CHEM 231

Class Examination **Tuesday 5 May 2009**

Name:

Time allowed: 90 minutes **Total marks:** 90

Instructions: Answer **ALL** questions. **Use the back of sheets if required.**

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1. (Total 20 marks)

(a) Explain what is meant by the term **quantised energy levels** as applied to the H atom.

(b) The following sets of quantum numbers describe an electron in which orbital?

(i) 2, 0, 0, +1/2

(ii) 4, 3, 2, -1/2

(iii) 3, 2, 2, -1/2

(iv) 3, 1, 0, +1/2

(c) What is the maximum number of electrons with the following quantum numbers in an atom? Show your working.

Specify the orbitals in which the electrons would be found.

(i) $n = 3$, $m_l = 1$

(ii) $n = 3$, $m_s = +1/2$

(d) State Hund's Rule and explain why isolated ground-state carbon atoms (C: Z = 6) are paramagnetic.

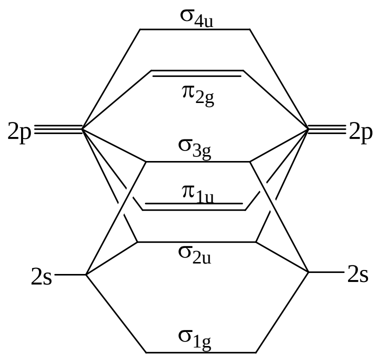
(e) Give the ground-state electron configuration and an excited-state electron configuration for Al^{3+} (Al: Z = 13).

2. (10 marks)

Explain why the energy of the electron in an excited state hydrogen atom is the same if the electron occupies either a 2s or 2p orbital whereas in a ground state carbon atom (C: Z = 6) the energy of an electron in the 2s orbital is lower than the energy of an electron in a 2p orbital. Use radial distribution function diagrams to aid your answer.

3. (Total 20 marks)

A molecular orbital (MO) energy level diagram appropriate for Li_2 to N_2 is shown below. Answer the following, with reference where appropriate, to the diagram. Assume z is the internuclear axis.



(a) (i) Explain the process of **linear combination of atomic orbitals.**

(ii) List all the molecular orbitals and state (based on the diagram above) whether they are either bonding, mainly bonding, antibonding or mainly antibonding. State the character of each orbital (e.g. σ_{2u} is mainly 2s antibonding in character etc).

(iii) Use Enclosure (Boundary) surface diagrams to show the formation of the σ_{1g} and σ_{2u} orbitals from the 2s orbitals.

(iv) Using the orbitals σ_{2g} and π_{2u} as examples, explain the labels 'g' and 'u'.

(v) Explain why the 2s orbitals are shown to be involved in the formation of the σ_{3g} but not in the formation of π_{1u} nor σ_{4u} orbitals.

(b) Use the MO energy level diagram to deduce the following properties of C_2 and C_2^{2-} (C: Z = 6).

(i) ground-state electron configurations

C_2:

C_2^{2-}:

(ii) bond orders

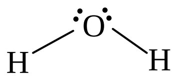
C_2:

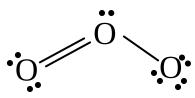
C_2^{2-}:

(iii) relative bond lengths

4. (Total 15 marks)

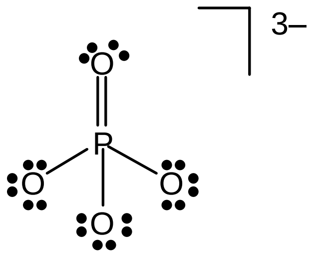
A Lewis dot diagram for water, H_2O, is shown below. Water is a bent (or angular) molecule with a bond angle of 104.5°. Outline the basic principles of Valence Shell Electron Pair Repulsion (VSEPR) theory, and use the theory to account for the geometry and bond angle of water (H: Z = 1; O: Z = 8). Predict, with brief explanation, whether ozone, also a bent molecule, has a larger or smaller bond angle than water.





5. (15 marks)

A Lewis Dot diagram for phosphate is shown below. Describe the bonding in PO_4^{3-} using Valence Bond theory. (P: [Ne] $3s^2 3p^3$; O: $1s^2 2s^2 2p^4$)



6. (10 marks)

Explain how the photosenstizing drugs, Visudyne and Photofrin, are used in photodynamic therapy to treat age-related macular degeneration and tumours (AMD), respectively. Your answer should include a brief description of the underlying principles of photodynamic therapy.