spherically symmetric, meaning independent of the angles  $\theta$  and  $\phi$ ; hint:  $\sin^2(x) + \cos^2(x) = 1$ .

b) (7 pt) Which of the following elements have a spherically symmetric electron distribution in the outer electronic level: O, Cl, Mn, Ca, Ni, Pd.

The wavefunction for the 1s hydrogen atom is given below:

1s level:

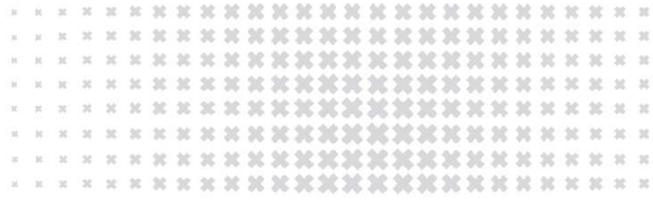
$$\psi(r, \theta, \phi) = R(r) \times Y(\theta, \phi) = 2 \left( \frac{Z}{a_0} \right)^{3/2} e^{-Zr/a_0} \times \left( \frac{1}{4\pi} \right)^{1/2}$$

Z = atom number,  $a_0$  (Bohr constant) = 52.9 pm, r = distance to the atom nucleus

c) (4 pt) The radial distribution function, P(r), is:  $P(r) = r^2 R^2(r)$ . Now show that the following is correct for the 1s orbital of the hydrogen atom:

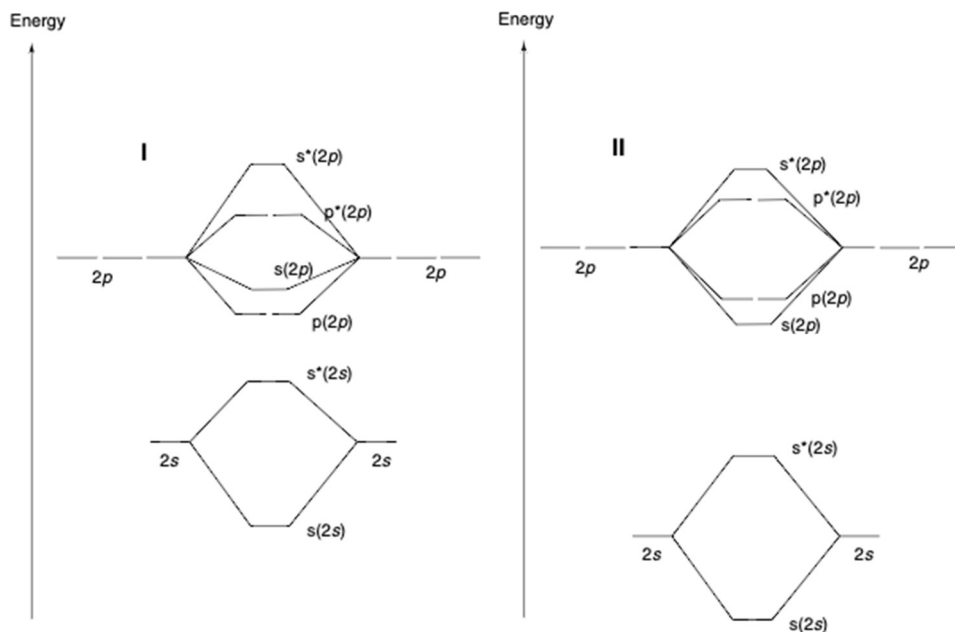
$$P(r) = \frac{4Z^3}{a_0^3} r^2 e^{-2Zr/a_0}$$

d) (4 pt) Sketch P(r) as a function of r for the 1s state of the hydrogen atom.



### Challenge 5 (MO theory) (17 points)

a) (7 pt) Below are two MO diagrams.



Use these MO diagrams to explain the following facts:

- i.  $B_2$  is paramagnetic (has unpaired electrons)
- ii.  $C_2$  is diamagnetic (no unpaired electrons)
- iii.  $O_2$  is paramagnetic (unpaired electrons)

b) (3 pt) Give the bond order for i)  $B_2$ , ii)  $C_2$ , iii)  $O_2$ .

c) (3 pt) Explain the following facts:

$C_2$ : bond length: 124 pm                      bond energy: 599 kJ/mol

$O_2$ : bond length: 121 pm                      bond energy: 494 kJ/mol

d) (4 pt) Draw the MO diagram of BN and give the bond order. Assume that orbital mixing does occur for this molecule! Is BN para- or diamagnetic?

$B.O = \frac{1}{2}(N - N^*)$ ,  $N$  = electrons in binding MOs,  $N^*$  = electrons in anti-binding MOs

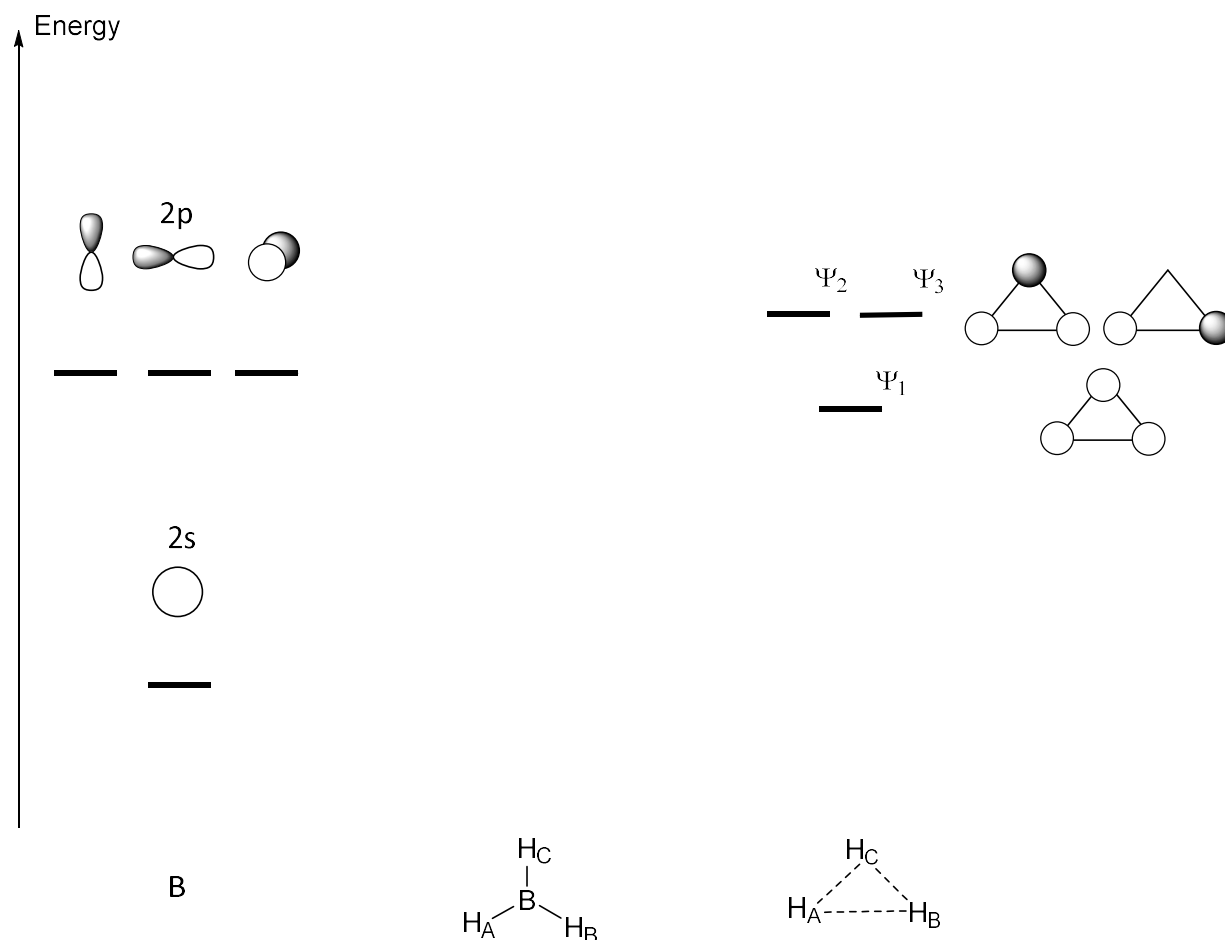


### Challenge 6 (Molecular Orbital Theory) (15 points)

Borane ( $\text{BH}_3$ ) is a strong Lewis acid that means its lowest unoccupied molecular orbital (LUMO) is susceptible for bonding with for example a lone pair of nitrogen in ammonia ( $\text{NH}_3$ ). In this exercise, we will find out which MO in borane is the LUMO.

- (3pt) Write down the Lewis structure of borane.
- (3pt) Do the hydrogen atoms lie in the same plane as B or is borane bent? Explain your answer.
- (6pt) Complete the MO diagram that is given below by forming the right combinations and by filling the MOs with electrons. Hint: draw the combinations.
- (3pt) Indicate in the MO diagram which MOs are bonding, non-bonding and antibonding. Specify which of the MO is the LUMO and which the HOMO (highest occupied molecular orbital).

The HOMO and LUMO are often the most important orbitals to consider when bonds are formed!



## Constants

$$h = 6.626 \cdot 10^{-34} \text{ J} \cdot \text{s}$$

$$c = 2.998 \cdot 10^8 \text{ m/s}$$

$$a_0 = 5.291 \cdot 10^{-11} \text{ m}$$

$$1 \text{ eV} = 1.602 \cdot 10^{-19} \text{ J}$$

$$m_e = 9.109 \cdot 10^{-31} \text{ kg}$$

$$m_p = 1.673 \cdot 10^{-27} \text{ kg}$$

**Periodic Table of the Elements**

Number		Symbol		Name		Mass	
1	1	H	Hydrogen	1.008			
2	2	He	Helium	4.003			
3	3	Li	Lithium	6.941			
4	4	Be	Beryllium	9.012			
5	5	B	Boron	10.811			
6	6	C	Carbon	12.011			
7	7	N	Nitrogen	14.007			
8	8	O	Oxygen	15.999			
9	9	F	Fluorine	18.998			
10	10	Ne	Neon	20.180			
11	11	Na	Sodium	22.990			
12	12	Mg	Magnesium	24.305			
13	13	Al	Aluminum	26.982			
14	14	Si	Silicon	28.086			
15	15	P	Phosphorus	30.974			
16	16	S	Sulfur	32.065			
17	17	Cl	Chlorine	35.453			
18	18	Ar	Argon	39.948			
19	19	K	Potassium	39.098			
20	20	Ca	Calcium	40.078			
21	21	Sc	Scandium	44.956			
22	22	Ti	Titanium	47.867			
23	23	V	Vanadium	50.942			
24	24	Cr	Chromium	51.996			
25	25	Mn	Manganese	54.938			
26	26	Fe	Iron	55.845			
27	27	Co	Cobalt	58.933			
28	28	Ni	Nickel	58.693			
29	29	Cu	Copper	63.546			
30	30	Zn	Zinc	65.38			
31	31	Ga	Gallium	69.723			
32	32	Ge	Germanium	72.631			
33	33	As	Arsenic	74.922			
34	34	Se	Selenium	78.971			
35	35	Br	Bromine	79.904			
36	36	Kr	Krypton	83.798			
37	37	Rb	Rubidium	85.468			
38	38	Sr	Strontium	87.62			
39	39	Y	Yttrium	88.906			
40	40	Zr	Zirconium	91.224			
41	41	Nb	Niobium	92.906			
42	42	Mo	Molybdenum	95.94			
43	43	Tc	Technetium	98.907			
44	44	Ru	Ruthenium	101.07			
45	45	Rh	Rhodium	102.906			
46	46	Pd	Palladium	106.42			
47	47	Ag	Silver	107.868			
48	48	Cd	Cadmium	112.414			
49	49	In	Indium	114.818			
50	50	Sn	Tin	118.711			
51	51	Sb	Antimony	121.760			
52	52	Te	Tellurium	127.6			
53	53	I	Iodine	126.904			
54	54	Xe	Xenon	131.29			
55	55	Cs	Cesium	132.905			
56	56	Ba	Barium	137.328			
57-71			Lanthanide Series				
57	57	La	Lanthanum	138.905			
58	58	Ce	Cerium	140.116			
59	59	Pr	Praseodymium	140.908			
60	60	Nd	Neodymium	144.243			
61	61	Pm	Promethium	144.913			
62	62	Sm	Samarium	150.36			
63	63	Eu	Europium	151.964			
64	64	Gd	Gadolinium	157.25			
65	65	Tb	Terbium	158.925			
66	66	Dy	Dysprosium	162.500			
67	67	Ho	Holmium	164.930			
68	68	Er	Erbium	167.259			
69	69	Tm	Thulium	168.934			
70	70	Yb	Ytterbium	173.055			
71	71	Lu	Lutetium	174.967			
72	72	Hf	Hafnium	178.49			
73	73	Ta	Tantalum	180.948			
74	74	W	Tungsten	183.84			
75	75	Re	Rhenium	186.207			
76	76	Os	Osmium	190.23			
77	77	Ir	Iridium	192.217			
78	78	Pt	Platinum	195.085			
79	79	Au	Gold	196.967			
80	80	Hg	Mercury	200.592			
81	81	Tl	Thallium	204.383			
82	82	Pb	Lead	207.2			
83	83	Bi	Bismuth	208.980			
84	84	Po	Polonium	[209]			
85	85	At	Astatine	[208.98]			
86	86	Rn	Radon	222.018			
87	87	Fr	Francium	[223]			
88	88	Ra	Radium	[226]			
89-103			Actinide Series				
89	89	Ac	Actinium	[227]			
90	90	Th	Thorium	232.038			
91	91	Pa	Protactinium	231.036			
92	92	U	Uranium	238.029			
93	93	Np	Neptunium	[237]			
94	94	Pu	Plutonium	244.064			
95	95	Am	Americium	[243]			
96	96	Cm	Curium	[247]			
97	97	Bk	Berkelium	[247]			
98	98	Cf	Californium	[251]			
99	99	Es	Einsteinium	[252]			
100	100	Fm	Fermium	[257]			
101	101	Md	Mendelevium	[258]			
102	102	No	Nobelium	[259]			
103	103	Lr	Lawrencium	[262]			

Alkali Metal

Alkaline Earth

Transition Metal

Basic Metal

Metalloid

Nonmetal

Halogen

Noble Gas

Lanthanide

Actinide