Laurence A Nafie

List of Publications by Citations

280 papers	10,460 citations	52 h-index	86 g-index
302 ext. papers	11,072 ext. citations	5.6 avg, IF	6.37 L-index

#	Paper	IF	Citations
280	Absolute configuration determination of chiral molecules in the solution state using vibrational circular dichroism. *Chirality*, **2003**, 15, 743-58	2.1	445
279	**2011**,		393
278	Vibrational circular dichroism. *Journal of the American Chemical Society*, **1976**, 98, 2715-2723	16.4	341
277	Infrared and Raman vibrational optical activity: theoretical and experimental aspects. *Annual Review of Physical Chemistry*, **1997**, 48, 357-86	15.7	272
276	Determination of absolute configuration of chiral molecules using vibrational optical activity: a review. *Applied Spectroscopy*, **2011**, 65, 699-723	3.1	221
275	Reorientation and Vibrational Relaxation as Line Broadening Factors in Vibrational Spectroscopy. *Journal of Chemical Physics*, **1972**, 57, 3145-3155	3.9	212
274	Tripeptides adopt stable structures in water. A combined polarized visible Raman, FTIR, and VCD spectroscopy study. *Journal of the American Chemical Society*, **2002**, 124, 14330-41	16.4	189
273	A confidence level algorithm for the determination of absolute configuration using vibrational circular dichroism or Raman optical activity. *ChemPhysChem*, **2011**, 12, 1542-9	3.2	156
272	Quantum Theory of the Intensities of Molecular Vibrational Spectra. *Journal of Chemical Physics*, **1970**, 52, 1576-1584	3.9	153
271	Vibronic coupling theory of infrared vibrational transitions. *Journal of Chemical Physics*, **1983**, 78, 7108-7116	3.9	135
270	Vibrational circular dichroism of 2,2,2-trifluoro-1-phenylethanol. *Journal of the American Chemical Society*, **1975**, 97, 3842-3843	16.4	132
269	Vibrational circular dichroism shows unusual sensitivity to protein fibril formation and development in solution. *Journal of the American Chemical Society*, **2007**, 129, 12364-5	16.4	126
268	Dual Polarization Modulation: A Real-Time, Spectral-Multiplex Separation of Circular Dichroism from Linear Birefringence Spectral Intensities. *Applied Spectroscopy*, **2000**, 54, 1634-1645	3.1	121
267	Theory of resonance Raman optical activity: the single electronic state limit. *Chemical Physics*, **1996**, 205, 309-322	2.3	116
266	The conformation of tetraalanine in water determined by polarized Raman, FT-IR, and VCD spectroscopy. *Journal of the American Chemical Society*, **2004**, 126, 2768-76	16.4	115
265	Direct observation and pH control of reversed supramolecular chirality in insulin fibrils by vibrational circular dichroism. *Chemical Communications*, **2010**, 46, 7154-6	5.8	109
264	Role of hydration in determining the structure and vibrational spectra of L-alanine and N-acetyl L-alanine N?-methylamide in aqueous solution: a combined theoretical and experimental approach. *Theoretical Chemistry Accounts*, **2008**, 119, 191-210	1.9	109

263	Vibrational circular dichroism in amino acids and peptides. 4. Vibrational analysis, assignments, and solution-phase Raman spectra of deuterated isotopomers of alanine. *Journal of the American Chemical Society*, **1982**, 104, 3329-3336	16.4	109
262	Fourier transform infrared vibrational circular dichroism. *Journal of the American Chemical Society*, **1979**, 101, 496-498	16.4	108
261	Preferred peptide backbone conformations in the unfolded state revealed by the structure analysis of alanine-based (AXA) tripeptides in aqueous solution. *Proceedings of the National Academy of Sciences of the United States of America*, **2004**, 101, 10054-9	11.5	106
260	Vibrational circular dichroism spectra of three conformationally distinct states and an unordered state of poly(L-lysine) in deuterated aqueous solution. *Biopolymers*, **1986**, 25, 1751-65	2.2	105
259	Is supramolecular filament chirality the underlying cause of major morphology differences in amyloid fibrils?. *Journal of the American Chemical Society*, **2014**, 136, 2302-12	16.4	103
258	Adiabatic molecular properties beyond the Born□Oppenheimer approximation. Complete adiabatic wave functions and vibrationally induced electronic current density. *Journal of Chemical Physics*, **1983**, 79, 4950-4957	3.9	100
257	Ab initio VCD calculation of a transition-metal containing molecule and a new intensity enhancement mechanism for VCD. *Journal of the American Chemical Society*, **2001**, 123, 11320-1	16.4	96
256	Theory of High Frequency Differential Interferometry: Application to the Measurement of Infrared Circular and Linear Dichroism via Fourier Transform Spectroscopy. *Applied Spectroscopy*, **1979**, 33, 130-135	3.1	95
255	The Structure of Alanine Based Tripeptides in Water and Dimethyl Sulfoxide Probed by Vibrational Spectroscopy. *Journal of Physical Chemistry B*, **2003**, 107, 358-365	3.4	87
254	Vibrational Optical Activity. *Applied Spectroscopy*, **1996**, 50, 14A-26A	3.1	86
253	Polarized laser Raman studies of biological polymers. *Journal of Chemical Physics*, **1969**, 51, 3993-4005	3.9	86
252	Chirality and diastereoselection of □□configured tetrahedral zinc complexes through enantiopure Schiff base complexes: combined vibrational circular dichroism, density functional theory, 1H NMR, and X-ray structural studies. *Inorganic Chemistry*, **2011**, 50, 11363-74	5.1	80
251	Experimental observation of resonance Raman optical activity. *Chemical Physics Letters*, **1998**, 287, 359-364	2.3	78
250	Optical activity in vibrational transitions: vibrational circular dichroism and Raman optical activity. *Accounts of Chemical Research*, **1979**, 12, 296-302	24.3	75
249	Dual circular polarization raman optical activity. *Chemical Physics Letters*, **1989**, 154, 260-266	2.5	73
248	Normal and reversed supramolecular chirality of insulin fibrils probed by vibrational circular dichroism at the protofilament level of fibril structure. *Biophysical Journal*, **2012**, 103, 522-531	2.9	72
247	Theory of Vibrational Circular Dichroism and Infrared Absorption: Extension to Molecules with Low-Lying Excited Electronic States. *Journal of Physical Chemistry A*, **2004**, 108, 7222-7231	2.8	72
246	Theory of natural Raman optical activity. *Molecular Physics*, **1991**, 72, 441-469	1.7	70

245	Spontaneous inter-conversion of insulin fibril chirality. *Chemical Communications*, **2012**, 48, 2837-9	5.8	69
244	A combined theoretical and experimental study of the structure and vibrational absorption, vibrational circular dichroism, Raman and Raman optical activity spectra of the L-histidine zwitterion. *Theoretical Chemistry Accounts*, **2008**, 119, 155-176	1.9	68
243	Scattered circular polarization Raman optical activity. *Chemical Physics Letters*, **1988**, 149, 367-374	2.5	68
242	Density Functional Theory Calculations of Vibrational Circular Dichroism in Transition Metal Complexes: Identification of Solution Conformations and Mode of Chloride Ion Association for (+)-Tris(ethylenediaminato)cobalt(III) *Journal of Physical Chemistry A*, **2002**, 106, 3560-3565	2.8	67
241	Vibrational circular dichroism in amino acids and peptides. 7. Amide stretching vibrations in polypeptides. *Biopolymers*, **1982**, 21, 2161-83	2.2	67
240	Tripeptides with ionizable side chains adopt a perturbed polyproline II structure in water. *Biochemistry*, **2004**, 43, 613-21	3.2	65
239	Role of Solvent and Secondary Doping in Polyaniline Films Doped with Chiral Camphorsulfonic Acid: Preparation of a Chiral Metal. *Chemistry of Materials*, **2002**, 14, 1430-1438	9.6	63
238	Stereochemical determination and bioactivity assessment of (S)-(+)-curcuphenol dimers isolated from the marine sponge Didiscus aceratus and synthesized through laccase biocatalysis. *Bioorganic and Medicinal Chemistry*, **2005**, 13, 5600-12	3.4	63
237	On the origin of the intensity of the resonant raman bands of differing polarization in heme proteins. *Chemical Physics Letters*, **1973**, 20, 563-568	2.5	63
236	Optically Active Nanostructured ZnO Films. *Angewandte Chemie - International Edition*, **2015**, 54, 15170-5	16.4	62
235	Experimental Measurement and Ab Initio Calculation of Raman Optical Activity of L-Alanine and Its Deuterated Isotopomers. *The Journal of Physical Chemistry*, **1995**, 99, 835-843		62
234	Dual and incident circular polarization Raman optical activity backscattering of (+)-trans-pinane. *Chemical Physics Letters*, **1991**, 180, 182-190	2.5	59
233	Direct observation of odd-even effect for chiral alkyl alcohols in solution using vibrational circular dichroism spectroscopy. *Journal of the American Chemical Society*, **2004**, 126, 194-8	16.4	58
232	Determination of the absolute configuration and solution conformation of gossypol by vibrational circular dichroism. *Chirality*, **2003**, 15, 196-200	2.1	58
231	Vibrational optical activity of oligopeptides. *Biopolymers*, **1995**, 37, 265-79	2.2	57
230	Vibrational circular dichroism in transition-metal complexes. 2. Ion association, ring conformation, and ring currents of ethylenediamine ligands. *Journal of the American Chemical Society*, **1986**, 108, 7255-7263	16.4	56
229	Vibrational circular dichroism in the mid-infrared using fourier transform spectroscopy. *Chemical Physics Letters*, **1982**, 90, 1-5	2.5	54
228	Determination of enantiomeric excess in samples of chiral molecules using fourier transform vibrational circular dichroism spectroscopy: simulation of real-time reaction monitoring. *Analytical Chemistry*, **2004**, 76, 6956-66	7.8	52

227	Time ordered diagrams for the resonant raman effect from molecular vibrations. *Chemical Physics Letters*, **1971**, 12, 131-136	2.5	52
226	Complete polarization measurements for non-symmetric Raman tensors: Symmetry assignments of ferrocytochrome C vibrations. *Journal of Raman Spectroscopy*, **1973**, 1, 455-464	2.3	51
225	Absolute configuration reassignment of two chromanes from Peperomia obtusifolia (Piperaceae) using VCD and DFT calculations. *Tetrahedron: Asymmetry*, **2010**, 21, 2402-2407		49
224	Electron Transition Current Density in Molecules. 1. Non-Born□Oppenheimer Theory of Vibronic and Vibrational Transitions. *Journal of Physical Chemistry A*, **1997**, 101, 7826-7833	2.8	49
223	Fourier transform vibrational circular dichroism from 800 to 10,000 cm□1: Near-IR-VCD spectral standards for terpenes and related molecules. *Vibrational Spectroscopy*, **2006**, 42, 254-272	2.1	49
222	Vibrational circular-dichroism spectroscopy of homologous cyclic peptides designed to fold into □ helices of opposite chirality. *Biointerphases*, **2011**, 6, 1-7	1.8	48
221	Vibrational circular dichroism in amino acids and peptides. 3. Solution- and solid-phase spectra of alanine and serine. *Journal of the American Chemical Society*, **1979**, 101, 6829-6837	16.4	48
220	The atom dipole interaction model of Raman optical activity: Reformulation and comparison to the general two-group model. *Journal of Chemical Physics*, **1979**, 70, 5582-5588	3.9	48
219	Determination of Absolute Configuration in Molecules with Chiral Axes by Vibrational Circular Dichroism: A C2-Symmetric Annelated Heptathiophene and a D2-Symmetric Dimer of 1,1□Binaphthyl. *Journal of Physical Chemistry A*, **2003**, 107, 7692-7696	2.8	47
218	Vibrational circular dichroism: an incisive tool for stereochemical applications. *Enantiomer*, **1998**, 3, 283-97		47
217	Amplified vibrational circular dichroism as a probe of local biomolecular structure. *Journal of the American Chemical Society*, **2014**, 136, 3530-5	16.4	46
216	Chlorofluoroiodomethane as a potential candidate for parity violation measurements. *Physical Chemistry Chemical Physics*, **2006**, 8, 79-92	3.6	46
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214	Theory of Raman scattering and Raman optical activity: near resonance theory and levels of approximation. *Theoretical Chemistry Accounts*, **2008**, 119, 39-55	1.9	45
213	VCD to determine absolute configuration of natural product molecules: secolignans from Peperomia blanda. *Organic and Biomolecular Chemistry*, **2012**, 10, 4208-14	3.9	44
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211	Infrared absorption and the Born□Oppenheimer approximation. II. Vibrational circular dichroism. *Journal of Chemical Physics*, **1977**, 67, 1501-1510	3.9	43
210	Fourier Transform Infrared Vibrational CircularDichroism: Improvements in Methodology and Mid-Infrared Spectral Results. *Applied Spectroscopy*, **1984**, 38, 20-26	3.1	42

209	Absolute configuration and selective trypanocidal activity of gaudichaudianic acid enantiomers. *Journal of Natural Products*, **2011**, 74, 1154-60	4.9	41
208	Dual source fourier transform polarization modulation spectroscopy: an improved method for the measurement of circular and linear dichroism. *Applied Spectroscopy*, **2004**, 58, 647-54	3.1	41
207	Comparison of IR and Raman forms of vibrational optical activity. *Faraday Discussions*, **1994**, 13-34; discussion 87-101	3.6	41
206	Velocity-gauge formalism in the theory of vibrational circular dichroism and infrared absorption. *Journal of Chemical Physics*, **1992**, 96, 5687-5702	3.9	41
205	Vibrational circular dichroism in the methine bending modes of amino acids and dipeptides. *Journal of the American Chemical Society*, **1988**, 110, 6970-6974	16.4	41
204	Enhanced vibrational circular dichroism via vibrationally generated electronic ring currents. *Journal of the American Chemical Society*, **1985**, 107, 6213-6222	16.4	41
203	Ring current mechanism of vibrational circular dichroism. *The Journal of Physical Chemistry*, **1986**, 90, 763-767		40
202	Racemization and geometrical isomerization of (2S,3S)-cyclopropane-1-13C-1,2,3-d3 at 407 .degree.C: kinetically competitive one-center and two-center thermal epimerizations in an isotopically substituted cyclopropane. *Journal of the American Chemical Society*, **1991**, 113, 1864-1866	16.4	39
201	Solvation-induced helicity inversion of pseudotetrahedral chiral copper(II) complexes. *Inorganic Chemistry*, **2015**, 54, 2193-203	5.1	38
200	Vibrational circular dichroism of amylose carbamate: structure and solvent-induced conformational changes. *Tetrahedron: Asymmetry*, **2008**, 19, 2111-2114		38
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195	Preparation of cruciferous phytoalexin related metabolites, (−)-dioxibrassinin and (−)-3-cyanomethyl-3-hydroxyoxindole, and determination of their absolute configurations by vibrational circular dichroism (VCD). *Tetrahedron Letters*, **2003**, 44, 6017-6020	2	37
194	Extension of fourier transform vibrational circular dichroism into the near-infrared region: continuous spectral coverage from 800 to 10 000 cm(-1). *Applied Spectroscopy*, **2004**, 58, 1057-64	3.1	37
193	Hydrogen Stretching Vibrational Circular Dichroism in Methyl Lactate and Related Molecules. *Journal of Physical Chemistry A*, **1999**, 103, 1523-1537	2.8	37
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191	Resonance raman studies of macrocyclic complexes. 2. Antiresonance and selective intensity enhancement in synthetic metal(II) porphyrin analogues. *Journal of the American Chemical Society*, **1976**, 98, 8007-14	16.4	36
190	Structure elucidation and absolute stereochemistry of isomeric monoterpene chromane esters. *Journal of Organic Chemistry*, **2011**, 76, 2603-12	4.2	35
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187	Electron Transition Current Density in Molecules. 2. Ab Initio Calculations for Electronic Transitions in Ethylene and Formaldehyde. *Journal of Physical Chemistry A*, **1998**, 102, 3352-3357	2.8	32
186	Synthesis and gas-phase vibrational circular dichroism of (+)-(S,S)-cyclopropane-1,2-2H2. *Journal of the American Chemical Society*, **1989**, 111, 1913-1915	16.4	31
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184	A New Scattered Circular Polarization Raman Optical Activity Instrument Equipped with a Charge-Coupled-Device Detector. *Applied Spectroscopy*, **1991**, 45, 18-25	3.1	31
183	Vibrational circular dichroism in the carbon-hydrogen and carbon-deuterium stretching modes of (S,S)-[2,3-2H2]oxirane. *Journal of the American Chemical Society*, **1987**, 109, 4727-4728	16.4	31
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179	Improved backscattering dual circular polarization raman optical activity spectrometer with enhanced performance for biomolecular applications. *Journal of Raman Spectroscopy*, **1997**, 28, 627-633	2.3	29
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169	Vibrational circular dichroism in amino acids and peptides. 5. Carbon-hydrogen, stretching vibrational circular dichroism and fixed partial charge calculations for deuterated isotopomers of alanine. *Journal of the American Chemical Society*, **1982**, 104, 3336-3342	16.4	28
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167	Localized molecular orbital calculations of vibrational circular dichroism. I. General theoretical formalism and CNDO results for the carbon□deuterium stretching vibration in neopentyl-1-d-chloride. *Journal of Chemical Physics*, **1981**, 75, 2935-2944	3.9	27
166	Calculation of excitation profiles from the vibronic theory of raman scattering. *Chemical Physics*, **1977**, 19, 303-311	2.3	27
165	Near-infrared and mid-infrared Fourier transform vibrational circular dichroism of proteins in aqueous solution. *Applied Spectroscopy*, **2010**, 64, 615-26	3.1	26
164	Observation and calculation of vibrational circular birefringence: a new form of vibrational optical activity. *Chirality*, **2009**, 21 Suppl 1, E277-86	2.1	26
163	Comparison of Step-Scan and Rapid-Scan Approaches to the Measurement of Mid-Infrared Fourier Transform Vibrational Circular Dichroism. *Applied Spectroscopy*, **1997**, 51, 504-507	3.1	26
162	Structure and absolute configuration of nyasol and hinokiresinol via synthesis and vibrational circular dichroism spectroscopy. *Journal of Natural Products*, **2005**, 68, 1603-9	4.9	26
161	Determination of the absolute configuration and solution conformation of the antifungal agents ketoconazole, itraconazole, and miconazole with vibrational circular dichroism. *Chirality*, **2005**, 17 Suppl, S101-8	2.1	26
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159	Vibrational circular dichroism in bis(acetylacetonato)(L-alaninato)cobalt(III). Isolated occurrences of the coupled oscillator and ring current intensity mechanisms. *Journal of the American Chemical Society*, **1985**, 107, 6205-6213	16.4	26
158	Simultaneous acquisition of all four forms of circular polarization Raman optical activity: results for □-pinene and lysozyme. *Journal of Raman Spectroscopy*, **2012**, 43, 89-94	2.3	25
157	Step-Scan Fourier Transform Vibrational Circular Dichroism Measurements in the Vibrational Region above 2000 cm□1. *Applied Spectroscopy*, **1997**, 51, 508-511	3.1	25
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149	Determination of the Absolute Configuration of (+)-Mirtazapine by Vibrational Circular Dichroism. *Helvetica Chimica Acta*, **2002**, 85, 1160	2	24
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142	Vibrational optical activity calculations using infrared and Raman atomic polar tensors. *Journal of Chemical Physics*, **1983**, 78, 27-31	3.9	23
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140	Stereochemical Aspects of Vibrational Optical Activity. *Topics in Stereochemistry*,113-206		23
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138	Vibrational circular dichroism spectra of lysozyme solutions: solvent effects on thermal denaturation processes. *Journal of Physical Chemistry B*, **2013**, 117, 2645-52	3.4	22

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135	Raman optical activity of biological molecules. *Vibrational Spectroscopy*, **1995**, 8, 231-239	2.1	22
134	Measurement of Vibrational Circular Dichroism Using a Polarizing Michelson Interferometer. *Applied Spectroscopy*, **1990**, 44, 5-7	3.1	22
133	Determination of Enantiomeric Excess in Deuterated Chiral Hydrocarbons by Vibrational Circular Dichroism Spectroscopy. *Applied Spectroscopy*, **1990**, 44, 235-238	3.1	22
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126	Subtle chirality in oxo- and sulfidorhenium(v) complexes. *Chemical Communications*, **2009**, 4841-3	5.8	20
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