

CONTENTS

	Page
Abstract.....	ii
Foreword.....	iii
I. INTRODUCTION.....	1
1.0. Purpose and objectives.....	1
2.0. Scope and limitations.....	1
3.0. Assumptions.....	2
4.0. Thermodynamic relations of a unimolecular first-order reaction.....	2
4.1. Thermodynamics of the transition state.....	2
4.2. Transition state theory and the rate constant.....	2
4.3. Transition state theory and the relations between the experimental activation energy and the enthalpy of activation.....	3
4.4. Transition state theory and the relations between the Arrhenius <i>A</i> -factor and the entropy of activation.....	3
4.5. Thermodynamics and the Arrhenius parameters of bond fission reactions.....	4
5.0. Thermochemical data sources.....	4
6.0. General index.....	4
7.0. Reaction sheet information.....	4
7.1. Reaction thermodynamics.....	5
7.2. Rate constants.....	5
7.3. Experimental information.....	5
7.4. References.....	5
7.5. Preferred values or evaluation.....	5
7.6. Comments.....	5
8.0. Glossary.....	6
8.1. Standard thermodynamic and kinetic symbols.....	6
8.2. Notations used in illustrations of transition state calculations.....	7
8.3. Symbols designating analytical methods and experimental rate measurement methods.....	7
9.0. Experimental errors.....	8
II. COMPLEX FISSIONS—MOLECULAR ELIMINATION REACTIONS.....	10
1.0. Four-center reactions.....	10
1.1. Transition state estimates of the <i>A</i> -factor of four-center elimination reactions.....	10
2.0. Three-center elimination reactions.....	12
3.0. Five-center elimination reactions.....	12
3.1. Evaluation.....	12
4.0. Six-center elimination reactions.....	12
4.1. Evaluation—transition state estimates of the <i>A</i> -factors of six-center elimination reactions.....	12
4.2. Ethyl acetate.....	14
III. CYCLIC COMPOUND REACTIONS.....	14
1.0. Characteristics.....	14
2.0. The biradical mechanism.....	14
3.0. General remarks concerning transition state calculations.....	15
4.0. Transition state estimates for cyclopropanes.....	15
4.1. <i>Cis</i> -1,2- <i>d</i> ₂ -cyclopropane.....	15
4.2. Vinylcyclopropane.....	16
4.3. <i>Trans</i> -1-methyl-2-vinylcyclopropane.....	17
5.0. Transition state estimates for cyclobutanes.....	18
5.1. Cyclobutane.....	18
5.2. <i>d</i> ₂ -methylene cyclobutane.....	18
6.0. Polycyclic compounds.....	19
6.1. Bicyclo[2.2.0]hexane→1,5-hexadiene.....	19
6.2. 1,3-Dimethylbicyclo[1.1.0]butane.....	20
IV. ISOMERIZATION REACTIONS (OTHER THAN CYCLIC COMPOUND REACTIONS).....	20
1.0. Cope rearrangements.....	20
2.0. "Ene" isomerizations.....	21
2.1. Transition state estimate of the <i>A</i> -factor for an "ene" isomerization.....	21

	Page
3.0. <i>Cis-trans</i> isomerizations.....	21
3.1. <i>Cis-but-2-ene</i>	21
3.2. Isostilbene.....	22
V. SIMPLE BOND FISSION REACTIONS	23
1.0. Characteristics.....	23
2.0. Reliability of the experimental data.....	24
3.0. Kinetic and thermodynamic complications in radical-radical recombination reactions...	25
4.0. Method of analysis.....	26
4.1. Illustrations of analysis methods.....	27
5.0. High and low <i>A</i> -factors in bond fission reactions.....	28
6.0. Rotational barriers in radicals and single shock tube kinetic results.....	29
6.1. Rotational barrier entropy corrections.....	30
7.0. Problems in the kinetics of azo compound decompositions.....	31
8.0. Problems in the amine and hydrazine decompositions.....	34
9.0. Summary of the calculated <i>A</i> -factors for radical-radical recombination reactions.....	36
VI. FREE RADICAL REACTIONS	37
1.0. Characteristics and reliability of the experimental data.....	37
2.0. Transition state estimates of the <i>A</i> -factors in radical decompositions.....	39
APPENDIX A. THERMODYNAMIC GROUP ADDITIVITIES	40
Table A-1. Hydrocarbons.....	40
Table A-2. Oxygen-containing compounds.....	41
Table A-3. Nitrogen-containing compounds.....	44
Table A-4. Halogen-containing compounds.....	46
Table A-5. Free radicals.....	48
APPENDIX B. FREQUENCIES USED IN TRANSITION STATE CALCULATIONS ...	51
Table B-1. Bond stretching frequencies.....	51
Table B-2. Bond angle bending frequencies.....	51
Table B-3. Bond torsion frequencies.....	51
Table B-4. Approximate entropies and heat capacities of bond vibrations.....	52
APPENDIX C. INTERNAL ROTATIONS	53
Table C-1. Entropies of free internal rotors as a function of temperature.....	53
Table C-2. Some characteristic torsion barriers, <i>V</i> (kcal/mole), to free rotation about single bonds for methyl groups.....	53
Table C-3. Some characteristic torsion barriers, <i>V</i> (kcal/mole), to free rotation about single bonds for groups larger than methyl.....	54
Table C-4. Decrease in entropy of free rotor as functions of barrier height (<i>V</i>), temperature (<i>T</i> °K), and partition function (<i>Q</i>).....	54
Table C-5. Molar heat capacity, <i>C_p</i> ^o (g/mole) as a function of barrier (<i>V</i>) temperature and partition function (<i>Q</i>).....	54
APPENDIX D. THERMODYNAMIC PROPERTIES OF FREE RADICALS	55
Table D-1. Preferred values of free radical heats of formation and their source.....	55
Table D-2. Calculated thermodynamic properties of free radicals: entropies and heat capacities.....	58
REFERENCES, to Sections I-VI and Appendices	61
DATA SHEETS	63
I. Complex fissions—molecular elimination reactions	63
<i>Four-center chlorides:</i>	
Chloroethane (ethyl chloride).....	65
1-Chloropropane (<i>n</i> -propyl chloride).....	66
1-Chlorobutane (<i>n</i> -butyl chloride).....	67
1-Chloropentane (<i>n</i> -pentyl chloride).....	68
1-Chloro-2-methylpropane (isobutyl chloride).....	69
2-Chloropropane (isopropyl chloride).....	70
2-Chloro-2-methylpropane (<i>t</i> -butyl chloride).....	71
2-Chlorobutane (<i>sec</i> -butyl chloride).....	72
2-Chloro-2-methylbutane (<i>t</i> -amyl chloride).....	73
Chlorocyclopentane (cyclopentyl chloride).....	74
Chlorocyclohexane (cyclohexyl chloride).....	75
1-Chloro-1-phenylethane (α -phenylethyl chloride).....	76
(-) Menthyl chloride.....	77
Neomenthyl chloride.....	78

	Page
Endo-2-chlorobornane (bornyl chloride).....	79
Exo-2-chlorobornane (isobornyl chloride).....	80
1,1-Dichloroethane (ethylidene dichloride).....	81
2,2-Dichloropropane.....	82
1,1-Dichloropropane.....	83
1,2-Dichloropropane.....	84
1,1,1-Trichloroethane.....	85
1-Chloro-1-methoxyethane (α -chloroethyl methyl ether).....	86
1-Chloro-1-ethoxyethane (α -chloroethyl ethyl ether).....	87
Trichloromethyl chloromethanoate (trichloromethyl chloroformate).....	88
<i>Four-center bromides:</i>	
Bromoethane (ethyl bromide).....	89
1-Bromopropane (<i>n</i> -propyl bromide).....	90
1-Bromobutane (<i>n</i> -butyl bromide).....	91
1-Bromopentane (<i>n</i> -pentyl bromide).....	92
1-Bromohexane (<i>n</i> -hexyl bromide).....	93
1-Bromo-2-methylpropane (isobutyl bromide).....	94
2-Bromopropane (isopropyl bromide).....	95
2-Bromobutane (<i>sec</i> -butyl bromide).....	96
4-Bromo-1-pentene.....	97
Bromocyclopentane (cyclopentyl bromide).....	98
Bromocyclohexane (cyclohexyl bromide).....	99
1-Bromo-1-phenylethane (α -phenylethyl bromide).....	100
2-Bromo-2-methylpropane (<i>t</i> -butyl bromide).....	101
2-Bromo-2-methylbutane (<i>t</i> -amyl bromide).....	102
2,3-Dimethyl-2-bromobutane.....	103
1,1-Dibromoethane (ethylidene dibromide).....	104
<i>Iodides:</i>	
Iodoethane (ethyl iodide).....	105
2-Iodopropane (isopropyl iodide).....	106
2-Iodobutane (<i>sec</i> -butyl iodide).....	107
2-Iodo-2-methylpropane (<i>t</i> -butyl iodide).....	108
<i>Others:</i>	
2-Methyl-2-propanol (<i>t</i> -butyl alcohol).....	109
2-Methyl-2-butanol (<i>t</i> -amyl alcohol).....	110
Methanoic acid (formic acid).....	111
Ethanoic acid (acetic acid).....	112
1,2-Ethanediamide (oxamide).....	113
Propanonitrile (ethyl cyanide).....	114
2-Methyl-2-aminopropane (<i>t</i> -butyl amine).....	115
Methanoloxime (formaldoxime).....	117
Ethanamide (acetamide).....	118
1,2-Ethanediamide (oxamide).....	119
Ethanethiol (ethyl mercaptan).....	120
2-Methyl-2-propanethiol (<i>t</i> -butyl mercaptan).....	121
2,2-Difluoroethyltrifluorosilane.....	122
2-Chloroethyltrichlorosilane.....	123
2-Chloroethylethylchlorosilane.....	124
2-Chloroethyldiethylchlorosilane.....	125
Ethene.....	126
<i>Three-center reactions:</i>	
Formyl fluoride.....	127
Trichloromethane (chloroform).....	128
Chlorodifluoromethane.....	129
<i>Five-center reactions:</i>	
Nitroethane.....	130
1-Nitropropane.....	131
2-Nitropropane.....	132
Isopropyl ether.....	133
1,1-Dimethyl-1-ethanesulfonyl chloride (trimethylmethanesulfonyl chloride).....	134

Six-center eliminations:

Alcohols:

	Page
3-Butene-1-ol (allylcarbinol).....	135
4-Pentene-2-ol (allylmethylcarbinol).....	136
2-Methyl-4-pentene-2-ol (allyldimethylcarbinol).....	137
3-Phenyl-3-butene-1-ol.....	138
4-Phenyl-3-butene-1-ol.....	139
1-Phenyl-4-ethyl-4-hydroxyhex-1-ene.....	140

Acids:

3-Butenoic acid.....	141
2,2-Dimethyl-3-butenic acid.....	142
2,2-Dimethyl- <i>trans</i> -3-pentenoic acid.....	143
2,2,3-Trimethyl-3-butenic acid.....	144
2,2-Dimethyl-3-ethyl-3-pentenoic acid.....	145
2-Methyl-2-(1-cyclopentyl) propionic acid.....	146
2-Methyl-2-(1-cyclohexenyl) propionic acid.....	147
2-Methyl-2-(1-cycloheptenyl) propionic acid.....	148

Esters:

Chloroformate esters:

Ethyl chloromethanoate (ethyl chloroformate).....	149
Isopropyl chloromethanoate (isopropyl chloroformate).....	151
Isobutyl chloromethanoate (isobutyl chloroformate).....	152
<i>sec</i> -Butyl chloromethanoate (<i>sec</i> -butyl chloroformate).....	153

Formic acid esters:

Ethyl methanoate (ethyl formate).....	154
Propyl methanoate (<i>n</i> -propyl formate).....	155
Isopropyl methanoate (isopropyl formate).....	156
<i>t</i> -Butyl methanoate (<i>t</i> -butyl formate).....	157

Primary acetic acid esters:

Ethyl ethanoate (ethyl acetate).....	158
1-Propyl ethanoate (<i>n</i> -propyl acetate).....	159
1-Butyl ethanoate (<i>n</i> -butyl acetate).....	160
Isobutyl ethanoate (2-methylpropyl acetate; isobutyl acetate).....	161
1-Pentyl ethanoate (<i>n</i> -pentyl acetate).....	162
2-Methylbutyl ethanoate (2-methylbutyl acetate).....	163
3-Methylbutyl ethanoate (γ -methylbutyl acetate).....	164
2-Ethylbutyl ethanoate (β -ethylbutyl acetate).....	165
2-Methoxyethyl ethanoate (β -methoxyethyl acetate).....	166
2-Ethoxyethyl ethanoate (β -ethoxyethyl acetate).....	167
2-Arylethyl ethanoates (<i>meta</i> or <i>para</i> substituted 2-phenylethyl acetates).....	168

Secondary acetic acid esters:

Isopropyl ethanoate (isopropyl acetate).....	169
<i>sec</i> -Butyl ethanoate (<i>sec</i> -butyl acetate).....	170
1-Methyl-3-butenyl ethanoate.....	171
1-Methylbutyl ethanoate (2-pentyl acetate).....	172
1-Ethylpropyl ethanoate (3-pentyl acetate).....	173
Cyclohexyl ethanoate (cyclohexyl acetate).....	174
1,2-Dimethylbutyl ethanoate (α,β -dimethyl- <i>n</i> -butyl acetate).....	175
1-Isopropyl-2-methylpropyl ethanoate (α -isopropyl β -methyl- <i>n</i> -propyl acetate).....	176
1-Methylhexyl ethanoate (2-heptyl acetate).....	177
1-Ethylpentyl ethanoate (3-heptyl acetate).....	178
1-Propylbutyl ethanoate (4-heptyl acetate).....	179
Endo-2-acetoxybornane (bornyl acetate).....	180
Exo-2-acetoxybornane (isobornyl acetate).....	181
1-Methyl-2-methoxyethyl ethanoate (1-methoxy-2-propyl acetate).....	182
1-Methyl-3-oxobutyl ethanoate.....	183
1-Phenylethyl ethanoate (α -phenylethyl acetate).....	184
1-Arylethyl ethanoates (1-phenylethyl derivatives).....	185
1,2-Diarylethyl ethanoates (<i>meta</i> or <i>para</i> substituted 1,2-diphenylethyl acetates).....	186
1-Methyl-2-chloroethyl ethanoate (1-chloroisopropyl acetate).....	187

	Page
1-Methyl-2-dimethylaminoethyl ethanoate; 2-dimethylamino-1-methyl ethyl ethanoate (β -dimethylamino-2-propylacetate).....	188
Tertiary acetic acid esters:	
<i>t</i> -Butyl ethanoate (<i>t</i> -butyl acetate).....	189
<i>t</i> -Pentyl ethanoate (<i>t</i> -amyl acetate).....	190
1,1,2-Trimethylpropyl ethanoate (2,3-dimethyl-2-butyl acetate).....	191
1,1-Dimethylbutyl ethanoate (1,1-dimethylbutyl acetate).....	192
1-Ethyl-1-methylpropyl ethanoate (1-ethyl-1-methylpropyl acetate).....	193
1-Methylcyclohexyl ethanoate (1-methylcyclohexyl acetate).....	194
<i>t</i> -Butyl chloroethanoate (<i>t</i> -butyl chloroacetate).....	195
<i>t</i> -Butyl dichloroethanoate (<i>t</i> -butyl dichloroacetate).....	196
Propionic acid esters:	
Ethyl propanoate (ethyl propionate).....	197
<i>t</i> -Butyl propanoate (<i>t</i> -butyl propionate).....	198
Ethyl-2,2-dimethylpropanoate (ethyl trimethylacetate).....	199
(-)-Menthyl benzoate.....	200
Diesters:	
Diacetic acid esters:	
Methylene diethanoate (methylene diacetate).....	201
Ethylidene diethanoate (ethylidene diacetate).....	202
Butylidene diethanoate (butylidene diacetate).....	203
Heptylidene diethanoate (heptylidene diacetate).....	204
Crotonylidene diethanoate (crotonylidene diacetate).....	205
Furfurylidene diethanoate (furfurylidene diacetate).....	206
2,2,2-Trichloro-1-ethylidene diethanoate.....	207
Dipropionic acid esters:	
Methylene dipropanoate.....	208
Ethylidene dipropanoate.....	209
Dibutyric acid esters:	
Methylene dibutanoate.....	210
Ethylidene dibutanoate.....	211
2,2,2-Trichloro-1-ethylidene dibutanoate.....	212
Carbonate esters:	
Methyl ethyl carbonate.....	213
Diethyl carbonate.....	214
X-1-phenylethyl methyl carbonates, X = ortho, meta, or para substitution.....	215
Miscellaneous ketones and anhydrides:	
Ethanoic anhydride (acetic anhydride).....	216
4-Hydroxy-4-methyl-2-pentanone.....	217
Ethers:	
1-Ethoxyethene (ethyl vinyl ether).....	218
Isopropoxyethene (vinyl isopropyl ether).....	219
<i>n</i> -Butyl vinyl ether.....	220
2. Cyclic compound reactions.....	221
Three-membered rings	
Alkylcyclopropanes:	
Cyclopropane.....	223
<i>trans</i> -1,2-Dideutero cyclopropane.....	224
Methylcyclopropane.....	225
<i>cis</i> - or <i>trans</i> -1,2-Dideutero-3-methylcyclopropane.....	226
<i>cis,trans</i> -1,2-Dideutero-3-methylcyclopropane.....	227
<i>cis</i> -1,2-Dimethylcyclopropane.....	228
<i>trans</i> -1,2-Dimethylcyclopropane.....	229
1,1-Dimethylcyclopropane.....	230
Ethylcyclopropane.....	231
<i>cis</i> -1-Ethyl-2-methylcyclopropane.....	232
<i>trans</i> -1-Ethyl-2-methylcyclopropane.....	232
<i>cis,trans</i> -1,2,3-Trimethylcyclopropane.....	233
1,1-Diethylcyclopropane.....	234
1,1,2,2-Tetramethylcyclopropane.....	235
Bicyclopropyl.....	236

<i>Vinylcyclopropanes:</i>	Page
Vinylcyclopropane.....	237
<i>cis</i> -1-Methyl-2-vinylcyclopropane.....	238
<i>trans</i> -1-Methyl-2-vinylcyclopropane.....	239
1-Methyl-1-vinylcyclopropane.....	240
Isopropenylcyclopropane.....	241
<i>trans</i> -1-Cyclopropyl-1-butene.....	242
1-Cyclopropyl-2-methyl-1-propene.....	243
1-Isopropenyl-1-methylcyclopropane.....	244
1,1-Dicyclopropylethene.....	245
1-Cyclopropyl-1-cyclopentene.....	246
<i>Halogen substituents:</i>	
Fluorocyclopropane.....	247
1,1-Difluorocyclopropane.....	248
1,1,2-Trifluorocyclopropane.....	249
1,1,2,2-Tetrafluorocyclopropane.....	250
Hexafluorocyclopropane (perfluorocyclopropane).....	251
Trifluoromethylcyclopropane.....	252
2,2,2-Trifluoro-1-ethylcyclopropane.....	253
Octafluorovinylcyclopropane (perfluorovinylcyclopropane).....	254
Decafluoroallylcyclopropane (perfluoroallylcyclopropane).....	255
Chlorocyclopropane.....	256
1,1-Dichlorocyclopropane.....	257
2,2-Dichloro-1-methyl-1-vinylcyclopropane (1-methyl-1-vinyl-2,2-dichlorocyclopropane).....	258
Bromocyclopropane.....	259
<i>Diazirines:</i>	
Dimethyldiazirine.....	260
3,3-Diethyldiazirine.....	261
3,3-Tetramethylenediazirine.....	262
3,3-Pentamethylenediazirine.....	263
Difluorodiazirine.....	264
<i>External double bonds:</i>	
Ethylidenecyclopropane.....	265
2-Methyl-1-methylenecyclopropane.....	265
<i>Others:</i>	
Oxirane (ethylene oxide).....	266
β , β -Dimethylcyclopropyl methyl ketone (2,2-dimethylcyclopropyl-1-ethanone).....	267
Perfluorooxirane (tetrafluorooxirane; tetrafluoroethylene oxide).....	268
<i>Cyclobutanes:</i>	
Cyclobutane.....	269
Methylcyclobutane.....	270
<i>trans</i> -1,2-Dimethylcyclobutane.....	271
<i>cis</i> -1,2-Dimethylcyclobutane.....	272
Ethylcyclobutane.....	273
<i>n</i> -Propylcyclobutane.....	274
Isopropylcyclobutane.....	275
Isopropenylcyclobutane.....	276
<i>Oxy substituents:</i>	
Oxetane (trimethylene oxide).....	277
3,3-Dimethyloxetane (3,3-dimethylketane).....	278
Cyclobutane carboxaldehyde.....	279
Ethanoylcyclobutane (methyl cyclobutyl ketone).....	280
Propionylcyclobutane (ethyl cyclobutyl ketone).....	281
Methyl cyclobutanecarboxylate.....	282
<i>External Double bond:</i>	
Cyclobutanone.....	283
Methylenecyclobutane.....	284
<i>Cyclobutenes:</i>	
Cyclobutene.....	285
1-Methyl-1-cyclobutene.....	286
3-Methyl-1-cyclobutene.....	287
1-Ethyl-1-cyclobutene.....	288

	Page
1,2-Dimethyl-1-cyclobutene.....	289
1,3-Dimethyl-1-cyclobutene.....	290
2,3-Dimethyl-1-cyclobutene.....	291
<i>trans</i> -1,2,3,4-tetramethyl-1-cyclobutene.....	292
<i>cis</i> -1,2,3,4-tetramethyl-1-cyclobutene.....	293
Fluorine substituents:	
Perfluorocyclobutene.....	294
Perfluorocyclobutane.....	295
<i>cis</i> -1,2-Dichlorohexafluorocyclobutane.....	296
(<i>cis</i> or <i>trans</i>)-1,2-Dichlorohexafluorocyclobutane.....	297
<i>cis</i> -Hexafluoro-1, 2- <i>bis</i> -trifluoromethylcyclobutane.....	298
<i>trans</i> -Hexafluoro-1, 2- <i>bis</i> -trifluoromethylcyclobutane.....	299
Decafluoro-1,2-dimethylcyclobutene.....	300
Five-Membered Rings	
Cyclopentene.....	301
1,5,5-Trimethyl-1,3-cyclopentadiene.....	302
2,5,5-Trimethyl-1,3-cyclopentadiene.....	303
2,5-Dihydrofuran.....	304
Pyrazoline.....	305
Methyl-substituted pyrazolines.....	306
Six-Membered Rings	
Cyclohexene.....	307
1-Methyl-1,4-cyclohexadiene.....	309
4-Methylcyclohexene.....	310
4-Vinylcyclohexene.....	311
1,4-Cyclohexadiene.....	312
1,4-Dioxane.....	313
1,3,5-Trioxane.....	314
2,4,6-Trimethyl-1,3,5-trioxane (paraldehyde).....	315
2,4,6-Tri- <i>n</i> -propyl-1,3,5-trioxane (para- <i>n</i> -butyraldehyde).....	316
2,4,6-Tri- <i>isopropyl</i> -1,3,5-trioxane (para- <i>isobutyraldehyde</i>).....	317
Other rings:	
Cycloheptatriene.....	318
1,5-Cyclooctadiene.....	319
Polycyclics:	
Spiropentane.....	320
Bicyclo[1.1.0]butane.....	321
1,3-Dimethylbicyclo[1.1.0]butane.....	322
Bicyclo[1.1.1]pentane.....	323
1,3-Dimethylbicyclo[1.1.1]pentane.....	324
Bicyclo[2.1.0]pent-2-ene.....	325
Bicyclo[2.1.0]pentane.....	326
<i>cis</i> -2-Methyl[2.1.0]bicyclopentane.....	327
<i>trans</i> -2-Methyl[2.1.0]bicyclopentane.....	327
Bicyclo[2.2.0]hexane.....	328
Bicyclo[3.1.0]hex-2-ene.....	329
Bicyclo[3.1.0]hexane.....	330
Bicyclo[2.1.1]hexane.....	331
Bicyclo[3.2.0]heptane.....	332
Bicyclo[3.2.0]hept-6-ene.....	333
Bicyclo[4.2.0]oct-7-ene.....	334
Bicyclo[2.2.1]hepta-2,5-diene.....	335
Bicyclo[2.2.1]hept-2-ene.....	336
2,3-Diazobicyclo[2.2.1]hept-2-ene.....	337
2,3-Diazobicyclo[2.2.2]oct-2-ene.....	338
Bicyclo[5.1.0]oct-2-ene.....	339
Cycloocta-1,4-diene.....	339
Tricyclo[3.3.0. ^{0,2,6}]octane.....	340
β -Pinene.....	341
Endo-dicyclopentadiene.....	342
Exo-dicyclopentadiene.....	343
Quadricyclo[2.2.1.0 ^{2,6} .0 ^{1,5}]heptane.....	344

	Page
Endo-bicyclo[2.2.1]hept-5-ene-2-carboxaldehyde (endo-5-norbornene-2-carboxaldehyde; endo-methylene-2.5-tetrahydrobenzaldehyde).....	345
3. Isomerization Reactions (Other Than Cyclic Compound Reactions)	
<i>cis</i> -1,2-Dideuteroethene.....	349
<i>trans</i> -1,2-Dichloroethene.....	350
<i>cis</i> -2-Butene.....	351
Perfluorobutadiene (hexafluorobutadiene).....	352
<i>trans</i> -Perfluoro-2-butene.....	353
<i>cis</i> -Perfluoro-2-butene.....	353
<i>cis</i> -1,2-Diphenylethene (isostilbene).....	354
Dimethyl- <i>cis</i> -1,2-ethendioate (dimethyl maleate).....	355
Methyl- <i>cis</i> -2-butenoate (methyl- <i>cis</i> crotonate).....	356
Methyl- <i>cis</i> -cinnamate.....	357
(<i>cis</i> -2-Butenenitrile) <i>cis</i> -crotonitrile.....	358
<i>cis</i> - β -Cyanostyrene.....	359
1,1,6,6- <i>t,t</i> -1,5-Hexadiene.....	360
1,5-Heptadiene.....	361
3-Methyl-1,5-hexadiene.....	362
3-Vinyloxy-1-propene (vinyl allyl ether).....	363
3-Isopropenoxy-1-propene (isopropenyl allyl ether).....	364
2-Methyl-3-vinyloxy-1-propene (2-methylallyl vinyl ether).....	365
1-Buten-3-yl vinyl ether.....	366
1,2,6-Heptatriene.....	367
<i>cis</i> -1,3,5-Hexatriene.....	368
<i>cis</i> -1,3,5-Hexadiene.....	369
2-Methyl- <i>cis</i> -1,3-pentadiene.....	370
4-Methyl-1,3-pentadiene.....	371
3,7-Dimethyl-1,6-octadiene.....	372
Methyl isocyanide.....	373
<i>p</i> -Tolyl isocyanide.....	374
(<i>l</i>)-2,2'-Diamino-6,6-dimethyldiphenyl racemization (<i>l, d</i>) isomer.....	375
<i>trans</i> -Difluorodiazine.....	376
Nitrosomethane.....	377
4. Simple Bond Fission Reactions	
Alkanes:	
Methane.....	381
Ethane.....	383
<i>n</i> -Butane.....	385
2,2-Dimethylpropane (neopentane).....	386
2,3-Dimethylbutane.....	388
2,2,3-Trimethylbutane.....	389
2,2,3,3-Tetramethylbutane (hexamethyl ethane).....	390
Alkenes and aromatics:	
Propene (propylene).....	391
1-Butene.....	392
2-Methyl-1-butene (2-methylpropene; isobutene).....	393
Toluene.....	394
Ethylbenzene.....	397
<i>n</i> -Propylbenzene.....	398
<i>n</i> -Butylbenzene.....	399
Isopropylbenzene (cymene).....	401
<i>t</i> -Butylbenzene.....	402
<i>p</i> -Isopropyltoluene (<i>p</i> -cymene).....	403
Dibenzyl (1,2-diphenylethane).....	404
<i>o</i> -Xylene.....	405
<i>m</i> -Xylene.....	406
<i>p</i> -Xylene.....	407
1,2-Methylnaphthalene (α and β -methylnaphthalene).....	408
Para, ortho, and meta fluorotoluenes.....	409
α , β , and γ -Picolines.....	410
Oxygen compounds:	
Acids:	
Phenylethanoic acid (phenylacetic acid).....	411

	Page
Diphenylethanoic acid (diphenylacetic acid).....	412
Peracetic acid.....	413
Ethers:	
Dimethyl ether.....	414
Diethyl ether.....	415
Ketones:	
Propanone (acetone).....	416
Acetophenone.....	417
1-Phenyl-2-propanone (benzyl methyl ketone).....	418
Benzophenone.....	419
1,3-Diphenyl-1,2-propanone (dibenzil ketone).....	420
1,2-Diphenyl-1,2-ethanedione (benzil).....	421
1,1,1-Trifluoro-2-propanone (trifluoroacetone).....	422
α,α,α -Trifluoroacetophenone.....	423
2,3-Butanedione (biacetyl).....	424
Esters:	
Benzylethanoate (benzyl acetate).....	425
Benzylbenzoate.....	426
Peroxides:	
Dimethyl peroxide.....	427
Diethyl peroxide.....	428
di- <i>n</i> -Propylperoxide.....	429
di- <i>t</i> -Butyl peroxide.....	430
Diethanoyl peroxide (diacetyl peroxide).....	432
Dipropanoyl peroxide (dipropionyl peroxide).....	433
Dibutanoyl peroxide (dibutyl peroxide).....	434
Hydroperoxides:	
Methyl hydroperoxide.....	435
Ethyl hydroperoxide.....	436
Isopropyl hydroperoxide.....	437
<i>t</i> -Butyl hydroperoxide.....	438
Amines:	
Hydrazine.....	439
Methylhydrazine.....	441
1,1-Dimethylhydrazine.....	442
Benzylamine (phenylaminomethane).....	443
<i>N</i> -Methylbenzylamine.....	444
Phenylhydrazine.....	445
<i>N</i> -Methylaniline.....	446
<i>N,N</i> -Dimethylaniline.....	447
Primary azo compounds:	
Azomethane.....	448
Hexafluoroazomethane (perfluoroazomethane).....	450
Azoethane.....	451
Azobutane.....	452
1,1'-Azoisobutane.....	453
Secondary azo compounds:	
Azoisopropane.....	454
2,2'-Azobutane.....	455
Methyl isopropyl diimide.....	456
Tertiary azo compound:	
2,2'-Azoisobutane.....	457
Complex azo compounds:	
Azotoluene.....	458
Tetramethyltetrazine.....	459
Tetraethyltetrazine.....	460
Cyanides:	
Propanonitrile (ethyl cyanide).....	461
2,2-Dimethylpropanonitrile (<i>t</i> -butyl cyanide).....	462
2-Methyl-2-phenylpropanonitrile (cumyl cyanide).....	463

	Page
Nitrites:	
Nitrit-methane (methyl nitrite).....	464
Nitritoethane (ethyl nitrite).....	466
1-Nitritopropane (<i>n</i> -propyl nitrite).....	467
2-Nitritopropane (isopropyl nitrite).....	468
1-Nitritobutane (<i>n</i> -butyl nitrite).....	469
Nitrates:	
Nitratomethane (methyl nitrate).....	470
Nitratoethane (ethyl nitrate).....	471
Collection of dinitrates, etc.....	472
Nitro compounds:	
Nitromethane.....	473
Nitroethane.....	475
Nitrotrichloromethane.....	476
Tetranitromethane.....	477
Other nitrogen compounds:	
Ethanoldoxime (acetaldoxime).....	478
Dimeric nitrosomethane.....	479
Dimeric-2-methyl-1-nitrosopropane (dimeric nitroisobutane).....	480
Diazomethane.....	481
Azidomethane (methyl azide).....	482
Azidoethane (ethyl azide).....	483
Sulfur compounds:	
Methanethiol (methyl mercaptan).....	484
Ethanethiol (ethyl mercaptan).....	485
Phenylmethanethiol (benzyl mercaptan).....	486
Thioanisole (phenylmethyl sulfide).....	487
Methyl benzyl sulfide.....	488
Methanysulfonylphenylmethane (benzyl methyl sulfone).....	489
Methanesulfonylmethane (dimethyl sulfone).....	490
3-Methanesulfonyl-1-propene (allyl methyl sulfone).....	491
Halides:	
Perfluoroethane.....	492
Perfluoropropene.....	493
Perfluoro-2-methyl-1-propene (perfluoroisobutene).....	494
Bromomethane (methyl bromide).....	495
Dibromomethane (methylene dibromide).....	496
Tetrabromoethane (carbon tetrabromide).....	497
Chlorobromomethane.....	498
Dichlorobromomethane.....	499
Trichlorobromomethane.....	500
Trifluorobromomethane.....	501
Tribromomethane.....	502
Bromobenzene.....	503
Substituted bromobenzenes.....	504
2- and 3-Bromopyridene.....	505
1- and 2-Bromonaphthalene (α - and β -bromonaphthalene).....	506
9-Bromophenanthrene and 9-bromoanthracene.....	507
2-Bromothiophene.....	508
3-Bromo-1-propene (allylbromide).....	509
Bromophenylmethane (benzyl bromide).....	511
Substituted bromo phenylmethanes (substituted benzylbromides).....	512
<i>p</i> -Bromomethyltoluene (<i>p</i> -xylyl bromide).....	513
ω , ω' -Dibromo- <i>para</i> -xylene.....	513
Benzoyl bromide.....	514
Chlorophenylmethane (benzyl chloride).....	515
Benzoyl chloride.....	516
Iodoethane (ethyl iodide).....	517
Metallic compounds:	
Dimethylmercury.....	518
Diethylmercury.....	520
Di- <i>n</i> -propylmercury.....	521

	Page
Di- <i>n</i> -butylmercury.....	522
Diisopropylmercury.....	523
Divinylmercury.....	524
Diphenylmercury.....	525
Phenylmercuric chloride.....	526
Phenylmercuric bromide.....	527
Phenylmercuric iodide.....	528
Dimethylcadmium.....	529
Dimethylzinc.....	530
Trimethylarsine.....	531
<i>tris</i> -(Trifluoromethyl)arsine.....	532
Trimethylbismuth.....	533
Trimethylgallium.....	534
Trimethylindium.....	535
Trimethylantimony.....	536
Trimethylthallium.....	537
Germane.....	538
Tetraethylgermane.....	539
Tetracarbonyl nickel (<i>o</i>) (nickel carbonyl).....	540
Tetraethyl lead.....	541
Silane.....	542
Tetramethylsilane (silicon tetramethyl).....	543
Tetraethylsilane (silicon tetraethyl).....	544
Tetra- <i>n</i> -propylsilane (silicon tetra- <i>n</i> -propyl).....	545
Hexamethyldisilane.....	546
Tetramethyl tin.....	547
Dichlorodimethylstannane (dimethyl tin dichloride).....	548
Boron:	
Diborane.....	549
Borine carbonyl.....	550
Trifluorophosphine borane.....	551
Inorganic nonmetal oxides:	
Dinitrogen oxide (nitrous oxide).....	553
Dinitrogen tetroxide.....	554
Dinitrogen pentoxide.....	555
Nitryl chloride.....	556
Nitroxylfluoride (fluorine nitrate).....	557
Chlorine nitrate (nitroxylchloride).....	558
Difluorine dioxide.....	559
Chloryl fluoride.....	561
Perchloryl fluoride.....	562
Dichlorine heptoxide.....	563
Perchloric acid.....	564
5. Free radical reactions	
Ethyl radical.....	567
<i>n</i> -Propyl radical.....	569
2-Deuteroisopropyl and isopropyl radical.....	572
Cyclobutyl radical.....	574
1-Buten-4-yl radical.....	575
<i>n</i> -Butyl radical.....	576
<i>sec</i> -Butyl radical (1-methyl-1-propyl radical).....	578
<i>t</i> -Butyl radical.....	580
Isobutyl radical.....	581
Cyclopentyl radical.....	583
Neopentyl radical.....	585
1-Methyl-1-pentyl radical (2-hexyl radical).....	586
Formyl radical.....	587
Hydroxymethyl radical.....	588
Acetyl radical.....	589
Epoxyethyl radical.....	591
Ethoxy radical.....	592

	Page
2-Oxo-1-propyl radical (acetyl radical).....	593
Isopropoxy radical.....	594
sec-Butoxy radical.....	596
<i>t</i> -Butoxy radical.....	597
1-Ethoxy-1-ethyl radical.....	600
4-Oxo-2-heptyl radical.....	602
Methyl peroxyethyl radical.....	603
Perfluoro- <i>t</i> -butoxy radical.....	604
2-Chloro-1-ethyl radical.....	605
1,2-Dichloro-1-ethyl radical.....	606
1,2,2-Trichloro-1-ethyl radical.....	507
1,1,2,2-Tetrachloro-1-ethyl radical.....	608
Pentachloroethyl radical.....	609
4-Chlorodifluoromethyl-2,5-cyclohexadienyl radical.....	610
2-Bromo-1-ethyl radical.....	611
<i>p</i> -(Bromomethyl) benzyl radical.....	613
Dimethylgallium radical.....	614
Methylindium diradical.....	615
Methylzinc radical.....	616
INDEX TO REACTANTS.....	617