

## LIST OF PUBLICATIONS OF JOSEF MICHL

B: Book          P: Patent          C: Communication          R: Review or Chapter in a Book

- P 1. Kopecký, J.; Michl, J. "Způsob výroby pyrrolo(2,3-d)-pyrimidinů", Czechoslovak patent no. 97821, August 11, 1959.
- C 2. Zuman, P.; Michl, J. "Role of Keto-Enol Tautomerism in the Polarographical Reduction of Some Carbonyl Compounds", *Nature* **1961**, 192, 655.
- C 3. Horák, V.; Michl, J.; Zuman, P. "A Contribution to the Studies of Elimination Reactions of Mannich Bases, Using Polarographic Method", *Tetrahedron Lett.* **1961**, 744.
- C 4. Zahradník, R.; Michl, J.; Koutecký, J. "Fluoranthene-like Hydrocarbons: MO-LCAO Study of Electronic Spectra, Charge-Transfer Spectra and Polarographic Reduction", *J. Chem. Soc.* **1963**, 4998.
5. Koutecký, J.; Hochman, P.; Michl, J. "Calculation of Electronic Spectra of Non-Alternant Conjugated Hydrocarbons by the Semiempirical Method of Limited Configuration Interaction", *J. Chem. Phys.* **1964**, 40, 2439.
6. Zahradník, R.; Michl, J.; Koutecký, J. "Tables of Quantum Chemical Data. II. Energy Characteristics of Some Non-Alternant Hydrocarbons", *Collect. Czech. Chem. Commun.* **1964**, 29, 1932.
7. Zahradník, R.; Michl, J.; Koutecký, J. "Tables of Quantum Chemical Data. III. Molecular Orbitals of Some Fluoranthene-like Hydrocarbons, Cyclopentadienyl, and Some of its Benzo and Naphtho Derivatives", *Collect. Czech. Chem. Commun.* **1964**, 29, 3184.
8. Zahradník, R.; Michl, J. "Electronic Structure of Non-Alternant Hydrocarbons, Their Analogues and Derivatives. Introductory Remarks", *Collect. Czech. Chem. Commun.* **1965**, 30, 515.
9. Zahradník, R.; Michl, J. "Electronic Structure of Non-Alternant Hydrocarbons, Their Analogues and Derivatives. I. A Theoretical Treatment of Reid's Hydrocarbons", *Collect. Czech. Chem. Commun.* **1965**, 30, 520.
10. Zahradník, R.; Michl, J. "Electronic Structure of Non-Alternant Hydrocarbons, Their Analogues and Derivatives. II. Odd-Numbered Polyenes with a Five-Membered Ring at Each End", *Collect. Czech. Chem. Commun.* **1965**, 30, 1060.
11. Zahradník, R.; Michl, J.; Pancíř, J. "Electronic Structure of Non-Alternant Hydrocarbons, Their Analogues and Derivatives. III. Ions of the Polyenylicyclopentadienyl Type", *Collect. Czech. Chem.*

*Commun.* **1965**, *30*, 2891.

12. Zahradník, R.; Michl, J. "Tables of Quantum Chemical Data. IV. Molecular Orbitals of Hydrocarbons of the Pentalene, Azulene and Heptalene Series", *Collect. Czech. Chem. Commun.* **1965**, *30*, 3173.
13. Zahradník, R.; Michl, J.; Jutz, C. "Electronic Structure of Non-Alternant Hydrocarbons, Their Analogues and Derivatives. IV. An HMO Study of Amino Derivatives of Fulvenes and Vinylogous Fulvenes", *Collect. Czech. Chem. Commun.* **1965**, *30*, 3227.
14. Michl, J. "A Note on the Absence of a Hypsochromic Shift in Protonated Aminofluoranthenes", *Spectrochim. Acta* **1965**, *21*, 2146.
15. Zahradník, R.; Michl, J. "Tables of Quantum Chemical Data. V. Molecular Orbitals of peri-Condensed Tricyclic Hydrocarbons", *Collect. Czech. Chem. Commun.* **1965**, *30*, 3529.
16. Zahradník, R.; Michl, J. "Tables of Quantum Chemical Data. VII. Molecular Orbitals of Indacene-like and Some peri-Condensed Tetracyclic Hydrocarbons", *Collect. Czech. Chem. Commun.* **1965**, *30*, 3550.
17. Zahradník, R.; Michl, J.; Kopecký, J. "Electronic Structure of Non-Alternant Hydrocarbons, Their Analogues and Derivatives. V. Indacene-like Hydrocarbons", *Collect. Czech. Chem. Commun.* **1966**, *31*, 640.
18. Michl, J.; Zahradník, R. "Electronic Structure of Non-Alternant Hydrocarbons, Their Analogues and Derivatives. VI. An HMO Study of Ions of the Cyclopentadienyl Series", *Collect. Czech. Chem. Commun.* **1966**, *31*, 1475.
19. Michl, J.; Zahradník, R.; Hochmann, P. "Electronic Structure of Non-Alternant Hydrocarbons, Their Analogues and Derivatives. VII. Electronic Spectra of Some Benzologs of the Cyclopentadienylum Cation", *J. Phys. Chem.* **1966**, *70*, 1732.
20. Michl, J.; Zahradník, R. "Electronic Structure of Non-Alternant Hydrocarbons, Their Analogues and Derivatives. VIII. A Note on the Electronic Spectrum of Acenaphthylene", *Collect. Czech. Chem. Commun.* **1966**, *31*, 2259.
21. Michl, J.; Zahradník, R. "Electronic Structure of Non-Alternant Hydrocarbons, Their Analogues and Derivatives. IX. A Note on the Electronic Spectrum of the Dibenzo[a,d]tropylium Cation", *Collect. Czech. Chem. Commun.* **1966**, *31*, 2311.
22. Zahradník, R.; Párkányi, C.; Michl, J.; Horák, V. "An HMO Correlation of the First Bands in the Electronic Spectra of Conjugated Hydrocarbon Ions", *Tetrahedron* **1966**, *22*, 1341.
23. Zahradník, R.; Michl, J.; Pancíř, J. "Electronic Structure of Non-Alternant Hydrocarbons, Their Analogues and Derivatives--X. Peri-Condensed Tetracyclic Systems", *Tetrahedron* **1966**, *22*, 1355.

24. Zahradník, R.; Michl, J. "Electronic Structure of Non-Alternant Hydrocarbons, Their Analogues and Derivatives. XI. HMO Energy Characteristics of Fluoranthene-like Hydrocarbons", *Collect. Czech. Chem. Commun.* **1966**, *31*, 3442.
25. Michl, J.; Zahradník, R. "Electronic Structure of Non-Alternant Hydrocarbons, Their Analogues and Derivatives. XII. Chemical Reactivity Indices of Fluoranthene and the Benzofluoranthenes", *Collect. Czech. Chem. Commun.* **1966**, *31*, 3453.
26. Michl, J.; Zahradník, R.; Simon, W. "Electronic Structure of Non-Alternant Hydrocarbons, Their Analogues and Derivatives. XIII. Relative Conjugative Power of the Isomeric Fluoranthyls Towards the Amino Group. Basicity.", *Collect. Czech. Chem. Commun.* **1966**, *31*, 3464.
27. Michl, J.; Boček, K.; Zahradník, R. "Electronic Structure of Non-Alternant Hydrocarbons, Their Analogues and Derivatives. XIV. Relative Conjugative Power of the Isomeric Fluoranthyls Towards the Amino and Nitro Groups. Infrared Characteristics", *Collect. Czech. Chem. Commun.* **1966**, *31*, 3471.
28. Michl, J.; Zahradník, R. "Electronic Structure of Non-Alternant Hydrocarbons, Their Analogues and Derivatives. XV. An HMO Study of the Amino, Nitro, and Aza Derivatives of Fluoranthene", *Collect. Czech. Chem. Commun.* **1966**, *31*, 3478.
29. Heilbronner, E.; Weber, J. P.; Michl, J.; Zahradník, R. "The Electronic Spectra of Acenaphthylene and Fluoranthene. A Comment on the Classification of Electronic Spectra", *Theor. Chim. Acta* **1966**, *6*, 141.
- C 30. Becker, R. S.; Michl, J. "Photochromism of Synthetic and Naturally Occurring 2H-Chromenes and 2H-Pyrans", *J. Am. Chem. Soc.* **1966**, *88*, 5931.
31. Michl, J.; Becker, R. S. "Separation of  $^1L_a$  Excitation Energies of Conjugated Hydrocarbons into Orbital Energy Difference and Two-Electron Term Contributions", *J. Chem. Phys.* **1967**, *46*, 3889.
32. Michl, J. "Electronic Structure of Non-Alternant Hydrocarbons, Their Analogues and Derivatives. XVIII. The Electronic Spectrum and Electron Affinity of Fluoranthene", *J. Mol. Spectrosc.* **1969**, *30*, 66.
33. Dewar, M. J. S.; Michl, J. "Synthesis and  $^{19}\text{F}$  NMR Spectra of Fluoroanthracenes, Fluoroacenaphthylenes, and Fluorofluoranthenes, and a Practical Synthesis of 7-Substituted Fluoranthenes", *Tetrahedron* **1970**, *26*, 375.
34. Michl, J. "Effects of Inductive Substituents on Electronic Spectra. Aza Analogs of Fluoranthene", *Theor. Chim. Acta* **1969**, *15*, 315.
35. Linderberg, J.; Michl, J. "On the Inherent Optical Activity of Organic Disulfides", *J. Am. Chem. Soc.* **1970**, *92*, 2619.

36. Thulstrup, E. W.; Michl, J.; Eggers, J. H. "Polarization Spectra in Stretched Polymer Sheets. II. Separation of  $\pi$ - $\pi^*$  Absorption of Symmetrical Molecules into Components", *J. Phys. Chem.* **1970**, *74*, 3868.
37. Michl, J.; Thulstrup, E. W.; Eggers, J. H. "Polarization Spectra in Stretched Polymer Sheets. III. Physical Significance of the Orientation Factors and Determination of  $\pi$ - $\pi^*$  Transition Moment Directions in Molecules of Low Symmetry", *J. Phys. Chem.* **1970**, *74*, 3878.
38. Michl, J.; Koutecký, J.; Becker, R. S.; Earhart, Jr., C. E. "A Note on the Parameters for Heteroatoms in Pariser-Parr-Pople (PPP) Calculations", *Theor. Chim. Acta* **1970**, *19*, 92.
- C 39. Kolc, J.; Michl, J. "Photochemical Synthesis of Matrix-Isolated Pleiadene", *J. Am. Chem. Soc.* **1970**, *92*, 4147.
- C 40. Michl, J.; Kolc, J. "A Photochemical Electrocyclic Reaction Requiring an Upper Triplet State", *J. Am. Chem. Soc.* **1970**, *92*, 4148.
41. Michl, J.; Jones, R. "Borazaro Analogues of Aromatic Hydrocarbons. I. Electronic Spectra", *Collect. Czech. Chem. Commun.* **1971**, *36*, 1233.
42. Michl, J. "Borazaro Analogues of Aromatic Hydrocarbons. II. Semiempirical Calculations", *Collect. Czech. Chem. Commun.* **1971**, *36*, 1248.
- C 43. Michl, J. "Energy Barriers in Photochemical Reactions. A Case for the Relevance of Woodward-Hoffmann-Type Correlations", *J. Am. Chem. Soc.* **1971**, *93*, 523.
44. Michl, J. "Photochemical Reactions of Large Molecules. I. A Simple Physical Model of Photochemical Reactivity", *Mol. Photochem.* **1972**, *4*, 243.
45. Michl, J. "Photochemical Reactions of Large Molecules. II. Application of the Model to Organic Photochemistry", *Mol. Photochem.* **1972**, *4*, 257.
46. Michl, J. "Photochemical Reactions of Large Molecules. III. Use of Correlation Diagrams for Prediction of Energy Barriers", *Mol. Photochem.* **1972**, *4*, 287.
47. Downing, J.; Michl, J. "Polarization Directions of Electronic Transitions in Large Conjugated Molecules of Low Symmetry", *Int. J. Quantum Chem.* **1972**, *6*, 311.
- C 48. Dvorák, V.; Kolc, J.; Michl, J. "Photochemical Generation of Keto-Ketene II from Cyclic Phthaloyl Peroxide. Indirect Evidence for Benzo- $\beta$ -propiolactone", *Tetrahedron Lett.* **1972**, 3443.
- C 49. Downing, J.; Dvorák, V.; Kolc, J.; Manzara, A.; Michl, J. "Direct Observation of a Doubly Excited State of Pleiadene", *Chem. Phys. Lett.* **1972**, *17*, 70.

- R 50. Michl, J. "Photochemical Reactions: Correlation Diagrams and Energy Barriers" in *Chemical Reactivity and Reaction Paths*; Klopman, G., Ed.; J. Wiley and Sons, Inc.: New York, 1974; Chapter 8, 301.
- R 51. Michl, J. "Physical Basis of Qualitative MO Arguments in Organic Photochemistry", *Topics in Current Chemistry* **1974**, 46, 1.
- R 52. Michl, J.; Downing, J. "Excited State Calculations on Large Molecules", in *Energy, Structure and Reactivity*; Smith, D. W., McRae, W. B., Eds.; John Wiley and Sons, Inc.: New York, 1974; 299.
- R 53. Michl, J. "Use of Correlation Diagrams for Interpretation of Organic Reactivity", in *Physical Chemistry*; Eyring, H., Henderson, D., Jost, W., Eds.; Academic Press, Inc.: New York, 1973; Vol. VII, Chapter 3, 125.
- C 54. Flynn, C. R.; Michl, J. "Photochemical Preparation of *o*-Xylylene from 1,4-Dihydrophthalazine in Rigid Glass", *J. Am. Chem. Soc.* **1973**, 95, 5802.
55. Kolc, J.; Michl, J. " $\pi$ - $\pi$  Biradicaloid Hydrocarbons. The Pleiadene Family. I. Photochemical Preparation from Cyclobutene Precursors", *J. Am. Chem. Soc.* **1973**, 95, 7391.
- C 56. Warnick, S. M.; Michl, J. "Magnetic Circular Dichroism: Semiempirical Calculation of B Terms Using the Perturbation Formula", *J. Chem. Phys.* **1974**, 60, 703.
57. Michl, J.; Eggers, J. H. "Polarization Spectra in Stretched Polymer Sheets--IV. Benzo[k]fluoranthene and Its Aza Analogs", *Tetrahedron* **1974**, 30, 813.
58. Downing, J. W.; Michl, J.; Jorgensen, P.; Thulstrup, E. W. "Selection of Configurations for SCF-CI Calculations of Spectral Properties and Comparison with TDHF Calculations. I. Convergence to CCI Results in PPP Calculations on  $S_0 \rightarrow S_x$  Transitions in  $6\pi$ -Electron Systems", *Theor. Chim. Acta* **1974**, 32, 203.
59. Kolc, J.; Michl, J. "Excited States of Dinaphth[de-1,2,3;d'e'-5,6,7]azulene: Polarized Absorption in Stretched Polymers and Magnetic Circular Dichroism", *J. Mol. Spectrosc.* **1974**, 51, 298.
- C 60. Labrum, J. M.; Kolc, J.; Michl, J. "Energy Barriers in Photochemical Reactions. Photochemical Conversion of 6b,12c-Dihydrocyclobuta[1,2-*a*:3,4-*a'*]bisacenaphthylene (Dehydroheptacyclene) to Dinaphth[de-1,2,3:d'e'-5,6,7]azulene", *J. Am. Chem. Soc.* **1974**, 96, 2636.
61. Muller, J. F.; Cagniant, D.; Chalvet, O.; Lavalette, D.; Kolc, J.; Michl, J. "Excited States of Benzo[4,5]cyclohepta[1,2,3-*de*]naphthalene and Its Heterocyclic Analogs. Polarization Directions and Magnetic Circular Dichroism", *J. Am. Chem. Soc.* **1974**, 96, 5038.
62. Flynn, C. R.; Michl, J. " $\pi$ , $\pi$ -Biradicaloid Hydrocarbons: *o*-Xylylene. Photochemical Preparation from 1,4-Dihydrophthalazine in Rigid Glass, Electronic Spectroscopy, and Calculations", *J. Am. Chem.*

*Soc.* **1974**, *96*, 3280.

63. Michl, J.; Thulstrup, E. W.; Eggers, J. H. "Polarization Spectra in Stretched Polymer Sheets. V. Excited States of Anthracene and Transition Moment Directions in Aminoanthracenes", *Ber. Bunsenges. Phys. Chem.* **1974**, *78*, 575.
64. Warnick, S. M.; Michl, J. "Use of Semiempirical Models for Calculation of B Terms in MCD Spectra. I. General Results and the Pariser-Parr-Pople (PPP) Model for Nonalternant Hydrocarbons", *J. Am. Chem. Soc.* **1974**, *96*, 6280.
65. Kolc, J.; Thulstrup, E. W.; Michl, J. "Excited Singlet States of Fluoranthene. I. Absorption, Linear and Magnetic Circular Dichroism, and Polarized Fluorescence Excitation of the Fluorofluoranthenes", *J. Am. Chem. Soc.* **1974**, *96*, 7188.
66. Michl, J. "Use of Semiempirical Models for Calculation of B Terms in MCD Spectra. II. The Pariser-Parr-Pople (PPP) Model: A Consequence of the Pairing Symmetry in  $\pi$  Systems with Alternant Skeletons", *J. Chem. Phys.* **1974**, *61*, 4270.
67. Flynn, C. R.; Michl, J. "Ethylene Iminocarbonate", *J. Org. Chem.* **1974**, *39*, 3442.
- R 68. Michl, J.; Poshusta, R. D. "Hydrogen Excimer - A Bound State of  $H_4$ ", in *The Exciplex*; Gordon, M.; Ware, W. R., Eds., Academic Press, Inc.: New York, 1975; p 145.
69. Michl, J.; Michl, J. "Use of Semiempirical Models for Calculation of B Terms in MCD Spectra. III. Pariser-Parr-Pople (PPP) Predictions for Dications and Dianions of Pentalene and Heptalene", *Tetrahedron* **1974**, *30*, 4215.
70. Michl, J.; Michl, J. "Use of Semiempirical Models for Calculation of B Terms in MCD Spectra. IV. Substituted Benzenes in the PPP Model", *J. Am. Chem. Soc.* **1974**, *96*, 7887.
71. Michl, J. "Model Calculations of Photochemical Reactivity", *Pure Appl. Chem.* **1975**, *41*, 507.
72. Thulstrup, E. W.; Case, P. L.; Michl, J. "Azulene: Polarized Absorption in Stretched Polymers and Magnetic Circular Dichroism", *J. Chem. Phys.* **1974**, *6*, 410.
73. Thulstrup, E. W.; Michl, J.; Jutz, C. "Measurement and SCF-CI PPP Calculation of Polarized Absorption and Magnetic Circular Dichroism of Azuleno[5,6,7-*cd*]phenalene", *J. Chem. Soc., Faraday Trans. 2* **1975**, *71*, 1618.
74. Michl, J.; Thulstrup, E. W. "Why Is Azulene Blue and Anthracene White? A Simple MO Picture", *Tetrahedron* **1976**, *32*, 205.
75. Thulstrup, E. W.; Nepraš, M.; Dvořák, V.; Michl, J. "Excited Singlet States of Fluoranthene. II. Linear Dichroism, Polarized Fluorescence Excitation, and Anodic Oxidation of the

- Aminofluoranthenes", *J. Mol. Spectrosc.* **1976**, *59*, 265.
76. Dvorák, V.; Michl, J. "Photoionization of Anions in Rigid Media: Absorption and Emission Spectroscopy of Cyclooctatetraene Radical Anion, Its Ion Pairs, and Triple Ions", *J. Am. Chem. Soc.* **1976**, *98*, 1080.
  77. Kratochvíl, V.; Kolc, J.; Michl, J. "Excited States of Dicyclohepta[cd,gh]pentalene: Linear Dichroism in a Stretched Polymer, Magnetic Circular Dichroism, and Calculations", *J. Mol. Spectrosc.* **1975**, *57*, 436.
  78. Kolc, J.; Downing, J. W.; Manzara, A. P.; Michl, J. " $\pi,\pi$ -Biradicaloid Hydrocarbons. The Pleiadene Family. II. A Doubly Excited State of Pleiadene", *J. Am. Chem. Soc.* **1976**, *98*, 930.
  79. Kolc, J.; Michl, J.; Vogel, E. "Excited States of Bridged [14]Annulenes with Anthracene Perimeter: Absorption, Polarized Emission, Linear Dichroism, and Magnetic Circular Dichroism", *J. Am. Chem. Soc.* **1976**, *98*, 3935.
  80. Gerhartz, W.; Poshusta, R. D.; Michl, J. "Excited Potential Energy Hypersurfaces of  $H_4$  at Trapezoidal Geometries. Relation to Photochemical  $2s + 2s$  Processes", *J. Am. Chem. Soc.* **1976**, *98*, 6427.
  - R 81. Michl, J. "Photochemistry", in *Semiempirical Methods of Electronic Structure Calculation. Part B: Applications*; Segal, G. A., Ed.; Plenum Press: New York, 1977; 99.
  82. Carr, R. V.; Kim, B.; McVey, J. K.; Yang, N. C.; Gerhartz, W.; Michl, J. "Photochemistry and Photophysics of 1,4-Dewarnaphthalene", *Chem. Phys. Lett.* **1976**, *39*, 57.
  83. Thulstrup, E. W.; Michl, J. "Electronic States of Acenaphthylene. Linear Dichroism in Stretched Polyethylene and Magnetic Circular Dichroism", *J. Am. Chem. Soc.* **1976**, *98*, 4533.
  84. Kolc, J.; Michl, J. "Electronic States of Pleiadiene (Cyclohepta[de]naphthalene). Linear Dichroism in Stretched Polyethylene and Magnetic Circular Dichroism", *J. Am. Chem. Soc.* **1976**, *98*, 4540.
  85. Michl, J. "Acenaphthylene and Pleiadiene (Cyclohepta[de]naphthalene): A Case of Approximate Orbital and State Cross-Pairing", *J. Am. Chem. Soc.* **1976**, *98*, 4546.
  86. Michl, J.; Muller, J. F. "Nonalternant Hydrocarbons: A Classification of Excited States in Acenaphthylene and Pleiadiene (Cyclohepta[de]naphthalene) Families", *J. Am. Chem. Soc.* **1976**, *98*, 4550.
  87. Thulstrup, E. W.; Michl, J. "Linear Dichroism and Magnetic Circular Dichroism of Acenaphth[1,2-a]acenaphthylene", *J. Mol. Spectrosc.* **1976**, *61*, 203.
  88. Michl, J. "Use of Semiempirical Models for Calculation of B Terms in MCD Spectra. Aromatic

- Hydrocarbons: Prediction of Substituent and Heteroatom Effects from PPP Model", *Chem. Phys. Lett.* **1976**, 39, 386.
89. Tseng, K. L.; Michl, J. "MCD Spectra of Diphenylmethyl Cation and Anion. A Test of the Pairing Theorem", *J. Am. Chem. Soc.* **1976**, 98, 6138.
90. Michl, J. " $\pi$ -Electron Systems: Recent Developments in Electronic Spectroscopy and the PPP Model", *Int. J. Quantum Chem.* **1976**, S10, 107.
91. Michl, J.; Michl, J. "Use of Semiempirical Models for Calculation of B Terms in MCD Spectra. VI. PPP Predictions for Double Ions of Even Alternant Hydrocarbons", *J. Chem. Phys.* **1976**, 17, 1.
92. Miller, R. D.; Kolc, J.; Michl, J. "The Photochemical Generation of Stable  $\sigma$ -Xylylene Derivatives by the Electrocyclic Ring Opening of Some Polycyclic Benzocyclobutene Derivatives", *J. Am. Chem. Soc.* **1976**, 98, 8510.
- R 93. Michl, J. "The Role of Biradicaloid Geometries in Organic Photochemistry", *Photochem. Photobiol.* **1977**, 25, 141.
- C 94. Michl, J. "Use of Semiempirical Models for Calculation of B Terms in MCD Spectra. PPP Model for  $[4N+2]$ annulenes: A Rule for Substituent and Heteroatom Effects", *Chem. Phys. Lett.* **1976**, 43, 457.
95. Hansen, P. E.; Berg, A.; Jakobsen, H. J.; Manzara, A. P.; Michl, J. " $^{13}\text{C}$ - $^{19}\text{F}$  Spin-Spin Coupling in Some Monofluorosubstituted Polycyclic Aromatic Hydrocarbons", *Org. Mag. Res.* **1977**, 10, 179.
96. Gerhartz, W.; Poshusta, R. D.; Michl, J. "Excited Potential Energy Hypersurfaces for  $\text{H}_4$ . II. 'Triply Right' ( $\text{C}_{2v}$ ) Tetrahedral Geometries. A Possible Relation to Photochemical 'Cross-Bonding' Processes", *J. Am. Chem. Soc.* **1977**, 99, 4263.
- C 97. Muller, J.-F.; Muller, D.; Dewey, H. J.; Michl, J. " $\pi,\pi$ -Biradicaloid Hydrocarbons: Spectral Characterization of Singlet and Triplet 1,3-Perinaphthadiyl and Observation of Thermal and Photochemical 2,3-Hydrogen Shifts", *J. Am. Chem. Soc.* **1978**, 100, 1629.
- C 98. Thulstrup, E. W.; Michl, J. "Excited Electronic States of Pyrene and Some Azapyrenes", *Spectrosc. Lett.* **1977**, 10, 435.
- R 99. Michl, J. "Magnetic Circular Dichroism of Cyclic  $\pi$ -Electron Systems", in *Molecular Optical Dichroism and Chemical Applications of Polarized Spectroscopy*, Proceedings of a Nobel Workshop in Lund, October 25-27, 1976; Nordén, B., Ed.; Lund University Press: Lund, Sweden, 1977; 124.
- C 100. Michl, J.; Thulstrup, E. W. "Linear Dichroism of Aromatic Molecules in Stretched Polyethylene", *Spectrosc. Lett.* **1977**, 10, 401.
- C 101. Michl, J. "Magnetic Circular Dichroism of Cyclic  $\pi$ -Electron Systems", *Spectrosc. Lett.* **1977**, 10,

- R 102. Thulstrup, E. W.; Downing, J. W.; Michl, J. "Excited Singlet States of Pyrene. Polarization Directions and Magnetic Circular Dichroism of Azapyrenes", in *Molecular Optical Dichroism and Chemical Applications of Polarized Spectroscopy*, Proceedings of a Nobel Workshop in Lund, October 25-27, 1976; Nordén, B., Ed.; Lund University Press: Lund, Sweden, 1977; 91.
103. Michl, J.; Thulstrup, E. W. "Linear Dichroism of Aromatic Molecules in Stretched Polyethylene", in *Molecular Optical Dichroism and Chemical Applications of Polarized Spectroscopy*, Proceedings of a Nobel Workshop in Lund, October 25-27, 1976; Nordén, B., Ed.; Lund University Press: Lund, Sweden, 1977; 35.
104. Dolbier, Jr., W. R.; Matsui, K.; Michl, J.; Horak, D. V. "2,2-Dimethylisoindene and 5,5-Dimethylbenzobicyclo[2.1.0]pent-2-ene", *J. Am. Chem. Soc.* **1977**, *99*, 3876.
105. Thulstrup, E. W.; Downing, J. W.; Michl, J. "Excited Singlet States of Pyrene. Polarization Directions and Magnetic Circular Dichroism of Azapyrenes", *Chem. Phys.* **1977**, *23*, 307.
106. Tseng, K. L.; Michl, J. "An Approach to Biradical-like Species. Spectroscopy of o-Xylylene in Argon Matrix", *J. Am. Chem. Soc.* **1977**, *99*, 4840.
107. Michl, J.; Castellan, A.; Souto, M. A.; Kolc, J. "Higher Excited States and Vibrationally Hot Excited States: How Important Are They in Organic Photochemistry in Dense Media?", in *Excited States in Organic Chemistry and Biochemistry*; Pullman, B., Goldblum, N., Eds.; D. Reidel Publishing Company: Dordrecht, Holland, 1977; 361.
108. Michl, J. "MCD of Cyclic  $\pi$ -Electron Systems. I. Algebraic Solution of the Perimeter Model for the A and B Terms of High-Symmetry Systems with a  $(4N+2)$ -Electron  $[n]$ Annulene Perimeter", *J. Am. Chem. Soc.* **1978**, *100*, 6801.
- R 109. Michl, J. book review of *Aspects of Organic Photochemistry* (W. H. Horspool, Academic Press: London, 1976), *J. Am. Chem. Soc.* **1978**, *100*, 1977.
110. Castellan, A.; Michl, J. "Magnetic Circular Dichroism of Cyclic  $\pi$ -Electron Systems. IV. Aza Analogs of Benzene", *J. Am. Chem. Soc.* **1978**, *100*, 6824.
111. Dvořák, V.; Manzara, A. P.; Michl, J. "Preparation, Nucleophilic Reactivity, NMR, UV and Fluorescence Spectroscopy, and Matrix Photoionization of a Li-TMEDA Salt of the Benzocyclobut[a]acenaphthylene Dianion", *Tetrahedron* **1978**, *34*, 2433.
112. Jonás, I.; Michl, J. "MCD Spectroscopy of Cyclic  $\pi$ -Electron Systems. VI. Pyridones and Related Heterocycles", *J. Am. Chem. Soc.* **1978**, *100*, 6834.
113. Otteson, D.; Jutz, C.; Michl, J. "MCD Spectroscopy of Cyclic  $\pi$ -Electron Systems. XV.

- Benzazulenes", *J. Am. Chem. Soc.* **1978**, *100*, 6882.
114. Kenney, III, J. W.; Herold, D. A.; Michl, J. "MCD Spectroscopy of Cyclic  $\pi$ -Electron Systems. XVI. Derivatives of Acenaphthylene", *J. Am. Chem. Soc.* **1978**, *100*, 6884.
115. Souto, M. A.; Otteson, D.; Michl, J. "MCD Spectroscopy of Cyclic  $\pi$ -Electron Systems. XVIII. Benzofluoranthenes", *J. Am. Chem. Soc.* **1978**, *100*, 6892.
116. Michl, J. "MCD of Cyclic  $\pi$ -Electron Systems. II. Algebraic Solution of the Perimeter Model for the B Terms of Systems with a  $(4N+2)$ -Electron  $[n]$ Annulene Perimeter", *J. Am. Chem. Soc.* **1978**, *100*, 6812.
117. Michl, J. "MCD of Cyclic  $\pi$ -Electron Systems. III. Classification of Cyclic  $\pi$  Chromophores with a  $(4N+2)$ -Electron  $[n]$ Annulene Perimeter and General Rules for Substituent Effects on the MCD Spectra of Soft Chromophores", *J. Am. Chem. Soc.* **1978**, *100*, 6819.
118. Vasák, M.; Whipple, M. R.; Michl, J. "MCD Spectroscopy of Cyclic  $\pi$ -Electron Systems. VII. Aza Analogs of Naphthalene", *J. Am. Chem. Soc.* **1978**, *100*, 6838.
119. Wallace, S. L.; Castellan, A.; Muller, D.; Michl, J. "MCD Spectroscopy of Cyclic  $\pi$ -Electron Systems. V. Derivatives of Pyridine", *J. Am. Chem. Soc.* **1978**, *100*, 6828.
120. Whipple, M. R.; Vasák, M.; Michl, J. "MCD Spectroscopy of Cyclic  $\pi$ -Electron Systems. VIII. Derivatives of Naphthalene", *J. Am. Chem. Soc.* **1978**, *100*, 6844.
121. Souto, M. A.; Michl, J. "MCD Spectroscopy of Cyclic  $\pi$ -Electron Systems. IX. Aminoquinolines and Aminoisoquinolines", *J. Am. Chem. Soc.* **1978**, *100*, 6853.
122. Otteson, D.; Michl, J. "MCD Spectroscopy of Cyclic  $\pi$ -Electron Systems. X. Quinolones, Isoquinolones, and Related Heterocycles", *J. Am. Chem. Soc.* **1978**, *100*, 6857.
123. Steiner, R. P.; Michl, J. "MCD Spectroscopy of Cyclic  $\pi$ -Electron Systems. XI. Derivatives and Aza Analogs of Anthracene", *J. Am. Chem. Soc.* **1978**, *100*, 6861.
124. Vasák, M.; Whipple, M. R.; Michl, J. "MCD of Cyclic  $\pi$ -Electron Systems. XII. Aza Analogs of Phenanthrene", *J. Am. Chem. Soc.* **1978**, *100*, 6867.
125. Vasák, M.; Whipple, M. R.; Berg, A.; Michl, J. "MCD of Cyclic  $\pi$ -Electron Systems. XIII. Derivatives of Pyrene", *J. Am. Chem. Soc.* **1978**, *100*, 6872.
126. Gerhartz, W.; Michl, J. "MCD of Cyclic  $\pi$ -Electron Systems. XIV. Derivatives of Azulene", *J. Am. Chem. Soc.* **1978**, *100*, 6877.
127. Dalgaard, G. P.; Michl, J. "MCD of Cyclic  $\pi$ -Electron Systems. XVII. Derivatives of Fluoranthene",

*J. Am. Chem. Soc.* **1978**, *100*, 6887.

128. Jonkman, H. T.; Michl, J.; King, R. N.; Andrade, J. D. "Low-Temperature Positive Secondary Ion Mass Spectrometry of Neat and Argon-Diluted Organic Solids", *Anal. Chem.* **1978**, *50*, 2078.
129. Jorgensen, N. H.; Pedersen, P. B.; Thulstrup, E. W.; Michl, J. "Semiempirical  $\pi$ -Electron Models for the Calculation of MCD B Terms for Systems with Approximate Alternant Pairing Symmetry. MCD of Biphenylene", *Int. J. Quantum Chem.* **1978**, *12S*, 419.
130. Souto, M. A.; Kolc, J.; Michl, J. "Upper and/or Hot Excited States in Organic Photochemistry in Dense Media. A Cycloreversion in a Polycyclic Cyclobutene", *J. Am. Chem. Soc.* **1978**, *100*, 6692.
131. Castellan, A.; Kolc, J.; Michl, J. " $\pi,\pi$ -Biradicaloid Hydrocarbons. The Pleiadene Family. IV. Involvement of Upper and/or Hot Excited Singlet and Triplet States in a Photochemical Conversion of a Polycyclic Cyclobutene to a Butadiene", *J. Am. Chem. Soc.* **1978**, *100*, 6687.
132. Steiner, R. P.; Michl, J. " $\pi,\pi$ -Biradicaloid Hydrocarbons. The Pleiadene Family. III. A Facile Symmetry-Forbidden Thermal Conversion of a Polycyclic Butadiene Moiety to a Cyclobutene", *J. Am. Chem. Soc.* **1978**, *100*, 6413.
- C 133. Jonkman, H. T.; Michl, J. "Secondary Ion Mass Spectrometry: A Tool for Identification of Matrix-isolated Species", *J.C.S., Chem. Commun.* **1978**, 751.
- R 134. Michl, J. "The Role of the Excited State in Organic Photochemistry", in *Excited States in Quantum Chemistry*; Nicolaides, C. A., Beck, D. R., Eds.; D. Reidel: Dordrecht, Holland, 1978; 417.
135. Steiner, R. P.; Miller, R. D.; Dewey, H. J.; Michl, J. "Photochemical Generation of 2,3-Napthoquinodimethane Derivatives: An Extremely Facile 'Forbidden' Thermal Reaction and Evidence for a Low-Energy Doubly Excited State", *J. Am. Chem. Soc.* **1979**, *101*, 1820.
- C 136. Zilm, K. W.; Conlin, R. T.; Grant, D. M.; Michl, J. "Low Temperature Natural-Abundance  $^{13}\text{C}$  NMR Spectroscopy of Matrix-Isolated Species. The Anisotropy of the Shielding Tensor in Ethylene", *J. Am. Chem. Soc.* **1978**, *100*, 8038.
137. Dolbier, Jr., W. R.; Matsui, K.; Dewey, H. J.; Horák, D. V.; Michl, J. "2,2-Dimethylisoidene and 5,5-Dimethylbenzobicyclo[2.1.0]pent-2-ene", *J. Am. Chem. Soc.* **1979**, *101*, 2136.
- C 138. Drahnak, T. J.; Michl, J.; West, R. "Dimethylsilylene,  $(\text{CH}_3)_2\text{Si}$ ", *J. Am. Chem. Soc.* **1979**, *101*, 5427.
- C 139. Jonáš, I.; Michl, J. "Simple Expressions for Polarized Raman Scattering by a Uniaxial Assembly of Partially Oriented Symmetrical Molecules", *J. Chem. Phys.* **1979**, *71*, 7.
140. Thulstrup, E. W.; Michl, J. "A Critical Comparison of Methods for Analysis of Linear Dichroism of Solutes in Stretched Polymers", *J. Phys. Chem.* **1980**, *84*, 82.

141. Downing, J. W.; Čížek, J.; Paldus, J.; Michl, J. "Multidimensional Interpolation by Polynomial Roots", *Chem. Phys. Lett.* **1979**, *67*, 377.
142. Souto, M. A.; Wallace, S. L.; Michl, J. "MCD of Cyclic  $\pi$ -Electron Systems. 19. Heterocyclic Analogs of the Indenide Anion", *Tetrahedron* **1980**, *36*, 1521.
143. Wallace, S. L.; Michl, J. "MCD of Cyclic  $\pi$ -Electron Systems. 20. Amino Derivatives of Indole, Azaindoles, and Purines", *Tetrahedron* **1980**, *36*, 1531.
- C 144. Conlin, R. T.; Miller, R. D.; Michl, J. "Adamantene", *J. Am. Chem. Soc.* **1979**, *101*, 7637.
145. Wallace, S. L.; Michl, J. "The Perimeter Model and Magnetic Circular Dichroism of Aceheptylene", *Isr. J. Chem.* **1980**, *20*, 253.
146. Thulstrup, E. W.; Michl, J. "Interpretation of Polarized Spectra", *J. Mol. Struct.* **1980**, *61*, 175.
147. Michl, J.; West, R. "Excited States of Oxocarbon Dianions", in *Oxocarbons*; West, R., Ed.; Academic Press: New York, 1980; Chapter 5, 79.
- R 148. Michl, J. "Electronic Structure of Aromatic  $\pi$ -Electron Systems as Reflected in Their MCD Spectra", *Pure Appl. Chem.* **1980**, *52*, 1549.
149. Jonkman, H. T.; Michl, J. "Secondary Ion Mass Spectrometry of Small Molecules Held at Cryogenic Temperatures", in *Springer Series in Chemical Physics 9, Secondary Ion Mass Spectrometry II*; Benninghoven, A., Ed.; Springer-Verlag: New York, 1979; 292.
150. Michl, J.; Thulstrup, E. W. "Polarized Spectroscopy of Partially Oriented Molecules. A General Formulation for Two-Photon Processes in Uniaxial Samples", *J. Chem. Phys.* **1980**, *72*, 3999.
151. Rich, J. D.; Drahnak, T. J.; West, R.; Michl, J. "Reversible Di- $\pi$ -Methane Rearrangements of Bicyclic Organosilicon Compounds", *J. Organomet. Chem.* **1981**, *212*, C1-C3.
152. Dewey, H. J.; Deger, H.; Frölich, W.; Dick, B.; Klingensmith, K. A.; Hohlneicher, G.; Vogel, E.; Michl, J. "Excited States of Methano-Bridged [10]-, [14]-, and [18]Annulenes. Evidence for Strong Transannular Interaction, and Relation to Homoaromaticity", *J. Am. Chem. Soc.* **1980**, *102*, 6412.
153. Zilm, K. W.; Conlin, R. T.; Grant, D. M.; Michl, J. "Low-Temperature Carbon-13 Magnetic Resonance of Solids. I. Alkenes and Cycloalkenes", *J. Am. Chem. Soc.* **1980**, *102*, 6672.
154. Waluk, J. W.; Michl, J. "Determination of Positional Isomers of Methylpyrenes and Other Polycyclic Aromatic Hydrocarbons by Magnetic Circular Dichroism", *Anal. Chem.* **1981**, *53*, 236.
155. Waluk, J. W.; Michl, J. "Magnetic Circular Dichroism of Cyclic  $\pi$ -Electron Systems. 21. The Trisulfur Trinitride Anion", *Inorg. Chem.* **1981**, *20*, 963.

156. Jonkman, H. T.; Michl, J. "Secondary Ion Mass Spectrometry of Small-Molecule Solids at Cryogenic Temperatures. I. Nitrogen and Carbon Monoxide", *J. Am. Chem. Soc.* **1981**, *103*, 733.
157. Downing, J. W.; Michl, J. "Interpolation of Multidimensional Potential Surfaces by Polynomial Roots", in *Potential Energy Surfaces and Dynamics Calculations*; Truhlar, D. G., Ed.; Plenum Press: New York, 1981; 199.
158. Drahnak, T. J.; Michl, J.; West, R. "Photoisomerization of Dimethylsilylene to 2-Silapropene and Thermal Reversion to Dimethylsilylene", *J. Am. Chem. Soc.* **1981**, *103*, 1845.
159. Zilm, K. W.; Beeler, A. J.; Grant, D. M.; Michl, J.; Chou, T.-C.; Allred, E. L. "Carbon-13 Magnetic Resonance Dipolar Spectroscopy. Orientation of the Chemical Shift Tensor in Cyclopropane", *J. Am. Chem. Soc.* **1981**, *103*, 2119.
160. Orth, R. G.; Jonkman, H. T.; Michl, J. "Secondary Ion Mass Spectrometry of Molecular Solids: A Source of Cluster Ions", *J. Am. Chem. Soc.* **1981**, *103*, 1564.
161. Waluk, J. W.; Vogel, E.; Michl, J. "Magnetic Circular Dichroism of Cyclic  $\pi$ -Electron Systems. 23. Monocyclic  $\pi$ -Excessive Nitrogen Heterocycles. 1,4-Dihydro-1,4-Diazocines", *J. Org. Chem.* **1981**, *46*, 3306.
162. West, R.; Downing, J. W.; Inagaki, S.; Michl, J. "Applications of MCD Spectroscopy: Excited States of Oxocarbon Dianions", *J. Am. Chem. Soc.* **1981**, *103*, 5073.
163. Radziszewski, J. G.; Michl, J. "Infrared Linear Dichroism of Solutes in Stretched Polyethylene Using Fourier-Transform Spectroscopy. Pyrene", *J. Phys. Chem.* **1981**, *85*, 2934.
164. Waluk, J. W.; Michl, J. "Applications of MCD Spectroscopy: Electronic Structure of the Thiotriazolium Cation,  $S_4N_3^+$ ", *Inorg. Chem.* **1982**, *21*, 556.
165. Pedersen, P. B.; Thulstrup, E. W.; Michl, J. "Magnetic Circular Dichroism of Cyclic  $\pi$ -Electron Systems. 24. Polarizations and Assignments in Some Pentacyclic and Hexacyclic Benzenoid Hydrocarbons", *J. Chem. Phys.* **1981**, *60*, 187.
166. Waluk, J. W.; Chivers, T.; Oakley, R. T.; Michl, J. "Magnetic Circular Dichroism of Cyclic  $\pi$ -Electron Systems. 22. Derivatives of the Trisulfur Trinitride Anion", *Inorg. Chem.* **1982**, *21*, 832.
167. Orth, R. G.; Jonkman, H. T.; Powell, D. H.; Michl, J. "Secondary Ion Mass Spectrometry of Small-Molecule Solids at Cryogenic Temperatures. II. Rare Gas Solids", *J. Am. Chem. Soc.* **1981**, *103*, 6026.
168. Vařák, M.; Downing, J. W.; Townsend, L. B.; Michl, J. "Magnetic Circular Dichroism of Cyclic  $\pi$ -Electron Systems - 25. Oxo Derivatives of Indazole, Benzimidazole and Purine", *Tetrahedron* **1982**, *38*, 1571.

169. West, R.; Fink, M. J.; Michl, J. "Tetramesityldisilene, a Stable Compound Containing a Silicon-Silicon Double Bond", *Science* **1981**, *214*, 1343.
- C 170. Dewey, H. J.; Michl, J. "Site-Selected Fluorescence of Bridged [14]Annulenes in Nitrogen Matrix", *J. Luminescence* **1981**, *24/25*, 527.
171. Walker, F. H.; Wiberg, K. B.; Michl, J. "[2.2.1]Propellane", *J. Am. Chem. Soc.* **1982**, *104*, 2056.
172. Dewey, H. J.; Miller, R. D.; Michl, J. "Enhancement of Through-Bond Coupling by Bond-Angle Distortion: Pyrazine", *J. Am. Chem. Soc.* **1982**, *104*, 5298.
173. Orth, R. G.; Jonkman, H. T.; Michl, J. "Secondary Ion Mass Spectrometry of Small-Molecule Solids at Cryogenic Temperatures. III. Nitrogen Oxides", *J. Am. Chem. Soc.* **1982**, *104*, 1834.
174. Plummer, B. F.; Michl, J. "Magnetic Circular Dichroism of Cyclic  $\pi$ -Electron Systems. 26. 6,7-Dihydroacenaphtho[5,6-cd][1,2,6]thiadiazine and Acenaphtho[5,6-cd][1,2,6]thiadiazine", *J. Org. Chem.* **1982**, *47*, 1233.
175. Strub, H.; Beeler, A. J.; Grant, D. M.; Michl, J.; Cutts, P. W.; Zilm, K. W. "Low-Temperature  $^{13}\text{C}$  Magnetic Resonance in Solids. II. Six  $\pi$ -Electron Ring Systems:  $\text{C}_7\text{H}_7^+$ ,  $\text{C}_6\text{H}_6$ , and  $\text{C}_5\text{H}_5^-$ ", *J. Am. Chem. Soc.* **1983**, *105*, 3333.
176. Michl, J.; Weeks, G. H. "Magnetic Circular Dichroism as an Analytical Tool for Substituted Polynuclear Aromatic Hydrocarbons", in *Polynuclear Aromatic Hydrocarbons: Physical and Biological Chemistry*; Sixth International Symposium, Battelle Press: Columbus, Ohio, 1982; 501.
177. Michl, J. Preface to a Tetrahedron Symposium in Print Number 4, "Biradicals", *Tetrahedron* **1982**, *38*, 735.
178. Orth, R. G.; Jonkman, H. T.; Michl, J. "Secondary Ion Mass Spectrometry of Small-Molecule Solids at Cryogenic Temperatures. IV. Carbon Dioxide, Carbonyl Sulfide, and Carbon Disulfide", *Int. J. Mass Spectrom. Ion Phys.* **1982**, *43*, 41.
179. Thulstrup, E. W.; Michl, J. "Orientation and Linear Dichroism of Symmetrical Aromatic Molecules Imbedded in Stretched Polyethylene", *J. Am. Chem. Soc.* **1982**, *104*, 5594.
180. Zilm, K. W.; Fink, M. J.; Grant, D. M.; West, R.; Michl, J. "Electronic Structure of the Silicon-Silicon Double Bond:  $^{29}\text{Si}$  Shielding Anisotropy in Tetramesityldisilene", *Organometallics* **1983**, *2*, 193.
181. Miller, R. D.; Wallraff, G.; Clecak, N.; Sooriyakumaran, R.; Michl, J.; Karatsu, T.; McKinley, A. J.; Klingensmith, K. A.; Downing, J. "Polysilanes: Solution Photochemistry and Deep UV Lithography", *Polym. Mater. Sci. Eng.* **1989**, *60*, 49.

182. Solum, M. S.; Zilm, K. W.; Michl, J.; Grant, D. M. "<sup>13</sup>C Line Shape Study of Two-Site Exchange in Solid Dimethyl Sulfone", *J. Phys. Chem.* **1983**, *87*, 2940.
183. Langkilde, F. W.; Thulstrup, E. W.; Michl, J. "The Effect of Solvent Environment on Molecular Electronic Transition Moment Directions: Symmetry Lowering in Pyrene", *J. Chem. Phys.* **1983**, *78*, 3372.
184. Michl, J.; Radziszewski, G. J.; Downing, J. W.; Wiberg, K. B.; Walker, F. H.; Miller, R. D.; Kovacic, P.; Jawdosiuk, M.; Bonačić-Koutecký, V.; "Highly Strained Single and Double Bonds", *Pure Appl. Chem.* **1983**, *55*, 315.
185. Klingensmith, K. A.; Püttmann, W.; Vogel, E.; Michl, J. "Applications of MCD Spectroscopy: MO Ordering and Transannular Interaction in 1,6-Methano[10]annulenes from Analysis of Substituent Effects", *J. Am. Chem. Soc.* **1983**, *105*, 3375.
186. Puebla, C.; Michl, J. "A New Concept in Optical Information Storage: Thermal Relaxation of Strain Birefringence", *Appl. Phys. Lett.* **1983**, *42*, 570.
187. Fink, M. J.; De Young, D. J.; West, R.; Michl, J. "Chemical Reactions of Tetramesityldisilene", *J. Am. Chem. Soc.* **1983**, *105*, 1070.
188. Frölich, W.; Dewey, H. J.; Deger, H.; Dick, B.; Klingensmith, K. A.; Püttmann, W.; Vogel, E.; Hohlneicher, G.; Michl, J. "Excited Singlet States of 'Hairpin' Polyenes," *J. Am. Chem. Soc.* **1983**, *105*, 6211.
189. Miller, R. D.; McKean, D. R.; Tompkins, T. L.; Clecak, N.; Willson, C. G.; Michl, J.; Downing, J. "Semiempirical Calculations of Electronic Spectra: Use in the Design of Mid-UV Sensitizers," in *Polymers in Electronics: American Chemical Society Symposium Series 242*, March 20-25, 1983; Davidson, T., Ed.; American Chemical Society: Washington, DC, 1984; 25.
190. Wiberg, K. B.; Walker, F. H.; Pratt, W. E.; Michl, J. "[2.1.1] Propellane. Reaction of 1,4-Diodobicyclo[2.1.1]hexane with *tert*-Butyllithium and with Potassium Atoms," *J. Am. Chem. Soc.* **1983**, *105*, 3638.
191. Wallraff, G. M.; Boyd, R. H.; Michl, J. "Conformational Mobility in the *trans*-Cycloheptene Copper(I) Triflate Complex," *J. Am. Chem. Soc.* **1983**, *105*, 4550.
192. Mitchell, M. B.; Guillory, W. A.; Michl, J.; Radziszewski, J. "Infrared Linear Dichroism of the T<sub>1</sub> State of Acridine in Stretched Polyethylene," *Chem. Phys. Lett.* **1983**, *96*, 413.
193. Langkilde, F. W.; Gisin, M.; Thulstrup, E. W.; Michl, J. "Alignment of Solutes in Stretched Polyethylene. Determination of the Five Second and Fourth Moments of the Orientation Distribution of 2-Fluoropyrene from Polarized Fluorescence. Additional Evidence for the Twisting of Weak Transition Moments by the Solvent Environment," *J. Phys. Chem.* **1983**, *87*, 2901.

194. Wallace, S. L.; Michl, J. "Photoisomerization of 1,4-Dewarnaphthalene in a Nitrogen Matrix: A Mechanistic Study," in *Photochemistry and Photobiology: Proceedings of the International Conference, January 10, 1983, University of Alexandria, Egypt, Vol. II*; Zewail, A. H., Ed.; Harwood Academic Publishers: Chur, Switzerland, 1983; Volume II, 1191.
195. Thulstrup, E. W.; Michl, J. "Optical Spectroscopy on Partially Oriented Samples," *Int. J. Quantum Chem.* **1983**, *17*, 471.
196. Arrington, C. A.; West, R.; Michl, J. "On the Thermal Interconversion of Matrix-Isolated Dimethylsilylene and 2-Silapropene. Their Reactions with Oxygen Atom Donors," *J. Am. Chem. Soc.* **1983**, *105*, 6176.
197. Arrington, C. A.; Klingensmith, K. A.; West, R.; Michl, J. "Polarized Infrared Spectroscopy of Matrix-Isolated Dimethylsilylene and 1-Methylsilylene," *J. Am. Chem. Soc.* **1984**, *106*, 525.
- C 198. Fink, M. J.; Michalczyk, M. J.; Haller, K. J.; West, R.; Michl, J. "The X-Ray Crystal Structure of Tetramesityldisilene," *J.C.S. Chem. Commun.* **1983**, *18*, 1010.
- R 199. Michl, J. "Secondary Ion Mass Spectrometry of Low-Temperature Solids," *Int. J. Mass Spectrom. Ion Phys.* **1983**, *53*, 255.
- C 200. Stulik, D.; Orth, R. G.; Jonkman, H. T.; Michl, J. "Secondary Ion Mass Spectrometry of Small-Molecule Solids at Cryogenic Temperatures. V. Oxygen," *Int. J. Mass Spectrom. Ion Phys.* **1983**, *53*, 341.
- C 201. Liang, J.; Michl, J. "Fast Atom and Fast Ion Bombardment of Solid Nitrogen Oxides: An FT-IR Study," *J. Am. Chem. Soc.* **1984**, *106*, 5039.
202. Beeler, A. J.; Orendt, A. M.; Cutts, P. W.; Grant, D. M.; Zilm, K. W.; Facelli, J. C.; Schindler, M. S.; Downing, J. W.; Kutzelnigg, W.; Michl, J. "Low-Temperature <sup>13</sup>C Magnetic Resonance in Solids. III. Linear and Pseudolinear Molecules," *J. Am. Chem. Soc.* **1984**, *106*, 7672.
203. Otteson, D.; Michl, J. "A Procedure for Gas-Phase Dehalogenation of Organic Dihalides with Alkali Metal Vapors Using Microwave and/or Ultrasound Excitation and Matrix Isolation of Products," *J. Org. Chem.* **1984**, *49*, 866.
204. Fink, M. J.; Haller, K. J.; West, R.; Michl, J. "Tetramesitylcyclodisiloxane: A Cyclic Siloxane with an Unusual Structure," *J. Am. Chem. Soc.* **1984**, *106*, 822.
205. Michalczyk, M. J.; West, R.; Michl, J. "Cis and Trans Isomers of Disilenes: Photochemical and Thermal Interconversions," *J. Am. Chem. Soc.* **1984**, *106*, 821.
206. Willson, G.; Miller, R.; McKean, D.; Clecak, N.; Tompkins, T.; Hofer, D. Michl, J.; Downing, J. "Design of a Positive Resist for Projection Lithography in the Mid-UV," *J. Polymer Eng. Sci.* **1983**,

23, 1004.

- R 207. Michl, J. "Magnetic Circular Dichroism of Aromatic Molecules," *Tetrahedron* **1984**, *40*, 3845.
- C 208. Bonačić-Koutecký, V.; Michl, J.; Köhler, J. "Prediction of Structural and Environmental Effects on the S<sub>1</sub>-S<sub>0</sub> Energy Gap and Jump Probability in Double-Bond *cis-trans* Photoisomerization. A General Rule," *Chem. Phys. Lett.* **1984**, *104*, 440.
209. Fink, M. J.; Michalczyk, M. J.; Haller, K. J.; Michl, J.; West, R. "X-Ray Crystal Structure for Two Disilenes," *Organometallics* **1984**, *3*, 793.
- C 210. Magnera, T. F.; David, D. E.; Tian, R.; Stulik, D.; Michl, J. "Triple-Quadruple Secondary Ion Mass Spectrometry of Low-Temperature Solids: Collision-Activated Dissociation of Large Cluster Ions," *J. Am. Chem. Soc.* **1984**, *106*, 5040.
211. Radziszewski, J. G.; Downing, J. W.; Jawdosiuk, M.; Kovacic, P.; Michl, J. "4-Azahomoadamant-3-ene: Spectroscopic Characterization and Photoresolution of a Highly Reactive Strained Bridgehead Imine," *J. Am. Chem. Soc.* **1985**, *107*, 594.
212. Downing, J. W.; Waluk, J. W.; Stanovnik, B.; Tisler, M.; Vercek, B.; Michl, J. "Applications of Magnetic Circular Dichroism: A Hammett-like Equation for Structural Work. Determination of Protonation Sites in Azaindolizines," *J. Org. Chem.* **1985**, *50*, 302.
- C 213. Michalczyk, M. J.; West, R.; Michl, J. "Formation of a Disiloxirane in the Oxidation of 1,2-Dimesityl-1,2-di-(*tert*)butyldisilaethylene," *Chem. Commun.* **1984**, *22*, 1525.
214. Michalczyk, M. J.; West, R.; Michl, J. "Kinetics of Thermal *cis-trans* Isomerizations in Disilenes", *Organometallics* **1985**, *4*, 826.
- C 215. Radziszewski, J. G.; Downing, J. W.; Wentrup, C.; Kaszynski, P.; Jawdosiuk, M.; Kovacic, P.; Michl, J. "2-Azaadamant-1-ene and 4-Azaprotadamant-3-ene", *J. Am. Chem. Soc.* **1984**, *106*, 7996.
- R 216. West, R.; Fink, M. J.; Michalczyk, M. J.; De Young, D. J.; Michl, J. "The Disilenes and Their Derivatives", in *Organosilicon and Bioorganosilicon Chemistry*, Sakurai, H., Ed.; Ellis Horwood, Ltd.: London, 1985; Part 1, Chapter 1, 3.
217. Facelli, J. C.; Orendt, A. M.; Grant, D. M.; Michl, J. "IGLO Calculations of the Antisymmetric Components of Nuclear Magnetic Shielding Tensors", *Chem. Phys. Lett.* **1984**, *112*, 147.
218. Michalczyk, M. J.; Fink, M. J.; Haller, K. J.; West, R.; Michl, J. "Structural and Chemical Properties of 1,3-Cyclodisiloxanes", *Organometallics* **1986**, *5*, 531.
219. Radziszewski, J. G.; Michl, J. "Symmetry Assignment of Vibrations in Anthracene, Phenazine, and Acridine from Infrared Dichroism in Stretched Polyethylene", *J. Chem. Phys.* **1985**, *82*, 3527.

- C 220. Bonačić-Koutecký, V.; Michl, J. "Charge-Transfer-Biradical Excited States: Relation to Anomalous Fluorescence. 'Negative'  $S_1 - T_1$  Splitting in Twisted Aminoborane", *J. Am. Chem. Soc.* **1985**, *107*, 1765.
- C 221. Radziszewski, J. G.; Downing, J. W.; Wentrup, C.; Kaszynski, P.; Jawdosiuk, M.; Kovacic, P.; Michl, J. "Geometrical Isomers of a Bridgehead Imine: (E)- and (Z)-2-Azabicyclo[3.2.1]oct-1-ene, and 2-Azabicyclo[2.2.2]oct-1-ene", *J. Am. Chem. Soc.* **1985**, *107*, 2799.
- R 222. Michl, J. "Organic Chemical Systems, Theory" in *Encyclopedia of Physical Science and Technology*; Meyers, R. A., Ed.; Academic Press, 1987; *10*, 1.
223. Michl, J. book review of *Reactive Molecules. The Neutral Reactive Intermediates in Organic Chemistry* (C. Wentrup, John Wiley and Sons: Chichester, 1984), *Angew. Chem.* **1986**, *25*, 295.
- C 224. Kirkor, E.; Gebicki, J.; Phillips, D. R.; Michl, J. "Incorporation of Neutral Molecules into Alkali Halides ("Salting"). Room-Temperature Composites from Normally Immiscible Components and Room-Temperature Matrix Isolation", *J. Am. Chem. Soc.* **1986**, *108*, 7106.
225. Michalczyk, M. J.; Fink, M. J.; De Young, D. J.; Carlson, C. W.; Welsh, K. M.; West, R.; Michl, J. "Organosilylenes and their Dimerization to Disilenes", *Silicon, Germanium, Tin, and Lead Compounds* **1986**, *9*, 75.
- C 226. Barrau, J.; Bean, D. L.; Welsh, K. M.; West, R.; Michl, J. "Photochemistry of a Matrix-isolated Geminal Diazide: Dimethylgermylene", *Organometallics* **1989**, *8*, 2606.
- C 227. Vančik, H.; Raabe, G.; Michalczyk, M. J.; West, R.; Michl, J. "Dimethylsilylene: A Trisilane and a Geminal Diazide as New Photochemical Precursors. Evidence for an Absorption Maximum Near 450 nm", *J. Am. Chem. Soc.* **1985**, *107*, 4097.
- B 228. Michl, J.; Thulstrup, E. W. *Spectroscopy with Polarized Light. Solute Alignment by Photoselection, in Liquid Crystals, Polymers, and Membranes*; VCH Publishers: Deerfield Beach, Florida, 1986.
229. Murthy, P. S.; Klingensmith, K. A.; Michl, J. "Optical Recording by a 823-nm GaAlAs Laser, Based on Stretched Polymer Birefringence Relaxation", *J. Appl. Polym. Sci.* **1986**, *31*, 2331.
230. Orendt, A. M.; Facelli, J. C.; Grant, D. M.; Michl, J.; Walker, F. H.; Dailey, W. P.; Waddell, S. T.; Schindler, M.; Kutzelnigg, W.; Wiberg, K. B. "Low Temperature  $^{13}\text{C}$  NMR Magnetic Resonance in Solids. 4. Cyclopropane, Bicyclo[1.1.0]butane and [1.1.1]Propellane", *Theor. Chim. Acta* **1985**, *68*, 421.
231. Bonačić-Koutecký, V.; Michl, J. "Photochemical Syn-Anti Isomerization of a Schiff Base: A Two-Dimensional Description of a Conical Intersection in Formaldimine", *Theor. Chim. Acta* **1985**, *68*, 45.

232. Bötcher, A.; Raabe, G.; Michl, J. "Magnetic Circular Dichroism of Cyclic  $\pi$ -Electron Systems. 27. Mesoionic Compounds", *J. Org. Chem.* **1985**, *50*, 5050.
- R 233. Raabe, G.; Michl, J. "Multiple Bonding to Silicon", *Chem. Rev.* **1985**, *85*, 419.
234. Facelli, J. C.; Orendt, A. M.; Beeler, A. J.; Solum, M. S.; Depke, G.; Malsch, K. D.; Downing, J. W.; Murthy, P. S.; Grant, D. M.; Michl, J. "Low-Temperature  $^{13}\text{C}$  Magnetic Resonance in Solids. 5. Chemical Shielding Anisotropy of the  $^{13}\text{CH}_2$  Group", *J. Am. Chem. Soc.* **1985**, *107*, 6749.
235. David, D. E.; Magnera, T. F.; Tian, R.; Michl, J. "KeV Energy Ion and Atom Bombardment of Low-Temperature Solids: Radiation Damage, Sputtering, and Mechanism", *Rad. Effects* **1986**, *99*, 731.
236. Weeks, G. H.; Adcock, W.; Klingensmith, K. A.; Waluk, J. W.; West, R.; Vasak, M.; Downing, J.; Michl, J. "A Probe for Substituent Hyperconjugative Power: Magnetic Circular Dichroism of the Benzene  $L_b$  Band", *Pure Appl. Chem.* **1986**, *58*, 39.
237. Raabe, G.; Vancik, H.; West, R.; Michl, J. "IR Transition Moment Directions in Matrix-Isolated Dimethylsilylene and 1-Methylsilene", *J. Am. Chem. Soc.* **1986**, *108*, 671.
- C 238. Zigler, S. S.; West, R.; Michl, J. "Observation of a Silanimine in an Inert Matrix and in Solution at Low Temperature", *Chem. Lett.* **1986**, 1025.
239. Magnera, T. F.; David, D. E.; Michl, J. "'Magic' Losses of One to Five  $\text{N}_2$  Molecules from Metastable  $\text{N}_{2n}^+$  Clusters," *Chem. Phys. Lett.* **1986**, *123*, 327.
240. David, D. E.; Magnera, T. F.; Tian, R.; Stulik, D.; Michl, J. "Cluster Ions from KeV-Energy Ion and Atom Bombardment of Frozen Gases," *Nuclear Instruments and Methods* **1986**, *B14*, 378.
241. Radziszewski, J. G.; Michl, J. "Fourier-Transform Infrared Linear Dichroism: Stretched Polyethylene as a Solvent in IR Spectroscopy, *J. Am. Chem. Soc.* **1986**, *108*, 3289.
242. Facelli, J. C.; Orendt, A. M.; Solum, M. S.; Depke, G.; Grant, D. M.; Michl, J. "Low Temperature  $^{13}\text{C}$  Magnetic Resonance in Solids. 6. Methine Carbons", *J. Am. Chem. Soc.* **1986**, *108*, 4268.
- P 243. Michl, J.; Puebla, C. "Optical Recording Method and Apparatus Utilizing Birefringent Materials", U.S. Patent No. 4,551,819, 1985.
244. Klein, H.-P.; Oakley, R. T.; Michl, J. "Magnetic Circular Dichroism of Cyclic  $\pi$ -Electron Systems. 28. Sulfur-Nitrogen Heterocycles", *Inorg. Chem.* **1986**, *25*, 3194.
- C 245. Fisher, J. J.; Penn, J. H.; Döhnert, D.; Michl, J. "Polarized IR Spectroscopy of a Triplet 1,3-Biradical: The Structure of a Methylene-Bridged 1,8-Naphthoquinodimethane", *J. Am. Chem. Soc.* **1986**, *108*, 1715.

- R 246. Bonačić-Koutecký, V.; Koutecký, J.; Michl, J. "Neutral and Charged Biradicals, Zwitterions, Funnels in  $S_1$ , and Proton Translocation: Their Role in Photochemistry, Photophysics, and Vision", *Angew. Chem. Internat. Ed. Engl.* **1987**, *26*, 170.
- C 247. Radziszewski, J. G.; Yin, T.-K.; Miyake, F.; Renzoni, G. E.; Borden, W. T.; Michl, J. "A Doubly Pyramidalized Olefin: Matrix Isolation Spectroscopy of Tricyclo[3.3.2.0]dec-3(7)-ene", *J. Am. Chem. Soc.* **1986**, *108*, 3544.
248. Wallraff, G. M.; Michl, J. "Low-Temperature Reactions of Copper(I) Triflate Complexes of *cis*- and *trans*-Cyclooctene and *cis*- and *trans*-Cycloheptene with Trimethyl Phosphite. Spectroscopic Evidence for Free *trans*-Cycloheptene", *J. Org. Chem.* **1986**, *51*, 1794.
- C 249. Sekiguchi, A.; Zigler, S. S.; West, R.; Michl, J. "Synthon for the Silicon-Silicon Triple Bond", *J. Am. Chem. Soc.* **1986**, *108*, 4241.
250. Solum, M. S.; Facelli, J. C.; Michl, J.; Grant, D. M. "Low-Temperature  $^{13}\text{C}$  Magnetic Resonance in Solids. 7. Methyl Carbons", *J. Am. Chem. Soc.* **1986**, *108*, 6464.
- C 251. Radziszewski, J. G.; Downing, J. W.; Michl, J.; Yin, T.-Y.; Renzoni, G. E.; Borden, W. T. "Thermal Reorganization of Two Pyramidalized Alkenes by Reverse Vinylcyclopropane Rearrangements", *J. Am. Chem. Soc.* **1987**, *109*, 820.
252. Borsch-Pulm, B.; Demmer, M.; Murthy, P. S.; Lex, J.; Schieb, T.; Vogel, E.; Hohlneicher, G.; Michl, J. "Excited States of Homobenzenoid Hydrocarbons. *Syn*- and *Anti*-1,6:7,12-Bis-methano[14]annulene", *J. Phys. Chem.* **1987**, *91*, 1382.
253. Radziszewski, J. G.; Burkhalter, F. A.; Michl, J. "Non-Destructive Photoorientation by Generalized Pseudorotation: A Quantitative Treatment", *J. Am. Chem. Soc.* **1987**, *109*, 61.
- C 254. Klingensmith, K. A.; Downing, J. W.; Miller, R. D.; Michl, J. "Electronic Excitation in Poly(di-*n*-hexylsilane)", *J. Am. Chem. Soc.* **1986**, *108*, 7438.
- P 255. Michl, J. "Methods for Making Solid Solutions from Normally Immiscible Components and for Modifying the Surface Structure of Solid Materials", U. S. Patent No. 4,599,462, 1986.
256. Urbassek, H. M.; Michl, J. "A Gas-Flow Model for the Sputtering of Condensed Gases", *Nuclear Instruments and Methods in Physics Research* **1987**, *B22*, 480.
257. Michl, J.; Thulstrup, E. W. "UV and IR Linear Dichroism: Polarized Light as a Probe of Molecular and Electronic Structure", *Acc. Chem. Res.* **1987**, *20*, 192.
258. Michl, J.; Radziszewski, J. G.; Downing, J. W.; Kopecký, J.; Kaszynski, P.; Miller, R. D. "Bridgehead Double Bonds", *Pure Appl. Chem.* **1987**, *59*, 1613.

259. Thulstrup, E. W.; Michl, J. "Stretched Polyethylene as a Solvent for Optical Spectroscopy", *Acta Phys. Polonica* **1987**, A71, 839.
260. Fisher, J. J.; Michl, J. "s-Cis vs. *Gauche* 1,3-Butadiene: Evidence for Planarity from Polarized Matrix-Isolation IR Spectroscopy", *J. Am. Chem. Soc.* **1987**, 109, 1056.
- C 261. Fisher, J. J.; Michl, J. "External and Internal Heavy-Atom Effects on the Rate of Spin-Forbidden Proton Tunneling in the Triplet Ground State Biradical, 1,3-Perinaphthadiyl," *J. Am. Chem. Soc.* **1987**, 109, 583.
- C 262. Magnera, T. F.; David, D. E.; Michl, J. "Dehydrogenation and Cracking of *n*-Butane with Gas-Phase Ni<sub>n</sub><sup>+</sup>, Pd<sub>n</sub><sup>+</sup>, and Pt<sub>n</sub><sup>+</sup> Cluster Ions," *J. Am. Chem. Soc.* **1987**, 109, 936.
263. Facelli, J. C.; Grant, D. M.; Michl, J. "Analysis of the IGLO Bond Contributions to the <sup>13</sup>C Shielding Tensors in the Local Bond Frame," *Int. J. Quantum Chem.* **1987**, 31, 45.
- C 264. Zigler, S. S.; Welsh, K. M.; West, R.; Michl, J. "Matrix Isolation of the First Silanediimine, N,N'-Bis(trimethylsilyl)silanediimine", *J. Am. Chem. Soc.* **1987**, 109, 4392.
265. Welsh, K. M.; Rich, J. D.; Michl, J.; West, R. "The Generation of Hexamethyl-1,4-Disilabenzene and Its Novel Thermal Chemistry", *J. Organomet. Chem.* **1987**, 325, 105.
- R 266. Facelli, J. C.; Grant, D. M.; Michl, J. "<sup>13</sup>C Shielding Tensors: Experimental and Theoretical Determination", *Acc. Chem. Res.* **1987**, 20, 152.
267. Michl, J., book review of *Introduction to Organic Photochemistry*; Doyle, J. D., *J. Am. Chem. Soc.* **1987**, 109, 4764.
- R 268. Michl, J.; Downing, J. W.; Karatsu, T.; Klingensmith, K. A.; Wallraff, G. M.; Miller, R. D. "Poly(di-*n*-hexylsilane) in Room-Temperature Solution: Photophysics and Photochemistry", in *Inorganic and Organometallic Polymers*, ACS Symposium Series 360, Zeldin, M., Wynne, K., Allock, H., Eds.; American Chemical Society: Washington, DC, 1988; Chapter 5, 61.
269. Radziszewski, J. G.; Arrington, C. A.; Downing, J. W.; Balaji, V.; Murthy, G. S.; Michl, J. "Vibrational Transition Moment Directions in Medium-Size Molecules: Experiment and Theory", *J. Mol. Structure (THEOCHEM)* **1988**, 163, 191.
270. Bonačić-Koutecký, V.; Schöffel, K.; Michl, J. "Critically Heterosymmetric Biradicaloid Geometries of Protonated Schiff Bases. Possible Consequences for Photochemistry and Photobiology", *Theor. Chim. Acta* **1987**, 72, 459.
- R 271. Magnera, T. F.; Balaji, V.; Michl, J.; Miller, R. D. "Polysilane Photochemistry and Laser Desorption Mass Spectrometry", in *Silicon Chemistry: Proceedings of the 8th International Symposium on Organosilicon Chemistry*; Corey, E. R.; Corey, J. Y.; Gaspar, P. P., Eds.; Ellis Horwood, Ltd.:

Chichester, England, 1988, Chapter 45, 491.

272. Balaji, V.; Michl, J. "New Strained Organic Molecules: Theory Guides Experiment", *Pure Appl. Chem.* **1988**, *60*, 189.
273. Kirkor, E. S.; David, D. E.; Magnera, T. F.; Michl, J. "A Simple Method for the Production of Controlled Electroplated Designs on a Metal Surface", *Langmuir* **1988**, *4*, 578.
274. Orendt, A. M.; Facelli, J. C.; Beeler, A. J.; Reuter, K.; Horton, W. J.; Cutts, P.; Grant, D. M.; Michl, J. "Low Temperature  $^{13}\text{C}$  Magnetic Resonance. 8. Chemical Shielding Anisotropy of Olefinic Carbons", *J. Am. Chem. Soc.* **1988**, *110*, 3386.
275. Orendt, A. M.; Michl, J.; Reiter, J. "On Triazoles. XIV.  $^{15}\text{N}$  NMR Study of Substituted 5-Amino-1,2,4-Triazoles", *Magnetic Resonance in Chemistry* **1989**, *27*, 1.
276. DeYoung, D. J.; Fink, M. J.; West, R.; Michl, J. "The Addition Reactions of Two Disilenes", *Main Group Metal Chemistry* **1987**, *10*, 19.
277. Murthy, P. S.; Michl, J. "Conformational Analysis by Infrared Linear Dichroism of Solutes in Stretched Polyethylene: The Twist Angle in Biphenyl and 4,4'-Dibromobiphenyl", *Collect. Czechoslovak Chem. Commun.* **1988**, *53*, 2366.
- R 278. Thulstrup, E. W.; Michl, J. "Polarized Absorption Spectroscopy of Molecules Aligned in Stretched Polymers", *Spectrochim. Acta* **1988**, *44A*, 767.
279. Klingensmith, K. A.; Dewey, H. J.; Vogel, E.; Michl, J. "Vibrational Structure of the  $^1\text{L}_b$  State of 1,6:8,13-Ethano[14]annulene. Transannular Interaction, the 'Mystery Band', and the Kekulé Vibration", *J. Am. Chem. Soc.* **1989**, *111*, 1539.
- C 280. Orendt, A. M.; Arnold, B. R.; Radziszewski, J. G.; Facelli, J. C.; Malsch, K. D.; Strub, H.; Grant, D. M.; Michl, J. " $^{13}\text{C}$  NMR and Polarized IR Spectra of Vicinally Labeled [ $^{13}\text{C}_2$ ]Cyclobutadiene in an Argon Matrix: Interconversion of Valence Tautomers", *J. Am. Chem. Soc.* **1988**, *110*, 2648.
281. Tian, R.; Facelli, J. C.; Michl, J. "Vibrational and Electronic Spectra of Matrix-Isolated  $\text{N}_3 \bullet$  and  $\text{N}_3^-$ ", *J. Phys. Chem.* **1988**, *92*, 4073.
282. Magnera, T. F.; Balaji, V.; Michl, J.; Miller, R. D.; Sooriyakumaran, R.; "Laser Desorption Mass Spectrometry of Polysilanes", *Macromolecules* **1989**, *22*, 1624.
283. Welsh, K. M.; Michl, J.; West, R. "The Photochemistry of Matrix-Isolated Di-*tert*-butyldiazidosilane. Observation of Di-*tert*-butylsilylene and N,N'-Di-*tert*-butylsilanediimine", *J. Am. Chem. Soc.* **1988**, *110*, 6689.
- R 284. Raabe, G.; Michl, J. "Multiple Bonds to Silicon", in *The Chemistry of Organic Silicon Compounds*,

- Patai, S., Rappoport, Z., Eds.; John Wiley & Sons Ltd.: Chichester, 1989; Chapter 17, 1015.
285. Gebicki, J.; Michl, J. "Radiolytic Generation of Organic Radical Anions Isolated in Argon Matrix", *J. Phys. Chem.* **1988**, *92*, 6452.
286. Kaszynski, P.; Michl, J. "A Practical Photochemical Synthesis of Bicyclo[1.1.1]pentane-1,3-dicarboxylic Acid", *J. Org. Chem.* **1988**, *53*, 4593.
- R 287. Thulstrup, E. W.; Michl, J. "Spectroscopic Applications of Molecular Alignment," in *Polarized Spectroscopy of Ordered Systems*; Samorí, B.; Thulstrup, E.W., Eds., Kluwer Academic: Dordrecht, The Netherlands, 1988; p. 1.
- R 288. Michl, J.; Thulstrup, E. W. "Applications of IR and UV-Visible Linear Dichroism," in *Polarized Spectroscopy of Ordered Systems*; Samorí, B.; Thulstrup, E. W., Eds., Kluwer Academic: Dordrecht, The Netherlands, 1988; p. 25.
- R 289. Michl, J.; Bonačić-Koutecký, V. "Biradicals and Biradicaloids: A Unified View", *Tetrahedron* **1988**, *44*, 7559.
- C 290. Kaszynski, P.; Michl, J. "[n]Staffanes: A Molecular-Size 'Tinkertoy' Construction Set for Nanotechnology. Preparation of End-functionalized Telomers and a Polymer of [1.1.1]Propellane", *J. Am. Chem. Soc.* **1988**, *110*, 5225.
291. Michl, J.; Downing, J. W.; Karatsu, T.; McKinley, A. J.; Poggi, G.; Wallraff, G. M.; Sooriyakumaran, R.; Miller, R. D. "Solution Photochemistry of Poly(dialkylsilane)s, a New Class of Photoresists", *Pure Appl. Chem.* **1988**, *60*, 959.
- C 292. McKinley, A. J.; Karatsu, T.; Wallraff, G. M.; Miller, R. D.; Sooriyakumaran, R.; Michl, J. "Photodegradation of Poly(dialkylsilane)s in Solution: the Persistent Radicals Have an Unexpected Structure", *Organometallics* **1988**, *7*, 2567.
293. Kirkor, E. S.; David, D. E.; Michl, J. "'Salted' Iron Pentacarbonyl: Molecular Isolation in Alkali Halide Solids", *J. Am. Chem. Soc.* **1990**, *112*, 139.
294. Tian, R.; Michl, J. "Fast-Particle Bombardment of Solid Nitrogen", *Faraday Discussions No. 86*, **1988**, 113.
- R 295. Michl, J. "Photochromism by Orientation", in *Photochromism - Molecules and Systems*, Bouas-Laurent, H.; Dürr, H., Eds.; Elsevier: Amsterdam, 1990; Chap. 27, p 919.
296. Wallraff, G. M.; Vogel, E.; Michl, J. "Bridged [14]Annulenes in Superacids: Protonation and Oxidation to Dications. Transannular Interaction and Homoaromaticity", *J. Org. Chem.* **1988**, *53*, 5807.

297. Kirkor, E.; Maloney, V. M.; Michl, J. "The Photochemistry of 'Salted' Quadricyclane and Norbornadiene: Alkali Halide Color Centers as Catalysts", *J. Am. Chem. Soc.* **1990**, *112*, 148.
- C 298. Tian, R.; Balaji, V.; Michl, J. "Evidence For a Cyclic Form of the Azide Anion", *J. Am. Chem. Soc.* **1988**, *110*, 7225.
- B 299. Klessinger, M.; Michl, J. *Lichtabsorption und Photochemie Organischer Moleküle*; Verlag Chemie: Weinheim, Federal Republic of Germany, 1990.
- C 300. Kaszynski, P.; Friedli, A. C.; Michl, J. "Mesogenic Properties of Telomers of [1.1.1]Propellane", *Mol. Cryst. and Liq. Cryst. Lett.* **1988**, *6*, 27.
- C 301. Karatsu, T.; Miller, R. D.; Sooriyakumaran, R.; Michl, J. "The Mechanism of the Photochemical Degradation of Poly(di-n-alkylsilanes) in Solution", *J. Am. Chem. Soc.* **1989**, *111*, 1140.
302. Magnera, T. F.; David, D. E.; Stulik, D.; Orth, R. G.; Jonkman, H. T.; Michl, J. "Production of Hydrated Metal Ions by Fast Ion or Atom Beam Sputtering. Collision-Induced Dissociation and Successive Hydration Energies of Gaseous Cu<sup>+</sup> with 1-4 Water Molecules", *J. Am. Chem. Soc.* **1989**, *111*, 5036.
303. Bonačić-Koutecký, V.; Schöffel, K.; Michl, J. "Neutral and Charged Biradicaloids, Funnels in S<sub>1</sub> and their Role in Photochemistry", in *Proceedings of the Workshop on Quantum Chemistry*, Girona, Spain, July 1988; Carbó, R., Ed.; Elsevier: Amsterdam, **1988**, p 297-326.
- R 304. Michl, J.; Kaszynski, P.; Friedli, A. C.; Murthy, G. S.; Yang, H.-C.; Robinson, R. E.; McMurdie, N. D.; Kim, T. "Harnessing Strain: From [1.1.1]Propellanes to Tinkertoys", in *Strain and Its Implications in Organic Chemistry*; de Meijere, A.; Blechert, S., Eds.; NATO ASI Series, Vol. 273; Kluwer Academic Publishers: Dordrecht, The Netherlands, **1989**; p 463.
- C 305. Friedli, A. C.; Kaszynski, P.; Michl, J. "Towards a Molecular-size Construction Set: 3,3<sup>(n-1)</sup>-Bisacetylthio[n]staffanes", *Tetrahedron Lett.* **1989**, *30*, 455.
- R 306. Arnold, B. R.; Michl, J. "Spectroscopy of Cyclobutadiene", in *Kinetics and Spectroscopy of Carbenes and Biradicals*, Platz, M. S., Ed., Plenum: New York, NY, **1990**.
307. Robinson, R. E.; Michl, J. "Chlorination of Bicyclo[1.1.1]pentane Derivatives", *J. Org. Chem.* **1989**, *54*, 2051.
- C 308. Magnera, T. F.; David, D. E.; Michl, J. "Gas-Phase Water and Hydroxyl Binding Energies for Monopositive First-Row Transition Metal Ions", *J. Am. Chem. Soc.* **1989**, *111*, 4100.
309. Miller, R. D.; Willson, C. G.; Wallraff, G. M.; Clecak, N.; Sooriyakumaran, R.; Michl, J.; Karatsu, T.; McKinley, A. J.; Klingensmith, K. A.; Downing, J. "Polysilanes: Photochemistry and Lithography", *Proceedings of the SPE Conference on Photopolymers: Principles, Processes, and Materials*,

Ellenville, N.Y., **1988**, p. 111.

- B 310. Thulstrup, E. W.; Michl, J. *Elementary Polarization Spectroscopy*; VCH Publishers: New York, N.Y., **1989**.
311. Bonačić-Koutecký, V.; Schöffel, K.; Michl, J. "Electronic States of Cyclobutadiene Heteroanalogs. Critical Biradicaloids", *J. Am. Chem. Soc.* **1989**, *111*, 6140.
- P 312. Michl, J.; Radziszewski, G. "Methods and Compositions for Recording Optical Information Employing Molecular Pseudorotation", U.S. Patent No. 4,789,965, December 6, 1988.
313. Radziszewski, J. G.; Waluk, J.; Michl, J. "Site-Population Conserving and Site-Population Altering Photoorientation of Matrix-Isolated Free-Base Porphine by Double Proton Transfer: IR Dichroism and Vibrational Symmetry Assignments", *Chem. Phys.* **1989**, *136*, 165.
314. Barrau, J.; Balaji, V.; Michl, J. "Matrix Isolation and IR Spectroscopy of Germanethione Me<sub>2</sub>Ge=S", *Organometallics*, **1989**, *8*, 2034.
- R 315. Miller, R. D.; Michl, J. "Polysilane High Polymers", *Chem. Rev.* **1989**, *89*, 1359.
316. Waluk, J.; Klein, H.-P.; Ashe, A. J. III; Michl, J. "Effective Electronegativities of Phosphorus, Arsenic, and Antimony in a  $\pi$  System. Evidence from Magnetic Circular Dichroism", *Organometallics* **1989**, *8*, 2804.
- C 317. Murthy, G. S.; Hassenrück, K.; Lynch, V. M.; Michl, J. "[n]Staffanes: The Parent Hydrocarbons", *J. Am. Chem. Soc.* **1989**, *111*, 7262.
- B 318. Michl, J.; Bonačić-Koutecký, V. *Electronic Aspects of Organic Photochemistry*, John Wiley and Sons, Inc.: New York, **1990**.
319. Miller, R. D.; Wallraff, G.; Clecak, N.; Sooriyakumaran, R.; Michl, J.; Karatsu, T.; McKinley, A. J.; Klingensmith, K. A.; Downing, J. "Polysilanes: Solution Photochemistry and Deep UV Lithography", *Polym. Eng. Sci.* **1989**, *29*, 882.
320. Radziszewski, J. G.; Michl, J. "Doubled Multiplexing in Fourier Transform Raman Spectroscopy", *J. Appl. Spectrosc.* **1990**, *44*, 414.
321. Höweler, U.; Chatterjee, P. S.; Klingensmith, K. A.; Waluk, J.; Michl, J. "Electronic States and Magnetic Circular Dichroism of Cyclic  $\pi$ -Systems with Antiaromatic Perimeters", *Pure Appl. Chem.* **1989**, *61*, 2117.
322. Balaji, V.; David, D. E.; Magnera, T. F.; Michl, J.; Urbassek, H. M. "Sputtering Yields of Condensed Rare Gases", *Nucl. Instr. and Meth.* **1990**, *B46*, 435.

- C 323. Hassenrück, K.; Radziszewski, J. G.; Balaji, V.; Murthy, G. S.; McKinley, A. J.; David, D. E.; Lynch, V. M.; Martin, H.-D.; Michl, J. "A Body-Diagonal Bond in Cubane: Can It Be Introduced?", *J. Am. Chem. Soc.* **1990**, *112*, 873.
324. Hassenrück, K.; Murthy, G. S.; Lynch, V. M.; Michl, J. "'Mixed Staffanes' as Intermediate Length Staffs for Molecular-size Tinkertoys. Parent Hydrocarbons and Terminal Diiodides Combining Bicyclo[1.1.1]pentane with Cubane or Bicyclo[2.2.2]octane Units", *J. Org. Chem.* **1990**, *55*, 1013.
- C 325. Michl, J.; Friedli, A. C.; Obeng, Y. S.; Bard, A. J. "[*n*]Staffanes - A Novel Rigid Spacer Structure for Electron and Energy Transfer Studies", Proceedings of the Sixth International Conference on Energy and Electron Transfer; Fiala, J.; Pokorný, J., Eds.; Charles University: Prague, Czechoslovakia, **1989**.
326. Friedli, A. C.; Lynch, V. M.; Kaszynski, P.; Michl, J. "Structures of Six Terminally Substituted [*n*]Staffanes, *n* = 1-4" *Acta Cryst. B* **1990**, *46*, 377.
327. Arnold, B. R.; Balaji, V.; Michl, J. "The Structure of Matrix-Isolated *s-cis*-1,3-Butadiene from Polarized IR Spectra: A Closer Look", *J. Am. Chem. Soc.* **1990**, *112*, 1808.
- C 328. Kaszynski, P.; Friedli, A. C.; McMurdie, N. D.; Michl, J. "Synthesis of Liquid Crystals Based on Bicyclo[1.1.1]pentane", *Mol. Cryst. Liq. Cryst.* **1990**, *191*, 193.
329. Magnera, T. F.; David, D. E.; Michl, J. "The First Twenty-eight Gas-Phase Proton Hydration Energies", *Chem. Phys. Lett.* **1991**, *182*, 363.
330. Kaszynski, P.; Friedli, A. C.; Michl, J. "Towards a Molecular-Size 'Tinkertoy' Construction Set. Methyl [*n*]Staffane-3-carboxylates, Dimethyl [*n*]Staffane-3,3<sup>(*n*-1)</sup>-dicarboxylates, and [*n*]Staffane-3,3<sup>(*n*-1)</sup>-dithiols from [1.1.1]Propellane", *J. Am. Chem. Soc.* **1992**, *114*, 601.
331. Royan, B. W.; Burford, N.; Waluk, J.; Michl, J. "Magnetic Circular Dichroism of Cyclic  $\pi$ -Electron Systems. 29. Bicyclic Phospholium and Arsolium Cations with P-S, As-S, P-N, and As-N  $p\pi$ - $p\pi$  Bonding", *Organometallics* **1990**, *9*, 1085.
- R 332. David, D. E.; Michl, J. "Sputtering of Condensed Gases by Nuclear Stopping: Chemical Aspects", *Progress in Solid-State Chemistry* **1989**, *19*, 283.
333. Magnera, T. F.; David, D. E.; Michl, J. "Metastable, Collision-Induced and Laser-Induced Decomposition of  $\text{Ar}_m\text{N}_{2n}^+$  (*m* = 0,1) Cluster Ions in the Gas Phase", *J. Chem. Soc., Faraday Trans.* **1990**, 2427.
- C 334. Michl, J. "The Relationship of Bonding to Electronic Spectra", *Acc. Chem. Res.* **1990**, *23*, 127.
335. Radziszewski, J. G.; Waluk, J.; Michl, J. "FT Visible Absorption Spectroscopy of Porphine in Noble Gas Matrices", *J. Mol. Spectrosc.* **1990**, *140*, 373.

- R 336. Michl, J.; Balaji, V. "Calculations of Photochemical Reactivity. Oligosilanes as an Illustration" in *Computational Advances in Organic Chemistry*; Ögretir, C., Csizmadia, I. G., Eds.; Kluwer: Dordrecht, The Netherlands, **1991**; 323.
- P 337. Michl, J.; Murthy, P. S. "Polymers and Dye Combinations and Methods for Their Use in Optical Recording", U.S. Patent No. 4,864,537, September 5, 1989.
338. Kaszynski, P.; McMurdie, N. D.; Michl, J. "Synthesis of Doubly Bridgehead-Substituted Bicyclo[1.1.1]pentanes. Radical Transformations of Bridgehead Halides and Carboxylic Acids", *J. Org. Chem.* **1991**, *56*, 307.
- C 339. Arnold, B. R.; Radziszewski, J. G.; Campion, A.; Perry, S. S.; Michl, J. "Raman Spectrum of Matrix-Isolated Cyclobutadiene. Evidence for Environmental Hindrance to Heavy-Atom Tunneling?", *J. Am. Chem. Soc.* **1991**, *113*, 692.
340. Klingensmith, K. A.; Klein, R. F. X.; Anderson, A. G.; Horak, V.; Michl, J. "Magnetic Circular Dichroism of Cyclic  $\pi$ -Electron Systems. 30. Thialene and Isothialene", *J. Mol. Struct. , (THEOCHEM.)* **1991**, *227*, 351.
341. Čársky, P.; Downing, J. W.; Michl, J. " $A_g$  Vibrational Levels of Cyclobutadiene on a New Potential Energy Surface", *Int. J. Quantum Chem.* **1991**, *40*, 415.
342. Radziszewski, J. G.; Waluk, J.; Nepraš, M.; Michl, J. "Fourier-Transform Fluorescence and Phosphorescence of Porphine in Rare-Gas Matrices", *J. Phys. Chem.* **1991**, *95*, 1963.
343. Arnold, B. R.; Balaji, V.; Downing, J. W.; Radziszewski, J. G.; Fisher, J. J.; Michl, J. "IR Polarization Directions in *s-trans*-1,3-Butadiene and the Average Topochemistry of the *s-cis* to *s-trans* Photoisomerization in Matrix Isolation", *J. Am. Chem. Soc.* **1991**, *113*, 2910.
344. Waluk, J.; Michl, J. "The Perimeter Model and Magnetic Circular Dichroism of Porphyrin Analogues", *J. Org. Chem.* **1991**, *56*, 2729.
345. Waluk, J.; Hemmi, G.; Sessler, J. L.; Michl, J. "Magnetic Circular Dichroism of Metallotexaphyrins", *J. Org. Chem.* **1991**, *56*, 2735.
346. McKinley, A. J.; Michl, J. "EPR-ENDOR Spectroscopy of Matrix-Isolated  $NH_3^+$  and  $CH_3$  Radicals", *J. Phys. Chem.* **1991**, *95*, 2674.
347. Sun, Y.-P.; Miller, R. D.; Sooriyakumaran, R.; Michl, J. "Fluorescence of Poly(di-*n*-alkylsilane)s in Room-Temperature Solution", *J. Inorg. Organomet. Polym.* **1991**, *1*, 3.
348. McKinley, A. J.; Karatsu, T.; Wallraff, G. M.; Thompson, D. P.; Miller, R. D.; Michl, J. "Solution Photochemistry of Poly(di-*n*-alkylsilane)s. An EPR-ENDOR Study of the Structure of the Persistent Radicals", *J. Am. Chem. Soc.* **1991**, *113*, 2003.

349. Balaji, V.; Michl, J. "Singlet Excitation in Polysilanes: *Ab initio* Calculations on Oligosilane Models", *Polyhedron* **1991**, *10*, 1265.
350. Waluk, J.; Müller, M.; Swiderek, P.; Köcher, M.; Vogel, E.; Hohlneicher, G.; Michl, J. "Electronic States of Porphyrenes", *J. Am. Chem. Soc.* **1991**, *113*, 5511.
- C 351. Davidson, I. M. T.; Michl, J.; Simpson, T. "Photochemistry of Permethyloligosilanes", *Organometallics* **1991**, *10*, 842.
352. Waluk, J.; Fetzer, J.; Hamrock, S. J.; Michl, J. "Evidence for Conformational Equilibrium in an Unsubstituted Benzenoid Hydrocarbon, Tetrabenz[a,c,d,f,l]perylene", *J. Phys. Chem.* **1991**, *95*, 8660.
- R 353. Michl, J. "The States of an Electron Pair and Photochemical Reactivity" in *Theoretical and Computational Models for Organic Chemistry*, Formosinho, S. J., Csizmadia, I. G., Arnaut, L. G., Eds.; Kluwer: Dordrecht, The Netherlands, **1991**; 207.
354. Zahradník, R.; Balaji, V.; Michl, J. "An SCF Study of Ten-Vertex and Twelve-Vertex Boranes and Heteroboranes", *J. Comp. Chem.* **1991**, *12*, 1147.
355. Friberg, S. E.; Kayali, I.; Kaszynski, P.; Michl, J. "Influence of 3-Pentyl-bicyclo[1.1.1]pentane-1-carboxylic Acid on a Simplified Stratum Corneum Lipid Structure", *Langmuir* **1992**, *8*, 996.
356. Brotin, T.; Waluk, J.; Desvergne, J.-P.; Bouas-Laurent, H.; Michl, J. "Electronic Absorption Properties of Symmetrical Dialkoxyanthracenes. Linear Dichroism and Magnetic Circular Dichroism", *Photochem. Photobiol.* **1992**, *55*, 335.
357. Sun, Y.-P.; Wallraff, G. M.; Miller, R. D.; Michl, J. "Models for Polysilane High Polymers. Room-temperature Solution Fluorescence Quenching in Linear Si<sub>10</sub>Me<sub>22</sub>, Si<sub>16</sub>Me<sub>34</sub>, and Poly(methylpropylsilane) by Carbon Tetrachloride", *J. Photochem. Photobiol.* **1992**, *62*, 333.
358. Magnera, T. F.; Michl, J. "Photodissociation of Ar<sub>n-m</sub>N<sub>2m</sub><sup>+</sup> Clusters (n=2 or 3, m=0-n)", *Chem. Phys. Lett.* **1992**, *192*, 99.
- C 359. Khabashesku, V. N.; Balaji, V.; Boganov, S. E.; Bashkirova, S. A.; Matveichev, P. M.; Chernyshev, E. V.; Nefedov, O. M.; Michl, J. "Matrix Isolation and Photochemical Interconversion of Silacyclopentadienes", *Mendeleev Commun.* **1992**, *1*, 38.
- R 360. Michl, J. "Solution Photophysics and Electronic Structure of Polysilanes", *Synth. Met.*, **1992**, *50*, 367.
- R 361. Michl, J.; Sun, Y.-P. "Electronic Structure, Photophysics and Photochemistry of Polysilanes", in *Polymeric Materials*, ACS Symposium Series 527, Reichmanis, E., O'Donnell, J.H., and Frank, C.W., Eds.; American Chemical Society: Washington, DC, **1993**; Chapter 10, p. 131.

362. Michl, J., "Singlet and Triplet States of an Electron Pair in a Molecule--A Simple Model", *J. Mol. Struct. (THEOCHEM.)* **1992**, 260, 299.
363. Sun, Y.-P.; Hamada, Y.; Huang, L. M.; Maxka, J.; Hsiao, J.-S.; West, R.; Michl, J. "Models for Polysilane High Polymers. I. Singlet Photophysics of Linear Permethylhexadecasilane (Si<sub>16</sub>Me<sub>34</sub>)", *J. Am. Chem. Soc.* **1992**, 114, 6301.
364. Sun, Y.-P.; Michl, J. "Models for Polysilane High Polymers. II. Photophysics of Linear Permethylhexasilane: A Low-Lying Franck-Condon Forbidden Excited Singlet State", *J. Am. Chem. Soc.*, **1992**, 114, 8186.
365. Obeng, Y. S.; Laing, M. E.; Friedli, A. C.; Yang, H. C.; Wang, D.; Thulstrup, E. W.; Bard, A. J.; Michl, J. "Self-Assembled Monolayers of Parent and Derivatized [n]Staffane-3,3<sup>(n-1)</sup>-Dithiols on Polycrystalline Gold Electrodes", *J. Am. Chem. Soc.*, **1992**, 114, 9943.
366. Hamrock, S. J.; Michl, J. "2,2-Dichloro[1.1.1]propellane", *J. Org. Chem.* **1992**, 57, 5027.
367. McKinley, A. J.; Ibrahim, P. N.; Balaji, V.; Michl, J. "Long-Range Spin Density Propagation in Saturated Hydrocarbons: 3-[n]Staffyl Radicals", *J. Am. Chem. Soc.*, **1992**, 114, 10631.
368. Burland, D. M.; Downing, J.; Michl, J. "A Two-State Model for the First Hyperpolarizability of Donor-Acceptor Substituted Systems", *Nonlinear Optics*, **1992**, 3, 195.
369. Čársky, P.; Michl, J. "Heavy-Atom Tunneling in Cyclobutadiene: *Ab Initio* Calculation of the Intensities of a<sub>g</sub> Raman Lines", *Theor. Chim. Acta*, **1992**, 84, 125.
- C 370. Plitt, H. S.; Michl, J. "Conformational Effects on  $\sigma$ -Conjugation: UV and IR Spectra of Matrix Isolated *trans*- and *gauche-n*-Si<sub>4</sub>Me<sub>10</sub>", *Chem. Phys. Lett.*, **1992**, 198, 400.
371. Gudipati, M. S.; Hamrock, S. J.; Balaji, V.; Michl, J. "Infrared Spectra of [n]Staffanes", *J. Phys. Chem.*, **1992**, 96, 10165.
372. Yang, H. C.; Magnera, T. F.; Lee, C.-M.; Bard, A. J.; Michl, J. "Rigid-Rod Langmuir-Blodgett Films from [n]Staffane-3-carboxylates", *Langmuir*, **1992**, 8, 2740.
373. Radziszewski, J. G.; Yin, T. -Y.; Renzoni, G. E.; Hrovat, D. A.; Borden, W. T.; Michl, J. "Matrix Isolation of Tricyclo[3.3.1.0<sup>3,7</sup>]non-3(7)-ene -- a Doubly Pyramidalized Alkene Predicted to Have a Nearly Tetrahedral Geometry at the Olefin Carbons", *J. Am. Chem. Soc.*, **1993**, 115, 1454.
374. Janecki, T.; Shi, S.; Kaszynski, P.; Michl, J. "[n]Staffanes with Terminal Nitrile and Isonitrile Functionalities and Their Metal Complexes", *Collect. Czech. Chem. Commun.*, **1993**, 58, 89.
375. Müller, J.; Baše, K.; Magnera, T. F.; Michl, J. "Rigid-Rod Oligo-*p*-Carboranes for Molecular Tinkertoys", *J. Am. Chem. Soc.*, **1992**, 114, 9721.

- R 376. Michl, J. "Formation of Charged Clusters by Sputtering of Frozen Gases", *Analisis*, **1992**, 20, 45s.
377. Magnera, T. F.; Michl, J. "O<sub>n</sub><sup>+</sup> Clusters Produced by Sputtering of Solid Oxygen", *Z. Phys. D - Atoms, Molecules and Clusters*, **1993**, 26, 93.
- B 378. Klessinger, M.; Michl, J. *Excited States and Photochemistry of Organic Molecules*, VCH Publishers: New York, NY, **1995**.
379. Gudipati, M. S.; Radziszewski, J. G.; Kaszynski, P.; Michl, J. "Bicyclo[3.2.2]non-1-ene: Matrix Isolation and Spectroscopic Characterization of a Moderately Strained Bridgehead Olefin", *J. Org. Chem.*, **1993**, 58, 3668.
- R 380. Michl, J. "Supramolecular Assemblies from 'Tinkertoy' Rigid-Rod Molecules" in *Mesomolecules: From Molecules To Materials*, Mendenhall, G. D., Liebman, J. F., and Greenberg, A., eds; Chapman & Hall, New York: **1995**, p. 132.
381. Radziszewski, J. G.; Kaszynski, P.; Littmann, D.; V. Balaji; Hess Jr., B. A.; Michl, J. "Twisted Si=N Bonds: Matrix Isolation of Bridgehead Silanimines", *J. Am. Chem. Soc.*, **1993**, 115, 8401.
382. Radziszewski, J. G.; Littmann, D.; Balaji, V.; Fabry, L.; Gross, G.; Michl, J. "Multiply Bonded Silicon: Matrix Isolation and Chemical Trapping of Products of Pyrolysis and Photolysis of Triazidophenylsilane", *Organometallics*, **1993**, 12, 4816.
383. Khabashesku, V. N.; Balaji, V.; Bogarov, S. E.; Nefedev, D. M.; Michl, J. "Matrix Isolation of Silacyclopentadienes: UV-Vis and IR Spectra and Photochemical Interconversion", *J. Am. Chem. Soc.*, **1994**, 116, 320.
384. Arnold, B. R.; Michl, J. "Ultraviolet and Polarized Infrared Spectroscopy of Matrix-Isolated Cyclobutadiene and Its Isotopomers", *J. Phys. Chem.*, **1993**, 97, 13348.
385. Magnera, T. F.; Sammond, D. M.; Michl, J. "Ground State Rotational Constant of Ar<sub>3</sub><sup>+</sup> by Rotational Depletion Coherence Spectroscopy", *Chem. Phys. Lett.*, **1993**, 211, 378.
386. Plitt, H.; Balaji, V.; Michl, J. "Localization of Singlet Excitation in Short Silicon Chains, Si<sub>2</sub>Me<sub>6</sub> to Si<sub>6</sub>Me<sub>14</sub>", *Chem. Phys. Lett.*, **1993**, 213, 158.
- R 387. Michl, J. "[n]Staffanes: Inert Rods for a Molecular Construction Set", *1995 McGraw Hill Yearbook of Science and Technology*, McGraw Hill, New York, p. 391.
388. Plitt, H. S.; Downing, J. W.; Raymond, M. K.; Balaji, V.; Michl, J. "Photophysics and Potential Energy Hypersurfaces of Permethylated Oligosilanes", *J. Chem. Soc. Faraday Trans.*, **1994**, 90, 1653.
389. Kramer, B.; Fleischhauer, J.; Michl, J. "Magnetischer Circular Dichroismus (MCD) von cyclischen π-Elektronensystemen mit 4N ± 1 Elektronen", *Z. Naturforsch.*, **1993**, 48a, 1243.

- R 390. Plitt, H. S.; Downing, J. W.; Teramae, H.; Raymond, M. K.; Michl, J. "Electronic Structure and UV Absorption Spectra of Permethylated Silicon Chains", *Polymeric Materials for Microelectronic Applications: Science and Technology*, ACS Symposium Series 579, Ito, H.; Tagawa, S.; Horie, K., Eds.; American Chemical Society: Washington, DC, 1994; Chapter 30, p. 376.
- R 391. Kaszynski, P.; Michl, J. "[n]Staffanes", in *Advances in Strain in Organic Chemistry, IV*. Halton, B., Ed.; JAI Press Inc., Greenwich, CT, 1995, p. 283.
392. Čársky, P.; Hrouda, V.; Michl, J. "Cubic-Grid Gaussian Basis Sets for Electron Scattering Calculations. I. Definition and Construction", *Int. J. Quant. Chem.*, **1995**, 53, 419.
393. Čársky, P.; Hrouda, V.; Michl, J. "Cubic-Grid Gaussian Basis Sets for Electron Scattering Calculations. II. Matrix Elements", *Int. J. Quant. Chem.*, **1995**, 53, 431.
394. Čársky, P.; Hrouda, V.; Michl, J.; Antic, D. "Cubic-Grid Gaussian Basis Sets for Electron Scattering Calculations. III. Effect of Basis Set Translation and Size on the Calculated Cross Section", *Int. J. Quant. Chem.*, **1995**, 53, 437.
395. Hrouda, V.; Polášek, M.; Čársky, P.; Michl, J. "Cubic-Grid Gaussian Basis Sets for Electron Scattering Calculations. IV. Differential Cross Section Averaging for Isotropic Samples", *Theor. Chim. Acta*, **1994**, 89, 401.
396. Teramae, H.; Michl, J. "Electronic States of Linear Tetrasilane and Polysilanes", *Mol. Cryst. Liq. Cryst.*, **1994**, 256, 149.
- R 397. Kaszynski, P.; Michl, J. "[1.1.1]Propellanes", in *The Chemistry of the Cyclopropyl Group*, Rappoport, Z., ed., John Wiley & Sons, Chichester, England, 1995, Vol. 2, p. 773.
- R 398. Michl, J. "The 'Molecular Tinkertoy' Approach to Materials", in *Applications of Organometallic Chemistry in the Preparation and Processing of Advanced Materials*, Harrod, J. F. and Laine, R. M., eds., Kluwer, Dordrecht, The Netherlands, **1995**, p. 243.
- R 399. Michl, J. "Synthesis of Giant Modular Structures", in *Chemical Synthesis: Gnosis to Prognosis*, Chatgililoglu, C. and Snieckus, V., eds., Kluwer, Dordrecht, The Netherlands, **1996**, p. 429.
- C 400. Albinsson, B.; Michl, J. "The Gauche, Ortho, and Anti Conformers of Perfluoro-*n*-butane: Matrix-Isolation IR Spectra", *J. Am. Chem. Soc.*, **1995**, 117, 6378.
401. Radziszewski, J.G.; Nepraš, M.; Balaji, V.; Waluk, J.; Vogel, E.; Michl, J. "Polarized IR Spectra of Photooriented Matrix-Isolated Free-Base Porphyrin Isotopomers", *J. Phys. Chem.* **1995**, 99, 14254.
402. Schöberl, U.; Magnera, T. F.; Harrison, R.; Fleischer, F.; Pflug, J. L.; Schwab, P. F. H.; Meng, X.; Lipiak, D.; Noll, B. C.; Allured, V. S.; Rudalevige, T.; Lee, S.; Michl, J. "Towards a Hexagonal Grid Polymer: Synthesis, Coupling, and Chemically Reversible Surface-Pinning of the Star Connectors,

- 1,3,5-C<sub>6</sub>H<sub>3</sub>(CB<sub>10</sub>H<sub>10</sub>CX)<sub>3</sub>", *J. Am. Chem. Soc.* **1997**, *119*, 3907.
403. Balaji, V.; David, D.; Tian, R.; Urbassek, H.; Michl, J. "keV-Energy Sputtering of Condensed Diatomic Gases", *J. Phys. Chem.* **1995**, *99*, 15565.
- P 404. Michl, J.; Kaszynski, P.; Friedli, A. C. "Compounds and Methods Based on [1.1.1]Propellane", U.S. Patent No. 5,405,550, April 11, 1995.
405. Albinsson, B.; Teramae, H.; Downing, J. W.; Michl, J. "Conformers of Saturated Chains: Matrix Isolation, Structure, IR and UV Spectra of *n*-Si<sub>4</sub>Me<sub>10</sub>", *Chem. Eur. J.* **1996**, *2*, 529.
- B 406. Michl, J.; Thulstrup, E. W. *Spectroscopy with Polarized Light. Solute Alignment by Photoselection, in Liquid Crystals, Polymers, and Membranes*, revised soft-cover edition; VCH Publishers: Deerfield Beach, Florida, **1995**.
407. Albinsson, B.; Michl, J. "The Anti, Ortho, and Gauche Conformers of Perfluoro-*n*-Butane: Matrix-Isolation IR Spectra and Calculations", *J. Phys. Chem.* **1996**, *100*, 3418.
408. Orendt, A. M.; Facelli, J. C.; Radziszewski, J. G.; Horton, W. J.; Grant, D. M.; Michl, J. "<sup>13</sup>C Dipolar NMR Spectrum of Matrix Isolated *o*-Benzyne-1,2-<sup>13</sup>C<sub>2</sub>", *J. Am. Chem. Soc.* **1996**, *118*, 846.
- R 409. Harrison, R. M.; Magnera, T. F.; Vacek, J.; Michl, J. "Towards Designer Solids", in *Modular Chemistry*, Michl, J., ed., Kluwer, Dordrecht, The Netherlands, **1997**, p 1.
410. Michl, J. "Spin-Orbit Coupling in Biradicals. 1. The 2-Electrons-in-2-Orbitals Model Revisited", *J. Am. Chem. Soc.* **1996**, *118*, 3568.
- C 411. King, B. T.; Janoušek, Z.; Grüner, B.; Trammel, M.; Noll, B. C.; Michl, J. "Dodecamethylcarba-closo-dodecaborate(-) Anion", CB<sub>11</sub>Me<sub>12</sub>", *J. Am. Chem. Soc.* **1996**, *118*, 3313.
412. Levin, M. D.; Kaszynski, P.; Michl, J. "Photochemical Synthesis of Bicyclo[1.1.1]pentane-1,3-dicarboxylic Acid", *Org. Syn.* **2000**, *77*, 249.
413. Albinsson, B.; Teramae, H.; Plitt, H. S.; Goss, L. M.; Schmidbaur, H.; Michl, J. "Matrix-Isolation IR and UV Spectra of Si<sub>3</sub>H<sub>8</sub> and Si<sub>4</sub>H<sub>10</sub>: Isomers and Conformers of Oligosilanes", *J. Phys. Chem.* **1996**, *100*, 8681.
414. Khabashesku, V. N.; Boganov, S. E.; Antic, D.; Nefedov, O. M.; Michl, J. "Matrix Isolation of Germacyclopentadienes: Direct Spectroscopic Evidence for Germylene-to-Germene Photochemical Interconversion", *Organometallics* **1996**, *15*, 4714.
415. DeLeeuw, S. W.; Solvaeson, D.; Ratner, M. A.; Michl, J. "Molecular Dipole Chains: Excitations and Dissipation", *J. Phys. Chem. B* **1998**, *102*, 3876.

416. Radziszewski, J. G.; Downing, J. W.; Gudipati, M. S.; Balaji, V.; Thulstrup, E. W.; Michl, J. "How Predictable Are IR Transition Moment Directions? Assignments of Vibrational Transitions in Propene and Deuterated Propenes", *J. Am. Chem. Soc.* **1996**, *118*, 10275.
417. Čársky, P.; Hroudá, V.; Polášek, M.; David, D. E.; Antic, D.; Michl, J. "Cubic-Grid Gaussian Basis Sets for Electron Scattering Calculations. VI. Applications to H<sub>2</sub>, H<sub>2</sub>O and CH<sub>4</sub>", *J. Phys. Chem. A* **1997**, *101*, 3754.
418. Michl, J.; Havlas, Z. "Spin-Orbit Coupling in Biradicals: Structural Aspects", *Pure Appl. Chem.* **1997**, *69*, 785.
419. Havlas, Z.; Michl, J. "Spin-Orbit Coupling in Organic Biradicals: Zero-Field Splitting in Triplet Tetramethyleneethane", *J. Mol. Struct. (THEOCHEM.)* **1997**, 398-399, 281.
- C 420. King, B. T.; Noll, B. C.; McKinley, A. J.; Michl, J. "Dodecamethylcarba-*closo*-dodecaboranyl (CB<sub>11</sub>Me<sub>12</sub>•), a Stable Free Radical", *J. Am. Chem. Soc.* **1996**, *118*, 10902.
421. Levin, M. D.; Hamrock, S. J.; Kaszynski, P.; Shtarev, A. B.; Levina, G. A.; Noll, B. C.; Ashley, M. E.; Newmark, R.; Moore, G. G. I.; Michl, J. "Preparation, Structure, and Properties of Symmetrically 1,3-Difunctionalized Penta- and Hexafluorobicyclo[1.1.1]pentanes", *J. Am. Chem. Soc.* **1997**, *119*, 12750.
- R 422. Michl, J. book review of *Molecular and Biomolecular Electronics* (R.R. Birge, Ed., Advances in Chemistry Series, 240; American Chemical Society: Washington, DC, 1994), *Int. J. Quant. Chem.*, **1997**, *62*, 237.
423. Magnera, T. F.; Peslherbe, L. M.; Körblová, E.; Michl, J. "The Organometallic 'Molecular Tinkertoy' Approach to Planar Grid Polymers", *J. Organomet. Chem.* **1997**, *548*, 83.
- R 424. Bernardi, F.; Olivucci, M.; Michl, J.; Robb, M. A. "Conical Intersections in the Theory of Organic Singlet Photochemistry", *The Spectrum* **1996**, *9*, 1.
425. Harrison, R. M.; Brotin, T.; Noll, B. C.; Michl, J. "Towards a Square Grid Polymer: Synthesis and Structure of Pedestal-Mounted Tetragonal Star Connectors, C<sub>4</sub>R<sub>4</sub>-Co-C<sub>5</sub>Y<sub>5</sub>", *Organometallics* **1997**, *16*, 3401.
426. Imhof, R.; Antic, D.; David, D. E.; Michl, J. "Conformational Effects in Photoelectron Spectra of Tetrasilanes", *J. Phys. Chem. A* **1997**, *101*, 4579.
- C 427. Imhof, R.; Teramae, H.; Michl, J. "Conformational Effects in UV Absorption Spectra of Tetrasilanes", *Chem. Phys. Lett.* **1997**, *270*, 500.
- R 428. Magnera, T. F.; Pecka, J.; Vacek, J.; Michl, J. "Synthesis and Handling of Single Sheets of a Covalent Monolayer Square Grid Polymer," in *Nanostructural Materials: Clusters, Composites, and Thin Films*, Moskovits, M.; Shalaev, V., Eds., ACS Symposium Series 679, American Chemical Society:

Washington, DC, **1997**, p. 213.

- C 429. Mazières, S.; Raymond, M. K.; Raabe, G.; Prodi, A.; Michl, J. "[2]Staffane Rod as a Molecular Rack for Unravelling Conformer Properties: Proposed Singlet Excitation Localization Isomerism in *anti,anti,anti*-Hexasilanes", *J. Am. Chem. Soc.* **1997**, *119*, 6682.
- C 430. Teramae, H.; Michl, J. "Geometry of the Localized  $\sigma\sigma^*$  Excited State of *n*-Tetrasilane", *Chem. Phys. Lett.* **1997**, *276*, 127.
431. Neumann, F.; Teramae, H.; Downing, J. W.; Michl, J. "Gauche, Ortho, and Anti Conformations of Saturated  $A_4X_{10}$  Chains: When Will all Six Conformers Exist?", *J. Am. Chem. Soc.* **1998**, *120*, 573.
432. Pospíšil, L.; Heyrovský, M.; Pecka, J.; Michl, J. "Towards a Hexagonal Grid Polymer: Interaction of Tentacled 1,3,5-Tricarboranylbenzene Derivatives with Mercury Surface," *Langmuir* **1997**, *13*, 6294.
433. Vacek, J.; Michl, J. "A Molecular 'Tinkertoy' Construction Kit: Computer Simulation of Molecular Propellers", *New J. Chem.* **1997**, *21*, 1259.
- B 434. Michl, J., ed., *Modular Chemistry, NATO ASI Series*, Vol. C499, Kluwer: Dordrecht, The Netherlands, **1997**.
- R 435. Neumann, F.; Michl, J. "Conformational Search: Linear Chains," in *The Encyclopedia of Computational Chemistry* Schleyer, P. v. R.; Allinger, N. L.; Clark, T.; Gasteiger, J.; Kollman, P. A.; Schaefer III, H. F.; Schreiner, P. R., Eds., Wiley: Chichester, England, **1998**, Vol. 1, p 556.
436. Zharov, I.; Saxena, A.; Michl, J.; Miller, R. D. "C-Hydroxydicarba-*closo*-dodecaboranes," *Inorg. Chem* **1997**, *36*, 6033.
437. Crespo, R.; Teramae, H.; Antic, D.; Michl, J. "Calculation of the Conformational Dependence of Valence and Rydberg States in *n*-Tetrasilane," *Chem. Phys.* **1999**, *244*, 203.
- R 438. Magnera, T. F.; Pecka, J.; Michl, J. "Synthesis of a Covalent Square Grid," In *Science and Technology of Polymers & Advanced Materials*, Prasad, P. N.; Mark, J. E.; Kandil, S. H.; Kafafi, Z. H., eds.; Plenum: New York, **1998**, p. 385.
439. Mazal, C.; Paraskos, A. J.; Michl, J. "Symmetric Bridgehead-to-Bridgehead Coupling of Bicyclo[1.1.1]pentanes and [*n*]Staffanes," *J. Org. Chem.* **1998**, *63*, 2116.
440. Raymond, M. K.; Magnera, T. F.; Zharov, I.; West, R.; Dreczewski, B.; Nozik, A. J.; Sprague, J.; Ellingson, R. J.; Michl, J.; "Low-Temperature Photophysics of Permethylated *n*-Heptasilane: The Borderline between Excitation Localization and Delocalization in a Conjugated Chain," in *Applied Fluorescence in Chemistry, Biology, and Medicine*, Rettig, W.; Strehmel, B.; Schrader, S., eds; Springer Verlag: Heidelberg, **1999**, p. 79.

- R 441. Michl, J.; "Magnetic Circular Dichroism of  $\pi$  Systems," in *The Encyclopedia of Computational Chemistry*, Schleyer P. v. R.; Allinger, N. L.; Clark, T.; Gasteiger, J.; Kollman, P. A.; Schaefer III, H. F.; Schreiner, P. R., Eds., Wiley: Chichester, England, **1998**, Vol. 3, p 1548.
- R 442. Pospíšil, L.; King, B. T.; Michl, J. "Voltammetry in Benzene Using Lithium Dodecamethylcarba-*closo*-dodecaborate,  $\text{LiCB}_{11}\text{Me}_{12}$ , as a Supporting Electrolyte: Reduction of  $\text{Ag}^{+}$ ", *Electrochim. Acta* **1998**, *44*, 103.
443. Havlas, Z.; Downing, J. W.; Michl, J. "Spin-Orbit Coupling in Biradicals. 2. *Ab Initio* Methodology and Application to 1,1-Biradicals: Carbene and Silylene", *J. Phys. Chem. A* **1998**, *102*, 5681.
444. Höweler, U.; Downing, J. W.; Fleischhauer, J.; Michl, J. "MCD of Non-Aromatic Cyclic  $\pi$ -Electron Systems. 1. The Perimeter Model for Antiaromatic 4*N*-Electron [*n*]Annulene Biradicals", *Perkin Transactions 2* **1998**, 1101.
445. Raymond, M. K.; Michl, J. "Quantum Confinement Induced Collapse of a Large to a Small Radius Self-Trapped Exciton in a Permethylated Polysilane Chain", *Int. J. Quant. Chem.* **1999**, *72*, 361.
- P 446. Michl, J.; King, B. T.; Janoušek, Z. "Weakly Nucleophilic Anions", U.S. Patent No. 5,731,470, March 24, 1998.
447. Fleischhauer, J.; Höweler, U.; Michl, J. "MCD of Non-Aromatic Cyclic  $\pi$ -Electron Systems. 2. The Perimeter Model for High-Symmetry 'Unaromatic' and 'Ambiaromatic' Molecules Derived from 4*N*-Electron [*n*]Annulenes", *Spectrochim. Acta* **1999**, *55A*, 585.
448. Havlas, Z.; Michl, J. "Spin-Orbit Coupling in Biradicals. 3. Heavy Atom Effects in Carbenes", *Collect. Czech. Chem. Commun.* **1998**, *63*, 1485.
449. Choi, C. H.; Kertesz, M.; Dobrin, S.; Michl, J. "Argon-Matrix-Isolation Raman Spectra and Density Functional Study of 1,3-Butadiene Conformers", *Theor. Chem. Accounts* **1999**, *102*, 196.
450. Albinsson, B.; Antic, D.; Neumann, F.; Michl, J. "The Conformers of *n*- $\text{Si}_5\text{Me}_{12}$ : A Comparison of *Ab Initio* and Molecular Mechanics Methods", *J. Phys. Chem. A* **1999**, *103*, 2184.
451. Grüner, B.; Janoušek, Z.; King, B. T.; Guan, H.-W.; Wang, C. H.; Vřetečka, V.; Michl, J. "Synthesis of 12-Substituted 1-Carba-*closo*-dodecaborate Anions and First Hyperpolarizability of the 12- $\text{C}_7\text{H}_6^+ - \text{CB}_{11}\text{H}_{11}^-$  Ylide", *J. Am. Chem. Soc.* **1999**, *121*, 3122. Erratum: *J. Am. Chem. Soc.* **2000**, *122*, 11274.
452. Brotin, T.; Pospíšil, L.; Fiedler, J.; King, B. T.; Michl, J. "Towards a Square Grid Polymer: Electrochemistry of Tentacled Tetragonal Star Connectors,  $\text{C}_4\text{R}_4\text{-Co-C}_5(\text{HgY})_5$ , on Mercury", *J. Phys. Chem. B* **1998**, *102*, 10062.
- R 453. Michl, J. "Optical Spectroscopy, Linear Polarization Theory", *Encyclopedia of Spectroscopy and*

*Spectrometry* **1999**, 1701.

454. Adcock, W.; Blokhin, A. V.; Elsey, G. M.; Head, N. H.; Krstic, A. R.; Levin, M. D.; Michl, J.; Munton, J.; Pinkhassik, E. Z.; Robert, M.; Savéant, J.-M.; Shtarev, A.; Stibor, I. "Manifestations of Bridgehead-Bridgehead Interactions in the Bicyclo[1.1.1]pentane System", *J. Org. Chem.* **1999**, *64*, 2618.
455. Magnera, T. F.; Michl, J. "Towards a More Regular Square Grid Polymer", *Atualidades de Físico-Química Orgânica* **1998**, 50.
456. King, B. T.; Noll, B. C.; Michl, J. "Cation- $\pi$  Interactions in the Solid State: Crystal Structures of  $M^+(\text{Benzene})_2\text{CB}_{11}\text{Me}_{12}^-$  ( $M = \text{Tl, Cs, Rb, K, Na}$ ) and  $\text{Li}^+(\text{Toluene})\text{CB}_{11}\text{Me}_{12}^-$ ", *Collect. Czech. Chem. Commun.*, **1999** *64*, 1001.
- R 457. Michl, J.; West, R. "Electronic Structure and Spectroscopy of Polysilanes", in *Silicon-Containing Polymers: The Science and Technology of their Synthesis and Applications*, Jones, R. G.; Ando, W.; Chojnowski, J., Eds., Kluwer Academic Publishers: Dordrecht, The Netherlands, 2000, p 499.
- R 458. Schwab, P. F. H.; Levin, M. D.; Michl, J. "Molecular Rods. 1. Simple Axial Rods", *Chem. Rev.* **1999**, *99*, 1863.
- P 459. Michl, J.; Magnera, T. F.; David, D. E.; Harrison, R. M. "Method of Assembly of Molecular-Sized Nets and Scaffolding", U.S. Patent 5,876,830, March 2, 1999.
460. Havlas, Z.; Michl, J. "Ab Initio Calculation of Zero-field Splitting and Spin-orbit Coupling in Ground and Excited Triplets of *m*-Xylylene", *J. Chem. Soc., Perkin Trans. 2* **1999**, 2299.
- R 461. Levin, M. D.; Kaszynski, P.; Michl, J. "Bicyclo[1.1.1]pentanes, [n]Staffanes, [1.1.1]Propellanes, and Tricyclo[2.1.0.0<sup>2,5</sup>]pentanes", *Chem. Rev.* **2000**, *100*, 169.
462. Ottosson, C. H.; Michl, J. "Conformers of *n*-Si<sub>6</sub>Me<sub>14</sub>: Ab Initio, Molecular Mechanics, and Additive Increment Methods", *J. Phys. Chem. A* **2000**, *104*, 3367.
463. Fogarty, H. A.; Ottosson, C. H.; Michl, J. "The Five Favored Backbone Conformations of *n*-Si<sub>4</sub>Et<sub>10</sub>: Cisoid, Gauche, Ortho, Deviant, and Transoid", *J. Mol. Struct. (Theochem)* **2000**, *506*, 243.
464. Zink, R.; Magnera, T. F.; Michl, J. "The Transoid, Ortho and Gauche Conformers of *n*-Si<sub>4</sub>Cl<sub>10</sub>: Mid-IR and Raman Matrix-Isolation Spectra", *J. Phys. Chem. A* **2000**, *104*, 3829.
465. Vacek, J.; Chocholousova, J.; Michl, J. "Calculations for a Gas-Flow Driven Molecular Rotor", *Proceedings of the HPCMP Users Group Conference*, Pittsburgh, PA, June 18-21, 2005, IEEE: Los Alamitos, CA, 2007, p 153.
466. Fleischhauer, J.; Höweler, U.; Michl, J. "MCD of Non-Aromatic Cyclic  $\pi$ -Electron Systems. 3. The

Perimeter Model for Low-Symmetry “Unaromatic” and “Ambiaromatic” Molecules Derived from 4*N*-Electron [*n*] Annulenes”, *J. Phys. Chem. A* **2000**, *104*, 7762. Erratum, *J. Phys. Chem. A* **2009**, *113*, 10866.

467. Fleischhauer, J.; Michl, J. “MCD of Non-Aromatic Cyclic  $\pi$ -Electron Systems. 4. Explicit Relations between Molecular Structure and Spectra”, *J. Phys. Chem. A* **2000**, *104*, 7776.
468. Shtarev, A. B.; Pinkhassik, E.; Levin, M. D.; Stibor, I.; Michl, J. “Partially Bridge-Fluorinated Dimethyl Bicyclo[1.1.1]pentane-1,3-dicarboxylates: Preparation and NMR Spectra”, *J. Am. Chem. Soc.* **2001**, *123*, 3484.
469. Fogarty, H. A.; Ottosson, C. H.; Michl, J. “Conformations of Oligosilanes with Ethyl and Methyl Substituents”, *J. Mol. Struct.* **2000**, *556*, 105.
- C 470. Zharov, I.; King, B. T.; Havlas, Z.; Pardi, A.; Michl, J. “Crystal Structure of  $n\text{-Bu}_3\text{Sn}^+\text{CB}_{11}\text{Me}_{12}^-$ ”, *J. Am. Chem. Soc.* **2000**, *122*, 10253.
- C 471. King, B. T.; Michl, J. “The Explosive “Inert” Anion  $\text{CB}_{11}(\text{CF}_3)_{12}^-$ ”, *J. Am. Chem. Soc.* **2000**, *122*, 10255.
472. Crespo, R.; Merchán, M.; Michl, J. “Electronic Excitation in a Saturated Chain: An MS-CASPT2 Treatment of the Anti Conformer of *n*-Tetrasilane”, *J. Phys. Chem. A* **2000**, *104*, 8593.
- C 473. Michl, J.; West, R. “Conformations of Linear Chains. Systematics and Suggestions for Nomenclature”, *Acc. Chem. Res.* **2000**, *33*, 821.
- R 474. Khabashesku, V. N.; Boganov, S. E.; Kudin, K. N.; Margrave, J. L.; Michl, J.; Nefedov, O. M. “Interconversions of the Silylene-to-Silene and Germylene-to-Germene Types: Direct Spectroscopic Studies and Calculations”, *Russian Chem. Bull.* **1999**, *48*, 2003.
475. Vacek, J.; Michl, J. “Molecular Dynamics of a Grid-Mounted Molecular Dipolar Rotor in a Rotating Electric Field”, *Proc. Natl. Acad. Sci. USA* **2001**, *98*, 5481.
- R 476. Zharov, I.; Michl, J. “Free and Complexed  $\text{R}_3\text{M}^+$  Cations (M = Ge, Sn, Pb)”, *Supplement: The Chemistry of Organo-Ge, Sn, and Pb Compounds* - Vol. 2, Ed. Z. Rappoport, **2002** Wiley: Chichester, UK, 633.
477. Tsuji, H.; Toshimitsu, A.; Tamao, K.; Michl, J. “UV, MCD, and LD Spectra of a Conformationally Constrained *ortho*-Tetrasilane: Support for the Avoided Crossing Model of Conformational Effects on Excited States”, *J. Phys. Chem. A* **2001**, *105*, 10246.
478. Franken, A.; King, B. T.; Rudolph, J.; Rao, P.; Noll, B. C.; Michl, J. “Preparation of [*closo*- $\text{CB}_{11}\text{H}_{12}$ ] by Dichlorocarbene Insertion into [*nido*- $\text{B}_{11}\text{H}_{14}$ ]”, *Collect. Czech. Chem. Commun.* **2001**, *66*, 1238.

479. David, D. E.; Balaji, V.; Urbassek, H. M.; Michl, J. "Sputtering of Condensed Polyatomic Gases by keV-Energy Ions", *Int. J. Mass Spect.* **2001**, *212*, 477.
- C 480. Moss, S.; King, B. T.; de Meijere, A.; Kozhushkov, S. I.; Eaton, P. E.; Michl, J. "LiCB<sub>11</sub>Me<sub>12</sub>: A Catalyst for Pericyclic Rearrangements", *Org. Lett.* **2001**, *3*, 2375.
481. Schwab, P. F. H.; Fleischer, F.; Michl, J. "Preparation of 5- and 5,5'-Brominated 2,2'-Bipyridines and 2,2'-Bipyrimidines", *J. Org. Chem.* **2002**, *67*, 443.
482. Zharov, I.; Michl, J.; Sherwood, M. H.; Sooriyakamarun, R.; Larson, C. E.; DiPietro, R. A.; Breyta, G.; Wallraff, G. M. "Mechanistic Studies of the Acidolysis Reactions Occurring in Silicon-Containing Bilayer Photoresists", *Chem. Mat.* **2002** *14*, 656.
483. Piqueras, M.; Crespo, R.; Michl, J., "Multiconfigurational Second-order Perturbation Calculation of the Electronic Absorption Spectrum of Trisilane, Si<sub>3</sub>H<sub>8</sub>", *Mol. Phys.* **2002**, *100*, 747.
- C 484. Havlas, Z.; Michl, J., "Prediction of an Inverse Heavy-Atom Effect in H-C-CH<sub>2</sub>Br: Bromine Substituent as a  $\pi$  Acceptor", *J. Am. Chem. Soc.* **2002**, *124*, 5606.
485. Tonne, J.; Prinzbach, H.; Michl, J., "Double Actinometry for Rigorous Evaluation of Quantum Yields of Clean Photoreversible Photochemical Reactions", *Photochem. Photophys. Sci.* **2002**, *1*, 105.
486. Fogarty, H. A.; Tsuji, H.; David, D. E.; Ottosson, C.-H.; Ehara, M.; Nakatsuji, H.; Tamao, K.; Michl, J., "Peralkylated Tetrasilanes: Conformational Dependence of the Photoelectron Spectrum", *J. Phys. Chem. A* **2002**, *106*, 2369.
- C 487. Dobkowski, J.; Wójcik, J.; Koźmiński, W.; Kołos, R.; Waluk, J.; Michl, J., "An Experimental Test of C-N Bond Twisting in the TICT State: Syn-Anti Photoisomerization in 2-(N-Methyl-N-isopropylamino)-5-cyanopyridine", *J. Am. Chem. Soc.* **2002**, *124*, 2406.
- R 488. King, B. T.; Zharov, I.; Michl, J. "Alkylated Carborane Anions and Radicals: Tools for Organic and Inorganic Chemists", *Chem. Innov.* **2001**, *31*, 23.
489. Honda, Y.; Hada, M.; Ehara, M.; Nakatsuji, H.; Downing, J.; Michl, J. "Relativistic Effects on Magnetic Circular Dichroism Studied by GUHF/SECI Method", *Chem. Phys. Lett.* **2002**, *355*, 219.
490. Magnera, T. F.; Michl, J. "Two-Dimensional Supramolecular Chemistry with Molecular Tinkertoys", *Proc. Nat. Acad. Sci. USA* **2002**, *99*, 4788.
491. Liu, K.; Avouris, P.; Bucchignano, J.; Martel, R.; Sun, S.; Michl, J. "Simple Fabrication Scheme for sub-10 nm Electrode Gaps Using Electron-Beam Lithography", *Appl. Phys. Lett.* **2002** *80*, 865.
492. Clarke, L. I.; Horinek, D.; Kottas, G. S.; Varaksa, N.; Magnera, T. F.; Hinderer, T. P.; Horansky, R. D.; Michl, J.; Price, J. C. "Dielectric Response of Chloromethylsilyl and Dichloromethylsilyl Dipolar

Rotors on Fused Silica Surfaces”, *Nanotechnology* **2002**, *13*, 533.

493. Varaksa, N.; Pospíšil, L.; Magnera, T. F.; Michl, J. “Self-Assembly of a Metal Ion Bound Monolayer of Trigonal Connectors on Mercury. An Electrochemical Langmuir Trough”, *Proc. Nat. Acad. Sci. USA* **2002**, *99*, 5012.
494. Schwab, P. F. H.; Noll, B. C.; Michl, J. "Synthesis and Structure of Trigonal and Tetragonal Connectors for a 'Tinkertoy' Construction Set," *J. Org. Chem.* **2002**, *67*, 5476.
495. Piqueras, M. C.; Merchán, M.; Crespo, R.; Michl, J. "Conformational Effects on the UV Absorption Spectrum of *n*-Tetrasilane: An MS-CASPT2 Treatment," *J. Phys. Chem. A* **2002**, *106*, 9868.
496. Schepers, T.; Michl, J. "Optimized Ladder C and Ladder H Models for Sigma Conjugation: Chain Segmentation in Polysilanes", *J. Phys. Org. Chem.* **2002**, *15*, 490.
- R 497. Michl, J.; "Historical Introduction", in *Conical Intersections: Electronic Structure, Dynamics, and Spectroscopy*, Domcke, W.; Yarkony, D. R.; Köppel, H., Eds. **2004** World Scientific: Singapore, ix.
498. Janoušek, Z.; Hilton, C.; Schreiber, P. J.; Michl, J. "C-Halogenation of the *closo*-[CB<sub>11</sub>H<sub>12</sub>]<sup>-</sup> Anion," *Collect. Czech. Chem. Commun.* **2002**, *67*, 1025.
- C 499. McKee, M. L.; Michl, J. "A Possible Reinterpretation of the Photoelectron Spectra of [CCl<sub>2</sub>]<sup>-</sup>, [CBr<sub>2</sub>]<sup>-</sup>, and [Cl<sub>2</sub>]<sup>-</sup>: A Role for Quartet Isodihalocarbene and/or Dihalocarbene Radical Anions?," *J. Phys. Chem. A* **2002**, *106*, 8495.
- R 500. Tsuji, H.; Michl, J.; Toshimitsu, A.; Tamao, K. “Synthetic Approach for Elucidation of Relationship between Photophysical Properties and Conformation of Oligosilanes”, *J. Synth. Org. Chem. Jpn.* **2002**, *60*, 762.
501. Berlin, Y. A.; Hutchison, G. R.; Rempala, P.; Ratner, M. A.; Michl, J. “Charge Hopping in Molecular Wires as a Sequence of Electron Transfer Reactions”, *J. Phys. Chem. A* **2003**, *107*, 3970.
502. Dobkowski, J.; Michl, J.; Waluk, J. "Electronic Spectroscopy and Photophysics of 2-(N-Methyl-N-isopropylamino)-5-cyanopyridine and Related Compounds", *Phys. Chem. Chem. Phys.* **2003**, *5*, 1027.
503. Casher, D. L.; Tsuji, H.; Sano, A.; Katkevics, M.; Toshimitsu, A.; Tamao, K.; Kubota, M.; Kobayashi, T.; Ottosson, H.; David, D. E.; Michl, J. "The Disilane Chromophore: Photoelectron and Electronic Spectra of Hexaalkyldisilanes and 1,(*n*+2)-Disila[*n.n.n*]propellanes", *J. Phys. Chem. A* **2003**, *107*, 3559.
504. Rempala, P.; Michl, J. “A Proposed Mechanism of [*closo*-CB<sub>11</sub>H<sub>12</sub>]<sup>-</sup> Formation by Dichlorocarbene Insertion into [*nido*-B<sub>11</sub>H<sub>14</sub>]<sup>-</sup>, A Computational Study by Density Functional Theory”, *Collect. Czech. Chem. Commun.* **2003**, *68*, 644.

505. Piqueras, M. C.; Crespo, R.; Michl, J. "The Transoid, Ortho, and Gauche Conformers of Decamethyl-*n*-tetrasilane,  $n\text{-Si}_4\text{Me}_{10}$ : Electronic Transitions in the Multistate Complete Active Space 2nd-Order Perturbation Theory Description", *J. Phys. Chem. A* **2003**, *107*, 4661.
- P 506. Hofer, D. C.; MacDonald, S. A.; Mahorowala, A. P.; Miller, R. D.; Michl, J.; Wallraff, G. M. "Hydroxycarborane photoresists and process for using same in bilayer thin film imaging lithography", US Patent 6,482,566, November 19, 2002.
507. Wang, B.; Zheng, X.; Michl, J.; Foley, E. T.; Hersam, M. C.; Bilić, A.; Crossley, M. J.; Reimers, J. R.; Hush, N. S. "An Azanorborene Anchor for Molecular-level Construction on Silicon(100)", *Nanotechnology* **2004**, *15*, 324.
- R 508. Tsuji, H.; Michl, J.; Tamao, K. "Recent Experimental and Theoretical Aspects of the Conformational Dependence of UV Absorption of Short Chain Peralkylated Oligosilanes", *J. Organomet. Chem.* **2003**, *685*, 9.
- R 509. Fogarty, H. A.; Casher, D. L.; Imhof, R.; Schepers, T.; Rooklin, D. W.; Michl, J. "Sigma Bonds: Electronic Structure, Photophysics, and Photochemistry of Oligosilanes", *Pure Appl. Chem.* **2003**, *75*, 999.
510. Rooklin, D. W.; Schepers, T.; Raymond-Johansson, M. K.; Michl, J. "Time-Dependent Density Functional Theory Treatment of the First UV Absorption Band in All-Transoid Permethyloligosilanes  $\text{Si}_n\text{Me}_{2n+2}$  ( $n = 2 - 8, 10$ )", *Photochem. Photophys. Sci.* **2003**, *2*, 511.
511. Horinek, D.; Michl, J. "Molecular Dynamics Simulation of an Electric Field Driven Dipolar Molecular Rotor Attached to a Quartz Glass Surface", *J. Am. Chem. Soc.* **2003**, *125*, 11900.
512. Mulcahy, M. E.; Berets, S. L.; Milosevic, M.; Michl, J. "Enhanced Sensitivity in Single-Reflection Spectroscopy of Organic Monolayers on Metal Substrates (pseudo-ATR)", *J. Phys. Chem. B* **2004**, *108*, 1519.
- R 513. Varaksa, N.; Magnera, T. F.; Michl, J. "Electrochemical Langmuir Trough", in *Dekker Encyclopedia of Nanoscience and Nanotechnology*, Schwarz, J. A.; Contescu, C.; Putyera, K., Eds., Marcel Dekker, Inc.: New York, **2004**, p. 1043.
- R 514. Havlas, Z.; Kývala, M.; Michl, J. "Spin-Orbit Coupling", in *Computational Methods in Photochemistry*, Kutateladze, A. G., Ed., CRC Press: Boca Raton, FL, **2005**, p. 111.
- C 515. Janoušek, Z.; Lehmann, U.; Častulík, J.; Čísařová, I.; Michl, J. "Li<sup>+</sup>-Induced  $\sigma$ -Bond Metathesis: Aryl for Methyl Exchange on Boron in a Methylated Monocarbododecaborate Anion", *J. Am. Chem. Soc.* **2004**, *126*, 4060.
- P 516. Michl, J.; Price, J. C.; Magnera, T. F. "Molecular Dipolar Rotors", US Patent 6,628,016, September 30, 2003.

517. Havlas, Z.; Kývala, M.; Michl, J. "Spin-Orbit Coupling in Biradicals. 4. Zero-Field Splitting in Triplet Nitrenes, Phosphinidenes, and Arsinidenes", *Collect. Czech. Chem. Commun.* **2003**, *68*, 2335.
- C 518. Zheng, X.; Mulcahy, M. E.; Horinek, D.; Galeotti, F.; Magnera, T. F.; Michl, J. "Dipolar and Non-Polar Altitudinal Molecular Rotors Mounted on a Au(111) Surface", *J. Am. Chem. Soc.* **2004**, *126*, 4540.
519. Fleischhauer, J.; Höweler, U.; Spanget-Larsen, J.; Raabe, G.; Michl, J. "MCD of Non-Aromatic Cyclic  $\pi$ -Electron Systems. 5. Biphenylene and its Aza Analogs", *J. Phys. Chem. A* **2004**, *108*, 3225.
520. Honda, Y.; Hada, M.; Ehara, M.; Nakatsuji, H.; Michl, J. "Theoretical studies on magnetic circular dichroism by the finite perturbation method with relativistic corrections", *J. Chem. Phys.* **2005**, *123*, 164113.
521. Caskey, D. C.; Shoemaker, R. K.; Michl, J. "Toward Self-Assembled Surface-Mounted Prismatic Altitudinal Rotors. A Test Case: Molecular Rectangle", *Org. Lett.* **2004**, *6*, 2093.
522. Zharov, I.; Weng, T.; Orendt, A. M.; Barich, D. H.; Penner-Hahn, J.; Grant, D. M.; Havlas, Z.; Michl, J. "Metal Cation - Methyl Interactions in  $\text{CB}_{11}\text{Me}_{12}^-$  Salts of  $\text{Me}_3\text{Ge}^+$ ,  $\text{Me}_3\text{Sn}^+$ , and  $\text{Me}_3\text{Pb}^+$ ", *J. Am. Chem. Soc.* **2004**, *126*, 12033.
523. Fogarty, H. A.; Imhof, R.; Michl, J. "Magnetic Circular Dichroism of Peralkylated Tetrasilane Conformers", *Proc. Natl. Acad. Sci.* **2004**, *101*, 10517.
524. Valášek, M.; Pecka, J.; Jindřich, J.; Calleja, G.; Craig, P. R.; Michl, J. "Oligomers of 'Extended Viologen', *p*-Phenylene-bis-4,4'-(1-aryl-2,6-diphenylpyridinium), as Candidates for Electron-Dopable Molecular Wires", *J. Org. Chem.* **2005**, *70*, 405.
525. Vyakaranam, K.; Körbe, S.; Divišová, H.; Michl, J. "A New Type of Intermediate,  $\text{C}^+(\text{BCH}_3)_{11}^- \leftrightarrow \text{C}(\text{BCH}_3)_{11}$ , in a Grob Fragmentation Coupled with Intramolecular Hydride Transfer. A Non-Classical Carbocation Ylide or a Carbenoid?", *J. Am. Chem. Soc.* **2004**, *126*, 15795.
526. Körbe, S.; Sowers, D. B.; Franken, A.; Michl, J. "Preparation of 1-*p*-Halophenyl and 1-*p*-Biphenyl Substituted Monocarbododecaborate Anions [*closo*-1-Ar- $\text{CB}_{11}\text{H}_{11}$ ] $^-$  by Insertion of Arylhalocarbenes into [*nido*- $\text{B}_{11}\text{H}_{14}$ ]", *Inorg. Chem.* **2004**, *43*, 8158.
527. David, D. E.; Popović, D. B.; Antic, D.; Michl, J. "A Multichannel Electron Energy Loss Spectrometer for Low-Temperature Condensed Films", *J. Chem. Phys.* **2004**, *121*, 10542.
528. Popović, D. B.; David, D. E.; Michl, J., Čurík, R.; Čársky, P. "Joint experimental and theoretical study of vibrationally inelastic electron scattering on propane", *J. Chem. Phys.* **2004**, *121*, 10551.
529. Havlas, Z.; Kývala, M.; Michl, J. "Spin-Orbit Coupling in Biradicals. 5. Zero-Field Splitting in Triplet Dimethylnitrenium, Dimethylphosphenium, and Dimethylarsenium Cations", *Mol. Phys.*

2005, 103, 407.

- R 530. Kottas, G. S.; Clarke, L. I.; Horinek, D.; Michl, J. "Artificial Molecular Rotors", *Chem. Rev.* **2005**, *105*, 1281.
531. Fleischhauer, J.; Raabe, G.; Klingensmith, K. A.; Höweler, U.; Chatterjee, P. K.; Hafner, K.; Vogel, E.; Michl, J. "MCD of Non-Aromatic Cyclic  $\pi$ -Electron Systems. Part 6: Pentalenes and Heptalenes", *Int. J. Quantum Chem.* **2005**, *102*, 925.
- R 532. Schwab, P. F. H.; Smith, J. R.; Michl, J. "Synthesis and Properties of Molecular Rods. 2. Zig-Zag Rods," *Chem. Rev.* **2005**, *105*, 1197.
- R 533. Michl, J. "Photophysics of Organic Molecules in Solution", in *Handbook of Photochemistry, Third Edition*, Montalti, M.; Credi, A.; Prodi, L.; Gandolfi, M. T., Eds. **2006** Marcel Dekker/CRC Press: Boca Raton, FL, p. 1.
534. Caskey, D. C.; Michl, J. "Toward Self-Assembled Surface-Mounted Prismatic Altitudinal Rotors. A Test Case: Trigonal and Tetragonal Prisms", *J. Org. Chem.* **2005**, *70*, 5442.
- R 535. Michl, J. "Foreword", in *Computational Photochemistry*, Olivucci, M., Ed. **2005** Elsevier: Amsterdam, The Netherlands, p. ix.
536. Piqueras, M. C.; Michl, J.; Crespo, R. "MS-CASPT2 Analysis of the UV Thermochromism of Octamethyltrisilane", *Mol. Phys.* **2006**, *104*, 1107.
- R 537. Magnera, T. F.; Michl, J. "Altitudinal Surface-Mounted Molecular Rotors", *Topics in Current Chemistry*, Kelly, T. R., Ed. **2005** Springer-Verlag: Berlin, Germany, p. 63.
538. Zharov, I.; Havlas, Z.; Orendt, A. M.; Barich, D. H.; Grant, D. M.; Fete, M. G.; Michl, J. "CB<sub>11</sub>Me<sub>11</sub> Boronium Ylides: Carba-*closo*-dodecaboranes with a Naked Boron Vertex", *J. Am. Chem. Soc.* **2006**, *128*, 6089.
539. Funston, A. Kirby, J. P.; Miller, J. R.; Pospíšil, L.; Fiedler, J.; Hromadová, M.; Gál, M.; Pecka, J.; Valášek, M.; Zawada, Z.; Rempala, P.; Michl, J. "One-Electron Reduction of an 'Extended Viologen', *p*-Phenylene-bis-4,4'-(1-aryl-2,6-diphenylpyridinium) Dication", *J. Phys. Chem. A* **2005**, *109*, 10862.
540. Caskey, D. C.; Wang, B.; Zheng, X.; Michl, J. "Self-Assembled Trigonal Prismatic Altitudinal Rotors with Triptycene Paddle Wheels", *Collect. Czech. Chem. Commun.* **2005**, *70*, 1970.
541. Horinek, D.; Michl, J. "Surface Mounted Altitudinal Molecular Rotors in Alternating Electric Field: Single-Molecule Parametric Oscillator Molecular Dynamics", *Proc. Natl. Acad. Sci.* **2005**, *102*, 14175.

542. Vyakaranam, K.; Janoušek, Z.; Eriksson, L.; Michl, J. "Preparation of Undecamethylated and Hexamethylated 1-Halocarpa-*closo*-dodecaborate Anions", *Heteroatom Chem.* **2006**, *17*, 217.
543. Vyakaranam, K.; Körbe, S.; Michl, J. "Air-Initiated Radical Polymerization of Lithium Salts of  $\omega$ -(Undecamethylcarba-*closo*-dodecaboran-1'-yl)alk-1-enes,  $\text{CH}_2=\text{CH}(\text{CH}_2)_{n-2}\text{C}(\text{BMe})_{11}^- \text{Li}^+$ ", *J. Am. Chem. Soc.* **2006**, *128*, 5680.
544. Horansky, R. D.; Magnera, T. F.; Price, J. C.; Michl, J. "Artificial Dipolar Molecular Rotors", in *Controlled Nanoscale Motion*, Lecture Notes in Physics, Vol. 711, Linke, H.; Månsson, A., Eds., Springer: Berlin and Heidelberg, 2007, p 303.
545. Göötz, B.; Popović, D. B.; David, D. E.; Michl, J.; Swiderek, P. "Depth and angular profiles of inelastic low energy electron scattering in condensed molecular samples", *J. Phys. Chem. B* **2006**, *110*, 5480.
546. Mazal, C.; Škarka, O.; Kaleta, J.; Michl, J. "Cis-endo-Bicyclo[1.1.1]pentane-1,2,3,4-tetracarboxylic Acid and Its Derivatives", *Org. Lett.* **2006**, *8*, 749.
547. Vyakaranam, K.; Barbour, J. B.; Michl, J. " $\text{Li}^+$ -Catalyzed Radical Polymerization of Simple Terminal Alkenes", *J. Am. Chem. Soc.* **2006**, *128*, 5610.
548. Pospíšil, L.; Fiedler, J.; Hromadová, M.; Gál, M.; Valášek, M.; Pecka, J.; Michl, J. "Search for a One-Electron Reduction of the Cation Radical of an "Extended Viologen", *p*-Phenylene-bis-4,4'-(1-Aryl-2,6-Diphenylpyridinium)", *J. Electrochem. Soc.* **2006**, *153*, E179.
549. Ehara, M.; Fukawa, S.; Nakatsuji, H.; David, D. E.; Pinkhassik, E. Z.; Levin, M. D.; Apostol, M.; Michl, J. "Through-Cage Coupling between Substituents: Synthesis and Valence Ionized States of Bridgehead Disubstituted Parent and Hexafluorinated Bicyclo[1.1.1]pentane Derivatives,  $\text{C}_5\text{X}_6\text{Y}_2$ ", *Chemistry - An Asian Journal* **2007**, *2*, 1007.
550. Paci, I.; Johnson, J. C.; Chen, X.; Rana, G.; Popović, D.; David, D. E.; Nozik, A. J.; Ratner, M. A.; Michl, J. "Singlet Fission for Dye-Sensitized Solar Cells: Can a Suitable Sensitizer Be Found?", *J. Am. Chem. Soc.* **2006**, *128*, 16546.
551. Vacek, J.; Horinek, D.; Michl, J. "Calculations of molecular rotors and motors", *Proceedings of the HPCMP Users Group Conference*, Nashville, TN, June 27-30, 2005, IEEE: Los Alamitos, CA, 2005, p 1.
552. Vacek, J.; Kobr, L.; Miller, J.; Michl, J.; "Design of a Fast Artificial Light-Absorption Driven Molecular Rotor", In *Foundations of Nanoscience: Self-Assembled Architectures and Devices*, Proceedings of the Second Annual Conference, Snowbird, UT, April 24-28, 2005; Reif, J., Ed.; ScienceTechnica: Durham, NC, 2005, p 233.
553. Vacek, J.; Chocholoušová, J.; Kobr, L.; Miller, J.; Michl, J. "Calculations of Light-Absorption Driven

Molecular Rotors”, *Proceedings of the HPCMP Users Group Conference*, Denver, CO, June 26-29, 2006; IEEE: Los Alamitos, CA, 2006, p 193.

554. Vacek, J.; Horinek, D.; Michl, J. “Molecular Dynamics of a Fast Artificial Electric-Field Driven Surface-Mounted Molecular Rotor: A Single-Molecule Parametric Oscillator”, In *Foundations of Nanoscience: Self-Assembled Architectures and Devices*, Proceedings of the Second Annual Conference, Snowbird, UT, April 24-28, 2005; Reif, J., Ed.; ScienceTechnica: Durham, NC, 2005, p 241.
555. Fogarty, H. A.; Ottosson, H.; Michl, J. “Calculation of Relative Energies of Permethylated Oligosilane Conformers in Vapor and in Alkane Solution”, *J. Phys. Chem. B* **2006**, *110*, 25485.
556. Pouwer, R. H.; Harper, J. B.; Vyakaranam, K.; Michl, J.; Williams, C. M.; Jessena, C. H.; Bernhardt, P. V. “Investigating Direct Alkynylation at the Bridgehead of Bicyclic Cages using Silver(I) acetylides”, *Eur. J. Org. Chem.* **2007**, 241.
557. Pospíšil, L.; Varaksa, N.; Magnera, T. F.; Brotin, T.; Michl, J. “Adsorption of Tentacled Tetragonal Star Connectors,  $C_4R_4-Co-C_5(HgX)_5$ , on Mercury”, *Langmuir* **2007**, *23*, 930.
558. King, B. T.; Körbe, S.; Schreiber, P. J.; Clayton, J.; Němcová, A.; Havlas, Z.; Vyakaranam, K.; Fete, M. G.; Zharov, I.; Ceremuga, J.; Michl, J. “The Sixteen  $CB_{11}H_nMe_{12-n}^-$  Anions with Five-fold Substitution Symmetry: Anodic Oxidation and Electronic Structure”, *J. Am. Chem. Soc.* **2007**, *129*, 12960.
559. Eriksson, L.; Vyakaranam, K.; Ludvík, J.; Michl, J. “Synthesis of the Isolable Biradicals  $^*(CH_3B)_{11}C-C\equiv C-C(BCH_3)_{11}^*$  and *trans*- $^*(CH_3B)_{11}C-CH=CH-C(BCH_3)_{11}^*$ ”, *J. Org. Chem.* **2007**, *72*, 2351.
560. Körbe, S.; Schreiber, P. J.; Michl, J. “Chemistry of the Carba-*closo*-Dodecaborate(-) Anion,  $CB_{11}H_{12}^-$ ”, *Chem Rev.* **2006**, *106*, 5208.
- C 561. Vyakaranam, K.; Havlas, Z.; Michl, J. “Aromatic Substitution with Hypercloso  $C(BCH_3)_{11}$ : a New Mechanism”, *J. Am. Chem. Soc.* **2007**, *129*, 4172.
562. Crespo, R.; Piqueras, M. C.; Michl, J. “Electronic Excitation in a *syn*-Tetrasilane: 1,1,2,2,3,3,4,4-Octamethyltetrasilacyclopentane”, *Theor. Chem. Acc.* **2007**, *118*, 81.
563. Vacek, J.; Michl, J. “Artificial Surface-Mounted Molecular Rotors: Molecular Dynamics Simulations”, *Adv. Funct. Mater.* **2007**, *17*, 730.
- P 564. Franken, A.; King, B. T.; Michl, J. “Preparation of Carborane Anions”, US Patent 7 161 040, January 9, 2007.
565. Munrow, M. R.; Subramanian, R.; Minei, A. J.; Antic, D.; MacLeod, M. K.; Michl, J.; Crespo, R.; Piqueras, M. C.; Izuha, M.; Ito, T.; Tatamitani, Y.; Yamanou, K.; Ogata, T.; Novick, S. E. “Rotational

spectra of gauche perfluoro-*n*-butane, C<sub>4</sub>F<sub>10</sub>; perfluoro-*iso*-butane, (CF<sub>3</sub>)<sub>3</sub>CF; and tris(trifluoromethyl)methane, (CF<sub>3</sub>)<sub>3</sub>CH”, *J. Mol. Spectrosc.* **2007**, *242*, 129.

566. Kjærsgaard, T.; Jansik, B.; Jørgensen, P.; Coriani, S.; Michl, J. “Gauge-Origin Independent Coupled Cluster Singles and Doubles Calculation of Magnetic Circular Dichroism of Azabenzenes and Phosphabenzene Using London Orbitals”, *J. Phys. Chem. A* **2007**, *111*, 11278.
567. Joseph, Y.; Peić, A.; Chen, X.; Michl, J.; Vossmeier, T.; Yasuda, A. “Vapor Sensitivity of Networked Gold-Nanoparticle Chemiresistors: The Importance of Flexibility and Resistivity of the Interlinkage”, *J. Phys. Chem. C* **2007**, *111*, 12855.
- R 568. Michl, J., Commentary. In *Molecular Quantum Mechanics: Analytic Gradients and Beyond*; A. G. Császár, G. Fogarasi, H. F. Schaefer III, P. G. Szalay, Eds.; Institute of Chemistry, Budapest, Hungary, 2007; p 311.
569. Čársky, P.; Čurík, R.; Pezler, B.; Michl, J. “Angular Distributions for Vibrationally Inelastic Nonresonant Scattering of Electrons by Molecules”, *J. Phys. Chem. A* **2007**, *111*, 12216.
570. Michl, J. “Li<sup>+</sup> Catalyzed Polymerization of Simple Alkenes”, *The Catalyst Rev. Newsletter* **2007**, *4*.
571. Michl, J.; Nozik, A. J.; Chen, X.; Johnson, J. C.; Rana, G.; Akdag, A.; Schwerin, A. F. “Toward singlet fission for excitonic solar cells”, in *Organic Photovoltaics VIII*, Kafafi, Z. H. and Lane, P. A., Eds. **2007** Proc. of SPIE Vol. 6656, p. 66560E1.
572. Michl, J. “Chemistry of the Three-Dimensionally Aromatic CB<sub>11</sub> Cage”, *Pure Appl. Chem.* **2008**, *80*, 429.
573. Caskey, D. C.; Yamamoto, T.; Addicott, C.; Shoemaker, R. K.; Vacek, J.; Hawkrige, A. M.; Muddiman, D. C.; Kottas, G. S.; Michl, J.; Stang, P. J. “Coordination-Driven Face-Directed Self-Assembly of Trigonal Prisms. Face-Based Conformational Chirality”, *J. Am. Chem. Soc.* **2008**, *130*, 7620.
574. Vacek, J.; Caskey, D. C.; Horinek, D.; Shoemaker, R. K.; Stang, P. J.; Michl, J. “Pyridine Ligand Rotation in Self-Assembled Trigonal Prisms. Evidence for Intra-Cage Solvent Vapor Bubbles?”, *J. Am. Chem. Soc.* **2008**, *130*, 7629.
575. Veis, L.; Čársky, P.; Pittner, J.; Michl, J. “Coupled Cluster Study of Polycyclopentanes: Structure and Properties of C<sub>5</sub>H<sub>2n</sub>, n = 0 - 4”, *Collect Czech. Chem. Commun.* **2008**, *73*, 1525.
576. Clayton, J. R.; King, B. T.; Zharov, I.; Fete, M. G.; Michl, J. “Salts of Dodecamethylcarba-*closo*-dodecaborate(-) Anion, CB<sub>11</sub>Me<sub>12</sub><sup>-</sup>, and the Radical Dodecamethylcarba-*closo*-dodecaboranyl, CB<sub>11</sub>Me<sub>12</sub><sup>•</sup>”, submitted for publication.
577. Michl, J. “Comment on molecular machines based on non-interlocking molecules (other than

- catenanes and rotaxanes)”, submitted for publication.
578. Winston, E. B.; Lowell, P. J.; Vacek, J.; Chocholoušová, J.; Michl, J.; Price, J. C. “Dipolar molecular rotors in the metal-organic framework crystal IRMOF-2”, *Phys. Chem. Chem. Phys.* **2008**, *10*, 5188.
579. Piqueras, M. C.; Crespo, R.; Michl, J. “Interpretation of the Electronic Spectra of Four Disilanes”, *J. Phys. Chem. A.*, **2008**, *112* 13095.
580. Michl, J. “The Eightieth Birthday of Professor Rudolf Zahradník”, *Collect. Czech. Chem. Commun.* **2008**, *73*, i.
- R 581. Michl, J. “Katalýza Radikálové Polymerace Jednoduchých Alkenů Lithiovými Kationty”, *Chem. Listy* **2008**, *102*, 873.
582. Volkis, V.; Mei, H.; Shoemaker, R. K.; Michl, J. “LiCB<sub>11</sub>(CH<sub>3</sub>)<sub>12</sub> Catalyzed Radical Polymerization of Isobutylene: Highly Branched Polyisobutylene and an Isobutylene - Ethyl Acrylate Copolymer”, *J. Am. Chem. Soc.* **2009**, *131*, 3132.
583. Vacek, J.; Chocholoušová, J.; Michl, J. “Calculations of Lithium<sup>+</sup> Carborane Complexes”, *Proceedings of the HPCMP Users Group Conference*, in press.
584. Oliva, J. M.; Serrano-Andrés, L.; Havlas, Z.; Michl, J. “On the Electronic Structure of a Dianion, a Radical Anion, and a Neutral Diradical Carborane Dimer”, *J. Mol. Struct.* **2009**, *912*, 13.
- P 585. Michl, J.; Vyakaranam, K.; Korbe, S. Catalysts for Radical Polymerization”, US Patent 2009/0069520 A1, March 12, 2009.
586. Michl, J.; Sykes, E. C. H. “Molecular Rotors and Motors: Recent Advances and Future Challenges”, *ACS Nano* **2009**, *3*, 1042.
587. Bande, A.; Michl, J. “Conformational Dependence of  $\sigma$ -Electron Delocalization in Linear Chains: Permethylated Oligosilanes”, *Chem. Eur. J.* **2009**, *15*, 8504.
- R 588. Oliva, J. M.; Serrano-Andrés, L.; Klein, D.; Schleyer, P., Michl, J. “Design of Carborane Molecular Architectures via Electronic Structure Computations”, *Int. J. Photoenergy*, published online Dec. 14, <http://dx.doi.org/10.1155/2009/292393>.
589. Mulcahy, M. E.; Magnera, T. F.; Michl, J. “Molecular Rotors on Au(111): Rotator Orientation from IR Spectroscopy”, *J. Phys. Chem. C* **2009**, *113*, 20698.
590. Greyson, E. C.; Vura-Weis, J.; Michl, J.; Ratner, M. A. “Singlet Fission in Organic Dimers: Maximizing the Triplet Yield within the Regime of Localized Excitation and Fast Coherent Electron Transfer”, *J. Phys. Chem. B.*, in press.

591. Schwerin, A. F.; Johnson, J. C.; Smith, M. B.; Sreearunothai, P.; Popović, D.; Černý, J.; Havlas, Z.; Paci, I.; Akdag, A.; MacLeod, M. K.; Chen, X.; David, D. E.; Ratner, M. A.; Miller, J. R.; Nozik, A. J.; Michl, J. "Toward Designed Singlet Fission: Electronic States and Photophysics of 1,3-Diphenylisobenzofuran", *J. Phys. Chem. A*, in press.
592. Joseph, Y.; Krasteval, N.; Chen, X.; Michl, J. "Flexible and Rigid Interlinked Gold-Nanoparticle Networks", submitted for publication.
593. Greyson, E. C.; Stepp, B. R.; Chen, X.; Schwerin, A. F.; Paci, I.; Smith, M. B.; Akdag, A.; Johnson, J. C.; Nozik, A. J.; Michl, J.; Ratner, M. A. "Singlet Exciton Fission for Solar Cell Applications: Energy Aspects of Inter-Chromophore Coupling", *J. Phys. Chem. B*, in press.
594. Michl, J. "Concluding Remarks: Physical Organic Chemistry", *Disc. Faraday Soc.*, in press.

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