

---

# INDEX

---

- Absorption, 331  
  dermal, 331  
  endocytosis, 331  
  gastrointestinal, 331  
  respiratory tract, 331
- Acid, 2, 85, 104–105, 130, 318–319  
  amino, 177–179, 241–242  
  ascorbic, 248–249  
  Bronsted–Lowry definition, 104, 106  
  fatty, 241, 258, 319  
  lactic, 152–153, 247–249, 251–252  
  Lewis definition, 106, 117, 163, 174  
  rain, 45, 50, 66  
  strong, 104, 129–130, 133  
  weak, 104–105, 129–130, 151, 153
- Activation energy, 160
- Adverse  
  effects, 327  
  outcome pathways (AOPs), 326, 337–338
- Air  
  Clean Air Act, 11, 44, 52, 67  
  pollution, 44–45, 51, 60, 136, 175
- Agricultural, 2, 10, 15–16, 53, 55–56, 236, 254, 258
- Alcohol, 2, 90, 101, 117, 163, 236, 247, 258
- Aldehydes, 49, 90, 101, 123, 163, 238
- Algae, 62–63, 239–240, 258–261, 343
- Alkanes, 85–86, 88–90, 174, 221, 246
- Alkenes, 85, 88–89, 117, 163, 172, 246
- Alkynes, 89
- Aluminum, 38, 53, 74–76, 83, 85, 106
- Amine, 92, 140
- Ammonia, 4, 105–106, 111, 174
- Anderson–Shultz–Flory distribution, 246
- Anions, 54, 84, 98–100, 102, 105, 114, 121, 128, 173
- Antibiotics, 2, 5, 170
- Aromatics, 3, 174, 249
- Arrhenius relation, 160–161
- Arsenic, 4, 11, 53, 59, 74–75
- Atom economy or utilization (Barry Trost), 24–26, 30, 115–117, 134–136, 162, 176, 295, 302, 310, 312–313
- Atomic  
  number, 74, 78, 82  
  radius, 74  
  structure, 77–78, 82  
  weight, 25, 74, 78–79, 112–113
- Bacteria, 4, 5, 31, 56, 175, 180, 251–253, 255, 327
- Base  
  Bronsted–Lowry definition, 104  
  Lewis definition, 106, 117  
  strong, 25, 105, 129–30, 133  
  weak, 105, 151
- Benzene, 3, 13, 93–94, 222, 226, 249–250, 327
- Bhopal (India), 4, 10, 14
- Biocatalysis, 5, 33, 170, 175–178
- Biodegradable  
  diesel, 258, 319  
  plastics, 30, 251–254  
  polymers, 102, 247
- Biodiesel, 67, 90, 105, 241, 252, 258–261, 319–320
- Biomarkers, 333, 338

- Biomass  
 biological process, 242–244  
 combustion, 100, 236  
 definition, 16, 17, 32, 60, 235–238, 261  
 sources, 60–61, 93, 238, 240, 266, 277,  
 284–285, 320  
 thermochemical treatment, 244–245, 247,  
 319–320  
 waste, 258–260
- Biorefinery, 60, 242–244, 260–261, 319–320
- Bisphenol A, 76
- Boyle's law, 198
- California, safer consumer products  
 regulation, 348
- Cancer, 4, 5, 9, 13, 22, 49, 51, 65, 179, 320,  
 334–335  
 species differences, 336–337
- Capital expenses, 290
- Carbohydrates, 236–238, 240, 243, 252
- Carbon cycle, 60, 236
- Carbon footprint, 17–18
- Carbon dioxide  
 absorption, 237, 252  
 dissolution, 52  
 production, 10, 32, 44, 49–50, 60, 100,  
 102–103, 111, 123, 134, 175, 236,  
 255, 257–259, 264, 267, 270, 274,  
 284, 317
- Carboxylic acid, 81, 91, 101, 333
- Carcinogens, 9, 11, 179, 335, 347
- Catalyst  
 chiral, 180  
 definition, 30, 102, 162–168  
 heterogeneous, 164–166, 173–175  
 homogeneous, 170–173  
 types, 33, 105, 134, 148, 156, 158–159,  
 191–192, 246, 248, 258, 304–305,  
 311, 318–319
- Cations, 54, 84, 98, 102, 105, 121, 128, 173
- Cellular  
 death  
 apoptosis, 334  
 necrosis, 334  
 responses  
 atrophy, 334  
 hyperplasia, 334  
 hypertrophy, 334
- Cellulose, 34, 183–184, 237–240, 243, 246,  
 255
- Changes  
 chemical, 30, 74, 100  
 physical, 30, 80, 100
- Charles' law, 198
- Chemical(s)  
 compostable, 252, 254  
 data poor, 326, 339, 341  
 exposure, 327  
 assessment, 330  
 dose, 329  
 effective, 329  
 internal, 331  
 lethal, 329  
 toxic, 329
- dose level  
 acceptable daily intake (ADI), 330  
 NOAEL, 329  
 LOAEL, 329  
 dose-response, 329–330
- of concern, 326, 335–336
- Chemistry  
 linked to toxicity  
 mechanistic domains, 338  
 structural alerts, 338  
 organic, 2, 90, 131  
 twenty-first century (green chemistry),  
 13–14, 18–19, 21–25, 28, 31–32,  
 34–35, 38, 40, 43, 60–62, 66, 68,  
 73, 99, 101–102, 104, 106, 135,  
 156, 159, 170, 176–177, 222, 235,  
 251, 267, 287–289, 292–300,  
 302–313, 316–322, 325–326, 339,  
 341, 346, 348, 350
- Chlorofluorocarbons (CFCs), 12, 46–47
- Cisplatin, 84
- Clean Air Act, 44
- Clean Water Act, 11, 52
- Climate change, 15–16, 46, 53, 66, 68, 285,  
 308, 311
- Coal, 3, 16, 35, 49–50, 57, 59–60, 88, 93,  
 102, 235, 237, 245, 251, 260,  
 263–266, 275, 278, 280, 282, 284,  
 286, 320
- Colloids, 102–103
- Combustion, 16, 39, 46, 49–50, 59–60,  
 100, 111, 142, 146–147, 175,  
 236–237, 242, 245, 257, 270,  
 275, 285
- Comparative Toxicogenomics Database  
 (CTD), 345

- Compounds  
  ionic, 81, 82, 94, 98–99, 118, 124, 126, 274  
  molecular, 81–82
- Comprehensive Environmental Response, Compensation and Liability Act (CERCLA), 11
- Conversion, 140
- Corn, 61, 67, 100–101, 183, 236, 238, 252–253, 255, 258, 286, 337
- Cracking, 3, 174, 226
- Critical point, 80, 217–219
- Crops, 2, 4, 10, 16, 44, 55, 60–61, 67, 236, 241, 243, 254–255, 258
- Cuyahoga River (Ohio), 8
- Deforestation, 55, 67, 236, 277
- Developed countries, 5, 12, 16, 18, 56
- Developing countries, 4, 12, 15–16, 18, 53, 55–56, 264, 277
- Dioxin, 9, 56
- Distribution, 102, 172, 256, 264–265, 285, 291–292, 303, 305, 313, 315, 330, 332, 335  
  coefficient, 222, 227–228
- Drugs, 2, 5–7, 33, 94, 104, 176–177, 179, 340, 348
- Earth Summit (Rio de Janeiro), 14, 15
- Ecotoxicity, 62
- Electrochemistry, 273
- Electrolyte, 124, 273
- Electronegativity, 94, 98
- Electrons, 79  
  transfer, 98, 118, 120  
  valence, 82–83, 88, 94, 277
- Elements, 14, 23, 25–26, 47, 53, 57, 64–65, 74–77, 79, 81–83, 85, 91, 98, 102, 115, 121–122, 144, 188, 197, 236, 269, 284, 292, 327
- Emergency Planning and Community Right-to-Know Act (EPCRA), 11
- Energy, 56–61  
  balance, 201, 203–204  
  impacts, 56–60  
  internal, 202  
  transfer, 21–30, 201–202  
    microwave, 190, 272  
    nuclear, 275
- Engineering  
  green, 19, 21–22, 34–35, 40, 43, 73, 287–289, 292–294, 305, 307–310, 313, 316–317, 321–322  
  reaction, 19, 139, 181
- Enthalpy, 160, 204, 215–217, 268–270  
  change, 214, 269
- Entropy, 210–214
- Environmental impact assessment, 65
- Environmental Protection Agency (EPA), 7, 11, 31–32, 34–35, 44–45, 51, 61–63, 67, 70, 265, 288, 330, 341–343, 346
- resources  
  ACTOR, 341–342  
  EPI Suite, 343  
  ExpoCastDB, 342  
  ToxCast, 342  
  ToxCastDB, 342  
  Virtual organs, 342
- Enzyme, 2, 117, 169, 176, 179–180, 255–256, 333
- Equation  
  Antoine, 220, 224, 227, 229  
  balancing, 109–110, 112  
  energy balance, 201, 203  
  van der Waals, 215  
  Van't Hoff, 232
- Equilibrium  
  chemical, 150–151, 162  
  flash calculation, 223, 227
- Ester, 91, 179, 258
- Esterification process for biodiesel production, 28, 172, 249, 258
- Ethanol  
  production from biomass, 254–255, 257  
  production from waste, 67, 183
- Ether, 50, 67, 91, 158
- European Center for the Validation of Alternative methods (ECVAM), 347
- Excretion, 333
- Exposure, 10, 13–14, 26–27, 51, 63, 69, 76–77, 91, 327–330, 332, 337–339, 341–343, 347, 349
- Fermentation, 2, 32, 34, 102, 180, 183, 185, 224, 238, 247–249, 252, 254–256, 320–321
- Fertilizers, 3, 4, 60, 66, 76, 237, 261
- Flex-fuel vehicles, 254, 256–257

- Fisher–Tropsch, 244, 246, 260
- Formula**
- condensed, 86, 89
  - molecular, 85–86, 109–111, 114, 184, 239
  - structural, 85–86, 88, 90–93
- Forces, intermolecular, 80, 81, 103
- Fossil**
- fuels, 60, 85, 237, 243, 259, 263–265, 275–276, 285
  - resources, 3, 29, 57, 66, 100–101, 135, 236–237, 242–243, 249, 261, 265–266, 279
- Free radicals, 47, 94, 339
- Future perspectives, 349–350
- tox-bioinformatics, 350
- Gas**
- ideal, 197–201
    - calculations, 205–210, 212–214
    - natural, 3, 16, 32, 50, 57–59, 135, 145, 226, 243, 245, 251, 263–264, 266, 275, 278, 284
    - real, 214–215
- Genego, 344
- Glucose**
- biocatalytic conversion, 249
  - conversion, 246–248
  - fermentation, 102, 247–248
- Green building action plan, 17
- Green chemistry principles, 24
- Green engineering principles, 25
- Greenhouse**
- emissions, 15–17, 46, 64–65, 67
  - gas, 236, 253, 264–265, 276, 278, 280, 282, 284–285, 308
- GREENSCOPE, 313, 316
- Group (or family)**, 74, 82–83, 85, 88, 94, 98, 106, 122, 125, 128
- functional, 30, 90–92, 101, 131, 134–135, 178, 247, 274, 343
- Hazard(ous), 7, 13–14, 22–23, 26–27, 31, 36, 40, 297, 311, 329–330, 348
- substances, 23–24, 30, 35, 106, 294, 326
  - traits, 326
- Heat**
- capacity, 206
  - definition, 202
- formation, 269–270
- reaction, 267–272
- transfer, 171, 203, 254, 288
- Henry's law**, 229
- Hess law**, 270–271
- Homeostasis**, 333
- Hudson River**, 9
- Hydrocarbons**, 3, 49, 85, 89, 100, 175, 226, 284
- Hydrogenation**, 33, 156, 163, 170, 172, 178, 192, 247–249
- Hydrogen**
- bonding, 81–82, 104
  - fuel cell, 285
- Ideal gas**, 199, 205
- Indoor air**, 51
- Insulin**, 5, 177
- Ion**
- monoatomic, 98, 121
  - polyatomic, 98, 99, 121, 128
  - spectator, 54, 118, 123, 126–127, 129, 131–134
- Ionic liquid**, 99, 159, 173, 318
- Irrigation**, 3, 4, 16, 53
- Isomers**, 135, 179
- structural, 238
- Isomerization**, 163, 246, 268
- Ketone**, 101, 116
- Kinetics**, 19, 139, 151, 153–159, 166–168, 174, 186, 288, 318, 336
- catalytic, 166
  - Michaelis–Menton, 169, 256
- Kyoto Protocol**, 216, 266
- Lead**, 6, 7, 11, 44–45, 53–54, 69, 74–75, 77, 84, 127, 175, 273, 332
- Life cycle**, 19, 23, 35, 37, 40, 60, 64, 69, 100, 243, 249, 255, 261, 287–289, 294–300, 306, 311, 315–316, 348
- Ligand**, 84, 134, 171–172, 178, 275
- Lignin**, 60, 236, 238, 240, 243
- Limiting reactant**, 141
- Lipid**, 236, 259, 331
- Love Canal (NY)**, 8
- Margin of safety (MOS)**, 329
- Mass**, law of conservation, 110, 112

- molar, 112–113, 137  
transfer, 164–166, 192–194
- Matter, 1, 16, 19, 44, 49, 52, 54–55, 73–74, 79, 100, 102–104, 110, 112, 122, 236, 238, 261, 333
- Mercury, 53, 59, 69, 75–76, 81, 84  
methyl, 76
- Metabolism  
bioactivation, 332  
first-pass, 331  
phase I, 332–333  
phase II, 332–333
- Metal  
center, 170–171, 274  
transition, 84
- Metalloids, 74–75
- Methyl isocyanate, 10
- Michaelis–Menton kinetics, 169, 256
- Microwave, 190, 272
- Mixture, 50, 62, 100, 102–104, 163, 174, 179–180, 200–201, 217, 220–222, 224–227, 236, 241, 244, 249, 254, 256–258, 284, 311, 320
- Mode of action (MOA), 326, 336
- Model(s); modeling  
compartmental, 332  
interoperability, 346  
quantitative structure-activity relationship (QSAR), 335, 343
- Mole, 112–113, 138, 149, 163, 188, 199–200, 205, 221–222, 225, 227–230, 232
- Molecules  
bio-derived, 243  
cyclic, 92–93  
diatomic, 81–82, 94, 110, 112, 175, 274, 284  
heteronuclear, 81–82, 94, 98  
homonuclear, 81, 94, 98
- Molecular weight, 49, 83, 91, 113–115, 172, 174, 177, 184, 206, 274
- Monod's equation, 256
- Monosaccharides, 238
- Montreal Protocol, 12, 46
- Neutrons, 78–79, 82
- New technologies, 340
- Nitrates, 4, 125, 127–128, 133
- Nitrogen cycle, 4
- Nonmetals, 74, 81, 94, 98
- Nucleus, 77–78, 81–82, 275
- OECD, 344
- Oil, 2, 3, 9, 14, 16, 28, 32, 49, 57, 59–60, 93, 104, 174, 236–237, 239, 241–243, 245, 251–253, 258–261, 263–266, 275, 277, 280, 282, 286, 291–292, 319, 337
- Olefins, 3, 171, 173
- Oxidation, 49–50, 84, 100, 111, 146, 148, 171, 175, 187, 230, 243, 247, 249, 274, 313  
aldehydes, 101  
half-reactions, 118–221  
numbers, 122–124, 126  
primary alcohols, 101  
secondary alcohols, 102
- Oxoanions, 99
- Oxygen, 44, 46–47, 49–50, 52–53, 67, 74–75, 81, 85, 89, 91, 94, 99–100, 110–112, 117, 121, 137, 141, 148–149, 187, 190, 229–230, 236–237, 243–246, 252, 254, 257, 270, 284–285, 318, 334
- Ozone, 11–12, 33, 44–49, 94, 141, 251  
depletion, 16, 65, 311, 313
- Partial pressure, 200
- Particles, 45, 50–51, 54, 73–74, 77–79, 103, 156, 167, 175, 178, 191–192, 194, 199
- Pathological adaption, 333
- Penicillin, 2, 5, 321
- Percent yield, 135–137
- Periodic table, 73–75, 79, 81–83, 85, 94, 112–113, 121–122
- Period, 83, 94, 122
- Pesticides, 3, 4, 10, 27, 30, 38, 55–56, 60, 66, 69, 237, 240, 261, 292, 346, 348
- Petroleum, 28, 30, 50, 57, 60, 77, 88, 174, 235, 246, 251, 258, 264–266, 319–320
- Petrochemicals, 2, 3, 174, 235, 240
- pH  
definition, 50, 52, 55, 105, 151–153, 169, 331  
scale, 105  
value, 106
- Pharmaceuticals, 5, 8, 30, 53, 174, 247, 320–321

- Phase  
 change, 80, 218  
 diagram, 80–81, 217–219
- Photochemistry, 45, 274
- Photosynthesis, 236–237, 252, 273–274
- Photovoltaic  
 cell, 274–275, 278  
 effect, 277
- Pollution prevention, 11–13, 19, 22–23,  
 30–31, 34, 43, 61–62, 294
- Polychlorinated biphenyls (PCBs), 9
- Polyethylene, 3, 85, 273  
 terephthalate, 28, 251, 318
- Polylactic acid, 247, 252
- Polymers, 32, 50, 101, 156, 171, 255, 260  
 biodegradable, 102  
 biological, 238
- Polymerization, 172, 174, 246, 248, 252, 318
- Polysaccharides, 238
- Process integration, 29
- Properties  
 chemical, 74, 77, 241, 331, 345  
 physical, 46, 80, 91
- Proteins, 32, 66, 236, 238, 241, 340, 345
- Protons, 78–79, 82, 98, 104–105, 331
- Raoult’s law, 221–223
- Rate, 2–4, 8, 12, 27, 38, 46, 55, 177, 235, 237,  
 281, 283, 290, 311, 312, 319, 332, 344  
 chemical reaction, 162, 164, 166, 192  
 definition, 139–143, 149, 151, 153  
 effect of concentration, 153–159  
 effect of temperature, 159–161  
 flow, 181–183, 185–187, 189–190, 193, 200  
 Langmuir–Hinshelwood, 166–168  
 Michaelis–Menton, 169, 256
- REACH, 346–347
- Reaction  
 addition with organic compounds, 116  
 electrophilic, 116  
 nucleophilic, 116, 338  
 combination (or synthesis or addition),  
 109, 115, 134  
 consecutive, 146–148, 164, 166  
 decomposition, 117  
 definition, 100–110  
 displacement (redox), 54, 118, 120, 126,  
 134, 273  
 effectiveness and efficiency, 135  
 elimination, 24, 117  
 exchange (or substitution), 54, 124,  
 126–129, 131–134  
 gas-forming, 131, 133, 229  
 heat, 267–272  
 neutralization (acid-base), 129–130, 133  
 parallel, 142, 144–147, 150  
 patterns, 115  
 precipitation, 124, 127–128, 133
- Reactor  
 batch, 154, 181–184, 189  
 continuous stirred tank, 184, 187  
 multiphase design, 191–194  
 packed bed, 190–192  
 plug flow (PFR), 157, 188–190  
 slurry, 192
- Regulations, 7, 11, 45, 52, 56, 61, 285, 306,  
 308, 348–349
- Renewable  
 feedstocks, 29, 32, 101, 236, 243, 293,  
 301, 319  
 materials, 19, 29, 40, 100, 116, 236, 251,  
 261, 266, 287  
 resources, 38, 40, 101, 235–236, 242–243,  
 261, 285, 289  
 sources of energy, 57–58, 275, 277, 280,  
 285, 315  
 geothermal, 275, 281–282, 284, 286  
 hydrogen technology, 284–285  
 hydropower, 275, 283–284  
 solar, 275–279, 282  
 wind, 279–281
- Residence time, 186
- Resources  
 finite, 235, 242  
 infinite, 235  
 perpetual, 235
- Resource Conservation and Recovery Act  
 (RCRA), 11
- Risk  
 assessment, 329, 338, 340, 346–347  
 characterization, 330  
 definition, 13–14  
 identification, 325  
 management, 329  
 risk/benefit, 328
- Salts, 4, 54, 77, 82, 99, 173–174, 230–231
- Selectivity, 30, 106, 135, 142, 144–145,  
 162–164, 170, 172, 174, 176, 178,  
 194, 272–274, 313

- Semiconductor, 277–278  
Silicon, 53, 74, 277–278  
Solar collectors, 276  
Solubility, 124, 172–173, 229–232, 333  
    rules (table), 125–128  
Solute, 103–105, 230–232  
Solutions  
    acidic, 52  
    basic, 52  
    definition, 102–103, 105  
    engineering, 39–41  
Solvent, 2, 26–28, 31–32, 35, 52, 91, 93, 102–104, 111, 139, 156, 159, 171–173, 228–233, 272, 302, 305, 310–311, 317–321  
Sonochemistry, 273  
Starch, 236, 238–240, 243, 251–252, 254–255  
States of matter, 79  
STITCH, 345  
Stoichiometric coefficient, 110, 119, 120, 125–126, 128, 141–142, 144, 147, 269, 279, 293  
Substance, 5, 31, 49, 55, 62–63, 66, 80, 102, 105–106, 118, 124, 199, 215, 221, 237, 251, 299, 327–329, 332–333, 347  
Superfund site, 9, 11  
Suspensions, 102–103  
Sustainability, 12, 14–18, 22, 37–39, 41, 43, 62, 68–70, 242, 244, 255, 265–266, 287–289, 292, 303, 305–311, 313–320, 322, 328, 346  
Sustainable process design, 310–311, 314, 316  
System(s)  
    biology, 326  
    closed, 199, 203–207, 209, 288  
    open, 204, 207, 214  
Sustainable development, definition, 38  
Thalidomide, 7  
Therapeutic index, 329  
Thermodynamics  
    first law, 201–207, 210, 212, 214  
    functions and applications, 267, 269  
    second law, 36, 210–213  
    system, definition, 197  
Threshold of toxicological concern (TTC), 326, 338  
Times Beach (Missouri), 9, 56  
Toluene, 3, 13, 222, 226–227, 274, 345  
Toxic, 6, 8  
    agents, 327  
        genotoxin, 327, 339  
        hepatotoxin, 327  
        poison, 327  
        toxicant, 327–329  
        toxin, 327  
    effects, 327  
        off-target, 335  
Release Inventory (TRI), 11  
Substances Control Act (TSCA), 11  
Toxicity, 10  
    cellular, 333  
    environmental, 325  
    neurotoxicity, 334  
Toxicology  
    basic principles, 326–329  
    computational, 326, 341  
    data  
        accidental or routine exposure, 328  
        animal studies, 328  
        cellular studies, 328, 335  
        gaps, 340  
    information  
        authoritative sources, 329  
        Open Tox, 339  
        ToxTree, 339  
        tutorial, 327  
    Toxicogenomics, 335  
    Toxicokinetics, 327, 330  
    Toxicodynamics, 330  
    Triglyceride, 241, 258  
    Triple point, 80, 217–218  
    Turnover number, 163  
Ultrasound, 273  
Urbanization, 53, 55, 236  
Volatile organic compounds (VOCs), 28, 50, 69, 102  
Water, Clean Water Act, 11, 52  
Wind turbines, 279–281  
Work, 202  
Yield, 141  
Zeolites, 172, 174