Index

synthesis of, 824

Boldface references refer to pages	Acetoacetic ester, alkylation of,	<i>N</i> -Acetylgalactosamine, structure of,
where terms are defined.	885–886	1024
a caa Alpha	ketones from, 885–886	<i>N</i> -Acetylglucosamine, biosynthesis
α, see Alpha	mixed aldol reactions of, 913	of, 846
ABS polymer, structure and uses of, 1247	Acetoacetyl CoA biosynthesis of	structure of, 1024
	Acetoacetyl CoA, biosynthesis of,	Acetylide anion, 325
Absorbance (LIV) 510	1101	alkylation of, 327–328
Absorbance (UV), 519	Acetone, electrostatic potential map	electrostatic potential map of, 326
Absorption spectrum, 436	of, 54, 56, 79	formation of, 325
Acesulfame-K, structure of, 1034	enol content of, 871	stability of, 326
sweetness of, 1033	hydrate of, 731	N-Acetylneuraminic acid, structure
Acetal(s), 742	industrial synthesis of, 722–723	of, 1024
from aldehydes, 742–744	pK_a of, 53, 877	Achiral, 144
from ketones, 742–744	uses of, 722	Acid, Brønsted–Lowry, 49
hydrolysis of, 743–744	Acetone anion, electrostatic potential	Lewis, 56 –58
mechanism of formation of,	map of, 55	organic, 54–55
743–744	resonance in, 45	strengths of, 50–51
Acetaldehyde, aldol reaction of,	Acetonitrile, electrostatic potential	Acid anhydride(s), 814
905–906	map of, 794	amides from, 835–836
bond angles in, 714	Acetophenone, ¹³ C NMR absorptions	electrostatic potential map of,
bond lengths in, 714	of, 758	820
electrostatic potential map of, 714,	structure of, 724	esters from, 835
820, 951	Acetyl ACP, structure of, 1169	from acid chlorides, 831
13C NMR absorptions of, 758	Acetyl azide, electrostatic potential	from carboxylic acids, 824
¹ H NMR spectrum of, 758	map of, 859	IR spectroscopy of, 851
Acetaminophen, molecular model of,	Acetyl chloride, electrostatic potential	naming, 815
27	map of, 820	NMR spectroscopy of, 852
synthesis of, 836	reaction with alcohols, 831	nucleophilic acyl substitution
Acetanilide, electrophilic aromatic	reaction with amines, 832	reactions of, 835–836
substitution of, 967	Acetyl CoA, see Acetyl coenzyme A	reaction with alcohols, 835
Acetate ion, bond lengths in, 42	Acetyl coenzyme A, carbonyl	reaction with amines, 835–836
electrostatic potential map of, 42,	condensation reactions of,	Acid bromide, enol of, 877
52, 55, 784	930	from carboxylic acid, 830
resonance in, 42–43	carboxylation of, 1170	Acid chloride(s), acid anhydrides
Acetic acid, bond angles in, 782	catabolism of, 1185–1190	from, 831
bond lengths in, 782	citric acid cycle and, 1185–1190	alcohols from, 833
dimer of, 782	fat catabolism and, 1162–1166	alcoholysis of, 831
dipole moment of, 38	fatty acids from, 1167–1173	amides from, 832
electrostatic potential map of, 52, 54	from pyruvate, 1181–1185	amines from, 960, 962
industrial synthesis of, 779	function of, 846	aminolysis of, 832
pK _a of, 51, 783	reaction with glucosamine, 846	carboxylic acids from, 830–831
properties of, 782	structure of, 1156	electrostatic potential map of, 820
protonation of, 59	thioester in, 846	esters from, 831
uses of, 779	Acetyl group, 724	from carboxylic acids, 823–824
Acetic acid dimer, electrostatic	Acetylene, bond angles in, 17	Grignard reaction of, 833
potential map of, 782	bond lengths in, 17, 317	hydrolysis of, 830–831
Acetic anhydride, electrostatic	bond strengths in, 17, 317	IR spectroscopy of, 851
potential map of, 820	electrostatic potential map of, 317	ketones from, 833–834
reaction with amines,	molecular model of, 16	naming, 815
835–836	pK_a of, 53, 326	NMR spectroscopy of, 852
reaction with monosaccharides,	sp hybrid orbitals in, 16	nucleophilic acyl substitution
1015–1016	structure of, 16–17, 316–317	reactions of, 830–834

pK_a of, 879

uses of, 314

Acid chloride(s)—cont'd Acyl group, 577, 712 Alcohol(s), 620 reaction with alcohols, 831 names of, 780 acetals from, 742-744 reaction with amines, 832 Acyl phosphate, 814 acidity of, 624-626 reaction with ammonia, 832 naming, 817 aldehydes from, 645-646 reaction with diorganocopper Acylation (aromatic), see alkenes from, 263-264, 641-643 reagents, 833-834 Friedel-Crafts reaction alkoxide ions from, 624 reaction with Gilman reagents, Adams, Roger, 277 alkyl halides from, 354–355, 833-834 Adams catalyst, 277 391-392, 639 reaction with Grignard reagents, Addition reaction, 184-185 α cleavage of, 431, 657 833 1,2-Addition reaction (carbonyl), biological dehydration of, 643 **751**–755 reaction with LiAlH₄, 833 boiling points of, 623 reaction with water, 830-831 1,2-Addition reaction (conjugated carbonyl compounds from, reduction of, 833 diene), 505 645-646 carboxylic acids from, 645-646 Acid halide(s), 814 1,4-Addition reaction (carbonyl), naming, 815 **751**–755 common names of, 622 nucleophilic acyl substitution 1,4-Addition reaction (conjugated dehydration of, 263-264, 641-643 electrostatic potential map of, 78 reactions of, 830-834 diene), 505 see also Acid chloride kinetic control of, 508-509 esters from, 644 Acidity, alcohols and, 624-626 thermodynamic control of, ethers from, 678-680 amines and, 951-952 508-509 from acid chlorides, 833 carbonyl compounds and, Adenine, electrostatic potential map from aldehydes, 630–631, 734–735 877-880 from alkenes, 269-274 of, 1132 carboxylic acids and, 782-784 molecular model of, 66 from carbonyl compounds, 630–636 phenols and, 624-626 protection of, 1142–1143 from carboxylic acids, 632-633, Acidity constant (K_a) , 50 structure of, 1129 827-828 Acid-base reactions, prediction of, Adenosine diphosphate (ADP), from esters, 632-633, 840-842 52 - 53structure and function of, 205, from ethers, 681-682 Acifluorfen, synthesis of, 710 1156-1157 from ketones, 630-631, 734-735 Acrolein, structure of, 724 Adenosine triphosphate (ATP), bond hybrid orbitals in, 18 Acrylic acid, p K_a of, 783 dissociation energy and, 204 hydrogen bonds in, 623 structure of, 780 coupled reactions and, 1157-1158 IR spectroscopy of, 443, 654 function of, 204-205 Activating group (aromatic ketones from, 645-646 mass spectrometry of, 431, 657 substitution), 581 reaction with glucose, 1158 acidity and, 787 structure and function of, 205, mechanism of dehydration of, 641-642 Activation energy, 206 1072, 1156-1157 reaction rate and, 206-207 S-Adenosylmethionine, from mechanism of oxidation of, 646 typical values for, 207 methionine, 694 naming, 621–622 Active site (enzyme), 210-211 function of, 396 NMR spectroscopy of, 655-656 citrate synthase, 1074 structure of, 1073 oxidation of, 645-647 hexokinase, 211 (S)-S-Adenosylmethionine, primary, 621 HMG-CoA reductase, 1204 stereochemistry of, 166 properties of, 623-627 Acyclic diene metathesis protecting group for, 648–650 Adipic acid, structure of, 780 polymerization (ADMET), 1252 ADMET, see acyclic diene metathesis reaction with acid, 641-642 mechanism of, 1251 polymerization, 1252 reaction with acid anhydrides, 835 Acyl adenosyl phosphate, from ADP, see Adenosine diphosphate reaction with acid chlorides, 831 carboxylic acids, 828-830 Adrenaline, biosynthesis of, 396 reaction with aldehydes, 742-744 mechanism of formation of, molecular model of, 175 reaction with alkenes, 680 828-830 structure of, 23 reaction with alkyl halides, Adrenocortical steroid, 1111 Acyl adenylate, from carboxylic acids, 678-679 -al, aldehyde name suffix, 723 reaction with ATP, 1156-1157 828-830 mechanism of formation of. Alanine, configuration of, 153-154 reaction with carboxylic acids, 828-830 electrostatic potential map of, 644, 824-826 Acyl azide, amines from, 960, 962 1045 reaction with Acyl carrier protein, function of, 1169 molecular model of, 26, 1044 chlorotrimethylsilane, 648-649 structure and properties of, 1046 reaction with CrO₃, 645-646 Acyl cation, electrostatic potential reaction with Dess-Martin map of, 578 titration curve for, 1051 Friedel-Crafts acylation reaction periodinane, 645–646 zwitterion form of, 56 and. 577-578 Alanylserine, molecular model of, reaction with Grignard reagents, resonance in, 577-578

reaction with HX, 354, 391–392, 639	NMR spectroscopy of, 757–758 oxidation of, 727	Kiliani–Fischer synthesis on, 1022 names of, 1010
reaction with ketones, 742–744	oximes from, 737–738	natural occurrence of, 1008
reaction with KMnO ₄ , 645	pK _a of, 879	oxidation of, 1020-1021
reaction with Na ₂ Cr ₂ O ₇ , 645–646	protecting groups for, 745	reaction with Br ₂ , 1020
reaction with NaH, 626	reaction with alcohols, 742–744	reaction with HCN, 1022
reaction with NaNH ₂ , 626	reaction with amines, 736–739	reaction with HNO ₃ , 1021
reaction with PBr ₃ , 355, 639	reaction with Br ₂ , 874–876	reaction with NaBH ₄ , 1020
reaction with POCl ₃ , 641–643	reaction with CrO ₃ , 727	reduction of, 1020
reaction with potassium, 626	reaction with	see also Carbohydrate,
reaction with SOCl ₂ , 355, 639	2,4-dinitrophenylhydrazine, 739	Monosaccharide
reaction with <i>p</i> -toluenesulfonyl	reaction with Grignard reagents,	Tollens' test on, 1020
chloride, 639–640	635, 735	uronic acids from, 1021
secondary, 621	reaction with H_2O , 731–732	Wohl degradation of, 1023
synthesis of, 629–636	reaction with HCN, 733	Aldosterone, structure and function
tertiary, 621	reaction with HX, 732–733	of, 1111
tosylates from, 639–640	reaction with hydrazine, 741–742	Algae, chloromethane from, 344
trimethylsilyl ethers of, 648–650	reaction with LiAlH ₄ , 630, 734	Alicyclic, 109
Alcoholysis, 821	reaction with NaBH ₄ , 630, 734	Aliphatic, 81
Aldaric acid, 1021	reaction with NH ₂ OH, 737–738	Alitame, structure of, 1034
from aldoses, 1021	reactivity of versus ketones,	sweetness of, 1033
Aldehyde, 722	729–730	Alkaloid(s), 63–64
acetals from, 742–744	reduction of, 630–631, 734	history of, 63
alcohols from, 630–631, 734–735	reductive amination of, 958–959	number of, 63
aldol reaction of, 905–906	Wittig reaction of, 746–748	Alkane(s), 80
alkanes from, 741–742	Wolff–Kishner reaction of,	boiling points of, 93
alkenes from, 746–748	741–742	branched-chain, 82
α cleavage of, 432, 759	Aldehyde group, directing effect of,	combustion of, 93
amines from, 958–959	588–589	conformations of, 98–99
biological reduction of, 631–632,	Alditol(s), 1020	dispersion forces in, 61, 93
750–751	from aldoses, 1020	from aldehydes, 741–742
bromination of, 874–876	Aldol reaction, 905–906	from alkyl halides, 356
Cannizzaro reaction of, 750	biological example of, 928–929	from Grignard reagents, 356
carbonyl condensation reactions	cyclohexenones from, 913–915	from ketones, 741–742
of, 905–906	cyclopentenones from, 913–915	general formula of, 81
carboxylic acids from, 727	dehydration in, 908–909	IR spectroscopy of, 442
common names of, 724	enones from, 908–909	isomers of, 81–82
cyanohydrins from, 733	equilibrium in, 906	mass spectrometry of, 428–429
2,4-dinitrophenylhydrazones from, 739	intramolecular, 913–915 mechanism of, 905–906	melting points of, 93 naming, 87–91
enamines from, 736–739	mixed, 912–913	Newman projections of, 94
enols of, 871–872	reversibility of, 905–906	normal (n), 82
enones from, 908–909	steric hindrance to, 906	parent names of, 83
from acetals, 743–744	uses of, 910–911	pK_a of, 326
from alcohols, 645–646	Aldolase, mechanism of, 928–929,	properties of, 92–94
from alkenes, 284–286	1177–1178	reaction with Br ₂ , 347
from alkynes, 321–322	type I, 928–929	reaction with Cl_2 , 93, 347–349
from esters, 725–726, 841	type II, 928–929	sawhorse representations of, 94
hydrate of, 727, 731–732	Aldonic acid(s), 1020	straight-chain, 82
imines from, 736–739	from aldoses, 1020–1021	Alkene(s), 222
IR spectroscopy of, 444, 756–757	Aldose(s), 1002	alcohols from, 269–274
mass spectrometry of, 431–432,	aldaric acids from, 1021	aldehydes from, 284–286
758–759	alditols from, 1020	alkoxymercuration of, 680
McLafferty rearrangement of, 431,	aldonic acids from, 1020	allylic bromination of, 350–351
758	Benedict's test on, 1020	biological addition reactions of,
mechanism of hydration of,	chain-lengthening of, 1022	294–295
731–732	chain-shortening of, 1023	bond rotation in, 229
mechanism of reduction of, 734	configurations of, 1008–1010	bromohydrins from, 267–269
naming, 723–724	Fehling's test on, 1020	bromonium ion from, 265–266

I-4 Index

alkene(s)—cont'd	reaction with OsO_4 , 283–284	see also Organohalide
cis-trans isomerism in, 229-230	reaction with ozone, 284–285	structure of, 346
cleavage of, 284–286	reaction with peroxyacids,	thiols from, 692
common names of, 228	281–282	Alkyl shift, carbocations and, 250
cyclopropanes from, 287–289	reaction with radicals, 291–292	Alkylamine(s), 944
1,2-dihalides from, 264–266	reduction of, 276–280	basicity of, 950
diols from, 282–284	Sharpless epoxidation of, 761	Alkylation (aromatic), 575 –577
electron distribution in, 195	Simmons–Smith reaction of,	see also Friedel–Crafts reaction
electrophilic addition reactions of,	288–289	Alkylation (carbonyl), 882–889
237–238	stability of, 234–236	acetoacetic ester, 885–886
electrostatic potential map of, 78,	steric strain in, 234–235	acetylide anions and, 327–328
194	synthesis of, 263–264	biological example of, 889–890
epoxides from, 281–282	uses of, 223	ester, 888
ethers from, 680	Alkoxide ion, 624	ketone, 887–890
E,Z configuration of, 231–232	solvation of, 625	lactone, 888
from alcohols, 263–264, 641–643	Alkoxymercuration, 680	
		malonic ester, 883–884
from aldehydes, 746–748	mechanism of, 680	nitrile, 888
from alkyl halides, 263	Alkyl group(s), 84	Alkylbenzene, biological oxidation
from alkynes, 322–325	directing effect of, 585–586	of, 597
from amines, 964–965	inductive effect of, 583	from aryl alkyl ketones, 599–600
from ketones, 746–748	naming, 84–85, 89–90	reaction with KMnO ₄ , 596–597
general formula of, 224	orienting effect of, 581	reaction with NBS, 597–598
halogenation of, 264–266	table of, 85	side-chain bromination of,
halohydrins from, 267–269	Alkyl halide(s), 344	597–598
hydration of, 269–274	alkenes from, 263	side-chain oxidation of, 596–597
hydroboration of, 272–274	amines from, 956–957	Alkylthio group, 693
hydrogenation of, 276–280	amino acids from, 1054	Alkyne(s), 314
hydroxylation of, 282–284	carboxylic acids from, 790	acetylide anions from, 325–326
hyperconjugation in, 235–236	coupling reactions of, 357–358	acidity of, 325–326
industrial preparation of, 223	dehydrohalogenation of, 263	aldehydes from, 321–322
IR spectroscopy of, 442–443	electrostatic potential map of, 78	alkenes from, 322–325
ketones from, 284–286	ethers from, 678–679	alkylation of, 327–328
Markovnikov's rule and, 240–241	from alcohols, 354–355, 391–392,	cleavage of, 325
mechanism of hydration of, 270	639	electrostatic potential map of, 78
naming, 226–227	from ethers, 681–682	from dihalides, 316
new naming system for, 227	Grignard reagents from, 355–356	hydration of, 319–321
nucleophilicity of, 195	malonic ester synthesis with,	hydroboration of, 321–322
old naming system for, 226–227	883–884	hydrogenation of, 322–323
organoboranes from, 272–274	naming, 345–346	IR spectroscopy of, 443
oxidation of, 281–286	phosphonium salts from, 747	ketones from, 319–321
oxymercuration of, 271–272	polarity of, 346	naming, 314–315
ozonolysis of, 284–285	polarizability of, 191	oxidation of, 325
pK _a of, 326	reaction with alcohols, 678–679	pK_a of, 326
polymerization of, 290–292	reaction with amines, 956	reaction with BH ₃ , 321–322
reaction with alcohols, 680	reaction with azide ion, 956–957	reaction with Br ₂ , 317–318
reaction with borane, 272–274	reaction with carboxylate ions,	reaction with Cl_2 , 317–318
reaction with	824	reaction with HBr, 317–318
N-bromosuccinimide, 350–351	reaction with Gilman reagents,	reaction with HCl, 317–318
reaction with Br ₂ , 264–266	357–358	reaction with KMnO ₄ , 325
reaction with carbenes, 287–289	reaction with HS ⁻ , 692	reaction with lithium, 323–325
reaction with Cl ₂ , 264–266	reaction with phthalimide ion,	reaction with NaNH ₂ , 325
reaction with halogen, 264–267	957	reaction with O_3 , 325
reaction with HBr, 238	reaction with sulfides, 694	reduction of, 322–325
reaction with HCl, 238	reaction with thiols, 693	structure of, 316–317
reaction with HI, 238	reaction with thiourea, 692	synthesis of, 316
reaction with hydrogen, 276–280	reaction with tributyltin hydride,	vinylic carbocation from, 318
reaction with KMnO ₄ , 285	370	vinylic halides from, 317–318
reaction with mercuric ion,	reaction with triphenylphosphine,	Alkynyl group, 315
271–272	747	Allene, heat of hydrogenation of, 259
		, , , , , , , , , , , , , , , , , , , ,

Allinger, Norman Louis, 132
Allose, configuration of, 1009
Allyl aryl ether, Claisen
rearrangement of, 683–684
Allyl carbocation, electrostatic
potential map of, 390
Allyl group, 228
Allylic, 350
Allylic bromination, 350–351
mechanism of, 350–351
Allylic carbocation, electrostatic
potential map of, 506
resonance in, 506
S _N 1 reaction and, 389–390
stability of, 506
Allylic halide, S _N 1 reaction and,
389–390
S_N 2 reaction and, 391
Allylic protons, ¹ H NMR spectroscopy
and, 474–475
Allylic radical, molecular orbital of,
351
resonance in, 351–352
spin density surface of, 352
stability of, 351–352
Alpha amino acid, 1045
see Amino acid
Alpha anomer, 1012
Alpha cleavage, alcohol mass
spectrometry and, 431, 657
aldehyde mass spectrometry and,
432, 759
amine mass spectrometry and,
431, 981–982
ketone mass spectrometry and,
432, 759
Alpha farnesene, structure of, 256
Alpha helix (protein), 1066 –1067
Alpha-keratin, molecular model of,
1067
secondary structure of, 1066–1067
Alpha-keto acid, amino acids from,
1054
reductive amination of, 1054
Alpha pinene, structure of, 222
Alpha substitution reaction, 718, 870
carbonyl condensation reactions
and, 907–908
evidence for mechanism of, 876
mechanism of, 874
Altrose, configuration of, 1009
Aluminum chloride, Friedel–Crafts
reaction and, 575
Amantadine, structure of, 139
Amide(s), 814
amines from, 844–845, 960–962
basicity of, 951
carboxylic acids from, 843–844
electrostatic potential map of, 820
erectiostatic potential map of, 620

from acid anhydrides, 835-836 from acid chlorides, 832 from carboxylic acids, 826-827 from esters, 840 from nitriles, 795–796 hydrolysis of, 843-844 IR spectroscopy of, 851 mechanism of hydrolysis of, 843-844 mechanism of reduction of, 845 naming, 816 nitriles from, 793-794 NMR spectroscopy of, 852 nucleophilic acyl substitution reactions of, 843-845 occurrence of, 842 pK_a of, 879 reaction with Br₂, 960, 961 reaction with LiAlH₄, 844–845 reaction with SOCl₂, 793–794 reduction of, 844-845 restricted rotation in, 1057 Amidomalonate synthesis, 1054 -amine, name suffix, 945 Amine(s), 944 acidity of, 951-952 alkenes from, 964-965 α cleavage of, 431, 981–982 basicity of, 948-950 chirality of, 165-166, 947 conjugate carbonyl addition reaction of, 753 electronic structure of, 947 electrostatic potential map of, 79 from acid chlorides, 960, 962 from acyl azides, 960, 962 from aldehydes, 958–959 from alkyl azides, 956-957 from alkyl halides, 956-957 from amides, 844-845, 960-962 from ketones, 958-959 from lactams, 845 from nitriles, 796 Henderson-Hasselbalch equation and, 954 heterocyclic, 946 Hofmann elimination of, 964-965 hybrid orbitals in, 17–18 hydrogen-bonding in, 948 IR spectroscopy of, 444, 979 mass spectrometry of, 431, 981-982 naming, 944-946 nitrogen rule and, 981-982 occurrence of, 944 odor of, 948 primary, 944 properties of, 948 purification of, 951

pyramidal inversion in, 947 reaction with acid anhydrides, 835-836 reaction with acid chlorides, 832 reaction with aldehydes, 736-739 reaction with alkyl halides, 956 reaction with carboxylic acids, 826-827 reaction with enones, 753 reaction with epoxides, 689-690 reaction with esters, 840 reaction with ketones, 736-739 secondary, 944 synthesis of, 955-962 tertiary, 944 uses of, 948 Amino acid(s), 1044 abbreviations for, 1046-1047 acidic, 1049 amidomalonate synthesis of, 1054 amphiprotic behavior of, 1045 basic, 1049 biosynthesis of, 1054 Boc derivatives of, 1062–1063 catabolism of, 1197-1201 configuration of, 1048-1049 electrophoresis of, 1053 enantioselective synthesis of, 1055 essential, 1049 esters of, 1062 Fmoc derivatives of, 1062-1063 from alkyl halides, 1054 from α -keto acids, 1054 from carboxylic acids, 1053 Henderson-Hasselbalch equation and, 1050-1051 isoelectric points of, 1046–1047 molecular weights of, 1046-1047 neutral, 1049 nonprotein, 1048 pKa's of, 1046-1047 protecting groups for, 1062-1063 reaction with di-tert-butyl dicarbonate, 1062-1063 reaction with ninhydrin, 1058 resolution of, 1054 synthesis of, 1053–1055 table of, 1046-1047 C-terminal, 1056 N-terminal, 1056 transamination of, 1198-1201 zwitterion form of, 1045 Amino acid analyzer, 1058–1059 Ion-exchange chromatography and, 1058-1059 Amino group, 945 directing effect of, 586-587 orienting effect of, 581 Amino sugar, 1024

p-Aminobenzoic acid, molecular	Anti periplanar geometry, 401	Friedel-Crafts alkylation of,
model of, 23	E2 reaction and, 401–402	575–577
Aminolysis, 821	molecular model of, 401	halogenation of, 567-571
Ammonia, dipole moment of, 38	Anti stereochemistry, 265	hydrogenation of, 599
electrostatic potential map of,	Antiaromaticity, 541	iodination of, 570–571
192	Antibiotic, β -lactam, 853–854	IR spectroscopy of, 443, 551
pK _a of, 53, 879	Antibonding molecular orbital, 20	naming, 535–537
reaction with acid chlorides, 832	Anticodon (tRNA), 1138	nitration of, 571–572
reaction with carboxylic acids,	Antisense strand (DNA), 1136	NMR ring current and, 552–553
826–827	Arabinose, configuration of, 1009	NMR spectroscopy of, 552–554
Ammonium cyanate, urea from, 1	Kiliani–Fischer synthesis on, 1022	nucleophilic aromatic substitution
Ammonium ion, acidity of,	Arachidic acid, structure of, 1090	reaction of, 592–593
949–950	Arachidonic acid, eicosanoids from,	oxidation of, 596–598
Amobarbital, synthesis of, 891	1097–1098	reduction of, 599
Amphetamine, structure of, 217	prostaglandins from, 188–189,	see also Aromaticity
synthesis of, 958	294–295, 1097–1098	sources of, 535
Amplitude, 435	structure of, 1090	sulfonation of, 572–573
Amylopectin, $1\rightarrow 6-\alpha$ -links in, 1029	Arecoline, molecular model of, 80	trisubstituted, 600-604
structure of, 1029	Arene(s), 536	UV spectroscopy of, 552
Amylose, $1\rightarrow 4-\alpha$ -links in, 1028	electrostatic potential map of, 78	Aromatic protons, ¹ H NMR
structure of, 1028	from arenediazonium salts, 970	spectroscopy and, 474–475
Anabolism, 1154	from aryl alkyl ketones, 599-600	Aromaticity, cycloheptatrienyl cation
fatty acids, 1167–1173	see also Aromatic compound	and, 544–545
glucose, 1191–1197	Arenediazonium salt(s), 968	cyclopentadienyl anion and,
Analgesic, 554	arenes from, 970	544–545
Androgen, 1110	aryl bromides from, 969	Hückel $4n + 2$ rule and, $541-543$
function of, 1110	aryl chlorides from, 969	imidazole and, 547
Androstenedione, structure and	aryl iodides from, 969	indole and, 550
function of, 1110	coupling reactions of, 972	ions and, 544–545
Androsterone, structure and function	from arylamines, 968–969	isoquinoline and, 550
of, 1110	nitriles from, 969	naphthalene and, 550
-ane, alkane name suffix, 83	phenols from, 970	polycyclic aromatic compounds
Anesthetics, dental, 63–64	reaction with arylamines, 972	and, 549–550
Angle strain, 114	reaction with CuBr, 969	purine and, 550
Angstrom, 3	reaction with CuCl, 969	pyridine and, 546–547
Anhydride, see Acid anhydride	reaction with CuCN, 970	pyrimidine and, 546–547
Aniline, basicity of, 950	reaction with Cu ₂ O, 970	pyrrole and, 547
electrostatic potential map of,	reaction with H ₃ PO ₂ , 970	quinoline and, 550
953	reaction with NaI, 969	requirements for, 541
from nitrobenzene, 572	reaction with phenols, 972	Arrow, electron movement and,
synthesis of, 572	reduction of, 970	44–45, 57–58, 197–199
Anilinium ion, electrostatic potential	substitution reactions of, 969–970	fishhook, 186, 291
map of, 953	Arginine, structure and properties of, 1047	<i>see also</i> Curved arrow Arsenic trioxide, LD ₅₀ of, 24
Anilinothiazolinone, Edman degradation and, 1059–1061		
	<i>epi</i> -Aristolochene, biosynthesis of, 261	Aryl alkyl ketone, reduction of, 599–600
Anionic polymerization, 1243 Anisole, electrostatic potential map	Aromatic compound(s), 534	Aryl boronic acid, Suzuki–Miyaura
of, 804	acylation of, 577–578	reaction of, 359
molecular model of, 676	alkylation of, 575–577	Aryl halide, S _N 2 reaction and,
¹³ C NMR spectrum of, 696	biological hydroxylation of,	379–380
Annulation reaction, 927–928	573–574	Suzuki–Miyaura reaction of, 359
[18]Annulene, electrostatic potential	bromination of, 567–569	Arylamine(s), 944
map of, 553	characteristics of, 541	basicity of, 950, 952–953
ring current in, 552–553	chlorination of, 570	diazotization of, 968–969
Anomer, 1012	coal tar and, 535	electrophilic aromatic substitution
Anomeric center, 1012	common names for, 535–536	of, 966–968
Ant, sex attractant of, 834	fluorination of, 570	from nitroarenes, 955
Antarafacial geometry, 1223	Friedel–Crafts acylation of,	reaction with arenediazonium
Anti conformation, 96	577–578	salts, 972
*		•

reaction with HNO₂, 968-969 Banana, esters in, 836 Benzenesulfonic acid, synthesis of, resonance in, 952 Barbiturates, 890–891 table of basicity in, 953 history of, 890 Benzodiazepine, combinatorial Ascorbic acid, see Vitamin C synthesis of, 891 library of, 605 Benzoic acid, ¹³C NMR absorptions Base, Brønsted-Lowry, 49 -ase, enzyme name suffix, 1070 in, 798 Asparagine, structure and properties Lewis, 56-59 pK_a of, 783 of, 1046 organic, 56 Aspartame, molecular model of, 27 strengths of, 50-51 substituent effects on acidity of, 787 structure of, 1034 Benzophenone, structure of, 724 Base pair (DNA), 1131–1132 sweetness of, 1033 electrostatic potential maps of, Benzoquinone, electrostatic potential Aspartic acid, structure and properties 1132 map of, 653 of, 1047 Benzoyl group, 724 hydrogen-bonding in, 1131–1132 Asphalt, composition of, 100 Base peak (mass spectrum), 426 Benzoyl peroxide, ethylene Aspirin, history of, 554 Basicity, alkylamines, 950 polymerization and, 291 LD₅₀ of, 24 amides, 951 Benzo[a]pyrene, carcinogenicity of, 549 amines, 948-950 molecular model of, 15 structure of, 549 synthesis of, 835 arylamines, 950, 952-953 Benzyl ester, hydrogenolysis of, 1062 toxicity of, 555 heterocyclic amines, 950 Benzyl group, 536 Asymmetric center, 145 nucleophilicity and, 381 Benzylic, 390 Atactic polymer, 1245 Basicity constant (K_b) , 949 Benzylic acid rearrangement, 867 -ate, ester name suffix, 816 Beeswax, components of, 1088–1089 Benzylic carbocation, electrostatic Atom, atomic mass of, 3 Benedict's test, 1020 potential map of, 390 atomic number of, 3 Bent bond, cyclopropane, 116 resonance in, 390 Benzaldehyde, electrostatic potential electron configurations of, 5 S_N1 reaction and, 389–390 map of, 583, 730 electron shells in, 4 Benzylic halide, S_N1 reaction and, isotopes of, 3 IR spectrum of, 756 389-390 orbitals in, 3-5 mixed aldol reactions of, 912 S_N2 reaction and, 391 quantum mechanical model of, 3-5 ¹³C NMR absorptions of, 758 Benzylic radical, resonance in, 598 Benzene, acylation of, 577-578 size of, 2 spin-density surface of, 598 structure of, 2-5 alkylation of, 575-577 Benzylpenicillin, discovery of, 853 Atomic mass, 3 bond lengths in, 539 structure of, 1 Atomic number (Z), 3 bromination of, 567–569 Benzyne, 595 Atomic weight, 3 chlorination of, 570 Diels-Alder reaction of, 595 electrostatic potential map of, 595 Atorvastatin, structure of, 1, 534 discovery of, 536 statin drugs and, 1203-1204 electrostatic potential map of, 43, evidence for, 595 ATP, see Adenosine triphosphate 539, 583 structure of, 595 Atrazine, LD₅₀ of, 24 fluorination of, 570 Bergström, Sune K., 1095 ATZ, see Anilinothiazolinone, Friedel-Crafts reactions of, Beta anomer, 1012 1059-1061 575-579 Beta-carotene, industrial synthesis of, Aufbau principle, 5 heat of hydrogenation of, 539 748 Avian flu, 1032 Hückel 4n + 2 rule and, 542 structure of, 222 iodination of, 570-571 UV spectrum of, 521 Axial bonds (cyclohexane), 120 drawing, 121 molecular orbitals of, 540-541 Beta-diketone, Michael reactions and, Azide, amines from, 956–957 nitration of, 571-572 922-923 reduction of, 956-957 ¹³C NMR absorption of, 554 Beta-keto ester, alkylation of, 885-886 Azo compound, 971 reaction with Br₂, 567-569 cyclic, 919-920 synthesis of, 972 reaction with Cl₂, 570 decarboxylation of, 886 uses of, 971 reaction with F-TEDA-BF₄, 570 Michael reactions and, 922-923 reaction with HNO_3 , 571–572 Azulene, dipole moment of, 558 pK_a of, 879 electrostatic potential map of, 558 reaction with H₂SO₄/HNO₃, 572 synthesis of, 919-920 structure of, 551 reaction with I₂, 570–571 Beta-lactam antibiotics, 853–854 resonance in, 43, 539-540 Beta-oxidation pathway, 1162-1167 stability of, 538-539 mechanisms in, 1162-1167 β , see Beta Backbone (protein), 1056 structure of, 538-541 steps in, 1162 Backside displacement, S_N2 reaction sulfonation of, 572 Beta-pleated sheet (protein), and, 376-377 toxicity of, 534 1066-1067 von Baeyer, Adolf, 114 UV absorption of, 520 molecular model of, 1067 Baeyer strain theory, 114 Benzenediazonium ion, electrostatic secondary protein structure and, Bakelite, structure of, 1256 potential map of, 972 1066-1067

Betaine, 747 S_N2 reaction, 396 reaction with carboxylic acids, Bextra, structure of, 562 thioester reduction, 847 876-877 BHA, synthesis of, 652 Biological substitution reactions, reaction with enolate ions, BHT, synthesis of, 652 diphosphate leaving group in, 881-882 395-396 Bicycloalkane, 130 reaction with ketones, 874-876 Biomass, carbohydrates and, 1000 Bimolecular, 376 reactions with aldoses, 1020 Bioprospecting, 251-252 Biodegradable polymers, 850, Bromo group, directing effect of, 1256-1257 Biosynthesis, fatty acids, 1167-1173 587-588 Biological acids, Biot, Jean Baptiste, 147 p-Bromoacetophenone, molecular Henderson-Hasselbalch Biotin, fatty acid biosynthesis and, model of, 466 equation and, 785-786 1170 ¹³C NMR spectrum of, 465 symmetry plane in, 466 Biological carboxylic acid derivative, stereochemistry of, 178 845-847 structure of, 1073 p-Bromobenzoic acid, p K_a of, 787 Bromocyclohexane, molecular model Biological mass spectrometry, Bird flu, 1032 Bisphenol A, epoxy resins from, 433-434 of, 122 Biological reaction, alcohol 697-698 ring-flip in, 122 dehydration, 264 polycarbonates from, 849-850 Bromoethane, electrostatic potential alcohol oxidation, 647 Block copolymer, 1248 maps of, 194 aldehyde reduction, 631-632, synthesis of, 1248 ¹H NMR spectrum of, 477 750-751 Boat conformation (cyclohexane), spin-spin splitting in, 477-478 Bromohydrin(s), 267 aldol reaction, 928–929 steric strain in, 119-120 alkene halogenation, 267 Boc (tert-butoxycarbonyl amide), from alkenes, 267-269 alkene hydration, 270-271 1062-1063 mechanism of formation of, 268 alkene hydrogenation, 280 amino acid derivatives of, 1062-1063 Bromomethane, bond length of, 346 α -substitution reaction, 889–890 Bond, covalent, 9-10 bond strength of, 346 molecular orbital theory of, 19-21 aromatic hydroxylation, 573-574 dipole moment of, 346 aromatic iodination, 571 pi, 14 electrostatic potential map of, 192 benzylic oxidation, 597 sigma, 10 Bromonium ion, 265 bromohydrin formation, 269 valence bond description of, 9–10 electrostatic potential map of, 266 carbonyl condensations, 928–930 Bond angle, 12 from alkenes, 265-266 carboxylation, 790 Bond dissociation energy (D), 203 stability of, 266 2-Bromopropane, ¹H NMR spectrum characteristics of, 210–212 table of, 204 Claisen condensation, 930 of, 478 Bond length, 10 Claisen rearrangement, 684, Bond rotation, alkanes, 94-95 spin-spin splitting in, 478 1229-1230 alkenes, 229 N-Bromosuccinimide, bromohydrin butane, 96-98 formation with, 268 comparison with laboratory reaction, 210-212 ethane, 94-95 reaction with alkenes, 268, conclusions about, 1202 propane, 96 350-351 conventions for writing, 211, 239 Bond strength, 10 reaction with alkylbenzenes, 597-598 decarboxylation, 1181–1185 Bonding molecular orbital, 20 dehydration, 643 Borane, electrophilicity of, 273 p-Bromotoluene, ¹H NMR spectrum electrophilic aromatic electrostatic potential map of, 273 of. 553 reaction with alkenes, 272-274 Brønsted-Lowry acid, 49 substitution, 571 elimination reactions, 407 reaction with alkynes, 321–322 conjugate base of, 49 energy diagram of, 209 reaction with carboxylic acids, 828 strengths of, 50-51 fat hydrolysis, 839-840 Boron trifluoride, electrostatic Brønsted-Lowry base, 49 Friedel-Crafts alkylation, 578-579 potential map of, 57, 194 conjugate acid of, 49 ketone alkylation, 889-890 Branched-chain alkane, 82 strengths of, 50-51 ketone reduction, 631-632, 750-751 Brown, Herbert Charles, 272 Breathalyzer test, 658 nucleophilic acyl substitution, Bridgehead atom (polycyclic Bupivacaine, structure of, 64 828-830 compound), 129 Butacetin, structure of, 865 nucleophilic substitutions, Broadband-decoupled NMR, 467 1,3-Butadiene, 1,2-addition reactions of, 505-506 395-396 Bromine, reaction with aldehydes, oxidation, 647 874-876 1,4-addition reactions of, 505-506 protein hydrolysis, 844 bond lengths in, 502 reaction with alkanes, 347 radical additions, 294-295 electrophilic addition reactions of, reaction with alkenes, 264-266 reduction, 631-632, 750-751 505-506 reaction with alkynes, 317–318 reductive amination, 959 reaction with aromatic electrostatic potential map of, 504 S_N1 reaction, 395–396 compounds, 567-569 heat of hydrogenation of, 503

molecular orbitals in, 503-504, 1215 polymerization of, 516 reaction with Br2, 506 reaction with HBr, 505-506 stability of, 502-504 UV spectrum of, 519 Butanal, 2-ethyl-1-hexanol from, 910-911 Butane, anti conformation of, 96 bond rotation in, 96-98 conformations of, 96-98 gauche conformation of, 97 molecular model of, 81 Butanoic acid, IR spectrum of, 798 1-Butanol, mass spectrum of, 657 2-Butanone, ¹³C NMR spectrum of, 465 3-Buten-2-one, electrostatic potential map of, 752 UV absorption of, 520 1-Butene, heat of hydrogenation of, 236 cis-2-Butene, heat of hydrogenation of, 235 molecular model of, 230, 234 steric strain in, 234-235 trans-2-Butene, heat of hydrogenation of, 235 molecular model of, 230, 234 Butoxycarbonyl (Boc) protecting group, 1062-1063 Butter, composition of, 1090 tert-Butyl alcohol, p K_a of, 625 tert-Butyl carbocation, electrostatic potential map of, 245 molecular model of, 244 Butyl group, 85 Butyl rubber polymer, structure and uses of, 1247 Butyllithium, electrostatic potential map of, 357 c (Speed of light), 435 C-terminal amino acid, 1056 Cadaverine, odor of, 948

c (Speed of light), 435
C-terminal amino acid, 1056
Cadaverine, odor of, 948
Caffeine, structure of, 32
Cahn–Ingold–Prelog sequence rules, 150–152
enantiomers and, 150–154
E,Z alkene isomers and, 231–232
Caine anesthetics, 63–64
Calicene, dipole moment of, 561
Camphor, molecular model of, 131
specific rotation of, 149
structure of, 1099
Cannizzaro reaction, 750
mechanism of, 750
Caprolactam, nylon 6 from, 1249

Capsaicin, structure of, 80 -carbaldehyde, aldehyde name suffix, 723 Carbamic acid, 1250 Carbanion, electrostatic potential map of, 326 stability of, 326 Carbene(s), 287 electronic structure of, 288 reaction with alkenes, 287-289 Carbenoid, 289 Carbinolamine, 736 Carbocaine, structure of, 64 Carbocation(s), 196 alkyl shift in, 250 E1 reaction and, 405 electronic structure of, 243-244 electrophilic addition reactions and, 196, 237-238 electrophilic aromatic substitution and, 568-569 electrostatic potential map of, 245, Friedel-Crafts reaction and, 576-577 Hammond postulate and, 248 hydride shift in, 249-250 hyperconjugation in, 245 inductive effects on, 245 Markovnikov's rule and, 241 rearrangements of, 249–250, 576-577 S_N1 reactions and, 389-390 solvation of, 393 stability of, 243-245, 390 vinylic, 318 Carbocation rearrangement, lanosterol biosynthesis and, 1113-1117 Carbohydrate(s), 1000 amount of in biomass, 1000 anomers of, 1011-1013 catabolism of, 1173-1181 classification of, 1001-1002 complex, 1001 essential, 1023-1025 Fischer projections and, 1004-1005 glycosides and, 1016-1018 $1 \rightarrow 4$ -links in, 1025–1026 name origin of, 1000 photosynthesis of, 1000-1001 see also Aldose, Monosaccharide Carbon atom, 3-dimensionality of, 6 ground-state electron configuration of, 5 tetrahedral geometry of, 6 Carbonate ion, resonance in, 47

-carbonitrile, nitrile name suffix, 781 Carbonyl compound(s), acidity of, 877-880 alcohols from, 630-636 alkylation of, 882-889 electrostatic potential map of, 79, from alcohols, 645–646 general reactions of, 714-719 IR spectroscopy of, 444 kinds of, 79, 712-713 mass spectrometry of, 431-432 Carbonyl condensation reaction, 719, 904-906 α -substitution reactions and, 907-908 biological examples of, 928-930 mechanism of, 904-905 Carbonyl group, 712 bond angles in, 714 bond length of, 714 bond strength of, 714 directing effect of, 588–589 inductive effect of, 583 orienting effect of, 581 resonance effect of, 584 structure of, 714 -carbonyl halide, acid halide name suffix, 815 -carbothioate, thioester name suffix, 816 -carboxamide, amide name suffix, 816 Carboxybiotin, fatty acid biosynthesis and, 1170 Carboxyl group, 779 -carboxylate, ester name suffix, 816 Carboxylate ion, reaction with alkyl halides, 824 resonance in, 784 Carboxylation, 790 biological example of, 790 -carboxylic acid, name suffix, 779 Carboxylic acid(s), 55, 778 acid anhydrides from, 824 acid bromide from, 830 acid chlorides from, 823-824 acidity of, 782-784 alcohols from, 632-633, 827-828 amides from, 826-827 amino acids from, 1053 biological, 785-786 bromination of, 876-877 common names of, 779-780 derivatives of, 814 dimers of, 782 dissociation of, 782-783 esters from, 824-826 from acid chlorides, 830-831 from alcohols, 645-646

Carbonic anhydrase, turnover

number of, 1069

Carboxylic acid(s)—cont'd	overview of, 1155	Chitin, structure of, 1031
from aldehydes, 727	protein, 1197–1201	Chloramphenicol, stereochemistry
from alkyl halides, 790, 883–884	pyruvate, 1181–1185	of, 181
from amides, 843–844	triacylglycerols, 1158–1167	Chlorine, reaction with alkanes, 93,
from esters, 837–840	Catalytic cracking, 101	347–349
from Grignard reagents, 790	Catalytic hydrogenation, see	reaction with alkenes, 264-266
from malonic ester, 883–884	Hydrogenation	reaction with alkynes, 317–318
from nitriles, 789–790, 795–796	Cation radical, mass spectrometry	reaction with aromatic
Hell-Volhard-Zelinskii reaction of,	and, 425–426	compounds, 570
876–877	Cationic polymerization, 1243	Chloro group, directing effect of,
hydrogen-bonding in, 782	Celebrex, 555	587–588
inductive effects in, 786–787	Celecoxib, NSAIDs and, 555	Chloroalkanes, dissociation enthalpy
IR spectroscopy of, 797–798	Cell membrane, lipid bilayer in, 1095	of, 244
naming, 779–780	Cellobiose, $1\rightarrow 4-\beta$ -link in, 1026	Chlorobenzene, electrostatic
NMR spectroscopy of, 798–799	molecular model of, 1026	potential map of, 583
nucleophilic acyl substitution	mutarotation of, 1026	¹³ C NMR absorptions of, 554
reactions of, 823–830	structure of, 1026	phenol from, 594
occurrence of, 778	Cellulose, $1\rightarrow 4-\beta$ -links in, 1028	p -Chlorobenzoic acid, p K_a of, 787
pK_a table of, 783	function of, 1028	2-Chlorobutanoic acid, pK_a of, 787
properties of, 782–784	structure of, 1028	3-Chlorobutanoic acid, pK_a of, 787
reaction with alcohols, 644,	uses of, 1028	4-Chlorobutanoic acid, pK_a of, 787
824–826	Cellulose nitrate, 1028	Chloroethane, dissociation enthalpy
reaction with amines, 826–827	Cephalexin, stereochemistry of, 181	of, 244
reaction with ammonia, 826–827	structure of, 854	Chloroform, dichlorocarbene from,
reaction with borane, 828	Cephalosporin, structure of, 854	287
reaction with Br ₂ , 876–877	Chain, Ernst, 853	LD ₅₀ of, 24
reaction with diazomethane, 866	Chain-growth polymer, 291–292,	Chloromethane, bond length of, 346
reaction with LiAlH ₄ , 632–633	847, 1242–1244	bond strength of, 346
reaction with PBr ₃ , 830	Chain reaction (radical), 188	dipole moment of, 346
reaction with SOCl ₂ , 823–824	Chair conformation (cyclohexane),	dissociation enthalpy of, 244
reduction of, 632–633, 827–828	118	electrostatic potential map of, 37,
synthesis of, 789–791	drawing, 119	190, 346
Carboxylic acid derivative(s), 814	molecular model of, 119	natural sources of, 344
biological, 845–847	see also Cyclohexane	2-Chloro-2-methylbutane,
electrostatic potential maps of,	Chemical Abstracts, 74	dissociation enthalpy of, 244
820	Chemical shift (NMR), 462	Chloropher of 75
interconversions of, 820–821	¹³ C NMR spectroscopy and,	p-Chlorophenol, pK _a of, 625
IR spectroscopy of, 851	464–465	Chlorophyll, biosynthesis of, 994
kinds of, 814	¹ H NMR spectroscopy and, 474–475	Chloroprene, polymerization of, 516
naming, 815–817	Chemical structure, drawing, 21–22	2-Chloropropane, dissociation
NMR spectroscopy of, 852 nucleophilic acyl substitution	Chevreul, Michel-Eugène, 1 Chiral, 144	enthalpy of, 244 Chlorosulfite, 823–824
reactions of, 820–821	Chiral drugs, 172–173	Chlorotrimethylsilane, bonds lengths
relative reactivity of, 819–821	Chiral environment, 171 –172	in, 649
table of names for, 817	prochirality and, 171–172	reaction with alcohols, 648–649
Cardiolipin, structure of, 1121	Chiral methyl group, 422	Cholecalciferol, structure of, 1232
Caruthers, Wallace Hume, 849	Chiral inchiyi gloup, 422 Chirality, amines and, 947	Cholestanol, structure of, 158
Carvone, chirality of, 146	cause of, 145	Cholesterol, amount of in body, 1203
structure of, 23	electrophilic addition reactions	biosynthesis of, 1112–1117
Caryophyllene, structure of, 1123	and, 296–298	carbocation rearrangements and,
Catabolism, 1154	naturally occurring molecules and,	250
acetyl CoA, 1185–1190	170–172	heart disease and, 1118
amino acids, 1197–1201	tetrahedral carbon and, 144–146	molecular model of, 1109
ATP and, 1156–1157	Chirality center, 145	specific rotation of, 149
carbohydrates, 1173–1181	detection of, 145–146	statin drugs and, 1203–1204
fats, 1158–1167	Fischer projections and, 1002–1005	stereochemistry of, 1109
fatty acids, 1162–1167	inversion of configuration of,	Cholic acid, molecular model of, 778
glucose, 1173–1181	373–374	Chorismate, Claisen rearrangement
glycerol, 1158–1161	<i>R,S</i> configuration of, 150–154	of, 1229–1230

Chromium trioxide, reaction with	Color, perception of, 522	Conjugated polyene, electrocyclic
aldehydes, 727	UV spectroscopy and, 521–522	reactions of, 1217–1222
Chrysanthemic acid, structure of, 108	Combinatorial chemistry, 605 –606	molecular orbitals of, 1215–1216
Chymotrypsin, peptide cleavage	kinds of, 605	Conjugated triene, electrocyclic
with, 1061	Combinatorial library, 605–606	reactions of, 1217
trans-Cinnamaldehyde, ¹ H NMR	Complex carbohydrate, 1001	Conjugation, ultraviolet spectroscop
spectrum of, 482	Computer chip, manufacture of,	and, 520
tree diagram for, 483	523–524	Conrotatory motion, 1219
cis–trans Isomers, 113	Concanavalin A, secondary structure	Consensus sequence (DNA), 1135
alkenes and, 229–230	of, 1066–1067	Constitutional isomers, 82
cycloalkanes and, 111–113 requirements for, 230	Concerted reaction, 1214 Condensation reaction, 908	kinds of, 82
Citanest, structure of, 64	Condensed structure, 21	Contraceptive, steroid, 1111 Cope rearrangement, 1229 –1230
Citrate, prochirality of, 1187	Cone cells, vision and, 522	suprafacial geometry of,
Citrate synthase, active site of, 1074	Configuration, 150	1229–1230
function of, 1071	assignment of, 150–154	Copolymer, 1246 –1248
mechanism of action of, 1071,	chirality centers and, 150–154	block, 1248
1074–1075	Fischer projections and, 1004	graft, 1248
molecular model of, 1074	inversion of, 373–374	table of, 1247
Citric acid, molecular model of, 27	R, 152	Copper(II) chloride, aromatic
Citric acid cycle, 1185–1190	S, 152	iodination and, 570–571
mechanisms in, 1187–1190	Conformation, 94	Coprostanol, structure of, 158
requirements for, 1187	anti, 96	Corn oil, composition of, 1090
result of, 1190	calculating energy of, 132	Coronary heart disease, cholesterol
steps in, 1186	eclipsed, 95	and, 1203–1204
Claisen condensation reaction,	gauche, 97	statin drugs and, 1203–1204
915 –917	staggered, 95	Coronene, structure of, 549
biological example of, 930	Conformational analysis	Cortisone, structure of, 108
intramolecular, 919–920	(cyclohexane), 127 –128	Couper, Archibald Scott, 6
mechanism of, 915-916	Conformer, 94	Coupled reactions, 1157–1158
mixed, 917–918	Coniine, chirality of, 147	ATP and, 1157–1158
Claisen rearrangement, 683–684,	molecular model of, 26	Coupling (NMR), 477
1229 –1230	Conjugate acid, 49	see also Spin–spin splitting
biological example of, 684,	Conjugate base, 49	Coupling constant, 478
1229–1230	Conjugate carbonyl addition	size of, 478
mechanism of, 683–684	reaction, 751 –755	use of, 478–479
suprafacial geometry of,	amines and, 753	Covalent bond(s), 7
1229–1230	enamines and, 925–926	bond angle in, 12
transition state of, 683–684	Gilman reagents and, 754–755	bond length in, 10
Clomiphene, structure of, 257	mechanism of, 752	bond strength in, 10
Clopidogrel, structure of, 32	Michael reactions and, 921–923	molecular orbital theory of, 19–21
Clostridium perfringens, DNA bases in,	water and, 753	polar, 34 –35
1131 Coal, structure of, 535	Conjugated compound, 500	rotation around, 94, 112 sigma, 10
Coal tar, compounds from, 535	Conjugated diene, 1,2-addition	valence bond theory of, 9–10
Cocaine, specific rotation of, 149	reactions of, 505–506 1,4-addition reactions of, 505–506	COX-2 inhibitors, 555, 1097
structure of, 63, 944	allylic carbocations from, 506	Cracking, steam, 223–224
structure of, 63, 944 structure proof of, 901	bond lengths in, 502	Crick, Francis H. C., 1131
synthesis of, 943	electrocyclic reactions of, 1217	Crotonaldehyde, structure of, 724
Coconut oil, composition of, 1090	electrophilic addition reactions of,	Crotonic acid, ¹³ C NMR absorptions
Coding strand (DNA), 1136	505–506	in, 798
CODIS, DNA fingerprint registry, 1146	electrostatic potential map of, 504	Crown ether, 690 –691
Codon (mRNA), 1137 –1138	heats of hydrogenation of, 503	electrostatic potential map of, 691
table of, 1137	molecular orbitals in, 503–504	$S_{\rm N}2$ reactions and, 691
Coenzyme, 212, 1071	polymers of, 516–517	solvation of cations by, 691
table of, 1072–1073	reaction with Br ₂ , 506	Crystallite, 1253
Coenzyme A, structure of, 846, 1072	reaction with HBr, 505–506	Crystallization, fractional, 161
Coenzyme Q, 653–654	stability of, 502–504	Cumene, phenol from, 650
Cofactor (enzyme), 1071	synthesis of, 501	Cumulene, structure of, 342

Curtius rearrangement, 960, 962 1,3-Cyclohexadiene, heat of strain energy of, 115 mechanism of, 962 hydrogenation of, 539 torsional strain in, 117 Curved arrow, electron movement UV absorption of, 520 Cyclopentanone, IR spectroscopy of, and, 44-45, 57-58 Cyclohexane, axial bonds in, guidelines for using, 197-198 120 - 122Cyclopentenones, from polar reactions and, 192, 197–199 barrier to ring flip in, 122 1,4-diketones, 913–915 Cyclopropane, angle strain in, 116 radical reactions and, 186, 291 bond angles in, 118 p-Cyanobenzoic acid, p K_a of, 787 chair conformation of, 118-119 bent bonds in, 116 Cyanocycline A, structure of, 793 from alkenes, 287-289 conformational analysis of, Cyanogenic glycoside, 793 126-128 molecular model of, 112, 116 Cyanohydrin(s), 733 1,3-diaxial interactions in, strain energy of, 115 from aldehydes, 733 124-125 torsional strain in, 116 from ketones, 733 drawing chair form of, 119 Cystathionine, cysteine from, 1213 Cysteine, biosynthesis of, 1213 mechanism of formation of, 733 equatorial bonds in, 120-122 uses of, 733-734 IR spectrum of, 451 disulfide bridges from, 1057 Cycloaddition reaction, 510, rate of ring-flip in, 460-461 structure and properties of, 1046 Cytosine, electrostatic potential map **1222**–1225 ring-flip in, 122 antarafacial geometry of, strain energy of, 115 of, 1132 1223-1225 twist-boat conformation of, 120 molecular model of, 66 cyclobutane synthesis and, 1225 Cyclohexane conformation, E2 protection of, 1142–1143 photochemical, 1225 reactions and, 403-404 structure of, 1129 see also Diels-Alder reaction Cyclohexanol, IR spectrum of, 654 stereochemical rules for, 1225 ¹³C NMR spectrum of, 655 D (Bond dissociation energy), 203 stereochemistry of, 1224-1225 Cyclohexanone, aldol reaction of, D (Debye), 37 suprafacial geometry of, 906 D Sugar, 1007 Fischer projections of, 1007 1223-1225 enol content of, 871 thermal, 1224 enolate ion of, 878 Dacron, structure of, 849 Cycloalkane(s), 109 IR spectrum of, 756 Darzens reaction, 942 ¹³C NMR absorptions of, 758 DCC (dicyclohexylcarbodiimide), 826 angle strain in, 114–115 Baever strain theory and, 114 Cyclohexene, heat of hydrogenation amide bond formation with, cis-trans isomerism in, 111-113 of, 539 826-827 heats of combustion of, 115 mechanism of amide formation IR spectrum of, 451 naming, 109-111 Cyclohexenones, from 1,5-diketones, with, 826-827 skeletal structures of, 109 peptide synthesis with, 1062-1063 913-915 strain energies of, 115 Cyclohexylamine, IR spectrum of, Deactivating group (aromatic 979 Cycloalkene, naming, 227–228 substitution), 581 Cyclohexylmethanol, ¹H NMR Cyclobutadiene, antiaromaticity of, acidity and, 787 542 spectrum of, 485 Debye (D), 37 electrostatic potential map of, 542 Cyclononane, strain energy of, 115 cis-Decalin, conformation of, 130 molecular model of, 130, 1108 Hückel 4n + 2 rule and, 542 Cyclooctane, strain energy of, 115 reactivity of, 542 Cyclooctatetraene, bond lengths in, trans-Decalin, conformation of, 130 Cyclobutane, angle strain in, 117 543 molecular model of, 130, 1108 conformation of, 117 dianion of, 546 Decarboxylation, 883 molecular model of, 117 electrostatic potential map of, β -keto esters and, 886 photochemical synthesis of, 1225 biological example of, 1181–1185 542-543 strain energy of, 115 Hückel 4n + 2 rule and, 542-543malonic esters and, 883-884 torsional strain in, 117 ¹H NMR absorption of, 553 pyruvate and, 1181-1185 reactivity of, 542 DEET, structure of, 865 Cyclodecane, strain energy of, 115 1,3-Cyclopentadiene, Diels-Alder 1,3,5,7,9-Cyclodecapentaene, Degenerate orbitals, 541 molecular model of, 543, 557 reactions of, 514 Degree of unsaturation, 224 Cycloheptane, strain energy of, 115 electrostatic potential map of, 974 calculation of, 224-226 pK_a of, 544 Cycloheptatriene, reaction with Br₂, Dehydration, 263 544-545 Cyclopentadienyl anion, aromaticity alcohol mass spectrum and, 657 Cycloheptatrienyl cation, aromaticity of, 544-545 alcohols, 263-264, 641-643 electrostatic potential map of, 545 aldol reaction and, 908-909 of, 544-545 electrostatic potential map of, 545 Hückel 4n + 2 rule and, 544-545biological example of, 264, 643 Hückel 4n + 2 rule and, 544-545Cyclopentane, angle strain in, 117 7-Dehydrocholesterol, vitamin D Cycloheptatrienylium bromide, conformation of, 117 from. 1232 synthesis of, 544-545 molecular model of, 117 Dehydrohalogenation, 263

Delocalized, 352 Dewar benzene, 1238 Diethyl ether, IR spectrum of, 695 Dextromethorphan, chirality of, 147 molecular model of, 676 Delta scale (NMR), 462 Denature (protein), 1068 Dextrorotatory, 148 synthesis of, 678 Dental anesthetics, 63-64 Dextrose, see Glucose Diethyl malonate, alkylation of, 883-884 Dialkylamine, p K_a of, 879 Deoxy sugar, 1024 Deoxyribonucleic acid (DNA), 1128 Diastereomers, 157 carboxylic acids from, 883-884 antisense strand of, 1136 kinds of, 164–165 Michael reactions and, 922-923 base-pairing in, 1131-1132 Diastereotopic protons (NMR), 473 pK_a of, 879 bases in, 1129 1,3-Diaxial interactions, 124-125 see also Malonic ester cleavage of, 1140 table of, 125 Diethyl propanedioate, see Diethyl consensus sequence in, 1135 Diazepam, degree of unsaturation in, malonate Digitoxigenin, structure of, 1125 double helix in, 1131-1132 224 3' end of, 1131 Diazomethane, reaction with Digitoxin, structure of, 1017 5' end of, 1131 Dihedral angle, 95 carboxylic acids, 866 exons in, 1136 Diazonio group, 969 Diiodomethane, Simmons-Smith Diazonium coupling reaction, 972 fingerprinting with, 1146–1147 reaction with, 288–289 Diisobutylaluminum hydride, heredity and, 1133 Diazoquinone-novolac resist, hydrogen-bonding in, 62, 523-524 reaction with esters, 841 1131-1132 Diazotization reaction, 968–969 structure of, 726 introns in, 1136 DIBAH, see Diisobutylaluminum Diisopropylamine, p K_a of, 878, lagging strand in, 1135 hydride 952 1,3-Diketone, p K_a of, 879 leading strand in, 1135 Dibutyl phthalate, use as plasticizer, major groove in, 1132 837 Dimethyl disulfide, bond angles in, minor groove in, 1132 Dichlorocarbene, electronic structure molecular model of, 62, 1132 Dimethyl ether, electrostatic of, 288 Okazaki fragments in, 1135 potential map of, 57, 677 electrostatic potential map of, 288 polymerase chain reaction and, from chloroform, 287 Dimethyl sulfide, molecular model 1145-1146 mechanism of formation of, 287 promotor sequence in, 1135 1,2-Dichloroethane, synthesis of, Dimethyl sulfoxide, electrostatic replication fork in, 1134 264-265 potential map of, 40 replication of, 1133–1135 cis-1,2-Dichloroethylene, electrostatic formal charges in, 40-41 S_N2 reaction and, 384 sense strand of, 1136 potential map of, 66 Dimethylallyl diphosphate, geraniol sequencing of, 1140-1141 trans-1,2-Dichloroethylene, electrostatic potential map of, biosynthesis and, 395-396 size of, 1129 structure of, 1130-1131 biosynthesis of, 1103–1105 synthesis of, 1142-1144 2,4-Dichlorophenoxyacetic acid, cis-1,2-Dimethylcyclohexane, transcription of, 1135–1136 synthesis of, 652 conformational analysis of, Watson-Crick model of, Dideoxy DNA sequencing, 1140-1141 126 - 1271131-1132 2',3'-Dideoxyribonucleotide, molecular model of, 126, 112 Deoxyribonucleotide, structures of, 1140-1141 trans-1,2-Dimethylcyclohexane, Dieckmann cyclization, 919-920 conformational analysis of, 1130 2'-Deoxyribose, structure of, 1129 mechanism of, 919-920 127 equilibrium forms of, 1031 Diels-Alder reaction, 510 molecular model of, 127, 112 1-Deoxyxylulose 5-phosphate characteristics of, 511–512 Dimethylformamide, S_N2 reaction pathway, terpenoid dienes in, 513-514 and, 384 biosynthesis and, 1099 dienophiles in, 511 2,2-Dimethylpropane, mass spectrum DEPT-NMR, 467-469 electrostatic potential map of, 510 of, 427 molecular model of, 82 uses of, 467-468 endo stereochemistry of, 512 DEPT-NMR spectrum, HOMO in, 1224 *N,N*-Dimethyltryptamine, LUMO in, 1224 electrostatic potential map of, 6-methyl-5-hepten-2-ol, 468 Dermabond, structure of, 1244 mechanism of, 510 Dess-Martin periodinane, alcohol s-cis diene conformation in, 2,4-Dinitrophenylhydrazone, 738 from aldehydes, 739 oxidations with, 645-646 513-514 reaction with alcohols, 645 stereochemistry of, 512, 1224 from ketones, 739 suprafacial geometry of, 1224 Diol, 282 structure of, 645 Detergent, structure of, 1093 Diene polymers, 516–517 1,2-Diol, cleavage of, 285-286 from alkenes, 282-284 Deuterium isotope effect, 400 vulcanization of, 517 E1 reaction and, 406 Dienophile, 511 from epoxides, 282-283, 686-687 requirements for, 511 reaction with HIO₄, 285-286 E2 reaction and, 400

Diorganocopper reagent, conjugate Drugs, approval procedure for, Electromagnetic radiation, 434-436 213-214 carbonyl addition reactions of, amplitude of, 435 754-755 chiral, 172-173 characteristics of, 435 reaction with acid chlorides, origin of, 213 energy of, 435-436 frequency of, 435 833-834 see also Gilman reagent E configuration, 231–232 kinds of, 434 Diovan, synthesis of, 359 assignment of, 231-232 wavelength of, 435 Dioxane, use of, 685 E1 reaction, 398, 405-406 Electromagnetic spectrum, 434 DiPAMP ligand, amino acid synthesis regions in, 434 carbocations and, 405 and, 1055 deuterium isotope effect and, Electron, lone-pair, 8 Diphosphate, as leaving group, 406 nonbonding, 8 395-396 kinetics of, 406 Electron configuration, ground Dipole moment (μ) , 37 mechanism of, 405 state, 5 halomethanes, 346 rate-limiting step in, 406 rules for assigning, 5 stereochemistry of, 406 polar covalent bonds and, 37-38 table of, 5 table of, 38 Electron movement, curved arrows Zaitsev's rule and, 406 Dipole-dipole forces, 60-61 E1cB reaction, 398, 406-407 and, 44-45, 57-58, 197-198 Dipropyl ether, ¹H NMR spectrum of, carbanion intermediate in, fishhook arrows and, 186, 291 696 406-407 Electron shell, 4 Disaccharide, 1025-1027 mechanism of, 406-407 Electron-dot structure, 7 $1\rightarrow$ 4-link in, 1025–1026 E2 reaction, 398, 399-402 Electronegativity, 35 synthesis of, 1029-1030 alcohol oxidation and, 646 inductive effects and, 36 Dispersion forces, 61 anti periplanar geometry of, polar covalent bonds and, 35-36 alkanes and, 93 401-402 table of, 35 Disrotatory motion, 1218 cyclohexane conformation and, Electrophile, 192 characteristics of, 197-198 Distortionless enhancement by 403-404 polarization transfer, see deuterium isotope effect and, 400 curved arrows and, 197-198 **DEPT-NMR** kinetics of, 400 electrostatic potential maps of, mechanism of, 400 192 Disulfide(s), 692 electrostatic potential map of, 79 menthyl chloride and, 404 examples of, 192 from thiols, 692 neomenthyl chloride and, 404 Electrophilic addition reaction, hybridization of, 19 rate law for, 400 **194**–196, **237**–238 carbocation rearrangements in, reduction of, 692 stereochemistry of, 401-402 thiols from, 692 Zaitsev's rule and, 403 249-250 Disulfide bridge, peptides and, Easter Island, rapamycin from, chirality and, 296-298 1057 251-252 energy diagram of, 206, 208, 238 Diterpene, 300 Eclipsed conformation, ethane and, Hammond postulate and, 248 Diterpenoid, 1098 95 intermediate in, 208 DMAPP, see Dimethylallyl molecular model of, 95 Markovnikov's rule and, 240-241 mechanism of, 195-196, diphosphate Edman degradation, 1059-1061 DMF, see Dimethylformamide mechanism of, 1059-1061 237-238 DMSO, see Dimethyl sulfoxide Eicosanoid(s), 1096-1098 regiospecificity of, 240-241 DMT (dimethoxytrityl ether), DNA biosynthesis of, 1097–1098 transition state in, 248 synthesis and, 1142 naming, 1096-1097 Electrophilic aromatic substitution DNA, see Deoxyribonucleic acid Elaidic acid, from vegetable oil, reaction, 566 DNA fingerprinting, 1146–1147 arylamines and, 966-968 1091 reliability of, 1147 Elastomer, 1255 biological example of, 571 characteristics of, 1255 inductive effects in, 583 STR loci and, 1146 kinds of, 566-567 Dopamine, molecular model of, cross-links in, 1255 $T_{\rm g}$ of, 1255 mechanism of, 568-569 957 Double bond. 13 Electrocyclic reaction, 1217–1222 orientation in. 580-581 electronic structure of, 14 conrotatory motion in, 1219 pyridine and, 976 disrotatory motion in, 1218 length of, 15 pyrrole and, 974–975 molecular orbitals in, 21 examples of, 1217-1218 resonance effects in, 584 HOMO and, 1219-1221 substituent effects in, 580-581 see also Alkene strength of, 14 photochemical, 1221-1222 Electrophoresis, 1052–1053 Double helix (DNA), 1131–1132 stereochemical rules for, 1222 DNA sequencing and, 1141 Doublet (NMR), 478 stereochemistry of, 1219-1222 Electrospray ionization (ESI) mass Downfield (NMR), 461 thermal, 1219-1220 spectrometry, 433

Electrostatic potential map, 36 cyclooctatetraene, 542-543 protonated methanol, 190 acetaldehyde, 714 1,3-cyclopentadiene, 974 purine, 978 acetamide, 820, 951 cyclopentadienyl anion, 545 pyridine, 546 acetate ion, 42, 52, 55, 784 cytosine, 1132 pyrimidine, 546 acetic acid, 52, 54 dichlorocarbene, 288 pyrrole, 547, 974 acetic acid dimer, 782 cis-1,2-dichloroethylene, 66 pyrrolidine, 974 trans-1,2-dichloroethylene, 66 acetic anhydride, 820 S_N2 reaction, 377 acetone, 54, 56, 79 Diels-Alder reaction, 510 sulfide, 79 acetone anion, 55 dimethyl ether, 57, 677 thioanisole, 804 acetonitrile, 794 dimethyl sulfoxide, 40 thioester, 820 acetyl azide, 859 *N,N*-dimethyltryptamine, 979 thiol, 79 acetyl chloride, 820 disulfide, 79 thymine, 1132 acetylene, 317 DNA base pairs, 1132 toluene, 585 electrophiles, 192 trifluoromethylbenzene, 585 acetylide anion, 326 acid anhydride, 820 enamine, 925 trimethylamine, 949 enol. 873 2,4,6-trinitrochlorobenzene, 592 acid chloride, 820 enolate ion, 878, 881 acyl cation, 578 vinylic anion, 326 adenine, 1132 ester, 820 vinylic carbocation, 318 alanine, 1045 ether, 78 water, 52 alcohol, 78 ethoxide ion, 784 zwitterion, 1045 alkene, 78, 194 ethyl carbocation, 245 Elimination reaction, 185, 397 alkyl halide, 78 ethylene, 75, 194 biological examples of, 407 alkyne, 78 ethylene oxide, 685 summary of kinds of, 407 allylic carbocation, 390, 506 fatty acid carboxylate, 1093 Embden-Meyerhof pathway, amide, 820 formaldehyde, 216, 730 1173-1181 amine, 79 see also Glycolysis formate ion, 784 amine hydrogen-bonding, 948 Grignard reagent, 356 Enamido acid, amino acids from, ammonia, 192 guanine, 1132 1055 aniline, 953 histidine, 1049 Enamine(s), 736 anilinium ion, 953 HSO_3^+ ion, 572 conjugate addition reactions of, hydrogen bond, 61, 623 anisole, 804 925-926 [18]annulene, 553 electrostatic potential map of, 925 hydronium ion, 192 arene, 78 hydroxide ion, 52, 192 from aldehydes, 736-739 azulene, 558 imidazole, 60, 547 from ketones, 736-739 benzaldehyde, 583, 730 isopropyl carbocation, 245 mechanism of formation of. benzene, 43, 539, 583 menthene, 75 738-739 methanethiol, 216 nucleophilicity of, 924-925 benzenediazonium ion, 972 benzoquinone, 653 methanol, 36, 54, 56, 190, 623 pH dependence of formation, 739 methoxide ion, 55, 627 benzyl carbocation, 390 reaction with enones, 925-926 benzyne, 595 methyl acetate, 820 Stork reaction of, 925-926 borane, 273 methyl anion, 326 Enantiomeric excess, 761 boron trifluoride, 57, 194 methyl carbocation, 245 Enantiomers, 143 bromoethane, 194 methyl thioacetate, 820 discovery of, 150 bromomethane, 192 9-methyladenine, 1149 resolution of, 161–163 bromonium ion, 266 methylamine, 56, 951 Enantioselective synthesis, 173, 1,3-butadiene, 504 N-methylguanine, 1149 760-761 3-buten-2-one, 752 methyllithium, 36, 190 Enantiotopic protons (NMR), 472 tert-butyl carbocation, 245 methylmagnesium iodide, 356 Endergonic, 201 butyllithium, 357 naphthalene, 550 Endergonic reaction, Hammond carbanion, 326 nitrile, 794 postulate and, 247 carbocation, 245, 288 nitronium ion, 572 Endo stereochemistry, Diels-Alder carbonyl compound, 79, 192 nucleophiles, 192 reaction and, 512 carboxylic acid derivatives, 820 1,3-pentadiene, 504 Endothermic, 202 chlorobenzene, 583 phenol, 583 -ene, alkene name suffix, 226 phenoxide ion, 627 Energy diagram, 206-207 chloromethane, 37, 190, 346 conjugated diene, 504 phosphate, 78 activation energy in, 206 crown ether, 691 polar covalent bonds and, 36 biological reactions and, 209 cyclobutadiene, 542 propenal, 511 electrophilic addition reactions cycloheptatrienyl cation, 545 propenenitrile, 511 and, 206, 208

Energy diagram—cont'd Epoxidation, enantioselective from alcohols, 644 endergonic reactions and, 206-207 method of, 761 from carboxylates, 824 exergonic reactions and, 206-207 Epoxide(s), 281 from carboxylic acids, 824-826 intermediates and, 208 acid-catalyzed cleavage of, hydrolysis of, 837-840 reaction coordinate in, 206 282–283, 686–688 IR spectroscopy of, 444, 851 transition state in, 206 base-catalyzed cleavage of, mechanism of hydrolysis of, Energy difference, equilibrium 689-690 838-839 position and, 123-124 1,2-diols from, 282-283, 686-687 mechanism of reduction of, 840-841 Enflurane, molecular model of, 147 from alkenes, 281-282 naming, 816 Enol, 319, 871 from halohydrins, 282 NMR spectroscopy of, 852 electrostatic potential map of, 873 mechanism of acid-catalyzed nucleophilic acyl substitution cleavage of, 282-283, 686-688 from acid bromides, 877 reactions of, 837-842 from aldehydes, 871-872 NMR spectroscopy of, 696 occurrence of, 836 from ketones, 871–872 reaction with acids, 282-283, partial reduction of, 841 mechanism of formation of, 686–688 pK_a of, 879 reaction with amines, 689-690 871-872 reaction with amines, 840 reactivity of, 873-874 reaction with base, 689-690 reaction with DIBAH, 841 Enolate ion, 872 reaction with Grignard reagents, reaction with Grignard reagents, alkylation of, 882–889 635, 842 electrostatic potential map of, 878, reaction with HX, 687-688 reaction with LDA, 888 reaction with LiAlH₄, 705 reaction with LiAlH₄, 632–633, halogenation of, 881-882 reduction of, 705 840-841 reaction with Br₂, 881–882 S_N 2 reactions of, 383 reduction of, 632-633, 840-841 synthesis of, 281-282 reactivity of, 881-882 saponification of, 838 resonance in, 878 Epoxy resin, preparation of, 697–698 uses of, 837 stability of, 878 prepolymer for, 697–698 Ester group, directing effect of, Enone, conjugate carbonyl addition 1,2-Epoxypropane, ¹H NMR spectrum 588-589 reactions of, 751-755 of, 696 Estradiol, structure and function of, from aldehydes, 908-909 Equatorial bonds (cyclohexane), 120 1110 from aldol reaction, 908–909 drawing, 121 Estrogen, 1110 from ketones, 908-909 Equilibrium constant (K_{eq}) , 200 function of, 1110 IR spectroscopy of, 757 free-energy change and, 201 Estrone, conformation of, 131 Michael reactions of, 922-923 Equilibrium position, energy structure and function of, 1110 molecular orbitals of, 909 difference and, 123-124 synthesis of, 927-928, 1240 reaction with amines, 753 Ergocalciferol, structure of, 1232 Ethane, bond angles in, 12 Ergosterol, UV absorption of, 532 reaction with enamines, 925-926 bond lengths in, 12 reaction with Gilman reagents, vitamin D from, 1232 bond rotation in, 94-95 754-755 Erythronolide B, structure of, 176 bond strengths in, 12 reaction with water, 753 Erythrose, configuration of, 1009 conformations of, 94-95 eclipsed conformation of, 95 synthesis of, 876 Eschenmoser, Albert, 333 Enthalpy change (ΔH) , 202 Essential amino acid, 1049 molecular model of, 13, 81 explanation of, 202 Essential carbohydrate, 1023–1025 rotational barrier in, 95 Entropy change (ΔS), 202 function of, 1024 sp^3 hybrid orbitals in, 12–13 explanation of, 202 Essential oil, 299 staggered conformation of, 95 Enzyme, **210**, **1068**–1070 Ester(s), 814 structure of, 12-13 torsional strain in, 95 active site in, 210–211 acid-catalyzed hydrolysis of, 839 classification of, 1070 alcohols from, 632-633, 840-842 Ethanol, history of, 658 naming, 1070 aldehydes from, 725-726, 841 industrial synthesis of, 270, Protein Data Bank and, 1076–1077 alkylation of, 888 620-621 amides from, 840 IR spectrum of, 436 rate acceleration of, 1068-1069 specificity of, 1069 aminolysis of, 840 LD_{50} of, 24 substrate of, 1069 base-catalyzed hydrolysis of, 838 metabolism of, 658 physiological effects of, 658 turnover number of, 1069 β -keto esters from, 919–920 X-ray crystal structures of, 447 carbonyl condensation reactions pK_a of, 51, 625 of, 915-917 Enzyme-substrate complex, 1069 toxicity of, 658 Ephedrine, structure of, 63 carboxylic acids from, 837-840 Ethene, see Ethylene Epichlorohydrin, epoxy resins from, electrostatic potential map of, 820 Ether(s), 676 697-698 from acid anhydrides, 835 alcohols from, 681-682 Epimer, 157-158 from acid chlorides, 831 alkyl halides from, 681-682

boiling points of, 677 bond angles in, 677 Claisen rearrangement of, 683-684 cleavage of, 681-682 electrostatic potential map of, 78 from alcohols, 678–680 from alkenes, 680 from alkyl halides, 678-679 IR spectroscopy of, 695 naming, 677 NMR spectroscopy of, 696 peroxides from, 678 properties of, 677-678 reaction with HBr, 681-682 synthesis of, 678-680 uses of, 676 Ethoxide ion, electrostatic potential map of, 784 Ethyl acetate, ethyl acetoacetate from, 916 ¹H NMR spectrum of, 852 Ethyl acetoacetate, mixed aldol reactions of, 913 see Acetoacetic ester Ethyl acrylate, ¹³C NMR absorptions in, 466 Ethyl alcohol, see Ethanol Ethyl benzoate, mixed Claisen condensation reaction of, 917-918 ¹³C NMR spectrum of, 492 Ethyl carbocation, electrostatic potential map of, 245 Ethyl formate, mixed Claisen condensation reaction of, 917-918 Ethyl group, 84 Ethylcyclopentane, mass spectrum of, 429 Ethylene, bond angles in, 14 bond lengths in, 14 bond strengths in, 14-15 Ethylene, electrostatic potential maps of, 194 electrostatic potential map of, 75 ethanol from, 270 heat of hydrogenation of, 236 hormonal activity of, 222 industrial preparation of, 223 molecular model of, 14 molecular orbitals of, 21, 1215 pK_a of, 326 polymerization of, 290–292 reaction with HBr, 194-196 sp² hybrid orbitals in, 13–14 structure of, 13–15 uses of, 223 Ethylene dichloride, synthesis of, 264-265

Ethylene glycol, acetals from, 745 manufacture of, 282 uses of, 282 Ethylene oxide, electrostatic potential map of, 685 industrial synthesis of, 685 uses of, 685 2-Ethyl-1-hexanol, synthesis of, 910-911 N-Ethylpropylamine, mass spectrum of, 982 Ethynylestradiol, structure and function of, 1111 von Euler, Ulf Svante, 1095 Exergonic, 201 Exergonic reaction, Hammond postulate and, 247 Exo stereochemistry, Diels-Alder reaction and, 512 Exon (DNA), 1136 Exothermic, 202

FAD, see Flavin adenine dinucleotide, FADH₂, Flavin adenine dinucleotide (reduced), 1163 Faraday, Michael, 536 Farnesyl diphosphate, biosynthesis of, 1105 Fat(s), 1089-1090 catabolism of, 1158-1167 composition of, 1090 hydrolysis of, 839-840, 1158-1161 saponification of, 1092 Fatty acid(s), 1089 acetyl CoA from, 1162-1167 anabolism of, 1167–1173 biosynthesis of, 1167–1173 catabolism of, 1162-1167 melting point trends in, 1091 number of, 1089 polyunsaturated, 1089 table of, 1090 Favorskii reaction, 901 Fehling's test, 1020 Fen-Phen, structure of, 962 crystallites in, 1255

Fen-Phen, structure of, 962
Fiber, 1255
crystallites in, 1255
manufacture of, 1255
Fieser, Louis F., 1010
Fingerprint region (IR), 439
First-order reaction, 386
Fischer, Emil, 1002, 1022
Fischer esterification reaction,

824–826 mechanism of, 824–825 Fischer projection, 1002–1005

Fischer projection, 1002–1005 carbohydrates and, 1004–1005 conventions for, 1003 D sugars, 1007
L, sugars, 1007
rotation of, 1003–1004
R,S configuration of, 1004
Fishhook arrow, radical reactions and, 186, 291
Flavin adenine dinucleotide,

biological hydroxylation and, 573–574 mechanism of, 1163–1164 structure and function of, 1072, 1163–1164

(reduced), structure of, 1163 Fleming, Alexander, 853 Flexibilene, structure of, 1123 Florey, Howard, 853

Flavin adenine dinucleotide

Fluorenylmethyloxycarbonyl (Fmoc) protecting group, 1062–1063 Fluorination (aromatic), 570 Fluoromethane, bond length of, 346

bond strength of, 346 dipole moment of, 346 Fluoxetine, molecular model of, 170 stereochemistry of, 170 synthesis of, 709

Fmoc (fluorenylmethyloxycarbonyl amide), 1062–1063 amino acid derivatives of,

1062–1063 Food, catabolism of, 1155 Food and Drug Administration (FDA),

213
Formal charge, 39–41
calculation of, 40–41
summary table of, 41

Formaldehyde, dipole moment of, 38 electrostatic potential map of, 216, 730

hydrate of, 731 industrial synthesis of, 722–723 mixed aldol reactions of, 912 reaction with Grignard reagents, 635

uses of, 722

Formate ion, bond lengths in, 784 electrostatic potential map of, 784 Formic acid, bond lengths in, 784 pK_a of, 783 Formyl group, **724** p-Formylbenzoic acid, pK_a of, 787

Fourier-transform NMR spectroscopy (FT-NMR), **463**–464 Fractional crystallization, resolution

and, 161 Fragmentation (mass spectrum),

426–429 Free radical, **187** *see also* Radical Free-energy change (ΔG), 201 Geminal (gem), 731 Glutamine, structure and properties standard, 201 Genome, size of in humans, 1135 of, 1046 Fremy's salt, 653 Gentamicin, structure of, 1031 Glutaric acid, structure of, 780 Frequency (ν) , 435 Geraniol, biosynthesis of, 395-396 Glutathione, function of, 692 Friedel-Crafts acylation reaction, Geranyl diphosphate, biosynthesis of, prostaglandin biosynthesis and, 577-578 1097-1098 acyl cations in, 577-578 monoterpenes from, 1106 structure of, 693 arylamines and, 967 Gibbs free-energy change (ΔG), 201 Glycal, 1030 mechanism of, 577-578 standard, 201 Glycal assembly method, 1030 Friedel-Crafts alkylation reaction, equilibrium constant and, 201 (+)-Glyceraldehyde, absolute **575**–577 Gilman reagent, 357 configuration of, 1006-1007 conjugate carbonyl addition arylamines and, 967 (−)-Glyceraldehyde, configuration of, biological example of, 578-579 reactions of, 754-755 153 - 154limitations of, 575-576 organometallic coupling reactions (R)-Glyceraldehyde, Fischer mechanism of, 575 of, 357-358 projection of, 1003 reaction with acid chlorides, polyalkylation in, 576 molecular model of, 1003 rearrangements in, 576-577 833-834 Glyceric acid, structure of, 780 Frontier orbitals, 1216 reaction with alkyl halides, Glycerol, catabolism of, 1158–1161 Fructose, anomers of, 1012–1013 357-358 sn-Glycerol 3-phosphate, naming of, furanose form of, 1012-1013 reaction with enones, 754-755 1161 sweetness of, 1033 Glass transition temperature Glycerophospholipid, 1094 (polymers), 1254 Glycine, structure and properties of, Fructose-1,6-bisphosphate aldolase, X-ray crystal structure of, 447 Glucocorticoid, 1111 1046 Fucose, biosynthesis of, 1043 Gluconeogenesis, 1191-1197 Glycoconjugate, 1019 structure of, 1024 mechanisms in, 1192-1197 influenza virus and, 1032 Fukui, Kenichi, 1216 overall result of, 1197 Glycogen, structure and function of, Fumaric acid, structure of, 780 steps in, 1192–1193 1029 Functional group, 74–79 Glucosamine, biosynthesis of, 1040 Glycol, 282, 686 carbonyl compounds and, 79 structure of, 1031 Glycolic acid, structure of, 780 electronegative atoms in, 78-79 Glucose, α anomer of, 1012 Glycolipid, 1019 importance of, 74-75 anabolism of, 1191-1197 Glycolysis, 1173–1181 IR spectroscopy of, 439–444 anomers of, 1012 mechanisms in, 1174-1181 multiple bonds in, 75, 78 β anomer of, 1012 overall result of, 1181 polarity patterns of, 191 biosynthesis of, 1191-1197 steps in, 1174-1175 table of, 76-77 catabolism of, 1173-1181 Glycoprotein, 1019 Functional RNAs, 1135 chair conformation of, 120, 128 biosynthesis of, 1019 Furan, industrial synthesis of, 973 configuration of, 1009 Glycoside, 1016 Furanose, 1012–1013 Fischer projection of, 1005 occurrence of, 1017 fructose and, 1012-1013 synthesis of, 1017-1018 from pyruvate, 1191–1197 glycosides of, 1016–1018 Glyptal, structure of, 1260 γ, see Gamma keto-enol tautomerization of, GPP, see Geranyl diphosphate Gabriel amine synthesis, 957 Graft copolymer, 1248 1175-1176 Koenigs-Knorr reaction of, synthesis of, 1248 Galactose, biosynthesis of, 1040 configuration of, 1009 1017-1018 Grain alcohol, 620 Wohl degradation of, 1023 molecular model of, 120, 128, 1012 Green chemistry, 409-410, 982-984 Gamma-aminobutyric acid, structure mutarotation of, 1013 ibuprofen synthesis by, 410 of, 1048 pentaacetyl ester of, 1015-1016 ionic liquids and, 982-984 Gamma rays, electromagnetic pentamethyl ether of, 1016 principles of, 409–410 spectrum and, 434 pyranose form of, 1011–1012 Grignard, François Auguste Victor, Ganciclovir, structure and function pyruvate from, 1173-1181 of. 1153 reaction with acetic anhydride, Grignard reaction, aldehydes and, Gasoline, manufacture of, 100-101 1015-1016 635 octane number of, 100-101 carboxylic acids and, 636 reaction with ATP, 1158 Gatterman-Koch reaction, 617 reaction with iodomethane, 1016 esters and, 635 Gauche conformation, 97 formaldehyde and, 635 sweetness of, 1033 ketones and, 635 butane and, 97 Williamson ether synthesis with, steric strain in, 97 limitations of, 636 Gel electrophoresis, DNA sequencing Glutamic acid, structure and mechanism of, 735 and, 1141 properties of, 1047 strategy for, 637

Grignard reagent, 355	exergonic reactions and, 247	electrocyclic reactions and,
alkanes from, 356	Markovnikov's rule and, 248	1219–1221
carboxylation of, 790	S _N 1 reaction and, 389	UV spectroscopy and, 518
carboxylic acids from, 790	Handedness, molecular, 143–146	Histamine, structure of, 989
electrostatic potential map of, 356	HDL, heart disease and, 1118	Histidine, electrostatic potential map
from alkyl halides, 355–356	Heart disease, cholesterol and, 1118	of, 1049
reaction with acids, 356	statin drugs and, 1203–1204	structure and properties of, 1047
reaction with aldehydes, 635, 735	Heat of combustion, 115	HMG-CoA reductase, active site in,
reaction with carboxylic acids, 636	Heat of hydrogenation, 235	1204
reaction with CO ₂ , 790	table of, 236	statin drugs and, 1203–1204
reaction with epoxides, 690	Heat of reaction, 202	HMPA, see,
reaction with esters, 635, 842	Helicase, DNA replication and, 1133	Hexamethylphosphoramide
reaction with formaldehyde, 635	Hell–Volhard–Zelinskii reaction,	Hoffmann, Roald, 1215
reaction with ketones, 635, 735	876–877	Hoffmann-LaRoche Co., vitamin C
reaction with nitriles, 796	amino acid synthesis and, 1053	synthesis and, 800–801
reaction with oxetanes, 708	mechanism of, 877	Hofmann elimination reaction,
Grubbs catalyst, olefin metathesis	Heme, biosynthesis of, 994	964–965
polymerization and, 1251	structure of, 973	biological example of, 965
Guanine, electrostatic potential map	Hemiacetal, 743	mechanism of, 964–965
of, 1132	Hemiketal, 743	molecular model of, 965
protection of, 1142–1143 structure of, 1129	Hemithioacetal, 1179	regiochemistry of, 964–965
Gulose, configuration of, 1009	Henderson–Hasselbalch equation,	Zaitsev's rule and, 964–965 Hofmann rearrangement, 960 –962
Guncotton, 1028	amines and, 954 amino acids and, 1050–1051	mechanism of, 960, 962
Gutta-percha, structure of, 516	biological acids and, 785 –786	HOMO, see Highest occupied
Gutta-perena, structure or, 510	Hertz (Hz), 435	molecular orbital
$\Delta H^{\circ}_{\text{hydrog}}$ (heat of hydrogenation),	Heterocycle, 546, 972	Homocysteine, structure of, 1048
235	aromatic, 546–548	Homolytic bond-breaking, 186
Hagemann's ester, synthesis of, 940	polycyclic, 977–978	Homopolymer, 1246
Halo group, directing effect of,	Heterocyclic amine, 946	Homotopic protons (NMR), 472
587–588	basicity of, 950	Honey, sugars in, 1027
inductive effect of, 583	names for, 946	Hormone, 1110
orienting effect of, 581	Heterolytic bond-breaking, 186	sex, 1110
resonance effect of, 584	Hevea brasieliensis, rubber from, 516	Hückel, Erich, 541
Haloalkane, see Alkyl halide	Hexachlorophene, synthesis of, 616,	Hückel $4n + 2$ rule, 541
Haloform reaction, 882	652	cyclobutadiene and, 542
Halogen, inductive effect of, 583	Hexamethylphosphoramide,	cycloheptatrienyl cation and,
resonance effect of, 584	$S_{ m N}2$ reaction and, 384	544–545
Halogenation, aldehydes and,	Hexane, IR spectrum of, 440	cyclooctatetraene and, 542–543
874–876	mass spectrum of, 428	cyclopentadienyl anion and,
alkenes and, 264–266	1,3,5-Hexatriene, molecular orbitals	544–545
alkynes and, 317–318	of, 1216	explanation of, 543
aromatic compounds and,	UV absorption of, 520	imidazole and, 547
567–571	1-Hexene, IR spectrum of, 440	molecular orbitals and, 543
biological example of, 267	2-Hexene, mass spectrum of, 430	pyridine and, 546–547
carboxylic acids and, 876–877	Hexokinase, active site in, 211	pyrimidine and, 546–547
ketones and, 874–876	molecular model of, 211	pyrrole and, 547
Halohydrin, 267	1-Hexyne, IR spectrum of, 440	Hughes, Edward Davies, 376
epoxides from, 282	High-density polyethylene, synthesis	Human fat, composition of, 1090
reaction with base, 282	of, 1246	Human genome, size of, 1135, 1142
Halomon, anticancer activity of,	High-molecular-weight polyethylene,	Humulene, structure of, 299
362–363	uses of, 1246 High-pressure liquid chromatography,	Hund's rule, 5
biosynthesis of, 267	amino acid analyzer and,	sp Hybrid orbitals, 16 –17 sp ² Hybrid orbitals, 14
Haloperoxidase, bromohydrin formation and, 269	1058–1059	sp^{2} Hybrid orbitals, 11–13
Hammond, George Simms, 247	Highest occupied molecular orbital	Hydrate, from aldehydes, 731–732
Hammond postulate, 247–248	(HOMO), 518 , 1216	from ketones, 731–732
carbocation stability and, 248	cycloaddition reactions and,	Hydration, alkene, 269 –274
endergonic reactions and, 247	1224–1225	alkyne. 319–321

Hydrazine, reaction with aldehydes,	Hydroxide ion, electrostatic potential	Infrared spectroscopy, 437–444
741–742	map of, 52, 192	acid anhydrides, 851
reaction with ketones, 741–742	Hydroxyacetic acid, pK_a of, 783	acid chlorides, 851
Hydride shift, 249–250	<i>p</i> -Hydroxybenzaldehyde, p K_a of, 628	alcohols, 443, 654
Hydroboration, alkene, 272–274	p -Hydroxybenzoic acid, p K_a of, 787	aldehydes, 444, 756–757
alkyne, 321–322	Hydroxyl group, directing effect of,	alkanes, 442
mechanism of, 274	586–587	alkenes, 442–443
regiochemistry of, 273-274,	inductive effect of, 583	alkynes, 443
484–485	orienting effect of, 581	amides, 851
stereochemistry of, 273–274	resonance effect of, 584	amines, 444, 979
Hydrocarbon, 81	Hydroxylation (alkene), 282–284	aromatic compounds, 443, 551
acidity of, 326	Hydroxylation (aromatic), 573–574	bond stretching in, 438
saturated, 81	Hyperconjugation, 235–236	carbonyl compounds, 444
unsaturated, 224	alkenes and, 235–236	carboxylic acid derivatives, 851
Hydrochloric acid, p K_a of, 51	carbocation stability and, 245	carboxylic acids, 797–798
Hydrocortisone, conformation of,		esters, 444, 851
136	Ibuprofen, chirality and, 173	ethers, 695
structure and function of, 1111	green synthesis of, 410	explanation of, 438
Hydrogen bond, 61 –62	molecular model of, 66, 173	fingerprint region in, 439–441
alcohols and, 623	NSAIDs and, 555	ketones, 444, 756–757
amines and, 948	stereochemistry of, 172–173	lactones, 851
biological consequences of, 62	synthesis of, 790	molecular motions in, 438
carboxylic acids and, 782	Idose, configuration of, 1009	nitriles, 798
DNA base pairs and, 1131–1132	Imidazole, aromaticity of, 547	phenols, 655
electrostatic potential map of, 61,	basicity of, 950, 975	regions in, 440–441
623	electrostatic potential map of, 60,	table of absorptions in, 439–441
Hydrogen molecule, bond length in, 10	547	vibrations in, 438
bond strength in, 10	Hückel $4n + 2$ rule and, 547	Infrared spectrum, benzaldehyde, 756
molecular orbitals in, 20	Imide(s), 957	butanoic acid, 798
Hydrogen peroxide, reaction with	hydrolysis of, 957	cyclohexane, 451
organoboranes, 272–273	Imine(s), 736	cyclohexanol, 654
[1,5] Hydrogen shift, 1228	from aldehydes, 736–739	cyclohexanone, 756
Hydrogenation, 276	from ketones, 736–739	cyclohexene, 451
alkenes, 276–280	mechanism of formation of,	cyclohexylamine, 979
alkynes, 322–323	736–737	diethyl ether, 695
aromatic compounds, 599	pH dependence of formation, 739	ethanol, 436
biological example of, 280	see also Schiff base	hexane, 440
catalysts for, 277	IND, see Investigational new drug, 213	1-hexene, 440
mechanism of, 277–278	Indole, aromaticity of, 550	1-hexyne, 440
stereochemistry of, 277–278	electrophilic substitution reaction	phenol, 655
steric hindrance and, 278–279	of, 978	phenylacetaldehyde, 445
trans fatty acids from, 279–280	structure of, 946	phenylacetylene, 446
vegetable oil, 1091	Indolmycin, biosynthesis of, 889–890	toluene, 551
Hydrogenolysis, benzyl esters and,	Inductive effect, 36, 583	Ingold, Christopher Kelk, 376
1062	alcohol acidity and, 625	Initiation step (radical reaction), 188
Hydrolase, 1070	carbocation stability and, 245	Insulin, disulfide bridges in, 1057
Hydrolysis, 821	carboxylic acid strength and,	structure of, 1057
amides, 843–844	786–787	Integration (NMR), 476
biological, 839–840, 844	electronegativity and, 36 electrophilic aromatic substitution	Intermediate, See Reaction
esters, 837–840	. The state of the	intermediate
fats, 839–840	and, 583 polar covalent bonds and, 36	Intoxilyzer test, 658
nitriles, 795–796	-	Intramolecular aldol reaction, 913–915
proteins, 844 Hydronium ion, electrostatic	Influenza virus, classification of, 1032	mechanism of, 914–915
Hydronium ion, electrostatic	glycoconjugates and, 1032	Intramolecular Claisen condensation,
potential map of, 192	Infrared radiation, electromagnetic	
Hydrophilic, 62 Hydrophobic, 62	spectrum and, 434	see Dieckmann cyclization
Hydroquinone, 653	energy of, 437 frequencies of, 437	Intron (DNA), 1136 Invert sugar, 1027
from quinones, 653	wavelengths of, 437	Investigational new drug (IND), 213
nom quinones, 000	wavelengths of, 10/	mresugational new drug (mvD), 213

Iodination (aromatic), 570–571 Iodoform reaction, 882	Isoquinoline, aromaticity of, 550 electrophilic substitution reaction	mechanism of hydration of, 731–732
Iodomethane, bond length of, 346	of, 978	mechanism of reduction of, 734
bond strength of, 346	Isotactic polymer, 1245	naming, 724
dipole moment of, 346	Isotope, 3	NMR spectroscopy of, 757–758
Ion pair, 388	IUPAC nomenclature, 87	oxidation of, 728
S _N 1 reaction and, 388	new system, 227–228	oximes from, 737–738
Ion-exchange chromatography,	old system, 227	pK _a of, 879
amino acid analyzer and,		protecting groups for, 745
1058–1059	J, see Coupling constant, 478	reaction with alcohols, 742–744
Ionic bond, 7		reaction with amines, 736–739
Ionic liquids, green chemistry and,	$K_{\rm a}$ (acidity constant), 50	reaction with Br ₂ , 874–876
982–984	K _b (basicity constant), 949	reaction with
properties of, 983	$K_{\rm eq}$ (equilibrium constant), 200	2,4-dinitrophenylhydrazine,
structures of, 982–983	Kekulé, Friedrich August, 6	739
IPP, see Isopentenyl diphosphate	Kekulé structure, 7	reaction with Grignard reagents,
IR, see Infrared	Keratin, α helix in, 1066–1067	635, 735
Iron, reaction with nitroarenes, 955	Kerosene, composition of, 100	reaction with HCN, 733
Iron(III) bromide, aromatic	Ketal, 742	reaction with H_2O , 731–732
bromination and, 568	see also Acetal	reaction with HX, 732–733
Iron sulfate, LD ₅₀ of, 24	Keto-enol tautomerism, 319,	reaction with hydrazine, 741–742
Isoamyl group, 90	871–872	reaction with KMnO ₄ , 728
Isobutane, molecular model of, 81	Ketone(s), 722	reaction with LDA, 888
Isobutyl group, 85	acetals from, 742–744	reaction with LiAlH ₄ , 630, 734
Isobutylene, polymerization of, 1243	acidity of, 877–880	reaction with lithium
Isoelectric point (pI), 1051–1052	alcohols from, 630-631, 734-735	diisopropylamide, 878
calculation of, 1052	aldol reaction of, 906	reaction with NaBH ₄ , 630, 734
table of, 1046–1047	alkanes from, 741–742	reaction with NH_2OH , 737–738
Isoleucine, metabolism of, 940	alkenes from, 746–748	reactivity versus aldehydes,
molecular model of, 159	alkylation of, 887–890	729–730
structure and properties of, 1046	α cleavage of, 432, 759	reduction of, 630–631, 734
Isomerase, 1070	amines from, 958–959	reductive amination of, 958–959
Isomers, 82	biological reduction of, 631–632,	Wittig reaction of, 746–748
alkanes, 81–82	750–751	Wolff–Kishner reaction of, 741–742
cis–trans cycloalkanes, 113	bromination of, 874–876	Ketone bodies, origin of, 1209
cis–trans alkenes, 229–230	carbonyl condensation reactions	Ketose, 1002
conformational, 94	of, 906	Kiliani, Heinrich, 1022
constitutional, 82	common names of, 724	Kiliani–Fischer synthesis, 1022
diastereomers and, 157	cyanohydrins from, 733	Kimball, George, 265
enantiomers and, 143–144	2,4-dinitrophenylhydrazones	Kinetic control, 508–509
epimers and, 157–158	from, 739	1,4-addition reactions and,
kinds of, 164–165	enamines from, 736–739	508–509
review of, 164–165	enols of, 871–872	Kinetics, 375
stereoisomers, 113	enones from, 908–909	E1 reaction and, 406
Isopentenyl diphosphate,	from acetals, 743–744	E2 reaction and, 400
biosynthesis of, 1099–1103	from acetoacetic ester, 885–886	S_N 1 reaction and, 386–387
geraniol biosynthesis and,	from acid chlorides, 833–834	S _N 2 reaction and, 375–376
395–396	from alkanes, 284, 286	Knoevenagel reaction, 941
isomerization of, 1103–1105	from alkenes, 284–286 from alkynes, 319–321	Knowles, William S., 760, 1055
terpenoids from, 1103–1106 Isoprene, heat of hydrogenation of,		Kodel, structure of, 1259 Koenigs–Knorr reaction, 1017 –1018
503	from nitriles, 796 hydrates of, 731–732	mechanism of, 1018
industrial synthesis of, 501	imines from, 736–739	neighboring-group effect in, 1018
structure of, 228	IR spectroscopy of, 444,	Krebs, Hans Adolf, 1185
UV absorption of, 520	756–757	Krebs, Halls Adolf, 1163 Krebs cycle, <i>see</i> Citric acid cycle
Isoprene rule, terpenes and, 299–300	mass spectrometry of, 431–432,	races cycle, see citile acid cycle
Isopropyl carbocation, electrostatic	758–759	L Sugar, 1007
potential map of, 245	McLafferty rearrangement of, 431,	Fischer projections of, 1007
Isopropyl group, 85	758	Labetalol, synthesis of, 948
100P10P11 810MP1 00	700	2000001, 0, 110110010 01, 7 10

Laboratory reaction, comparison with Lexan, structure and uses of, 849-850, cycloaddition reactions and, biological reaction, 210-212 1224-1225 Lactam(s), 845 Lidocaine, molecular model of, 102 LUMO, see Lowest unoccupied amines from, 845 structure of, 64 molecular orbital Ligase, 1070 Lyase, 1070 reaction with LiAlH₄, 845 Lactic acid, configuration of, 153 Light, plane-polarized, 147-148 Lycopene, structure of, 501 enantiomers of, 143 speed of, 435 Lysergic acid diethylamide, structure molecular model of, 145 Limonene, biosynthesis of, 261, 1106 of, 989 resolution of, 162–163 Lysine, structure and properties of, biosynthesis of, 1106 structure of, 780 enantiomers of, 170 Lactone(s), 837 molecular model of, 170 Lysozyme, MALDI-TOF mass alkylation of, 888 odor of enantiomers of, 170 spectrum of, 433-434 IR spectroscopy of, 851 Lindlar catalyst, 323 p*I* of, 1052 reaction with LDA, 888 Line-bond structure, 7 Lyxose, configuration of, 1009 Lactose, molecular model of, 1027 $1\rightarrow 4$ -Link, 1025 occurrence of, 1027 Linoleic acid, structure of, 1090 Magnetic field, NMR spectroscopy Linolenic acid, molecular model of, structure of, 1027 and, 457-458 1091 Magnetic resonance imaging, 486 sweetness of, 1033 Lagging strand, DNA replication and, structure of, 1090 uses of, 486 1135 Lipase, mechanism of, 1158-1161 Major groove (DNA), 1132 Lanosterol, biosynthesis of, Lipid, 1088 MALDI mass spectrometry, 433 classification of, 1088 1112-1117 Maleic acid, structure of, 780 carbocation rearrangements and, Lipid bilayer, 1095 Malic acid, structure of, 780 1115, 1117 Lipitor, structure of, 1, 534 Walden inversion of, 372–373 structure of, 300 statin drugs and, 1203-1204 Malonic ester, carboxylic acids from, Lipoamide, structure and function of, Lapworth, Arthur, 733 883-884 Lard, composition of, 1090 1184 decarboxylation of, 883-884 Latex, rubber from, 516 Lipoic acid, structure and function of, pK_a of, 879 1073, 1184 Laurene, synthesis of, 902 Malonic ester synthesis, 883-884 Lauric acid, structure of, 1090 Lipoprotein, heart disease and, 1118 intramolecular, 884 Lithium, reaction with alkynes, LD₅₀, 24 Maltose, $1\rightarrow 4-\alpha$ -link in, 1026 molecular model of, 1026 table of, 24 323-325 LDA, see Lithium diisopropylamide Lithium aluminum hydride, reaction mutarotation of, 1026 LDL, heart disease and, 1118 with carboxylic acids, 632-633 structure of, 1026 Le Bel, Joseph Achille, 6 reaction with esters, 632-633 Manicone, synthesis of, 834 Leading strand, DNA replication and, reaction with ketones and Mannich reaction, 943 1135 aldehydes, 630 Mannose, biosynthesis of, 1040 Leaving group, 382 Lithium diisopropylamide (LDA), chair conformation of, 128 biological reactions and, formation of, 878 configuration of, 1009 395-396 properties of, 878 molecular model of, 128 S_N1 reaction and, 391–392 Marcaine, structure of, 64 reaction with cyclohexanone, 878 S_N2 reactions and, 382–383 Margarine, manufacture of, 279–280, reaction with esters, 888 Leucine, biosynthesis of, 941, 1213 reaction with ketones, 878, 888 metabolism of, 940 reaction with lactones, 888 Markovnikov, Vladimir Vassilyevich, structure and properties of, 1046 reaction with nitriles, 888 Leukotriene E₄, structure of, 1096 Markovnikov's rule, 240-241 Lithium diorganocopper reagent, see Leuprolide, structure of, 1083 Gilman reagent alkene additions and, 240-241 Levorotatory, 148 Lithocholic acid, structure of, 1109 alkyne additions and, 317 Lewis, Gilbert Newton, 7 Locant, IUPAC naming and, 87-88 carbocation stability and, 241, Lewis acid, 56-58 243-245 Lone-pair electrons, 8 examples of, 58 Loratadine, structure of, 255, 570 Hammond postulate and, 248 reactions of, 57-58 Lotaustralin, structure of, 793 hydroboration and, 273-274 Lewis base, 56-59 Lovastatin, biosynthesis of, 515 oxymercuration and, 271 examples of, 59 statin drugs and, 1203-1204 Mass number (A), 3 reactions of, 58-59 structure of, 515 Mass spectrometer, double-focusing, Lewis structure, 7 Low-density polyethylene, synthesis resonance and, 42-43 exact mass measurement in, 427 of, 1246 Lewis Y hexasaccharide, synthesis of, Lowest unoccupied molecular orbital kinds of, 425 1030 operation of, 425-426 (LUMO), 518, 1216

Mass spectrometry (MS), 424	aldehyde oxidation, 727	E1 reaction, 405
alcohols, 431, 657	aldehyde reduction, 734	E1cB reaction, 406–407
aldehydes, 431-432, 758-759	aldol reaction, 905–906	E2 reaction, 400
alkanes, 428–429	aldolase catalyzed reactions,	Edman degradation, 1059–1061
α cleavage of alcohols in, 431	928–929, 1177–1178	electrophilic addition reaction,
α cleavage of amines in, 431	alkane chlorination, 347–348	195–196, 237–238
amines, 431, 981–982	alkene epoxidation, 281–282	electrophilic aromatic
base peak in, 426	alkene halogenation, 265–266	substitution, 568–569
biological, 433–434	alkene hydration, 270	enamine formation, 738–739
carbonyl compounds, 431–432	alkene polymerization, 291–292	enol formation, 871–872
cation radicals in, 425–426	alkoxymercuration, 680	ester hydrolysis, 838–839
dehydration of alcohols in, 431	alkylbenzene bromination,	ester reduction, 840–841
electron-impact ionization in,	597–598	FAD reactions, 1163–1164
425–426	alkyne addition reactions,	fat catabolism, 1162–1166
electrospray ionization in, 433	317–318	fat hydrolysis, 1158–1161
fragmentation in, 426-429	alkyne hydration, 319–320	Fischer esterification reaction,
ketones and, 431–432, 758–759	alkyne reduction with Li/NH ₃ ,	824–825
MALDI ionization in, 433	324–325	Friedel-Crafts acylation reaction,
McLafferty rearrangement in, 431,	α -bromination of ketones,	577–578
758	874–876	Friedel-Crafts alkylation reaction,
molecular ion in, 426	α -substitution reaction, 874	575
nitrogen rule and, 981–982	allylic bromination, 350–351	glycolysis, 1173–1181
parent peak in, 426	amide formation with DCC,	Grignard carboxylation, 790
soft ionization in, 427	826–827	Grignard reaction, 735
time-of-flight, 433	amide hydrolysis, 843–844	Hell–Volhard–Zelinskii reaction,
Mass spectrum, 426	amide reduction, 845	877
1-butanol, 657	amino acid transamination,	Hofmann elimination reaction,
computer matching of, 428	1198–1201	964–965
2,2-dimethylpropane, 427	aromatic bromination, 568–569	Hofmann rearrangement, 960,
ethylcyclopentane, 429	aromatic chlorination, 570	962
N-ethylpropylamine, 982	aromatic fluorination, 570	hydroboration, 274
hexane, 428	aromatic iodination, 570–571	hydrogenation, 277–278
2-hexene, 430	aromatic nitration, 571–572	imine formation, 736–737
interpretation of, 426–429	aromatic sulfonation, 572	intramolecular aldol reaction,
lysozyme, 434	base-catalyzed epoxide cleavage,	914–915
methylcyclohexane, 429	689	isopentenyl diphosphate
5-methyl-2-hexanone, 759	base-catalyzed ester hydrolysis,	biosynthesis, 1099–1103
2-methylpentane, 450	838	ketone hydration, 731–732
2-methyl-2-pentanol, 432	β -oxidation pathway, 1162–1166	ketone reduction, 734
2-methyl-2-pentene, 430	biological hydroxylation, 573–574	Koenigs–Knorr reaction, 1018
propane, 426	biotin-mediated carboxylation,	Michael reaction, 921–922
Maxam–Gilbert DNA sequencing,	1170	mutarotation, 1013
1140	bromohydrin formation, 268	nitrile hydrolysis, 795–796
McLafferty rearrangement, 431, 758	bromonium ion formation, 265	nucleophilic acyl substitution
Mechanism (reaction), 186	Cannizzaro reaction, 750	reaction, 819
acetal formation, 743–744	carbonyl condensation reaction,	nucleophilic addition reaction,
acetylide alkylation, 327	904–905	728
acid chloride formation with	citrate synthase, 1074–1075	nucleophilic aromatic substitution
SOCl ₂ , 823–824	Claisen condensation reaction,	reaction, 592–593
acid-catalyzed epoxide cleavage,	915–916	olefin metathesis polymerization,
282–283, 686–688	Claisen rearrangement, 683–684	1251
acid-catalyzed ester hydrolysis,	conjugate carbonyl addition	diorganocopper conjugate
839	reaction, 752	addition, 755
alcohol dehydration with acid,	Curtius rearrangement, 962	organometallic coupling reaction,
641–642	cyanohydrin formation, 733	358–359
alcohol dehydration with POCl ₃ ,	dichlorocarbene formation, 287	oxidative decarboxylation,
642–643	Dieckmann cyclization reaction,	1181–1185
alcohol oxidation, 646	919–920 Diele Alder reaction, 510	oxymercuration, 271–272
aldehyde hydration, 731–732	Diels–Alder reaction, 510	phenol from cumene, 650–651

Mechanism (reaction)—cont'd polar reactions, 190–193 prostaglandin biosynthesis, structure of, 12 294-295 radical reactions, 187-189 reductive amination, 958 Robinson annulation reaction, Sandmeyer reaction, 970 saponification, 838 S_N1 reaction, 386–387 pK_a of, 625 S_N 2 reaction, 376–377 Stork enamine reaction, 925 Suzuki-Miyaura reaction, 359 toxicity of, 620 Williamson ether synthesis, uses of, 620 678-679 Wittig reaction, 746-747 model of, 557 Wolff-Kishner reaction, 741-742 Meerwein-Ponndorf-Verley reaction, from, 694 772 Meerwein's reagent, 707 Melmac, structure of, 1260 Melt transition temperature 1046 (polymers), 1254 Menthene, electrostatic potential map of, 75 functional groups in, 75 787 Menthol, chirality of, 147 molecular model of, 118 structure of, 118 Menthyl chloride, E1 reaction of, 406 map of, 820 E2 reaction of, 404 Mepivacaine, structure of, 64 Mercapto group, 691 Mercuric trifluoroacetate, alkoxymercuration with, 680 Mercurinium ion, 271 map of, 326 Merrifield, Robert Bruce, 1064 stability of, 326 Merrifield solid-phase peptide synthesis, 1064-1066 Meso compound, 159 plane of symmetry in, 159–160 Messenger RNA, 1135 Methyl group, 84 codons in, 1137-1138 chiral, 422 translation of, 1137-1139 Mestranol, structure of, 342 Meta (m) prefix, 537 Meta-directing group, 581 Metabolism, 1154 Methacrylic acid, structure of, 780 Methamphetamine, synthesis of, 994 structure of. 18 Methandrostenolone, structure and function of, 1111 Methane, bond angles in, 12 bond lengths in, 12 bond strengths in, 12 chlorination of, 347-348 molecular model of, 12, 81 Methyl shift, carbocations and, pK_a of, 326

reaction with Cl₂, 187–188 sp^3 hybrid orbitals in, 11–12 Methanethiol, bond angles in, 18, dipole moment of, 38 electrostatic potential map of, 36, 54, 56, 190, 216, 623 industrial synthesis of, 620 molecular model of, 18, 19 polar covalent bond in, 36 sp^3 hybrid orbitals in, 18 1,6-Methanonaphthalene, molecular Methionine, S-adenosylmethionine biosynthesis of, 770 molecular model of, 156 structure and properties of, Methoxide ion, electrostatic potential map of, 55, 627 p-Methoxybenzoic acid, pK_a of, *p*-Methoxypropiophenone, ¹H NMR spectrum of, 480 Methyl acetate, electrostatic potential ¹³C NMR spectrum of, 458 ¹H NMR spectrum of, 458 Methyl α -cyanoacrylate. polymerization of, 1244 Methyl anion, electrostatic potential Methyl carbocation, electrostatic potential map of, 245 Methyl 2,2-dimethylpropanoate, ¹H NMR spectrum of, 476 directing effect of, 585-586 inductive effect of, 583 orienting effect of, 581 Methyl phosphate, bond angles in, molecular model of, 18 Methyl propanoate, ¹³C NMR spectrum of, 467 Methyl propyl ether, ¹³C NMR spectrum of, 696 Methyl salicylate, as flavoring agent,

Methyl thioacetate, electrostatic potential map of, 820 9-Methyladenine, electrostatic potential map of, 1149 Methylamine, bond angles in, 17 dipole moment of, 38 electrostatic potential map of, 56, 951 molecular model of, 18 sp^3 hybrid orbitals in, 17–18 Methylarbutin, synthesis of, 1017-1018 p-Methylbenzoic acid, p K_a of, 787 2-Methylbutane, molecular model of, 2-Methyl-2-butanol, ¹H NMR spectrum of, 481 Methylcyclohexane, 1,3-diaxial interactions in, 124–125 conformations of, 124-125 mass spectrum of, 429 molecular model of, 124, 146 1-Methylcyclohexanol, ¹H NMR spectrum of, 485 2-Methylcyclohexanone, chirality of, molecular model of, 146 1-Methylcyclohexene, ¹³C NMR spectrum of, 471 N-Methylcyclohexylamine, ¹³C NMR spectrum of, 980 ¹H NMR spectrum of, 980 Methylene group, 228 Methylerythritol phosphate pathway, terpenoid biosynthesis and, 1099 N-Methylguanine, electrostatic potential map of, 1149 6-Methyl-5-hepten-2-ol, DEPT-NMR spectra of, 468 5-Methyl-2-hexanone, mass spectrum of, 759 Methyllithium, electrostatic potential map of, 36, 190 polar covalent bond in, 36 Methylmagnesium iodide, electrostatic potential map of, N-Methylmorpholine N-oxide, reaction with osmates, 283-284 2-Methylpentane, mass spectrum of, 450 2-Methyl-3-pentanol, mass spectrum of. 432 2-Methyl-2-pentene, mass spectrum of, 430 p-Methylphenol, p K_a of, 625 2-Methylpropane, molecular model

2-Methyl-1-propanol, ¹³ C NMR	cyclohexane ring flip, 122	propane conformations, 96
spectrum of, 469	cyclopentane, 117	pseudoephedrine, 175
2-Methylpropene, heat of	cyclopropane, 112, 116	serylalanine, 1056
hydrogenation of, 236	cytosine, 66	staggered ethane conformation, 95
Metoprolol, synthesis of, 690	<i>cis</i> -decalin, 130, 1108	stearic acid, 1090
Mevacor, structure of, 515	trans-decalin, 130, 1108	steroid, 1107
Mevalonate, decarboxylation of, 1102	diethyl ether, 676	sucrose, 1027
Mevalonate pathway, terpenoid	dimethyl disulfide, 19	syn periplanar geometry, 401
biosynthesis and, 1099–1103	<i>cis</i> -1,2-dimethylcyclohexane, 126	Tamiflu, 132
Micelle, 1092 –1093	trans-1,2-dimethylcyclohexane,	testosterone, 130
Michael reaction, 921 –923	127	tetrahydrofuran, 676
acceptors in, 922–923	cis-1,2-dimethylcyclopropane, 112	threose, 147
donors in, 922–923	<i>trans</i> -1,2-dimethylcyclopropane,	trimethylamine, 947
mechanism of, 921–922	112	tRNA, 1138
partners in, 922–923	dimethylpropane, 82	twist boat cyclohexane, 120
Robinson annulation reactions		
	DNA, 62, 1132	vitamin C, 800
and, 927	dopamine, 957	Molecular orbital, 19
Microwaves, electromagnetic	eclipsed ethane conformation, 95	allylic radical, 351
spectrum and, 434	enflurane, 147	antibonding, 20
Mineralocorticoid, 1111	ethane, 13, 81	benzene, 540–541
Minor groove (DNA), 1132	ethylene, 14	bonding, 20
Mitomycin C, structure of, 998	fluoxetine, 170	1,3-butadiene, 503–504, 1215
Mixed aldol reaction, 912–913	glucose, 120, 128	conjugated diene, 503–504
Mixed Claisen condensation reaction,	(R)-glyceraldehyde, 1003	conjugated enone, 909
917–918	hexokinase, 211	degenerate, 541
Molar absorptivity (UV), 519	Hofmann elimination, 965	ethylene, 1215
Molecular ion (M ⁺), 426	ibuprofen, 66, 173	1,3,5-hexatriene, 1216
Molecular mechanics, 132	isobutane, 81	Molecular orbital (MO) theory, 19-21
Molecular model, acetaminophen, 27	isoleucine, 159	Hückel $4n + 2$ rule and, 543
acetylene, 16	lactic acid, 145	Molecular weight, mass spectral
adenine, 66	lactose, 1027	determination of, 426–427
adrenaline, 175	lidocaine, 102	Molecule(s), 7
alanine, 26, 1044	(–)-limonene, 170	condensed structures of, 21
alanylserine, 1056	(+)-limonene, 170	electron-dot structures of, 7
α helix, 1067	linolenic acid, 1091	Kekulé structures of, 7
<i>p</i> -aminobenzoic acid, 23	maltose, 1026	line-bond structures of, 7
anisole, 676	mannose, 128	skeletal structures of, 21–22
anti periplanar geometry, 401	menthol, 118	Molozonide, 284
arecoline, 80	meso-tartaric acid, 160	Monomer, 289
aspartame, 27	methane, 12, 81	Monosaccharide(s), 1001
aspirin, 15	methanethiol, 19	anomers of, 1011–1013
β -pleated sheet, 1067		configurations of, 1008–1010
	methanol, 18	
<i>p</i> -bromoacetophenone, 466	1,6-methanonaphthalene, 557	cyclic forms of, 1011–1013
bromocyclohexane, 122	methionine, 156	essential, 1023–1025
butane, 81	methyl phosphate, 18	esters of, 1015–1016
<i>cis</i> -2-butene, 230, 234	methylamine, 18	ethers of, 1016
trans-2-butene, 230e, 234	2-methylbutane, 82	Fischer projections and,
tert-butyl carbocation, 244	methylcyclohexane, 124, 146	1004–1005
camphor, 131	2-methylcyclohexanone, 146	glycosides of, 1016–1018
cellobiose, 1026	2-methylpropane, 81	hemiacetals of, 1011–1013
chair cyclohexane, 119	naphthalene, 65	osazones from, 1042
cholesterol, 1109	Newman projections, 94	oxidation of, 1020–1021
cholic acid, 778	norbornane, 131	phosphorylation of, 1019
citrate synthase, 1074	omega-3 fatty acid, 1091	reaction with acetic anhydride,
citric acid, 27	oseltamivir phosphate, 132	1015–1016
coniine, 26	pentane, 82	reaction with iodomethane, 1016
cyclobutane, 117	phenylalanine, 102	reduction of, 1020
1,3,5,7,9-cyclodecapentaene, 543,	piperidine, 966	see also Aldose
557	propane, 81	Monoterpene, 300
	* * '	* .

Monoterpenoid, 1098 thioesters, 816 pK_a of, 879 Moore, Stanford, 1058 thiols, 691 reaction with Grignard reagents, Morphine, biosynthesis of, 997 Naphthalene, aromaticity of, 550 specific rotation of, 149 electrostatic potential map of, 550 reaction with LDA, 888 structure of, 63 Hückel 4n + 2 rule and, 550 reaction with LiAlH₄, 796 MRI, see Magnetic resonance molecular model of, 65 reduction of, 796 ¹³C NMR absorptions of, 554 imaging, 486 synthesis of, 793-794 mRNA, see Messenger RNA orbitals picture of, 550 Nitrile group, directing effect of, MS, see Mass spectrometry reaction with Br₂, 549 588-589 Mullis, Kary Banks, 1145 resonance in, 549 inductive effect of, 583 Multiplet (NMR), 476 Naproxen, NSAIDs and, 555 orienting effect of, 581 resonance effect of, 584 table of, 479 structure of, 33 Muscalure, synthesis of, 358 Natural gas, composition of, 100 Nitrile rubber polymer, structure and Natural product, 251 Mutarotation, 1013 uses of, 1247 glucose and, 1013 drugs from, 213 Nitro compound, Michael reactions mechanism of, 1013 number of, 251 and, 922-923 NBS, see N-Bromosuccinimide Mycomycin, stereochemistry of, 181 Nitro group, directing effect of, Mylar, structure of, 849 NDA, see New drug application, 214 588-589 *myo*-Inositol, structure of, 139 Neighboring-group effect, 1018 inductive effect of, 583 Myrcene, structure of, 299 Neomenthyl chloride, E2 reaction of, orienting effect of, 581 Myristic acid, catabolism of, 1166 404 resonance effect of, 584 Neopentyl group, 90 Nitroarene, arylamines from, 955 structure of, 1090 S_N2 reaction and, 379 reaction with iron, 955 n (normal), 82 Neoprene, synthesis and uses of, 516 reaction with SnCl₂, 955 n + 1 rule, 478 New drug application (NDA), 214 reduction of, 955 Nitrobenzene, aniline from, 572 N-terminal amino acid, 1056 New molecular entity (NME), number Naming, acid anhydrides, 815 of, 213 reduction of, 572 acid chlorides, 815 Newman, Melvin S., 94 synthesis of, 572 Newman projection, 94 p-Nitrobenzoic acid, p K_a of, 787 acid halides, 815 acyl phosphate, 817 molecular model of, 94 Nitrogen, hybridization of, 17–18 alcohols, 621-622 Nicotinamide adenine dinucleotide, Nitrogen rule of mass spectrometry, 981-982 aldehydes, 723-724 biological oxidations with, 647 biological reductions with, aldoses, 1010 Nitronium ion, 571–572 alkanes, 87-91 631-632 electrostatic potential map of, 572 alkenes, 226-227 reactions of, 751 *p*-Nitrophenol, pK_a of, 625 alkyl groups, 84-85, 89-90 structure of, 751, 1072 Nitrous acid, reaction with amines, alkyl halides, 345–346 Nicotinamide adenine dinucleotide 968-969 alkynes, 314-315 phosphate, biological NME, see New molecular entity, 213 alphabetizing and, 91 reductions and, 280 NMO, see N-Methylmorpholine Nicotine, structure of, 28, 944 amides, 816 N-oxide amines, 944-946 Ninhydrin, reaction with amino NMR, see Nuclear magnetic resonance aromatic compounds, 535-537 acids, 1058 Node. 4 carboxylic acid derivatives, Nitration (aromatic), 571-572 Nomenclature, see Naming 815-817 Nitric acid, pK_a of, 51 Nomex, structure of, 1259 carboxylic acids, 779-780 Nitrile(s), 781 Nonbonding electrons, 8 cycloalkanes, 109-111 alkylation of, 888 Noncovalent interaction, 60-62 amides from, 795-796 cycloalkenes, 227-228 Nonequivalent protons, spin-spin eicosanoids, 1096-1097 amines from, 796 splitting and, 482–483 enzymes, 1070 carboxylic acids from, 789-790, tree diagram of, 483 esters, 816 795-796 Nootkatone, chirality of, 146 ethers, 677 electrostatic potential map of, 794 Norbornane, molecular model of, 131 heterocyclic amines, 946 from amides, 793-794 Norepinephrine, adrenaline from, from arenediazonium salts, 969 396 ketones, 724 new IUPAC system for, 227-228 hydrolysis of, 789-790, 795-796 biosynthesis of, 597 IR spectroscopy of, 798 Norethindrone, structure and nitriles, 781 old IUPAC system for, 227 ketones from, 796 function of, 1111 naming, 781 Normal (n) alkane, 82 phenols, 622 prostaglandins, 1096-1097 naturally occurrence of, 793 Norsorex, synthesis of, 1253 sulfides, 693 NMR spectroscopy of, 798 Novocaine, structure of, 64

Novolac resin, 523–524 Noyori, Ryoji, 760	¹³ C Nuclear magnetic resonance spectrum, acetaldehyde, 758	acid anhydrides, 835–836 acid chlorides, 830–834
NSAID, 554	acetophenone, 758	acid halides, 830–834
Nuclear magnetic resonance	anisole, 696	amides, 843–845
spectrometer, field strength of,	benzaldehyde, 758	carboxylic acids and, 823–830
458	benzoic acid, 798	esters, 837–842
operation of, 460	<i>p</i> -bromoacetophenone, 465	kinds of, 821
Nuclear magnetic resonance	2-butanone, 465, 758	mechanism of, 819
spectroscopy (NMR), 456	crotonic acid, 798	reactivity in, 819–821
acid anhydrides, 852	cyclohexanol, 655	Nucleophilic addition reaction, 715 ,
acid chlorides, 852	cyclohexanone, 758	728 –730
alcohols, 655–656	ethyl benzoate, 492	acid catalysis of, 731–732
aldehydes, 757–758	methyl acetate, 458	base catalysis of, 731–732
allylic protons and, 474–475	methyl propanoate, 467	mechanism of, 728
amides, 852	methyl propyl ether, 696	steric hindrance in, 729
amines, 979–980	1-methylcyclohexene, 471	trajectory of, 729
aromatic compounds, 552–554	<i>N</i> -methylcyclohexylamine, 980	variations of, 729
aromatic protons and, 474–475	2-methyl-1-propanol, 469	Nucleophilic aromatic substitution
calibration peak for, 462	1-pentanol, 464	reaction, 592 –594
carboxylic acid derivatives, 852	propanenitrile, 798	mechanism of, 592-593
carboxylic acids, 798–799	propanoic acid, 798	Nucleophilic substitution reaction, 373
chart for, 461	propionic acid, 798	biological examples of, 395–396
¹³ C chemical shifts in, 464–465	¹ H Nuclear magnetic resonance	see S _N 1 reaction, S _N 2 reaction
¹ H chemical shifts in, 474–475	spectrum, acetaldehyde, 758	summary of, 407–408
coupling constants in, 478	bromoethane, 477	Nucleophilicity, 380
delta scale for, 462	2-bromopropane, 478	basicity and, 381
DEPT-NMR and, 467-469	<i>p</i> -bromotoluene, 553	table of, 381
diastereotopic protons and, 473	trans-cinnamaldehyde, 482	trends in, 381
enantiotopic protons and, 472	cyclohexylmethanol, 485	Nucleoside, 1128
energy levels in, 458	dipropyl ether, 696	Nucleotide, 1128
epoxides, 696	1,2-epoxypropane, 696	3' end of, 1131
esters, 852	ethyl acetate, 852	5' end of, 1131
ethers, 696	methyl acetate, 458	Nucleus, size of, 2
field strength and, 457–458	methyl 2,2-dimethylpropanoate,	Nylon, 847 –849
FT-NMR and, 463–464	476	manufacture of, 849
homotopic protons and, 472	<i>p</i> -methoxypropiophenone, 480	naming, 849
integration of, 476	2-methyl-2-butanol, 481	uses of, 849
ketones, 757–758	1-methylcyclohexanol, 485	Nylon 6, structure of, 848
multiplets in, 477–479	N-methylcyclohexylamine, 980	synthesis of, 1249
n+1 rule and, 478	phenylacetic acid, 799	Nylon 6,6, structure of, 849
nitriles, 798	1-propanol, 656	synthesis of, 1249
overlapping signals in, 482	toluene, 482	Nylon 10,10, uses of, 1259
¹³ C peak assignments in, 467–469	Nuclear spin, common nuclei and,	
¹ H peak size in, 483–484	458	Ocimene, structure of, 256
phenols, 656	NMR and, 456–457	Octane number (fuel), 100–101
principle of, 456–458	Nucleic acid, 1128	Octet rule, 6
proton equivalence and, 471–473	see Deoxyribonucleic acid,	-oic acid, carboxylic acid name suffix,
pulsed, 463–464	Ribonucleic acid	779
radiofrequency energy and, 457–458	Nucleophile(s), 192 characteristics of, 197–198	Okazaki fragments, DNA replication and, 1135
ring current and, 552–553	curved arrows and, 197–198	-ol, alcohol name suffix, 622
shielding in, 458	electrostatic potential maps of,	Olah, George Andrew, 266
signal averaging in, 463–464	192	Olefin, 222
spin-flips in, 457	examples of, 192	Olefin metathesis polymerization,
spin–spin splitting in, 477–480	S_N 1 reaction and, 392	1251–1253
time scale of, 460–461	S _N 2 reaction and, 380–381	Grubbs catalyst for, 1251
uses of ¹³ C, 470–471	Nucleophilic acyl substitution	kinds of, 1252
uses of ¹ H, 484–485	reaction, 717, 818–819	mechanism of, 1251
vinylic protons and, 457–458	abbreviated mechanism for, 1169	Oleic acid, structure of, 1090

Oligonucleotide, 1142	Organometallic coupling reaction,	PAM resin, solid-phase peptide
synthesis of, 1142–1144	357–359	synthesis and, 1065
Olive oil, composition of, 1090	Organopalladium compound,	<i>Para</i> (<i>p</i>) prefix, 537
Omega-3 fatty acid, 1089	Suzuki-Miyaura reaction of, 359	Paraffin, 92
molecular model of, 1091	Organophosphate, bond angles in, 18	Parallel synthesis, 605
-one, ketone name suffix, 724	hybrid orbitals in, 18	Parent peak (mass spectrum), 426
-onitrile, nitrile name suffix, 781	Orlon, structure and uses of, 293	Partial charge, 35
Optical activity, 147–149	Ortho (o) prefix, 537	Pasteur, Louis, enantiomers and, 150
measurement of, 148	Ortho- and para-directing group, 581	resolution of enantiomers and,
Optical isomers, 150	Osazone, 1042	161
Optically active, 148	-ose, carbohydrate name suffix, 1002	Patchouli alcohol, structure of, 1099
Orbital, 3	Oseltamivir phosphate, mechanism	Paternity, DNA test for, 1146–1147
energies of, 4	of, 1032–1033	Pauli exclusion principle, 5
hybridization of, 11–18	molecular model of, 132	Pauling, Linus Carl, 11
shapes of, 3–4	structure of, 32	PCR, see Polymerase chain reaction,
p Orbital, nodes in, 4	Osmate, 283	1145–1146
shape of, 3–4	Osmium tetroxide, reaction with	PDB, see Protein Data Bank,
d Orbital, shape of, 4	alkenes, 283–284	1076–1077
s Orbital, shape of, 3	toxicity of, 283	Peanut oil, composition of, 1090
Organic chemicals, number of, 74	Oxalic acid, structure of, 780	Pedersen, Charles John, 690
toxicity of, 24–25	Oxaloacetic acid, structure of, 780	Penicillin, discovery of, 853
Organic chemistry, 1	Oxaphosphatane, 746	Penicillin V, specific rotation of, 149
foundations of, 1–2	Oxetane, reaction with Grignard	stereochemistry of, 172
Organic compound(s), elements	reagents, 708	Penicillium notatum, penicillin from,
found in, 2	Oxidation, 281	853
number of, 1	alcohols, 645–647	Pentachlorophenol, synthesis of, 652
oxidation level of, 361	aldehydes, 727	1,4-Pentadiene, electrostatic potential
polar covalent bonds in, 190–191	aldoses, 1020–1021	map of, 504
size of, 1	alkenes, 281–286	Pentadienyl radical, resonance in, 47
Organic foods, 24–25	biological, 647	Pentalene, 561
Organic reactions, chirality and,	organic, 360	Pentane, molecular model of, 82
296–298	phenols, 653	2,4-Pentanedione, pK_a of, 880
conventions for writing, 239	sulfides, 694	2,4-Pentanedione anion, resonance
kinds of, 184–185	thiols, 692	in, 46
Organic synthesis, enantioselective,	Oxidation level, table of, 361	1-Pentanol, ¹³ C NMR spectrum of, 464
760–761	Oxidative decarboxylation, pyruvate	
strategy of, 329	catabolism and, 1181–1185	Pentobarbital, synthesis of, 891
Organoborane, from alkenes,	steps in, 1182	Pentose phosphate pathway, 1208,
272–274	Oxidoreductase, 1070	1210–1211 Pepsin, p <i>I</i> of, 1052
reaction with H ₂ O ₂ , 272–273	Oxime, 738 from aldebydes and lectones, 727, 729	
Organocopper reagent, see	from aldehydes and ketones, 737–738	Peptide(s), 1044 amino acid sequencing of,
Diorganocopper reagent,	Oxirane, 281	1059–1061
Gilman reagent Organodiphosphate, biological	Oxo group, 725 Oxycodone, structure of, 1	backbone of, 1056
substitution reactions and,	OxyContin, structure of, 1	covalent bonding in, 1056–1057
395–396	Oxyfluorfen, synthesis of, 594	disulfide bonds in, 1057
Organohalide(s), 344	Oxygen, hybridization of, 18	Edman degradation of, 1059–1061
biological uses of, 362–363	Oxymercuration, 271 –272	reaction with
naturally occurring, 362–363	mechanism of, 271–272	phenylisothiocyanate,
number of, 362	regiochemistry of, 271	1059–1060
reaction with Gilman reagents,	Ozone, preparation of, 284	solid-phase synthesis of, 1064–1066
357–358	reaction with alkenes, 284–285	synthesis of, 1062–1066
see also Alkyl halide	reaction with alkynes, 325	Peptide bond, 1056 –1057
uses of, 344	Ozonide, 284	DCC formation of, 826–827,
Organomagnesium halide, see	danger of, 285	1062–1063
Grignard reagent		restricted rotation in, 1057
Organomercury compounds, reaction	Paclitaxel, structure of, 333	Pericyclic reaction, 1214
with NaBH ₄ , 271–272	Palmitic acid, structure of, 1090	frontier orbitals and, 1216
Organometallic compound, 356	Palmitoleic acid, structure of, 1090	kinds of, 1214
-		

stereochemical rules for, 1231	Phenylacetylene, IR spectrum of, 446	PITC, see Phenylisothiocyanate,
Woodward–Hoffmann rules for, 1215–1216	Phenylalanine, biosynthesis of, 684, 1229–1230	1059–1060 p <i>K</i> _a , 5 0
Periodic acid, reaction with 1,2-diols,	molecular model of, 102	table of, 51
285–286	pK_a of, 52	Planck equation, 435–436
Periplanar, 401	structure and properties of, 1046	Plane of symmetry, 144
Perlon, structure of, 848	Phenylisothiocyanate, Edman	meso compounds and, 159–160
Peroxide, 678	degradation and, 1059–1060	Plane-polarized light, 147 –148
Peroxyacid, 281	Phenylthiohydantoin, Edman	Plasmalogen, structure of, 1121
reaction with alkenes, 281–282	degradation and, 1059–1061	Plastic, recyclable, 1256–1257
PET, <i>see</i> Polyethylene terephthalate,	Phosphate, electrostatic potential	see also Polymer
1254	map of, 78	Plasticizer, 837, 1254
Petit, Rowland, 542	Phosphatidic acid,	structure and function of, 1254
Petroleum, catalytic cracking of, 101	glycerophospholipids from,	toxicity of, 1254
composition of, 100	1094	Plavix, structure of, 32
gasoline from, 100–101	Phosphatidylcholine, structure of,	Plexiglas, structure of, 293
history of, 100	1094	Poison ivy, urushiols in, 621
refining of, 100–101	Phosphatidylethanolamine, structure	Polar aprotic solvent, 383
reforming of, 101	of, 1094	S _N 1 reaction and, 393
Pfu DNA polymerase, PCR and, 1145	Phosphatidylserine, structure of, 1094	$S_{ m N}2$ reaction and, 383–384
Pharmaceuticals, approval procedure	Phosphine(s), chirality of, 166	Polar covalent bond, 34 –35
for, 213–214	Phosphite, DNA synthesis and, 1143	dipole moments and, 37–38
origin of, 213	oxidation of, 1144	electronegativity and, 35–36
Phenol(s), 620	Phospholipid, 1094 –1095	electrostatic potential maps and,
acidity of, 624–626	classification of, 1094	36
Bakelite from, 1256	Phosphopantetheine, coenzyme A	inductive effects and, 36
Dow process for, 650	from, 846, 1156	Polar reaction, 187 , 190–193
electrophilic aromatic substitution	Phosphoramidite, DNA synthesis	characteristics of, 190–193
reactions of, 652	and, 1143	curved arrows in, 192, 197–199
electrostatic potential map of, 583	Phosphoria acid at a final file	electrophiles in, 192
from arenediazonium salts, 970	Phosphoric acid, pK_a of, 51	example of, 194–196
from chlorobenzene, 594	Phosphorus, hybridization of 18	nucleophiles in, 192
from cumene, 650 hydrogen bonds in, 623	Phosphorus, hybridization of, 18 Phosphorus oxychloride, alcohol	Polarimeter, 148 Polarizability, 191
IR spectroscopy of, 655	dehydration with, 641–643	Poly(ethylene terephthalate),
IR spectrum of, 655	Phosphorus tribromide, reaction with	structure of, 1254
mechanism of synthesis of,	alcohols, 355, 639	Poly(glycolic acid), biodegradability
650–651	Photochemical reaction, 1217	of, 1257
naming, 622	Photolithography, 523 –524	uses of, 850
NMR spectroscopy of, 656	resists for, 523–524	Poly(hydroxybutyrate),
oxidation of, 653	Photon, 435	biodegradability of, 1257
phenoxide ions from, 624	energy of, 435–436	uses of, 850
pK _a of, 625	Photosynthesis, 1000–1001	Poly(lactic acid), biodegradability of,
properties of, 623–627	Phthalates, use as plasticizers, 837	1257
quinones from, 653	Phthalic acid, structure of, 780	uses of, 850
reaction with arenediazonium	Phthalimide, Gabriel amine synthesis	Poly(methyl methacrylate), uses of,
salts, 972	and, 957	293
uses of, 621, 650, 652	Phylloquinone, biosynthesis of,	Poly(vinyl acetate), uses of, 293
Phenolic resin, 1256	578–579	Poly(vinyl butyral), uses of, 1260
Phenoxide ion, 624	Pi (π) bond, 14	Poly(vinyl chloride), plasticizers in,
electrostatic potential map of, 627	acetylene and, 16	1254
resonance in, 627	ethylene and, 14	uses of, 293
Phentermine, synthesis of, 962	molecular orbitals in, 21	Polyacrylonitrile, uses of, 293
Phenyl group, 536	Picometer, 3	Polyalkylation, Friedel–Crafts
Phenylacetaldehyde, aldol reaction	Picric acid, synthesis of, 650	reaction and, 576
of, 906	Pinacol rearrangement, 672	Polyhutadiona synthesis of 516
IR spectrum of, 445 Phenylacetic acid, ¹ H NMR spectrum	Pineapple, esters in, 836 Pineriding, molecular model of, 966	Polybutadiene, synthesis of, 516
of, 799	Piperidine, molecular model of, 966 structure of, 946	vulcanization of, 517 Polycarbonate, 849–850, 1249
01, 777	structure or, 740	1 orycarbonate, 049-030, 1249

Polycyclic aromatic compound, 549 aromaticity of, 549–550	Polysaccharide(s), 1028–1029 synthesis of, 1029–1030	Propanenitrile, ¹³ C NMR absorptions in, 798
Polycyclic compound, 129	Polystyrene, uses of, 293	Propanoic acid, ¹³ C NMR absorptions
bridgehead atoms in, 129 conformations of, 129–130	Polytetrafluoroethylene, uses of, 293 Polyunsaturated fatty acid, 1089	in, 798 1-Propanol, ¹ H NMR spectrum of,
Polycyclic heterocycle, 977–978	Polyurethane, 1250	656
Polyester, 847	foam, 1250	Propenal, electrostatic potential map
manufacture of, 849	kinds of, 1250	of, 511
uses of, 849	stretchable, 1250	Propene, see Propylene
Polyethylene, crystallites in, 1253	Polyynes, occurrence of, 314	Propenenitrile, electrostatic potential
high-density, 1246	Posttranslational modification,	map of, 511
high-molecular-weight, 1246	protein, 1142	Propionic acid, see Propanoic acid
kinds of, 1246	Potassium nitrosodisulfonate,	Propyl group, 85
low-density, 1246	reaction with phenols, 653	Propylene, heat of hydrogenation of,
synthesis of, 291–292	Potassium permanganate, reaction	236
ultrahigh-molecular-weight, 1246	with alcohols, 645	industrial preparation of, 223
uses of, 293 Ziegler–Natta catalysts and, 1246	reaction with alkenes, 285 reaction with alkylbenzenes,	uses of, 223 Prostaglandin(s), 1095 –1098
Polyimide, structure of, 862	596–597	biosynthesis of, 294–295,
Polymer(s), 289	reaction with ketones, 728	188–189, 1097–1098
atactic, 1245	Pravachol, structure of, 107	functions of, 188, 1095–1096
biodegradable, 850, 1256–1257	Pravadoline, green synthesis of, 983	naming, 1096–1097
biological, 289–290	Pravastatin, structure of, 107	occurrence of, 1095
chain-growth, 291 –292,	statin drugs and, 1203–1204	see also Eicosanoid
1242–1244	Prepolymer, epoxy resins and,	Prostaglandin E ₁ , structure of, 108,
classification of, 1242	697–698	1096
crystallites in, 1253	Prilocaine, structure of, 64	Prostaglandin E ₂ , biosynthesis of,
elastomer, 1255	Primary alcohol, 621	1097–1098
fiber, 1255	Primary amine, 944	Prostaglandin F_{2a} , structure of, 114
glass transition temperature of,	Primary carbon, 86	Prostaglandin H ₂ , biosynthesis of,
1254	Primary hydrogen, 86	188–189, 1097–1098
isotactic, 1245	Primary structure (protein), 1066	Prostaglandin I ₂ , structure of, 1096
kinds of, 1254	pro-R prochirality center, 167–168	Protecting group, 648
melt transition temperature of, 1254	<i>pro-S</i> prochirality center, 167 –168 Problems, how to work, 26	alcohols, 648–650 aldehydes, 745
plasticizers in, 1254	Procaine, structure of, 30, 64	ketones, 745
recycling codes for, 1257	Prochirality, 167 –169	nucleic acid synthesis and,
representation of, 1242	assignment of, 167–168	1142–1143
step-growth, 847 –850,	chiral environments and, 171–172	peptide synthesis and, 1062–1063
1248–1250	naturally occurring molecules and,	Protein(s), 1044
syndiotactic, 1245	168–169	α helix in, 1066–1067
table of, 293	re descriptor for, 167	backbone of, 1056
thermoplastic, 1254	si descriptor for, 167	biosynthesis of, 1137–1139
thermosetting resin, 1256	Prochirality center, 167–168	denaturation of, 1068
van der Waals forces in, 1253	pro-R, 167–168	isoelectric point of, 1052
Polymerase chain reaction (PCR),	pro-S, 167–168	mechanism of hydrolysis of, 844
1145–1146	Progesterone, structure and function	number of in humans, 1137
amplification factor in, 1145	of, 1110	primary structure of, 1066
<i>Pfu</i> DNA polymerase in, 1145 <i>Taq</i> DNA polymerase in, 1145	structure of, 501 Progestin, 1110	quaternary structure of, 1066 secondary structure of,
Polymerization, anionic, 1243	function of, 1110	1066–1067
cationic, 1243	Proline, biosynthesis of, 959	see also Peptide
mechanism of, 291–292	structure and properties of, 1046	C-terminal amino acid in, 1056
Ziegler–Natta catalysts for,	Promotor sequence (DNA), 1135	N-terminal amino acid in, 1056
1245–1246	Propagation step (radical), 188	tertiary structure of, 1066, 1068
Polypropylene, polymerization of,	Propane, bond rotation in, 96	Protein Data Bank (PDB), 1076–1077
1245	conformations of, 96	downloading structures from,
stereochemical forms of, 1245	mass spectrum of, 426	1076
uses of, 293	molecular model of, 81, 96	number of structures in, 1076

Protic solvent, 383	reaction with thiamin	Reaction intermediate, 208
S_N 1 reaction and, 393	diphosphate, 1181–1183	Reaction mechanism, 186
S_N 2 reaction and, 383–384	Pyruvate dehydrogenase complex,	Reaction rate, activation energy and,
Proton equivalence, ¹ H NMR	1181	206–207
spectroscopy and, 471–473	Pyruvic acid, structure of, 780	Rearrangement reaction, 185
Protonated methanol, electrostatic	Olomo structure of OC1	Reducing sugar, 1020
potential map of, 190	Qiana, structure of, 861	Reduction, 277
Protosteryl cation, lanosterol biosynthesis and, 1114, 1117	Quantum mechanical model, 3–5 Quartet (NMR), 477	acid chlorides, 833
Prozac, structure of, 170	Quaternary ammonium salt, 945	aldehydes, 630–631, 734 aldoses, 1020
Pseudoephedrine, molecular model	Hofmann elimination and,	alkene, 276–280
of, 175	964–965	alkyne, 322–325
PTH, see Phenylthiohydantoin,	Quaternary carbon, 86	amides, 844–845
1059–1061	Quaternary structure (protein), 1066	arenediazonium salt, 970
Purine, aromaticity of, 550	Quetiapine, structure of, 31	aromatic compounds, 599–600
electrostatic potential map of, 978	Quinine, structure of, 550, 977	carboxylic acids, 632–633,
nucleotides from, 1129	Quinoline, aromaticity of, 550	827–828
structure of, 978	electrophilic substitution reaction	disulfides, 692
Pyramidal inversion, amines and, 947	of, 978	esters, 632–633, 840–841
energy barrier to, 947	Lindlar catalyst and, 323	ketones, 630–631, 734
Pyranose, 1011 –1013	Quinone(s), 653	lactams, 845
glucose and, 1011–1012	from phenols, 653	nitriles, 796
Pyridine, aromaticity of, 546–547, 976	hydroquinones from, 653	organic, 360
basicity of, 950, 976	reduction of, 653	quinones, 653
dipole moment of, 976–977	Description 152	Reductive amination, 958 –959
electrophilic substitution reactions of, 976	R configuration, 152	amino acid synthesis and, 1054
,	assignment of, 152 R group, 86	biological example of, 959
electrostatic potential map of, 546 Hückel $4n + 2$ rule and, 546–547	Racemate, 161	mechanism of, 958 Refining (petroleum), 100–101
Pyridoxal phosphate, amino acid	Racemic mixture, 161	Regiospecific, 240
catabolism and, 1198	Radical, 187	Registry of Mass Spectral Data, 428
imines from, 736	reactivity of, 187	Relenza, mechanism of, 1032–1033
structure of, 30, 1073	stability of, 349, 351	Replication (DNA), 1133 –1135
Pyridoxamine phosphate,	Radical chain reaction, 188	direction of, 1134–1135
transamination and, 1198	initiation steps in, 188	error rate during, 1135
Pyrimidine, aromaticity of, 546–547	propagation steps in, 188	lagging strand in, 1135
basicity of, 950, 977	termination steps in, 188	leading strand in, 1135
electrostatic potential map of, 546	Radical reaction(s), 187–189	Okazaki fragments in, 1135
Hückel $4n + 2$ rule and, $546-547$	addition, 187	replication fork in, 1134
nucleotides from, 1129	biological example of, 294–295	Replication fork (DNA), 1134
Pyrrole, aromaticity of, 547, 973–974	characteristics of, 188	Residue (protein), 1056
basicity of, 950, 973	fishhook arrows and, 186	Resist, photolithography and,
electrophilic substitution reactions	prostaglandin biosynthesis and,	523–524
of, 974–975	188–189, 1097–1098	Resolution (enantiomers), 161–163
electrostatic potential map of, 547, 974	substitution, 187 Radio waves, electromagnetic	Resonance, 42 –46 acetate ion and, 42–43
Hückel $4n + 2$ rule and, 547	spectrum and, 434	acetone anion and, 45
industrial synthesis of, 973	Radiofrequency energy, NMR	acyl cations and, 577–578
Pyrrolidine, electrostatic potential	spectroscopy and, 457–458	allylic carbocations and, 506
map of, 974	Rapamycin, discovery of, 252	allylic radical and, 351–352
structure of, 946	structure of, 251	arylamines and, 952
Pyrrolysine, structure of, 1048	Rate equation, 376	benzene and, 43, 539–540
Pyruvate, acetyl CoA from,	Rate-determining step, 386	benzylic carbocation and, 390
1181–1185	Rate-limiting step, 386	benzylic radical and, 598
catabolism of, 1181–1185	Rayon, 1028	carbonate ion and, 47
from glucose, 1173-1181	Re prochirality, 167	carboxylate ions and, 784
glucose from, 1191–1197	Reaction (polar), 187, 190–193	enolate ions and, 878
oxidative decarboxylation of,	Reaction (radical), 187–189	Lewis structures and, 42–43
1181–1185	Reaction coordinate, 206	naphthalene and, 549

Resonance—cont'd	ROMP, see ring-opening metathesis	Serylalanine, molecular model of,
pentadienyl radical and, 47	polymerization, 1252	1056
2,4-pentanedione anion and, 46	rRNA, see Ribosomal RNA	Sesquiterpene, 300
phenoxide ions and, 627	Rubber, production of, 516	Sesquiterpenoid, 1098
Resonance effect, electrophilic	structure of, 516	Sex hormone, 1110
aromatic substitution and, 584	vulcanization of, 517	Sharpless, K. Barry, 760
Resonance form, 43	, , , , , , , , , , , , , , , , , , , ,	Sharpless epoxidation, 761
drawing, 45–46	S configuration, 152	Shell (electron), 4
electron movement and, 43–45	assignment of, 152	capacity of, 4
rules for, 43–45	s-cis conformation, 513	Shielding (NMR), 458
stability and, 45	Diels–Alder reaction and, 513–514	Si prochirality, 167
three-atom groupings in, 46	Saccharin, structure of, 1034	Sialic acid, 1024
Resonance hybrid, 43	sweetness of, 1033	Side chain (amino acid), 1048
Restriction endonuclease, 1140	Safrole, structure of, 707	Sigma (σ) bond, 10
number of, 1140	Samuelsson, Bengt, 1095	symmetry of, 10
palindrome sequences in, 1140	Sandmeyer reaction, 969 –970	Sigmatropic rearrangement, 1226–1230
Retin A, structure of, 259	mechanism of, 970	antarafacial geometry of, 1227
Retinal, vision and, 522	Sanger, Frederick, 1063	examples of, 1228–1230
Retrosynthetic analysis, 329	Sanger dideoxy DNA sequencing,	[1,5] hydrogen shift and, 1228
Rhodium, aromatic hydrogenation	1140-1141	notation for, 1227
catalyst, 599	Sanger's reagent, 592	stereochemical rules for, 1227
Rhodopsin, isomerization of, 522	β -Santalene, structure of, 299	suprafacial geometry of, 1227
vision and, 522	Saponification, 838, 1092	vitamin D and, 1232
Ribavirin, structure of, 561	mechanism of, 838	Signal averaging, FT-NMR
Ribonucleic acid (RNA), 1128	Saran, structure and uses of,	spectroscopy and, 463–464
bases in, 1129	1246–1247	Sildenafil, structure of, 973
biosynthesis of, 1135–1136	Sativene, synthesis of, 902	Silver oxide, Hofmann elimination
3' end of, 1131	Saturated, 81	reaction and, 964–965
5' end of, 1131	Saturated hydrocarbon, 81	Simmons–Smith reaction, 288–289
kinds of, 1135	Sawhorse representation, 94	Simple sugar, 1001
messenger, 1135	SBR polymer, structure and uses of,	Simvastatin, structure of, 107
ribosomal, 1135	1247	Single bond, 13
size of, 1130	Schiff base, 736, 1177	electronic structure of, 12–13
small, 1135	see also Imine	length of, 12
structure of, 1130–1131	Scurvy, vitamin C and, 800	see also Alkane
transfer, 1135	sec-, name prefix, 85	strength of, 12
translation of, 1137–1139	sec-Butyl group, 85	Sirolimus, structure of, 251
Ribonucleotide(s), structures of,	Secobarbital, synthesis of, 891	Skeletal structure, 21
1130	Second-order reaction, 376	rules for drawing, 21–22
Ribose, configuration of, 1009	Secondary alcohol, 621	Skunk scent, cause of, 692
Ribosomal RNA, 1135	Secondary amine, 944	Small RNAs, 1135
function of, 1135	Secondary carbon, 86	S _N 1 reaction, 385 –388
Ring current (NMR), 552	Secondary hydrogen, 86	biological examples of, 395–396
[18]annulene and, 552–553	Secondary metabolite, 251	carbocation stability and, 389–390
Ring-expansion reaction, 901	number of, 251	characteristics of, 389–394
Ring-flip (cyclohexane), 122	Secondary structure (protein),	energy diagram for, 387
energy barrier to, 122	1066–1067	epoxide cleavage and, 688
		ion pairs in, 388
molecular model of, 122	Sedoheptulose, structure of, 1002	-
Ring-opening metathesis	Selenocysteine, structure of, 1048	kinetics of, 386
polymerization (ROMP), 1252	Semiconservative replication (DNA),	leaving groups in, 391–392
Risk, chemicals and, 24–25	1134	mechanism of, 386–387
RNA, see Ribonucleic acid	Sense strand (DNA), 1136	nucleophiles and, 392
Roberts, Irving, 265	Sequence rules, 150–152	racemization in, 387–388
Robinson annulation reaction,	<i>E,Z</i> alkene isomers and, 231–232	rate law for, 386
927–928	enantiomers and, 150–154	rate-limiting step in, 386–387
mechanism of, 927	Serine, biosynthesis of, 1212	solvent effects on, 392–393
Rod cells, vision and, 522	structure and properties of, 1047	stereochemistry of, 387–388
Rofecoxib, NSAIDs and, 555	Seroquel, structure of, 31	substrate structure and, 389–390
structure of, 1	Serum lipoprotein, table of, 1118	summary of, 394

S _N 2 reaction, 376 –377	Specific rotation, 148–149	$S_{ m N}$ 1 reaction and, 387–388
allylic halides in, 391	table of, 149	S_N 2 reactions and, 376–377
amines and, 956	Sphingomyelin, 1094–1095	Stereogenic center, 145
benzylic halides in, 391	Sphingosine, structure of, 1095	Stereoisomers, 112
biological example of, 396	Spin density surface, allylic radical,	kinds of, 164–165
characteristics of, 378–385	352	number of, 156
crown ethers and, 691	benzylic radical, 598	properties of, 160
electrostatic potential maps of,	Spin-flip, NMR spectroscopy and, 457	Stereospecific, 288, 512
377	Spin–spin splitting, 477	Stereospecific numbering, sn-glycerol
energy diagrams for, 385	alcohols and, 656	3-phosphate and, 1161
epoxide cleavage and, 383, 688, 689	bromoethane and, 477–478 2-bromopropane and, 478	Steric hindrance, S_N 2 reaction and, 378–379
inversion of configuration in,	n + 1 rule and, 478	Steric strain, 97
376–377	¹³ C NMR spectroscopy and, 480	cis alkenes and, 234–235
kinetics of, 375–376	¹ H NMR spectroscopy and,	substituted cyclohexanes and,
leaving groups and, 382–383	477–480	124–125
mechanism of, 376–377	nonequivalent protons and,	Steroid(s), 1107 –1111
nucleophiles in, 380–381	482–483	adrenocortical, 1111
rate law for, 376	origin of, 477–478	anabolic, 1111
solvent effects and, 383–384	rules for, 479	androgens, 1110
stereochemistry of, 376–377	tree diagrams and, 483	biosynthesis of, 1112–1117
steric hindrance in, 378–379	Split synthesis, 605–606	cis A–B ring fusion in, 1108
substrate structure and, 378–380	Squalene, epoxidation of, 1112–1113	conformation of, 1107
summary of, 384–385	from farnesyl diphosphate, 1112	contraceptive, 1111
table of, 381 tosylates and, 382	steroid biosynthesis and, 1112–1113	estrogens, 1110 glucocorticoid, 1111
Williamson ether synthesis and,	Squalene oxide, cyclization of, 1114,	mineralocorticoid, 1111
678–679	1116–1117	molecular model of, 1107
Soap, 1092–1093	Staggered conformation, ethane and,	numbering of, 1107
history of, 1092	95	progestins, 1110
manufacture of, 1092	molecular model of, 95	stereochemistry of, 1108–1109
mechanism of action of, 1093	Stannous chloride, reaction with	synthetic, 1111
micelles of, 1092–1093	nitroarenes, 955	trans A–B ring fusion in, 1108
Sodium amide, reaction with	Starch, $1\rightarrow 4-\alpha$ -links in, 1028	Stork enamine reaction, 925–926
alcohols, 626	structure of, 1028	advantages of, 926
Sodium bisulfite, osmate reduction	Statin drugs, heart disease and,	mechanism of, 925
with, 283	1203–1204	STR loci, DNA fingerprinting and,
Sodium borohydride, reaction with	mechanism of action of,	1146
ketones and aldehydes, 630	1203-1204	Straight-chain alkane, 82
reaction with organomercury	sales of, 106	Strecker synthesis, 999
compounds, 271–272	structure of, 107	Structure, condensed, 21
Sodium chloride, dipole moment of,	Steam cracking, 223–224	electron-dot, 7
38	Steam distillation, 299	Kekulé, 7
Sodium cyclamate, LD ₅₀ of, 24	Stearic acid, molecular model of,	Lewis, 7
Sodium hydride, reaction with	1090	line-bond, 7
alcohols, 626	structure of, 1090	skeletal, 21
Solid-phase peptide synthesis,	Stein, William, 1058	Strychnine, LD ₅₀ of, 24
1064–1066	Step-growth polymer, 847 –850,	Styrene, anionic polymerization of,
PAM resin in, 1065	1248–1250	1244 Substituent 87
Wang resin in, 1065 Solvation, 383	table of, 848 Stereocenter, 145	Substituent, 87 Substituent effect, additivity of,
carbocations and, 393	Stereochemistry, 94, 112	590
S _N 2 reaction and, 383	absolute configuration and, 154	electrophilic aromatic substitution
Solvent, polar aprotic, 383	Diels–Alder reaction and, 512	and, 580–581
protic, 383	E1 reaction and, 406	explanation of, 582–589
S _N 1 reaction and, 392–393	E2 reaction and, 401–402	summary of, 589
S_N 2 reaction and, 383–384	electrophilic addition reactions	Substitution reaction, 185
Sorbitol, structure of, 1020	and, 296–298	Substrate (enzyme), 1069
Spandex, synthesis of, 1250	R,S configuration and, 150–154	Succinic acid, structure of, 780

Sucralose, structure of, 1034 Tautomer, 319, 871 Thioester(s), 814 sweetness of, 1033 Taxol, structure of, 333 biological reduction of, 847 Sucrose, molecular model of, 1027 Tazobactam, 867 electrostatic potential map of, 820 specific rotation of, 149 Teflon, structure and uses of, 293 naming, 816 structure of, 1027 Template strand (DNA), 1136 pK_a of, 879 Thiol(s), 676, 691-693 sweetness of, 1033 Terephthalic acid, synthesis of, 596 Sugar, complex, 1001 Termination step (radical), 188 disulfides from, 692 D, 1007 Terpene, 299-300 electrostatic potential map of, 79 L, 1007 Terpenoid, 299-300, 1098-1106 from alkyl halides, 692 see also Aldose, Carbohydrate biosynthesis of, 299–300, hybridization of, 19 simple, 1001 1098-1106 naming, 691 Sulfa drug, 968 classification of, 300, 1098 odor of, 692 synthesis of, 573 isoprene rule and, 299-300 oxidation of, 692 Sulfanilamide, structure of, 573 mevalonate biosynthetic pathway pK_a of, 625 synthesis of, 968 for, 1099-1103 polarizability of, 191 Sulfathiazole, structure of, 968 tert-, name prefix, 85 reaction with alkyl halides, 693 Sulfide(s), 676, 693–695 tert-Amyl group, 90 reaction with Br2, 692 electrostatic potential map of, 79 tert-Butyl group, 85 reaction with NaH, 693 from thiols, 693 Tertiary alcohol, 621 sulfides from, 693 naming, 693 Tertiary amine, 944 thiolate ions from, 693 oxidation of, 694 Tertiary carbon, 86 Thiolate ion, 693 reaction with alkyl halides, 694 Thionyl chloride, reaction with Tertiary hydrogen, 86 sulfoxides from, 694 Tertiary structure (protein), 1066, alcohols, 355, 639 Sulfonation (aromatic), 572-573 1068 reaction with amides, 793-794 Sulfone, 694 Testosterone, conformation of, 130 reaction with carboxylic acids, from sulfoxides, 694 molecular model of, 130 823-824 Sulfonium ion(s), 694 structure and function of, 1110 Thiophene, aromaticity of, 548 chirality of, 166 Tetracaine, structure of, 995 Thiourea, reaction with alkyl halides, Sulfoxide(s), 694 Tetrahedral geometry, conventions 692 from sulfides, 694 for drawing, 6 Threonine, stereoisomers of, 156 oxidation of, 694 Tetrahydrofolate, structure of, 1073 structure and properties of, 1047 Tetrahydrofuran, as reaction solvent, Threose, configuration of, 1009 Sunshine vitamin, 1232 molecular model of, 147 Super glue, structure of, 1244 263 Suprafacial geometry, 1223 molecular model of, 676 Thromboxane B₂, structure of, 1096 Suture, polymers in, 850 Tetramethylsilane, NMR spectroscopy Thymine, electrostatic potential map Suzuki-Miyaura reaction, 359 and, 462 of, 1132 mechanism of, 359 Thermodynamic control, 508–509 structure of, 1129 Sweeteners, synthetic, 1033-1034 1,4-addition reactions and, Thyroxine, biosynthesis of, 571 Swine flu, 1032 508-509 structure of, 1048 Time-of-flight (TOF) mass Symmetry plane, 144 Thermoplastic polymer, 1254 Symmetry-allowed reaction, 1215 characteristics of, 1254 spectrometry, 433 Symmetry-disallowed reaction, 1215 examples of, 1254 Titration curve, alanine, 1051 Syn periplanar geometry, 401 $T_{\rm g}$ of, 1254 TMS, see Tetramethylsilane, molecular model of, 401 uses of, 1254 Trimethylsilyl ether Syn stereochemistry, 273 Thermosetting resin, 1256 Tollens' test, 1020 Syndiotactic polymer, 1245 cross-linking in, 1256 Toluene, electrostatic potential map Synthase, 1167 uses of, 1256 of, 585 Synthesis, strategy of, 329 Thiamin diphosphate, p K_a of, 1183 IR spectrum of, 551 reaction with pyruvate, 1181-1183 ¹³C NMR absorptions of, 554 Table sugar, see Sucrose structure of, 1183 ¹H NMR spectrum of, 482 Tagatose, structure of, 1002 ylide from, 1183 Toluene-2,4-diisocyanate, Talose, configuration of, 1009 Thiamin, structure of, 549, 975, 1073 polyurethanes from, 1250 thiazolium ring in, 549 p-Toluenesulfonyl chloride, reaction Tamiflu, mechanism of, 1032–1033 molecular model of, 132 Thiazole, basicity of, 975 with alcohols, 639-640 thio-, thioester name suffix, 816 Torsional strain, 95 structure of, 32 Thioacetal, synthesis of, 770 Tosylate, 373-374 Tamoxifen, structure of, 257 Thioanisole, electrostatic potential from alcohols, 639-640 synthesis of, 771 Tag DNA polymerase, PCR and, 1145 map of, 804 S_N 2 reactions and, 382, 640 Tartaric acid, stereoisomers of, 159 -thioate, thioester name suffix, 816 uses of, 640

Toxicity, chemicals and, 24–25 tRNA, see Transfer RNA Valsartan, synthesis of, 359 Trans fatty acid, from vegetable oil, Van der Waals force, polymers and, Trypsin, peptide cleavage with, 1061 from hydrogenation of fats, Tryptophan, p K_a of, 52 van't Hoff, Jacobus Hendricus, 6 structure and properties of, 1047 279-280 Vegetable oil, 1089–1090 Transamination, 1198-1201 Turnover number (enzyme), 1069 composition of, 1090 mechanisms in, 1198-1201 Twist-boat conformation hydrogenation of, 279–280, 1091 steps in, 1198-1201 (cyclohexane), 119–120 Veronal, synthesis of, 890 Transcription (DNA), 1135-1136 steric strain in, 119–120 Vestenamer, synthesis of, 1252–1253 antisense strand and, 1136 molecular model of, 120 Vicinal, 316, 686 consensus sequence and, 1135 Tyrosine, biosynthesis of, 643 Vinyl group, 228 catabolism of, 1211 Vinyl monomer, 292 promoter sequence and, 1135 sense strand and, 1136 iodination of, 571 Vinylcyclopropane, rearrangement structure and properties of, 1047 Transfer RNA, 1135 of, 1237 anticodons in, 1138-1139 Vinylic anion, electrostatic potential function of, 1138-1139 Ubiquinones, function of, 654 map of, 326 molecular model of, 1138 structure of, 653 stability of, 326 Ultrahigh-molecular-weight Vinylic carbocation, electronic shape of, 1138 Transferase, 1070 polyethylene, uses of, 1246 structure of, 318 Transition state, 206 Ultraviolet light, electromagnetic electrostatic potential map of, Hammond postulate and, 247 spectrum and, 434 318 from alkynes, 318 Translation (RNA), **1137**–1139 wavelength of, 517–518 Tranyleypromine, synthesis of, 962 Ultraviolet spectroscopy, 517–520 stability of, 318 Tree diagram (NMR), 483 absorbance and, 519 Vinylic halide, alkynes from, 316 Triacylglycerol, 1089 S_N2 reaction and, 379–380 aromatic compounds, 552 catabolism of, 1158-1167 conjugation and, 520 Vinylic protons, ¹H NMR Trialkylsulfonium ion(s), alkylations HOMO-LUMO transition in, 518 spectroscopy and, 474-475 with, 694 molar absorptivity and, 519 Vinylic radical, alkyne reduction and, 324-325 chirality of, 166 Ultraviolet spectrum, benzene, 520 Tributyltin hydride, reaction with β -carotene, 521 Vioxx, 1, 555 alkyl halides, 370 1,3-butadiene, 519 Visible light, electromagnetic Tricarboxylic acid cycle, see Citric 3-buten-2-one, 520 spectrum and, 434 acid cycle 1,3-cyclohexadiene, 520 Vision, chemistry of, 522 Trifluoroacetic acid, pK_a of, 783 ergosterol, 532 retinal and, 522 Trifluoromethylbenzene, electrostatic 1,3,5-hexatriene, 520 Vitalistic theory, 1 potential map of, 585 isoprene, 520 Vitamin, 799 Triglyceride, see Triacylglycerol, 1089 Unimolecular, 386 Vitamin A, industrial synthesis of, Trimethylamine, bond angles in, 947 Unsaturated, 224 323 bond lengths in, 947 Unsaturated aldehyde, conjugate structure of, 62 electrostatic potential map of, 949 addition reactions of, 751-755 synthesis of, 748 molecular model of, 947 Vitamin B₁, structure of, 975 Unsaturated ketone, conjugate Trimethylsilyl ether, cleavage of, 649 addition reactions of, 751-755 Vitamin B_{12} , structure of, 333 from alcohols, 648-649 Unsaturation, degree of, 224 synthesis of, 333 synthesis of, 648-649 Upfield, (NMR), 461 Vitamin C, industrial synthesis of, Trimetozine, synthesis of, 832 Uracil, structure of, 1129 800-801 2,4,6-Trinitrochlorobenzene, Urea, from ammonium cyanate, 1 molecular model of, 800 electrostatic potential map of, Urethane, 1250 scurvy and, 800 Uric acid, pK_a of, 805 stereochemistry of, 178 Uronic acid, 1021 Triphenylphosphine, reaction with structure of, 62 alkyl halides, 747 from aldoses, 1021 uses of, 800 Triple bond, 16 Urushiols, structure of, 621 Vitamin D, sigmatropic electronic structure of, 16 UV, see Ultraviolet rearrangements and, 1232 Vitamin K_1 , biosynthesis of, length of, 17 see also Alkyne Valence bond theory, 9-10 578-579 Valence shell, 6 strength of, 17 Viton polymer, structure and uses of, Triplet (NMR), 477 Valganciclovir, structure and function 1247 Trisubstituted aromatic compound, VLDL, heart disease and, 1118 of, 1153 synthesis of, 600-604 Valine, structure and properties of, Volcano, chloromethane from, 344 Vulcanization, 517 Triterpenoid, 1098 1047

I-36 Index

Walden, Paul, 372 Walden inversion, 372–375 Wang resin, solid-phase peptide synthesis and, 1065 Water, acid-base behavior of, 50 dipole moment of, 38 electrostatic potential map of, 52 nucleophilic addition reaction of, 731-732 pK_a of, 51–52 reaction with aldehydes, 731-732 reaction with ketones, 731-732 Watson, James Dewey, 1131 Watson-Crick DNA model, 1131-1132 Wave equation, 3 Wave function, 3 molecular orbitals and, 19-20 Wavelength (λ), 435 Wavenumber, 437 Wax, 1088-1089 Whale blubber, composition of, 1090 Whitmore, Frank C., 249 Wieland-Miescher ketone, synthesis of, 938

Williamson ether synthesis, 678–679 carbohydrates and, 1016 mechanism of, 678-679 Willstätter, Richard, 542 Winstein, Saul, 388 Wittig reaction, 746–748 mechanism of, 746-747 uses of, 747-748 vitamin A synthesis using, 748 Wohl degradation, 1023 Wöhler, Friedrich, 1 Wolff-Kishner reaction, 741-742 mechanism of, 741-742 Wood alcohol, 620 Woodward, Robert Burns, 333, 1215 Woodward-Hoffmann rules, 1215-1216

X rays, electromagnetic spectrum and, 434 X-Ray crystallography, 447 X-Ray diffractometer, 447 o-Xylene, ozonolysis of, 559 Xylocaine, structure of, 64 Xylose, configuration of, 1009 -yl, alkyl group name suffix, 84
-yl phosphate, acyl phosphate name suffix, 817
Ylide, 746
-yne, alkyne name suffix, 314

Z configuration, 231–232 assignment of, 231-232 Zaitsev, Alexander M., 397 Zaitsev's rule, 397 alcohol dehydration and, 641 E1 reaction and, 406 E2 reaction and, 403 Hofmann elimination and, 964-965 proof for, 470-471 Zanamivir, mechanism of, 1032–1033 Zeisel method, 708 Ziegler–Natta catalyst, 1245 Zinc-copper, Simmons-Smith reaction and, 288-289 Zocor, structure of, 107 Zwitterion, 1045 electrostatic potential map of, 1045

Structures of Some Common Functional Groups

Name	Structure*	Name ending	Example
Alkene (double bond)	c=c (-ene	H ₂ C=CH ₂ Ethene
Alkyne (triple bond)	_C = C—	-yne	HC≡CH Ethyne
Arene (aromatic ring)		None	Benzene
Halide	(X = F, Cl, Br, I)	None	CH ₃ CI Chloromethane
Alcohol	C OH	-ol	CH ₃ OH Methanol
Ether	C C	ether	CH ₃ OCH ₃ Dimethyl ether
Monophosphate	C 0 P 0 O	phosphate	CH ₃ OPO ₃ ²⁻ Methyl phosphate
Diphosphate		diphosphate	CH ₃ OP ₂ O ₆ ³⁻ Methyl diphosphate
Amine	c N:	-amine	CH ₃ NH ₂ Methylamine
Imine (Schiff base)	:N = C C	None	NH CH ₃ CCH ₃ Acetone imine
Nitrile	–C≡N	-nitrile	CH ₃ C <mark>≡N</mark> Ethanenitrile
Thiol	C SH	-thiol	CH ₃ SH Methanethiol
*The bonds whose connections aren't specified are assumed to be attached to carbon or hydrogen atoms in the rest of the molecule.			

Name	Structure*	Name ending	Example
Sulfide	C S C	sulfide	CH ₃ SCH ₃ Dimethyl sulfide
Disulfide	c S S C	disulfide	CH ₃ SSCH ₃ Dimethyl disulfide
Sulfoxide	0 ⁻ c s ⁺ c	sulfoxide	O ⁻ + CH ₃ SCH ₃ Dimethyl sulfoxide
Aldehyde	O C H	-al	O CH ₃ CH Ethanal
Ketone	C C C	-one	O CH ₃ CCH ₃ Propanone
Carboxylic acid	O OH	-oic acid	O CH ₃ COH Ethanoic acid
Ester	C C C	-oate	O CH ₃ COCH ₃ Methyl ethanoate
Thioester	C C S C	-thioate	O CH ₃ CSCH ₃ Methyl ethanethioate
Amide	C C N	-amide	O CH ₃ CNH ₂ Ethanamide
Acid chloride	C CI	-oyl chloride	CH ₃ CCI Ethanoyl chloride
Carboxylic acid anhydride		-oic anhydride	O O CH ₃ COCCH ₃ Ethanoic anhydride
*The bonds whose connections aren't specified are assumed to be attached to carbon or hydrogen atoms in the rest of the molecule.			