

Laurence A Nafie

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Conformational Variability Correlation Prediction of Transmissibility and Neutralization Escape Ability for Multiple Mutation SARS-CoV-2 Strains using SSSCPreds. <i>ACS Omega</i> , 2021 , 6, 19323-19329	3.9	5
279	Isolation, Total Synthesis, and Absolute Configuration Determination of Renoprotective Dimeric -Acetyldopamine-Adenine Hybrids from the Insect. <i>Organic Letters</i> , 2020 , 22, 5726-5730	6.2	5
278	Vibrational optical activity: From discovery and development to future challenges. <i>Chirality</i> , 2020 , 32, 667-692	2.1	29
277	SSSCPreds: Deep Neural Network-Based Software for the Prediction of Conformational Variability and Application to SARS-CoV-2. <i>ACS Omega</i> , 2020 , 5, 30556-30567	3.9	3
276	Recent advances in linear and nonlinear Raman spectroscopy. Part XIV. <i>Journal of Raman Spectroscopy</i> , 2020 , 51, 2354-2376	2.3	3
275	Recent advances in linear and nonlinear Raman spectroscopy. Part XIII. <i>Journal of Raman Spectroscopy</i> , 2019 , 50, 1783-1806	2.3	2
274	Recent advances in linear and nonlinear Raman spectroscopy. Part XII. <i>Journal of Raman Spectroscopy</i> , 2018 , 49, 1874-1906	2.3	8
273	Vibrational Optical Activity in Chiral Analysis 2018 , 201-247		3
272	Vibrational Optical Activity: From Small Chiral Molecules to Protein Pharmaceuticals and Beyond 2018 , 421-469		7
271	A Vibrational Circular Dichroism Microsampling Accessory: Mapping Enhanced Vibrational Circular Dichroism in Amyloid Fibril Films. <i>Applied Spectroscopy</i> , 2017 , 71, 1117-1126	3.1	16
270	Unravelling a Direct Role for Polysaccharide β -Strands in the Higher Order Structure of Physical Hydrogels. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 4603-4607	16.4	19
269	Unravelling a Direct Role for Polysaccharide β -Strands in the Higher Order Structure of Physical Hydrogels. <i>Angewandte Chemie</i> , 2017 , 129, 4674-4678	3.6	5
268	Raman Optical Activity, Theory 2017 , 891-899		1
267	Origin of enhanced VCD in amyloid fibril spectra: Effect of deuteration and pH. <i>Chirality</i> , 2017 , 29, 469-475	4.5	16
266	Recent advances in linear and non-linear Raman spectroscopy. Part XI. <i>Journal of Raman Spectroscopy</i> , 2017 , 48, 1692-1717	2.3	13
265	Vibrational CD Spectrometers 2017 , 524-533		
264	Recent advances in linear and non-linear Raman spectroscopy. Part X. <i>Journal of Raman Spectroscopy</i> , 2016 , 47, 1548-1565	2.3	12

263	Substrate-Determined Diastereoselectivity in an Enzymatic Carbonylation. <i>ChemBioChem</i> , 2016 , 17, 1207-1210	3	3
262	Three-Dimensional Chemical Structure Search Using the Conformational Code for Organic Molecules (CCOM) Program. <i>Chirality</i> , 2016 , 28, 370-5	2.1	3
261	Solvation-induced helicity inversion of pseudotetrahedral chiral copper(II) complexes. <i>Inorganic Chemistry</i> , 2015 , 54, 2193-203	5.1	38
260	Rapid Filament Supramolecular Chirality Reversal of HET-s (218-289) Prion Fibrils Driven by pH Elevation. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 8521-5	3.4	18
259	Supramolecular chirality in peptide microcrystals. <i>Chemical Communications</i> , 2015 , 51, 89-92	5.8	28
258	Recent advances in linear and non-linear Raman spectroscopy. Part IX. <i>Journal of Raman Spectroscopy</i> , 2015 , 46, 1173-1190	2.3	13
257	Optically Active Nanostructured ZnO Films. <i>Angewandte Chemie</i> , 2015 , 127, 15385-15390	3.6	18
256	Optically Active Nanostructured ZnO Films. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 15170-516.4	5.6.4	62
255	The transition from the native to the acid-state characterized by multi-spectroscopy approach: study for the holo-form of bovine lactalbumin. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2014 , 1844, 593-606	4	21
254	Is supramolecular filament chirality the underlying cause of major morphology differences in amyloid fibrils?. <i>Journal of the American Chemical Society</i> , 2014 , 136, 2302-12	16.4	103
253	Amplified vibrational circular dichroism as a probe of local biomolecular structure. <i>Journal of the American Chemical Society</i> , 2014 , 136, 3530-5	16.4	46
252	Recent advances in linear and nonlinear Raman spectroscopy. Part VIII. <i>Journal of Raman Spectroscopy</i> , 2014 , 45, 1326-1346	2.3	21
251	Recent advances in linear and nonlinear Raman spectroscopy. Part VII. <i>Journal of Raman Spectroscopy</i> , 2013 , 44, 1629-1648	2.3	17
250	Data mining of supersecondary structure homology between light chains of immunoglobulins and MHC molecules: absence of the common conformational fragment in the human IgM rheumatoid factor. <i>Journal of Chemical Information and Modeling</i> , 2013 , 53, 584-91	6.1	8
249	Levels of supramolecular chirality of polyglutamine aggregates revealed by vibrational circular dichroism. <i>FEBS Letters</i> , 2013 , 587, 1638-43	3.8	27
248	Vibrational circular dichroism spectra of lysozyme solutions: solvent effects on thermal denaturation processes. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 2645-52	3.4	22
247	Physical chemistry: handedness detected by microwaves. <i>Nature</i> , 2013 , 497, 446-8	50.4	21
246	Analysis of the molten globule state of bovine lactalbumin by using vibrational circular dichroism. <i>Vibrational Spectroscopy</i> , 2012 , 60, 68-72	2.1	22

245	Simultaneous acquisition of all four forms of circular polarization Raman optical activity: results for α -pinene and lysozyme. <i>Journal of Raman Spectroscopy</i> , 2012 , 43, 89-94	2.3	25
244	Recent advances in linear and nonlinear Raman spectroscopy. Part VI. <i>Journal of Raman Spectroscopy</i> , 2012 , 43, 1845-1863	2.3	23
243	Infrared Vibrational Optical Activity: Measurement and Instrumentation 2012 , 115-146		9
242	Normal and reversed supramolecular chirality of insulin fibrils probed by vibrational circular dichroism at the protofilament level of fibril structure. <i>Biophysical Journal</i> , 2012 , 103, 522-531	2.9	72
241	Further monoterpene chromane esters from <i>Peperomia obtusifolia</i> : VCD determination of the absolute configuration of a new diastereomeric mixture. <i>Tetrahedron Letters</i> , 2012 , 53, 6051-6054	2	17
240	Simultaneous resonance Raman optical activity involving two electronic states. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 7329-36	2.8	36
239	VCD to determine absolute configuration of natural product molecules: secolignans from <i>Peperomia blanda</i> . <i>Organic and Biomolecular Chemistry</i> , 2012 , 10, 4208-14	3.9	44
238	Experimental and theoretical polarized Raman linear difference spectroscopy of small molecules with a new alignment method using stretched polyethylene film. <i>Analytical Chemistry</i> , 2012 , 84, 1394-401	7.8	8
237	Spontaneous inter-conversion of insulin fibril chirality. <i>Chemical Communications</i> , 2012 , 48, 2837-9	5.8	69
236	Albendazole sulfoxide enantiomers: preparative chiral separation and absolute stereochemistry. <i>Journal of Chromatography A</i> , 2012 , 1230, 61-5	4.5	24
235	Vibrational circular-dichroism spectroscopy of homologous cyclic peptides designed to fold into β helices of opposite chirality. <i>Biointerphases</i> , 2011 , 6, 1-7	1.8	48
234	Chirality and diastereoselection of μ_2 -configured tetrahedral zinc complexes through enantiopure Schiff base complexes: combined vibrational circular dichroism, density functional theory, ^1H NMR, and X-ray structural studies. <i>Inorganic Chemistry</i> , 2011 , 50, 11363-74	5.1	80
233	Determination of absolute configuration of chiral molecules using vibrational optical activity: a review. <i>Applied Spectroscopy</i> , 2011 , 65, 699-723	3.1	221
232	2011 ,		393
231	Overview of Vibrational Optical Activity 2011 , 1-34		2
230	Vibrational Frequencies and Intensities 2011 , 35-69		
229	Appendix A: Models of VOA Intensity 2011 , 335-343		
228	Appendix B: Derivation of Probability and Current Densities from Multi-Electron Wavefunctions for Electronic and Vibrational Transitions 2011 , 345-351		

227	Appendix C: Theory of VCD for Molecules with Low-Lying Excited Electronic States 2011 , 353-361		
226	Appendix D: Magnetic VCD in Molecules with Non-Degenerate States 2011 , 363-368		
225	Instrumentation for Vibrational Circular Dichroism 2011 , 169-204		
224	Instrumentation for Raman Optical Activity 2011 , 205-232		1
223	Measurement of Vibrational Optical Activity 2011 , 233-259		1
222	Calculation of Vibrational Optical Activity 2011 , 261-292		
221	Molecular Chirality and Optical Activity 2011 , 71-94		1
220	Theory of Vibrational Circular Dichroism 2011 , 95-130		
219	Applications of Vibrational Optical Activity 2011 , 293-333		1
218	Recent advances in linear and nonlinear Raman spectroscopy. Part V. <i>Journal of Raman Spectroscopy</i> , 2011 , 42, 2049-2068	2.3	18
217	A confidence level algorithm for the determination of absolute configuration using vibrational circular dichroism or Raman optical activity. <i>ChemPhysChem</i> , 2011 , 12, 1542-9	3.2	156
216	Structure elucidation and absolute stereochemistry of isomeric monoterpene chromane esters. <i>Journal of Organic Chemistry</i> , 2011 , 76, 2603-12	4.2	35
215	Absolute configuration and selective trypanocidal activity of gaudichaudianic acid enantiomers. <i>Journal of Natural Products</i> , 2011 , 74, 1154-60	4.9	41
214	Theory of Raman Optical Activity 2011 , 131-167		1
213	Raman Optical Activity, Theory* 2010 , 2397-2405		1
212	Vibrational CD Spectrometers* 2010 , 2899-2909		1
211	Near-infrared and mid-infrared Fourier transform vibrational circular dichroism of proteins in aqueous solution. <i>Applied Spectroscopy</i> , 2010 , 64, 615-26	3.1	26
210	Direct observation and pH control of reversed supramolecular chirality in insulin fibrils by vibrational circular dichroism. <i>Chemical Communications</i> , 2010 , 46, 7154-6	5.8	109

209	Structure and absolute configuration of ginkgolide B characterized by IR- and VCD spectroscopy. <i>Chirality</i> , 2010 , 22, 217-23	2.1	14
208	Observation of resonance electronic and non-resonance-enhanced vibrational natural Raman optical activity. <i>Journal of Raman Spectroscopy</i> , 2010 , 41, 1563-1565	2.3	28
207	Recent advances in linear and nonlinear Raman spectroscopy. Part IV. <i>Journal of Raman Spectroscopy</i> , 2010 , 41, 1566-1586	2.3	14
206	Absolute configuration reassignment of two chromanes from <i>Peperomia obtusifolia</i> (Piperaceae) using VCD and DFT calculations. <i>Tetrahedron: Asymmetry</i> , 2010 , 21, 2402-2407		49
205	Structural determination of molecular stereochemistry using VCD spectroscopy and a conformational code: absolute configuration and solution conformation of a chiral liquid pesticide, (R)-(+)-malathion. <i>Chirality</i> , 2009 , 21 Suppl 1, E172-80	2.1	12
204	Observation and calculation of vibrational circular birefringence: a new form of vibrational optical activity. <i>Chirality</i> , 2009 , 21 Suppl 1, E277-86	2.1	26
203	A revised conformational code for the exhaustive analysis of conformers with one-to-one correspondence between conformation and code: application to the VCD analysis of (S)-ibuprofen. <i>Journal of Organic Chemistry</i> , 2009 , 74, 1231-6	4.2	22
202	Subtle chirality in oxo- and sulfidorhenium(v) complexes. <i>Chemical Communications</i> , 2009 , 4841-3	5.8	20
201	Vibrational circular dichroism analysis reveals a conformational change of the baccatin III ring of paclitaxel: visualization of conformations using a new code for structure-activity relationships. <i>Journal of Organic Chemistry</i> , 2008 , 73, 2367-72	4.2	24
200	Vibrational Circular Dichroism: A New Tool for the Solution-State Determination of the Structure and Absolute Configuration of Chiral Natural Product Molecules. <i>Natural Product Communications</i> , 2008 , 3, 1934578X0800300	0.9	12
199	Theory of Raman scattering and Raman optical activity: near resonance theory and levels of approximation. <i>Theoretical Chemistry Accounts</i> , 2008 , 119, 39-55	1.9	45
198	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. <i>Theoretical Chemistry Accounts</i> , 2008 , 119, 155-176	1.9	68
197	Reduction of linear birefringence in vibrational circular dichroism measurement: use of a rotating half-wave plate. <i>Theoretical Chemistry Accounts</i> , 2008 , 119, 69-79	1.9	23
196	Role of hydration in determining the structure and vibrational spectra of L-alanine and N-acetyl L-alanine N ² -methylamide in aqueous solution: a combined theoretical and experimental approach. <i>Theoretical Chemistry Accounts</i> , 2008 , 119, 191-210	1.9	109
195	Isotopic difference spectra as an aide in determining absolute configuration using vibrational optical activity: vibrational circular dichroism of ¹³ C- and ² H-labelled nonamethoxy cyclotrimeratrylene. <i>Chirality</i> , 2008 , 20, 673-80	2.1	10
194	Raman optical activity of flagellar filaments of <i>Salmonella</i> : Unusually intense ROA from L-type self-assembled protein filaments and their possible higher level chiral organization. <i>Vibrational Spectroscopy</i> , 2008 , 48, 65-68	2.1	15
193	Vibrational circular dichroism of amylose carbamate: structure and solvent-induced conformational changes. <i>Tetrahedron: Asymmetry</i> , 2008 , 19, 2111-2114		38
192	Vibrational circular dichroism shows unusual sensitivity to protein fibril formation and development in solution. <i>Journal of the American Chemical Society</i> , 2007 , 129, 12364-5	16.4	126

191	Structural and optical isomers of nonamethoxy cyclotrimeratrylene: separation and physical characterization. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 10507-16	2.8	13
190	HPLC separation and VCD spectroscopy of chiral pyrazoles derived from (5R)-dihydrocarvone. <i>Tetrahedron: Asymmetry</i> , 2007 , 18, 1911-1917		10
189	Applications of Vibrational Optical Activity in the Pharmaceutical Industry 2007 ,		2
188	Near-infrared excited Raman optical activity. <i>Applied Spectroscopy</i> , 2007 , 61, 1103-6	3.1	22
187	Fourier transform near-infrared vibrational circular dichroism used for on-line monitoring the epimerization of 2,2-dimethyl-1,3-dioxolane-4-methanol: A pseudo racemization reaction. <i>Chirality</i> , 2006 , 18, 775-82	2.1	18
186	Determination of the absolute configuration and solution conformation of a novel disubstituted pyrrolidine acid A by vibrational circular dichroism. <i>Chirality</i> , 2006 , 18, 746-53	2.1	20
185	Chlorofluoroiodomethane as a potential candidate for parity violation measurements. <i>Physical Chemistry Chemical Physics</i> , 2006 , 8, 79-92	3.6	46
184	Synthesis and vibrational circular dichroism of enantiopure chiral oxorhenium(V) complexes containing the hydrotris(1-pyrazolyl)borate ligand. <i>Inorganic Chemistry</i> , 2006 , 45, 10230-9	5.1	28
183	Vibrational optical activity in chiral analysis 2006 , 505-544		15
182	Vibrational Circular Dichroism 2006 ,		1
181	Raman spectroscopic study on the L-type straight flagellar filament of Salmonella. <i>Vibrational Spectroscopy</i> , 2006 , 42, 192-194	2.1	6
180	Two-dimensional vibrational circular dichroism correlation spectroscopy: pH-induced spectral changes in l-alanine. <i>Journal of Molecular Structure</i> , 2006 , 799, 226-238	3.4	17
179	Fourier transform vibrational circular dichroism from 800 to 10,000 cm ⁻¹ : Near-IR-VCD spectral standards for terpenes and related molecules. <i>Vibrational Spectroscopy</i> , 2006 , 42, 254-272	2.1	49
178	Structure and absolute configuration of nyasol and hinokiresinol via synthesis and vibrational circular dichroism spectroscopy. <i>Journal of Natural Products</i> , 2005 , 68, 1603-9	4.9	26
177	Enantiomeric excess determination by fourier transform near-infrared vibrational circular dichroism spectroscopy: simulation of real-time process monitoring. <i>Applied Spectroscopy</i> , 2005 , 59, 1114-24	3.1	20
176	Stereochemical determination and bioactivity assessment of (S)-(+)-curcuphenol dimers isolated from the marine sponge <i>Didiscus aceratus</i> and synthesized through laccase biocatalysis. <i>Bioorganic and Medicinal Chemistry</i> , 2005 , 13, 5600-12	3.4	63
175	Determination of the Atropisomeric Stability and Solution Conformation of Asymmetrically Substituted Biphenyls by Means of Vibrational Circular Dichroism (VCD). <i>Helvetica Chimica Acta</i> , 2005 , 88, 2302-2314	2	6
174	Phase equilibrium in poly(rA).poly(rU) complexes with Cd ²⁺ and Mg ²⁺ ions, studied by ultraviolet, infrared, and vibrational circular dichroism spectroscopy. <i>Biopolymers</i> , 2005 , 78, 275-86	2.2	13

173	Determination of the absolute configuration and solution conformation of the antifungal agents ketoconazole, itraconazole, and miconazole with vibrational circular dichroism. <i>Chirality</i> , 2005 , 17 Suppl, S101-8	2.1	26
172	Preferred peptide backbone conformations in the unfolded state revealed by the structure analysis of alanine-based (AXA) tripeptides in aqueous solution. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2004 , 101, 10054-9	11.5	106
171	Solution conformations of cyclosporins and magnesium-cyclosporin complexes determined by vibrational circular dichroism. <i>Biopolymers</i> , 2004 , 73, 163-77	2.2	23
170	Conformational determination of [Leu]enkephalin based on theoretical and experimental VA and VCD spectral analyses. <i>Physical Chemistry Chemical Physics</i> , 2004 , 6, 2434	3.6	15
169	Tripeptides with ionizable side chains adopt a perturbed polyproline II structure in water. <i>Biochemistry</i> , 2004 , 43, 613-21	3.2	65
168	Direct observation of odd-even effect for chiral alkyl alcohols in solution using vibrational circular dichroism spectroscopy. <i>Journal of the American Chemical Society</i> , 2004 , 126, 194-8	16.4	58
167	Theory of Vibrational Circular Dichroism and Infrared Absorption: Extension to Molecules with Low-Lying Excited Electronic States. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 7222-7231	2.8	72
166	Determination of enantiomeric excess in samples of chiral molecules using fourier transform vibrational circular dichroism spectroscopy: simulation of real-time reaction monitoring. <i>Analytical Chemistry</i> , 2004 , 76, 6956-66	7.8	52
165	The conformation of tetraalanine in water determined by polarized Raman, FT-IR, and VCD spectroscopy. <i>Journal of the American Chemical Society</i> , 2004 , 126, 2768-76	16.4	115
164	Dual source fourier transform polarization modulation spectroscopy: an improved method for the measurement of circular and linear dichroism. <i>Applied Spectroscopy</i> , 2004 , 58, 647-54	3.1	41
163	Extension of fourier transform vibrational circular dichroism into the near-infrared region: continuous spectral coverage from 800 to 10 000 cm ⁻¹ . <i>Applied Spectroscopy</i> , 2004 , 58, 1057-64	3.1	37
162	An Unexpected Atropisomerically Stable 1,1-Biphenyl at Ambient Temperature in Solution, Elucidated by Vibrational Circular Dichroism (VCD). <i>Helvetica Chimica Acta</i> , 2003 , 86, 3141-3155	2	16
161	Determination of the absolute configuration and solution conformation of gossypol by vibrational circular dichroism. <i>Chirality</i> , 2003 , 15, 196-200	2.1	58
160	Absolute configuration determination of chiral molecules in the solution state using vibrational circular dichroism. <i>Chirality</i> , 2003 , 15, 743-58	2.1	445
159	The structure of tri-proline in water probed by polarized Raman, Fourier transform infrared, vibrational circular dichroism, and electric ultraviolet circular dichroism spectroscopy. <i>Biopolymers</i> , 2003 , 71, 558-68	2.2	38
158	Preparation of cruciferous phytoalexin related metabolites, (1R)-dioxibassinin and (1R)-3-cyanomethyl-3-hydroxyoxindole, and determination of their absolute configurations by vibrational circular dichroism (VCD). <i>Tetrahedron Letters</i> , 2003 , 44, 6017-6020	2	37
157	Structural studies on McN-5652-X, a high-affinity ligand for the serotonin transporter in mammalian brain. <i>Bioorganic and Medicinal Chemistry</i> , 2003 , 11, 2463-70	3.4	18
156	Determination of molecular stereochemistry using vibrational circular dichroism spectroscopy: absolute configuration and solution conformation of 5-formyl-cis, cis-1,3,5-trimethyl-3-hydroxymethylcyclohexane-1-carboxylic acid lactone. <i>Chemical Record</i> , 2003 , 3, 112-9	6.6	18

155	Determination of Absolute Configuration in Molecules with Chiral Axes by Vibrational Circular Dichroism: A C ₂ -Symmetric Annulated Heptathiophene and a D ₂ -Symmetric Dimer of 1,1'-Binaphthyl. <i>Journal of Physical Chemistry A</i> , 2003 , 107, 7692-7696	2.8	47
154	erythro-1-Naphthyl-1-(2-piperidyl)methanol: synthesis, resolution, NMR relative configuration, and VCD absolute configuration. <i>Journal of Organic Chemistry</i> , 2003 , 68, 7308-15	4.2	30
153	The Structure of Alanine Based Tripeptides in Water and Dimethyl Sulfoxide Probed by Vibrational Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 358-365	3.4	87
152	Observation of Fourier transform near-infrared vibrational circular dichroism to 6150 cm ⁻¹ . <i>Applied Spectroscopy</i> , 2003 , 57, 1245-9	3.1	25
151	Vibrational absorption spectra, DFT and SCC-DFTB conformational study and analysis of [Leu]enkephalin. <i>Physical Chemistry Chemical Physics</i> , 2003 , 5, 1295-1300	3.6	21
150	(R)-(+)- and (S)-(-)-1-(9-Phenanthryl)ethylamine: Assignment of Absolute Configuration by CD Tweezer and VCD Methods, and Difficulties Encountered with the CD Exciton Chirality Method. <i>European Journal of Organic Chemistry</i> , 2002 , 2002, 1788-1796	3.2	25
149	Determination of the Absolute Configuration of (-)-Mirtazapine by Vibrational Circular Dichroism. <i>Helvetica Chimica Acta</i> , 2002 , 85, 1160	2	24
148	Determination of the absolute configuration of a key tricyclic component of a novel vasopressin receptor antagonist by use of vibrational circular dichroism. <i>Chirality</i> , 2002 , 14, 215-9	2.1	18
147	Role of Solvent and Secondary Doping in Polyaniline Films Doped with Chiral Camphorsulfonic Acid: Preparation of a Chiral Metal. <i>Chemistry of Materials</i> , 2002 , 14, 1430-1438	9.6	63
146	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). <i>Journal of Physical Chemistry A</i> , 2002 , 106, 3560-3565	2.8	67
145	Tripeptides adopt stable structures in water. A combined polarized visible Raman, FTIR, and VCD spectroscopy study. <i>Journal of the American Chemical Society</i> , 2002 , 124, 14330-41	16.4	189
144	The Use of Dual Polarization Modulation in Vibrational Circular Dichroism Spectroscopy. <i>ACS Symposium Series</i> , 2002 , 79-88	0.4	4
143	A new chiral oxathiane: synthesis, resolution and absolute configuration determination by vibrational circular dichroism. <i>Tetrahedron: Asymmetry</i> , 2001 , 12, 2605-2611		19
142	A chiral 1,4-oxazin-2-one: asymmetric synthesis versus resolution, structure, conformation and VCD absolute configuration. <i>Tetrahedron: Asymmetry</i> , 2001 , 12, 2703-2707		21
141	Ab initio VCD calculation of a transition-metal containing molecule and a new intensity enhancement mechanism for VCD. <i>Journal of the American Chemical Society</i> , 2001 , 123, 11320-1	16.4	96
140	Vibrational Optical Activity of Pharmaceuticals and Biomolecules 2000 ,		2
139	Vibrational transition current density in (2S,3S)-oxirane-d ₂ : visualizing electronic and nuclear contributions to IR absorption and vibrational circular dichroism intensities. <i>Journal of Molecular Structure</i> , 2000 , 550-551, 123-134	3.4	7
138	Dual Polarization Modulation: A Real-Time, Spectral-Multiplex Separation of Circular Dichroism from Linear Birefringence Spectral Intensities. <i>Applied Spectroscopy</i> , 2000 , 54, 1634-1645	3.1	121

137	Vibrational Transition Current Density in (S)-Methyl Lactate: Visualizing the Origin of the Methine-Stretching Vibrational Circular Dichroism Intensity. <i>Journal of Physical Chemistry A</i> , 2000 , 104, 3944-3951	2.8	20
136	Raman Optical Activity, Theory 1999 , 1976-1985		1
135	Hydrogen Stretching Vibrational Circular Dichroism in Methyl Lactate and Related Molecules. <i>Journal of Physical Chemistry A</i> , 1999 , 103, 1523-1537	2.8	37
134	Vibrational CD Spectrometers 1999 , 2391-2402		3
133	Experimental observation of resonance Raman optical activity. <i>Chemical Physics Letters</i> , 1998 , 287, 359-364	3.6	78
132	Electron Transition Current Density in Molecules. 2. Ab Initio Calculations for Electronic Transitions in Ethylene and Formaldehyde. <i>Journal of Physical Chemistry A</i> , 1998 , 102, 3352-3357	2.8	32
131	Vibrational circular dichroism: an incisive tool for stereochemical applications. <i>Enantiomer</i> , 1998 , 3, 283-97		47
130	Electron Transition Current Density in Molecules. 3. Ab Initio Calculations for Vibrational Transitions in Ethylene and Formaldehyde. <i>Journal of the American Chemical Society</i> , 1997 , 119, 10620-10626	16.4	33
129	Infrared and Raman vibrational optical activity: theoretical and experimental aspects. <i>Annual Review of Physical Chemistry</i> , 1997 , 48, 357-86	15.7	272
128	Comparison of Step-Scan and Rapid-Scan Approaches to the Measurement of Mid-Infrared Fourier Transform Vibrational Circular Dichroism. <i>Applied Spectroscopy</i> , 1997 , 51, 504-507	3.1	26
127	Step-Scan Fourier Transform Vibrational Circular Dichroism Measurements in the Vibrational Region above 2000 cm ⁻¹ . <i>Applied Spectroscopy</i> , 1997 , 51, 508-511	3.1	25
126	Electron Transition Current Density in Molecules. 1. Non-BornOppenheimer Theory of Vibronic and Vibrational Transitions. <i>Journal of Physical Chemistry A</i> , 1997 , 101, 7826-7833	2.8	49
125	Improved backscattering dual circular polarization raman optical activity spectrometer with enhanced performance for biomolecular applications. <i>Journal of Raman Spectroscopy</i> , 1997 , 28, 627-633	2.3	29
124	Resonance and Non-Resonance Raman Optical Activity in Pharmaceutical Analgesic Molecules 1997 , 459-460		4
123	Step-Scan Fourier Transform Vibrational Circular Dichroism Spectra of Pharmaceutical Molecules 1997 , 461-462		
122	Comparison of Fourier-Transform Vibrational Circular Dichroism and Multichannel-detected Raman Optical Activity 1997 , 807-808		
121	Optical Design and Sampling Methods for the Measurement of Vibrational Circular Dichroism with a Nicolet Magna FT-IR Spectrometer 1997 , 803-805		
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