

Chemistry 549 - Advanced Physical Chemistry II: Atoms and Molecules

Department of Chemistry, University of Alabama

Fall Semester 2005, Academic Year 2005-2006

Subject: Quantum Mechanics applied to Atoms and Molecules

Meetings: MWF 11:00-11:50 am, Shelby 251

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TextbooksIra N. Levine, *Quantum Chemistry*, Fifth Edition (Prentice-Hall, Englewood Cliffs, NJ, 1999);**Coverage:**

1. **Molecular Orbital Section: Theory and Applications**
 - 1.1. Classical waves and time-independent Schrodinger equation
 - 1.2. Quantum mechanics of simple systems
 - 1.3. One-electron atom and ions
 - 1.4. Postulates of quantum mechanics
 - 1.5. Variational method
 - 1.6. Huckel method
 - 1.7. Extended Huckel method
 - 1.8. SCF-LCAO-MO
 - 1.9. Semiempirical methods (INDO, MINDO, AM1, PM3)
 - 1.10. Ab initio methods (Gaussian) and molecular mechanics
 - 1.11. Use computer lab to construct and calculate molecules
2. **Spectroscopy**
 - 2.1. UV and Fluorescence spectroscopy
 - 2.2. Infrared and Raman spectroscopy
 - 2.3. Microwave and X-ray photoelectron spectroscopy
 - 2.4. Principles of magnetic resonance
 - 2.5. NMR in solids
 - 2.6. NMR in liquids (spin-spin coupling)
 - 2.7. EPR of radicals in solution
 - 2.8. EPR of trapped radicals in solids
 - 2.9. EPR of molecules in triplet state

Prerequisites:

Grading System: Two 1-hour exams (100 points each). One molecular orbital calculation project, 100 points. One final exam, 200 points. Total points 500. Homework will be assigned, graded, and returned. If less than 30% of the homework is handed in, loss of one letter grade will occur (A to B, B to C, etc.).

Exams (and final exam) will be closed book, closed notes. However, you may bring into the examination one sheet, one-sided, 8.5 x 11 inches, of formulas and data, pencil, and an electronic calculator (programmable or not). You can bring three such pages to the final examination.

Homework: Problem sets are assigned, heavily recommended, collected on the days designated, and graded. The homework problems are DUE TO BE FINISHED by the date at which they are listed

SCHEDULE (forty-five 50-minute periods):

Wed Aug. 24. : Schrodinger equation (Levine Ch. 1)

Fri	Aug. 26.	:	
Mon.	Aug. 28.	:	Levine Chapter 1: all problems##
Wed.	Aug. 30.	:	Particle in a box (Levine Ch. 2)
Fri.	Sep. 2.	:	Levine Chapter 2: all problems ## Operators (Levine Ch. 3)
Mon.	Sep. 5.	:	Labor Day Holiday. No class.
Wed.	Sep. 7.	:	Levine #3.1, 3.2, 3.7, 3.8, 3.9, 3.10, 3.11, 3.12, 3.13, 3.15, 3.16, 3.17, 3.18, 3.20, 3.21, 3.22, 3.23, 3.24, 3.27, 3.28, 3.30, 3.31, 3.36, 3.39, 3.42 (a) through (f) ## Harmonic oscillator (Levine Ch.4)
Fri	Sep. 9.	:	Levine #4.1, 4.2, 4.3, 4.6, 4.12, 4.13, 4.16, 4.19, 4.20, 4.22, 4.24, 4.26, 4.27, 4.29 ##
Mon	Sep. 12.	:	Angular momentum (Levine Ch. 5)
Wed.	Sep. 14.	:	Levine #5.2, 5.4, 5.5, 5.7, 5.9, 5.10, 5.12, 5.13, 5.14, 5.15, 5.16, 5.19, 5.20, 5.21, 5.25, 5.26, 5.31 ##
Fri.	Sep. 16.	:	Hydrogen atom (Levine Ch. 6)
Mon.	Sep. 19.	:	Levine #6.2, 6.4, 6.5, 6.7, 6.8, 6.10, 6.12, 6.13, 6.15, 6.18, 6.19, 6.24, 6.27, 6.29, 6.30, 6.33, 6.34, 6.35, Laguerre problem (from IV edition), 6.46, 6.47 ##)
Wed.	Sep. 21.	:	Theorems of quantum mechanics (Levine Ch. 7)
Fri.	Sep. 23.	:	Variational method (Levine Ch. 8) Levine #7.1, 7.3, 7.5 (a) and (b), 7.9, 7.10, 7.16, 7.18, 7.20, 7.21, 7.24, 7.26, 7.27, 7.37, 7.38, 7.39, 7.40, 7.45, 7.46, 7.50, 7.53, 7.55, 7.57, 7.58, 7.61 (a) through (j) ##
Mon.	Sep. 26.	:	First Hour Examination: Levine Chapters 1-7
Wed.	Sep. 28.	:	Levine # 8.3, 8.17, 8.18, 8.19, 8.23, 8.27, 8.34, 8.39, 8.40 ## Perturbation theory (Levine Ch. 9)
Fri.	Sep. 30.	:	
Mon.	Oct. 3.	:	Levine #9.1, 9.2, 9.5 ## Electron spin (Levine Ch. 10)
Wed.	Oct. 5.	:	Levine #10.1, 10.6, 10.7, 10.9, 10.12, 10.15, 10.18, 10.19, 10.21 ## Many-electron atoms (Levine Ch. 11)
Fri.	Oct. 7.	:	
Mon.	Oct. 10.	:	Levine #11.1, 11.6, 11.15, 11.18, 11.19, 11.20, 11.23, 11.28, 11.30 ##
Wed.	Oct. 12.	:	Molecular symmetry (Levine Ch. 12)
Fri.	Oct. 14.	:	Levine #12.2, 12.3, 12.4, 12.5, 12.6, 12.7, 12.8, 12.9, 12.10, 12.14, 12.17, 12.18, 12.19, 12.20, 12.21, 12.22, 12.23, 12.24, 12.25, 12.26, 12.27 ## Diatomic molecules (Levine Ch. 13)
Mon.	Oct. 17.	:	
Wed.	Oct. 19.	:	Levine (V) #13.1, 13.2, 13.3, 13.14, 13.42, 13.45, 13.50, 13.63 ## Use microcomputers to construct and calculate molecules
Fri.	Oct. 21.	:	
Mon.	Oct. 24.	:	Ab initio theory of polyatomic molecules (Levine Ch.15)
Wed.	Oct. 26.	:	Decide what to compute in your project
Fri.	Oct. 28.	:	Semiempirical treatments of polyatomic molecules (Levine Ch. 16)
Mon.	Oct. 31.	:	
Wed.	Nov. 2.	:	
Fri.	Nov. 4.	:	UV and fluorescence spectroscopy
Mon.	Nov. 7.	:	Second Hour Examination: Levine Chapters 7-16
Wed.	Nov. 9.	:	
Fri.	Nov. 11.	:	Infrared and Raman spectroscopy
Mon.	Nov. 14.	:	Microwave spectroscopy
Wed.	Nov. 16.	:	X-ray photoelectron spectroscopy (XPS)
Fri.	Nov. 18.	:	

Mon. Nov. 21. : NMR in liquids (spin-spin coupling)
Wed. Nov. 23. : **Thanksgiving Holiday – no class**
Fri. Nov. 25. : **Thanksgiving Holiday – no class**
Mon. Nov. 28. : Principles of magnetic resonance. NMR in solids
Wed. Nov. 30. : EPR of radicals in solution
Fri. Dec. 2. : EPR of molecules in triplet state
Mon. Dec. 5. :
Wed. Dec. 7. : **Present project results**
Fri. Dec. 9. :

Tue Dec. 13. 8:00 a.m.-10:30 a.m.: **FINAL EXAM (cumulative; 2.5 hrs):**