

**UNIVERSITY OF CALGARY
DEPARTMENT OF CHEMISTRY
COURSE OUTLINE
FALL 2015**

1. COURSE: CHEMISTRY 701.23. Electronic Structure Methods Applied to Transition Metal Chemistry

LEC	DAYS	TIME	ROOM	INSTRUCTOR	OFFICE	PHONE	EMAIL	OFFICE HOURS
L01	MWF	9:00-9:50am	SB 324	Dr. Thurbide	SB219	220 5370	thurbide@ucalgary.ca	MW 11-1

D2L course name: CHEM 701.23 L01 - (FALL 2015) – Electronic Structure Methods Applied to Transition Metal Chemistry

Departmental Office: SA 229, 220-5341, info@chem.ucalgary.ca

- 2. PREREQUISITES:** Chemistry B.Sc. or equivalent (<http://www.ucalgary.ca/pubs/calendar/current/chemistry.html#6525>).

Note: The calendar description and the Faculty of Science policy on prerequisites and antirequisites is described in section 3.5 C. of the online University Calendar (<http://www.ucalgary.ca/pubs/calendar/current/sc-3-5.html>). Students are responsible to ensure that they meet all prerequisite requirements for each course in which they are registered. Students who do not meet these requirements will be deleted from the course.

- 3. GRADING:** The University policy on grading and related matters is described sections F.1 and F.2 of the online University Calendar (<http://www.ucalgary.ca/pubs/calendar/current/f.html>). In determining the overall grade in the course the following weights will be used:

Assignment 1	30%
Assignment 2	30%
Critical term paper	40%

Total	100%

The marks for each of the course components will be recorded as a numerical score and combined as shown above to arrive at the total numerical score which will then be converted to a letter grade to be reported to the Registrar.

Grading Scale:

A+	A	A-	B+	B	B-
95% - 100%	90% - 94%	85% - 89%	80% - 84%	75% - 79%	70% - 74%
C+	C	C-	D+	D	F
65% - 69%	60% - 64%	55% - 59%	50% - 54%	45% - 49%	0% - 44%

- 4. MISSED COMPONENTS OF TERM WORK:** The regulations of the Faculty of Science pertaining to this matter are found in the Faculty of Science area of the Calendar in section 3.6: <http://www.ucalgary.ca/pubs/calendar/current/sc-3-6.html>. It is the student's responsibility to familiarize himself/herself with these regulations. See also <http://www.ucalgary.ca/pubs/calendar/current/e-3.html>.
- 5. TEXTBOOK:** *No single textbook. Readings will be drawn from Computational Chemistry and Molecular Modeling: Principle and Applications. K.I. Ramachandran, DeepaGopakumar, Krishnan Namboori. 2008. Springer Berlin Heidelberg. A few selected papers from the research literature will also be considered.*
- 6. EXAMINATION POLICY:** Any examinations will be open book. Students should also read the Calendar, Section G, on Examinations: <http://www.ucalgary.ca/pubs/calendar/current/g.html>.

7. **WRITING:** In this course, the quality of the student's writing will be a factor in their evaluation. See also <http://www.ucalgary.ca/pubs/calendar/current/e-2.html>.

8. OTHER IMPORTANT INFORMATION FOR STUDENTS:

- (a) **ACADEMIC MISCONDUCT:** (cheating, plagiarism, or any other form) is a very serious offence that will be dealt with rigorously in all cases. A single offence may lead to disciplinary probation or suspension or expulsion. The Faculty of Science follows a zero tolerance policy regarding dishonesty. Please read the sections of the University Calendar under K. Student Misconduct (<http://www.ucalgary.ca/pubs/calendar/current/k.html>) to inform yourself of definitions, processes and penalties.
- (b) **ACADEMIC INTEGRITY:** Do you know what "honesty in academics" is? Check the University website at: <http://www.ucalgary.ca/honesty/>
- (c) **ASSEMBLY POINTS: in case of emergency during class time. Be sure to FAMILIARIZE YOURSELF with the information at <http://www.ucalgary.ca/emergencyplan/assemblypoints>.**
- (d) **ACADEMIC ACCOMMODATION POLICY:** Students needing an Accommodation because of a Disability or medical condition should contact Student Accessibility Services in accordance with the Procedure for Accommodations for Students with Disabilities available at http://www.ucalgary.ca/policies/files/policies/procedure-for-accommodations-for-students-with-disabilities_0.pdf. Students needing an Accommodation in relation to their coursework or to fulfil requirements for a graduate degree, based on a Protected Ground other than Disability, should communicate this need, preferably in writing, to the Associate Head of Chemistry, Dr. Ashley Causton, by email ahugchem@ucalgary.ca or phone (403) 220-5353.
- (e) **SAFEWALK:** Campus Security will escort individuals day or night (<http://www.ucalgary.ca/security/safewalk>). Call **220-5333** for assistance. Use any campus phone, emergency phone or the yellow phones located at most parking lot pay booths.
- (f) **FREEDOM OF INFORMATION AND PRIVACY:** This course is conducted in accordance with the Freedom of Information and Protection of Privacy Act (FOIPPA). As one consequence, **students should identify themselves on all written work by placing their name on the front page and their ID number on each subsequent page.** For more information see also <http://www.ucalgary.ca/secretariat/privacy>.
- (g) **STUDENT UNION INFORMATION:**
VP Academic: **Phone:** 220-3911 **Email:** suvpaca@ucalgary.ca.
SU Faculty Rep: **Phone:** 220-3913 **Email:** sciencerep@su.ucalgary.ca
Website: <http://www.su.ucalgary.ca/>
Student Ombuds Office: 403 220-6420 Email ombuds@ucalgary.ca <http://ucalgary.ca/provost/students/ombuds>
- (h) **INTERNET and ELECTRONIC COMMUNICATION DEVICE Information.** You can assume that in all classes that you attend, **your cell phone should be turned off.** Also, communication with other individuals, via laptop computers, Blackberries or other devices connectable to the Internet is not allowed in class time unless specifically permitted by the instructor. If you violate this policy you may be asked to leave the classroom. Repeated abuse may result in a charge of misconduct.