Index

Α

absorbance, 457. See also infrared (IR) absorption absorption, matrix effect, 361 accepted reference value (ARV), 43 (table) accuracy, 43 (table), 116, 406 added internal standard method, 368-369 additive elements, 145, 147 (table), 187, 188, 582, 601 administrative reviews, 84 aerosol, 174 (table), 174-175, 176, 214, 215. See also nebulizers Aids to Analysis, 106-107 algorithms, 364-370 alkali elements, 178 alternative fuel standard (AFS), 625 aluminum, 194, 254-255 amines, 500, 501 analyte, 223 analytical chemistry, 208 Analytical Chemistry Journal, 209 analytical instrumentation, 27 (table) analytical performance, 53 (table) analytical techniques, 3, 211 (table). See also specific techniques analyzer, 258, 292-293, 398, 399, 405, 406 (table), 410-411 mercury, 571, 573 (table), 573-575 *See also specific types* analyzing crystal, 351-354, 353 (table), 356 Anderson-Darling (AD) statistic, 80, 82 anions, 503-504, 505, 506 (figure) ANOVA, 43 (table) aqueous metallic standards, 139 aqueous solution, 178, 191, 223 argon, 358 arsenic compounds, 246 ashing, 164, 191-192, 194 (figure), 228, 608

asphaltenes, 189 aspiration rate, 171, 173 (table) assignable cause, 43 (table) assigned test value (ATV), 43 (table) ASTM Committee E13, 481 ASTM International Committee D02, 3, 146, 598, 600 **ASTM Proficiency Test Programs** (PTP), 56-57 (table), 116, 146 (table), 386–389, 551 (table), 553-554, 598 ASTM Research Report RR-D02, 552 ASTM Standard Guide D7372, 57 ASTM test methods, 26, 32 (table), 34 (table), 36 (table), 69-70 (table), 122, 128, 129-130 (table), 131 atomic absorption spectrometry and, 145 (table), 145-146 chromatography and, 523-524 crude oil and, 607 energy dispersive X-ray florescence and, 385-386, 386-389 inductively coupled plasmaatomic emission spectrometry and, 185-190, 187 (table) ion chromatography and, 506-509, 507 (figure), 508 (figure), 510 wavelength dispersion X-ray spectrometry and, 371 See also specific test methods ASTM ULSD ILCP Program, 554-558, 555 (table), 556 (table), 557 (table), 613, 637-638 atmospheric pressure ionization (API) projects, 293 atom/ion intensity ratio, 182 atomic absorption spectrometry (AAS), 4, 7 (table), 135-137, 136 (figure), 147, 148-153 (table) application, 142–145, 143 (table) ASTM test methods, 145 (table), 145-146

calibration and, 33–34, 34 (table), 1.38 - 140crude oil and, 610, 610 (table) differentiation, 157 flame conditions in, 140 (table) instruments, 140-141 interference, 137-138 lubricants, 144 (table) measurements, 152-153 (table), 610 (table), 611 (table) of metals, 139 (table) sample introduction, 138 used oil and, 586 See also graphic furnace atomic absorption spectrometry (GFAAS) atomic emissions detector, 527-528, 527 (figure), 528 (figure) atomic fluorescence spectroscopy (AFS), 246, 280, 283 instrumentation, 247-153, 248-250 (figure), 253 (figure), 258 mercury and, 262-267, 263 (figure), 272, 279-280, 283, 569 on-line technique, 576 atomic spectroscopic techniques, 151 (table), 612 (table). See also specific techniques atomization, 156-164, 161 (table), 163 (figure), 166, 167 atomizer, 135 attenuated total reflectance (ATR), 482-483, 482 (figure) auto suppressor, 497-499 automotive fuels, 223-228. See also specific fuel autosampler, 162

В

B100, 626 background absorption interferences, 137 barite, 222 barium, 116, 217 barium sulfate, 502 beam filter, 387, 379 (figure) Beer's Law, 135, 485 bias, 43 (table), 75, 91-92. See also relative bias binary blends, 320 biodiesel. See also biofuel biofuel, 17, 18 (table), 23, 227-228, 456-457, 457 (figure), 600, 625-626 economics of, 626-628 interlaboratory crosscheck programs and, 637-638 production, 626-628 sources, 626 sulfur and, 559–561 testing and, 628-637, 629 (table), 637 (table) bitumen, 436-437, 437 (figure), 438 (figure) blank determination, 40 Bloom, N. S., 567, 576 boiling point, 289, 301, 303, 448 (table), 519–522, 521 (figure) Botto, R. I., 208 Bouquet, M., 295-296 box and whisker graphs, 82 (table), 92, 98-100, 99 (figure) Bragg's law, 353, 394 (figure), 394 "breaking radiation," 374 Bremsstrahlung, 374 burner system, 140 Burnett, J., 295-296 Bush, George W., 625

С

calcium, 89 (figure) calibration, 24, 25 (table), 25–27, 29 (figure), 43 (table), 65, 112 in atomic absorption spectrometry (AAS), 33–34, 34 (table) in gas chromatography, 39–40, 520, 521, 533 (figure) in graphite furnace atomic absorption spectrometry (GFAAS), 160–162 in inductively coupled plasma– atomic emission spectrometry (ICP-AES) and, 34–35, 181–182

in infrared analysis, 38-39, 487, 488 mercury and, 262 in monochromatic wavelength dispersive X-ray fluorescence and, 400-401, 402 in neutron activation analysis (NAA), 36 in nuclear magnetic resonance (NRM) analysis, 39 photometric test methods and, 32, 32 (table) procedures, 26-27 sulfur, 35 temperature measuring devices and. 28 wavelength dispersive X-ray spectrometry and, 370-371 X-ray fluorescence (XRF) spectrometry test methods and, 36-38. 36-37 (table) calibration blends, 325 (table) calibration coke gas requirements, 325 calibration curve, 33, 34, 35, 37-38, 264 (figure), 303, 400, 404 (figure), 534 (figure) calibration cylinders, 339 (table) calibration documentation, 32 calibration frequency, 30-31 calibration gas cylinder requirements, 334, 336 (table) calibration gases, 332 (table) calibration mixture, 39-40 calibration practices, 48-49 calibration reference material, 114-116, 115 (table), 116-117 calibration requirements, 320-323 calibration schedule. See calibration frequency calibration solutions, 181–182 calibration standards, 25 (table), 26, 29-30, 43 (table), 113 (table), 114, 135, 137, 138 californium, 418 calorific value, 340 capability, 103. See also test method capability trends; TPI_{industry}

carbon, 426 (table), 434, 452, 455-456, 455 (figure), 456 (figure), 459, 461 (figure), 461 (table), 462 (figure) carbon balance, 338 carbon fraction parameters, 445 (table) carbon particle emission, 183 carbonyl functionalities, 474 (table) cation analysis, 502 (figure) caustic washing, 502, 504 (figure) cellulose ethanol. 627 certification methods, 116 certified reference material (CRM), 25 (table), 43 (table), 113 (table) channeltron. 314 characteristic radiation, 350-351, 356 charts. See quality control charts check standard, 25 (table), 44 (table), 113 (table) Chemical Analysis: A Series of Monographs on Analytical Chemistry and Its Applications, 209chemical interferences, 137 chemical shift anisotropy (CSA), 458 chemical shift ranges, 425 (table), 426 (table) chemical speciation, 220 chemical suppression, 497–499, 497 (figure), 498 (figure) chloride, 335, 634-636 chlorine, 400 (table), 401 (table) chromatogram, 272 (figure) chromatographic atomic spectrometric methods, 269 chromatography, 4-5, 511, 523-524 gasoline analysis and, 519 hydrocarbon analysis and, 515-519 instrumentation and, 511-514, 522-523, 524-530 simulated distillation and, 519-523, 520 (table) See also specific types class I apparatus, 27 class II apparatus, 27 class III apparatus, 27

cleaning, 157 coal, 437-439, 439 (figure), 459-461 mercury in, 565, 570-571, 571 (table), 572 (table) coal combustion residues, 570-571 Cochran test, 61 coke oven gas, 324 coke production process, 323-328, 324 (table), 326-327 (table), 329 (figure) Coker mid-distillate, 485 (figure) cold vapor atomic absorption spectrophotometry (CVAAS), 142, 142 (table), 569, 570 collection optic, 398 (table), 399 (figure) collimators, 354 combustion air requirement index (CARI), 342 combustion ion chromatography, 506-509, 507 (figure), 508 (figure) Combustion IP Prep Station, 508, 506-509, 507 (figure), 508 (figure) commercial condensate, 267-280, 267-268 (table) common cause, 44 (table) compensation methods, 370 composition-property relations, 448 (table), 452 (table) Compton correction, 362-364, 370 condensate samples, 265, 266, 272 condition monitoring, 488-492 conductivity detector, 497-499 conostan mercury standard, 266 consensus values, 127 (table) continuous improvement, 79, 87 (figure) continuum absorption, 159 control chart, 31, 44 (table), 48 (table) control limits, 44 (table) copper, 628-629 corn, 627 correlation spectroscopy, 432 (figure) Council of European Nations (CEN) Interlaboratory Study, 552, 553 (table) cross check, 54-55, 75, 148 (table), 405, 407 (table)

cross talk, 321, 321 (table) crude oil, 145–146, 165 (table), 217-220, 300-301 (table), 302 (figure), 414 (figure), 441, 450, 621 (table) analysis, 607-620 gas chromatography and, 515, 516 (figure) inductively coupled plasmaatomic emission spectrometry (ICP-AES) analysis of, 189-194, 191 (table), 192 (table), 193 (table), 194 (table) mercury in, 571–572, 572 (table) reference material, 620-621 sampling and, 607–610, 607 (table) sulfur in, 541, 542 (table) trace elements, 505-507, 506 (table) crystal optics, 394-397

D

D1688A, 628-629 D2445, 290, 307-308 (table) D2622, 105, 543, 546, 630-631 D2650, 289 D2786, 290 D2789, 290 D3239, 290 D4294, 385, 546-547 D4806, 628 D4814, 628 D4927, 547 D4951, 548, 630 D5185, 548, 592 D5292-99, 452 D5453, 549 D5708, 609 (table) D5798, 628 D5863, 609 (table) D6259, 64 D6299, 64 D6300, 64 D6445, 386 D6481, 386 D6617, 64-65 D6667, 550

D6708, 65 D6751, 628 D7039, 548, 633-634 D7171, 435 D7212, 386 D7220, 386 D7372, 74 D7414, 601 D7415, 601 D7417, 601 D7590, 601 D7624, 601 D7691, 609 (table) data distributions, 86. See also histograms data normality checks, 86 De Jongh algorithm, 366–367 degrees of freedom, 44 (table) density of mixture, 342 detection limit, 44 (table), 142, 142 (table), 147, 149-150 (table) graphite furnace atomic absorption spectroscopy and, 162 in hydrocarbons, 199 inductively coupled plasmaatomic emission spectrometry (ICP-AES) and, 179 (table), 193 (figure) mercury testing and, 266-267 detector, 141, 378-382, 411, 412, 511 chromatography and, 524-530 conductivity, 497-499 infrared, 481 in wavelength-dispersive X-ray fluorescence (WD-XRF) spectrometry, 355-357 See also specific detectors detector filter. 379 diesel, 163, 389, 406 (table), 430 (figure), 431 (figure), 433 (figure), 441-442, 445-446, 451 (figure), 534 (figure), 541, 543 (table) diffraction, 352 (figure), 352 diffuse reflectance measurement, 483 (figure) diffusion, 435 dilution rate, 227

diphenylmercury (DPM), 264, 265 direct dilution, 189, 191 direct injection high-efficiency nebulizer (DIHEN), 225 direct injection high-efficiency nebulizer-inductively coupled plasma isotope dilution mass spectrometry, 225 dispersive systems, 477-478 distortionless enhancement by polarization transfer (DEPT), 431-432 Dixon test, 61 doubly curved crystal (DCC), 392, 393-398 drift correction monitors, 38 drinking water, 503 Dryfus, S., 217, 218 Dumarey equation, 274 duplicate intralaboratory test results, 61 - 62Duyck, 217, 220

E

E1301, 74 electrolytic eluent, 495 electron impact ionization, 289, 312 (figure) electron impact-mass spectrometry (EI-MS), 291-292 electron-hole pair, 380 electronic transitions, 376 (figure) electrothermal atomic absorption spectrometry (ETAAS), 223 electrothermal vaporization (ETV), 215element loss, 158, 159 element oxides, 158-159 elemental analysis, 216 (table) elemental determinations, 210 elemental distribution, 193 (table) elemental properties, 158 eluent, 494-495, 499 emission interferences, 137 emissions, 35, 541 Energy Policy Act (2005), 625-626 energy-dispersive X-ray fluorescence spectrometer, 287 (table), 377

(figure), 377-382, 378 (figure), 380 (figure), 381 (figure), 382 (figure), 383 (figure), 384 (figure) engineers, 208 enhancement, matrix effect, 361-362 environmental degredation, 627 Environmental Protection Agency (EPA), 389, 554, 558, 565, 568, 571, 574 equipment, 28, 29 (table). See also instrumentation; temperature measuring device equivalent precision, 61, 63 ethanol, 625, 626-627 interlaboratory crosscheck and, 637-638 testing and, 628, 629 (table), 630-637 ethanol-gasoline blend, 559-560, 561 (table), 626 ethylene cracker effluent gas analysis, 328-330. 330-333 ethylene cracking furnace, 330 (figure) ethylene oxide, 335 (table), 337 (table) excitation optics, 397, 398 (table) exploration, 502 explosion-proof, 280

F

Faraday cup, 313, 313 (figure) fatty acid methyl esters (FAME), 456-457, 458, 549, 600 filter furnace. 166 filter-based infrared spectrophotometer, 479 final blend gasoline analysis, 519 fit for use, 44 (table) flagged data, 84-85 flame atomic absorption spectrometry (FAAS), 223 flame ionization detector (FID), 511 flame photometric detector, 528-530, 529 (figure) flame source, 140 flow counter gas proportional detector, 355, 357-358

fluid catalytic cracker (FCC), 428 (figure), 450 fossil fuels, 118, 233-236 Fourier-transform (FT) instruments, 47, 478-479, 479 (figure), 489 (figure) Fourier-transform infrared spectroscopy (FT-IR), 235, 489-492, 594-598 fragmentation, 333 (table), 337 (table) free carbon index (FCI), 455-456 free induction decay (FID), 424-425 F-test, 81, 83, 93, 94 fuel gas production gas analysis, 340-346 fuel gas sources, 343-345 (table) fuel oils, 163, 181 (table), 186 (table) fume hoods, 177 fundamental parameter method, 362

G

Gallegos, E. J., 294-295 gamma ray measurements, 410-412, 414 (figure) gas amplification factor, 357 gas chromatogram, 522 (figure), 523 (figure), 524 (figure) gas chromatographer, 511–512, 512 (figure) gas chromatography analysis, 12 (table), 12-14, 39-40, 446-447, 449, 449 (figure). See also specific techniques gas chromatography-atomic fluorescent spectrometry (GC-AFS), 272 gas chromatography-inductively coupled plasma-mass spectrometry (GC-ICP-MS), 226, 230, 232, 270 gas chromatography-mass spectrometry (GC-MS), 211, 297-311 gas chromatography-mass spectrometry-florescent indicator (GC-MS-FID), 302 (figure), 307-308 (table)

gas chromatography-microwave induced plasma-atomic emission spectrometry (GC-MIP-AES), 269 gas displacement pump, 176 (figure) gas feed furnace effluent, 331 gas-filled detector, 380 gasoline, 145, 163, 196, 197, 200 (table), 201-202, 428 (figure), 450, 516 (figure), 516 (table), 519 GC-field ionization mass spectrometry (GC-FIMS), 523-524 generic laboratory equipment, 29 (table) goniometer, 354-355 good laboratory practice (GLP), 44 graphite furnace, 16, 159, 166, 167 (figure) graphite furnace atomic absorption spectrometry (GFAAS), 156, 161 (table), 166-167, 585 applications, 162-166 crude oil and, 610 instrumentation, 156-158, 159 - 160interferences, 158-159 measurements, 161 (table) procedures, 160-162 graphs, 82 (table), 100-102, 101 (figure), 102 (figure) Grating spectrophotometer, 477 (figure) Gray, A. L., 211 group type analysis, 304-305 (table) guard column, 495-496

Η

health hazard, 236 heat stable salts (HSS), 500, 501 (table), 501 (figure) heavy oil analysis, 191 (table), 192–193, 450–451 hexamethyldisiloxane (HMS), 203 hexanes, 198 (figure), 199 (table), 200 (table) high field nuclear magnetic resonance (NRM) spectroscopy, 429–434, 443–462

high performance liquid chromatography, 229, 230, 531, 531-532 (table), 532-534 high performance liquid chromatography-inductively coupled plasma-mass spectrometry (HLPC-ICP-MS), 230 high vacuum chamber, 317 (figure) high-resolution Ge(Li) detector, 411 high-resolution mass spectrometry, 293-297, 295 (table) high-resolution nuclear magnetic resonance (NRM) spectroscopy, 427-429, 439-443, 440 (figure), 441 (figure), 442 (figure), 443-457 histograms, 82 (table), 86-91, 87-91 (figure) historical statistics, 93 hollow cathode lamps, 140 Houk, R. S., 211 Hwang, J. D., 567-568 hydrocarbon feedstock, 309-310 (table) hydrocarbons, 195-201, 221, 232 (figure) infrared (IR) absorption detailed analysis and, 515-519, 517 (table), 518 (table) infrared (IR) and, 475-477 liquid, 268-270, 277-280, 282 (figure) mercury in, 258-259, 262, 268–270, 277–280, 281 (figure) type analysis, 299-300 (table), 532 types, 446 vaporization of, 264 (table) See also crude oil; separation mechanisms hydrodemetalization, 229 hydrotreating heavy vacuum gas oil (HVGO), 309, 309-310 (table) hyperpure germanium detector, 411

I

ICP Information Newsletter, 209 ICP-MS detection system, 530, 530 (figure) ID-ETV-ICP-MS, 235

in torch vaporization (ITV), 215 Indian Oil Corporation, 446-447, 449 inductively coupled plasma-atomic emission spectrometry (ICP-AES), 7 (table), 66-67, 170, 174 crude oil and, 616, 616 (table), 617 (table) detection limits and, 179 (table) petroleum industry methods and, 185 - 204short term precision and, 180 (table) solvent selection and, 170-171, 172, 174 (table), 174-175, 204 - 205used oil and, 588, 591-594, 591 (table) See also organic inductively coupled plasma-atomic emission spectrometry (ICP-AES) inductively coupled plasma-atomic emission spectrometry (ICP-AES) test methods, 34-35, 66-67 (table) inductively coupled plasma-mass spectrometry (ICP-MS), 192-193, 209, 210, 223-224, 236 books, 212-214 (table) crude oil analysis and, 217-220, 610-613, 612 (table), 617 (table) fossil fuels and, 233-236 historical development and, 210-211, 214-216 metal determination, 221-223 specialization analysis and, 229-232 influence coefficient algorithms, 364 - 370infrared (IR), 473, 475-477, 476 (figure). See also infrared spectroscopic analysis infrared (IR) absorption, 473-476, 481 infrared detector, 481 infrared spectroscopic analysis, 11 (table), 38-39, 69, 473-477, 484-488, 489-492 instrumentation and, 477-481

sampling and, 481–484 injection, 495 inspection, 42 instrumental neutron activation analysis (INAA), 222, 411, 412 (table), 413, 420, 572-573 instrumentation atomic absorption spectrometry (AAS) and, 135–137, 136 (table). 140-141. See also atomic absorption spectrometry atomic florescent spectrometry and, 247-248, 251 (figure), 253 (figure), 258 energy-dispersive X-ray fluorescence spectrometry and, 377-382, 377 (figure), 378 (figure), 380 (figure), 381 (figure), 383 (figure) graphite furnace atomic absorption spectrometry (GFAAS) and, 156-158, 159-160, 160-162 inductively coupled plasmaatomic emission spectrometry (ICP-AES) and, 66, 176-178, 195-197, 197 (figure) inductively coupled plasma-mass spectrometry (ICP-MS) and, 211, 214, 216 infrared spectroscopic analysis and, 477-481 ion chromatography and, 494-500, 495 (figure) mass spectrometry and, 287-289, 288 (figure), 315-318, 316 (figure), 317 (figure) monochromatic wavelength dispersive X-ray fluorescence and, 392-397 nebulization and, 195-197, 199-201 nuclear magnetic resonance (NRM) spectroscopy, 426–434 X-ray fluorescence (XRF) spectrometry and, 349, 351 (figure), 351-360

interferences, 66, 137

graphite furnace atomic absorption spectrometry (GFAAS) and, 158–159

monochromatic wavelength dispersive X-ray technology and, 403–404, 405 (table)

- organic inductively coupled plasma-atomic emission spectrometry (ICP-AES) and, 183–185
- sulfur and, 547, 548
- interlaboratory crosscheck programs, 589–601. See also ASTM ULSD ILCP
- interlaboratory test results, 61-63
- internal standard method, 364, 368

internal standards (IS), 183-184

- International Union of Pure and Applied Chemistry (IUPAC), 138
- intertechnique comparison, 147 (table)
- Intralaboratory Cross Check Program (ILCP), 75, 76, 77–78 (table), 79, 80 (table), 94, 97 (figure), 119, 122, 613, 637–638
- investigations, 84, 85 (table)
- ion chromatograph, 494–500, 495 (figure), 496 (figure). *See also* ion chromatography (IC)
- ion chromatography (IC), 494–500, 495 (figure), 514, 523, 636 (table) combustion, 506–509, 507 (figure), 508 (figure) methods, 500–509, 509–510
 - (table)
- *See also* ion chromatograph ion masses, 291 (table)
- ion trap mass spectrometers, 316
- ionization, 289–290, 293, 312–313, 357 ionization interferences, 137 ionization modes, 298 ionization technique, 289–290 Iowa, 627
- IP value, 314–315
- iron, 216, 605, 607
- irradiation, 36, 410–412

isotope dilution-inductively coupled plasma-mass spectrometry, 225

isotope dilution mass spectrometry (IDMS), 578

isotope dilution-cold vaporinductively coupled plasma-mass spectrometry (ID-CV-ICP-MS), 577-578

J

jet fuel, 9 (figure), 585

Johann geometry, 395 (figure), 395–396

Johansson geometry, 395 (figure) Joint Oil Analysis Program (JOAP),

585

Journal of Analytical Atomic Spectrometry (JAAS), 209

Κ

Kelly, W. R., 118 Kirchoff, Gustav, 4

L

laboratory capability, 51-52, 54 laboratory precision, 51-52, 74, 128, 130 (table), 131 laboratory quality management, 48 - 57laboratory records, 82 (table) laboratory staff, 84 laboratory standards, 53. See also reference material Lachance (Cola) algorithm, 367–368 Lachance-Traill algorithm, 364–365 laser ablation (LA), 215 laser ablation-inductively coupled plasma-isotope dilution mass spectrometry, 225-226 LC analysis, 14 (table) LC-ELSD, 303 (table) lead, 143-144, 162, 227, 234-235 Lienemann, C. P., 220, 221 light absorption, 136 light rare earth elements (REEs), 218 light source, 136 "like dissolves like," 171 linear regression, 400

liquid chromatography, 512–514, 513 (figure), 533 (figure) high performance, 531, 531-532 (table), 532-534 liquid feed furnace effluent, 331 (table) liquid petroleum gas (LPG), 500, 502 liquid-state nuclear magnetic resonance (NRM) spectroscopy, 443-457 logarithmic spiral doubly curved crystal (DCC), 396-397 log-spiral collection optics, 398 low field nuclear magnetic resonance (NRM) spectroscopy, 427-429, 434-443, 436 (figure) low flow nebulizers, 197, 199-200 low-resolution nuclear magnetic resonance (NRM) spectroscopy, 426-427 low-resolution quantitative methods, 289 - 293lube additives, 71 (table) lube oil, 89 (figure), 125–126 (table), 127 (table), 128 (table), 299 (table) calibration resource material, 122-123, 127-128 lubricating oils, 122-123, 127-128, 144 (table), 147 (table), 148 (table), 164, 187-190, 193-194, 228-229, 388 (table), 543 (table), 593 Lumex method, 575 L'Vov, Boris, 156

Μ

magnet systems, 426 magnetic field, 160, 424, 426, 434– 439, 439–443, 443–462 magnetic mass spectrometers, 292 magnetic-sector mass spectrometers, 316 mass balances, 28 mass doublets, 295 (table) mass spectra, 21 mass spectrometry, 287, 320–323, 500 analysis and, 323–346 gas chromatography, 297–311

high resolution, 293-297, 295 (table) instrumentation and, 287-289, 288 (figure), 315-318, 315 (figure), 316 (figure), 317 (figure) low resolution, 289-293 principles, 311-315, 312 (figure), 313 (figure), 314 (figure) sampling techniques, 318-319, 319 (figure) See also process mass spectrometry; *specific types* matrix correction, 362-370, 403 (figure), 404 (table) matrix effects, 360-371, 401-403, 576. See also interference matrix elimination, 504-506 matrix interferences, 137, 183-184 "matrix matched," 182 matrix modifiers, 159, 190, 191 mean, 83, 105-107 mean (X) graphs, 100-102, 101 (figure), 102 (figure) measurement compatibility, 112 membrane sampling system, 319 mercury, 246, 247, 252, 261 (figure), 565-567, 566 (table), 579 (table), 580 analytical methodology, 568, 572 - 578collection efficiency of, 258 (table) commercial condensate and, 267-268, 267 (table), 268-280 in hydrocarbons, 258–259, 262, 277-280, 281 (figure) instrumentation for, 270-273 in natural gas, 253-258, 257 (figure), 260 (table), 261-267, 267 - 283on-line determination, 273-275 in petrochemicals, 253-255, 260 (table), 261 (table), 262-267 in petroleum products, 569-572. See also specific fuels sampling, 567, 568 speciation, 269-273 storage, 567-568

See also atomic florescent spectrometry (AFS), instrumentation mercury analyzer, 258 mercury speciation, 577 (table) mercury values, 219-220 metal concentration, 33, 613 (table), 614 (table) metal determination, 135, 142-143, 146 (table). See also atomic absorption spectrometry (AAS) metals, 72 (table) calibration and, 33 trace, 145. See also trace elements wear, 144, 188 See also specific metal method development, 112 micellar electrokinetic capillary chromatograph (MECC) method, 230 Michelson interferometer, 478, 478 (figure), 479 microchannel plate, 313-314, 314 (figure) microemulsions, 192, 218 microwave digestion, 190, 191, 194, 219.233 middle distillates, 292 middle-distillate fuels, 189 molecular absorption, 159, 160 molecular weight, 306 (table) molybdenum, 203 (figure) monochromatic wavelengthdispersive X-ray fluorescence (MWD-XRF), 392, 393 (figure), 405 - 408doubly curved crystal (DCC) and, 393-397 focused beam and. 392-393 sulfur and. 548 sulfur chlorine and, 398-401, 398 (table), 399 (table) monochromator, 135, 136, 141 Morrison, G. H., 118 Moseley, Henry, 374 motor oil, 582-584 MS analysis, 8 (table)

multichannel gamma ray analyzer, 410–411 multicollector (MC), 216 multiple linear regression (MLR), 450 multivariate calibration techniques, 322–323

Ν

Nadkarni, R. A., 70, 118, 174, 224 naphthas, 194-195, 201-204, 202 (figure), 203 (figure), 203 (table), 204 (table), 220 naphthenes, 515, 518 (table) natural gas, 246-247, 256 (figure), 500. 502 condensate, 267, 268, 269-270 liquid, 275-277, 277 (figure), 278 (figure) mercury in, 253-259, 260 (table), 261 (figure), 262-267, 267-283, 569-570. See also mercury sampling techniques and, 256 - 258See also atomic florescent spectrometry (AFS) Natural Institute of Science and Technology (NIST), 45 (table), 554-555, 620-621 calibration standards and, 30 reference materials, 120-122 (table) standard reference material and, 54, 55 (table), 217-218. See also standard reference material near infrared (NIR) spectrophotometer, 484 nebulizers, 141, 175-176, 178, 188, 195-197, 214-215 low flow, 197-200 See also specific types neuron activation analysis, 118 neurotoxin, 227 neutron activation analysis (NAA), 36, 410-412, 413 (figure), 419 (table) crude oil and, 617, 618 (table) fast, 414-418, 416 (table) radiochemical, 412-413 substoichiometric, 418

neutron source, 418 nickel, 163 (figure), 164, 198 (figure), 216, 605, 607 Nippon Instrument Corporation's (NIC) mercury analyzer, 573-575 NIST SRM 1848, 588, 593 (table) NIST Standard Reference Material 1848, 123 (table), 124 (table) nitration, 491 (figure) nitric oxide (NO), 297 nitrogen, 417, 605 nitrogen chemiluminescence detector, 525 (figure), 526 (figure), 526-527 nonspecific absorption, 159-160 non-spectroscopic techniques, 16 (table) NP-LC, 532 NRM analysis, 10 (table) nuclear magnetic resonance (NRM) spectroscopy, 423-426, 229 (figure), 430 (figure), 431 (figure), 447 (figure), 451 (figure), 453 (figure), 462-463 instrumentation and, 429-434 low field, 427-429, 434-439, 439 - 443low-resolution, 426-427 high field, 429-434, 443-462 high-resolution, 427-429, 439-443, 440 (figure), 441 (figure), 442 (figure), 443-457 nuclear magnetic resonance (NRM) spectroscopy parameters, 39, 443-447, 445 (table), 446 (table), 453-454, 458-459

0

off-gas sampling, 334 (figure), 337 (table) offshore oil, 218 oil analysis, 17 (table). *See also specific oil* olefins, 515 on-line analysis, 323, 324, 328 on-line sulfur determination, 558–559 ¹H. *See* nuclear magnetic resonance (NRM) spectroscopy organic inductively coupled plasmaatomic emission spectrometry (ICP-AES), 170–175, 171 (table) analysis procedures, 178-183, 181 (table), 186 (table) detection limits, 179 (table) inferences, 183-185 instrumentation and, 175-178 See also inductively coupled plasma-atomic emission spectrometry (ICP-AES) organic liquids, 199 (table) organomercurial compounds, 269, 270-271, 272 (table) organometallic standards, 33, 139, 144 organo-silicon compounds, 202, 216 - 217outliers, 45 (table), 60-61 out-of-statistical-control data, 45 (table), 50, 51 oxidation, 489 (figure), 490 (figure) oxygen, 177-178, 195, 217, 417

Ρ

"particle size independent" method, 188-189 peak profiles, 160-161 pentanes, 198 (figure) performance improvements, 53 (table) peristaltic pump, 66-67, 175, 176 (table) petroleum coke, 194 petroleum products. See specific products phosphate antiwear additives, 601 phosphino-polycarboxylates (PPCA), 222-223 phosphorus, 164, 222, 632 phosphorus compounds, 528-529 photoelectric process, 350-351 photometric test methods, 32, 32 (table) photomultiplier tube, (PMT), 525 PIONA multidimensional analyzer, 516, 517 (table), 518 (table) pipelines, 254

- platinum group elements (PGEs), 234
- pneumatic nebulizers, 175, 221
- pneumation, 197, 200-201
- point-focusing doubly curved crystal optics, 395
- polarization, 382, 383 (figure)
- polars, 171
- polyethylene, 338, 339 (table), 339–340
- polyethylene production gas analysis, 338–340, 341 (table)
- polytetrafluoroethylene (PTFE), 257
- pooled limit of quantization (PLOQ), 45 (table)
- pooled standard deviation, 81
- porphyrins, 605-606
- Practice for Applying Statistical Quality Assurance Techniques to Evaluate Analytical Measurement System Performance (D6299), 64
- Practice for Determination of a Pooled Limit of Quantization (D6259), 64
- Practice for Determination of Precision and Bias for Use in Test Methods for Petroleum Products and Lubricants (D6300), 64
- Practice for Laboratory Bias Detection Using Single Test Result (D6617), 64–65
- Practice for Statistical Assessment and Improvement of the Expected Agreement Between Two Test Methods That Purport to Measure the Same Property of a Material (D6708), 65
- precision, 45 (table), 74, 94, 128–131, 130 (table), 322
 - crude oil and, 613 (table), 614 (table), 619 (table) mercury testing and, 265–266 sulfur and, 630–637, 634 (table), 635 (table)
 - See also precision ratio (PR); precision test program (PTP)
- precision ratio (PR), 45 (table), 49
- preventative action, 52
- problem solving, 208, 210 (table)

process capacity index (CpK), 44 (table) process mass spectrometry, 311-315 instrumentation and, 315-318, 315 (figure), 316 (figure), 317 (figure) sampling techniques, 318-319, 319 (figure) process nuclear magnetic resonance (NRM) instrumentation, 427-429 product specification, 63 proficiency test programs (PTP), 74-75, 76-84, 84-97, 98-110, 116 proficiency test programs (PTP) report, 82 (table) proficiency test programs (PTP) toolkit, 79, 82 (table) proficiency testing, 45 (table), 75 proportional counter, 380 (table), 384 (figure) proton chemistry, 430 (figure) proton types, 425, 444 (table) PSA method, 575-576 pulse height selection, 356–357 pumping device, 175, 315 (figure) pyrolysis, 157, 160 pyrolysis curve, 163 (figure), 164

Q

quadrupole inductively coupled plasma-mass spectrometry (QICP-MS). 215 quadrupole mass analyzers, 292–293 qualitative analysis, infrared, 484–485 qualitative wavelength-dispersive X-ray fluorescence (WD-XRF) spectrometry analysis, 352 quality assurance, 42, 48, 45 (table). See also laboratory quality management; quality control; quality protocols; statistical data handling quality components, 65-73 quality control, 42, 45 (table), 53, 54 quality control charts, 50, 51, 82 (table) quality control frequency, 49, 50 (table)

quality control sample, 46 (table), 49–50 quality control standard, 113 (table), 114 quality disputes, 61–63 quality index, 46 (table) quality management, 46 (table) quality protocols, 65–73 quantitative analysis, 360–362, 485–486 quantitative wavelength–dispersive X-ray fluorescence (WD-XRF) spectrometry analysis, 352 quantum detector, 481

R

radiochemical neutron activation analysis (RNAA), 413-413 radioelement, 415 radioisotope, 277 rare earth elements (REEs), 218 Rasberry-Heinrich algorithm, 365-360 Rayleigh scattering, 362–363 readouts, 142 recovery performance, 264, 265 (figure), 265, 266 (table) reference composition, 366 reference material (RM), 25 (table), 30, 46 (table), 53-54, 112, 113 (table), 114-116, 115 (figure), 120–122 (table) calibration, 114–116, 115 (table), 116-117 crude oil and, 620-621, 621 (table) National Institute of Science and Technology (NIST) and, 120-122 (table) storage, 115 (table) sulfur determination and, 561, 561-563 (table) See also reference material (RM) values: reference standards reference material (RM) values, 116-117 referenced standards, 40-41 (table), 48, 108–110 (table)

refining, 500-502 Reformulated Gasoline Program, 224 relative bias, 46 (table), 98 relative standard deviation (RSD), 104-105, 105 (figure), 105-107, 106 (figure), 107 (figure) renewable fuels standard (RFS), 62.5 repeatability, 31, 46 (table), 61-62, 405, 408 (figure) replicate testing, 61 representative sample, 46 (table) representative sampling, 64-65 reproducibility (R), 46 (table), 405, 408 (figure), 555, 556-557, 557 (table) residual fuel oil, 117, 118 (table), 119 (table), 145–146, 233 inductively coupled plasmaatomic emission spectrometry (ICP-AES) analysis of, 189-194, 191 (table), 192 (table), 193 (table), 194 (table) resolving power (RP), 293–294 reststrahlen, 482 result tables and statistical summary, 82 (table) reverse phase liquid chromatography (RP-LC), 513-514 robust statistics, 82 (table) root cause investigation guide, 82 (table) rotating disc electrode emission spectrometry, 586, 588 rounding-off, 59-60, 61 (table) Rowland circle, 394–395 (figure) R_{these data}, 103 run chart, 46 (table)

S

Saint Pierre, 228 salt monitoring, 501 (figure). *See also* heat stable salts (HSS) sample analysis, 161–162, 182–183 sample dilution, 188, 190 sample distribution, 79 sample introduction, 138

sample preparation technique, 190-192. 504-509 sample solution, 136 sample storage, 37 sampling, 64-65, 65 (table), 256-258, 257 (table) crude oil and, 607-610, 607 (table) infrared. 481-484 sampling system, 274 (figure), 274, 278 (figure), 584-585 saturation vapor pressure, 174 (table) scan/selective ion monitoring (SIM), 287 scattering crystal, 382 scintillating crystal, 359 scintillation detector, 355, 359-360 scrubbing, 500 selenite (Se-IV), 230 selenocyanate (SeCN), 230 semiconductor detector, 380-381 separation column, 495-496, 511 separation mechanism, 512, 513. See also separation column short-term precision, 180 (table) Si, 203, 203 (table), 204 (table) sigma detection limits, 198 (figure) signal-to-noise ratio, 382, 383 silicon, 144, 194, 201-204, 417-418 "silicon crisis," 201 silicon-drift detector (SDD), 381, 381 (figure) simulated distillation, 519-523, 520 (table) single pulse excitation (SPE) MAS, 457-459 single-channel analyzer (SCA), 399 (figure) site precision, 47 (table), 97 size exclusion chromatography (SEC), 229 slurry analysis, 166 S-O compounds, 549 (table), 633 (table) SOA standard, 49, 50 sodium, 216, 605, 606 software, 275

solid state nuclear magnetic resonance (NRM) spectroscopy, 433-434, 457-462, 460 (table), 463 (table) solvent aspiration rate, 172 (table), 173 (table) solvent selection, 170-171, 172-174 (table), 174-175 solvents, 162 sour gases, 500 soybeans, 627 speciated isotope dilution mass spectrometry (SIDMS), 278 speciation, 229, 269 spectral interference calibration, 182 spectral interferences, 137 spectral residuals, 486-487 spectrochemical analysis, 3. See also specific methods spectrometer considerations, 178 spectrometers, 38-39, 292, 298, 315-316, 316 (figure), 317-318, 349, 351 (table), 351-360, 428-429, 429 (figure). See also specific types spectrophotometers, 477-481, 477 (figure) spectroscopic methods, 17, 18-22 (table). 23 spectroscopic techniques, 15-16 (table), 17 (table), 621 (table), 622 (table). See also specific techniques spectroscopy, 3-4 spike compounds, 225, 226 spike recovery, 203 (table), 204 (table) spray chambers, 176-177, 178, 184, 201 stability test, 321-322 standard addition method, 138 standard deviation, 47 (table), 81, 83-84, 94, 105-107. See also relative standard deviation standard error of the mean, 80-81 Standard Guide for Analysis and Interpretation of Proficiency Test Program Results (D7372), 74

Standard Guide for Proficiency Testing by Interlaboratory Comparisons (E1301), 74 standard reference material (SRM), 47 (table), 53, 54, 113 (table), 117 - 119crude oil and. 620-621 genesis of, 19, 122 graphite furnace atomic absorption spectroscopy and, 162 from the National Institute of Science and Technology, 578, 579 (table) ware metal and, 592 (table) Standard Test Method for Aromatic Carbon Contents of Hydrocarbon Oils by High Resolution Nuclear Resonance Spectroscopy (D5292-99). 452 Standard Test Method for Aromatic Types Analysis of Gas-Oil Aromatic Fractions by High Ionizing Voltage Mass Spectrometry (D3239), 290 Standard Test Method for Chemical Composition of Gases by Mass Spectrometry (D260), 289 Standard Test Method for Hydrocarbon Type Analysis of Gas-Oil Saturates Fractions by High Ionizing Voltage Mass Spectrometry (D2789), 290 Standard Test Method for Hydrocarbon Types in Low Olefinic Gasoline by Mass Spectrometry (D2789), 290 Standard Test Method for Hydrocarbon Types in Middle Distillates by Mass Spectrometry (D2445), 290 Standard Test Method for Hydrogen Content of Middle Distillate Petroleum Products by Low-Resolution Pulsed Nuclear Magnetic Resonance Spectroscopy (D7171), 435 state-of-statistical-control chart, 47 (table)

statistical data handling, 57-65 statistical quality control (SQC), 47 (table) statistical run rules. 50-52 statistics, 82 (table) steam cracking, 328 stoichiometric air requirement, 342 storage. See reference material, storage; sample storage substoichiometric RNAA, 418 sulfate, 491 (figure), 634-635 sulfonate recovery, 633 (table) sulfur, 15-16 (table), 99-100, 541-542, 605, 619, 619 (table), 620 (table), 630-638 in biofuels. 559–560 certified reference materials and, 561 in crude oil, 541, 542 (table) in diesel, 87 (figure), 88 (figure), 90 (figure), 91 (figure), 97 (figure), 116, 451, 453 (table) emissions, 224 in fossil fuels, 235, 541-542 in fuel oil, 216-217, 230, 541 interlaboratory studies and, 552-553 in jet fuel, 99 (figure) on-line determination and, 558-559 oxides, 224 proficiency testing and, 553-554 relative standard deviation and, 103 (figure), 107 (figure) in RFG, 103 (figure) speciation, 526 (table) test methods and, 542-551, 545 (table), 550 (table), 551 (table), 555 (table) in ULSD, 92 (figure), 93, 94 (figure), 95 (figure) See also ASTM ULSD ILCP Program; sulfur determination sulfur calibration, 35 sulfur chemiluminescence detection (SCD), 231 sulfur chemiluminescence detector, 524-526, 525 (figure), 526 (figure)

sulfur determination, 384, 387, 389 (table), 389, 631–632, 633–634, 634 (table). *See also* sulfur sulfur oxides, 541–542 supercritical fluid chromatography (SFC), 514, 531, 535 (figure), 536 suppressed conductivity detection, 503 (figure) suppressor, 497–499 surrogate mixtures, 488

Т

T measurements, 435 temperature measuring device, 28 terminology, 43-48 (table) test method capability trends, 103, 104 test methods biofuels and, 628-637 chromatography and, 523-524 comparison, 128 crude oil and, 608, 608 (table), 609, 609 (table) energy dispersive X-ray florescence and, 385-386, 386-389 graphite furnace atomic absorption spectroscopy and, 164-166 ion chromatography and, 506-509, 507 (figure), 508 (figure), 510 (table) liquid chromatography and, 531-532 (table) mercury and, 566, 569 (table), 570 nuclear magnetic resonance (NMR) spectroscopy and, 440-441, 446-447, 449, 449 (figure) PIONA analyzer and, 517 (table) sulfur determination and, 542-551, 544 (table), 545 (table), 550 (table), 551 (table), 555 (table), 628-637 used oil and, 585-598, 591 (table), 596 (table), 599 (table), 602 (table) See also ASTM test methods; specific test methods

test performance index (TPI), 47 (table), 49, 50 (table), 52 (table) test result rounding, 59 test results, 59, 61-63 testing frequency, 49, 64 tetraethyllead (TEL), 197 tetralin, 184, 185 (figure), 193 (figure), 194 (figure), 202 tetramethylsilane (TMS), 202-204 thermal conductivity detector (TCD), 511 thermal ionization mass spectrometry (TIMS), 216 thermal properties, 158 ¹³C. See nuclear magnetic resonance (NRM) spectroscopy $^{34}\text{S}/^{32}\text{S}$ isotope ratio, 225, 235 time domain nuclear magnetic resonance (NRM) spectroscopy, 426-427 time-of-flight mass spectrometers, 298, 316, 317 (figure) time-of-flight mass spectrometry (TOF-MS), 215 timers. 28 tolerance, 30-31 toolkit. See proficiency test programs (PTP) toolkit torches. 177 total diaromatics, 306 (table) total ion chromatogram (TIC), 298 toulene solutions, 202, 203, 204 (table), 263-264 TPI_{industry}, 82 (table), 95-97, 96 (table), 97 (table), 103-104, 103 (figure), 104 (figure) trace contaminate analysis, 507 (figure) trace elements, 117, 118 (table), 119 (table), 145, 160, 165 (table), 219, 220, 411 crude oil and, 605-607, 607 (table). See also metal trace metals, 145, 194-195, 216-217, 221 - 223traceability, 25 (table), 26, 48, 112 transmittance, 475 trimethylarsine (TMAs), 246

troubleshooting, 208 true value, 47 (table) T-test, 82 (table), 83, 84 tube furnace, 258

U

ultrasonic nebulizers (USN), 176, 177 (figure), 195-197, 196 (figure) ultraviolet florescence (UV-FL), 549, 550 ultraviolet/visible light absorbance (UV/Vis), 500 uncertainty, 75 uncontrolled variables. 106 United States, 627-628 universal calibration, 195-196 used oil, 582, 602 crosscheck programs and, 598-601, 598 (table) sampling, 584-585 testing, 585-598, 591 (table), 596 (table), 599 (table), 602 (table) USN microporous membrane desolvator (USN-MMD), 195, 197 (figure)

V

vacuum distillates, 163 vacuum gas oil (VGO), 450 vacuum system, 211, 287, 314-315, 317 (figure) vanadium, 216, 217, 236, 605, 607 vapor pressure osmometry (VPO), 300 vaporization, 264 (table) vaporization chamber, 262, 264 variance, 47 (table) verification, 24-25 versatility, 288 viscosity, 143, 455 viscosity index (VI), 145 volatile elements, 166 volatile hydrocarbons. See hydrocarbons volatility, 171, 174, 194-195, 204 (table) volumetric glassware, 28

W

Walsh, Sir Alan, 4, 135 wavelength, 160, 198 (figure), 352-354, 363, 611, 611 (table). See also wavelength-dispersive X-ray fluorescence (WD-XRF) spectrometry wavelength dispersive X-ray fluorescence (WD-XRF) spectrometry, 349, 351-360 matrix effects and, 361-370, 371 (table) sulfur and, 543, 546, 547 wear metals, 144, 188, 582, 583 (table), 584 (table), 587 (table), 589, 589-590 (table), 592 (table), 595 (table) weld crack, 255 (figure) Winter Conference on Plasma Spectrochemistry, 208, 209-210 Wilhelm, Robert, 4 Wilhelm, S. M., 566 Wobbe index, 340 WSD spectrometer, 351 (figure)

Χ

X-ray attenuation, 349-350 X-ray cups, 38 X-ray diffraction, 352 X-ray fluorescence (XRF) spectrometry, 36-38, 36-37 (table), 376 (figure), 391 ASTM test methods and, 385-386, 386-389 crude oil and, 617-620, 620 (table) principles, 374-377, 375 (figure), 376 (figure) sulfur and, 544, 546, 548 See also energy-dispersive X-ray fluorescence spectrometer; wavelength dispersive X-ray fluorescence (WD-XRF) spectrometry X-ray fluorescence analysis, 9 (table), 68-69. See also wavelength dispersive X-ray fluorescence (WD-XRF) spectrometry; X-ray fluorescence (XRF) spectrometry

X-ray fluorescence test methods, 36–38, 68 (table), 69 X-ray source, 377 X-ray transmission (XRT) instrumentation, 559 X-ray tube, 359–360, 378, 378 (figure), 392 xylene, 183-184, 184 (figure), 202

Ζ

Zeeman effect, 160, 575 Z-score, 75, 82 (table), 92–95, 94 (figure), 97 (table)