

Contents

<i>Preface to the Third Edition</i>	xi
<i>Acknowledgments</i>	xiii
<i>Photo and Figure Credits</i>	xiv
 <i>1~Using Computations in Chemical Research</i>	 1
<i>What is Electronic Structure Theory?</i>	3
<i>Example Research Problem: Vitamin E</i>	4
Selecting the Initial Calculations.....	6
<i>Planning and Carrying Out Calculations</i>	7
The Theoretical Model Progression: Model Chemistries	8
Chemical Models and Real Molecules.....	15
Predicting Properties of Interest.....	17
Modeling the Chemical Environment	20
Combining Calculations with Experiments	22
<i>Atomic Units</i>	28
<i>Advanced Topics</i>	29
Treating Post-Third Row Elements	29
Numerical Integration & Grids	30
Density Fitting Basis Sets	31
 <i>2~Getting Started with Calculations</i>	 33
<i>First Steps: An Energy Calculation on Formaldehyde</i>	35
Setting Up and Running Calculations	36
EXAMPLE 2.1: FORMALDEHYDE ENERGY, MOLECULAR ORBITALS & ATOMIC CHARGES	36
Understanding the Gaussian Input File.....	44
<i>Gaussian Calculation Results</i>	46
Interpreting Energies & Energy Differences.....	47
Dipole and Higher Multipole Moments.....	48
Molecular Orbitals	49
Atomic Charge Distribution	51
<i>More about Energies and Orbitals</i>	52
When Energies Can & Cannot be Compared	52
EXAMPLE 2.2: COMPARING FORMALDEHYDE AND ACETONE.....	52
EXAMPLE 2.3: 1,2-DICHLORO-1,2-DIFLUOROETHANE CONFORMER ENERGIES	53
Modeling Open Shell Systems	53
Biorthogonalized Orbitals.....	54
EXAMPLE 2.4: COMPARING CANONICAL & BIORTHOGONALIZED ORBITALS	55
EXAMPLE 2.5: SPIN POLARIZATION IN HETEROSUBSTITUTED ETHENE RADICALS	55
<i>Minimizing Molecular Structures: Opt+Freq Calculations</i>	57
EXAMPLE 2.6: FORMALDEHYDE OPTIMIZATION & FREQUENCY CALCULATION	58
Thermal Energy Corrections	59

Clean vs. Optimize	59
EXAMPLE 2.7: CLEANING VS. OPTIMIZING ANILINE	59
EXAMPLE 2.8: ACETALDEHYDE/OXIRANE ISOMERIZATION ENERGY	61
<i>Modeling Large Systems: Gaussian's ONIOM Facility</i>	61
EXAMPLE 2.9: QM:QM CALCULATIONS ON TWO VITAMIN E STRUCTURES	62
<i>Exercises</i>	65
EXERCISE 2.1: COMPARING ETHYLENE AND FORMALDEHYDE	65
EXERCISE 2.2: OPTIMIZING CHROMIUM HEXACARBONYL	66
EXERCISE 2.3: ATOMIC CHARGE ANALYSIS FOR DIZINCOCENE	66
EXERCISE 2.4: COMPARING ETHYLENE AND FLUOROETHYLENE	67
EXERCISE 2.5: TWO MORE HETEROSUBSTITUTED ETHENE RADICALS	67
EXERCISE 2.6: THE GROUND STATE OF O ₂	69
EXERCISE 2.7: ONIOM CALCULATIONS ON VITAMIN E-RELATED MOLECULES	69
<i>Advanced Topics & Exercises</i>	71
Wavefunction Stability	71
ADVANCED EXAMPLE 2.10: OXYGEN STABILITY CALCULATIONS	72
ADVANCED EXERCISE 2.8: OZONE WAVEFUNCTION STABILITY	72
Comparing Model Chemistries for Accuracy	73
ADVANCED EXERCISE 2.9: BOND ENTHALPIES OF SECOND & THIRD ROW HYDRIDES	73
ADVANCED EXERCISE 2.10: BUTANE ENTHALPY OF ISOMERIZATION	75
ADVANCED EXERCISE 2.11: MALONALDEHYDE OPTIMIZATION	77
Exploring Basis Sets in Depth	78
ADVANCED EXERCISE 2.12: THE PO BOND LENGTH: THE BASIS SET LIMIT	78
ADVANCED EXERCISE 2.13: BASIS SET DEFINITIONS	79
Understanding CPU Resource Requirements	81
ADVANCED EXERCISE 2.14: CPU USAGE BY PROBLEM SIZE	81
<i>3~Geometry Optimizations</i>	85
<i>Potential Energy Surfaces</i>	87
<i>Locating Stationary Points on the PES</i>	88
Optimization Convergence Criteria	88
Examining Optimization Results	89
EXAMPLE 3.1: OPTIMIZING DECAMETHYLZINCOCENENE	90
EXAMPLE 3.2: OPTIMIZING COBALT(III) ACETYLACETONATE	96
<i>Locating Transition Structures</i>	97
EXAMPLE 3.3: LOCATING A TRANSITION STRUCTURE WITH QST2	98
EXAMPLE 3.4: TRANSITION STRUCTURE FOR VINYL AZIDE DECOMPOSITION	99
<i>Characterizing Stationary Points</i>	102
EXAMPLE 3.5: EXPLORING THE C ₃ H ₅ F POTENTIAL ENERGY SURFACE	104
<i>Interpreting Normal Mode Information</i>	106
EXAMPLE 3.6: AZIDE DECOMPOSITION: CONCERTED VS. STEPWISE MECHANISMS	106
<i>Exercises</i>	110
EXERCISE 3.1: COMPARING STRUCTURES IN THE VINYL SERIES	110
EXERCISE 3.2: COMPARING C ₆₀ O ISOMERS	112
EXERCISE 3.3: LOCATING A TRANSITION STRUCTURE ON THE GEH ₄ PES	114
EXERCISE 3.4: MODELING HYDROGEN SHIFTS IN C ₃ H ₅ F	115
<i>Advanced Topics & Exercises</i>	116
Strategies for Handling Difficult Optimization Cases	116
ADVANCED EXAMPLE 3.7: APPROACHES TO THE ACETALDEHYDE-VINYL ALCOHOL TS	118
ADVANCED EXERCISE 3.5: PROTONATION & PROTON TRANSFERS IN ALLENES	126
ADVANCED EXERCISE 3.6: PERIODIC TRENDS IN TRANSITION METAL COMPLEXES	134

ADVANCED EXERCISE 3.7: $\text{HCO}(\text{CO})_4$ ISOMERS	134
ADVANCED EXERCISE 3.8: OPTIMIZING THE BOND LENGTH OF HF	135
ADVANCED EXERCISE 3.9: SEARCHING FOR A SYMMETRIC MINIMUM.....	136

4~Predicting Chemical Properties.....139

Frequency Calculation Results: IR and Raman Spectra.....143

Scaling Frequencies.....144

EXAMPLE 4.1: IR SPECTRUM OF FORMALDEHYDE; RAMAN SPECTRUM OF BENZENE145

Understanding & Interpreting Frequency Data.....148

Applications of IR and Raman Spectroscopy148

EXAMPLE 4.2: DETECTING C_{60} IN INTERSTELLAR SPACE148

EXAMPLE 4.3: RAMAN CRIME SOLVING: IDENTIFYING SUBSTANCES ON CURRENCY.....150

Substituting Isotopes.....153

EXAMPLE 4.4: SUBSTITUTING DEUTERIUM IN FORMALDEHYDE.....154

Modeling Thermochemistry.....154

Why & How to Model Thermochemical Quantities.....155

EXAMPLE 4.5: THERMOCHEMISTRY CALCULATIONS ON SMALL MOLECULES155

Compound Model Chemistries for High Accuracy Energies157

EXAMPLE 4.6: USING & EVALUATING HIGH ACCURACY MODEL CHEMISTRIES160

Predicting Spectra: NMR.....161

EXAMPLE 4.7: ^{13}C NMR EXTREMES: METHANE, BENZENE, METHYL CATION.....162

Viewing NMR Data in GaussView and WebMO163

Conformational Searching and Boltzmann Averaging164

EXAMPLE 4.8: TRIMETHYLPENTANEDIOL ^{13}C SPECTRUM164

Exercises.....170

EXERCISE 4.1: FREQUENCIES OF STRAINED HYDROCARBONS.....170

EXERCISE 4.2: CARBONYL STRETCH BY SUBSTITUENT172

EXERCISE 4.3: ISOTOPE SUBSTITUTION EFFECTS ON BENZENE'S RAMAN SPECTRUM173

EXERCISE 4.4: NMR PROPERTIES OF ALKANES, ALKENES & ALKYNES.....174

EXERCISE 4.5: ^{13}C SHIFTS IN NITROANILINES: A SURPRISE DEVIATION FROM ADDITIVITY175

EXERCISE 4.6: THE ^{13}C NMR SPECTRUM OF PROPELLANE178

EXERCISE 4.7: AZULENE/NAPHTHALENE HEAT OF ISOMERIZATION WITH CBS-QB3.....179

EXERCISE 4.8: COST & ACCURACY OF CBS-QB3 vs. G3/G4: BENZENE HEAT OF COMBUSTION.....179

EXERCISE 4.9: C_{60}O ISOMERS REVISITED.....180

EXERCISE 4.10: PROTON NMR OF CHLOROCYCLOHEXANE CONFORMATIONS.....182

Advanced Topics & Exercises.....182

More About Computing Vibrational Properties182

ADVANCED EXAMPLE 4.9: RAMAN SPECTRA OF SMALL WATER CLUSTERS 1.....185

ADVANCED EXERCISE 4.11: RAMAN SPECTRA OF SMALL WATER CLUSTERS 2186

ADVANCED EXERCISE 4.12: FORMALDEHYDE ANHARMONIC FREQUENCY ANALYSIS.....187

ADVANCED EXERCISE 4.13: ANHARMONIC ANALYSIS OF CARBONYL STRETCH189

Materials Properties: Polarizability, Hyperpolarizability & Gamma.....190

ADVANCED EXERCISE 4.14: PREDICTING NONLINEAR OPTICAL PROPERTIES190

ADVANCED EXERCISE 4.15: PREDICTING GAMMA FOR POLYACETYLENES.....191

Highly Accurate Thermochemistry & Wavefunction Stability196

ADVANCED EXAMPLE 4.10: THE WAVEFUNCTION FOR THE CN CATION.....196

5~Modeling Chemistry in Solution.....199

Continuum Models of Solvation201

Cavity Shapes202

Escaped Charge and the Electrostatic Equations202

Setting Up Solvation Calculations with Gaussian.....	203
EXAMPLE 5.1: METHYL LACTATE CONFORMERS IN METHANOL.....	204
<i>Properties in Solution</i>	206
EXAMPLE 5.2: FORMALDEHYDE IR SPECTRUM IN ACETONITRILE.....	206
EXAMPLE 5.3: VITAMIN E OXIDATION MODEL IN SOLUTION.....	206
Predicting Thermodynamic Quantities.....	207
<i>Predicting Free Energies in Solution: The SMD Method</i>	207
EXAMPLE 5.4: FREE ENERGY OF SOLVATION FOR ACETIC ACID IN CHLOROFORM.....	208
Alternate Solvation Models Based on SMD.....	209
<i>Exercises</i>	211
EXERCISE 5.1: FORMALDEHYDE FREQUENCIES IN CYCLOHEXANE.....	211
EXERCISE 5.2: FURFURALDEHYDE CONFORMERS IN VARIOUS SOLVENTS.....	211
EXERCISE 5.3: METHYL LACTATE IN WATER.....	213
EXERCISE 5.4: A MENSCHUTKIN REACTION.....	214
EXERCISE 5.5: COMPARING FREE ENERGIES OF SOLVATION.....	215
<i>Advanced Topics & Exercises</i>	216
Including Explicit Solvent Molecules.....	216
ADVANCED EXAMPLE 5.5: METHYL ACETATE HYDROLYSIS WITH EXPLICIT WATERS.....	217
ADVANCED EXERCISE 5.6: HYDROLYSIS REACTANT AND PRODUCT COMPLEXES.....	219
More About Free Energies in Solution.....	222
ADVANCED EXAMPLE 5.6: THE COMPONENTS OF FREE ENERGIES IN SOLUTION.....	224
<i>6~Studying Reaction Mechanisms</i>	227
<i>Visualizing Surfaces to Understand Reactivity</i>	229
EXAMPLE 6.1: DIELS-ALDER REGIOSELECTIVITY.....	229
EXAMPLE 6.2: REACTIVITY OF Al_5O_4^-	232
EXAMPLE 6.3: INDANE AND TETRALIN.....	234
<i>Studying Potential Energy Surfaces</i>	236
EXAMPLE 6.4: ROTATIONAL ISOMERIZATION IN ALLYL CATION.....	236
Potential Energy Surface Scans.....	238
EXAMPLE 6.5: SCAN CALCULATIONS: ROTATIONAL ISOMERIZATION.....	241
EXAMPLE 6.6: BOND DISSOCIATION IN METHANE.....	243
Reaction Paths.....	244
Running IRC Calculations.....	244
EXAMPLE 6.7: STUDYING THE H_2CO POTENTIAL ENERGY SURFACE.....	247
<i>Isodesmic Reactions</i>	250
EXAMPLE 6.8: CO_2 ENTHALPY OF FORMATION.....	250
Limitations of Isodesmic Reactions & Hess's Law.....	251
EXAMPLE 6.9: TESTING HESS'S LAW.....	251
<i>Exercises</i>	252
EXERCISE 6.1: ELECTRON DENSITIES OF SUBSTITUTED BENZENES.....	252
EXERCISE 6.2: RELAXED SCANS: ROTATIONAL BARRIERS IN ACETOPHENONES.....	255
EXERCISE 6.3: THE H_2CO POTENTIAL ENERGY SURFACE.....	256
EXERCISE 6.4: THE SILICON CATION + SILANE POTENTIAL ENERGY SURFACE.....	258
EXERCISE 6.5: ISODESMIC REACTIONS.....	262
EXERCISE 6.6: HEAT OF FORMATION FOR TETRAFLUOROSILANE.....	263
<i>Advanced Topics and Exercises</i>	265
ADVANCED EXERCISE 6.7: METHYL ACETATE HYDROLYSIS REVISITED.....	265
Scanning Multiple Variables.....	267
ADVANCED EXAMPLE 6.10: THE O_3 POTENTIAL ENERGY SURFACE.....	267
ADVANCED EXERCISE 6.8: STUDYING KETO-ENOL TAUTOMERISM.....	268

S_N2 Reactions	271
ADVANCED EXAMPLE 6.11: A SIMPLE S_N2 REACTION	272
ADVANCED EXERCISE 6.9: LEAVING GROUP EFFECTS IN ETHYL HALIDE S_N2 REACTIONS	273
7~Predicting Spectra	275
<i>NMR Spectroscopy: Beyond Chemical Shifts</i>	278
NMR Shielding Tensor Components.....	278
EXAMPLE 7.1: NMR SHIELDING SUBSTITUENT EFFECTS IN SUBSTITUTED ACETYLENES	278
NMR Spin-spin Coupling Constants.....	279
EXAMPLE 7.2: SPIN-SPIN COUPLING CONSTANTS	281
<i>Vibrational Circular Dichroism</i>	281
EXAMPLE 7.3: ABSOLUTE CONFIGURATION OF CAMPHOR.....	283
Conformational Averaging.....	284
EXAMPLE 7.4: VCD SPECTRUM OF DESFLURANE.....	285
<i>Raman Optical Activity</i>	289
EXAMPLE 7.5: OBSERVING α -PINENE EPOXIDATION WITH ROA.....	290
Solvent Effects on VCD and ROA Spectra.....	292
EXAMPLE 7.6: EPICHLORHYDRIN ROA SPECTRUM: GAS PHASE VS. CYCLOHEXANE.....	292
EXAMPLE 7.7: MODELING ROA SPECTRA IN WATER.....	294
<i>Optical Rotations</i>	295
EXAMPLE 7.8: OPTICAL ROTATIONS: SUBSTITUTED OXIRANES.....	296
Modeling ORD in Solution	297
<i>A Final Note on Boltzmann Averaging</i>	298
<i>Exercises</i>	299
EXERCISE 7.1: NMR SHIELDING TENSORS: SUBSTITUENT EFFECTS.....	299
EXERCISE 7.2: SPIN-SPIN COUPLING CONSTANTS: THREE MEMBERED RING SYSTEMS	300
EXERCISE 7.3: SPIN-SPIN COUPLING CONSTANTS: HIGHLY STRAINED SYSTEMS	300
EXERCISE 7.4: ABSOLUTE CONFIGURATION OF FENCHONE	301
EXERCISE 7.5: DISTINGUISHING PRODUCTS WITH VCD.....	302
EXERCISE 7.6: (R)-3-METHYLCYCLOHEXANONE VCD SPECTRUM	304
EXERCISE 7.7: α -PINENE OXIDE DIASTEREOMERS	305
EXERCISE 7.8: CONFORMATION ELUCIDATION OF A CHIRAL DRUG	305
EXERCISE 7.9: EPICHLORHYDRIN ROA SPECTRUM IN ACETONITRILE	309
EXERCISE 7.10: LACTAMIDE ROA SPECTRUM IN WATER	310
EXERCISE 7.11: INDUCED CHIRALITY: CAMPHOR VCD SPECTRUM IN CHLOROFORM	313
EXERCISE 7.12: OPTICAL ROTATIONS: SUBSTITUTED OXIRANES.....	316
EXERCISE 7.13: SOLVENT EFFECTS ON ORD: EPICHLOROHYDRIN	317
<i>Advanced Topics and Exercises</i>	319
Microwave Spectroscopy and Hyperfine Coupling Constants.....	319
ADVANCED EXERCISE 7.14: 1,1-DIFLUOROPROP-2-YNYL RADICAL	322
ADVANCED EXERCISE 7.15: PROP-2-YNYL RADICAL HYPERFINE COUPLING	323
ADVANCED EXERCISE 7.16: CF^+ IN INTERSTELLAR SPACE	324
ADVANCED EXERCISE 7.17: HYPERFINE COUPLING CONSTANTS: ARSENIC COMPOUNDS.....	324
8~Modeling Excited States.....	327
<i>Chemistry and Light: Excited States</i>	329
Model Chemistries for Modeling Excited States	330
<i>Predicting Vertical Transition Energies & UV/Visible Spectra</i>	331
EXAMPLE 8.1: BENZENE EXCITATION ENERGIES	332
Determining the Symmetry of an Excited State.....	334
Oscillator Strengths.....	335

EXAMPLE 8.2: MODELING DYES FOR SOLAR CELLS.....	336
EXAMPLE 8.3: EXCITED STATES OF $V(H_2O)_6^{2+}$	339
Natural Transition Orbitals.....	341
High Accuracy Excited States	342
EXAMPLE 8.4: TITANIUM OXIDE EXCITED STATES.....	342
<i>Electronic Circular Dichroism</i>	344
EXAMPLE 8.5: PLUMERICIN ECD	344
<i>Predicting Fluorescence: Optimizing Excited State Geometries</i>	347
EXAMPLE 8.6: DMABN EXCITED STATE GEOMETRY	
<i>Exercises</i>	350
EXERCISE 8.1: EVALUATING DYES FOR DSSC DEVICES	350
EXERCISE 8.2: EXCITED STATES OF VANADIUM-WATER COMPLEXES.....	353
EXERCISE 8.3: HIGH ACCURACY EXCITED STATES: TITANIUM OXIDE.....	355
EXERCISE 8.4: ECD RESULTS ANALYZED IN CONJUNCTION WITH VCD & OR	358
EXERCISE 8.5: DMABN EXCITED STATE GEOMETRY IN SOLUTION.....	359
EXERCISE 8.6: MODELING FLUORESCENCE OF NANOFIBERS	362
<i>Advanced Topics & Exercises</i>	364
Franck-Condon Analysis.....	364
ADVANCED EXAMPLE 8.7: FRANCK-CONDON ANALYSIS: A UV ABSORPTION SPECTRUM.....	366
ADVANCED EXERCISE 8.7: FRANCK-CONDON ANALYSIS: ACROLEIN	369
ADVANCED EXERCISE 8.8: ABSORPTION SPECTRUM OF ANOTHER DIPHENYL COMPOUND	370
Modeling Emission with State-Specific Solvation.....	371
ADVANCED EXAMPLE 8.8: STUDYING FLUORESCENCE IN COUMARIN 153.....	373
ADVANCED EXERCISE 8.9: ACETALDEHYDE ABSORPTION & EMISSION.....	377
ADVANCED EXERCISE 8.10: COUMARIN 153 EMISSION IN DMSO	379
Studying Ground States & Excited States with CASSCF.....	380
ADVANCED EXERCISE 8.11: ACTIVE SPACE FOR BENZENE	383
ADVANCED EXAMPLE 8.9: BENZENE CASSCF SINGLE POINT ENERGY CALCULATION	384
Locating Conical Intersections.....	386
ADVANCED EXERCISE 8.12: CASSCF STUDY OF BENZENE→BENZVALENE	386
Restricted Active Space SCF (RASSCF)	390
ADVANCED EXERCISE 8.13: RASSCF STUDY OF CYCLOPENTADIENE EXCITED STATES	390
<i>9~Advanced Modeling Techniques</i>	399
<i>Preparing ONIOM Input for Biological Systems</i>	401
Locating and Selecting PDB Files.....	402
Understanding PDB Files.....	404
PDB File Pitfalls.....	406
TUTORIAL: PREPARING A GAUSSIAN INPUT FILE FOR GFP.....	408
<i>Relativistic Effects</i>	437
EXAMPLE 9.1: THE GEOMETRY OF METAL HEXAFLUORIDE COMPOUNDS.....	438
EXAMPLE 9.2: ^{17}O NMR CHEMICAL SHIFTS IN TRANSITION METAL-OXO COMPLEXES	439
<i>Weakly Bound Complexes: Dispersion & Counterpoise Corrections</i>	440
EXAMPLE 9.3: MODELING METHANE DIMER	440
EXAMPLE 9.4: MODELING PHENOL DIMER	442
<i>Electronic Spin Organization in Molecular Systems</i>	444
Two Examples of Open Shell Species.....	445
EXAMPLE 9.5: NITROGEN MOLECULE AND NITROGEN DIANION.....	445
EXAMPLE 9.6: A REACTION INVOLVING RADICAL SPECIES	445
Antiferromagnetic Coupling.....	447
EXAMPLE 9.7: MODELING ANTIFERROMAGNETISM IN FERREDOXINS	447
Spin States on the Potential Energy Surface.....	449

EXAMPLE 9.8: SCANNING THE POTENTIAL ENERGY SURFACE OF 2,6-PYRIDYNE	449
Exercises	452
EXERCISE 9.1: M-F BOND LENGTHS IN METAL HEXAFLUORIDE COMPOUNDS	452
EXERCISE 9.2: ^{17}O NMR CHEMICAL SHIFTS IN TRANSITION METAL-OXO COMPLEXES	453
EXERCISE 9.3: COUNTERPOISE CORRECTIONS: METHANE DIMER	454
EXERCISE 9.4: STUDYING PHENOL DIMER WITH 6-311+G(2d,p)	455
EXERCISE 9.5: OXYGEN MOLECULE AND OXYGEN DICATION	456
EXERCISE 9.6: METHYL RADICAL ADDITION TO CYANOETHENE.....	457
EXERCISE 9.7: CARBON NANOTUBES.....	457
EXERCISE 9.8: MODELING THE BIRADICAL 2,6-PYRIDYNE	460
 10~The Theoretical Background	463
Mathematics & Quantum Mechanics	465
Schrödinger's Equation and the Molecular Hamiltonian.....	467
Restriction on the Wavefunction	469
Hartree-Fock Theory	470
Molecular Orbitals and Basis Sets	470
Electron Spin Operators	471
Constructing the Hartree-Fock Wavefunction.....	472
The Variational Principle and the Self-Consistent Field (SCF) Approach.....	473
The Roothaan-Hall Equations	474
EXERCISE 10.1: CALCULATION OF THE HARTREE-FOCK ENERGY	476
Open Shell Systems & Unrestricted Wavefunctions	478
Electron Correlation Methods	481
Configuration Interaction	482
Coupled Cluster Theory	483
EXERCISE 10.2: SIZE CONSISTENCY: HELIUM ATOM CLUSTER.....	483
The Triples Correction to CCSD	484
Møller-Plesset Perturbation Theory.....	485
EXERCISE 10.3: CORRELATION ENERGIES OF A WATER MOLECULE.....	486
Density Functional Theory	486
Hybrid Functionals	488
EXERCISE 10.4: PROTON AFFINITY OF METHYL ANION	489
EXERCISE 10.5: HCN GEOMETRY AND FREQUENCIES.....	491
Long-Range Corrections	492
Double Hybrid Functionals	492
Dispersion	492
EXERCISE 10.6: ARGON DIMER BINDING ENERGY	493
Integration Grids and DFT Calculations	494
EXERCISE 10.7: COMPARING INTEGRATION GRIDS.....	495
Petersson's Complete Basis Set Extrapolation	496
Excited State Methods	497
Complete Active Space SCF.....	499
 References	503
 Molecule Index	523
Index	527