

Glossary of Symbols and Abbreviations

Mathematical notation

\exists	there exists
\forall	for all
$\{x P\}$	the set of elements x having the property P
$x \in X$	x is an element of the set X
$A \subset B$	A is a subset (subgroup) of the set (group) B
$A \triangleleft B$	A is an invariant subgroup of the group B
$a_i b_i \equiv \sum_i a_i b_i$	Summation convention for repeated indices i, j, k, \dots
ϵ_{ijk}	Antisymmetric unit tensor: $\epsilon_{ijk} = +1$ if $(ijk) = (xyz)$ or any cyclic permutation thereof; $\epsilon_{ijk} = -1$ if $(ijk) = (yxz)$ or any cyclic permutation thereof; $\epsilon_{ijk} = 0$ otherwise.
$(a \wedge b)_i = \epsilon_{ijk} a_j b_k$	vector product

Abbreviations:

NRM	Nonrigid molecule
SRMM	Semirigid molecular model
IR	Irreducible representation
PI	Permutation - inversion
CNPI	Complete nuclear permutation - inversion
PPT	Primitive period transformation

References

1. Longuet-Higgins, H.C., 1963, *Molec. Phys.*, 6, 445.
2. Buck, B., Biedenharn, L.C., & Cusson, R.Y., 1979, *Nucl. Phys.*, A317, 205.
3. Sutcliffe, B.T., 1979, Lectures presented at NATO ASI 'Quantum Dynamics of Molecules', Cambridge, England.
4. Makushkin, Yu. S., & Ulenikov, O.N., 1977, *J. Mol. Spec.*, 68, 1.
5. Sørensen, G.O., 1979, *Topics in Current Chemistry*, 82, 99.
6. Wilson, E.B., Decius, J.C., & Cross, P.C., 1955, *Molecular Vibrations* (McGraw-Hill).
7. Louck, J.D., 1976, *J. Mol. Spec.*, 61, 107.
8. Meyer, R., & Gunthard, Hs. H., 1968, *J. Chem. Phys.*, 49, 1510.
9. Eckart, C., 1935, *Phys. Rev.*, 47, 552.
10. Sayvetz, A., 1939, *J. Chem. Phys.*, 7, 383.
11. Judd, B.R., 1975, *Angular Momentum Theory for Diatomic Molecules* (Academic).
12. Husson, N., 1975, *Annls Phys.*, 9, 271.
13. Meyer, F.O., & Redding, R.W., 1978, *J. Mol. Spec.*, 70, 410.
14. Hilico, J.-C., Berger, H., & Loete, M., 1976, *Can. J. Phys.*, 54, 1702.
15. Pascaud, E., & Poussigue, G., 1978, *Can. J. Phys.*, 56, 1577.
16. Gulshani, P., 1979, *Can. J. Phys.*, 57, 998.
17. Louck, J.D., & Galbraith, H.W., 1976, *Rev. Mod. Phys.*, 48, 69.
18. Nielsen, H.H., 1951, *Rev. Mod. Phys.*, 23, 90.
19. Howard, B.J., & Moss, R.E., 1970, *Mol. Phys.*, 19, 433.
20. Born, M., & Oppenheimer, R., 1927, *Ann. Physik*, 84, 457.
- 20a. Kiselev, A.A., 1978, *Can. J. Phys.*, 56, 615.
21. Özkam, I., & Goodman, L., 1979, *Chem. Rev.*, 79, 275.
22. Jørgensen, F., & Pedersen, T., 1974, *Mol. Phys.*, 27, 33.
23. Pedersen, T., 1978, Unpublished Report, University of Copenhagen.
24. Podolsky, B., 1928, *Phys. Rev.*, 32, 812.
25. Wilson, E.B., & Howard, J.B., 1936, *J. Chem. Phys.*, 4, 260.
26. Watson, J.K.G., 1968, *Mol. Phys.*, 15, 479.
27. Watson, J.K.G., 1970, *Mol. Phys.*, 19, 465.
28. Whittaker, E.T., 1929, *Analytical Dynamics* (Cambridge).
29. Malhiot, R.J., & Ferigle, S.M., 1954, *J. Chem. Phys.*, 22, 717.
30. Herold, H., & Ruder, H., 1974, *J. Phys.*, G5, 341.
31. Woolley, R.G., 1976, *Adv. Phys.*, 25, 27.
32. Woolley, R.G., 1978, *J. Am. Chem. Soc.*, 100, 1073.
33. Woolley, R.G., 1979, *Israel J. Chem.*, 18, No. 4.
34. Dalton, B.J., & Nicholson, P.D., 1975, *Int. J. Quant. Chem.*, 9, 525.
35. Liehr, A.D., 1963, *Prog. Inorg. Chem.*, 5, 385.
36. Goldstein, H., 1950, *Classical Mechanics* (Addison-Wesley).
37. Gulshani, P., & Rowe, D.J., 1976, *Can. J. Phys.*, 54, 970.
38. Peric, M., 1977, *Mol. Phys.*, 34, 1675.
39. Natanson, G.A., & Adamov, M.N., 1974, *Vest. Leningr. Univ.*, No. 10, 24; Jørgensen, F., 1978, *Int. J. Quant. Chem.*, 24, 55.
40. Quade, C.R., 1976, *J. Chem. Phys.*, 64, 2783.
41. Hoy, A.R., Mills, I.M., & Strey, G., 1972, *Mol. Phys.*, 24, 1265.
42. Barakat, R., 1979, *Mol. Phys.*, 38, 1655.
43. Kroto, H.W., 1975, *Molecular Rotation Spectra* (Wiley).
44. Essen, H., 1978, *Am. J. Phys.*, 46, 983.
45. Jørgensen, F., 1978, Thesis, University of Copenhagen.
46. Rowe, D.J., & Rosensteel, G., 1979, *J. Math. Phys.*, 20, 465.
47. Casimir, H.B.G., 1931, *Rotation of a Rigid Body in Quantum Mechanics* (Walters).
48. Bauder, A., Meyer, R., & Gunthard, Hs. H., 1974, *Mol. Phys.*, 28, 1305.
49. Ezra, G.S., 1979, *Mol. Phys.*, 38, 863.
50. Hougen, J.T., Bunker, P.R., & Johns, J.W.C., 1970, *J. Mol. Spec.*, 34, 136.
51. Hougen, J.T., 1964, *Can. J. Phys.*, 42, 1920.
52. Hougen, J.T., 1965, *Can. J. Phys.*, 43, 935.
53. Bunker, P.R., 1967, *J. Chem. Phys.*, 47, 718.
54. Papousek, D., & Spirko, V., 1976, *Topics Current Chem.*, 68, 59.
55. Russeger, P., & Brickmann, J., 1975, *J. Chem. Phys.*, 62, 1086.

56. Gilles, J.M.F., & Philippot, J., 1972, *Int. J. Quant. Chem.*, 6, 225.
57. Kreglewski, M., 1978, *J. Mol. Spec.*, 72, 1.
58. Hougen, J.T., & Redding, R.W., 1971, *J. Mol. Spec.*, 37, 366.
59. Sarka, K., 1971, *J. Mol. Spec.*, 29, 66.
60. Bauder, A., & Gunthard, Hs. H., 1976, *J. Mol. Spec.*, 60, 290.
61. Berry, R.S., 1979, Lectures presented at NATO ASI 'Quantum Dynamics of Molecules', Cambridge, England.
62. Abraham, F.F., 1974, *Homogeneous Nucleation Theory* (Academic).
63. Kendrick, J., & Hillier, I.H., 1977, *Mol. Phys.*, 33, 635.
64. Martin, R.L., & Davidson, E.R., 1978, *Mol. Phys.*, 35, 1713.
- 64a. Gerber, W.H., & Schumacher, E., 1978, *J. Chem. Phys.*, 69, 1692.
65. Berry, R.S., 1960, *J. Chem. Phys.*, 32, 933.
66. Whitesides, G.M., & Mitchell, H.L., 1969, *J. Am. Chem. Soc.*, 91, 5384.
67. Berry, R.S., *Personal Communication*.
68. Dalton, B.J., 1966, *Mol. Phys.*, 11, 265.
69. Dalton, B.J., 1971, *J. Chem. Phys.*, 54, 4745.
70. Brocas, J., & Fastenakel, D., 1975, *Mol. Phys.*, 30, 193; Dalton, B.J., Brocas, J., & Fastenakel, D., 1976, *Mol. Phys.*, 31, 1887; Fastenakel, D., & Brocas, J., 1980, *Mol. Phys.*, 40, 361; Brocas, J., Fastenakel, D., and Buschen, J., 1980, *Mol. Phys.*, 41, 1163.
71. Trindle, C., Data, S.N., & Bouman, T.D., 1977, *Int. J. Quant. Chem.*, 11, 627.
72. Curtiss, C.F., Hirschfelder, J.O., & Adler, F.T., 1950, *J. Chem. Phys.*, 18, 1638.
73. Eckart, C., 1934, *Phys. Rev.*, 46, 384.
74. Van Vleck, J.H., 1935, *Phys. Rev.*, 47, 487.
75. Bohr, A., 1976, *Rev. Mod. Phys.*, 48, 365.
76. Fabre de la Ripelle, M., & Navarro, J., 1979, *Ann. Phys.*, 123, 185.
77. Kramer, P., & Moshinsky, M., 1968, *in Group Theory and its Applications*, Vol. I, edited by E.M. Loebl (Academic).
78. Smirnov, Yu. F., & Shitikova, K.V., 1977, *Sov. J. Part. Nucl.*, 8, 344.
79. Bosanac, S., & Murrell, J.N., 1973, *Mol. Phys.*, 26, 349.
80. Wallace, R., 1979, *Chem. Phys.*, 37, 93.
81. Kellmann, M.E., & Berry, R.S., 1976, *Chem. Phys. Lett.*, 42, 327.
82. Amar, F., Kellmann, M.E., & Berry, R.S., 1979, *J. Chem. Phys.*, 70, 1973; Amar, F., Kellmann, M.E., & Berry, R.S., 1980, *J. Chem. Phys.*, 73, 2387; Ezra, G.S., & Berry, R.S., 1981, *J. Chem. Phys.*, to be published.
83. Harter, W.G., Patterson, C.W., & da Paixao, F.J., 1978, *Rev. Mod. Phys.*, 50, 37.
84. Wigner, E.P., 1930, *Nachr. Ges. Wiss. Göttingen*, page 133; Brestler, C.J., 1923, *Dissertation* (Utrecht).
85. Herzberg, G., 1945., *Infrared and Raman Spectra of Polyatomic Molecules* (Van Nostrand).
86. Wilson, E.B., 1934, *J. Chem. Phys.*, 2, 432.
87. Wilson, E.B., 1935, *J. Chem. Phys.*, 3, 276.
88. Wilson, E.B., 1935, *J. Chem. Phys.*, 3, 818.
89. Hougen, J.T., 1962, *J. Chem. Phys.*, 37, 1433.
90. Hougen, J.T., 1963, *J. Chem. Phys.*, 39, 358.
91. Hougen, J.T., 1971, *J. Chem. Phys.*, 55, 1122.
92. Hougen, J.T., 1975, *MTP International Review of Science*, Vol. 3 (Physical Chemistry Series 2), page 75.
93. Mills, I.M., 1964, *Mol. Phys.*, 7, 549.
94. Bunker, P.R., & Papousek, D., 1969, *J. Mol. Spec.*, 32, 419.
95. Oka, T., 1973, *J. Mol. Spec.*, 48, 503.
96. Bunker, P.R., 1975, *Vibrational Spectroscopy and Structure*, Vol. 3, edited by J.R. Durig (Marcel Dekker).
97. Bunker, P.R., 1979, *Molecular Symmetry and Spectroscopy* (Academic).
98. Moret-Bailly, J., 1965, *Cahier Phys.*, 178, 253.
99. Moret-Bailly, J., 1974, *J. Mol. Spec.*, 50, 483.
100. Hougen, J.T., 1974, *J. Mol. Spec.*, 50, 485.
101. Jahn, J.A., 1938, *Proc. R. Soc. A*, 168, 469.
102. Michelot, F., Bobin, B., & Moret-Bailly, J., 1979, *J. Mol. Spec.*, 76, 374.
103. Cantrell, C.D., 1976, *in Physics of Quantum Electronics*, Vol. 4 (Addison-

- Wesley).
104. Cantrell, C.D., & Galbraith, H.W., 1975, *J. Mol. Spec.*, 58, 158.
 105. Berger, H., 1977, *J. de Phys.*, 38, 1371.
 106. Fano, U., & Chang, E.S., 1972, *Phys. Rev.*, A6, 173.
 107. Harter, W.G., & Patterson, C.W., 1976, *A Unitary Calculus for Electronic Orbitals*, Lecture Notes in Physics 49 (Springer Verlag).
 108. Lathouwers, L.L., 1978, *Phys. Rev.* A18, 2150.
 109. Herzberg, G., 1950, *Spectra of Diatomic Molecules* (Van Nostrand).
 110. Townes, C.H., & Schawlow, A.L., 1955, *Microwave Spectroscopy* (McGraw-Hill).
 111. Pfeifer, P., 1979, Preprint ETH-Zurich.
 112. Gilles, J.M.F., & Philippot, J., 1978, *Int. J. Quant. Chem.*, 14, 299.
 113. Flurry, R.L., & Siddall, T.H., 1978, *Mol. Phys.*, 36, 1309.
 114. Pack, R.T., & Hirschfelder, J.O., 1968, *J. Chem. Phys.*, 49, 4009.
 115. Wigner, E.P., 1959, *Group Theory* (Academic).
 116. Watson, J.K.G., 1967, *J. Chem. Phys.*, 46, 1935.
 117. Levy-Leblond, J.M., 1971, *in* *Group Theory & its Applications*, Vol. 2, edited by E.M. Loeb1 (Academic).
 118. Watson, J.K.G., 1965, *Can. J. Phys.*, 43, 1996.
 119. Herzberg, G., 1966, *Electronic Spectra and Electronic Structure* (Van Nostrand).
 120. McWeeny, R., 1963, *Symmetry* (Pergamon).
 121. Butler, P.R., 1975, *Phil. Trans. R. Soc.*, 277, 545.
 122. Bunker, P.R., 1973, *J. Mol. Spec.*, 48, 181.
 123. Altmann, S.L., 1967, *Proc. R. Soc. A*, 298, 184.
 124. Altmann, S.L., 1971, *Mol. Phys.*, 21, 587.
 125. Altmann, S.L., 1977, *Induced Representations in Crystals and Molecules* (Academic).
 126. Natanson, G., 1976, *Opt. Spectrosc.*, 41, 18.
 127. Dellepiane, G., Gussoni, M., & Hougen, J.T., 1973, *J. Mol. Spec.*, 47, 515.
 128. Watson, J.K.G., & Merer, A.J., 1973, *J. Mol. Spec.*, 47, 499.
 129. Dyke, T.R., Howard, B.J., & Klemperer, W.A., 1972, *J. Chem. Phys.*, 56, 2442.
 130. Dyke, T.R., 1977, *J. Chem. Phys.*, 66, 492.
 131. Quack, M., 1977, *Mol. Phys.*, 34, 477.
 132. Metropoulos, A., & Chiu, Y-N., 1978, *J. Chem. Phys.*, 68, 5607.
 133. Hougen, J.T., 1965, *Pure Appl. Chem.*, 11, 481.
 134. Frei, H., Meyer, R., Bauder, A., & Gunthard, Hs. H., 1976, *Mol. Phys.*, 32, 43.
 135. Frei, H., Groner, P., Bauder, A., & Gunthard, Hs. H., 1978, *Mol. Phys.*, 36, 1469.
 136. Stone, A.J., 1964, *J. Chem. Phys.*, 41, 1568.
 137. Watson, J.K.G., 1971, *Mol. Phys.*, 21, 577.
 138. Woodman, C.M., 1970, *Mol. Phys.*, 19, 753.
 139. Serre, J., 1968, *Int. J. Quant. Chem.*, 2S, 107.
 140. Serre, J., 1974, *Adv. Quantum Chem.*, 8, 1.
 141. Wilson, E.B., Lin, C.C., & Lide, D.R., 1955, *J. Chem. Phys.*, 23, 136.
 142. Natanson, G.A., & Adamov, M.N., 1974, *Vestn. Leningr. Gos. Univ. No. 4*, 22.
 143. Fleming, J.W., & Banwell, C.N., 1969, *J. Mol. Spec.*, 31, 378.
 144. Turrel, G., 1970, *J. Mol. Struct.*, 5, 245.
 145. Nourse, J.G., & Mislow, K., 1975, *J. Am. Chem. Soc.*, 97, 4571.
 146. McIntosh, H., 1960, *J. Mol. Spec.*, 5, 269.
 147. McIntosh, H., 1963, *J. Mol. Spec.*, 10, 51.
 148. Dreizler, H., 1968, *Fortchr. Chem. Forsch.*, 10, 59.
 149. Natanson, G.A., & Adamov, M.N., 1970, *Vestn. Leningr. Univ. No. 4*, 50.
 150. Gunthard, Hs.H., Bauder, A., & Frei, H., 1979, *Topics in Current Chemistry*, 81, 7.
 151. Balasubramanian, K., 1980, *J. Chem. Phys.*, 72, 665.
 152. Coxeter, H.S.M., & Moser, W.O.J., 1972, *Generators and Relations for Discrete Groups* (Springer).
 153. Magnus, W., Karrass, A., & Solitar, D., 1976, *Combinatorial Group Theory* (Dover).
 154. Natanson, G.A., 1979, *Opt. Spectrosc.*, 47, 137.
 155. Bunker, P.R., 1965, *Mol. Phys.*, 9, 257.
 156. Bunker, P.R., 1964, *Mol. Phys.*, 8, 81.

157. Bunker, P.R., 1965, *Mol. Phys.*, 9, 247.
158. Hamada, Y., Hirawaka, A.Y., Tamagake, K., & Tsuboi, M., 1970, *J. Mol. Spec.*, 35, 420.
159. Flurry, R.L., 1975, *J. Mol. Spec.*, 56, 88.
160. Flurry, R.L., & Abdulnur, S.F., 1976, *J. Mol. Spec.*, 63, 33.
161. Littlewood, D.E., 1950, *The Theory of Group Characters* (Oxford, Clarendon).
162. Wallace, R., 1979, *Chem. Phys.*, 37, 285.
163. Gust, D., & Mislow, K., 1973, *J. Am. Chem. Soc.*, 95, 1353.
164. Bunker, P.R., 1979, *Lecture Notes in Chemistry*, 12, 38.
165. Brink, D.M., & Satchler, G.R., 1968, *Angular Momentum* (Clarendon).
166. Rose, M.E., 1957, *Elementary Theory of Angular Momentum* (Wiley).
167. Dirac, P.A.M., 1958, *The Principles of Quantum Mechanics* (Clarendon).
168. Van Vleck, J.H., 1951, *Rev. Mod. Phys.*, 23, 213.
169. Howard, B.J., & Brown, J.M., 1976, *Mol. Phys.*, 31, 1517.
170. McIntosh, H.V., 1971, *in Group Theory and its Applications*, Vol. 2, edited by E.M. Loebel (Academic).
171. Stone, A.J., 1975, *Mol. Phys.*, 29, 1461.
172. Fox, K., & Ozier, I., 1970, *J. Chem. Phys.*, 52, 5044.
173. Mead, C.A., 1974, *Topics in Current Chemistry*, 49, 1.
174. Altmann, S.L., 1963, *Phil. Trans. R. Soc.*, A255, 216.
175. Bradley, C.J., & Cracknell, A.P., 1972, *The Mathematical Theory of Symmetry in Solids* (Clarendon).
176. Fritzer, H.P., 1976, *Lecture Notes in Physics*, 50, 348.
177. Fritzer, H.P., 1979, *in Recent Advances in Group Theory and their Applications to Spectroscopy*, edited by J.C. Donini (Plenum: NATO ASI series).
178. Metropoulos, A., & Chiu, Y-N., 1979, *Chem. Phys.*, 42, 61.
179. Klein, D.J., 1975, *in Group Theory and its Applications*, Vol. 3, edited by E.M. Loebel (Academic).
180. Seligman, T.H., 1979, *Lecture Notes in Chemistry*, 12, 178.
181. Louck, J.D., 1979, *Lecture Notes in Chemistry*, 12, 57.
182. Dress, A., 1979, *Lecture Notes in Chemistry*, 12, 77.
183. Natanson, G.A., & Adamov, M.N., 1976, 'New Aspects in the Symmetry Theory of Polyatomic Molecules' (Translated from *Fiz. Molek. (USSR)*, Los Alamos translation LA-TR-77-32); Natanson, G.A., 1978, *Fiz. Molek. (USSR)*, No. 6, 3.
184. Ezra, G.S., 1981, *Mol. Phys.*, 43, 773.
185. Frei, H., Bauder, A., & Gunthard, Hs.H., 1981, *Mol. Phys.*, 43, 785.
186. Melvin, M., 1956, *Rev. Mod. Phys.*, 28, 18.
187. Boyle, L.L., & Walker, J.R., 1977, *Int. J. Quant. Chem.*, 12 S2, 157.
188. Odutola, J.A., Alvis, D.L., Curtis, C.W., & Dyke, T.R., 1981, *Mol. Phys.*, 42, 267.
189. Ezra, G.S., 1981, Submitted for publication.
190. Weber, A., 1980, *J. Chem. Phys.*, 73, 3952.
191. Renkes, G.D., 1981, *Chem. Phys.*, 57, 261.

M. F. O'Dwyer, J. E. Kent, R. D. Brown

Valency

Heidelberg Science Library

2nd edition. 1978. 150 figures. XI, 251 pages

ISBN 3-540-90268-6

Distribution rights for Australia and
New Zealand: Holt-Saunders PTY. Ltd.,
Artarmon, N.S.W.

Contents: Gross Atomic Structure. –
Atomic Theory. – Many-Electron Atoms. –
Molecular Theory and Chemical Bonds. –
The Solid State. – Experimental Methods of
Valency.

This textbook is designed for use by advanced first year freshman chemistry students as well as physical chemistry students in their sophomore and junior years. It covers SI units and the concept of energy, and the structure and theory of atoms, using wave mechanics and graphs to define atomic orbitals and the meaning of quantum numbers, for both hydrogen atoms as well as many-electron atoms. Periodic trends such as ionization and orbital energies are emphasized and explained through atomic theory.

The book also covers molecular theory and the chemical bond using a model approach. Electrostatic models for ionic compounds and transition metal complexes and a molecular orbital are included together with valencebond and Sidgwick-Powell models for covalent compounds. Problems and appendices are provided to enable readers to deepen their comprehension of the subject.



Springer-Verlag
Berlin
Heidelberg
New York

THEORETICA CHIMICA ACTA

an International Journal
of Theoretical Chemistry

ISSN 0040-5744

Title No. 214

Edenda curat: Hermann Hartmann, Mainz

Adiuvantibus: R. D. Brown, Clayton; K. Fukui, Kyoto;
R. Gleiter, Heidelberg; F. Grein, Fredericton;
E. A. Halevi, Haifa; G. G. Hall, Nottingham;
M. Kotani, Tokyo; A. Neckel, Wien; E. E. Nikitin,
Moskwa; H. Primas, Zürich; B. Pullman, Paris;
E. Ruch, Berlin; K. Ruedenberg, Ames; C. Sandorfy,
Montreal; M. Simonetta, Milano; A. Veillard, Straß-
bourg; R. Zahradník, Praha

Today, theory and experiment are inseparably bound. Every chemical experiment is preceded by reflection and careful consideration, and the results are interpreted according to chemical theories and perceptions.

The editors of **Theoretica Chimica Acta** therefore wish to emphasize the wide-ranging program reflected in the policy of their journal:

“**Theoretica Chimica Acta** accepts manuscripts in which the relationships between individual chemical and physical phenomena are investigated. In addition, experimental research that presents new theoretical viewpoints is desired.”

Theoretica Chimica Acta offers experimental chemists increased space for the publication of discussion of the goals of their work, the significance of their findings, and the concepts on which their experimental work is based. Such discussions contribute significantly to mutual understanding between theoreticians and experimentalists and stimulate both new reflections and further experiments.

Subscription information and/or sample copies available upon request. Please send your order or request to Springer-Verlag, Journal Promotion Department, P. O. Box 105280, D-6900 Heidelberg 1, FRG



Springer
International
