Maastricht Science Programme

INTRODUCTION TO CHEMISTRY

(SCI1004)



http://www.ufh.ac.za/departments/pac/

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General

Meeting time: Period 2

Meeting place:

Coordinator: Dr. Burgert Blom (burgert.blom@maastrichtuniversity.nl)

Required Course Materials

Textbook: "Chemistry³: Introducing inorganic, organic and physical chemistry" Burrows, Holman, Parsons, Pilling, Price. Second Edition, Oxford University Press

Course Description and Objectives

This lecture course will serve as an introduction to the chemical sciences. The course will provide the student with all fundamental chemical knowledge necessary to continue with further study in the areas of chemistry and biology. The course will be focused on the understanding of chemistry through examples and applications relevant to the life sciences.

Course Specific Objectives:

- To give the student the ability to recognize chemical compounds and to understand their basic physical and chemical properties.
- To enable the student to understand the basic physical chemistry of fundamental importance to most natural processes such as thermodynamics and acid/base behavior
- To provide the student with sufficient background for further study in advanced courses in chemistry and other natural sciences
- To present the student with current developments in chemistry and their impact on society, the environment, and industry

Course Procedures

The class will consist of 1/3 lectures and 2/3 tutorial sessions. Lectures will be highly interactive and attendance is extremely encouraged. Students are asked to read the book chapters associated with each lecture, if possible before coming to lecture in order to improve your participation. The topics covered in tutorials may or may not be discussed in lecture. Exams are comprehensive and will test on knowledge acquired from lecture, tutorials, and book chapters.

- Participate! This is extremely important in your learning experience. There is no wrong answer; inaccurate answers will alert the instructor to concepts that need to be explained again!
- Ask questions. There is no such thing as a silly question. Instructor answers to the
 questions will help to deepen your understanding as well as the understanding of
 your fellow classmates.
- Come to class! Attendance is highly encouraged as the information presented in lecture will not be made available elsewhere.
- Take notes. Writing things down will help to cement the new knowledge in your mind.
- Think. The purpose of this class is not to regurgitate material but to understand the concepts underlying chemistry.

Course Requirements

The following represent the points of assessment and evaluation that will be used in this course:

- One open-question midterm exam on lectures 1, 2 and 3, to take place during week 4. 35%
- One open-question final exam on ALL lectures to take place during exam week: 45%
- Tutorial grade: 20% (questions will be given weekly from the textbook as the course progresses)
- In case of a failing overall grade in this class, but a pass on attendance, a resit of the final will be permitted. The grade obtained in the resit will be substituted for the grade of the final exam.

Attendance:

This course has an 85% attendance requirement. If the student fails to meet the 85% requirement but has 70% attendance, the student is required to request an additional assignment in order to have the possibility to pass the course. In order to be granted an additional assignment, the student must prove that he had valid reasons for ALL absences.

Failure to meet with 70% attendance requirement will result in a Failing grade in attendance. A student with a fail on attendance is not entitled to a resit exam.

In case of a failing overall grade in this class, but a pass on attendance, a resit of the final will be permitted.

Resit:

In order to be eligible for a resit exam, a student must have:

- Met the attendance requirement of the course, or been allowed to make up for it by means of an additional assignment and
- Made a fair attempt to fulfill all requirements of the assessment. The course coordinator evaluates whether an attempt can indeed be considered 'fair'

Course Schedule 2017

This schedule is tentative and flexible. It may be modified and adjusted each week according to the instructor's consideration.

Week 1 Introduction to the course

Lecture 1: Elements, atoms, and molecules;

Quantum numbers and orbitals; The Aufbau Principle.

Drawing Lewis Structures and Molecular Geometry; Hybridization.

Chapter 3, 5

Task 1 Periodicity: Pre Discussion/Post Discussion

Task 2 Bond-type triangles: Pre Discussion

Week 2 Lecture 2: Chemical Reactions and molar calculations (*Chapter 1*)

Task 2: Post Discussion

Task 3 Water: Pre Discussion/Post Discussion

Task 4 Redox Reactions: Pre Discussion

Week 3 Lecture 3: Gases and kinetics (Chapter 8 and 9)

Task 4: Post Discussion

Task 5 Buffers: Pre Discussion

Week 4 <u>Midterm Examination on Lectures 1, 2 and 3 and Tasks 1-4</u>

Lecture 4: Acid Base Chemistry (*Chapter 7*)

Task 5 Buffers: Post Discussion

Task 6 Hess's Law: Pre Discussion

Midterm Revision

Week 5 Lecture 5: Thermodynamics (Chapter 13, Chapter 14)

Task 6: Post Discussion

Task 7 Reaction rates: Pre Discussion (Chapter 7)

Week 6 Lecture 6: Electrochemistry (*Chapter 16*)

Task 7: Post Discussion

Final tutorial: Review for exam

Week 7 Exam on ALL lectures

TASKS

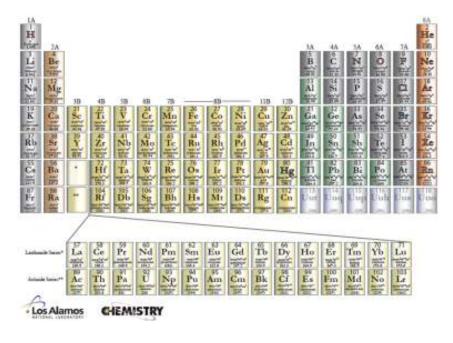
Periodicity

The quest to classify and organize elements in a coherent manner went from Lavoisier's classification of 33 elements into gases, metals, non-metals, and earths to Dmitri Mendeleev's periodic table.

A basis for the table used today, Mendeleev's constructed his table by noticing that certain elements have similar properties. By grouping elements into chemical families, Mendeleev was forced to leave gaps in the table where he predicted new elements would be discovered. Mendeleev's deep understanding of the nature of atoms and elements meant that all his predictions were accurate! All the missing elements have been discovered. Furthermore, elements that have been synthetically manufactured can also be classified in the same system!

When used properly, the periodic table is an extremely powerful tool. A simple reading can give the atomic number, atomic mass, and physical state of the element. Knowledge of the s, p, d, and f blocks can lead to a quick assignment of electronic configurations. Understanding the table's group and period layout provides information on the chemical family of the elements, as well as their stability and their reactivity.

Furthermore, periodic trends such as atomic size, electron affinity, ionization energy, and electronegativity provide explanations for most of the chemical behavior and reactivity patterns of the elements.



VSEPR and Beyond

VSEPR Theory (Valence Shell Electron Pair Repulsion) enables the prediction of the geometry of molecules containing exclusively main-group elements pretty well. It does not work for transition metal containing complexes, unfortunately, and there more progressive bonding theories and models, such as molecular orbital theory which are required.

Starting from a Lewis structure, one can predict the shape of the molecule by simply counting the number of electron or bonding pairs around the central atom. Many people confuse this, and confuse the "electron pair geometry" with the "molecular geometry" and this leads to confusion. To get the right Lewis formula, one must always move the valence electrons around of the atoms so that one tries to get the octet configuration for each atom. For heavier elements (period 2 and onwards) the expanded, or extended octet is possible, for example SF₆ where the S atom has a total of 12 electrons around it (6 bonding pairs).

The electron pair geometry is the starting point. Electron pairs can be lone pairs, or bonding pairs. Once one knows how many of these are around the central atom, one can figure out the molecular geometry by seeing how many of these electron pairs are lone pairs, and how many are bonding pairs.

Without the correct Lewis structure, however, one can never predict the correct geometry, so it is essential that one gets the Lewis formula right! We can also predict the hybridization once we know the geometry: for example, AX_4 will be sp^3 hybridised (irrespective of whether the electron pairs are lone or bonding pairs); AX_6 will be d^2sp^3 hybridised, and so on.

This neat and tidy theory, therefore really enables one using very simple ideas to accurately predict shape, geometry, and hybridization and is very important in introductory chemistry, but has severe limitations! Molecular orbital theory is a more rigorous theory to explain bonding, and can in contrast to VSEPR be used in explaining bonding in transition metals complexes.

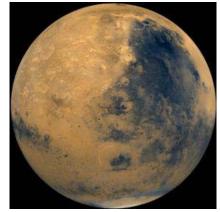


Fig 1. G. N. Lewis, the American chemist after whom Lewis structures are named. He made many contributions in chemistry, including acids and bases and the discovery of the covalent bond.

Water

"The Curiosity rover's landing site on Mars, Gale Crater, used to hold a lake, scientists announced on Monday at the American Geophysical Union (AGU) meeting in San Francisco. And on Tuesday researchers analyzing photographs taken by the Mars Reconnaissance Orbiter (MRO) reported that liquid water appears to be darkening the slopes of mountains near the Martian equator—the first time strong indications of present-day water have been seen in this region."

- From: New Signs of Water on Mars Ramp Up Search for Life, *Scientific American*, December 11, 2013



The discovery of water on the red giant is exciting because it gives rise to the possibility that life could have existed – or could exist – in the planet. The existence of water in abundance on Earth is what differentiates our planet from any other in the solar system. By looking at molecules with similar size and composition, such as CH₄ (methane – natural gas), it is evident that if it wasn't for its unique properties –resulting from its structure and composition- it would not be possible for water to exist in a liquid state under normal Terran atmospheric conditions – nor would ice behave the way that it does.

This would be problematic, since water is the solvent of life – dissolving the various



electrolytes and nutrients needed by cells. Water is also the main component of blood, helping to deliver oxygen to cells and carry waste material away from them. When dealing with solutions, it is important to be able to measure their concentration, and for aqueous solution the most important concentration unit is molarity.

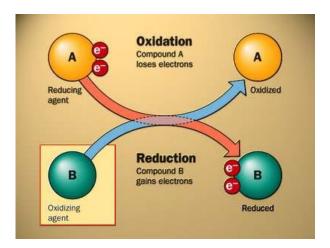
Understanding concentration and its dependence on mass and volume is important for biological purposes, because concentration gradient drives processes such as osmosis and diffusion.

Redox Reactions

The interconversion of NAD to NADH, NADP to NADPH or FAD⁺ to FADH₂ has important biological functions. These molecules are electron carriers, used to transport electrons between different compartments in the cell – for example during cellular respiration. The reactions undergone during these interconversions are redox reactions.

Redox reactions are an important class of chemical reactions. The word Redox is a condensation of the terms reduction and oxidation, which refer to the way in which electrons move when these reactions take place. Because in redox reactions electrons can be considered as "reactants" and "products", balancing can be a little tricky and it is important to understand how it is properly done. The reaction of NAD⁺ with H⁺ to give NADH is a good example.

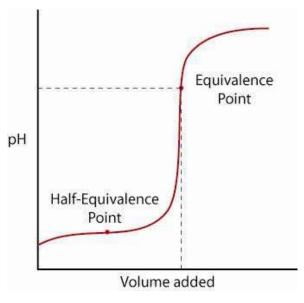
Redox reactions like the one above can be broken into the oxidation half reaction and the reduction half reaction. These reactions can be assigned potentials, measured against a standard hydrogen electrode. The size and sign of the potential indicates the likelihood of the reduction or oxidation reaction to take place. Therefore, these potentials can be used to identify good reducing agents and good oxidizing agents.



Buffers

Human cells can only survive in a very narrow pH range, around 7.4. In fact, acidosis and alkalosis are two diseases that occur when blood pH inside the body becomes unbalanced. There are many biological reactions happening inside the body during which protons are exchanged. This should significantly and constantly alter blood's pH, but it seems unaffected and remains stable. Blood is able to resist significant changes in its pH because it is a buffered solution.

The best way to understand buffers is by looking at the titration of a weak acid (or a weak base) with a strong base (or a strong acid). Titration curves such as the one shown in Figure 1 provide a lot of information. By looking at a titration curve, one can figure out where the buffering region is and therefore what the buffer capacity is. One can also learn what the acid's pKa is, and in which region of the curve the buffer fails. The half-equivalence and equivalence points are special points that also provide useful information, especially if one considers that the properties of the buffer depend on the ratio between the acid and its conjugate base. It is also curious to note that for these type of titrations, the pH at the equivalence point is not 7.



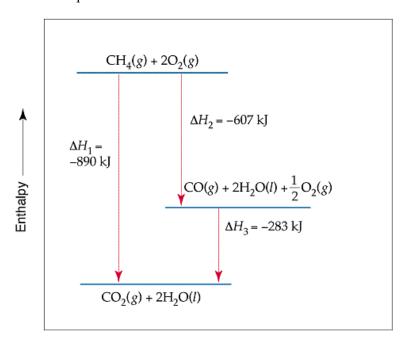
A titration curve

An important tool when dealing with buffers is the Henderson-Hasselbach equation. This equation allows for the prediction of pH changes in buffered systems without the need for elaborate calculations.

Hess's Law

Energy is a state function. This means that the change of energy going from one particular set of reactants to one particular set of products should always be the same whether the reaction takes place in one step or in a series of steps. Hess's Law takes advantage of this property in order to allow us to calculate changes in enthalpies of reaction. For example, it can be used to calculate the enthalpy change of the reaction of nitrogen with oxygen to form nitrogen dioxide if we know what the change in enthalpy of the reaction of nitrogen with oxygen to form nitrogen oxide is 180 KJ, and the change in enthalpy of the decomposition of nitrogen dioxide into oxygen and nitrogen monoxide is 112 KJ. It is important to keep in mind that any manipulations done to the reactions must be reflected in their enthalpies as well.

Hess's law is important to understand when calculating the enthalpy change of a reaction based on standard enthalpies of formation.



Hess's Law for the combustion of methane

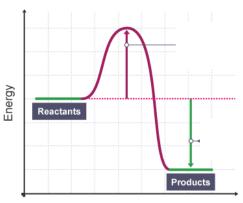
Reaction Rates

Both inside and outside of biological systems, different reactions take place at different speeds; equations can be written to describe their rates. For the reaction of A with B in order to form C, the general rate equation has the form Rate = $k[A]^x[B]^y$. Different reactions depend differently on the concentrations of the reactants, and based on this dependence they are known as zero, first, or second order reactions. The rate equation can be integrated to give rise to individual equations that can be used to obtain information such as the half-life or the concentration at time t. A good way to understand the different rates is by looking at plots of each order.

Knowing how fast a reaction happens gives no information on whether or not it will actually happen. For example, the combustion of carbon

$$C + O_2 \longrightarrow CO_2$$

is very thermodynamically favored – but a tree does not spontaneously catch fire. This is because, like all reactions –whether exothermic or endothermic- the combustion of carbon requires activation energy in order to happen. The activation energy, together with the reaction enthalpy can be shown graphically in a reaction progress curve. Reaction



Reaction progress

progress curves are useful because they can also allow us to visualize the pathway of the reaction – including how many intermediates and transition states are present, and can be used to understand how and why a catalyst accelerates a reaction.

Nature's most important catalysts are called enzymes. Enzymes accelerate all types of reactions in living organisms by binding a substrate to their active sites. The rate equation used to understand ezyme kinetics is known as the Michalis-Menten equation. This equation can be used, among other things, to figure out the strength of binding of the substrate to the enzyme and the maximum rate at which the enzyme can work.

