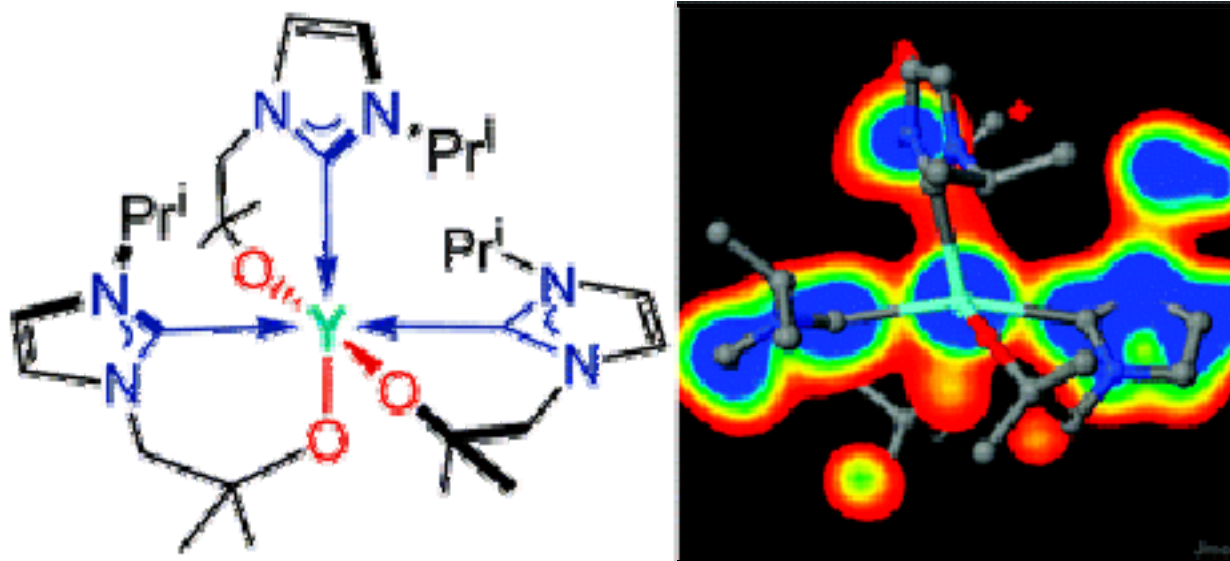


An Introduction to Inorganic Chemistry CHMB31H3 at UTSC



Comparisons between Yttrium and Titanium N-Heterocyclic Carbene Complexes in the Search for Early Transition Metal NHC Backbonding Interactions; Arnold, P. A. et al. *Inorganic Chemistry* ASAP article, Sept. 4 2008

Dr. Gillian Goring

Office Hours

Monday 1 pm - 2 pm SW-506E

Thursday 2 pm - 3pm SW-506E

Open hours:

Thursday 4 pm - 5:30 pm SW-506E

Friday 10:30 am - 12:30 pm SW-506E

Lectures

Tuesday: 2:00 pm – 4:00 pm (SW-143)

Friday: 2:00 pm - 3:00 pm (SW-309)

Email: gillian.goring@utoronto.ca

Subject line: INOR or B31

Introduction to the Course

Textbook: Inorganic Chemistry 3rd edition
by Catherine E. Housecroft and Alan G.
Sharpe

- ✓ Other editions are acceptable but there may not always be reference to them during the lecture.
- ✓ There is one copy of the third edition on reserve in the UTSC library.
- ✓ There may or may not be a solution manual available for this course.
- ✓ Course overview will be given next lecture.

Marking Scheme

✓ Short quizzes during class	10%
✓ Assignment #1	10%
✓ Term test #1	15%
✓ Assignment #2	10%
✓ Term test #2	15%
✓ Poster Presentations	10%
✓ Final exam	30%

Course lectures will be available on the course **intranet**. I recommend that everyone prints out a copy of the notes and bring them to the lecture. **You will really struggle if you don't have the notes.** You will need to scribble and add things to the notes during class.

Course Expectations

from course calendar

- ❖ Fundamentals of *coordination, solid state* and *descriptive* Inorganic Chemistry.
- ❖ Structures, bonding and reactivity of **transition metal coordination compounds**; *solid state structures* and *energetics*; selected chemistry of non-transition elements.
- ❖ Examples will be taken from environmental and biologically important inorganic compounds.
- Prerequisite: CHMA10H and CHMA11
You have to have passed these courses before you take this course!

Course Expectations

- ❖ I want to ensure that you are learning at a continuous pace with new ideas being reinforced by short quizzes and assignment questions.
- ❖ I hope that the pace is a good speed and I DO WELCOME feedback (positive or negative or suggestions) any time either in the envelope on my door or in person.
- ❖ Also remind me if I am talking *TOO fast* as I know that new material is intense and an incoherent professor makes it worst.

How things will work?

- Each week there will be a brief snapshot of your knowledge and progress to see how you are retaining the new material.
- These brief snapshots will usually appear as a
 - ✓ short quiz
 - ✓ turning in a question from the suggested problems
 - ✓ Breaks (10 minutes) will be taken half way through the class to stretch and ask questions.
- Remember if you are thinking about a particular question, others are as well, and would appreciate if you asked the question.

THERE ARE NO STUPID QUESTIONS !!!

A chemist is a chemist is a chemist.

- Gertrude Stein

- ❖ Some main divisions

analytical physical organic inorganic
theoretical biochemical

- ❖ Some basic equipment

computers glassware chemical compounds
analysis techniques (HPLC, GC, NMR, MS, IR)

- ❖ Are we really studying the same thing over and over again?

- ❖ Some concepts will reappear between courses but there are definite distinctions.

A Brief History of Inorganic Chemistry -1

- ❖ Organic chemistry
 - ❖ carbon and its reactions
- ❖ Inorganic chemistry
 - ❖ all other elements
- ❖ Could you become an inorganic specialist in the early 1800s or 1900s?

A Brief History of Inorganic Chemistry -2

- ❖ 1743 only 13 elements
- ❖ 1794 up to 28 elements
- ❖ Antoine Lavoisier (1743 – 1749)
 - ❖ Balances were produced
 - ❖ Some reproducible mass measurements
 - ❖ Master chemistry knowledge to date
 - ❖ Beheaded during the French Revolution



A Brief History of Inorganic Chemistry -3

- ❖ Early to Mid 1800s
 - ❖ Inaccurate determination of mass
 - ❖ Analyzed quantitatively some minerals and ores
 - ❖ 11 new elements found since 1794
 - ❖ Electrolysis of salt reactions found 6 new elements
 - ❖ Reactions with reducing agents and acids found 11 more elements

A Brief History of Inorganic Chemistry -4

- ❖ 1860 1st International Chemical Congress (Germany)
 - ❖ Accurate atomic weights were established
 - ❖ Total 66 elements discovered
 - ❖ Dalton's atomic theory well established
 - ❖ Avogadro's idea about the existence of diatomic molecular gases
- ❖ Dalton – Avogadro controversy (1811 to 1860) dealing with atomic theory
- ❖ Element symbol controversy resolved by Jöns Jakob Berzelius (Sweden)
 - ❖ System we use today
 - ❖ Divide elements into organic and inorganic

A Brief History of Inorganic Chemistry -5

- ❖ patents developing for industrial inorganic chemistry
 - ❖ 1824 (Portland cement)
 - ❖ 1831 (contact process development for making H_2SO_4)
 - ❖ 1843 (phosphate fertilizer industry)
 - ❖ 1851 (diaphragm cell for electrolytic generation of Cl)
- ❖ Other developments
 - ❖ 1859 spectroscopy development
 - ❖ 1879 to 1886 found 8 lanthanides
 - ❖ 1886 fluorine isolated by Ferdinand Moissan
 - ❖ 1890s inert gases isolated by William Ramsay and others

A Brief History of Inorganic Chemistry -6

- ❖ Establishment of periodic table
 - ❖ Johann Döbereiner and John Newlands attempts
 - ❖ Dobereiner based on ‘triads’ of elements
 - ❖ Newlands suggested “laws of octaves” groups of 7
 - ❖ 1869 Dmitri Mendeleev (Russian) presented a periodic table with spots assigned for elements yet to be discovered

A Brief History of Inorganic Chemistry -7

- ❖ 1900 Planck energy is in quanta ($E=h\nu$)
- ❖ Early 1900s Einstein, Thomson, Rutherford, de Broglie, Pauli, Schrödinger advances
- ❖ 1920s 90 elements known
- ❖ 1923 Lewis structures
- ❖ 1931 valence-bond theory
- ❖ Early 1930s molecular orbital theory
- ❖ 1933 crystal field theory
- ❖ Discoveries in early 1900 to 1950 became revised through new research in the 1950 to 2000s

Week 1 Lecture 1

Basic concepts ATOMS (Chapter 1)

What is an atom and what are its components?

- ❖ An atom is:
 - ❖ Electrons negatively charged 9.109×10^{-31}
 - ❖ Protons positively charged 1.673×10^{-27}
 - ❖ Neutrons neutrally charged 1.675×10^{-27}
- ❖ Nucleus has protons and neutrons
- ❖ In an element (number of = number of)
- ❖ Electrons surround nucleus
- ❖ Radius of nucleus is 10^{-15} m
- ❖ Radius of atom is 30 pm to 300 pm

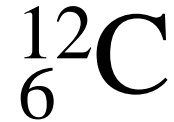
What is an atomic number?

- ❖ Z atomic number (# protons = # electrons)
- ❖ A mass number (# protons + # electrons)
- ❖ E elemental symbol
- ❖ A – Z Number of neutrons



What is relative atomic mass?

- ❖ Atomic mass is $1/12^{\text{th}}$ the mass of $^{12}_6\text{C}$ atom
 - ❖ 1.660×10^{-17} kg
 - number (# protons = # electrons)
- ❖ Relative atomic mass is relative to $^{12}_6\text{C} = 12.000$



Classical Quantum Theory -1

- ❖ Electron can behave as
 - ❖ A particle (1900 to 1925)
 - ❖ interpretation of atomic spectra
 - ❖ assignment of electronic configuration
 - ❖ A wave
 - ❖ basis of stereochemistry
 - ❖ methods of calculating the properties of molecules

Classical Quantum Theory -2

- ❖ Energy released in particular size called **QUANTA** and are influenced by the **wavelength**

- ❖ $\Delta E = h\nu$ E in Joules; ν in s^{-1} or Hz

- ❖ $c = \lambda\nu$ λ in m; ν in s^{-1} or Hz

- ❖ $\Delta E = hc/\lambda$

- ❖ each quanta of energy is related to a prominent visible line in the emission spectra of an element

Classical Quantum Theory -3

- ❖ Light interacts with element in its ground state
- ❖ An electron gets promoted to an excited state
- ❖ As electron returns towards ground state, it can undergo allowed and forbidden transitions
- ❖ Some of the allowed transitions will result in the release of a photon of light which may be seen in one of the following series of lines
 - ❖ Lyman series is in the UV
 - ❖ Balmer series is in the visible
 - ❖ Paschen, Brackett and Pfund series are in the IR

Classical Quantum Theory -4

- ❖ Niels Bohr one electron atoms (Hydrogen)
 - ❖ stationary states of energy (ground state energy) where electron can exist must be constant
 - ❖ circular orbits around the nucleus (s atomic orbitals)
 - ❖ **principle quantum number** n is 1
 - ❖ influenced by angular momentum
 - ❖ centrifugal force
 - ❖ If electron moves then the force holding the electron to the nucleus must be less than the force attracting it to outer atomic orbitals at higher energy levels

Classical Quantum Theory -5

- ❖ Ionization of an atom
- ❖ Ionization energy
- ❖ IE expressed in per mole of atoms (using Avogadro's number)
- ❖ Difficult to do these types of calculations with any other atoms other than He^+
- ❖ Knowledge of Bohr radius calculations is not required but do be aware of what the various terms do mean
- ❖ Equations 1.6 to 1.10 in 3rd edition (Bohr's theory of the atomic spectrum of hydrogen)

de Broglie's relationship

- ❖ Recall
 - ❖ electron could be a particle or a wave
- ❖ Wave-particle duality
- ❖ de Broglie relationship relates that particle (electron) having momentum mv does have an associated wavelength λ

$$\lambda = h / mv$$

- ❖ h is
- ❖ m is
- ❖ v is
- ❖ λ is

Can an electron be in two places at once?

- ❖ Recall
 - ❖ **Uncertainty principle**
 - ❖ do we know the momentum and position of an electron at the same time?
 - ❖ probability of finding the electron in a particular volume of space (atomic orbital)
 - ❖ need to deal with wavefunction equations (ψ)
 - ❖ let's meet and greet the Schrödinger equation!

Schrödinger's equation -1

- ❖ Sum of energy (E) Kinetic E + Potential E = Total E

$$-\left(\hbar^2 / 2m\right)\left(d^2\Psi / dx^2\right) + V\Psi = E\Psi$$

- ❖ $\hbar/2\pi =$

- ❖ $m =$

- ❖ kinetic energy =

- ❖ potential energy =

- ❖ Electrons move in 3D so need to work with 3D values
 - ❖ so there are angular and radial parts to ψ

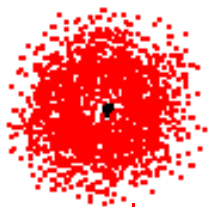
$$\psi_{\text{cartesian}}(x,y,z) \equiv \psi_{\text{radial}}(r)\psi_{\text{angular}}(\theta,\phi) \equiv R(r)A(\theta,\phi)$$

Schrödinger's equation -2

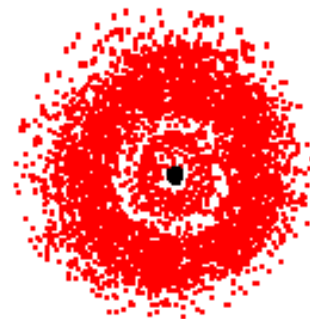
- ❖ Region where electron is located is the atomic orbital
- ❖ Energy values are associated with each ψ
- ❖ Quanta of energy arise from Schrödinger equation
 - ❖ principle quantum number
 - ❖ orbital quantum number
 - ❖ spin quantum number
 - ❖ magnetic spin quantum number
- ❖ radial components depend on n and l
- ❖ angular components depend on l and m_l

Atomic orbitals -1

- ❖ “ n ” determines the energy of a particle (electron with mass m) confined within a 1-D box
- ❖ electron can move anywhere in box (orbital)
- ❖ Radial component = surface boundary of volume
- ❖ Angular component = shape of volume
 - ❖ in s orbitals
 - ❖ angular component is independent of angles (θ, ϕ) and is a constant value
 - ❖ symmetric about the nucleus



1s orbital with black dot being the nucleus



2s orbital with black dot being the nucleus

Atomic orbitals -2

- ❖ “ l ” determines the shape of atomic orbital
- ❖ Types of orbitals arise from shapes and symmetries
 - ❖ s orbital $l = 0$
 - ❖ p orbital $l = 1$
 - ❖ d orbital $l = 2$
 - ❖ f orbital $l = 3$
- ❖ m_l has values between $-l$ to $+l$
- ❖ How does this translate into the number of orbitals?

Atomic orbitals -2

- ❖ s orbital $l = 0$ 1 orbital / 1 energy (E_1)
 - ❖ p orbital $l = 1$ 3 orbitals / 1 energy (E_2)
 - ❖ d orbital $l = 2$ 5 orbitals / 1 energy (E_3)
 - ❖ f orbital $l = 3$ 7 orbitals / 1 energy (E_4)
-
- ❖ Energy values are
 - ❖ different for each orbital shape
 - ❖ higher in value with more orbitals
 - ❖ degenerate within the same orbital

**But what about the electron in the orbital?
Or the particle in the box?**

But what about the electron in the orbital?

Or the particle in the box?

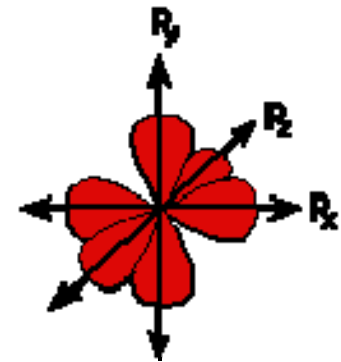
- ❖ Electron follows the path of a wave at a particular energy level “ n ”
- ❖ Probability of finding electron near nucleus is less likely and it is probably further away (ie. 53 pm from nucleus)
- ❖ At higher “ n ”, electron will move faster as the wave and has further distance to travel as there is more volume to explore and more volumes of the same energy to explore
- ❖ How do you describe these degenerate orbital volumes?

p Atomic orbitals

- ❖ “*p*” has 3 degenerate orbitals of equal energy
- ❖ 1 node for $n = 2$
- ❖ Orbital must have region near nucleus where electron is rarely found
- ❖ Known as nodal plane which passes through the nucleus
- ❖ Angular part of Schrodinger’s equation dictates shape



2p orbital with black dot being the nucleus



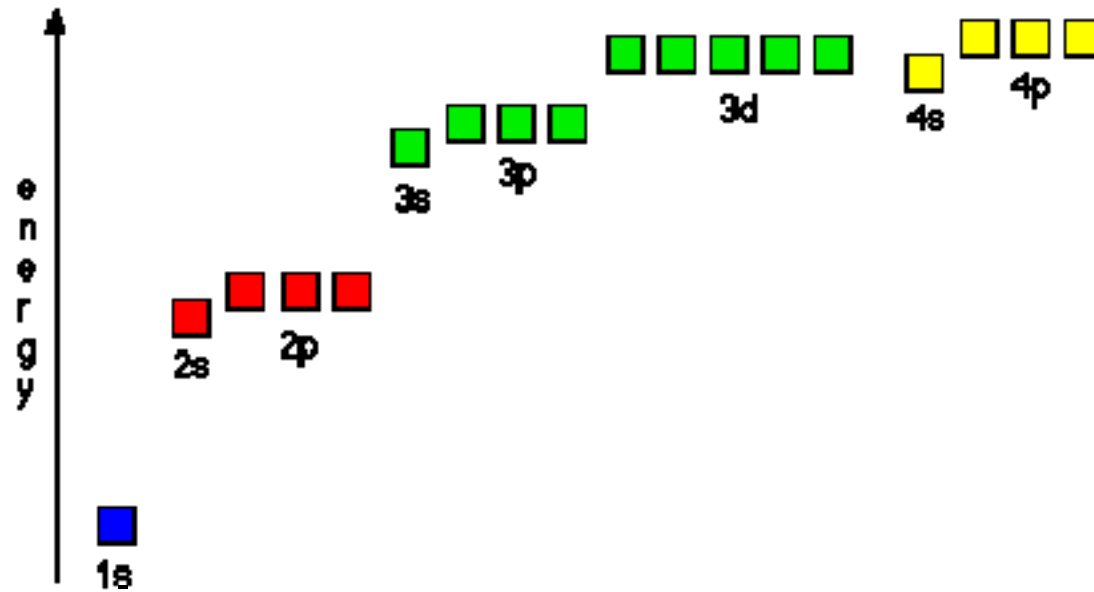
p Atomic orbitals

- ❖ Let's draw the nodal planes for the three degenerate *p* atomic orbitals

d Atomic orbitals

- ❖ “*d*” has 5 degenerate orbitals of equal energy
- ❖ 2 nodes for $n = 3$
 - ❖ 2 nodes = 2 nodal planes
 - ❖ Node must be near nucleus
 - ❖ Volume and orientation of orbitals are of interest here
 - ❖ d_{yz} , d_{xy} , d_{xz} , dz^2 , dx^2-y^2
- ❖ See figure 1.11 in text of the representation of the five degenerate *d* atomic orbitals

Energy level diagram



Aufbau principle

- ❖ Uses ground state electron configuration of an element
- ❖ How do we fill up the orbitals?
 - ❖ Lowest energy first (1s, 2s etc)
 - ❖ One electron per degenerate orbital, then electrons can be paired
- ❖ Core electrons are those located in completely filled orbitals in the lower energy quantum levels to their nearest noble gas configuration
- ❖ Zr $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^2$
- ❖ or [Kr] $5s^2 4d^2$

Review

- ❖ Definition and components of atoms
- ❖ Schrödinger's equation and its application to atomic orbitals
- ❖ The shape and characteristics of atomic orbitals at $n=1$ to $n=4$
- ❖ Uses ground state electron configuration of an element
- ❖ Next time
 - ❖ Trends in the periodic table

Remember to get the lecture notes for next week. You have to print them from the intranet.