

PUBLICATIONS - SAMUEL KRIMM

1. Stein, R.S., Krimm, S. and Tobolsky, A.V. "An Investigation of the Relationship Between Polymer Structure and Mechanical Properties. III. A Thermodynamic and Optical Analysis of the Behavior of Polyethylene, Polyvinyl Chloride and Lactoprene" *Text. Res. J.* 19, 8-22 (Jan. 1949).
2. Krimm, S. and Tobolsky, A.V. "X-ray Pattern of Polystyrene as a Function of Temperature" *J. Polymer. Sci.* 6, 667-668 (May 1951).
3. Krimm, S. and Tobolsky, A.V. "Quantitative X-ray Studies of Order in Amorphous and Crystalline Polymers. Quantitative X-ray Determination of Crystallinity in Polyethylene" *J. Polymer Sci.* 7, 57-76 (July 1951).
4. Krimm, S. and Tobolsky, A.V. "Quantitative X-ray Studies of Order in Amorphous and Crystalline Polymers. Scattering from Various Polymers and a Study of the Glass Transition in Polystyrene and Polymethyl Methacrylate" *Text. Res. J.* 21, 805-822 (Nov. 1951).
5. Krimm, S. and Stein, R.S. "An X-ray Spectrometer for Polymer Studies" *Rev. Sci. Instr.* 22, 920-925 (Dec. 1951).
6. Krimm, S. "Orientation of Crystallites in Stretched Polyethylene" *J. Appl. Phys.* 23, 287 (Feb. 1952).
7. Krimm, S. "X-ray Studies of Crystalline and Amorphous Order in High Polymers" *J. Phys. Chem.* 57, 22-25 (Jan. 1953).
8. Krimm, S. "Infrared Dichroism in the 13.8μ Band of $n\text{-C}_{36}\text{H}_{74}$ Single Crystals and Polyethylene" *J. Chem. Phys.* 22, 567-568 (Mar. 1954).
9. Liang, C.Y., Sutherland, G.B.B.M. and Krimm, S. "Selection Rules and Frequencies of the Skeletal Vibrations of Long Chain Polymers in the Crystalline State" *J. Chem. Phys.* 22, 1468-1469 (Aug. 1954).
10. Krimm, S. "Frequency Shift of the CO Stretching Band in Polypeptides and Proteins" *J. Chem. Phys.* 23, 1371-1372 (July 1955).
11. Krimm, S. "The Structure of Feather Keratin" in Symposium on the Utilization of Chicken Feathers as Filling Materials, National Academy of Sciences-National Research Council, Mar. 1956, pp. 26-34.
12. Krimm, S. and Schor, R. "Structure of Feather Keratin" *J. Chem. Phys.* 24, 922-923 (Apr. 1956).
13. Liang, C.Y., Krimm, S. and Sutherland, G.B.B.M. "Infrared Spectra of High Polymers. I. Experimental Methods and General Theory" *J. Chem. Phys.* 25, 543-548 (Sept. 1956).

14. Krimm, S., Liang, C.Y. and Sutherland, G.B.B.M. "Infrared Spectra of High Polymers. II. Polyethylene" *J. Chem. Phys.* 25, 549-562 (Sept. 1956).
15. Liang, C.Y. and Krimm, S. "Infrared Spectra of High Polymers. III. Polytetrafluoroethylene and Polychlorotrifluoroethylene" *J. Chem. Phys.* 25, 563-571 (Sept. 1956).
16. Krimm, S., Liang, C.Y. and Sutherland, G.B.B.M. "Assignment of the OH In-Plane Deformation Frequency" *J. Chem. Phys.* 25, 778 (Sept. 1956).
17. Krimm, S. and Liang, C.Y. "Infrared Spectra of High Polymers. IV. Polyvinyl Chloride and Polyvinylidene Chloride" *J. Polymer Sci.* 22, 95-112 (Oct. 1956).
18. Krimm, S., Liang, C.Y. and Sutherland, G.B.B.M. "Infrared Spectra of High Polymers. V. Polyvinyl Alcohol" *J. Polymer Sci.* 22, 227-247 (Nov. 1956).
19. Liang, C.Y. and Krimm, S. "Orientation in Polyethylene Terephthalate Film" *J. Chem. Phys.* 27, 327-328 (July 1957).
20. Jensen, L.H., Krimm, S., Parrish, R.G. and Wood, D.L. "The Crystal Structure of N,N'-Hexamethylenebispropionamide" *Acta Cryst.* 10, 528-533 (Aug. 1957).
21. Liang, C.Y. and Krimm, S. "Infrared Dichroism of Mutually Perpendicular Normal Modes in Oriented High Polymers" *J. Chem. Phys.* 27, 1437-1438 (Dec. 1957).
22. Liang, C.Y. and Krimm, S. "Infrared Spectra of High Polymers. VI. Polystyrene" *J. Polymer Sci.* 27, 241-254 (Jan. 1958).
23. Liang, C.Y. and Krimm, S. "Infrared Spectra of High Polymers. VII. Polyacrylonitrile" *J. Polymer Sci.* 31, 513-522 (Sept. 1958).
24. Krimm, S. and Liang, C.Y. "Infrared Spectra of High Polymers. VIII. Polyvinyl Nitrate" *J. Appl. Phys.* 29, 1407-1411 (Oct. 1958).
25. Krimm, S., Berens, A.R., Folt, V.L. and Shipman, J.J. "Assignment of the C-Cl Stretching Modes in the Infrared Spectrum of Polyvinyl Chloride" *Chem. and Ind.* 1512-1513 (Nov. 1958).
26. Krimm, S., Berens, A.R., Folt, V.L. and Shipman, J.J. "Carbon-Chlorine Stretching Modes of Polyvinyl Chloride" *Chem. and Ind.* 433 (Mar. 1959).
27. Krimm, S. "Infrared Spectra and the Structure of High Polymers" *SPE Journal* 15, 797-804 (Sept. 1959).
28. Liang, C.Y. and Krimm, S. "Infrared Spectra of High Polymers. IX. Polyethylene Terephthalate" *J. Mol. Spectrosc.* 3, 554-574 (Oct. 1959).
29. Krimm, S. "Note on the Infrared Dichroism of Axially Oriented Polymers" *J. Chem. Phys.* 32, 313 (Jan. 1960).
30. Krimm, S. "Approximate Isotopic Frequency Rule and Its Application to the Spectra of Complex Molecules", *J. Chem. Phys.* 32, 1780-1783 (June 1960).

31. Krimm, S., "Infrared Spectra of High Polymers" Fortschritte der Hochpolymeren-Forschung (Advances in Polymer Science) 2, 51-172 (Aug. 1960).
32. Krimm, S. "Structure of Frizzle Mutant Feather Keratin" J. Mol. Biol. 2, 247-249 (Oct. 1960).
33. Krimm, S. "Polymers: Theory and Interpretation of Spectra" in The Encyclopedia of Spectroscopy, Reinhold Publishing Corporation, New York, 1960, pp. 535-544.
34. Schor, R. and Krimm, S. "Studies on the Structure of Feather Keratin. I. X-ray Diffraction Studies and Other Experimental Data" Biophys. J. 1, 467-487 (July 1961).
35. Schor, R. and Krimm, S. "Studies on the Structure of Feather Keratin. II. A β -Helix Model for the Structure of Feather Keratin" Biophys. J. 1, 489-515 (July 1961).
36. Wilson, P.R., Krimm, S. and Stein, R.S. "An Optical Diffractometer Analysis of Light Scattering Patterns Obtained from Polyethylene Films" J. Phys. Chem. 65, 1749-1754 (Oct. 1961).
37. Onishi, T. and Krimm, S. "Origins of Characteristic Bands in the Infrared Spectra of Isotactic Polystyrene and Isotactic Poly(Ring-d₅ Styrene)" J. Appl. Phys. 32, 2320-2325 (Nov. 1961).
38. Krimm, S. "Structure of Alpha-Keratin" Nature 192, 810-811 (Dec. 1961).
39. Krimm, S. "Determination of Chain Unit Structure, Stereoregularity, and Irregularity by Infrared Spectroscopy" in Unsolved Problems in Polymer Science, ed. Frank R. Mayo, ASD Technical Report 62-283, Committee on Macromolecular Chemistry, National Academy of Sciences-National Research Council, Mar. 1962, pp. 64-66.
40. Westover, C.J., Tiffany, M.L. and Krimm, S. "Studies on the Structure of Feather Keratin. III. Optical Rotatory Dispersion of Soluble Feather Keratin" J. Mol. Biol. 4, 316-318 (Apr. 1962).
41. Krimm, S. "Infrared Spectra and Chain Conformation of Proteins", J. Mol. Biol. 4, 528-540 (June 1962).
42. Enomoto, S. and Krimm, S., "Elastic Moduli of Helical Polypeptide Chain Structures" Biophys. J. 2, 317-326 (July 1962).
43. Folt, V.L., Shipman, J.J. and Krimm, S. "Characterization of Tacticity in High Polymers" J. Polymer Sci. 61, S17-S20 (Sept. 1962).
44. Krimm, S. "The Crystal Structure of Poly(Bisphenol-A Carbonate)" J. Polymer Sci. 61, S40-S41 (Oct. 1962).

45. Shipman, J.J., Folt, V.L. and Krimm, S. "Characteristic Infrared Frequencies of Rotational Isomers of Alkyl Chlorides" *Spectrochim. Acta.* 18, 1603-1613 (Dec. 1962).
46. Krimm, S., Folt, V.L., Shipman, J.J. and Berens, A.R. "Infrared Spectra and Assignments for Polyvinyl Chloride and Deuterated Analogs" *J. Polymer Sci.* A1, 2621-2650 (Aug. 1963).
47. Krimm, S. "Infrared Spectra of Solids: Dichroism and Polymers" in *Infrared Spectroscopy and Molecular Structure*, ed. M. Davies, Elsevier Publishing Co., Amsterdam, 1963, Chapter VIII, pp. 270-310.
48. Krimm, S. and Enomoto, S. "Infrared Studies of Conformational Changes in Polyvinyl Chloride" *J. Polymer Sci.* A2, 669-678 (Feb. 1964).
49. Krimm, S. "Recent Developments in the Vibrational Spectroscopy of High Polymers" *J. Polymer Sci.* C7, 3-18 (1964).
50. Krimm, S., Folt, V.L., Shipman, J.J. and Berens, A.R. "Conformation-Sensitive Infrared Carbon-Chlorine Bands of Polyvinyl Chloride" *J. Polymer Sci.* B2, 1009-1013 (Nov. 1964).
51. Tiffany, M.L. and Krimm, S. "Studies on the Structure of Feather Keratin. IV. Solubilization Effects of Mercuric Salts" *J. Mol. Biol.* 10, 199-201 (Nov. 1964).
52. Krimm, S., Shipman, J.J., Folt, V.L. and Berens, A.R. "Infrared Evidence for Solid State Constraints on Chain Conformations in Poly(Vinyl Chloride)" *J. Polymer Sci.* B3, 275-278 (Apr. 1965).
53. Opaskar, C.G. and Krimm, S. "Tetrahedral Approximation in Normal Coordinate Calculations of High Polymers" *Spectrochim. Acta* 21, 1165-1166 (June 1965).
54. Krimm, S. and Bank, M.I. "Assignment of the 71 cm^{-1} Band in Polyethylene" *J. Chem. Phys.* 42, 4059-4060 (1 June 1965).
55. Ramachandran, G.N., Venkatachalam, C.M., and Krimm, S. "Stereochemical Criteria for Polypeptide and Protein Chain Conformations. III. Helical and Hydrogen-Bonded Polypeptide Chains" *Biophys. J.* 6, 849-876 (Nov. 1966).
56. Krimm, S. "Antiparallelism of Chains in Polyglycine II" *Nature* 212, 1482-1483 (Dec. 24, 1966).
57. Tasumi, M. and Krimm, S. "Crystal Vibrations of Polyethylene" *J. Chem. Phys.* 46, 755-766 (15 Jan. 1967).
58. Krimm, S., Tasumi, M. and Opaskar, C.G. "Planarity of the Carbon Chain in Crystalline Polyethylene" *J. Polymer Sci.* B5, 105-111 (Jan. 1967).
59. Krimm, S. and Anderson, T.F. "Structure of Normal and Contracted Tail Sheaths of T4 Bacteriophage" *J. Mol. Biol.* 27, 197-202 (28 July 1967).

60. Opaskar, C.G. and Krimm, S. "A Force Field for Secondary Chlorides" *Spectrochim. Acta* 23A, 2261-2278 (Aug. 1967).
61. Krimm, S., Kuroiwa, K. and Rebane, T. "Infrared Studies of C–H···O=C Hydrogen Bonding in Polyglycine II" in *Conformation of Biopolymers*, ed. G.N. Ramachandran, Academic Press, London and New York, 1967, pp. 439-447.
62. Enomoto, S., Opaskar, C.G. and Krimm, S. "Infrared Spectrum and Structure of Poly[3,3-bis (chloromethyl) oxacyclobutane]" *J. Polymer Sci.* C16, 2263-2276 (1967).
63. Krimm, S. "Small-Angle Equatorial Diffraction in Fibrous Proteins" in *Small-Angle X-ray Scattering*, ed. H. Brumberger, Gordon and Breach, New York, 1967, pp. 157-167.
64. Krimm, S. and Kuroiwa, K. "Low Temperature Infrared Spectra of Polyglycines and C–H···O=C Hydrogen Bonding in Polyglycine II" *Biopolymers* 6, 401-407 (Mar. 1968).
65. Shipman, J.J., Folt, V.L. and Krimm, S. "Comments on 'The Rotational Isomers of the Monohalogeno-substituted Derivatives of n-Pentane and n-Octane' " *Spectrochim. Acta* 24A, 437-438 (Apr. 1968).
66. Tasumi, M. and Krimm, S. "Vibrational Analysis of Chain Folding in Polyethylene Crystals" *J. Polymer. Sci. A2*, 6, 995-1010 (May 1968).
67. Krimm, S. "Infrared Spectroscopy and Polymer Structure" *Pure and Applied Chemistry* 16, 369-387 (1968).
68. Krimm, S. and Mark, J.E. "Conformations of Polypeptides with Ionized Side Chains of Equal Length" *Proc. Natl. Acad. Sci. USA* 60, 1122-1129 (Aug. 1968).
69. Tiffany, M.L. and Krimm, S. "New Chain Conformations of Poly(glutamic acid) and Polylysine" *Biopolymers* 6, 1379-1382 (Sept. 1968).
70. Krimm, S. "C–H···O=C Hydrogen Bonding in Proteins" in *Symposium on Fibrous Proteins Australia 1967*, ed. W.G. Crewther, Butterworths, Australia, 1968, pp. 84-85.
71. Bank, M.I. and Krimm, S. "Lattice Frequency Studies of Crystalline and Fold Structure in Polyethylene" *J. Appl. Phys.* 39, 4951-4958 (Oct. 1968).
72. Yamadera, R. and Krimm, S. "Force Fields for Nitriles" *Spectrochim. Acta* 24A, 1677-1686 (Nov. 1968).
73. Tiffany, M.L. and Krimm, S. "Circular Dichroism of Poly-L-Proline in an Unordered Conformation" *Biopolymers* 6, 1767-1770 (Dec. 1968).
74. Opaskar, C.G. and Krimm, S. "Influence of Defects on the Infrared Spectra of Polymers" *J. Polymer Sci. A2*, 7, 57-76 (Jan. 1969).

75. Mark, J.E. and Krimm, S. "Low-Energy Conformations of Isotactic Vinyl Chains Having Charged Side Chains of Equal Length" *Macromolecules* 2, 175-177 (Mar.-Apr. 1969).
76. Tiffany, M.L. and Krimm, S. "Circular Dichroism of the 'Random' Polypeptide Chain" *Biopolymers* 8, 347-359 (Sept. 1969).
77. Bank, M.I. and Krimm, S. "Infrared Study of Lamellar Linking by Cilia in Polyethylene Single-Crystal Mats" *J. Appl. Phys.* 40, 4248-4253 (Oct. 1969).
78. Bank, M.I. and Krimm, S. "Mixed-Crystal Infrared Study of Chain Folding in Crystalline Polyethylene" *J. Polymer Sci. A2*, 7, 1785-1809 (Oct. 1969).
79. Krimm, S., Mark, J.E. and Tiffany, M.L. "Influence of Counter-Ions on the Helical Conformations of Charged Polypeptide Chains" *Biopolymers* 8, 695-697 (Nov. 1969).
80. Bank, M.I. and Krimm, S. "Mixed Crystal Infrared Study of Chain Segregation in Polyethylene" *Polymer Letters* 8, 143-148 (Mar. 1970).
81. Warriar, A.V.R. and Krimm, S. "Intermolecular Vibrations in Liquid Secondary Chlorides" *J. Chem. Phys.* 52, 4316-4317 (15 Apr. 1970).
82. Warriar, A.V.R. and Krimm, S. "Intermolecular Interactions in Crystalline Poly(vinyl chloride)" *Macromolecules* 3, 709-710 (Sept.-Oct. 1970).
83. Kikuchi, Y. and Krimm, S. "Infrared Studies of the Role of Monoclinic Structure in the Deformation of Polyethylene" *J. Macromol. Sci.-Phys.* B4, 461-472 (Sept. 1970). [Also in Plastic Deformation of Polymers, ed. A. Peterlin, Marcel Dekker, Inc., New York, 1971, pp. 1-12.]
84. Jakes, J. and Krimm, S. "A Valence Force Field for the Amide Group" *Spectrochim. Acta* 27A, 19-34 (Jan. 1971).
85. Jakes, J. and Krimm, S. "Normal Coordinate Analyses of Molecules with the Amide Group" *Spectrochim. Acta.* 27A, 35-63 (Jan. 1971).
86. Krimm, S. and Jakes, J. "Vibrational Spectrum of Cyclic C₃₄H₆₈ and Chain Folding in Polyethylene Single Crystals" *Macromolecules* 4, 605-609 (Sept.-Oct. 1971).
87. Krimm, S. and Venkatachalam, C.M. "Free Energy Calculations of the Interactions of Helical Poly(L-Proline) with Water" *Proc. Natl. Acad. Sci. USA* 68, 2468-2471 (Oct. 1971).
88. Harget, P.J. and Krimm, S. "Direct Analysis of Small-Angle Equatorial X-ray Scattering from Fibrous Systems. I. Expressions for the Intensity and Patterson Function" *Acta. Cryst.* A27, 586-596 (Nov. 1971).
89. Johnston, N. and Krimm, S. "An Infrared Study of Unordered Poly-L-Proline in CaCl₂ Solutions" *Biopolymers* 10, 2597-2605 (Dec. 1971).

90. Ronish, E.W. and Krimm, S. "CNDO Calculations of Side Chain-Main Chain Angular Dependence in Paraffin and Peptide Chains" *J. Chem. Phys.* 56, 3175-3176 (15 Mar. 1972).
91. Krimm, S. and Ching, J.H.C. "Infrared Spectra of Polyethylene-Poly(ethylene-d₄) Mixed-Crystal Systems" *Macromolecules* 5, 209-211 (Mar.-Apr. 1972).
92. Harget, P.J. and Krimm, S. "Direct Analysis of Small-Angle Equatorial X-ray Scattering From Fibrous Systems. II. Methods of Extracting Physical Parameters Describing the Scattering System" *J. Polymer Sci. A2*, 10, 919-936 (May 1972).
93. Abe, Y. and Krimm, S. "Normal Vibrations of Crystalline Polyglycine I" *Biopolymers* 11, 1817-1839 (Sept. 1972).
94. Abe, Y. and Krimm, S. "Normal Vibrations of Polyglycine II" *Biopolymers* 11, 1841-1853 (Sept. 1972).
95. Ronish, E.W. and Krimm, S. "Theoretical Calculation of the Circular Dichroism of Unordered Polypeptide Chains" *Biopolymers* 11, 1919-1928 (Sept. 1972).
96. Krimm, S. and Abe, Y. "Intermolecular Interaction Effects in the Amide I Vibrations of β -Polypeptides" *Proc. Natl. Acad. Sci. USA* 69, 2788-2792 (Oct. 1972).
97. Tiffany, M.L. and Krimm, S. "Effect of Temperature on the Circular Dichroism Spectra of Polypeptides in the Extended State" *Biopolymers* 11, 2309-2316 (Dec. 1972).
98. Tiffany, M.L. and Krimm, S. "Extended Conformations of Polypeptides and Proteins in Urea and Guanidine Hydrochloride" *Biopolymers* 12, 575-587 (Mar. 1973).
99. Wilkes, C.E., Folt, V.L. and Krimm, S. "Crystal Structure of Poly(vinyl chloride) Single Crystals" *Macromolecules* 6, 235-237 (Mar.-Apr. 1973).
100. Venkatachalam, C.M. and Krimm, S. "Theoretical Studies of the Interactions of Polypeptides with Small Molecules. Aspects of Conformation of Polyproline in Solution" in Conformation of Biological Molecules and Polymers, ed. E.D. Bergmann and B. Pullman, Israel Academy of Sciences and Humanities, Jerusalem, 1973, pp. 141-154.
101. Moore, W.H., Ching, J.H.C., Warrior, A.V.R. and Krimm, S. "Assignment of Torsion and Low Frequency Bending Vibrations of Secondary Chlorides" *Spectrochim. Acta* 29A, 1847-1858 (Oct. 1973).
102. Moore, W.H. and Krimm, S. "Calculated Intermolecular Interactions in Secondary Chlorides" *J. Chem. Phys.* 59, 5195-5196 (1 Nov. 1973).

103. Moore, W.H. and Krimm, S. "A Complete General Valence Force Field for Secondary Chlorides" *Spectrochim. Acta* 29A, 2025-2042 (Dec. 1973).
104. Harget, P.J. and Krimm, S. "Macromolecular Structure and Organization of Alpha Keratin" *Biopolymers* 13, 257-273 (Feb. 1974).
105. Venkatachalam, C.M., Price, B.J. and Krimm, S. "Theoretical Analysis of Pyrrolidine Ring Puckering and the Conformational Energies of Proline and 5-Methylproline Dimers" *Macromolecules* 7, 212-220 (Mar.-Apr. 1974).
106. Moore, W.H. and Krimm, S. "Vibrational Analyses of 2,4-Dichloro-pentane and 2,4,6-Trichloroheptane" *J. Mol. Spectrosc.* 51, 1-26 (Apr. 1974).
107. Krimm, S. and Tiffany, M.L. "The Circular Dichroism Spectrum and Structure of Unordered Polypeptides and Proteins" *Israel J. Chem.* 12 (1-2), 189-200 (1974).
108. Krimm, S. "Infrared Studies of Chain Organization in Crystalline Polyethylene" in Proceedings of the International Symposium on Macromolecules, Rio de Janeiro, July 26-31, 1974, ed. E.B. Mano, Elsevier Scientific Publishing Co., Amsterdam, 1974, pp. 107-130.
109. Krimm, S., Ching, J.H.C. and Folt, V.L. "Mixed-Crystal Infrared Study of Chain Organization in Polyethylene Crystallized under Orientation and Pressure" *Macromolecules* 7, 537-538 (July-Aug. 1974).
110. Ronish, E.W. and Krimm, S. "The Calculated Circular Dichroism of Polyproline II in the Polarizability Approximation" *Biopolymers* 13, 1635-1651 (Aug. 1974).
111. Stamatoff, J.B., Krimm, S. and Harvie, N.R. "X-ray Diffraction Studies of Human Erythrocyte Membrane Structure" *Proc. Natl. Acad. Sci. USA* 72, 531-534 (Feb. 1975).
112. Stamatoff, J.B., Krimm, S. and Harvie, N.R. "X-ray Diffraction Studies of the Human Erythrocyte Membrane" in Erythrocyte Structure and Function, ed. G.J. Brewer, Alan R. Liss, Inc., New York, 1975, pp. 507-512.
113. Venkatachalam, C.M., Price, B.J. and Krimm, S. "A Theoretical Estimate of the Energy Barriers Between Stable Conformations of the Proline Dimer" *Biopolymers* 14, 1121-1132 (June 1975).
114. Moore, W.H. and Krimm, S. "The Vibrational Spectrum of Crystalline Syndiotactic Poly(vinyl chloride)" *Die Makromolekulare Chemie, Suppl.* 1, 491-506 (June 1975).
115. Ching, J.H.C. and Krimm, S. "Mixed-Crystal Infrared Studies on Melt-Crystallized Polyethylene" *J. Appl. Phys.* 46, 4181-4184 (Oct. 1975).
116. Hsu, S.L., Moore, W.H. and Krimm, S. "A Vibrational Analysis on Crystalline *Trans*-1,4-Polybutadiene" *J. Appl. Phys.* 46, 4185-4193 (Oct. 1975).

117. Ching, J.H.C. and Krimm, S. "Mixed-Crystal Infrared Studies of Annealed Poly(ethylene) Single Crystals" *Macromolecules* 8, 894-897 (Nov.-Dec. 1975).
118. Moore, W.H. and Krimm, S. "Transition Dipole Coupling in Amide I Modes of β -Polypeptides" *Proc. Natl. Acad. Sci. USA* 72, 4933-4935 (Dec. 1975).
119. Hsu, S.L. and Krimm, S. "A Raman Study of the Phase Transition in Crystalline *Trans*-1,4-Polybutadiene" *J. Polymer Sci. Polym. Phys. Ed.* 14, 521-529 (Mar. 1976).
120. Hsu, S.L., Krimm, S., Krause, S. and Yeh, G.S.Y. "Longitudinal Acoustic Mode in Isotactic Polypropylene" *J. Polymer Sci. Polym. Lett. Ed.* 14, 195-200 (Apr. 1976).
121. Stamatoff, J.B. and Krimm, S. "Phase Determination of X-ray Reflections for Membrane-Type Systems with Constant Fluid Density" *Biophys. J.* 16, 503-516 (May 1976).
122. Hsu, S.L., Moore, W.H. and Krimm, S. "Vibrational Spectrum of the Unordered Polypeptide Chain: A Raman Study of Feather Keratin" *Biopolymers* 15, 1513-1528 (Aug. 1976).
123. Hsu, S.L. and Krimm, S. "Longitudinal Acoustic Mode in Polymers" *J. Appl. Phys.* 47, 4265-4270 (Oct. 1976).
124. Moore, W.H. and Krimm, S. "Vibrational Analysis of Peptides, Polypeptides, and Proteins. I. Polyglycine I" *Biopolymers* 15, 2439-2464 (Dec. 1976).
125. Moore, W.H. and Krimm, S. "Vibrational Analysis of Peptides, Polypeptides, and Proteins. II. β -Poly(L-alanine) and β -Poly(L-alanyl-glycine)" *Biopolymers* 15, 2465-2483 (Dec. 1976).
126. Rabolt, J.F., Moore, W.H. and Krimm, S. "Vibrational Analysis of Peptides, Polypeptides, and Proteins. 3. α -Poly(L-alanine)" *Macromolecules* 10, 1065-1074 (Sept.-Oct. 1977).
127. Hsu, S.L., Ford, G.W. and Krimm, S. "Longitudinal Acoustic Mode in Polymers. II. Solution of the General Composite Perturbed Elastic Rod" *J. Polym. Sci. Polym. Phys. Ed.* 15, 1769-1778 (Oct. 1977).
128. Hsu, S.L. and Krimm, S. "Longitudinal Acoustic Mode in Polymers: Applications of the General Theory to Planar Zigzag Methylene Chains" *J. Appl. Phys.* 48, 4013-4018 (Oct. 1977).
129. Krimm, S. "Raman Studies of the Longitudinal Acoustic Mode in Polymers" *Indian J. Pure Appl. Phys.* 16, 335-343 (Mar. 1978).
130. Snyder, R.G., Hsu, S.L. and Krimm, S. "Vibrational Spectra in the C-H Stretching Region and the Structure of the Polymethylene Chain" *Spectrochim. Acta* 34A, 395-406 (Apr. 1978).

131. Krimm, S. and Hsu, S.L. "Longitudinal Acoustic Mode in Polymers. IV. LAM-3 of the General Perturbed Rod and Applications to Paraffins and Polymers" *J. Polym. Sci. Polym. Phys. Ed.* **16**, 2105-2114 (Dec. 1978).
132. Bandekar, J. and Krimm, S. "Vibrational Analysis of Peptides, Polypeptides, and Proteins: Characteristic Amide Bands of β -turns" *Proc. Natl. Acad. Sci. USA* **76**, 774-777 (Feb. 1979).
133. Bandekar, J. and Krimm, S. "Vibrational Analysis of Peptides, Polypeptides, and Proteins. VII. Normal Modes and Vibrational Spectra of a Type I Beta-Turn Tetrapptide" in Peptides: Structure and Biological Function. Proceedings of the Sixth American Peptide Symposium, ed. E. Gross and J. Meienhofer, Pierce Chemical Col., Rockford, IL, 1979, pp. 241-244.
134. Krimm, S. and Cheam, T.C. "Mixed-Crystal Infrared Studies of Chain Organization in Solution-Crystallized Polyethylene" *Disc. Faraday Soc.* **68**, 244-250 (1979).
135. Chang, C. and Krimm, S. "Longitudinal Acoustic Mode in Polymers. V. Nature of Perturbing Forces in n-Paraffins and Polymers" *J. Polym. Sci. Polym. Phys. Ed.* **17**, 2163-2170 (Dec. 1979).
136. Krimm, S. and Bandekar, J. "Vibrational Analysis of Peptides, Polypeptides, and Proteins. V. Normal Vibrations of β -Turns" *Biopolymers* **19**, 1-29 (Jan. 1980).
137. Bandekar, J. and Krimm, S. "Vibrational Analysis of Peptides, Polypeptides, and Proteins. VI. Assignment of β -Turn Modes in Insulin and Other Proteins" *Biopolymers* **19**, 31-36 (Jan. 1980).
138. McCaughan, L. and Krimm, S. "X-ray and Neutron Scattering Density Profiles of the Intact Human Red Blood Cell Membrane" *Science* **207**, 1481-1483 (28 Mar. 1980).
139. Cheam, T.C. and Krimm, S. "Mixed-Crystal Infrared Studies of Chain-Folding in Polyethylene Single Crystals: Low-Temperature and Molecular Weight Studies" *J. Polym. Sci. Polym. Phys. Ed.* **19**, 423-447 (Mar. 1981).
140. Diem, H.E. and Krimm, S. "Quantitative Analysis of Binary Mixtures. I. General Method" *Appl. Spectroscopy* **35**, 421-428 (July-Aug. 1981).
141. Maxfield, F.R., Bandekar, J., Krimm, S., Evans, D.J., Leach, S.J., Nemethy, G. and Scheraga, H.A. "Conformation of Cyclo(L-alanyl-glycyl- ϵ -aminocaproyl), a Cyclized Dipeptide Model for a β -Bend. 3. Infrared and Raman Spectroscopic Studies" *Macromolecules* **14**, 997-1003 (July-Aug. 1981).

142. Garrell, R.L., Shaw, K.D. and Krimm, S. "Coverage-Dependent Surface Enhanced Raman Spectra of Halide Ions on Colloidal Silver" *J. Chem. Phys.* 75, 4155-4157 (15 Oct. 1981).
143. Dwivedi, A.M. and Krimm, S. "Vibrational Analysis of Peptides, Polypeptides, and Proteins. X. Poly(glycine I) and Its Isotopic Derivatives" *Macromolecules* 15, 177-185 (Jan.-Feb. 1982).
144. Dwivedi, A.M. and Krimm, S. "Vibrational Analysis of Peptides, Polypeptides, and Proteins. XI. β -Poly(L-alanine) and Its N-Deuterated Derivative" *Macromolecules* 15, 186-193 (Jan.-Feb. 1982); *ibid* 16, 340 (Feb. 1983).
145. McCaughan, L. and Krimm, S. "Biochemical Profiles of Membranes from X-ray and Neutron Diffraction" *Biophys. J.* 37, 417-426 (Feb. 1982).
146. Bandekar, J., Evans, D.J., Krimm, S., Leach, S.J., Lee, S., McQuie, J.R., Minasian, E., Nemethy, G., Pottle, M.S., Scheraga, H.A., Stimson, E.R. and Woody, R.W. "The Conformations of Cyclo(L-alanyl-L-alanyl- ϵ -aminocaproyl) and of Cyclo(L-alanyl-D-alanyl- ϵ -aminocaproyl); Cyclized Dipeptide Models for Specific Types of β -Bends" *Int. J. Peptide Protein Res.* 19, 187-205 (Feb. 1982).
147. Tasumi, M., Takeuchi, H., Ataka, S., Dwivedi, A.M. and Krimm, S. "Normal Vibrations of Proteins: Glucagon" *Biopolymers* 21, 711-714 (Mar. 1982).
148. Krimm, S. and Dwivedi, A.M. "Infrared Spectrum of the Purple Membrane: Clue to a Proton Conduction Mechanism?" *Science* 216, 407-408 (23 Apr. 1982).
149. Krimm, S. and Dwivedi, A.M. "Vibrational Analysis of Peptides, Polypeptides, and Proteins. XII. Fermi Resonance Analysis of the Unperturbed ND Stretching Fundamental in Polypeptides" *J. Raman Spectrosc.* 12, 133-137 (Apr. 1982).
150. Jing, X. and Krimm, S. "Mixed-Crystal Infrared Studies of Chain Folding in Polyethylene Single Crystals. Effect of Crystallization Temperature" *J. Polym. Sci. Polym. Phys. Ed.* 20, 1155-1173 (July 1982).
151. Dwivedi, A.M. and Krimm, S. "Vibrational Analysis of Peptides, Polypeptides, and Proteins. XV. Crystalline Polyglycine II" *Biopolymers* 21, 2377-2397 (Dec. 1982).
152. Krimm, S. "Vibrational Analysis of Conformation in Peptides, Polypeptides, and Proteins" *Biopolymers* 22, 217-225 (Jan. 1983).
153. Garrell, R.L., Shaw, K.D. and Krimm, S. "Surface Enhanced Raman Spectroscopy of Halide Ions on Colloidal Silver: Morphology and Coverage Dependence" *Surface Sci.* 124, 613-624 (Jan. 1983).
154. Shaw, K.D., Garrell, R.L. and Krimm, S. "Surface Enhanced Raman Spectroscopy of Halide Ions on Colloidal Silver: Simulation of Silver-Halide Ion Spectra" *Surface Sci.* 124, 625-637 (Jan. 1983).

155. Jing, X. and Krimm, S. "Mixed-Crystal Infrared Studies of Chain Folding in Melt-Crystallized Polyethylene" *J. Polym. Sci. Polym. Lett. Ed.* 21, 123-130 (Feb. 1983).
156. Jing, X. and Krimm, S. "Vibrational Analysis of 2,3-Dichlorobutanes" *Spectrochim. Acta* 39A, 251-260 (Mar. 1983).
157. Chang, C. and Krimm, S. "Longitudinal Acoustic Mode in Polymers: Influence of Defects" *J. Appl. Phys.* 54, 5526-5540 (Oct. 1983).
158. Krimm, S. and Chang, C. "Nitric Acid Etching Studies of Compositional Heterogeneity in Mixed-Crystal Polyethylene Single Crystals" *J. Polym. Sci. Polym. Lett. Ed.* 21, 907-911 (Nov. 1983).
159. Chang, C. and Krimm, S. "Mixed-Crystal Infrared Study of Chain Mobility in Untreated and Nitric-Acid-Treated Polyethylene Single Crystals" *J. Polym. Sci. Polym. Lett. Ed.* 21, 913-917 (Nov. 1983).
160. Naik, V.M. and Krimm, S. "Vibrational Analysis of Peptides, Polypeptides, and Proteins. XVII. Normal Modes of Crystalline Pro-Leu-Gly-NH₂, a Type II β -Turn" *Int. J. Peptide Protein Res.* 23, 1-24 (Jan. 1984).
161. Naik, V.M. and Krimm, S. "Vibrational Analysis of the Structure of Crystalline Gramicidin A" *Biophys. J.* 45, 109-112 (Jan. 1984).
162. Dwivedi, A.M. and Krimm, S. "Vibrational Analysis of Peptides, Polypeptides, and Proteins. 19. Force Fields for α -Helix and β -Sheet Structures in a Side-Chain Point-Mass Approximation" *J. Phys. Chem.* 88, 620-627 (Feb. 2, 1984).
163. Dwivedi, A.M. and Krimm, S. "Vibrational Analysis of Peptides, Polypeptides, and Proteins. XVIII. Conformational Sensitivity of the α -Helix Spectrum: α _I- and α _{II}-Poly(L-alanine)" *Biopolymers* 23, 923-943 (May 1984).
164. Cheam, T.C. and Krimm, S. "Vibrational Analysis of Crystalline Diketopiperazine - I. Raman and I.R. Spectra" *Spectrochim. Acta* 40A, 481-501 (June 1984).
165. Cheam, T.C. and Krimm, S. "Vibrational Analysis of Crystalline Diketopiperazine - II. Normal Mode Calculations" *Spectrochim. Acta* 40A, 503-517 (June 1984).
166. Cheam, T.C. and Krimm, S. "Transition Dipole Interaction in Polypeptides: *Ab Initio* Calculation of Transition Dipole Parameters" *Chem. Phys. Lett.* 107, 613-616 (15 June 1984).
167. Sengupta, P.K., Krimm, S. and Hsu, S.L. "Vibrational Analysis of Peptides, Polypeptides, and Proteins. XXI. β -Calcium-Poly(L-glutamate)" *Biopolymers* 23, 1565-1594 (Aug. 1984).

168. Dwivedi, A.M., Krimm, S. and Malcolm, B.R. "Vibrational Analysis of Peptides, Polypeptides, and Proteins. XXIV. Conformation of Poly(α -aminoisobutyric Acid)" *Biopolymers* 23, 2025-2065 (Oct. 1984).
169. Chang, C. and Krimm, S. "Longitudinal Acoustic Mode in Polymers. VII. Surface Structure from Swelling Studies of Freeze-Dried Polyethylene Single Crystals" *J. Polym. Sci. Polym. Phys. Ed.* 22, 1871-1884 (Nov. 1984).
170. Naik, V.M., Krimm, S., Denton, J.B., Nemethy, G. and Scheraga, H.A. "Vibrational Analysis of Peptides, Polypeptides, and Proteins. XXVII. Structure of Gramicidin S from Normal Mode Analyses of Low-Energy Conformations" *Int. J. Peptide Protein Res.* 24, 613-626 (Dec. 1984).
171. Naik, V.M. and Krimm, S. "The Structure of Crystalline and Membrane-Bound Gramicidin A by Vibrational Analysis" *Biochem. Biophys. Res. Comm.* 125, 919-925 (Dec. 28, 1984).
172. Sengupta, P.K. and Krimm, S. "Raman and Normal Mode Studies of the Polypeptide Chain Conformations in Crystalline Magnesium and Calcium Poly(L-glutamate)s" *Spectrochim. Acta* 41A, 205-207 (Jan./Feb. 1985).
173. Cheam, T.C. and Krimm, S. "Infrared Intensities of Amide Modes in N-Methylacetamide and Poly(glycine I) from *Ab Initio* Calculations of Dipole Moment Derivatives of N-Methylacetamide" *J. Chem. Phys.* 82, 1631-1641 (15 Feb. 1985).
174. Sengupta, P.K. and Krimm, S. "Vibrational Analysis of Peptides, Polypeptides, and Proteins. XXXII. α -Poly(L-glutamic Acid)" *Biopolymers* 24, 1479-1491 (Aug. 1985).
175. Bandekar, J. and Krimm, S. "Vibrational Analysis of Peptides, Polypeptides, and Proteins. XXXI. Cyclo (D-Phe-L-Pro-Gly-D-Ala-L-Pro), a γ -Turn Pentapeptide" *Int. J. Peptide Protein Res.* 26, 158-165 (Aug. 1985).
176. Bandekar, J. and Krimm, S. "Vibrational Analysis of Peptides, Polypeptides, and Proteins. XXX. Normal Mode Analysis of γ -Turns" *Int. J. Peptide Protein Res.* 26, 407-415 (Oct. 1985).
177. Murthy, N.S., Szollosi, A.B., Sibilica, J.P. and Krimm, S. "Structure of Iodide Ion Arrays in Iodinated Nylon 6 and the Chain Orientation Induced by Iodine in Nylon 6 Films" *J. Polymer Sci. Polym. Phys. Ed.* 23, 2369-2376 (Nov. 1985).
178. Naik, V.M. and Krimm, S. "Vibrational Analysis of the Structure of Gramicidin A. I. Normal Mode Analysis" *Biophys. J.* 49, 1131-1145 (June 1986).
179. Naik, V.M. and Krimm, S. "Vibrational Analysis of the Structure of Gramicidin A. II. Vibrational Spectra" *Biophys. J.* 49, 1147-1154 (June 1986).

180. Datye, V.K. and Krimm, S. "Lattice Dynamics and Specific Heat of α -Helical Poly(L-alanine)" *J. Chem. Phys.* 84, 6989-6996 (15 June 1986).
181. Krimm, S. "Infrared Spectroscopy of Polymers" in Encyclopedia of Materials Science and Engineering, ed. Michael B. Bever, Pergamon Press, Oxford, 1986, pp. 2305-2310.
182. Chang, C. and Krimm, S. "Longitudinal Acoustic Mode in Polymers. VIII. Nature of Mass Perturbations in Terminally Brominated Paraffins" *J. Polym. Sci. Polym. Phys. Ed.* 24, 1373-1381 (July 1986).
183. Krimm, S. and Bandekar, J. "Vibrational Spectroscopy and Conformation of Peptides, Polypeptides, and Proteins" *Adv. Protein Chem.* 38, 181-364 (1986).
184. Cheam, T.C. and Krimm, S. "Vibrational Properties of the Peptide N-H Bond as a Function of Hydrogen-Bond Geometry: An *Ab Initio* Study" *J. Mol. Struct.* 146, 175-189 (Aug. 1986).
185. Krimm, S. "Vibrational Analysis of Protein Structure" in Protein Structure, Folding, and Design, ed. Dale L. Oxender, Alan R. Liss, Inc., New York, 1986, pp. 237-241.
186. Krimm, S. "Peptides and Proteins" in Biological Applications of Raman Spectroscopy: Vol. 1 - Raman Spectra and The Conformation of Biological Macromolecules, ed. T.G. Spiro, John Wiley & Sons, 1987, Chap. 1, pp. 1-45.
187. Sengupta, P.K. and Krimm, S. "Raman and Normal-Mode Studies of the Extended-Helix Conformation in Polypeptide Chains" *Biopolymers* 26, S99-S107 (1987).
188. Dybal, J., Cheam, T.C. and Krimm, S. "C=O Stretch Mode Splitting in the Formic Acid Dimer: Electrostatic Models of the Intermonomer Interaction" *J. Mol. Struct.* 159, 183-194 (June 1987).
189. Krimm, S. "Spectra and Structure of Polypeptides" in Vibrational Spectra and Structure, Vol. 16, ed. J.R. Durig, Elsevier, 1987, Chap. 1, pp. 1-72.
190. Cheam, T.C. and Krimm, S. "Vibrational Analysis of Cyclo(D-Ala-L-Ala) in Two Crystalline Forms. Effect of Structure on Peptide Group and CH Modes" *Spectrochim. Acta* 44A, 185-208 (Feb. 1988).
191. Bandekar, J. and Krimm, S. "Vibrational Spectroscopy of L-Valyl-Glycyl-Glycine, a Parallel-Chain β Structure" *Biopolymers* 27, 885-908 (June 1988).
192. Bandekar, J. and Krimm, S. "Normal Mode Spectrum of the Parallel-Chain β -Sheet" *Biopolymers* 27, 909-921 (June 1988).
193. Zhao, W., Bandekar, J. and Krimm, S. "Dependence of Disulfide Vibrational Frequencies on Internal Rotation Geometry: An *Ab Initio* and Normal Mode Study of Dimethyl Disulfide" *J. Am. Chem. Soc.* 110, 6891-6892 (28 Sept. 1988).

194. Dybal, J. and Krimm, S. "Dipole Derivatives and Infrared Intensities of the Ester Group. An *Ab Initio* and Force Field Study of Methyl Acetate" *J. Mol. Struct.* 189, 383-392 (31 Oct. 1988).
195. Song, S., Asher, S.A., Krimm S. and Bandekar, J. "Assignment of a New Conformation-Sensitive UV Resonance Raman Band in Peptides and Proteins" *J. Am. Chem. Soc.* 110, 8547-8548 (Dec. 7, 1988).
196. Krimm, S. "Determination of Polypeptide Chain Conformation by Normal Mode Analysis of Vibrational Spectra" in *Spectroscopy of Biological Molecules-New Advances*, ed. E.D. Schmid, F.W. Schneider, and F. Siebert, John Wiley & Sons, 1988, pp. 19-24.
197. Dwivedi, A.M., Krimm, S. and Mierson, S. "Vibrational Force Field and Normal Mode Analysis of N,N-Dimethylacetamide" *Spectrochim. Acta* 45A, 271-279 (Feb. 1989).
198. Cheam, T.C. and Krimm, S. "*Ab Initio* Force Fields of Glycine Dipeptide in C₅ and C₇ Conformations" *J. Mol. Struct.* 193, 1-34 (Feb. 1989).
199. Murthy, N.S., Stamm, M., Sibilica, J.P. and Krimm, S. "Structural Changes Accompanying Hydration in Nylon 6" *Macromolecules* 22, 1261-1267 (Mar. 1989).
200. Song, K. and Krimm, S. "Mixed-Integer and Fractional-Integer Chain Folding in Crystalline Lamellae of Poly(ethylene oxide): A Raman Longitudinal Acoustic Mode Study" *Macromolecules* 22, 1504-1505 (Mar 1989).
201. Krimm, S., Song, S. and Asher, S.A. "Amide V Overtone Assignment of a Conformation-Sensitive Band in the UV Resonance Raman Spectra of Peptides and Proteins" *J. Am. Chem. Soc.* 111, 4290-4294 (June 7, 1989).
202. Cheam, T.C. and Krimm, S. "*Ab Initio* Force Fields of Alanine Dipeptide in C₅ and C₇ Conformations" *J. Mol. Struct. (Theochem)* 188, 15-43 (June 1989).
203. Krimm, S. "Infrared, Raman, and Normal Mode Studies of Structure in Peptides and Proteins", *Seventh International Conference on Fourier Transform Spectroscopy*, ed. David G. Cameron, *Proc. SPIE Vol. 1145*, 4-9 (1989).
204. Sundius, T., Bandekar, J. and Krimm, S. "Vibrational Analysis of Crystalline Triglycine" *J. Mol. Struct.* 214, 119-142 (Dec. 1989).
205. Song, K. and Krimm, S. "Raman Longitudinal Acoustic Mode (LAM) Studies of Folded-Chain Morphology in Poly(ethylene oxide)(PEO). I. Normal Mode Analysis of LAM of a Helical-Chain Oligomer of PEO" *J. Polym. Sci. Polym. Phys. Ed.* 28, 35-50 (Jan. 15, 1990).
206. Song, K. and Krimm, S. "Raman Longitudinal Acoustic Mode (LAM) Studies of Folded-Chain Morphology in Poly(ethylene oxide) (PEO). II. Normal Mode

- Analysis of Folded-Chain Structures of PEO" J. Polym. Sci. Polym. Phys. Ed. 28, 51-61 (Jan. 15, 1990).
207. Song, K. and Krimm, S. "Elastic Modulus of Poly(ethylene oxide) Determined from the Raman Longitudinal Acoustic Mode" J. Polym. Sci. Polym. Phys. Ed. 28, 63-69 (Jan. 15, 1990).
208. Dybal, J. and Krimm, S. "Normal-Mode Analysis of Infrared and Raman Spectra of Crystalline Isotactic Poly(methyl methacrylate)" *Macromolecules* 23, 1301-1308 (Mar. 5, 1990).
209. Cheam, T.C. and Krimm S., "*Ab Initio* Force Fields of Alanine Dipeptide in Four Non-Hydrogen Bonded Conformations" J. Mol. Struct. (Theochem) 206, 173-203 (Mar. 1990).
210. Song, K. and Krimm, S. "Raman Longitudinal Acoustic Mode (LAM) Studies of Folded-Chain Morphology in Poly(ethylene oxide) (PEO). III. Chain Folding in PEO as a Function of Molecular Weight" *Macromolecules* 23, 1946-1957 (April 2, 1990).
211. Zhao, W. and Krimm, S. "Vibrational Studies of the Disulfide Group in Proteins. Part II. *Ab Initio* Force Fields and Normal Mode Frequencies of Dimethyl, Methyl Ethyl, and Diethyl Disulfides" J. Mol. Struct. 224, 7-20 (July 1990).
212. Chough, S.H. and Krimm, S. "Vibrational Analysis of 2,3,4-Trichloropentanes" *Spectrochim. Acta* 46A, 1405-1418 (Oct. 1990).
213. Chough, S.H. and Krimm, S. "Vibrational Analysis of 2,2,3-Trichlorobutane and a Force Field for 2,2-Dichloropropane" *Spectrochim. Acta* 46A, 1419-1430 (Oct. 1990).
214. Chough, S.H. and Krimm, S. "Comprehensive Force Field for Multiply-Chlorinated Hydrocarbons" *Spectrochim. Acta* 46A, 1431-1438 (Oct. 1990).
215. Zhao, W., Bandekar, J. and Krimm, S. "Vibrational Studies of the Disulfide Group in Proteins. III. A Simplified *Ab Initio* Force Field for Diethyl Disulfide and SS and CS Stretch Frequency - Conformation Correlations for Diisobutyl Disulfide" J. Mol. Struct. 238, 43-54 (Oct.1, 1990).
216. Mirkin, N.G. and Krimm, S. "Vibrational Dynamics of the *Cis* Peptide Group" J. Am. Chem. Soc. 112, 9016-9017 (Nov. 21, 1990).
217. Mirkin, N.G. and Krimm, S. "Conformers of *Trans*-N-Methylacetamide. *Ab Initio* Study of Geometries and Vibrational Spectra" J. Mol. Struct. 242, 143-160 (Jan. 1991).
218. Qian, W., Bandekar, J. and Krimm, S. "Vibrational Analysis of Crystalline Tri-L-Alanine" *Biopolymers* 31, 193-201 (Feb. 5, 1991).

219. Song, S., Asher, S.A., Krimm, S. and Shaw, K.D. "Ultraviolet Resonance Raman Studies of *Trans* and *Cis* Peptides: Photochemical Consequences of the Twisted π^* State" *J. Am. Chem. Soc.* 113, 1155-1163 (Feb. 13, 1991).
220. Palmö, K., Pietilä, L.-O. and Krimm, S. "Construction of Molecular Mechanics Energy Functions by Mathematical Transformation of *Ab Initio* Force Fields and Structures" *J. Comput. Chem.* 12, 385-390 (Mar. 1991).
221. Palmö, K., Pietilä, L.-O. and Krimm, S. "Conversion of *Ab Initio* Force Fields and Structures to Molecular Mechanics Energy Functions" *Computers Chem.* 15, 249-250 (July-Sept. 1991).
222. Qian, W., Zhao, W. and Krimm, S. "Vibrational Studies of the Disulfide Group in Proteins. IV. SS and CS Stretch Frequencies of Known Peptide and Protein Disulfide Bridges" *J. Mol. Struct.* 250, 89-102 (October 1, 1991).
223. Mirkin, N.G. and Krimm, S. "Conformers of *Cis*-N-Methylacetamide. *Ab Initio* Study of Geometries and Vibrational Spectra" *J. Mol. Struct. (Theochem)* 236, 97-111 (Nov. 1, 1991).
224. Mirkin, N.G. and Krimm, S. "*Ab Initio* Analysis of Hydrogen-Bonded *Trans*- and *Cis*-N-Methylacetamide" *J. Am. Chem. Soc.* 113, 9742-9747 (Dec. 18, 1991).
225. Hong, J.W., Lando, J.B., Koenig, J.L., Chough, S.H. and Krimm, S. "Normal-Mode Analysis of Infrared and Raman Spectra of Poly(vinyl fluoride)" *Vibrational Spectroscopy* 3, 55-66 (March 1992).
226. Qian, W. and Krimm, S. "Vibrational Studies of the Disulfide Group in Proteins. V. Correlation of SS Stretch Frequencies with the CCSS Dihedral Angle in Known Protein Disulfide Bridges" *Biopolymers* 32, 321-326 (April 1992).
227. Qian, W. and Krimm, S. "Vibrational Studies of the Disulfide Group in Proteins. VI. General Correlations of SS and CS Stretch Frequencies with Disulfide Bridge Geometry" *Biopolymers* 32, 1025-1033 (Aug. 1992).
228. Qian, W. and Krimm, S. "Vibrational Studies of the Disulfide Group in Proteins. VII. Normal Mode Analysis of the Raman Spectra of Erabutoxin, γ -II Crystallin and Immunoglobulin" *J. Raman Spectroscopy* 23, 517-521 (Oct. 1992).
229. Palmö, K., Pietilä, L.-O. and Krimm, S. "Treatment of Redundancies Among Internal Coordinates in Optimizing Molecular Mechanics Force Constants" *J. Comput. Chem.* 13, 1142-1150 (Nov. 1992).
230. Qian, W. and Krimm, S. "Conformation Dependence of the SH and CS Stretch Frequencies of the Cysteine Residue" *Biopolymers* 32, 1503-1518 (Nov. 1992).
231. Murthy, N.S., Minor, H., Bednarczyk, C. and Krimm, S. "Structure of the Amorphous Phase in Oriented Polymers" *Macromolecules* 26, 1712-1721 (March 1993).

232. Palmö, K., Pietilä, L.-O. and Krimm, S. "Optimization of Parameters of Nonbonded Interactions in a Spectroscopically Determined Force Field" *Computers Chem.* 17, 67-72 (March 1993).
233. Qian, W. and Krimm, S. "Energetics of the Disulfide Bridge: An *Ab Initio* Study" *Biopolymers* 33, 1591-1603 (Oct. 1993).
234. Krimm, S. "Reflections on Herman F. Mark" *J. Polymer Sci.: Polymer Symposia* 75, 193-194 (1993).
235. Qian, W. and Krimm, S. "Dipole Derivative Distribution: A Useful Adjunct to the Potential Energy Distribution" *J. Phys. Chem.* 97, 11578-11579 (Nov. 11, 1993).
236. Palmö, K., Mirkin, N.G., Pietilä, L.-O. and Krimm, S. "Spectroscopically Determined Force Fields for Macromolecules. I. *n*-Alkane Chains" *Macromolecules* 26, 6831-6840 (Dec. 20, 1993).
237. Mirkin, N.G. and Krimm, S. "*Ab Initio* Studies of the Conformation Dependence of the Spectra of Stable Conformers of *n*-Pentane and *n*-Hexane" *J. Phys. Chem.* 97, 13887-13895 (Dec. 23, 1993).
238. Kim, I. and Krimm, S. "Tilted-Chain Lamellar Morphology in Initially Crystallized Low Molecular Weight Poly(ethylene oxide) from Raman Longitudinal Acoustic Mode Spectra" *Macromolecules* 27, 5232-5234 (Aug. 29, 1994).
239. Qian, W. and Krimm, S. "Vibrational Analysis of Glutathione" *Biopolymers* 34, 1377-1394 (Oct. 1994).
240. Qian, W. and Krimm, S. "*Ab Initio* Force Field for the Carboxyl Group of Glutathione Derived from Hydrogen-Bonded Glycine" *J. Phys. Chem.* 98, 9992-10000 (Oct. 6, 1994).
241. Chen, X.G., Schweitzer-Stenner, R., Krimm, S., Mirkin, N.G. and Asher, S.A. "N-Methylacetamide and Its Hydrogen-Bonded Water Molecules are Vibrationally Coupled" *J. Am. Chem. Soc.* 116, 11141-11142 (Nov. 30, 1994).
242. Krimm, S. and Reisdorf, Jr., W.C. "Understanding Normal Modes of Proteins" *Faraday Discuss.* 99, 181-197 (1994).
243. Chen, X.G., Schweitzer-Stenner, R., Asher, S.A., Mirkin, N.G., and Krimm, S. "Vibrational Assignments of *trans*-N-Methylacetamide and Some of Its Deuterated Isotopomers from Band Decomposition of IR, Visible, and Resonance Raman Spectra" *J. Phys. Chem.* 99, 3074-3083 (March 9, 1995).
244. Chen, X.G., Asher, S.A., Schweitzer-Stenner, R., Mirkin, N.G., and Krimm, S. "UV Raman Determination of the $\pi\pi^*$ Excited State Geometry of *N*-Methylacetamide: Vibrational Enhancement Pattern" *J. Am. Chem. Soc.* 117, 2884-2895 (Mar. 15, 1995).

245. Mirkin, N.G. and Krimm, S. "Structure of *Trans*-N-Methylacetamide: Planar or Non-Planar Symmetry?" J. Mol. Struct. (Theochem) 334, 1-6 (April 20, 1995).
246. Krimm, S. "Future Directions for Vibrational Spectroscopy in Polymer Science" Trends in Polymer Science 3, 144-145 (May 1995).
247. Reisdorf, Jr., W.C. and Krimm, S. "Infrared Dichroism of Amide I and Amide II Modes of α_I - and α_{II} -Helix Segments in Membrane Proteins" Biophys. J. 69, 271-273 (July 1995).
248. Palmö, K. and Krimm, S. "Chain Elastic Modulus of Polyethylene: A Spectroscopically Determined Force Field (SDFF) Study" J. Polym. Sci. Polym. Phys. Ed. 34, 37-45 (Jan. 1996).
249. Reisdorf, Jr., W.C. and Krimm, S. "Infrared Amide I' Band of the Coiled Coil" Biochemistry 35, 1383-1386 (Feb. 6, 1996).
250. Mirkin, N.G. and Krimm, S. "Ab Initio Vibrational Analysis of Isotopic Derivatives of Aqueous Hydrogen-Bonded *trans*-N-Methylacetamide" J. Mol. Struct. 377, 219-234 (Apr. 15, 1996).
251. Qian, W. and Krimm, S. "Origin of the C=O Stretch Mode Splitting in the Formic Acid Dimer" J. Phys. Chem. 100, 14602-14608 (Aug. 29, 1996).
252. Kim, I. and Krimm, S. "Raman Longitudinal Acoustic Mode Studies of a Poly(ethylene oxide) Fraction during Isothermal Crystallization from the Melt" Macromolecules 29, 7186-7192 (Oct. 21, 1996).
253. Palmö, K. and Krimm, S. "Energetics Analysis of Syndiotactic Polypropylene Crystal Structure" Macromolecules 29, 8549-8550 (Dec. 16, 1996).
254. Kim, I. and Krimm, S. "Raman Longitudinal Acoustic Mode Studies of Poly(ethylene oxide) and α,ω -Methoxylated Poly(ethylene oxide) Fractions during Isothermal Crystallization from the Melt" J. Polym. Sci. B.: Polym. Phys. 35, 1117-1126 (May 1997).
255. Asher, S.A., Li, P., Chi, Z., Chen, X.G., Schweitzer-Stenner, R., Mirkin, N.G., and Krimm, S. "Reply to Comment on 'Vibrational Assignments of *trans*-N-Methylacetamide and Some of Its Deuterated Isotopomers from Band Decomposition of IR, Visible and Resonance Raman Spectra'" J. Phys. Chem. A. 101, 3992-3994 (May 22, 1997).
256. Mannfors, B., Pietilä, L.-O., Palmö, K., Sundius, T., and Krimm, S. "Molecular Mechanics Potential Energy Functions from Vibrational Spectroscopy and Quantum Chemistry" J. Mol. Struct. 408/409, 63-69 (June 1, 1997).
257. Qian, W. and Krimm, S. "A Model for the Intermolecular Interactions of the Hydrogen Bond That Incorporates Its Spectroscopic Properties" J. Phys. Chem. A. 101, 5825-5827 (Aug. 14, 1997).

258. Lee, S.-H. and Krimm, S. "Polarized Raman Spectra of Oriented Films of α -Helical Poly(L-alanine) and its N-Deuterated Analogue" *J. Raman Spectrosc.* 29, 73-80 (Jan. 1998).
259. Schweitzer-Stenner, R., Sieler, G., Mirkin, N.G., and Krimm, S. "Intermolecular Coupling in Liquid and Crystalline States of *trans*-N-Methylacetamide Investigated by Polarized Raman and FT-IR Spectroscopies" *J. Phys. Chem. A.* 102, 118-127 (Jan. 1, 1998).
260. Qian, W. and Krimm, S. "Electrostatic Model for the Interaction Force Constants of the Formic Acid Dimer" *J. Phys. Chem. A.* 102, 659-667 (Jan. 15, 1998).
261. Lee, S.-H. and Krimm, S. "General Treatment of Vibrations of Helical Molecules and Application to Transition Dipole Coupling in Amide I and Amide II Modes of α -Helical Poly(L-alanine)" *Chem. Phys.* 230, 277-295 (May 1, 1998).
262. Palmo, K. and Krimm, S. "Electrostatic Model for Infrared Intensities in a Spectroscopically Determined Molecular Mechanics Force Field" *J. Comput. Chem.* 19, 754-768 (May 1998).
263. Palmo, K., Mirkin, N.G., and Krimm, S. "Spectroscopically Determined Force Fields for Macromolecules. 2. Saturated Hydrocarbon Chains" *J. Phys. Chem. A.* 102, 6448-6456 (Aug. 6, 1998).
264. Lee, S.-H. and Krimm, S. "Ab Initio-Based Vibrational Analysis of α -Poly(L-alanine)" *Biopolymers* 46, 283-317 (Oct. 15, 1998).
265. Krimm, S. and Palmo, K. "Intensities of Infrared and Raman Bands" in *Encyclopedia of Computational Chemistry*, John Wiley and Sons, New York, 1998, pp. 1361-1363.
266. Lee, S.-H., Mirkin, N.G., and Krimm, S. "A Quantitative Anharmonic Analysis of the Amide A Band in α -Helical Poly(L-alanine)" *Biopolymers* 49, 195-207 (March 1999).
267. Krimm, S. "Vibrational Spectroscopy of Polypeptides" in *Modern Polymer Spectroscopy* ed. G. Zerbi, Wiley-VCH, Weinheim, 1999, Chap. 5, pp. 239-285.
268. Lee, S.-H., Palmo, K., and Krimm, S. "New Out-of-Plane Angle and Bond Angle Internal Coordinates and Related Potential Energy Functions for Molecular Mechanics and Dynamics Simulations" *J. Comput. Chem.* 20, 1067-1084 (July 30, 1999).
269. Qian, W., Mirkin, N.G., and Krimm, S. "A Spectroscopically Effective Molecular Mechanics Model for the Intermolecular Interactions in the Hydrogen-Bonded N-Methylacetamide Dimer" *Chem. Phys. Lett.* 315, 125-129 (Dec. 17, 1999)

270. Krimm, S. "Interpreting Infrared Spectra of Peptides and Proteins" in Infrared Analysis of Peptides and Proteins. Principles and Application, ed. Bal Ram Singh, ACS Symposium Series 750, American Chemical Society, Washington, DC, 2000, pp. 38-53.
271. Mannfors, B., Sundius, T., Palmo, K., Pietila, L.-O., and Krimm, S. "Spectroscopically Determined Force Fields for Macromolecules. Part 3. Alkene Chains" *J. Mol. Struct.* 521, 49-75 (2000).
272. Krimm, S. "C.V. Raman: A Personal Note" in Raman Scattering in Materials Science, eds. W.H. Weber and R. Merlin, Springer, Berlin, 2000, pp. 446-447.
273. Mirkin, N.G. and Krimm, S. "Ab Initio Analysis of the Vibrational Spectra of Conformers of Some Branched Alkanes" *J. Mol. Struct.* 550-551, 67-91 (5 Sept. 2000).
274. Mannfors, B., Palmo, K., and Krimm, S. "A New Electrostatic Model for Molecular Mechanics Force Fields" *J. Mol. Struct.* 556, 1-21 (2000).
275. Lee, S.-H., Palmo, K., and Krimm, S. "A New Formalism for Molecular Dynamics in Internal Coordinates" *Chem. Phys.* 265, 63-85 (2001).
276. Qian, W. and Krimm, S. "Spectroscopically Determined Molecular Mechanics Model for the Intermolecular Interactions in Hydrogen-Bonded Formic Acid Dimer Structures" *J. Phys. Chem. A* 105, 5046-5053 (May 24, 2001).
277. Lee, S.-H., Palmo, K., and Krimm, S. "The Casimir-Eckart Condition and the Transformation of Dipole Moment Derivatives Revisited" *J. Mol. Struct. (Theochem)* 546, 217-230 (16 July 2001).
278. Lee, S.-H., Palmo, K., and Krimm, S. "A New Method to Calculate B-Matrix Elements for External Rotations with Application to the B-Matrix Internal Coordinate Molecular Dynamics Formalism" *Chem. Phys. Lett.* 342, 643-651 (20 July 2001).
279. Mannfors, B., Mirkin, N.G., Palmo, K., and Krimm, S. "A Polarizable Electrostatic Model of the N-Methylacetamide Dimer" *J. Comput. Chem.* 22, 1933-1943 (Dec. 2001).
280. Palmo, K. and Krimm, S. "Energetics Analysis of Forms I-IV Syndiotactic Polypropylene Crystal Structures" *Macromolecules* 35, 394-402 (Jan. 15, 2002).
281. Mirkin, N.G. and Krimm, S. "Amide III Mode φ, ψ Dependence in Peptides: A Vibrational Frequency Map" *J. Phys. Chem. A* 106, 3391-3394 (Apr. 11, 2002)
282. Qian, W. and Krimm, S. "Vibrational Spectroscopy of Hydrogen Bonding: Origin of the Different Behavior of the C-H \cdots O Hydrogen Bond" *J. Phys. Chem. A* 106, 6628-6636 (July 18, 2002).
283. Lee, S.-H., Palmo, K., and Krimm, S. "Internal Coordinate Molecular Dynamics

- Based on the Spectroscopic B-Matrix” in Computational Methods for Macromolecules: Challenges and Applications, eds. Tamar Schlick and Hin Hark Gan, Springer-Verlag, Berlin Heidelberg New York, 2002, pp. 104-128.
284. Qian, W. and Krimm, S. “C-H \cdots O and O-H \cdots O Hydrogen Bonding in Formic Acid Dimer Structures: A QM/MM Study Confirms the Common Origin of Their Different Spectroscopic Behavior” *J. Phys. Chem. A* 106, 11663-11671 (Nov. 28, 2002).
 285. Palmo, K., Mannfors, B., and Krimm, S. “Balanced Charge Treatment of Intramolecular Electrostatic Interactions in Molecular Mechanics Energy Functions” *Chem. Phys. Lett.* 369, 367-373 (Feb. 17, 2003).
 286. Palmo, K., Mannfors, B., Mirkin, N.G., and Krimm, S. “Potential Energy Functions: From Consistent Force Fields to Spectroscopically Determined Polarizable Force Fields” *Biopolymers* 68, 383-394 (Mar. 2003).
 287. Mannfors, B., Mirkin, N.G., Palmo, K., and Krimm, S. “Analysis of the Pyramidalization of the Peptide Group Nitrogen: Implications for Molecular Mechanics Energy Functions” *J. Phys. Chem. A* 107, 1825-1832 (Mar. 20, 2003).
 288. Mirkin, N.G. and Krimm, S. “Structural Dependence of NH Stretch Mode Frequency Shifts in Amide and Peptide Systems” *J. Phys. Chem. A* 108, 5438-5448 (June 24, 2004).
 289. Mirkin, N.G. and Krimm, S. “Are Amide Mode Infrared Frequency Shifts in Crystalline α -Nylon-6 at Low Strains Due to Changes in Nitrogen Pyramidalization?” *Macromolecules* 37, 6660-6661 (Aug. 24, 2004).
 290. Palmo, K. and Krimm, S. “Theoretical Basis and Accuracy of a Non-Iterative Polarization Protocol in Molecular Mechanics Energy Function Calculations” *Chem. Phys. Lett.* 395, 133-137 (Sept. 2004).
 291. Mirkin, N.G. and Krimm, S. “A New Vibrational Spectroscopic Tool for the Determination of Peptide Conformation: The Isotope-Edited C $^{\alpha}$ H $^{\alpha}$ Stretch Mode” *J. Phys. Chem. A* 108, 10923-10924 (Dec. 16, 2004).
 292. Qian, W. and Krimm, S. “Limitations of the Molecular Multipole Expansion Treatment of Electrostatic Interactions for C-H \cdots O and O-H \cdots O Hydrogen Bonds and Application of a General Charge Density Approach” *J. Phys. Chem. A* 109, 5608-5618 (June 30, 2005).
 293. Lee, S.-H., Palmo, K., and Krimm, S. “WIGGLE: A New Constrained Molecular Dynamics Algorithm in Cartesian Coordinates” *J. Comput. Phys.* 210, 171-182 (20 Nov. 2005).
 294. Colvin, M.E., Cramer, C.J., Dykstra, C.E., Jensen, J.H., Krimm, S., Rivail, J.-L., Thakkar, A.J., and Yañez, M. “Molecular Quantum Mechanics to Biodynamics:

- Essential Connections” *J. Mol. Struct. (Theochem)* **764**, 1-8 (30 May 2006).
295. Lee, S.-H., Wang, J., Krimm, S., and Chen, Z. “Irreducible Representation and Projection Operator Application to Understanding Nonlinear Optical Phenomena: Hyper-Raman, Sum Frequency Generation, and Four-Wave Spectroscopy” *J. Phys. Chem. A* **110**, 7035-7044 (June 8, 2006).
296. Qian, W. and Krimm, S. “Charge Density Treatment of the Molecule-Charge Interaction and Its Relation to the Electrical Component of Hydrogen Bonding: Accuracy and Distance Dependence” *J. Mol. Struct. (Theochem)* **766**, 93-104 (15 Aug. 2006).
297. Palmo, K., Mannfors, B., Mirkin, N.G., and Krimm, S. “Inclusion of Charge and Polarizability Fluxes Provides Needed Physical Accuracy in Molecular Mechanics Force Fields” *Chem. Phys. Lett.* **429**, 628-632 (5 Oct. 2006).
298. Lee, S.-H., Palmo, K., and Krimm, S. “A Comparative Study of Molecular Dynamics in Cartesian and in Internal Coordinates: Dynamical Instability in the Latter Caused by Nonlinearity of the Equations of Motion” *J. Comput. Phys.* **28**, 1107-1118 (30 Apr. 2007).
299. Mirkin, N.G. and Krimm, S. “Conformation Dependence of the C^αD^α Stretch Mode in Peptides. 1. Isolated Alanine Peptide Structures” *J. Phys. Chem. A* **111**, 5300-5303 (June 21, 2007).
300. Palmo, K. and Krimm, S. “Group Polarization Model for Molecular Mechanics Energy Functions” *J. Chem. Theory Comput.* **3**, 2120-2127 (Nov. 2007).
301. Mirkin, N.G. and Krimm, S. “Peptide C^αD^α Stretch Frequencies in a Hydrated Conformation Are Perturbed Mainly by C^α-D^α...O Hydrogen Bonding” *J. Phys. Chem. B* **112**, 15627-15628 (4 Dec. 2008).
302. Mannfors, B., Palmo, K., and Krimm, S. “Spectroscopically Determined Force Field for Water Dimer: Physically Enhanced Treatment of Hydrogen Bonding in Molecular Mechanics Energy Functions” *J. Phys. Chem. A* **112**, 12667-12678 (11 Dec. 2008).
303. Mirkin, N.G. and Krimm, S. “Conformation Dependence of the C^αD^α Stretch Mode in Peptides. II. Explicitly Hydrated Alanine Peptide Structures” *Biopolymers* **91**, 791-800 (Sept. 2009).
304. Mirkin, N.G. and Krimm, S. “Conformation Dependence of the C^αD^α Stretch Mode in Peptides: Side-Chain Influence in Dipeptide Structures” *Biopolymers* **93**, 1065-1071 (Dec. 2010).
305. Mirkin, N.G. and Krimm, S. “Water Interaction Differences Determine the Relative Energetic Stability of the Polyproline II Conformation of the Alanine Dipeptide in Aqueous Environments” *Biopolymers* **97**, 789-794 (Oct. 2012).

