# INDEX


**A**

*ab initio* 39,424,426,430,455,470,485,655,661, 711
abiotic
  attenuation 1579
  degradation 1175
  process 1151
absorbance 343
absorption capacity 1635
acceptor number 566
acetaldehyde 1131
acetic acid 9,506,829
acetone 341-342,640,829,847,849,854,881,906, 959,1149,1508
acetonitrile 2,13
acetophenone 819
acid/base
  character 580
  interaction 3,565,570,584,683,689
  properties 617
acidic groups 348
acidity 585,806,1053
acids 574
acoustic
  dissipation 364
  wave admittance analysis 342
acrylics 848
acrylonitrile 787
activated carbon 1509,1513,1543,1634
  service life 1531
activation
  energy 778,807
  theory 362
activity coefficient 177,282
  at infinite dilution 164
adhesion 14,339,570
adhesives 581,847,849,851,1638
  anaerobic 847
  chemically reactive 847
  polychloroprene 849
  pressure-sensitive 851
  UV-curable 847
adsorbent 1509
  inner surface area 1510
adsorption 570,1151
  capacity 1510
  enthalpy 1509
  fundamentals 1509
  heat 1526
  isotherm 1510
  kinetics 1509,1511
  preferential 274
adsorption-desorption 1160
adsorptive power 1510
aerosolization 354
aerospace 852,1640
AFM 569,706
agar 710
aggregate mass 689
  vesicular 690
aggregates 506,580,697
aggregation 565,570,578,689,697
agitation speed 798
agriculture 1640
air 1149
  contaminants, standard 925
  velocity 1526
airflow 353-354
airways 1082
Alagona approach 444
alcohol consumption 1396
alcohols 127,137,806,828,880
alkahest 7
alkalinity 1053
alkanes 127
N-alkylpyridinium 1468
allergic effects 1319
  potential 1320
Allerhand-Schleyer scale 588
p-allylanisole 826
allylation 811
altitude 1191
alumina 1513
aluminum stearate 693
amine 510
aminoacids 23
ammonia 16
amobarbital 286
amorphous
  phase 351
  structure 348
amphiphiles 691
amphotericity 577
n-amyl acetate 848-849
n-amyl ketone 849
analytical ultracentrifuge 186
anemia 1376

anhydrous form 282
aniline 9
  point 102,1056
anisole 819
annealing 254
anthraquinone 701
antifungal properties 881
antigens 1361
antiparallel orientation 12
Antoine equation 389
apolar 875,884
approximation, two-body 37
aprotic 762-763,798,811,813,829
aquifer 1572
Arrhenius description 573
asphalt 855
  processing 1640
association
  heteromolecular 505-507
  number 692,689
  self 350
asthma 1328
atomic surface tension 482
ATP 866
attenuation capacity 1163
autoignition temperature 1054
automotive 851
  finishing 1641
  industry 958
  maintenance 1641
  painting operations 1641
autoprotolysis 524
Axilrod-Teller term 453

**B**

bacteria
  Gram-positive 862
  solvent-tolerant 859
Bader charges 444
barbituric acid 286
Barker-Henderson approach 749
barotropic effect 1425
barrier properties 693
basicity 585
bathochromic shift 590,592,602
battery electrolytes 1472
Beer law 353
Benard cells 412
benzene 1,39,105,127,342,697-698,812,817,
  829,848,882,952,957,1127,1133,1334
  exposure 1365
benzonitrile 794
benzyl alcohol 778,854
benzyl cyanide 815
BET 1510
binding energy 754
binodal 131,148,184,191-192,400,408
bioavailability 1130
biocatalysis 875
biodegradation 1151
  first-order 1153
  potential 1054
biofilm 1624
biological
  membrane 866,870
  monitoring 1080
biomarker 1375
bioreactor 1624
biosphere 856
biotic process 1151
biotransformation 859,1133,1618
biphenyls 287,301
bleaching 344
blends 184,694
blistering 956
blisters 1131
Blodgett-Langmuir film 496
blood 1081
blue shift 639
blush resistor 956
boiling
  point 1055
  temperature 15
Boltzmann factor 476,655
bond
  covalent 16
  energy 16
  intermolecular 345
  strength 849
Bondi approach 126
Bootstrap model 791
Born
  approach 482
  equation 769
  formula 677
  model 769
  radius 771
  term 652
  theory 133,738
Born-Kirkwood-Onsager expansion 665
Born-Oppenheimer approximation 422
Bose-Einstein statistics 429
boson 429
boundary
  condition 312
  surface 419
Brannon-Peppas equation 348
breakdown voltage 1059
breakthrough time 342,1631,1633,1635
breath monitoring 1079
breathing 1634
Brillouin theorem 659
Bristow-Watson method 246
bromine index 1055

bromobenzene 691-692,784
1-bromobutane 811
Brönsted equation 587
Brooker scale 590
Brownian dynamics 472
bubble
collapse 360
dynamics 356,366
formation 354
growth 360
small 363
surface 364
Buckhingam
formula 682
potential 459
burning, sustained 1069
butabarbital 286
1-butanol 545,694,854
2-butanol 694
t-butanol 694,1397
2-butanone 794,854
butyl acetate 848,881
butyl glycol 880
t-butyl methyl ether 2
2-butylhexanol 848
γ-butyrolactone 696

## C

calorific value 1056
calorimeter 243,1056
calorimetric study 540
capillary
condensation 1510,1524
effect 379
force 365
carbon dioxide 2,39,688,897
carbon tetrachloride 591,648,697,754,827,1133, 1382,1396
carbonyl
frequency 698
group 842
stretching frequency 567
stretching mode 349
carcinogen 1367
classification 1322
carcinogenic 2,1133
carcinogenicity 1132,1321
Car-Parrinello simulation 470
carrageenan 710
cartridge 1636
catalysis, triphase 830
catalyst 1467
phase 826
phase transfer 824
separation 828
catalytic
oxidation 1508
reaction 2
catheters 956
cation radius 771
cavitation 371
free energy 11,17
cavity 284,366
boundary 498
collapsing 366
ellipsoidal 680
field 682
formation 292,648,663
molecular 480
radius 717,769
shape 482,652,662,665
surface 21,284,484
surface area 284
volume 648
cell
membrane 860
multiplication 1176
physiology 866
toluene-adapted 862
cellophane 1535
cellulose 127,694
acetate butyrate 881
chain
dimension 706,711
flexibility 127,273
rigid 127
segment 345
separation 128
topology 709,711
transfer 779
chair conformation 711
Chako formula 680
charge
density 709
distribution 132
transfer 463,586,780,782
complex 571
state 641
Charnahan-Starling equation 762
chemical 344
composition 419
equilibrium 1
potential 101,149,159,198,307,341,344-345, 575
reaction rate 132
reactivity 1,737,739,741,743,745,747,749, 751,753,755,757,759,761,763,765, 767,769,771,773,775
resistance 339
shift 591
chemisorption 1509
chlorinated hydrocarbons 827
chlorobenzene 506,794,810,812,830
1-chlorobutane 811

1-chlorooctane 826
chlorofluorocarbons 853,1189
chromatographic separation 2
chromophore 589,592
chromosomal changes 1375
chromosomes 1376
circulation cell 1625
clathrates 1130
Clausius-Clapeyron equation 244
Clausius-Mosotti
  relation 680
  theory 738
Clean Air Act 929
Clean Water Act 932
cleaners 1644
cleaning 853,894,957
  processes 1508
cleavage 702
climate forcing 1192
clothing 339
  materials 1631
  protective 342
cloud point 101,184,189-190,271,273,408,695
Cluff-Gladding method 334
coagulation bath 695
coal 952
  tar 855
coatings 386,565,963,1169,1555,1557
  environmental performance 965
  multilayer 35
  waterborne 352-353
coefficient
  hydrodynamic interaction 685
  mutual 340-341
  of diffusion 354
  of volumetric absorption 353
  self-diffusion 340-341,344
coffee 1441
cohesion energy 115,261
coil
  conformation 709
  dimension 273
  expansion 268
coil coating 880,1641
collisions 419
color 1056
colorimetric analysis 1056
combustion 1056
cometabolism 1582
compatibility 318
compatibilizer 693
complex formation 556
complexation 780,782,824
composites 1642
compressibility 126,200
  factor 244
  isothermal 648
Compton scattering 757
condensation 852
conductivity
  electrical 516,1126
  thermal 354
configuration 18
  interaction 431,658
conformation 18,25,707,710,788
conformational state 706
conformer 506,711
  energy 530
  equilibrium 530
  form 532
  stability 531
  transformation energy 531
conformic equilibrium 506
construction industry 1648
  products 855
contact angle 565
containers 693
continuum dielectric theory 133
continuum models 479
convective movement 1151
conversion 798
copolymer 686
copolymerization 779
  model 781
corrosion 339,852,1057
cosmetics 881,1319,1643
COSMO 481,484
cosolvency 267,793
  criterion 320
cosolvent 282,284-286,288,867,1175
  power 269
Coulomb
  contribution 444
  hole 430
  integral 448
  law 430,875
  term 459
Coulombic
  attraction 575
  interaction 439,451,574,727
Coupled-Cluster theory 431
coupling reactivity 816
covalence 463
cranial nerve 1328
cresol 957
  meta 590
crew-cut 690
critical
  behavior 191
  molar volume 340
  point 191-192,202
  region 214
  scattering, pulse-induced 184
  solution temperature 129

temperature 193
crosslink density 128
crosslinked elastomer 130
crosslinks 128,331,701
distance 345
cross-propagation reaction 786,790
cryoscopy 147,149,188
crystal
energy 282
lattice 1,1130
surface 1130
texture 1118
crystalline phase 350
crystallinity 351,694
degree 352
crystallization 348,567,694
crystals 694
curing time 343
cybotactic 585
cavity 585
region 584,608
cyclodextrin 294
cyclohexane 105,185,188,506,591,701,810, 826-827
cyclohexanone 698,704,813,956,1131,1165
cyclopentanone 956
cytochrome 1099,1112,1356,1379,1394

**D**

Dalton law 364
Deborah number 339-340
Debye
longitudinal relaxation time 136
model 134
relaxation model 137
relaxation time 134
Debye-Hückel approximation 728
decaffeination 1441
n-decane 810,812,830
Dee-Walsh equation 203
defect, stress-related 386
defects 388
deformation 344
history 360
degreasing 1227,1233
dehydrobromination 826
dehydrogenase 1356
dehydrohalogenation 827,1572
de-icing fluids 853
DelPhi 481
demixing 176,184,189 - 190,206,273,695
density 505,516,521,1057
density-functional theory 574
deprotonation 33
dermal exposure 1079
dermatitis 881
des Cloizeaux Law 308
desorption 566
free energy 569
DFT 481
dialysis 956
dibromomethane 807
p-dichlorobenzene 699
1,2-dichloroethane 127,686,819,1133
dichloromethane 686,692,694-695,698,701,810, 812-813,815-817,819,827,826,829,956, 1396,1398
dichroism 592
dielectric constant 25,115,190,454,459,479,487, 652,738,754,763,781,829,875
continuum 584,649,663
response function 133
surface 494
continuum theory 674
enrichment 613
Diels-Alder 1470
diethyl ether 2
di-2-ethyl hexyl phthalate 686
diethylaniline 815
differential refractometer 158
diffusion 339
coefficient 38,310,351,388,1152,1157,1509
control 779
distance 346,348,1526
elastic 340
equation 307
gradient 339
molecular 1082
rate 344,350
time 340
translational 779
diffusive transport 340
diffusivity 341
dilute 282
dilution ratio 102,1058
dimeric interaction 425
2,3-dimethyl-butane 341
1,3-dimethyl-2-imidazolidinone 1136
N,N-dimethylacetamide 694,1135,1400
dimethyl-benzene 854
N,N-dimethylformamide 127,188,694-695,956, 1135,1170,1400
dimethylsulfoxide 302,507,694,709
Dimroth-Reichardt
scale 588
value 281
1,4-dioxane 686,691,694,709,956,1401
dip
coating 956
molding 956
diphenyl ether 2
diphenylhydantoin 286
dipolar moment 15

term 750
dipole moment 12,298,506,585,641,653,754, 763,807,875
dipole-dipole forces 584
interaction 12,138,528,530-531
permanent 767
Dirac function 662
dispersion 13
forces 454,649
disproportionation 783
dissociation 508
dissolution spontaneous 127
dissolving power 1422
distillation units 962
diurnal 1195
DMF 754
DNA 454
dodecane 826
domain
amorphous 350
crystalline 350
Dong-Winnick scale 589
donor
complex 785
number 566,738
donor-acceptor
approach 744
interaction 574,584
properties 527
reactions 571
Doppler broadening 644
double-liner system 1165
Drago
scale 591
equation 569
driveway sealer 855
driving force 339
drug acceptability 1130
degradation 1131
dry cleaners 1091
dry cleaning 883,1189
dryer 353 - 354,387
drying 339,565
conditions 386,1118
convection 353
defects 409
rate 396
technology 386
time 351
DTA 190
Dubois-Bienvenue scale 590
dye reduction 1100
dyes 1169
dynamic light scattering 689

**E**

ebulliometry 147,149,167
ecosystem 1617
ecotoxicity 1170
ecotoxicological effects 1185
effluents 1149
efflux pump 863
eigenfunction 427
eigenvalue 420
Einstein's equation 684
elastic linkage 361
elasticity potential 128
electron
affinity 574
cloud 469
transfer reaction 765
transport 1099
electron beam curing 880
electronegativity 754
equalization 444
electronic
nose 1222
state 462
transition 291,655
electronic industry 894,1644
electronic-vibrational spectra 639
electron-pair acceptors 3
donation 571
donors 3
electrophilic species 782
electrostatic
forces 649
interaction 12,453,541,651-652
potential 481
electrostatics 480
electrosynthesis 1473
elongational flow 360
embryotoxicity 1133,1334
Emergency Planing Act 933
emission 1149
limit value 1214
enantiomeric ratio 877
enantioselectivity 858,877
encephalopathy 1327
energy
consumption 388
minimum 18
of activation 341
potential 345
enhancement factor 1429
enthalpy 566-567,755
conformational 254
differential 195
evaporation 243,1509
exothermic 567
molar 345

of melting 346
entropic contribution 722
entropy 130
component 332
conformational 257
dilution 195
hydration 760
ideal 105
environmental fate 1149,1151,1153,1155,1157, 1159,1161,1170
laws 924
enzymatic
factors 1317
reaction 857,874
enzymes 857,872,1395
epoxy 847
equidensity 21
equilibrium
chemical process 528
constant 788
equipotential 21
ESR 2,700,790
ethanol 286,694,701,847,882
ethers 127
2-ethoxyhexyl acetate 848
ethyl acetate 342,694,816,827,881
ethyl benzene 341-342,854
N-ethyl carbazole 816
ethyl ether 810
ethyl formate 1131
ethylene glycol ether 1169
eutectic point 1465
eutectics 1466
EVA 347
evaporation
rate 353-354,956,1059
cooling 354
Ewald approach 487
excimer 268
exciplex 752,766 - 767
excitation energy 641
excited state 2
explosive limits 388,1060
exposure parameters 1315
extraction 1058,1068,1442
efficiency 940
process 2
temperature 943
extrusion 956

## F

factor of chain expansion 685
fermentation 1584,1599
Fermi hole 430
Fermi-Dirac statistics 428
fermion 428
fetotoxicity 1338
fiber 695,1535,1645
diffraction 708
fibrosis 1394
Fick law 1084,1151
Fickian kinetics 340
film 693
casting 956
thickness 354
filters 1633
Fixman theory 728
flammability limits 1060
flanges 962
flash point 1060
flocculation 14
Flory equation 308
Flory matrix 723
Flory-Huggins
equation 365,389
interaction parameter 112,151,321,345,347, 569
theory 154,793,1125
Flory-Orwoll-Vrij model 199,206
Flory-Rehner
equation 128,321,331
theory 344
fluorescence 342,610,689
intensity 692
recovery 344
fluorescent radiation 701
fluorination 693
fluorine 693
fluorocarbon resin 880
foam-enhanced remediation 1626
folding rate 350
food 709,923
industry 1128
safety 934
force
field 451
repulsive 14
formaldehyde 1190
resin 881
formation heat 790
formic acid 591
fractionation 689
Franck-Condon
principle 291,752
state 644 - 645,654,658
free energy of mixing 345
free volume 125
freedom, degree 199-200,433,470,715
free-volume theory 339,353
freezing point 1061
frequency shift 699
Freundlich
equation 1152
isotherm 1510,1525,1575

Friedel-Crafts alkylation 1468
frontier orbital interaction 574
FTIR 2,342-343,396,565,570,698,756,759
fuel, sulfur 1056
fugacity 149,
  coefficient 170,195,207
furniture 1169,1205,1222-1223,1646
future trends 946,1637

## G

gas cleaning 1507
gas chromatography 1062,1064,1116,1135,
  1228,1562
gas tank 693
gasoline 1169
Gaussian chain 685
Gay-Berne potential 458
GC-IR 1131
GC-MS 1131
gel 333,344,707,710
  stable 194
  structure 698
gelation 697
genetic
  component 1361
geometry change 450
Gibbs
  energy of mixing 124
  free energy 101,148,152,191,705
Gibbs-Dugem-Margulis equation 157,553
glass transition temperature 176,254,340,
  348-349,703
glassy state 350
gloss 704
gloves 1631-1632
  surgical 956
glycerol 286
glycol ester 880
glycol ethers 1169
goniometer 689
grafting
  efficiency 703
green
  chemistry 1422
  strength 849
greenhouse gases 1189
ground transportation 950
groundwater 1150,1163,1571,1599
  well 1623
Grunwald-Winstein scale 587
Gutmann concept 738

## H

habit 1119
hair spray 881
halorespiration 1582
Hammond-Stokes relation 39
Hansen solubility 112
  parameters 106,264,695
hard sphere
  diameter 746
  potential 14,37
hard-core cell 201
hardness absolute 575
Hartree-Fock
  approximation 484
  description 430
  equation 665
  method 655
  procedure 423
  theory 661,666
hazard communication standard 926
hazardous wastes 1548
health and safety laws 924
heart 1415
heat
  capacity 254,1460
  conductivity 392
  dissipation 363
  flow 354
  of vaporization 387
  transport 1
Helmholtz free energy 493,566
hematopoietic effect 1365
hematoxicity 1365
Henry
  constant 173,177,206,213,1155
  law 148,389,1125,1150,1578
  diagram 112
hepatotoxicity 1337,1379,1385,1393
hepatoxins 1396
n-heptane 590,697,848,1126
herbicides 1102
hexamethylphosphoric triamide 2
n-hexane 2,127-128,323,590,697,812,828,
  848-849,1127
Hildebrand theory 124
Hildebrand-Scatchard
  equation 104
  hypothesis 345
hole 339-340
HOMO 571,573-574,789
homomorph 585-586,593,600
homopolymerization 777-778
homopropagation 778
homotactic interaction 722
Hook law 160
Hookean energy 732
hops 1441
HPLC 759
HSGC 154-155,167,178
Huggins equation 246
Hughes-Ingold theory 745

humidity 852
relative 353
Huyskens-Haulait-Pirson approach 103
hybridization 754
hydrate 282
hydrocarbons 102,941,1361,1617
hydrodynamic interaction 361
hydrodynamics 356
hydrogen
bond 15,683,709,760
bonding 111,573,584,613,703,740,1126
hydrolase 858
hydroperoxide 700
hydrophilicity 830
hydrophobic 866
effect 16,285,758,760
interaction 11,16,282
hydrophobicity 758,760,830,875
parameter 286
hydroxyl group 806
radicals 1559
hypernetted chain approximation 461,465
hypsochromic
sensitivity 607
shift 590,607,609
hypsochromism 588

I

IGC 148-149,154-155,164,166,177,565-566
immune system 1356,1367
incineration 880
infrared absorption 111
ingestion 1079
inhalation 1079,1316,1355
initiation 777
injection molding 956
ink 1647
inorganic chemicals 950
interaction
charge transfer 16
constant 566
dimeric 424
electrostatic 16
intermolecular 639
parameter 345
polymer-solvent 1125
potential 455
trimeric 424
interatomic force 470
interface 339,565
air-solvent 288
intermolecular
bonding 755
distance 12
forces 1
interaction 37,261
internal gradient 386
intersolute 282
effect 282,293
ion association 546
ion-dipole interaction 528,545
ionic
associate 507
liquid 2,1459
melts 616
radius 768
ion-ion interaction 528
ionization 816
iron and steel industry 951
irradiation 1131
isobutanol 351
isomerization 506,826
equilibrium 530
iosoctane 347
isopiestic measurement 158
isopleth diagram 1194
isopropanol 302,848,851,881,906,1397
isotactic 578
isotropic liquid 1465

J

Jackob number 376
joint filling 855
jump unit 339-340

K

Kapustinskii equation 1461
Kauri number 101
Kelvin equation 1510
ketones 880
kidney
disease 1355,1357,1359-1361,1655
function 1359
kinetic rate 807
Kirkwood
factor 754,762
theory 738
Kirkwood-Riseman-Zimm model 361
Kitaura-Morokuma decomposition scheme 429
knots 691
Knudsen method 245
Kohlemann-Noll theory 360
Kohn-Sham equation 471
Kosower scale 589

L

labeling 1062
laboratory hoods 962
laminar thickness 694
laminates 1642
land disposal 1149
Langevin dynamics 472
Langmuir
isotherm 1510,1575

method 245
laser 689
lattice-hole theory 203
LCST 198,268,372,380,384,1424
leachate concentration 1165
leather 1222
Leffler-Grunwald operator 285
Lennard-Jones
energy 749
interaction 138
potential 37,40,458,462,467,477
solvent 748
lethality 1176
leukemia 1365
Lewis
acidity 740
basicity 738
definition 571,617
donor 705
number 376,392
parameter 565
lifetime 654,1190
Lifshitz-van der Waals interaction 565
light absorption 2,680
limonene 864
linear
response 133
response theory 133
lipase 878
lipophilic contamination 898
liposomes 860
liquid
compressibility 356
constrained 495
crystals 485
general condition 357
motion 365
Newtonian 356
surface 493
system 419
lithology 1627
liver 1379,1393
function 1394
London
dispersion 469
equation 718
formula 447,672
Lorentz-Lorenz relation 680
LUMO 571,573-574,789
lungs 1082
Lux-Flood definition 573,618
lyophilization 874

## M

macroscopic level 1
Manning theory 729
Marangoni number 413
Mark-Houwink equation 363,728
Markov chain theory 475
Martin correlation 362,390
mass transfer 387,816
material degradation 1632
Maxwell
element 361
equation 358
model 360
Mayo-Lewis model 780
mechanical
equilibrium 307
toughness 339
medical
applications 955
devices 955
melting 253
melts 200
membrane 689
cytoplasmatic 863
morphology 694
memory effect 357
Menschutkin reaction 1,9,30,742,745
menstruum 8
menstruum universale 7
Mercedes-Benz logo 761
mesomorphic solid 1465
mesophase 1465
mesopores 1513
metabolites 1317,1356
metal cation 450
metal casting 957
methane 208
methanol 188,286,341-342,547,694,826,829,957,1131
4-methyl-2-pentanone 854
N-methyl-2-pyrrolidone 398,686,694-695,698,778,841,847,956
2-methyl-pentane 341
methyl acetate 342,694,881,1131
methyl chloroform 1396
methyl ethyl ketone 127,129,687,842,847,849,854,881,952,956
methyl glycol acetate 881
methyl isobutyl ketone 703,881
1-methyl naphthalene 688
methylcyclopentane 129
1-methylimidizole 1460
micelles 690
microbial membrane 860
microcoulometry 1065
microdomains 350
microfiltration 694
microflora 1620
microorganisms 857,865
growth 1176
solvent resistant 865

survival 1176
micropores 1513
microscopy 689
microstructure 386
Millington equation 1152
mineral spirits 847-848,855,950
mining 1169
miscibility gap 268,273
mitochondria 1112
mixing
configurational entropy 124
entropy 124,292
free energy 104
model
classical 419
continuum 17,20,25,133
electrostatic 9
free volume 196
iceberg 16
lattice 198
lattice-fluid 196
supermolecule 18,22
molar
cohesive energy 103
volume 516,521
molecular
arrangement 698
design 36
dynamics 18,472
ensemble design 36
mass 345
mechanics 450
model 698
motion 254
orbital 423
orbital theory 571
orientation 752
packing 752
sieves 1513-1514
theory 361
toxicity 860
weight 343,351-352,689,703
molecule-molecule interaction 475
Møller-Plesset
perturbation 670
theory 431
treatment 671
molten salt 1459
Momany approach 444
monoclinic 1119
monomer
emission ratio 268
feed 781
monomer-monomer complex 785
Monte Carlo 17,19,37,208,472,476,662,723,760
morphological
feature 690
structure 689
morphology 339
of skin 339
Mulliken charges 444
mutagenicity 1132

**N**

nail polish 881
remover 881
nanofibers 691
nanospheres 690
nanostructures 689
naphtha 848,854,881,950,957,1233
naphthalene 288,302
natural attenuation 1571,1573,1575,1577,1579,
1581,1583,1585,1587,1589,1591,1593,
1595,1597,1599,1601,1603,1605,1607,
1609,1611,1613,1615
navy 1472
nephropathy 1359
nephrotoxicology 1356
Nernst layer 831
nervous system 1407
network 331
networks 710
neuropathy 1328
neuropsychological assessment 1329
neurotoxicity 1132
neutron scattering 185,698,756
small angle 147
Newton-Euler equation 37
Newtonian viscosity 361
nitrile rubber 848
nitrobenzene 641,819-820
nitrocellulose 848,881,1646
nitroethane 1400
nitromethane 754
nitroparaffins 1400
2-nitropropane 1400
NMR 2,342,351,388,705-706,713,759,788,
793,1432
$^{1}$H-NMR 1135
shift 738
nondipolar 754
nonpolar 827
surface area 286
non-solvents 177
Norrish type II 701
nucleic acids 16
nucleophilic
agent 807
species 782
nucleophilicity 813
number of arms 689
Nusselt number 392

## O

octane 127,185
1-octanol 287-288
octupolar 754
odor 851,1219
  hedonic tone 1221
  in industrial plants 1222
  in materials 1222
  intensity 1220
  testing 1063
  unit 1220,1223
odorant concentration 1220
oils 923
Oldroyd equation 358,361
olfactometer 1223
Onsager
  cavity radius 654
  dipolar term 653
  model 651,667
  reaction field 654
  theory 655,715
Onsager-Bottcher theory 682
opalescence, critical 190
operation cost 1508
optical clarity 339
orbital radius 574
organic acids 16
organic chemical industry 962
orientational order 762
Ornstein-Zernike
  equation 464
  theory 490
Orofino-Flory theory 726
orthorhombic 1119
Osawa concept 729
OSHA standards 925
osmometry 147,149,154,168,195,267
  membrane 178,183
Ostvald-Freundlich equation 1491
oxidation degree 618
oxygen, singlet 702
ozone 1189,1192,1267
  depletion 1192
  precursor 1189
  production 1196
  tropospheric 1190

## P

pacemaker 956
packing density 746
Padé approximation 750
paints 354,581,709,1169,1235,1555,1557
  emissions 1559
  industry 1063
painting 950
paper 1647
Papirer's equation 566
partial pressure 1150
partition coefficient 288,291,860,875,1082, 1149,1153
partitioning 2,867
patching 855
patent literature 1637
Pauli
  exclusion principle 427-430
  repulsion 649
Pauling crystal radius 770
PDAC 445
Pekar factor 766
Peklet number 363
PEL 925,1079
penetration 1422
perchloroethylene 914,956,1057
Percus-Yevick approximation 461,465
perfluorohexane 2
performance 1422
perichromism 2
permeability 693,860,1631
temperature effect 1632
permeation
  flux 694
  number 1631
permittivity 505-506,513,517-518,531,540,669
perturbation theory 436,461
pervaporation membrane 693
pesticides 1169
PET 688
pH 297,348,688,1064
pharmaceutical 709,1552
  industry 1468
  product 1119
  substances 282,1129,1135
pharmacopoeia 1129
phase
  boundary 344
  diagram 129-130
  homogenization 190
  separation 125,190,386
    thermally-induced 694
  toxicity 860
  transfer, catalyst 824
  transition 1420
phenol-formaldehyde resin 847
phenomenological model 288
phospholipids 860
photochemistry 1194
photodegradation 1151
photoefficiency 1559
photoionization 133
photolysis 701,1175,1192
photooxidation 700,1175
photoreactor 1563
photoresists 701,1546

photosensitizers 701
photostabilization 702
phytoremediation 1622
pickling 952,957
piezoelectric method 163
pinholes 956
Piola tensor 306
pipeline coatings 855
plasma cleaning 897
plasticizer 856
plasticizing action 701
plastisol 847
PLUME 1164
p-nitrophenol 699
Poisson equation 480
polar 750,754,760,807,824,842,897
  bond 754
  character 586
  liquids 693
  solvation 746
polarity 2,9,288,531,577,584-585,610,700,745, 803,813,815,875
  effect 780,782
  index 527
  parameter 288
  scale 584,588
polarity-polarizability scale 584
polarizability 298,584,655,740,749,785
polarizable continuum model 481
polarization 12,133,428,486
  effect 459
  orientational 669
poly(acrylic acid) 687
poly(amide-imide) 841
poly(ethylene glycol) 206
poly(ethylene oxide) 186,687,699
poly(vinyl methyl ether) 185
poly(vinylidene fluoride) 693
polyacrylonitrile 127,694
polyaddition 841,963
polyamide 694
polyamides 694,847
polyaniline 703,1126
polybutadiene 127
polybutylene 848
polycarbonate 694,700,820
polychloroprene 127,848-849
polycondensation 818,820,841,963
polycrystalline particles 1118
polydimethylsiloxane 185,206,704
polydispersity 154
polyelectrolyte 454
polyester 880-881
polyesters 694,847
polyether 818
polyetheretherketone 348-349,699
polyetherimide 694
polyethersulfone 694
polyethylene 128-129,693,701-702
polyethylene glycol 808,817,826
polyethylmethacrylate 103
polyimide 692,694,702,841,847
polyisobutylene 685,848
polyisobutylmethacrylate 103
polyisoprene 127
polymer
  coil 271,779
  drying 350
  segment 339
  semicrystalline 350
  solubility 198
polymerization 842
  free radical 777
polymers 253
polymethylmethacrylate 127,269,343,568,570, 578,686,1437
polymorph 755
polymorphic transition 1119
polymorphism 709
polyolefins 694
  telechelic 694
polyphenylene 685
polyphenyleneoxide 694
polypropylene 693
polypyrrole 568
polysaccharides 706-707,709,711,713,715,717, 719,721,723,725,727,729,731,733,735,1654
polysiloxanes 273
polystyrene 127,129,186,188,269,342,344,686, 698
  atactic 128
  isotactic 128,697
  syndiotactic 697-698
polysulfides 818,848,853
polysulfonate 818
polysulfone 694
polyurethanes 331,346,354,694,847-848,850, 855,956,1640
polyvinylacetate 185,351-352,848
polyvinylalcohol 127
polyvinylchloride 127,129,691-692,698,880
pore
  diameter 1509,1524
  size 694
  system 1513
porins 862
porosity 1118
porous
  matrices 1422
  membrane 694
potential energy surface 422
potentiometric titration 619
powder coating 881
Poynting correction 171,1429

Prandtl number 392
Prausnitz theory 208
pregnancy 1333,1335,1337,1339,1341,1343, 1345,1347,1349,1351,1353,1655
pressure
drop 1526
partial 353
pressure-temperature relationship 1420
Prigogine
approximation 199
cell model 200
theory 125
Prigogine-Flory-Patterson
equation 202
theory 199-200,207
primer 705,881
printing 1169,1647
probability function 430
process safety management 927
propagation 778
heat 787,790
pathway 785
radical 793
step 780,782
1-propanol 545,694
2-propanol 694
propyl acetate 342
propylene carbonate 591
propylene glycol ether 1169
protagonism 15
protection 1631
protective equipment 1080
proteins 16,754,866
protic 745,752,762,798,813,829
protolysis 524
proton
influx 860
leakage 860
transfer 507
proton-donor function 510
pulmonary blood vessels 1082
pulping 1647
pump valves 962
pupil dilatation 1222
purity 1065
pycnometer 1057
pyridine 507

**Q**

QM/MM 478
quadrupolar 754
forces 753
quantum
description 419
level 18
number 430
yield 702

**R**

radiant energy 353
radicals 700,782
lifetime 701
stability 790
radius of gyration 684-685,689,691
Raman 756
Raoult law 154,196,365,372,389,613,794
activity coefficient 877
Rayleigh
factor 182
ratio 689
time 363
reaction
endothermic 1
field 481,651-652
field approach 487
nucleophilic 9
rate 798,807,811,815-816
reactive barriers 1628
reactivity 700
reactors 962
recrystallization 2,1130
recycling 880
red shift 752
refractive index 158,190,740,1066
regional scale 1193
regulations 1267,1269,1271,1273,1275,1277, 1279,1281,1283,1285,1287,1289,1291, 1293,1295,1297,1299,1301,1303,1305, 1307,1309
in Europe 1311,1313
regulatory approaches 1199
Reichardt scale 740
reinforcing 339
relaxation
enthalphy 254
segmental 346
spectrum 361
time 133,340,358,361,654
relief devices 962
reproductive
toxicity 1169
toxicology 1353
reptation 344
repulsion 14
residence time 387
residual stress 339
resistance specific 1059
resistive heating 1626
resistivity 1058
resorcinol 699
Resource Conservation Act 932
respirator 1633
respirators 1371

respiratory
physiology 1081
protection 1633
respirometer 1099
retardation time 358
retention volume 566
retroreflective coating 881
rewind station 387
Reynolds number 366,370
rheological
equation 356
properties 683,704
Rider approach 122
rigid spheres 14
ring deformation 711
RISM 466
rod-like micelles 690
Röntgen model 755
rotamer 591
energy 531
rotation 711
barrier 532
freedom 1477
Rouse theory 361
rubber 847
elasticity 148
natural 342
nitrile 342
rubbery state 349
Runge-Kutta-Gill method 393

## S

sample collectors 962
Sanchez-Lacombe
equation 201
theory 207
SANS 185-186,706
SAPT 440
SAXS 184-185,706
scaled-particle theory 461
Scatchard equation 263
Scatchard-Hildebrand theory 197
scattered intensity 689
scattering angle 689
Schlieren photography 186
Schrödinger equation 420,482,656-657,663,671, 674,676
sealants 847-849,851,855
seals 962
second viral coefficient 689
sedimentation velocity 186
segment
fraction 200
size 200
statistical 361
selectivity 694
self-consistent field 423
self-diffusion coefficient 38
self-remediation 1622
SEM 689
semiconductor 1546
shear modulus 347
Sherwood number 392
shoe industry 849
shrinkage 354
silica gel 1513
silicones 847-848
Simha-Somcynsky equation 203
similia similibus solvuntor 8
simulated-annealing 470
simulation 137
numerical 132
skeletal structure 806
skin 1631
absorption 1355
layer thickness 697
protective devices 1371
Slater determinant 669
small molecule 339
Small method 261
Smidsrød-Haug approach 729
Snyder's polarity 851
Soave-Redlich-Kwong eqaution 213
soil 1149,1157
contamination 1617
solar cell 1476
solid matrix 339
solubility 16
behavior 3
demands 318
equilibrium 282
parameter 103,111,198,243,253,261,347
relative 285
supercritical pressure 1425
solute 684
electrostatic field 133
mass concentration 684
polarization 11
pure 282
surface area 286
solute-solute interaction 282,292,301
solute-solvent interaction 455,481
solution 768
dilute 362
free energy 285
inhomogeneous 148
lattice 125
processing 956
solvation 282,759-760,807
continuum 482
dynamics 133
effect 283
energy 133,505,528,639,657,667
free energy 132

function 137
preferential 613
process 133
selective 538
shell 17,132,284,288,301,450
solvatochromic 288
analysis 609
dyes 660,705
shift 639,655,660,665,674,677,738
solvatochromism 2,590,593,601,610,751
negative 602
solvent
acidity 607
activity 146,194,207
adsorbed on crystal faces 1116
allergen 1319
basicity 600
binary 505,513
cavity 288,291
chemical potential 125
choice 872-873,875,877,879
cleaning 952
concentration 388
cost 657
crystalline 346
definition 1201,1234
degradation 700
diffusion 344,353
donor 787
effect 281
emission 1232
evaporation time 697
expansibility 747
explicit effect 780
exposure 1078
extraction 923
extraction process 935
flux 342
good 569,685
hydrophilic 1152
implicit effect 780
interaction 1130
ionizing power 587
loss 931
maximum contaminant level 1164
maximum permissible concentration 1164
metabolism 1317
mixed 505
mixture 267,281,352,683
motions 133,137
movement 339
neurotoxicity 1327
occluded 1116
oxidation 1559
partitioning 1067,1152
penetration 1631
polarity 3,593,610,702,705
polarity scale 588
poor 569
power 101
probe 585-586
quality 346
recovery 1507,1509,1511,1513,1515,1517,
1519,1521,1523,1525,1527,1529,1531,
1533,1535,1537,1539,1541,1543
reduction 847
removal 386
replacement 847
residual 349,1125,1129
retention 570
route of entry 1355
selection 1
separation 693
solubility 1150
state 345
symmetric 318
toxicity 1097,1132
traces 701
transport 3
transport phenomena 339
treated 1556
uptake 348
vapor phase 196
solvent activity
data 198
solvents 1150
applications 1507
binary 318
chlorinated 1572
classification 1235
cleaning 1056
critical properties 1420
diffusion 305
new 1637
oxygenated 694
polar 683
residual 1067
spent 1555
theta 685
use 847
solvent-solute interaction 282
solvent-solvent interaction 282,284,455
solvent-tolerant bacteria 859
solvolysis 297
rate 584,587
solvophobic effect 285
sorption isotherm 177
sorption-desorption hysteresis 177
spatial ordering 419
scale 1191
specific gravity 1057
specification 1068
spectral
band 639

broadening 643
line 639
shift 585,639
spectroscopy
dielectric 581
UV 689
spillages 962,1149
spin 430
spinodal 131,148,183-184,190-192,400,408
spin-spin interaction 530
spontaneous abortion 1343
Spriggs law 362
stability 700
stabilization 700
starlike 690
Staverman relation 203
steam-enhanced extraction 1628
stereochemical evidence 789
stereocomplex 578
stereoregularity 578
steric
properties 785
repulsion 448
Stockmayer
fluid 138,767
model 462
Stockmayer-Casassa relation 180
stoichiometric equilibrium 283
Stokes shift 592,612
storage tanks 962
strain, solvent-tolerant 862
strands 691
stress cracking 1059
tensor 356
stripping 853,950
reactor 1623
styrene 1385
styrene-butadiene copolymer 848
styrene-butadiene-styrene 848
subsurface contamination 1617
suit materials 1633
sulfur dioxide 853
supercritical
fluid 2,202
technology 1420
$CO_2$ 854
supermolecule approach 674
surface
crazing 700
distribution 569
energy 566
free energy 565
inhomogeneity 566
isopotential 653
layers 339
lubricity 956
modifier 565
solubility 1131
tension 14,284,288,301,352,364,567,570, 648,690,898,901-902,1460
surfactant-aided remediation 1625
surgical gloves 956
Svedberg equation 187
swell ratio 309
swelling 128,305,339,565
binary solvents 318
data 327
equilibrium 128,130,189,308,318,344-345, 348
extreme 320
kinetics 310,347
maximum 326
mode 312
pressure 195,346
stage 313
syndiotactic 578
synergistic effect 267
system free energy 132

**T**

tableting 1552
tacticity 778
tautomeric equilibrium 506
tautomerism 1,33
Taylor diffusion coefficient 1432
tear strength 850
TEM 689
temperature 341,349,353,798,852
temperature-shift factor 362
teratogenic 1334
teratogenicity 1132,1336,1341
teratology 1337
termination 779
1,1,2,2-tetrachloroethane 1396,1398
tetrachloroethylene 348,1149,1334,1336,1388, 1396, 1399
tetrachloromethane 2,813
tetrahedric coordination 16
tetrahydrofuran 347,569,686,694,696,700-701, 754,956,1401
texture 1119
TGA 396,1134
theophylline 282
thermal
capacity 126
desorption 1626
expansion 190,198
oxidation 1508
thermochromic coefficient 752
thermodynamic 360
equilibrium 148,157-158,176
work of adhesion 565
thermolysis 702
thickness 343,353

change 350
time scale 339
time-temperature superposition 362
titanium dioxide 1559
TLV 1079
toluene 127,185,188,334,341-342,344,347,365, 686,704,794,816,826-827,829-830,847-849, 851,854,881,952,957,959,1328,1334,1336, 1385,1388
tomography 1628
torsional angle 711
Toth isotherm 1437
toxcicodynamics 1315
toxic residues 339
Toxic Substances Control Act 933
toxicokinetics 1315
transesterification 877
transfer reaction 779
transition state 9,786,807
tribological properties 339
1,1,1-trichloroethane 854,914,959,1138,1398
1,1,2-trichloroethane 695,1396
trichloroethylene 854,914,952,1328,1387,1396, 1399
triethylamine 30
trinitrotoluene 1400
Trouton
entropy 762
rule 762
tubes 956
TWA 925

U

UCST 268-269,272,1424
Uhlig model 284
ultrafiltration 694
ultrasonic absorption 190
unimolecular heterolysis 1
unit cell 755
uptake
dermal 1316
routes 1315
UV 788
curing 880
radiation 853
UV/Vis 2

V

van der Waals
dispersion 469
envelope 673
equation 467
equation of state 1423
forces 16,1477,1509
interaction 451,875
radius 663
repulsion 647
solid 653
sphere 662
surface 21,445,663,721
volume 206
van Oss-Good's expression 565
van't Hoff parameters 558
vapor
data 161
degreasing 1056, 1233
measurement 147,149,154
pressure 157,262,365,1069
solubility 1084
vaporization
energy 198
entropy 762,765
heat 15,261
vapor-liquid equilibrium 198
varnishes 344,583,1169,1235
velocity field 356
vents 962
vibronic transitions 589
N-vinylpyrrolidone 703
viscoelasticity 357
viscosity 351,505,515,517,683,844,1069,1432, 1460
intrinsic 268,684,687
measurement 689
Newtonian 684
relative 685
specific 684,692
VOC 854,959,1196,1201,1546
calculation 1069
calculation methods 1205-1209
definition 1202,1241,1267
emission 388,848
exempt 1070
Vogel-Tammann-Fulcher equation 1474
volume
excluded 273,689
fraction 308,345,347,350
free 274,340-341
hydrodynamic 272
molar 341-342,345
vorticity 360
Vrentas-Duda theory 353,388

W

wash plant 1556
wastes 1163
water 15,137,1149
waterproofing 855
wave function 423
Wertheim pertubation theory 208,750
wettability 570
wetting 496,898,902
index 916
Wilke-Chang equation 38

wood coatings 1646
workplace
monitoring 1079
regulations 925
wound dressing 956

## X

XPS 565,567,569
X-ray 708,756,770
small angle scattering 147
xylene 127,186,341,696,700-701,847-848,851, 854,881,952,959,1385

## Y

yellowing 881
Yvon-Born-Green approximation 461

## Z

Z scale 589
zeolites 495,1514
Zimm
plot 183
equation 689
zwitterion 1471