

Index

- Abegg, R., 50
Academy of Sciences, 32, 64, 120, 202, 207, 237
Academy's Committee on Science and Public Policy, 237, 238
Accuracy, 5, 142, 152, 157, 209, 210, 223, 227–228, 233, 234, 236, 239, 242, 245
Activation, 23–24, 99, 102
Adiabatic transition, 36, 43
Advanced Research Projects Agency (ARPA), 238
Affinity, 6, 29, 32, 54, 77, 121, 123, 125, 181, 255
Air Force Cambridge Research Center, 220
Alvarez, L., 88
American Chemical Society, 18, 68, 69, 202
American Institute of Physics, 218
Americans, 85, 88, 98, 99, 101–102, 156, 160–161, 203
Ammonia, 152, 160
Analogy/ies, 10, 22, 36, 40–41, 43, 58, 70, 88, 119–120, 124, 154, 168, 172, 194, 209–210, 215, 254
Analytic calculations, 24, 224
Anderson, P. W., 208
Annus Mirabilis, 61
Antiparallel, 16–17, 65, 72, 181
Antisymmetry, 28, 89, 152
Appel, K., 212, 260
Appleton, E., 138
Appropriation, 54–55, 184, 246, 249, 250, 255, 257
Approximation(s), 3, 56, 58, 62, 65–68, 77, 79, 81, 84–85, 91–92, 95–96, 101–102, 105, 111, 115, 131–132, 139–141, 160, 166, 170–171, 177, 199, 201, 208–209, 215, 218, 221, 223–227, 230–231, 233, 236, 238, 252
Hartree-Fock, 236
Hückel LCAO, 201
methods, 96, 105, 115, 131–132, 139, 141, 171, 225
Pariser-Parr-Pople (PPP), 224
self-consistent field, 139–140
zero differential overlap, 224
Arbitrariness, 70, 73, 117–118, 180
Argon, 137–138
Armaments Research Department, 227
Armit, J. W., 30
Armstrong, H. E., 78, 109, 250
Army Research Office, 220
Arndt, F. G., 78
Aromatic molecules, 25, 30, 55, 148, 206, 232
Arrhenius, S., 149–249
Arsem, W. C., 51
Atom(s), 10, 14–16, 18–25, 27, 30, 32, 36, 39, 41–44, 46, 48–60, 62–68, 70–78, 80–81, 83–86, 88–94, 99–101, 103, 107, 109–111, 114, 121, 132–133, 135–141, 143–144, 146–151, 153, 157–158, 160, 162–164, 168–169, 172, 179, 182, 194, 202, 206, 210,

- Atom(s) (cont.)
 212, 217–219, 234, 238, 247, 249, 251–252,
 255–256, 259
 cubic, 49–53
 separated, 36, 43–44, 46, 57, 73, 76, 80, 91,
 143, 210
 united, 36, 43–44, 46, 57, 58, 73, 128, 144,
 172
 Atomic structure, 18, 21, 26, 50, 53–54, 133,
 155
Aufbau, 3, 6, 39, 128, 144
- Balliol College, Oxford, 167
 Barnett, M. P., 203, 204, 260
 Barriol, J., 190, 193, 198
 Baudet, Jeanne, 190
 Bauer, E., 191–192
 Bayer, A., 78
 Beaven, H. C., 158–159
 Benzene, 27, 30, 55, 78–80, 110, 117, 124,
 146–147, 152, 161–163, 167, 178–179, 195,
 206, 221, 224
 Bergmann, E., 195
 Berlin, T. H., 203
 Berthier, G., 190, 196
 Berthod, Hélène, 190
 Besnainou, Sylvette, 190
 Bethe, H., 95, 154
 Binuclear orbit, 10, 55–58, 133
 Biology, 2, 126, 138, 174, 193, 201–202,
 217–219, 239, 253, 255, 260–261
 Birge, R. T., 39, 41, 61, 69, 70, 87
 Bishop, R., 256
 Bjerrum, N., 11, 13–14
 Blackett, P. M. S., 154
 Bloch, F., 90–91
 Bohr, N., 6, 10–11, 19, 27, 34, 39, 43, 48, 50,
 53, 55, 57, 61, 89–90, 93–94, 107, 128, 133,
 138–139, 151
 Bohr's atomic model, 53–54
 Bond(s), 9, 14, 17–18, 22–23, 25, 28–29, 37,
 50, 51–53, 58, 61–68, 70, 72–80, 83, 85–86,
 91–93, 96, 99, 101–103, 108–109, 111,
 114–115, 117–119, 124–125, 146–147, 149,
 151–152, 161–169, 171–173, 177–178,
 180–182, 184, 190, 192–196, 201, 206,
 233–235, 242, 251
 angles, 67–68, 77, 168
 chemical, 3, 14–15, 25, 31, 47, 50–53, 55,
 57–58, 61, 64–65, 67–69, 73, 75–79, 83–84,
 86, 90, 102, 104–105, 108, 115–121, 125,
 128, 132, 145, 149, 152, 166–167, 178,
 181–182, 188–189, 192–194, 199, 205, 230,
 251
 covalent, 2, 31, 73, 76, 83, 108, 145–146,
 251
 directional character of, 66, 77
 direction of, 66, 168
 double, 25, 27–29, 50, 52, 74, 78, 81, 124,
 146, 149, 161–162, 167, 195
 electron-pair, 47, 53, 57–58, 64–66, 68, 73,
 75, 81, 84, 145, 167, 206, 250
 energy, 66, 76–77, 80, 102, 124, 206
 homopolar bond, 14, 17, 37
 length, 163, 165, 166, 231
 nature of chemical, 15, 47, 50, 53, 57, 61,
 64, 69, 73, 76, 77, 79, 86, 105, 115–121,
 125, 128, 132, 145, 167, 178, 180, 189, 251
 nonpolar, 50, 51, 53, 107
 one electron, 74
 order, 162, 163, 168–169, 182, 189, 203,
 206, 231
 partial ionic character of, 76, 78, 251
 π , 29
 polar, 50, 53
 shared electron, 55, 75, 122
 σ , 29
 single, 50, 52, 76, 78, 169
 stability, 32
 three-electron, 74–75, 78, 251
 two-electron, 51
 Bonding power, 44, 45, 69, 70
 Born, M., 12–13, 16, 22, 26, 34, 55, 87–90,
 94, 98, 103, 136, 145, 161, 165
 Boron Hydrides, 74, 152
 Bose-Einstein statistics, 135

- Boulder Conference, 183, 197–199, 201, 223, 226, 228, 230–231, 235
Boundary/ies, 2, 6, 47, 57, 77, 131, 234, 237, 261
Boys, S. F., 207, 209, 227–230, 260
Bragg, Sir L., 55, 134
Bragg, W. H., 55, 62, 132, 145, 147, 154
Brakel, J. Van, 257
Bray, W. C., 48
Bridgman, P. W., 61, 91, 112, 115
Brillouin, L., 194
Brion, Hélène, 190, 194
British Association for the Advancement of Science, 18, 107, 131, 143, 145, 153, 249, 250
Brodetsky, S., 158
Brooks, H., 237
Buckingham, D., 18
Burrau, O., 17, 20, 58, 59
Bush, V., 141, 150
Butadiene, 152, 196, 254
Butlerov, A. M., 121

Calais, J. P., 212, 260
Calculation(s), 3, 5, 9, 10, 12, 15, 20, 24–25, 30, 32–33, 37, 57–59, 64, 71, 75, 80–81, 83–85, 88–90, 93, 95–96, 100–101, 103, 114–115, 120, 126, 132, 136–140, 143, 148–150, 152–153, 155–157, 161–167, 172, 176, 180, 182, 185, 187, 189, 193, 195, 197, 199, 202–211, 220–224, 227–234, 236–241, 245–246, 252–254, 261
ab initio, 5, 126, 172, 197, 204, 222, 225, 229, 239, 242
analytical, 5, 116, 255
semiempirical, 5, 84, 206, 221, 227, 229, 241
Calculators/calculating machines, 204–205, 212, 222, 228, 230, 254
California Institute of Technology, 39, 55, 110
Cancérisation par les Substances Chimiques et Structure Moléculaire, 199, 200
Carbon, 24, 28, 66–67, 79, 112, 147, 149, 162, 168, 180
Carbon atom, 24, 27, 30, 63, 66–67, 78, 162, 168, 179
Carcinogenesis, 193, 199, 200
Carcinogenic activity, 189, 200
Cavendish Professor of Experimental Physics, 134
Censor's Office, 156
Center of Material Sciences and Engineering, 209
Centre de Chimie Théorique, 187, 190, 193
Centre de Mécanique Ondulatoire Appliquée, 193, 198
Centre Européen de Calculs Atomiques et Moléculaires, 196
Centre Inter-regional de Calcul Électronique, 196
Centre National de la Recherche Scientifique, 190, 245. *See also* CNRS
Chair of Quantum Chemistry, 216
Chapman, S., 136, 173
Chemical combination, 19, 50, 52, 83
Chemical Elements and their Compounds, 107
Chemical fact, 24, 77, 108, 125, 133, 251
Chemical force, 24, 32, 121
Chemical formula, 23–24
Chemical physics, 27, 105–106, 112–115, 217, 235
Chemical problems, 3, 9, 16, 18, 25–26, 29, 56, 69, 87, 96, 105, 107, 109, 115, 117, 132, 176, 183–184, 199, 218, 239–241, 245–246, 249
Chemical reaction, 9, 21, 23, 43, 106, 146, 149
Chemical reactivity, 49, 124, 169, 200, 206, 254
Chemical Reviews, 30, 64, 88, 101
Chemical Society, 106, 107, 111, 151
Chemical thermodynamics, 247–249, 257–258
Chemistry, 2–9, 12, 17–20, 22–27, 29, 31–33, 36–37, 39–40, 44, 46–49, 53, 55–56, 65, 68,

- Chemistry (cont.)
- 73, 77–78, 81, 84, 86–87, 91–94, 96, 98, 102, 104–109, 111–119, 121, 123, 125–129, 131–133, 135–136, 138, 143–145, 147–148, 151–153, 158–160, 162, 164, 167–171, 173–177, 180–185, 187–193, 195–205, 209–210, 212–214, 216–218, 222, 224–234, 236–243, 245–261
 - computational, 217, 235
 - and computers, 217
 - inorganic, 18, 33, 53, 126, 148–149, 260
 - and mathematics, 183
 - organic, 21, 25, 30–31, 67, 78–79, 106–109, 112–113, 118–120, 122–123, 133, 147, 149, 162, 168, 172, 188, 195, 198–200, 225, 227, 231, 235, 237, 239, 241–242, 250, 252, 254
 - philosophy of, 5, 247, 261
 - physical, 9, 13, 27, 30, 32, 48, 77, 87, 106, 107, 112, 113–114, 116, 134, 167–168, 192, 205, 235, 249–250
 - role of theory in, 247, 253, 255, 261
 - Second Instrumental Revolution in, 261
 - structural, 3, 77, 109, 111, 126, 144, 178, 225, 231
 - theoretical, 18, 33, 126, 131, 145, 148–150, 166, 170, 173–174, 177–178, 182–185, 187, 190–193, 196–197, 199–200, 247, 250–251
 - theoretical particularity of, 255
 - Chemists' culture, 19, 38, 47, 65, 107, 120, 122–123, 128
 - Circulation, 197, 207, 214, 260
 - Clark, G. L., 19
 - Classical physics, 16, 28, 120, 145, 205
 - Claus, A., 78, 80
 - Clementi, E., 217–218, 243, 260
 - Clifton College, 158
 - Closed shell, 20, 30, 43, 83, 101, 238
 - Clusters of issues, 2–5, 7, 246
 - CNRS, 190–191, 193, 196, 245, 254
 - Colby, W. F., 39
 - Colloque de la Liaison Chimique, 191, 195.
 - See also* Conference, Paris
- Complex spectra, 90, 93, 95, 140
- Compounds, 19–20, 22, 30, 40, 52, 65, 67, 74–75, 78, 80, 101, 107, 112, 126, 147–149, 188, 195–196, 200, 245
- aromatic, 26–27, 30, 78, 102, 125
- benzenoid, 26–27, 30, 195
- covalent, 75, 148
- nonpolar, 50, 52, 75
- polar, 49, 50, 52, 75
- Compressibility, 61, 137
- Compromise(s), 122, 213, 233
- Compton, A. H., 35, 45, 62, 112–113, 209
- Computer(s), 2, 4–5, 7, 126–127, 132, 153, 157–158, 183, 187, 193, 195–196, 199, 204, 207, 209, 213, 215–219, 221–235, 237–243, 245–246, 251–254, 261
- and ab initio computations, 221–222, 226, 233
- and cultures of quantum chemistry, 187, 225
- EDSAC, 157, 228
- hardware, 187, 222, 240–241, 254
- high speed, 2, 157, 224
- program(s), 5, 126, 218, 222–223, 228, 230–232, 235, 237, 239, 241
- and semiempirical approximations, 215, 223, 226
- software, 187, 222, 240–241, 254
- technology, 187, 209, 221–223
- Computing Laboratory, 150, 173, 253
- Concept(s), 1–3, 18, 21, 23, 27, 37, 41, 44, 47, 51–52, 56, 70, 73, 75, 77, 84, 97, 108, 110–111, 114, 117–119, 121–122, 124–125, 133, 139, 143, 149, 163, 166–169, 173, 175–176, 180–183, 185, 189, 192, 194, 197, 212, 214, 219, 227, 231, 233–234, 246, 248, 251–253, 255–257, 259, 261
- chemical, 86, 109, 117, 168, 184, 190, 193, 206, 215, 234, 240, 242, 259
- resonance, 75, 117–119, 124, 149, 166, 251
- Conceptual framework, 24, 125, 219, 246

- Conceptual scheme, 42, 69, 84, 85
Condon, E. U., 58, 59, 62, 90, 217
Conference(s), 1–3, 126, 144, 146–147, 187, 192, 199, 202–208, 217, 221, 230–234, 237, 238–241, 246, 256
Boulder, 183, 197–199, 201, 223, 226, 228, 230–231, 235
on Computational Support for Theoretical Chemistry, 1, 187, 237
in Jerusalem, 195, 197
Nikko, 210
Paris, 126, 187, 192, 203
Sanibel Island, 126, 216–217, 236, 241
Shelter Island, 126, 202–206, 208–211, 221, 230
in Sweden, 197
Texas (Molecular Quantum Mechanics Conference), 221, 233
Conference on Computational Support for Theoretical Chemistry, 1, 187, 237
Configuration Interaction, 92, 171, 196, 206, 208, 210–211, 224, 236
Conjugated systems, 80, 168, 169, 195, 197, 199
Connant, J. B., 121
Consensus, 3, 5, 38, 105, 110, 172, 181, 240, 246, 259
Contexts, 3, 48, 54–55, 219
Contingency, 4, 38, 128
Contingent, 4, 6–7, 246, 256
Coolidge, A. S., 215, 222
Correlation diagram, 46, 83
Coulson, C. A., 1–4, 121, 131–132, 134, 141, 148, 150, 154, 158–185, 189, 191–193, 196, 199, 201, 203–208, 210, 212, 214, 219, 225–227, 229–230, 232–235, 242–243, 249–250, 253, 259, 260
Courant, R., 34
Craig, D. P., 170–171, 175, 206
Crawford, B. L., 203, 206–207, 260
Crick, F., 141
Criterion/a, 4–6, 28, 30, 45, 63, 65–68, 76, 78, 117, 143, 161, 164, 171, 250
Crystal(s), 26, 34, 55, 62, 67–68, 76, 88, 91, 96, 112–114, 136–137, 147–148, 168, 192, 204, 208, 209–210, 212, 219, 221, 251, 260
Culture(s), 4–5, 13, 19, 37–38, 47, 65, 105, 107, 120, 122, 123, 125, 128, 158, 173, 177, 184, 187, 212, 222, 225, 227, 229–230, 235, 246–248, 253–259
Cunningham, E., 134
Dalton, J., 149
Darwin, C. G., 134
Daudel, Pascaline, 191
Daudel, R., 4, 168, 187–190, 192–194, 198–199, 202, 219, 230, 260
de Broglie, L., 188, 193–194, 198–200
Debye, P., 26–27, 34, 89, 108, 113, 145
Del-squared V Club, 135, 138
Department of Theoretical Chemistry, University of Cambridge, 227
Determinant, 62, 87, 89–92, 140, 169, 236
Dewar, J., 78–80, 175
Diamagnetism, 54, 97, 99
Diatom project, 223, 231
Dickinson, R. G., 55
Dielectric constant, 31, 56, 112
Differential analyzer, 141–143, 150, 154, 157
Dilute solutions, 26, 149
Dirac, P. A. M., 9, 13, 20, 35, 37, 45, 61, 89, 90–91, 94, 96, 131, 135, 138, 145, 150, 154, 157, 159, 176, 185, 207, 208, 223, 256
Disciplinary, 2, 5, 27, 47, 77, 87, 97, 105, 131, 210, 214, 217, 219, 243, 261
Disciplinary emergence, 3, 7
Discourse, 6, 7, 239, 255, 256, 257
Dissertation, 26, 31, 34, 40, 48, 88, 94, 136, 139, 160, 190, 195, 213, 227
Eigenfunction(s), 24, 30, 57–60, 66–68, 75, 81, 110, 140
Eigenvalues, 60, 140, 163
Eistert, B., 78
Electrodynamics, 11, 97, 98, 104, 204

- Electron(s), 9, 10–11, 15–18, 20, 21–23, 25, 27–28, 30, 32, 33, 36, 41–45, 47, 49–60, 62, 64–75, 77–78, 80–81, 83–86, 88–92, 95, 97, 100, 101, 103, 110, 117, 122, 125–126, 128, 131–133, 135, 139–141, 143–146, 149–153, 161–164, 166, 168–169, 172, 181–182, 193–194, 200, 203, 205–206, 210, 215, 220–224, 228, 233–234, 236–240, 250–251, 255–256
 bonding, 64, 70–73
 charge density, 20, 189, 231, 233
 delocalized, 193
 jump, 11
 K , 193
 L , 22, 193
 localized, 167
 nonbonding, 44, 70, 83
 orbital, 10, 76, 172, 103
 outer, 10, 56
 $p\sigma$, 73
 pairing of, 55, 70, 72, 131, 145, 146
 π , 28, 30, 153, 162, 163, 171, 172, 206, 224
 promoted, 44, 70, 71, 72
 promotion, 41
 ring, 10, 30
 S , 62, 71–72, 90, 101
 $s\sigma$, 71
 σ , 193, 238
 spin, 16, 25, 28, 36, 54, 56, 70, 89
 unpaired, 28, 65, 70, 72, 74
 unpromoted, 44
Electronegativity/ies, 76–77, 180, 251
Electronic computers, 2, 5, 157, 215–216, 229–230, 232–235, 242
Electronic structure, 28, 41, 46, 56, 67, 75, 80–81, 95, 110, 125, 133, 138, 144, 146, 149, 160, 162, 189, 190, 194, 200, 203, 206, 213, 215, 225, 227, 228, 251, 254
Electronic Theory of Valency, The, 107
Elementary Wave Mechanics, 104
 Energy, 11, 13, 15–17, 19–21, 23, 25, 28, 30–33, 41, 43–46, 48, 54, 58–59, 61–62, 64, 66, 70–77, 79–80, 92, 93–94, 102, 110, 120, 124, 127, 134, 140, 143, 146, 149, 161–165, 168–169, 171, 176, 180, 194, 204, 206, 209, 232, 238, 241
 cohesive, 204, 210
 of formation, 19, 64, 76, 80
 potential, 28, 31, 44, 75, 140
 of promotion, 44, 71
 resonance, 58, 74, 79, 80, 96, 120, 124, 149, 161
 total, 21, 31, 44, 58, 72, 76, 124, 140, 163
Epistemological, 29, 30, 38, 48, 112, 255–256, 259
Equation, 4, 5, 9, 16–17, 21, 34, 62, 64, 66, 96, 97, 113, 134, 138–142, 150, 154, 158, 166, 169, 177, 206–207, 245, 248
Schrödinger, 3, 17, 19–20, 22, 33, 37, 43, 57, 62, 111, 125, 128, 140, 166, 183, 215, 228, 236
 secular, 62, 169, 209, 210
Essec Prize of the French League Against Cancer, 200
ETH, 26
Ethylene, 28, 124, 147, 152, 161, 167, 178
Europe, 36, 42, 55–57, 61, 87–89, 94–95, 103, 202, 205, 208, 222, 223
European Office of Air Research and Development Command, 213
Everitt, C. W. F., 16
Ewald, P. P., 13, 14, 27
Exchange, 15–18, 22, 54, 59, 80, 90, 98, 103, 114, 118, 141, 154, 157, 163, 167, 190, 205, 208, 224, 240, 241, 260
Excited state, 24, 43, 147, 171, 194, 222, 228, 254
Exclusion principle, 15–18, 20, 25, 32–34, 37, 42, 44, 54, 58–59, 70, 81, 128, 149, 153. *See also Pauli principle; Pauli exclusion principle*
Explanation, 1–3, 9, 12, 16, 20–21, 30, 42, 49, 54–55, 58, 62, 64, 66, 72, 75, 85, 94, 97, 101, 108, 111–112, 114, 126, 128, 131, 133,

- 143–144, 146, 148–149, 161, 180, 182, 192, 195, 200, 201, 205, 252, 253
Eyring, H., 103, 203, 207, 214, 217
- Faculty Board of Mathematics, 150
Fairbank, W. M., 16
Fajans, K., 87
Faraday Society, 106, 107, 111, 132, 133, 143, 146, 147, 172–173
Ferromagnetism, 91, 147
First World War, 26, 40, 134, 188
Fischer, Inga, 171, 197, 212
Fock, V., 140, 164, 206, 211, 221, 236
Fowler, R. H., 18, 94, 106, 131–136, 138–139, 145–146, 157, 159, 160
Franck, J., 16, 34
Free radicals, 79, 146, 162
Fröman, A., 212, 260
Fry, H., 21
Fues, E., 31
- Gale, H. A., 45
Gallipoli, 134
Garner, W. E., 143
Gaunt, J. A., 135
Geiger, M., 12
General Chemistry, 119
Generalization(s), 23, 41, 65, 70, 75, 101, 150, 203, 250
George Fisher Baker Non-resident Professor/Lecturer, 108, 116
Goudsmidt, S., 57
Graphical method, 33, 142
Great War, 134, 136, 138
Ground state, 15, 22, 28, 66, 92, 94, 99, 101, 110, 144, 164, 171, 215, 222, 228, 233, 234
Group theory, 6, 17, 22–25, 30, 37–38, 89–91, 93, 95–97, 100, 104, 141, 161, 190, 191, 205
Györgyi, A. S., 200
- Habilitation, 26, 27, 32
Hacking, I., 6
- Hall, G. G., 152, 212, 229, 260
Harkins, W. D., 40, 87
Hartree, D. R., 3, 88–89, 131, 134–135, 138–142, 153–158, 164, 183, 185, 206, 211, 221, 234, 236, 260
Hartree, W., 134, 138, 155, 157
Heilbron, J., 17
Heisenberg, W., 12–13, 15, 18, 27, 34, 45, 88–89, 91–92, 94, 135–136, 138–139, 145–147
Heitler, W., 2–3, 6, 12–18, 20–23, 25, 36–37, 39, 42, 45, 47, 57–60, 64–65, 68–72, 79, 81, 83, 86–87, 89–93, 97–105, 114, 116–117, 127, 131, 141, 143–144, 147, 152, 161, 189, 198, 205, 215, 219, 222, 230, 241, 243, 256, 260
Heitler-London (1927) paper, 18, 37, 64, 101, 127, 152, 205, 230, 256
Helium atom, 18, 57–58, 60, 65, 72, 88–89, 94, 194
Hellmann, H., 31–33, 37, 131, 260
Henri, V., 145, 190
Herzberg, K., 13, 172
Heuristic, 29, 68, 100, 118, 166, 181
Heurlinger, T., 11
High-speed computing, 157, 222
High temperatures, 34, 241
Hilbert, D., 13, 26
Hill, A. V., 134, 138
Hinshelwood, C., 121, 170
Hirschfelder, J. O., 203, 212, 219
Historical, 2–6, 37, 125, 149, 177, 230, 251, 255–257, 259
Historiography, 4, 245, 247
Hoffman, R., 254
Honl, H., 12
Hückel, E., 25–31, 37, 79–81, 87, 96, 102, 119–121, 131, 147–148, 162, 170, 172, 189, 199, 210, 220, 221, 224, 226, 237, 260
Hückel, W., 31
Hückel LCAO approximation, 201
Hulthén, A., 213
Humboldt University, 13

- Hund, F., 3, 27–28, 30, 34, 36–37, 39, 41–43, 45, 81, 83, 85, 87, 89, 91–93, 97, 100, 103, 128, 131, 143, 147–148, 172, 260
- Husserl, E., 12–13
- Hybridization, 60, 62, 64, 77, 146, 167, 180, 182, 206, 251
- Hydrogen atom, 14–16, 18, 23, 57, 59, 60, 72, 91–92, 133, 168
- Hydrogen molecule, 10, 12, 14–15, 17–21, 57–60, 65, 71, 81, 85, 91–93, 96, 101, 125, 205, 222
- ion, 10, 17, 20–21, 58, 85
- Hylleraas, E. A., 88, 217, 218
- Imagination, 89, 157, 181, 182, 231
- Imperial Chemical Industries, 97
- Imperial College, 136, 227
- Inaugural lecture, 157, 176, 183, 184, 229, 246
- Indistinguishability, 52, 54, 59–60, 74, 141, 193
- Ingold, C. K., 78, 121
- Inorganic chemistry, 18, 33, 53, 126, 148, 149, 260
- Institut de Biologie Physico-Chimique, 193, 200
- Institut du Radium, 188, 189, 190, 193
- Institute for Advanced Study, 17
- Institute for Theoretical Physics, Copenhagen, 13
- Institute of Molecular Biophysics, 201, 217
- Institute of Technology, Hannover, 31
- Institute of Technology, Stuttgart, 31
- Instrument, 5, 17, 114, 132, 156–158, 187, 231, 239, 242, 245, 249, 254, 261
- Integral(s), 60, 89, 93, 134, 137, 141, 161, 169, 202–203, 206–207, 210, 214, 222, 224, 228, 230, 237–238, 240, 245
- Coulomb, 15, 163
- exchange, 15, 80, 90, 163, 205, 224
- four-center, 203
- molecular, 126, 176, 203–210, 222, 225, 232
- overlap, 15, 68, 180, 203, 220
- repulsion, 224
- three-center, 162
- two-center, 203, 207
- International Conference in Physics 1934, 146, 147
- International Education Board, 13–14
- International Journal of Quantum Chemistry*, 218, 241
- International Union of Pure and Applied Physics, 147, 205, 208
- Internuclear, 16, 21, 32, 36, 44, 46, 57, 83, 92, 171, 209, 218
- Interpretation, 11, 13, 17, 19, 24, 34, 37, 40, 42, 46–47, 50, 69, 85, 95, 101, 108, 110, 135, 139, 145, 151–153, 166–169, 206, 215, 219, 225, 232, 259
- chemical facts, 24, 108
- Introduction to Chemical Physics*, 105, 112–114
- Introduction to Quantum Mechanics with Applications to Chemistry*, 119, 251
- Introduction to Theoretical Physics*, 113
- Intuition, 116, 119, 177, 180, 182, 194, 231
- Ionization, 31, 54, 140, 194, 223
- Isomer(s), 52, 78, 111
- Jacobi, C. G. J., 13
- James, H. M., 215, 222
- Jansen, L., 219
- Japan Society for Promotion of Science, 205
- Jerusalem Symposia in Quantum Chemistry and Biochemistry, 195, 197
- Jewish, 12, 13, 31, 32, 193
- John Humphrey Plummer Professorship of Inorganic Chemistry, 148
- John Simon Guggenheim Memorial Foundation Fellowship (Guggenheim Fellowship), 55, 58, 89, 95
- Joliot-Curie, F., 188, 191, 198, 200
- Joliot-Curie, Irène, 188, 200
- Jordan, P., 13, 34
- Jost, W., 32, 33

- Journal, 2, 4, 12, 20, 56, 61, 68–69, 73, 77, 102, 165, 200, 204–205, 208, 218–219, 240–241, 250, 256
Journal of Chemical Physics, 77, 81, 160, 165, 218, 236
Journal of the American Chemical Society, 61, 73, 77, 178
Julg, A., 190, 196, 198
- Kant, I., 22
Kapitza Club, 135
Karachalios, A., 25
Karpov Institute, 32, 33
Kasha, M., 201, 217
Kekulé, F. A., 78–80, 117, 119, 124, 149, 181
Kemble, E., 11, 39–40, 45, 61, 87, 94
Kimball, G. E., 203, 214
Kinetic theory, 11, 113, 134, 137, 145, 148
Klein, O., 213
Kopineck, H. J., 207
Kossel, W., 16, 31
Kotani, M., 204, 205, 207–208, 210, 212, 219, 260
Kramers, H. A., 61, 89, 90, 93, 95, 135, 220
Kronig, R., 100–101, 136, 220
Kuhn, T., 86
Kurti, N., 97
- Laboratory, 45, 48–49, 51, 55, 98, 107, 112, 127, 134, 150, 157–158, 167–168, 170, 173, 193, 196, 209, 213, 215–216, 219, 224–225, 228, 231, 239, 242, 247, 248, 253–254
Brookhaven National, 238
Cavendish, 61, 135
IBM Research, 217
Jefferson Physical, 40
Mallinckrodt Chemical, 215
Marine Biological, 200–201
of Molecular Structure and Spectra (LMSS), 126, 202, 216, 219, 220, 222, 231, 253
Ryerson, 45
Lacassagne, A., 188, 190, 200
- La Chimie Théorique et ses Rapports avec la Théorie Corpusculaire Moderne*, 188
Ladenburg, A., 78
Lamb, A. B., 61, 73
Language, 4, 10, 13, 19, 24, 30, 43, 69, 81, 85, 101, 105–106, 109, 112, 116, 122, 152, 167, 193, 214–215, 223, 225, 246, 255
Lapworth, A., 78, 132
Larmor, J., 249
LCAO (linear combination of atomic orbitals), 83–85, 201, 222
Le Bel, J. A., 149
Legitimization, 2–3, 5, 105, 192, 239, 255, 259, 260
Lennard-Jones, J. E., 28, 83, 93, 98, 103, 121, 131–132, 134, 136–138, 141, 143–146, 148–153, 159–162, 164–165, 169–170, 172, 183, 185, 191, 204, 225, 227, 260
Les Théories Électroniques de la Chimie Organique, 199
Lewis, G. N., 10, 16, 18–19, 30, 39, 44, 47–55, 57, 64, 65, 70, 74, 75, 77–78, 80, 83, 87, 101, 107–108, 110, 116, 122, 126, 128, 132–133, 143, 152, 181, 243, 247, 248, 249, 250
Lindemann, F., 97
Lindenberg, J., 212, 260
Lindsay, R. B., 154, 155
Loge, 193–195
London, F., 2–4, 6, 12–25, 36–37, 39, 42, 45, 47, 57, 58–60, 64–65, 68–72, 79, 81, 83, 86–87, 90–93, 97–106, 110, 114, 116, 117, 127, 131, 141, 143–144, 147, 152, 161, 189, 191, 198, 205, 213, 215, 222, 230, 241, 243, 256, 260
London, H., 97
Longuet-Higgins, H. C., 168–170, 191, 225, 227, 235, 250, 252
Loomis, F. W., 39, 45
Lord Kelvin (William Thomson), 141
Löwdin, P. O., 1–2, 4, 197, 204–219, 224, 230, 232, 243, 253, 260
Lowry, T. M., 78, 132, 133, 227

- Lucas, H., 78, 131
 Lucasian Professor in Natural Philosophy, 131
- MacInnes, D. A., 202–204, 206
 Macroscopic quantum phenomenon, 98, 105
 Magnetism, 54, 94, 134, 159
 Manifesto, 218, 228
 Many-body problem, 22, 23
 Margenau, H., 203
 Massachusetts Institute of Technology (MIT),
 40, 48, 62, 87, 112–113, 141, 156, 202, 204,
 209, 211, 217, 222, 225, 228, 253
 Mathematical chemistry, 18, 113
 Mathematical equivalence, 87, 164
 Mathematical Institute, 173, 210, 253
 Mathematical Laboratory, 150, 157, 228, 253,
 254
 Mathematical physics, 27, 34, 131, 133–134,
 136, 143, 154, 157, 174, 204, 205
 Mathematical problem, 20, 164, 210
 Mathematical techniques, 132, 145, 184, 201,
 204
 Mathematical Tripos, 138
 Mathematics, 2, 5, 12–13, 34, 37, 49, 105,
 110, 122, 128, 132–134, 136, 149, 150, 154,
 158–159, 161, 164, 168, 173, 174–178, 183,
 188, 200, 205, 218, 227, 229, 249–250,
 253–254, 257, 261
 applied, 1, 3, 31, 33, 131–133, 153, 173–175,
 183–185, 210, 226–227, 229, 230, 235, 246
 in chemistry, 49, 132, 258
 role of, 49, 176, 255
 Matrix mechanics, 12–13, 17, 20
 Matsen, F. A., 221
 Mayer, J. E., 117, 203, 208
 Mayer, Maria Goeppert, 212
 Mayot, M., 190
 McCrea, W., 18, 135
 McWeeny, R., 168, 219, 227, 229–230, 260
 Mecke, R., 41
 Meckler, A., 208–209, 228
 Meeting(s), 2–3, 18, 27, 42, 56, 62, 68–69, 84,
 88, 107, 108, 121, 126, 131–133, 143–148,
 155, 172, 184, 191–192, 197, 202–204, 206,
 208–210, 212, 217–218, 230–232, 241–243,
 246, 250, 253, 260
 1928 Bunsen Gessellschaft, 108
 1923 Faraday Society, 107, 132, 133
 Meissner, W., 97
 Mendelssohn, K., 97
 Mesomerism, 78, 117, 120, 189
 Metallurgy, 114, 149
 Methane, 22–23, 62, 93, 95–96, 152, 160,
 162, 168, 205, 228
 Method(s), 7, 9, 17, 20–21, 23–24, 26, 30,
 32–33, 40, 42–43, 47, 52, 59–60, 62, 68,
 70–72, 75, 79–81, 83–86, 88, 90–93, 95–96,
 101, 103–106, 108–109, 111–112, 114–115,
 117–119, 123–125, 131–132, 134–143,
 146–151, 153–154, 158–167, 169–173,
 177–181, 184, 189, 192, 195–197, 199–205,
 208–212, 214–215, 217, 219–222, 225–226,
 229–230, 235–242, 245, 248–250, 252–253,
 259–261
 empirical, 58–59, 165
 LCAO-MO, 236
 LCAO-MO-SCF, 222
 molecular orbital, 30, 84–86, 91–93, 96, 101,
 118–119, 123–125, 146–149, 151, 161–162,
 178, 181, 195, 196, 201, 209–210
 nonempirical, 199, 210
 quantitative, 192, 196
 self-consistent field, 88, 153–154, 158, 164,
 196
 semiquantitative, 82, 202
 valence bond, 91–93, 103, 115, 118,
 124–125, 146–147, 149, 161, 165, 177,
 180–181, 196, 201
 Millikan, R. A., 94
 Milne, E. A., 134, 173, 174
 Minimizing energy, 15, 168
 MIT, 40, 48, 62, 87, 112–113, 141, 156, 202,
 204, 209, 211, 217, 222, 225, 228, 253
 Models, 6, 10, 29, 30, 51, 53, 55, 62, 78, 112,
 175, 210, 252
 Moffitt, W., 168, 204

- Molecular calculations, 136, 193, 206, 237
Molecular fields, 136–138
Molecular orbital theory, 30, 68, 75, 79, 84–86, 91–93, 96, 101, 109, 118–119, 122–125, 146–147, 149–151, 158, 160–164, 166–168, 170–171, 177–178, 181, 184, 189, 190, 192, 195–196, 201, 209–210, 220–221, 235. *See also* Method, molecular orbital
Molecular point of view, 73, 85
Molecule(s), 3–4, 6, 10–11, 16, 18–19, 21, 23, 25–26, 29–30, 32, 34, 36, 39–45, 47–49, 51–56, 58, 62, 64–81, 83–88, 90–95, 99–101, 107–109, 111, 113–115, 117–119, 121, 124–126, 128, 132–133, 135, 137, 143–153, 160–164, 166, 168–169, 171–173, 177, 188–190, 192–196, 199–202, 205–206, 208–210, 212, 215, 217–219, 222–225, 227–228, 230, 232–238, 240, 242, 247, 251–252, 254, 260
classification of, 95, 146
diatomic, 10–11, 15, 36, 40, 41–43, 46–47, 57–58, 83, 93, 144, 149, 172, 222, 223
ethylene, 124, 152
fulvene, 195, 196
heteropolar, 223, 251
 H_3 , 222
isosteric, 40–41
naphthalene, 80, 224
odd, 54, 74
polyatomic, 23, 26, 47, 58, 68, 73, 81, 83, 90, 95, 144, 146–147, 161–162, 205, 215, 237
as united atoms, 43, 44
water, 10, 66
Monk, G. S., 45
Mormann, T., 13
Mott, N., 98, 135, 154, 159, 204
Moureau, H., 190
Mulliken, R. S., 3, 6, 14, 20, 27–28, 30, 34, 36–37, 39–47, 61, 67–73, 81, 83–88, 91–95, 97–98, 100–101, 103, 125–128, 131, 141, 143–144, 151, 159, 161, 164, 167, 172, 180, 191–192, 196, 202–204, 206–208, 210–214, 216–223, 225–226, 230–231, 235, 242–243, 253, 260
Mulliken, S. P., 40
National Academy of Sciences Committee on Scientific Conferences, 202
National Physical Laboratory, 134
National Research Council, 39–40, 55, 94
National Research Council Report on the Spectra of Diatomic Molecules, 40
National Science Foundation, 217, 220, 230
National Socialist German Workers' Party, 27
Natural sciences, 2, 4, 106, 219
Nature, 41, 99, 109–110, 131, 135, 143, 154, 178
Nazi, 32, 97–98, 156
Néel, L., 208
Neon, 137–138, 160
Nernst, W., 48, 97, 249
Nesbet, R. K., 228
Networking, 3, 197–198, 218, 259, 260
New York Chapter of the National Council of Arts, Sciences and Professions, The, 121
Nitrogen, 22, 74, 106, 137, 147
Nobel prize, 17, 125, 152, 225, 231, 260
Nomenclature, 41, 133, 144, 210, 225
Nonvisualizable, 29, 120
Noyes, A. A., 48, 55–56, 87, 112, 132
Nuclear motion, 36, 40
Nuclear physics, 134, 147, 221
Numerical analysis, 141, 219, 237
Numerical solution, 140, 142, 158, 243, 245
Nikko Symposium, 196, 208, 221, 226
Ochsenfeld, R., 97
Odiot, S., 190
Office of Naval Research (ONR), 202, 220
Ohno, K., 212
Optimists, 93, 97, 201, 210, 242
Orbital(s), 10, 15, 28, 29, 36, 43, 57, 60, 62, 67, 76, 77, 83–86, 89–91, 93, 99, 101, 103, 109, 123, 128, 139, 144, 146, 149–153, 158,

- Orbital(s) (cont.)
 161, 163, 170, 172–173, 180–181, 189–190,
 194, 209, 211, 221–224, 228, 233, 235,
 237
 binuclear, 21, 57
 Gaussian type (GTO), 235
 localized, 83, 91
 molecular, 4, 6, 30, 34, 37, 39, 42–43, 58,
 60, 62, 68, 71, 75, 79, 83–86, 91, 92–93, 96,
 101, 103, 109, 114, 118, 119, 122–126, 128,
 144, 146–147, 149–153, 158, 160–168,
 170–172, 177–181, 184, 189, 190, 192,
 195–197, 199, 201, 209–210, 220, 221–222,
 235–236
 Slater type (STO), 209, 222, 228, 235, 237
 Orbital angular momentum, 36, 149
 Ordnance Board, 134
Organic Chemistry of Nitrogen, 106
 Oseen, C. W., 11
 Ostwald, W., 48, 106, 249, 258
 Overlapping, 29, 30, 63, 66, 68, 75–76, 94,
 114, 161, 167–168, 233
 Oxygen, 28, 74–75, 99, 144, 209
- Page, L., 39
 Paramagnetism, 28, 74, 85, 144
 Parameters, 89, 165, 171, 207, 210, 235, 238,
 242, 245, 247–249, 254, 258
 Pariser, R., 199, 224–226, 230–231, 237, 260
 Parr, R., 199, 202–203, 206–208, 224–226,
 230–231, 237, 260
 Parson, A. L., 51
 Pauli, W., 15–18, 20, 25, 29, 32–34, 37, 42,
 44, 54, 58–59, 70, 89, 92, 128, 135, 204
 Pauli exclusion principle, 16, 20, 34, 37, 42,
 70
 Pauling, L., 3, 4, 6, 14, 18, 20, 21, 23, 29–30,
 32, 36, 39, 47, 55–69, 73–81, 83, 85, 87–89,
 92, 94, 96–102, 104–106, 109–113,
 115–121, 123–126, 128, 131, 145, 152, 161,
 167, 177–178, 180–181, 184, 189, 191–192,
 195–196, 204, 214–216, 219, 225, 243,
 250–251, 260
 Pauli principle, 15, 17–18, 20, 25, 32–33, 44,
 58, 59, 128
 Pauncz, R., 219
 Peierls, R., 92, 154
 Periodic table, 20, 42, 46, 51, 77, 223
 Perrin, J., 188, 192, 193
Perspectives in Organic Chemistry, 118
 Perturbation, 23, 28, 36, 58, 59, 62, 79, 101,
 139, 149, 169, 238
 Pessimists, 93, 97, 210, 242
 Pfander, A., 12
 Philosophical problems, 5, 6, 255
 Philosophy, 12, 97, 106, 115, 131, 259
 Philosophy of chemistry, 5, 247, 261
 Philosophy of science, 5, 12–13
 Physical chemistry, 9, 13, 27, 30, 32, 48, 77,
 87, 106, 107, 112–114, 116, 134, 167, 168,
 192, 205, 235, 249, 250
 Physical law, 9, 33, 104
Physical Review, 61, 63, 69, 77, 79, 81, 90, 156
 Physical Society, 42, 46, 62, 88, 147, 157
 Pippard, A. B., 16
 Pitzer, K. S., 204
 Platt, J. R., 220, 222, 260
 Plummer Chair of Mathematical Physics, 134
 Polanyi, M., 191
 Polyatomic molecules, 23, 26, 47, 58, 68, 73,
 81, 83, 90, 95, 144, 146, 147, 161, 162,
 205, 237
 Polyelectronic atoms, 24, 57, 141
 Pople, J., 152, 224–229, 231, 236–237, 260
 Practices, 1, 2, 4, 113, 120, 199, 230, 232,
 235, 238, 242, 248, 253–254, 257–258, 261
 Pragmatism, 21, 65, 115, 116, 131, 252
 Prandtl, L., 26
 Primas, H., 257
 Privatdozent, 34, 56
Proceedings of the National Academy of Sciences,
 64, 207
 Professor of Mathematical Physics, 131, 157
 Pseudopotential, 32, 33
 Pullman, Alberte (née Bucher), 4, 168,
 188–193, 195–202, 218, 230, 245

- Pullman, B., 4, 188, 190–191, 193, 195–202, 212, 229, 230
- Quantization, 10, 11, 63–64, 66–68
- Quantum biochemistry, 193, 195, 197, 200, 260
- Quantum biology, 126, 217, 260
- Quantum chemistry, 1–7, 9, 12, 17–18, 25, 29, 31–34, 36–37, 39, 48, 55, 61, 65, 81, 86–87, 92–93, 96, 104–106, 108, 112, 114–116, 118–119, 121, 123, 125–129, 131–134, 143–144, 147–148, 153, 158, 160, 162, 164, 167, 171, 173, 175, 177, 180–182, 184–185, 187–193, 195–202, 204, 209–219, 221–222, 225–227, 229–235, 237–243, 245–247, 250–255, 257–261
- applications of, 252
- characteristics of, 232
- computational, 185, 228, 229
- cultures of, 187, 225
- discourse of, 239, 255
- hyperbola of, 230, 236
- nature of, 219, 233
- as a quasi-laboratory science, 219
- status of, 2, 105, 108, 123, 246
- Quantum Chemistry Group, 211–214, 216, 225, 254
- Quantum Chemistry Program Exchange (QCPE), 241
- Quantum Mechanical Calculations, 3, 9, 143, 165, 231, 241, 252
- Quantum Mechanics of Organic Molecules*, 118
- Quantum number, 25, 36, 41–45, 64, 66, 70, 72–73, 144
- Quantum theory, old, 36, 39, 43, 54–56, 94, 133, 139
- Quantum Theory of Radiation*, 98
- Quantum Theory Project, 216–217
- Ramsey, J., 257
- Randall, M., 48
- Ransil, B. J., 222, 223, 231, 235, 260
- Rauschning, H., 156
- Reductionism, 5, 104, 115, 256, 257, 258
- Relativity, 9, 12, 26, 47, 48, 134, 154
- Report of the Commission of the Institute of Organic Chemistry of the Academy of Sciences USSR, 120
- Resonance, 15, 21, 23–24, 58–60, 66, 67, 73–80, 96, 106, 110–112, 115, 117–121, 123–125, 128, 146, 149, 151, 153, 161–162, 165–167, 169–170, 173, 177, 180–182, 185, 189, 195, 231, 251
- among several valence bond structures, 80, 146
- extension of, 121
- hybrid, 124
- ontological status of, 120–121, 124, 181
- quantum mechanical, 15, 24, 75, 79, 109
- Resonance theory, 4, 6, 106, 109, 110–112, 115, 119, 121–126, 167, 180, 189, 215, 251
- arbitrary character of, 126
- extension of, 121
- manmade character of, 124
- popularization of, 106
- Reviews of Modern Physics*, 69, 218
- Rhetoric, 122, 184
- Richards, T. W., 48
- Richmond, H. W., 134
- Robertson, R., 132, 133
- Robinson, R., 30, 78
- Rockefeller Foundation, 191, 202
- Rodebush, W., 19
- Roothaan, C. C. J., 196, 203–204, 207, 219–223, 236, 260
- Roscoe, H. E., 249
- Ross, I. G., 206
- Rouse Ball Chair of Applied Mathematics, 173, 210
- Roux, M., 190
- Royal Society of London, 97, 106, 153, 170
- Rüdenberg, K., 204, 207, 222, 224
- Rule of eight, 20, 49, 52, 74
- Rumer, G., 23, 90, 102
- Rumpf, P., 190

- Rutherford, E., 50, 107, 109, 134
 Rydberg, J., 11, 41
- Sanibel Island Conferences, 216
 Saunders, F. A., 34, 40, 41
 Scerri, E., 257
 Scheler, M., 12
 Scherr, W. C., 222, 260
 Schmidt, O., 188
 Schrödinger, E., 12, 14, 16, 18, 20, 22, 24, 42, 55–57, 94, 125, 139
 Schrödinger equation, 3, 17, 19, 20, 22–33, 37, 43, 57, 62, 111, 125, 128, 140, 166, 183, 215, 228, 236
 Schützenberger, P., 249
 Schwarzschild, K., 11
 Self-consistent field, 88, 139–141, 153–154, 158, 161, 164, 194, 196, 206, 222, 224, 238
 Semiempirical, 3, 5, 7, 24, 31–33, 68, 75–76, 84, 103, 116, 126, 128, 171, 173, 199, 206, 215, 219–227, 229, 235–236, 238, 241–243 calculations, 5, 84, 206, 227, 229, 241
 Shannon, C. E., 194
 Shared electrons, 10, 55, 57, 83–84, 133, 144, 181
 Shelter Island Conference, 126, 202–206, 208–211, 221, 230
 Sherman, A., 37, 46, 93, 96–97, 160, 201, 210, 235, 242
 Sherman, J., 80
 Shortley, G. H., 90
 Shull, H., 204, 207, 212, 219, 260
 Sidgwick, N. V., 100, 106–112, 132, 133, 167
 Simon, F. E., 97
 Simplicity, 162, 181, 184, 201, 215, 233
 Simplification(s), 44, 59, 64, 66, 79, 85, 90, 150, 164, 165, 224,
 Slater, J. C., 29–31, 36, 45, 61–63, 67, 79–81, 83, 87–93, 95, 97–99, 101–102, 105, 112–115, 117, 140–141, 147, 154–156, 161, 202, 204, 206, 208–213, 216–219, 222, 225–226, 228, 230, 235, 237, 243, 253, 260
 Smiles, S., 138
 Smithells, A., 250
 Sokolov, N. D., 121
 Solid-State and Molecular Theory Group, 208–209, 216–217, 253
Some Physical Properties of the Covalent Link in Chemistry, 108, 167
 Sommerfeld, A., 11–13, 16, 27, 55–57, 94, 121
 Soviet Union, 31–33, 120
 Spectra, 10–12, 34, 36, 39–43, 46–47, 66, 68–70, 72, 84–85, 90, 93–95, 107, 126, 128, 135, 139–140, 143–146, 159, 172–173, 195, 202, 216, 219–222, 225, 231, 253
 diatomic, 40, 47
 line, 41, 94
 Spectroscopy, 10–13, 34, 36, 39, 40, 54, 112, 143
 Spherical symmetry, 36, 164
 Spin, 15–18, 20–23, 25, 28, 34, 36, 54, 56, 58, 60, 65, 70, 72, 83, 89, 90–91, 93, 99, 146, 181, 194, 210, 211, 256
 Spin theory of valence, 25, 72
 Sponer, Hertha, 34, 41, 204
 St. John's College, Cambridge, 138
 Stationary state, 110, 139, 149
 Statistical mechanics, 113–114, 134–135, 138–169
 Stein, Gertrude, 86
 Stereochemical, 29, 149
 Strong electrolytes, 26, 27, 135
 Structural formula, 21, 25, 50, 78, 109, 149, 150
 Structure(s), 9, 18, 21, 23–24, 26, 28, 30, 34, 36, 40–42, 45–50, 53–57, 67–68, 75, 77–81, 92, 95, 98, 101, 106–114, 117, 119–121, 123–127, 132–133, 138, 140–153, 155, 160, 162, 165–168, 173–175, 180, 182, 188–190, 193–194, 199–203, 206, 209, 213, 215–216, 219–222, 224–225, 227–228, 230–232, 237–238, 249, 251, 253–255
 covalent, 75, 182
 ionic, 75, 182
 Kekulé, 79–80, 117, 119, 124

- Lewis, 77–78, 110
resonance, 189
single valence bond, 78, 80, 119
Style of reasoning, 6, 7, 51, 64, 80, 86, 97, 98, 129, 209, 214, 218, 242, 246, 259
Subdiscipline, 1, 2, 4, 6–7, 81, 105, 115, 123, 127, 131, 147, 173, 177, 188, 197, 198, 199, 201, 245, 246, 252, 261
Sugiura, Y., 205, 222
Superconductivity, 23, 97, 104
Superfluidity, 23, 100, 104
Superfluids, 105
Sutton, L., 110, 167, 191, 204
Swedish Natural Science Research Council, 212–213
Swirles, Bertha, 135, 154
Symmetry, 16, 20, 22, 24, 36, 62, 140, 143, 146, 149, 158, 164, 172
Symposium on *Aspects de la Chimie Quantique Contemporaine*, 254
Syrkin, Ya., 32
- Tables of Molecular Integrals*, 208, 222, 225
Tautomerism, 50, 78, 110, 112, 117
Technische Hochschule Stuttgart, 13
Tetrahedral, 23, 62, 66–67, 81, 149, 160, 162, 168, 180
carbon, 27, 30, 63, 67
Texas Symposium, 197
Textbook(s), 2, 3, 32, 48, 105, 106, 108, 112–114, 116, 119, 122, 125, 132, 176, 178, 184, 188, 195, 197–201, 210, 214, 243, 246, 260
Cancérisation par les Substances Chimiques et Structure Moléculaire, 199, 200
General Chemistry, 119
Introduction to Chemical Physics, 105, 112–114
Introduction to Quantum Mechanics with Applications to Chemistry, 119, 251
Introduction to Theoretical Physics, 113
La Chimie Théorique et ses Rapports avec la Théorie Corpusculaire Moderne, 188
- Les Théories Électroniques de la Chimie Organique*, 199
Nature of the Chemical Bond, The, 105, 116–120, 125, 128, 132, 167, 178, 189
Partisan, 122
Quantum Biochemistry, 199, 201
Quantum Chemistry, 33, 198, 214
Quantum Mechanics of Organic Molecules, 118
Some Physical Properties of the Covalent Link in Chemistry, 108, 167
Theoretical Chemistry, 148–149, 198
Theory of Resonance and its Application to Organic Chemistry, The, 106, 122
Thermodynamics and the Free Energy of Chemical Substances, 48
Valence, 48–49, 53, 107, 132, 176–178, 181, 184, 199, 210, 229
Theorems, 25, 31, 38, 116, 145, 174, 250
Theoretical Chemistry, 1, 18, 33, 126, 131, 145, 148–150, 166, 170, 173–174, 177–178, 182–185, 187, 190–193, 196–200, 225, 227, 231, 235, 237, 239, 241–242, 250, 252, 254
Theoretical Physics, 13, 27, 31, 33–34, 39, 55, 94, 98–99, 112–114, 116, 135–136, 138, 153, 156, 169, 170, 173–174, 176, 205, 208
Theoretical Traditions, 9, 251
Theory, 4, 6, 9, 11–13, 17–27, 29–34, 36–39, 41–43, 45, 48–59, 61–62, 64, 66, 68–70, 72, 75, 78–79, 81, 83, 85, 87, 89, 90–91, 93–104, 106–126, 128, 132–137, 139–141, 143, 145–151, 153–154, 158, 160–168, 170–171, 173, 176–178, 180, 182–184, 189–192, 195, 198–199, 201, 205–206, 208–209, 211, 215–221, 224–225, 229, 235, 237–238, 242–243, 247–251, 253–258, 261
building, 4, 57, 117–118, 258
chemical, 70, 108, 115, 145, 180, 182, 247, 249, 251
descriptive, 220
Lewis's, 53, 70, 83, 101, 107

- Theory (cont.)
- magnetochemical, 54
 - molecular orbital, 68, 75, 79, 85, 109, 122, 150–151, 158, 160–164, 166–168, 171, 177, 184, 189–190, 192, 201, 220, 221, 235
 - perturbation, 59, 62, 79, 139, 149, 238
 - phenomenological, 41
 - physical, 54, 64, 108, 139, 145, 247, 249
 - role of, 5, 247, 253, 255, 261
 - qualitative, 119
 - quantitative, 220
 - semiempirical, 220
 - structure/al, 21, 108–109, 111, 119, 122–126, 128, 184, 251, 255,
 - valence, 18–19, 25, 42, 45, 48, 50, 55, 68–73, 75, 78, 81, 83–85, 93, 95–96, 101, 103, 107, 109, 118, 128, 132–133, 145–147, 176–177, 202, 206, 251
- Theory of Atomic Spectra, The*, 90
- Theory of Electric and Magnetic Susceptibilities, The*, 94
- Theory of Resonance and its Application to Organic Chemistry, The*, 106, 122
- Theory of Spectra and Atomic Constitution*, 107
- Thermodynamics and the Free Energy of Chemical Substances*, 48
- Thomson, J. J., 49–51, 132, 249
- Thought forms, 1, 2, 6, 234, 261
- Tiselius, A., 213
- Tolman, R., 87
- Townes, C. H., 208
- Trinity College, Cambridge, 133–134, 136, 159, 160
- Triplet State, 28, 209
- Ufford, C. W., 204
- Ultraviolet, 11, 28, 144, 161
- University, 3, 11–13, 16–17, 27, 31, 37, 45, 61, 93, 94, 107, 138, 143, 158, 164–165, 168, 170, 173, 175, 190, 196, 204–205, 207, 212–213, 216–217, 220–222, 224, 228, 233, 246, 253
- American, 40
- of Bristol, 98, 136, 143, 158
- of California at Berkeley, 19, 39, 48, 51
- of California at Los Angeles, 122
- of Cambridge, 131, 138, 148, 159, 170, 222, 227, 253
- of Chicago, 39, 40, 45, 122, 202, 206, 221–223
- of Chicago Computation Center, 221
- Cornell, 108, 116, 254
- of Florida, 213, 216
- of Frankfurt, 34
- of Gottingen, 12, 26, 34, 136
- Harvard, 39, 48, 121, 215
- of Jena, 34
- Johns Hopkins, 45
- of Kiel, 31
- of Leipzig, 27
- of London, 121, 169, 176
- of Manchester, 55, 136, 142, 153
- of Marburg, 27
- of Michigan, 39
- of Munich, 12–13
- of Nebraska, 48
- New York, 39, 40, 45
- of Oxford, 1, 106, 168, 182, 210
- of Rostock, 34
- of Tokyo, 205
- Tokyo Imperial, 204
- of Uppsala, 1, 204, 213–214, 253
- of Utrecht, 135
- Yale, 39, 50
- of Zurich, 12
- Unshared electrons, 57, 75, 83, 144
- U. S. Air Force, 213
- U. S. military agencies, 213
- Usefulness, 65, 68, 79, 117–118, 126, 167, 182, 199, 249
- Valadalen Summer School, 126, 214
- Valence, 1, 4, 6, 19–25, 28–30, 32, 36–37, 40–42, 45, 47–50, 52–55, 59, 61–62, 65, 67–73, 75, 78–81, 83–85, 87–88, 90–93,

- 95–96, 99–103, 107, 109, 114–115, 117–119, 121, 123–125, 128, 131–133, 143–147, 149–151, 160–162, 164–165, 168, 171–172, 176–178, 180–181, 184, 189–190, 192–193, 195–196, 199, 201–202, 206, 210, 229, 235, 251
contra, 50
directed, 63, 67, 81, 149, 151
normal, 50
saturation, 18
Valence and the Structure of Atoms and Molecules, 48, 107, 132
Valence bond (VB) method, 91–93, 103, 115, 118, 124–125, 146–147, 149, 161, 165, 177, 180–181, 196, 201
Van der Waals forces, 14–16, 25, 145
Van't Hoff, J., 29–30, 149, 247–249
Van Vleck, J. H., 18, 20, 36–37, 46, 62, 81, 84–85, 87–90, 93–98, 100, 102, 128, 160, 162–163, 201, 204, 208, 210, 217, 235, 242–243, 260
Variational method, 140, 149, 163, 171
Veterinary College, Hannover, 31
Visualizability, 13, 19, 25, 29, 120, 129, 177, 232–233, 258
- Waller, I., 208, 213
Watson, J., 200
Wave function, 15–17, 20–21, 59–60, 62–63, 66, 68, 76, 79, 85, 89–92, 97, 139–141, 149, 152, 157–158, 161, 163–164, 171, 177, 180, 189, 202, 211, 217, 222–225, 227, 233–234, 236, 252
Wave mechanics, 24, 37, 56, 92, 104, 109, 111–112, 114, 135, 139, 145, 149, 150, 176
Weizmann, C., 195, 197
Wentzel, G., 56, 94, 222
Werner, A., 67, 149
Weyl, H., 17, 23, 88, 141
Wheeler, B. I., 48
Wheland, G. W., 79, 80, 101, 106, 118, 120–124, 178, 195, 204
Whittaker, J. M., 135
- Wiener, N., 88
Wigner, E., 22, 23, 86, 89, 90, 92, 141
Wilkes, M. V., 157, 228
Wilson, A. H., 135
Wilson, C. T. R., 154
Wilson, E. B., 18, 116, 207, 214, 251, 252
Wood, R. W., 45
- Zeitschrift für Physik*, 56, 136
- We thank Antonia Pavli for help with the index.