

SUBJECT INDEX

- Alkali-halide dimer structure 23
Asymmetric Tunnelling 68, **84**, 93
- Barrier heights 7, 16, 24, 72, 93, **104**, 105, 109, 116, 117, 118
Barrier to pseudorotation 196
Bending in two rotor molecules 134, 138, 142, 145, 147
Brønsted coefficient **104**, 105, 106, 114, 118
- Carbocation structure **9**
Cyanide structure **19**, 24
Collisional fine structure 237
Concept of feasibility **72**
Conformational dependence 98, 116, 118
Conformational functions **102**
- Deltahedron **159**, 161, 162, 163, 164
Deltahedron deformations **164**
Double rotation plus bending mode **134**, **138**, **145**, **147**
Double rotation plus torsion mode **139**, **147**
Double rotation plus wagging mode **135**, **145**
dsd mechanism 153, **159**, 162, 166, 167, 169, 174, 176, 177, 178
dsd invariant isomers 170, 171, 177, 178, 179
dsd non-invariant isomers 170, 171, 177
Dynamic NMR 153, 163
Dynamic stereochemistry 156
Dynamics of non-linear coupled oscillators 250, 251, 259
- Eckart-Sayvetz coordinates **48**, 49, 51, 57, 59, 60, 63
Electronic predissociation 204, **234**, **237**, 238, 239, 240
Energy redistribution 204, 216, 250
Energy transfer 250
- Feasibility 68, **72**
- Fermi resonance 266
Floppy molecules (see Non-rigid molecules)
Full Nonrigid Molecule Groups **124**
Fundamental Fermi resonance 264
Fundamental Fermi vectors 266
- Generalized valley approximation 53, 54, 56
- Half-collision 237, 238
Heptacoordinate complexes 153, 155, 160, 168
Heptacoordinate stereochemistry 153, 159
- Inorganic complexes **18**, 26, 31, 34, 39, 41
Internal resonances 250
Internal rotation 7, 9, 13, 62, 92, 98, 100, 102, 113, 118, 122, 127
Intrinsic internal paths 48, 53, 55, 63
Intramolecular relaxation 204
Intramolecular dynamics 203
Intramolecular energy redistribution 250
- Large amplitude displacement variables 75
Large amplitude internal variables 48, 53, 57, 58, 59, 60, 61, 62, 63
Large amplitude motion 8, 9, 37, 53, 54, 68, 93, 121, 124
Large amplitude oscillations 251
Least square bond lengths 58
Least square large amplitude internal variables 58, 59, 60
Lifetime 2, 3, 205, 207, 213, 214, 315
Linewidths 205, 213, 214, 215, 217, 219, 220
Local potential **102**, 104
Longuet-Higgins theory 3, 5, 67, 68, 72, 122, 123, 124, 133, 150
- Metal hydride complex structure 23
Molecular Symmetry Groups 6, 68, **72**, 122, 150

- Monorotor molecules (see Single Rotor Molecules)
- Non-deltahedron deformations **164**
- Non-rigid Molecules **3, 8, 9, 18, 23, 42, 47, 53, 67, 93, 121, 122, 126, 150**
- Non-rigid Molecule Groups **68, 75, 121, 122, 123, 126**
- Non-resonant Fermi vector **250, 263, 266, 276, 293**
- Normal vibrations **47, 60, 61, 62, 63**
- Permutation groups **4, 69, 154, 156**
- Permutation-Inversion groups **4, 5, 59, 61, 62, 63, 67, 69, 122, 123, 133, 154, 156**
- Permutational analysis **153, 154, 160**
- Photofragmentation **204**
- Photodissociation **234, 236**
- Potential energy functions **98, 106, 117, 127, 129, 132, 193, 194, 198, 199, 204**
- Potential energy operators **75, 124, 127**
- Potential energy surfaces **8, 25, 69, 73, 76, 85, 123, 196**
- Reaction path **50, 78, 79, 81, 157**
- Restricted Non-rigid Molecule Groups **124, 125, 129**
- Resonance surfaces **250, 254, 256, 257, 304**
- Resonance widths **251, 285, 305**
- Resonant Fermi vector **250, 263, 264, 265, 293, 297**
- Ring puckering **50, 123, 181, 183, 185, 186, 187, 188**
- Ring puckering in cycloalkane ketones **185, 186, 187, 188**
- Ring puckering potential energy functions **186, 189**
- Rotational contours **189**
- Rotational isomerism **98, 99**
- Rotational predissociation **204, 218, 219, 225, 227**
- Single rotor molecules **98, 102, 118, 127**
- Semirigid model **2, 23, 50, 55, 60, 62**
- Stationary states **2, 70**
- Sub-resonances **251, 252, 259, 264, 290, 295, 299, 301**
- Sub-resonant coupling **260, 274**
- Sub-resonant Fermi vectors **266**
- Super-resonances **263**
- Super-resonant Fermi vectors **266, 293**
- Symmetry eigenvectors **121, 128, 129, 131, 133, 137, 139, 140, 141, 143, 144, 148**
- Torsional force constants **98, 111, 113, 118**
- Torsional potential energy curves **110, 112, 115, 117**
- Torsion in two rotor molecules **139, 147**
- Trajectory **52, 53, 212, 213, 229, 235, 269, 270, 271, 272, 273, 274, 275, 293, 299, 304**
- Transition states (TS) **10, 76, 78, 79, 80, 86, 87, 157, 158, 168**
- Tunnelling **35, 51, 67, 71, 72, 73, 76, 84**
- Tunnelling splitting **13, 30, 71, 72, 84, 85**
- Two rotor Molecules **128**
- van der Waals complexes **214, 218, 234, 237, 240**
- Vibrational predissociation **204, 228, 214, 215, 216, 226, 228**
- Wagging in cycloalkane ketones **193, 194, 200**
- Wagging in two rotor molecules **135, 145**

TOPICS IN
MOLECULAR ORGANIZATION AND ENGINEERING

Honorary Chief Editor: W. N. Lipscomb, Harvard, U.S.A.

Executive Editor: Jean Maruani, Paris, France

1. J. Maruani (ed.): *Molecules in Physics, Chemistry, and Biology*.
Vol. 1: General Introduction to Molecular Sciences. 1988
ISBN 90-277-2596-9
2. J. Maruani (ed.): *Molecules in Physics, Chemistry, and Biology*.
Vol. 2: Physical Aspects of Molecular Systems. 1988
ISBN 90-277-2597-1
3. J. Maruani (ed.): *Molecules in Physics, Chemistry, and Biology*.
Vol. 3: Electronic Structure and Chemical Reactivity. 1989
ISBN 90-277-2598-5
4. J. Maruani (ed.): *Molecules in Physics, Chemistry, and Biology*.
Vol. 4: Molecular Phenomena in Biological Sciences. 1989
ISBN 90-277-2599-3
5. E. Schoffeniels and D. Margineanu: *Molecular Basis and Thermodynamics of Bioelectrogenesis*. 1990
ISBN 0-7923-0975-8
6. A. Lund and M. Shiotani (eds.): *Radical Ionic Systems. Properties in Condensed Phases*. 1991
ISBN 0-7923-0988-X
7. P.I. Lazarev (ed.): *Molecular Electronics. Materials and Methods*. 1991
ISBN 0-7923-1196-5
8. E. Rizzarelli and T. Theophanides (eds.): *Chemistry and Properties of Biomolecular Systems*. 1991
ISBN 0-7923-1393-3
9. L.A. Montero and Y.G. Smeyers (eds.): *Trends in Applied Theoretical Chemistry*. 1992
ISBN 0-7923-1745-9
10. M.T. Pope and A. Müller (eds.): *Polyoxometalates: From Platonic Solids to Anti-Retroviral Activity*. 1994
ISBN 0-7923-2421-8
11. N. Russo, J. Anastassopoulou and G. Barone (eds.): *Properties and Chemistry of Biomolecular Systems*. 1994
ISBN 0-7923-2666-0
12. Y.G. Smeyers (ed.): *Structure and Dynamics of Non-Rigid Molecular Systems*. 1994
ISBN 0-7923-2774-8