

Contents

	<i>Preface</i>	<i>page xv</i>
	<i>Acknowledgments</i>	<i>xvii</i>
	<i>Acknowledgments for permissions to use illustrations</i>	<i>xviii</i>
1	Fuels and the global carbon cycle	1
	Notes	8
2	Catalysis, enzymes, and proteins	10
	2.1 Catalysis	10
	2.2 Proteins	11
	2.3 Enzymes	13
	Notes	17
3	Photosynthesis and the formation of polysaccharides	19
	3.1 Water splitting in photosynthesis	20
	3.2 Carbon dioxide fixation	24
	3.3 Glucose, cellulose, and starch	27
	Notes	32
4	Ethanol	35
	4.1 Fermentation chemistry	35
	4.2 Commercial production of ethanol via fermentation	38
	4.3 Ethanol as a motor vehicle fuel	42
	4.4 Issues affecting possible large-scale production of fuel ethanol	47
	4.5 Cellulosic ethanol	48
	Notes	49
5	Plant oils and biodiesel	53
	5.1 Biosynthesis of plant oils	53
	5.2 Direct use of vegetable oils as diesel fuel	57
	5.3 Transesterification of plant oils	59
	5.4 Biodiesel	62
	Notes	66

6	Composition and reactions of wood	69
6.1	Wood combustion	78
6.2	Wood pyrolysis	79
6.2.1	Charcoal	79
6.2.2	Methanol	81
6.3	Wood gasification	82
6.4	Wood saccharification and fermentation	83
	Notes	84
7	Reactive intermediates	87
7.1	Bond formation and dissociation	87
7.2	Radicals	89
7.2.1	Initiation reactions	89
7.2.2	Propagation reactions	91
7.2.3	Termination reactions	94
7.3	Radical reactions with oxygen	95
7.4	Carbocations	97
7.5	Hydrogen redistribution	100
	Notes	101
8	Formation of fossil fuels	103
8.1	Diagenesis: from organic matter to kerogen	104
8.2	Catagenesis: from kerogen to fossil fuels	109
8.3	Catagenesis of algal and liptinitic kerogens	111
8.4	Catagenesis of humic kerogen	117
8.5	Summary	127
	Notes	128
9	Structure–property relationships among hydrocarbons	132
9.1	Intermolecular interactions	132
9.2	Volatility	134
9.3	Melting and freezing	142
9.4	Density and API gravity	145
9.5	Viscosity	148
9.6	Water solubility	151
9.7	Heat of combustion	152
9.8	The special effects of aromaticity	156
	Notes	158
10	Composition, properties, and processing of natural gas	161
10.1	Gas processing	164
10.1.1	Dehydration	164
10.1.2	Gas sweetening	166

10.1.3	Separation of C ₂ ⁺ hydrocarbons	168
10.2	Natural gas as a premium fuel	170
	Notes	171
11	Composition, classification, and properties of petroleum	174
11.1	Composition	174
11.1.1	Alkanes	174
11.1.2	Cycloalkanes	175
11.1.3	Aromatics	177
11.1.4	Heteroatomic compounds	179
11.1.5	Inorganic components	180
11.2	Classification and properties of petroleum	181
11.2.1	API gravity	181
11.2.2	Carbon preference index	181
11.2.3	Age–depth relationships	182
11.2.4	Composition relationships	183
11.3	Asphalts, oil sands, and other unconventional oils	187
	Notes	189
12	Petroleum distillation	192
12.1	Desalting	193
12.2	Principles of distillation	194
12.3	Refinery distillation operations	198
12.3.1	Atmospheric-pressure distillation	198
12.3.2	Vacuum distillation	199
12.4	Introduction to petroleum distillation products	200
12.4.1	Gasoline	200
12.4.2	Naphtha	201
12.4.3	Kerosene	201
12.4.4	Diesel fuel	202
12.4.5	Fuel oils	202
12.4.6	Lubricating oils	203
12.4.7	Waxes	203
12.4.8	Asphalt	204
	Notes	204
13	Heterogeneous catalysis	206
13.1	Catalytic materials	207
13.1.1	The active species	207
13.1.2	The support	207
13.1.3	The promoter	209
13.1.4	Preparation	209
13.2	Adsorption on catalyst surfaces	210
13.3	Mechanisms of catalytic reactions	216

13.4	Measures of catalyst performance	217
13.5	Surface effects on catalysts	219
	Notes	221
14	Catalytic routes to gasoline	224
14.1	Gasoline combustion	224
14.2	Specifications and properties of gasoline	229
14.3	Refinery routes to enhanced yield and quality	231
14.4	Alkylation and polymerization	232
14.5	Catalytic cracking	234
	14.5.1 Cracking catalysts	235
	14.5.2 Cracking reactions	241
	14.5.3 Practical aspects	243
14.6	Catalytic reforming	245
	14.6.1 Reforming catalysts	245
	14.6.2 Reforming reactions	246
	14.6.3 Practical aspects	249
14.7	Methanol to gasoline	251
	Notes	253
15	Middle distillate fuels	256
15.1	Middle distillate fuel products	256
	15.1.1 Kerosene	256
	15.1.2 Jet fuel	256
	15.1.3 Diesel fuel	260
	15.1.4 Fuel oils	265
15.2	Hydroprocessing	266
	15.2.1 Hydrodesulfurization	267
	15.2.2 Hydrodenitrogenation	272
	15.2.3 Hydrodemetallation	273
	15.2.4 Hydrofining	273
	15.2.5 Hydrocracking	274
	15.2.6 Hydrogenation	276
	15.2.7 Sources of hydrogen	277
	Notes	278
16	Thermal processing in refining	281
16.1	Thermal cracking	281
16.2	Visbreaking	284
16.3	Coking processes	286
	16.3.1 Delayed coking	287
	16.3.2 Fluid coking and Flexicoking	292
	Notes	293

17	Composition, properties, and classification of coals	295
	17.1 Classification of coal by rank	295
	17.2 The caking behavior of bituminous coals	298
	17.3 Elemental composition	299
	17.4 The macromolecular structures of coals	306
	17.5 Coals as heterogeneous solids	312
	17.6 Physical properties	314
	Notes	320
18	The inorganic chemistry of coals	323
	18.1 The origin of inorganic components in coals	324
	18.2 Inorganic composition of coals	324
	18.3 Minerals in coals and their reactions	326
	18.4 Coal cleaning	329
	18.5 Behavior of inorganic components during coal utilization	334
	Notes	340
19	Production of synthesis gas	342
	19.1 Steam reforming of natural gas	342
	19.2 Partial oxidation of heavy oils	344
	19.3 Coal and biomass gasification	345
	19.3.1 Fundamentals of the carbon–steam and related reactions	346
	19.3.2 Coal gasification processes	352
	19.3.3 Fixed-bed gasification	354
	19.3.4 Fluidized-bed gasification	356
	19.3.5 Entrained-flow gasification	357
	19.3.6 Underground coal gasification	359
	19.3.7 Biomass gasification	360
	Notes	361
20	Gas treatment and shifting	363
	20.1 Gas clean-up	363
	20.2 Acid gas removal	365
	20.3 The water gas shift	371
	Note	373
21	Uses of synthesis gas	375
	21.1 Fuel gas	375
	21.2 Methanation	375
	21.3 Methanol synthesis	378
	21.4 Fischer–Tropsch synthesis	381
	21.5 Kölbel reaction	389

21.6	Oxo synthesis	390
21.7	Gas to liquids	391
21.8	The potential of synthesis gas chemistry	392
	Notes	393
22	Direct production of liquid fuels from coal	396
22.1	Pyrolysis	396
22.2	Solvent extraction	398
22.3	Direct coal liquefaction	402
	22.3.1 Principles	402
	22.3.2 Direct liquefaction processing	406
	Notes	413
23	Carbonization and coking of coal	415
23.1	Thermal decomposition of coals	415
23.2	Low- and medium-temperature carbonization	417
23.3	The special case of bituminous coals	418
23.4	Chemistry of coke formation	420
23.5	Industrial production of metallurgical coke	426
	Notes	432
24	Carbon products from fossil and biofuels	435
24.1	Activated carbons	435
24.2	Aluminum-smelting anodes	440
24.3	Carbon blacks	443
24.4	Graphites	445
	24.4.1 Natural graphite	445
	24.4.2 Graphitization processes	446
	24.4.3 Electrodes	447
	24.4.4 High-density isotropic graphites	449
	Notes	450
25	Carbon dioxide	453
25.1	Carbon capture and storage	455
	25.1.1 Algae	455
	25.1.2 Biochar	457
	25.1.3 Chemical uses of CO ₂	459
	25.1.4 Coalbed methane recovery	460
	25.1.5 Enhanced oil recovery	461
	25.1.6 Mineral carbonation	462
	25.1.7 Photocatalysis	464

Contents

xiii

25.1.8	Underground injection	466
25.1.9	Urea synthesis	467
25.2	Conclusions	468
	Notes	469
	<i>Index</i>	472