Petr BouÅ

List of Publications by Year
in descending order

173 papers	5,738 citations	61984 43 h-index	110387 64 g-index
178 all docs	178 docs citations	178 times ranked	3398 citing authors

#	Article	IF	Citations
1	Transfer of molecular property tensors in cartesian coordinates: A new algorithm for simulation of vibrational spectra. Journal of Computational Chemistry, 1997, 18, 646-659.	3.3	224
2	Empirical modeling of the peptide amide I band IR intensity in water solution. Journal of Chemical Physics, 2003, 119, 11253-11262.	3.0	189
3	Gauge-Origin Independent Density-Functional Theory Calculations of Vibrational Raman Optical Activity. Journal of Physical Chemistry A, 2002, 106, 7448-7455.	2.5	162
4	Partial optimization of molecular geometry in normal coordinates and use as a tool for simulation of vibrational spectra. Journal of Chemical Physics, 2002, 117, 4126-4132.	3.0	119
5	Gold nanoclusters with bright near-infrared photoluminescence. Nanoscale, 2018, 10, 3792-3798.	5.6	113
6	Ab initio quantum mechanical models of peptide helices and their vibrational spectra. Biopolymers, 2002, 65, 45-59.	2.4	107
7	Computational Analysis of Solvent Effects in NMR Spectroscopy. Journal of Chemical Theory and Computation, 2010, 6, 288-299.	5.3	106
8	Through-space transfer of chiral information mediated by a plasmonic nanomaterial. Nature Chemistry, 2015, 7, 591-596.	13.6	105
9	Ab initio simulations of the vibrational circular dichroism of coupled peptides. Journal of the American Chemical Society, 1993, 115, 9602-9607.	13.7	103
10	Demonstration of the Ring Conformation in Polyproline by the Raman Optical Activity. Journal of the American Chemical Society, 2006, 128, 2438-2443.	13.7	94
11	Explicit versus Implicit Solvent Modeling of Raman Optical Activity Spectra. Journal of Physical Chemistry B, 2011, 115, 4128-4137.	2.6	92
12	Vibrational Spectral Simulation for Peptides of Mixed Secondary Structure:â€‰ Method Comparisons with the Trpzip Model Hairpin. Journal of Physical Chemistry B, 2005, 109, 23687-23697.	2.6	90
13	Conformational Flexibility ofl-Alanine Zwitterion Determines Shapes of Raman and Raman Optical Activity Spectral Bands. Journal of Physical Chemistry A, 2006, 110, 4689-4696.	2.5	90
14	Proline Zwitterion Dynamics in Solution, Glass, and Crystalline State. Journal of the American Chemical Society, 2006, 128, 13451-13462.	13.7	82
15	Empirical solvent correction for multiple amide group vibrational modes. Journal of Chemical Physics, 2005, 122, 144501.	3.0	81
16	Raman Optical Activity of Methyloxirane Gas and Liquid. Journal of Physical Chemistry Letters, 2011, 2, 498-502.	4.6	75
17	Applications of chiroptical spectroscopy to coordination compounds. Coordination Chemistry Reviews, 2015, 284, 1-18.	18.8	74
18	Simulations of oligopeptide vibrational CD: Effects of isotopic labeling. Biopolymers, 2000, 53, 380-395.	2.4	73

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19	Recent Trends in Chiroptical Spectroscopy: Theory and Applications of Vibrational Circular Dichroism and Raman Optical Activity. ChemPlusChem, 2020, 85, 561-575.	2.8	73
20	Determining the Absolute Configuration of Two Marine Compounds Using Vibrational Chiroptical Spectroscopy. Journal of Organic Chemistry, 2012, 77, 858-869.	3.2	71
21	Enantiomeric Discrimination by Surfaceâ€Enhanced Raman Scatteringâ€“Chiral Anisotropy of Chiral Nanostructured Gold Films. Angewandte Chemie - International Edition, 2020, 59, 15226-15231.	13.8	70
22	Inspecting chiral molecules by Raman optical activity spectroscopy. RSC Advances, 2014, 4, 57125-57136.	3.6	68
23	Structure and Vibrational Motion of Insulin from Raman Optical Activity Spectra. Analytical Chemistry, 2012, 84, 2440-2451.	6.5	64
24	Ab Initio Modeling of Amide I Coupling in Antiparallel Î²-Sheets and the Effect of 13C Isotopic Labeling on Infrared Spectra. Journal of Physical Chemistry B, 2005, 109, 5348-5357.	2.6	62
25	Anharmonic effects in IR, Raman, and Raman optical activity spectra of alanine and proline zwitterions. Journal of Chemical Physics, 2007, 126, 224513.	3.0	61
26	Transferability of Various Molecular Property Tensors in Vibrational Spectroscopy. Journal of Chemical Theory and Computation, 2012, 8, 977-985.	5.3	60
27	Formation and structure of the potassium complex of valinomycin in solution studied by Raman optical activity spectroscopy. Physical Chemistry Chemical Physics, 2010, 12, 11021.	2.8	57
28	Interpretation of Raman and Raman Optical Activity Spectra of a Flexible Sugar Derivative, the Gluconic Acid Anion. Journal of Physical Chemistry A, 2009, 113, 3594-3601.	2.5	56
29	First-Principles Predictions of Vibrational Raman Optical Activity of Globular Proteins. Journal of Physical Chemistry Letters, 2015, 6, 3314-3319.	4.6	56
30	Computational evaluation of the coupled oscillator model in the vibrational circular dichroism of selected small molecules. Journal of the American Chemical Society, 1992, 114, 9100-9105.	13.7	55
31	Ramachandran Plot for Alanine Dipeptide as Determined from Raman Optical Activity. Journal of Physical Chemistry Letters, 2013, 4, 2763-2768.	4.6	55
32	Measurement and Calculation of Absolute Rotational Strengths for Camphor, Î±-Pinene, and Borneol. Journal of Physical Chemistry A, 1998, 102, 102-110.	2.5	54
33	Bâ€™Z Conformational Transition of DNA Monitored by Vibrational Circular Dichroism. Ab Initio Interpretation of the Experiment. Journal of Physical Chemistry B, 2002, 106, 12623-12634.	2.6	53
34	Measurement and Calculation of the Raman Optical Activity of Î±-Pinene and trans-Pinane. Collection of Czechoslovak Chemical Communications, 1997, 62, 1384-1395.	1.0	51
35	Vibrational circular dichroism of tetraphenylporphyrin in peptide complexes? A computational study. , 2000, 12, 191-198.		51
36	Comparison of Quantitative Conformer Analyses by Nuclear Magnetic Resonance and Raman Optical Activity Spectra for Model Dipeptides. Journal of Physical Chemistry A, 2008, 112, 8633-8640.	2.5	51

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37	Spectroscopic Detection of DNA Quadruplexes by Vibrational Circular Dichroism. Journal of the American Chemical Society, 2011, 133, 15055-15064.	13.7	50
38	Convergence Properties of the Normal Mode Optimization and Its Combination with Molecular Geometry Constraints. Collection of Czechoslovak Chemical Communications, 2005, 70, 1315-1340.	1.0	50
39	Contribution of transition dipole coupling to amide coupling in IR spectra of peptide secondary structures. Vibrational Spectroscopy, 2006, 42, 63-73.	2.2	49
40	Detection of Circularly Polarized Luminescence of a Csâ€Eu^{III} Complex in Raman Optical Activity Experiments. Angewandte Chemie - International Edition, 2015, 54, 14933-14936.	13.8	49
41	Detection of Sugars via Chirality Induced in Europium(III) Compounds. Analytical Chemistry, 2016, 88, 8878-8885.	6.5	49
42	Comparison of the numerical stability of methods for anharmonic calculations of vibrational molecular energies. Journal of Computational Chemistry, 2007, 28, 1617-1624.	3.3	48
43	Insight into vibrational circular dichroism of proteins by density functional modeling. Physical Chemistry Chemical Physics, 2018, 20, 4926-4935.	2.8	48
44	A cluster model of liquid water and its IR spectroscopic response. Chemical Physics Letters, 2002, 365, 82-88.	2.6	45
45	Identification of Lanthanide(III) Luminophores in Magnetic Circularly Polarized Luminescence Using Raman Optical Activity Instrumentation. Analytical Chemistry, 2017, 89, 5043-5049.	6.5	44
46	Vibrational Optical Activity of (3S,6S)-3,6-Dimethyl-1,4-dioxane-2,5-dione. Journal of the American Chemical Society, 1996, 118, 10285-10293.	13.7	43
47	Simulation of the Raman Optical Activity ofl-Alanylâ˜l-Alanine. Journal of Physical Chemistry A, 2001, 105, 6362-6368.	2.5	43
48	Simulations of vibrational spectra from classical trajectories: Calibration withab initioforce fields. Journal of Chemical Physics, 2007, 127, 084502.	3.0	43
49	Monitoring the Backbone Conformation of Valinomycin by Raman Optical Activity. ChemPhysChem, 2011, 12, 1509-1518.	2.1	41
50	Chiral sensing of amino acids and proteins chelating with Eu^{III}complexes by Raman optical activity spectroscopy. Physical Chemistry Chemical Physics, 2016, 18, 23803-23811.	2.8	40
51	A Complete Set of NMR Chemical Shifts and Spinâ˜Spin Coupling Constants forl-Alanyl-l-alanine Zwitterion and Analysis of Its Conformational Behavior. Journal of the American Chemical Society, 2005, 127, 17079-17089.	13.7	38
52	Correction of Vibrational Broadening in Molecular Dynamics Clusters with the Normal Mode Optimization Method. Journal of Physical Chemistry B, 2012, 116, 336-342.	2.6	38
53	On the influence of the water electrostatic field on the amide group vibrational frequencies. Journal of Chemical Physics, 2004, 121, 7545.	3.0	37
54	Detection of Molecular Chirality by Induced Resonance Raman Optical Activity in Europium Complexes. Angewandte Chemie - International Edition, 2012, 51, 11058-11061.	13.8	37

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55	Theoretical Modeling of the Surface-Enhanced Raman Optical Activity. Journal of Chemical Theory and Computation, 2012, 8, 1714-1720.	5.3	37
56	Geometry and Solvent Dependence of the Electronic Spectra of the Amide Group and Consequences for Peptide Circular Dichroism. Journal of Physical Chemistry A, 2006, 110, 4702-4711.	2.5	36
57	Two Spectroscopies in One: Interference of Circular Dichroism and Raman Optical Activity. Angewandte Chemie - International Edition, 2020, 59, 21895-21898.	13.8	35
58	Specific circularly polarized luminescence of Eu(iii), Sm(iii), and Er(iii) induced by N-acetylneuraminic acid. Chemical Communications, 2018, 54, 1790-1792.	4.1	34
59	DNA Oligonucleotideâ^'cis-Platin Binding:Â Ab Initio Interpretation of the Vibrational Spectra. Journal of Physical Chemistry A, 2007, 111, 9714-9723.	2.5	33
60	Interpretation of Synchrotron Radiation Circular Dichroism Spectra of Anionic, Cationic, and Zwitterionic Dialanine Forms. Journal of Physical Chemistry A, 2007, 111, 2750-2760.	2.5	33
61	Porphyrin Protonation Studied by Magnetic Circular Dichroism. Journal of Physical Chemistry A, 2012, 116, 778-783.	2.5	32
62	Theoretical Modeling of Peptide Î±-Helical Circular Dichroism in Aqueous Solution. Journal of Physical Chemistry A, 2011, 115, 1734-1742.	2.5	31
63	Tracking of the Polyproline Folding by Density Functional Computations and Raman Optical Activity Spectra. Journal of Physical Chemistry B, 2011, 115, 15079-15089.	2.6	31
64	Computation of magnetic circular dichroism by sumâ€overâ€states summations. Journal of Computational Chemistry, 2013, 34, 1531-1539.	3.3	31
65	Binding of Lanthanide Complexes to Histidineâ€Containing Peptides Probed by Raman Optical Activity Spectroscopy. Chemistry - A European Journal, 2018, 24, 8664-8669.	3.3	31
66	Vibrational Raman optical activity of 1â€phenylethanol and 1â€phenylethylamine: Revisiting old friends. Chirality, 2009, 21, E4-12.	2.6	30
67	Europium (III) as a Circularly Polarized Luminescence Probe of DNA Structure. Scientific Reports, 2019, 9, 1068.	3.3	30
68	RNA Structural Forms Studied by Vibrational Circular Dichroism:Â Ab Initio Interpretation of the Spectra. Journal of Physical Chemistry B, 2004, 108, 3899-3911.	2.6	29
69	Matrix formulation of the surface-enhanced Raman optical activity theory. Journal of Chemical Physics, 2007, 126, 136101.	3.0	29
70	Tight Î²-turns in peptides. DFT-based study of infrared absorption and vibrational circular dichroism for various conformers including solvent effects. Theoretical Chemistry Accounts, 2008, 119, 81-97.	1.4	29
71	Solvent Dependence of theN-Methylacetamide Structure and Force Field. Journal of Physical Chemistry A, 2009, 113, 9727-9736.	2.5	29
72	<scp>l</scp>-Alanyl-<scp>l</scp>-alanine Conformational Changes Induced by pH As Monitored by the Raman Optical Activity Spectra. Journal of Physical Chemistry A, 2009, 113, 7760-7768.	2.5	29

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73	CH Stretching Region: Computational Modeling of Vibrational Optical Activity. Journal of Chemical Theory and Computation, 2013, 9, 3096-3108.	5.3	29
74	Simulation of Raman and Raman optical activity of saccharides in solution. Physical Chemistry Chemical Physics, 2020, 22, 1983-1993.	2.8	29
75	Solvated States of Poly-<scp>l</scp>-alanine Î±-Helix Explored by Raman Optical Activity. Journal of Physical Chemistry A, 2014, 118, 3655-3662.	2.5	28
76	Simulations of Structure and Vibrational Spectra of Deoxyoctanucleotides. Journal of Physical Chemistry B, 2005, 109, 20579-20587.	2.6	27
77	Intense chirality induction in nitrile solvents by a helquat dye monitored by near resonance Raman scattering. Chemical Communications, 2016, 52, 6257-6260.	4.1	27
78	Transfer and Amplification of Chirality Within the â€œRing of Fireâ€•Observed in Resonance Raman Optical Activity Experiments. Angewandte Chemie - International Edition, 2019, 58, 16495-16498.	13.8	27
79	Applications of the Cartesian coordinate tensor transfer technique in the simulations of vibrational circular dichroism spectra of oligonucleotides. Chirality, 2010, 22, E96-E114.	2.6	26
80	Simulation of Raman optical activity of multi-component monosaccharide samples. Physical Chemistry Chemical Physics, 2016, 18, 2130-2142.	2.8	26
81	Chirality in Peptide Vibrations: Ab Initio Computational Studies of Length, Solvation, Hydrogen Bond, Dipole Coupling, and Isotope Effects on Vibrational CD. ACS Symposium Series, 2002, , 50-64.	0.5	25
82	Structure of supramolecular astaxanthin aggregates revealed by molecular dynamics and electronic circular dichroism spectroscopy. Physical Chemistry Chemical Physics, 2018, 20, 18038-18046.	2.8	25
83	Quantitative analysis of sugar composition in honey using 532â€nm excitation Raman and Raman optical activity spectra. Journal of Raman Spectroscopy, 2016, 47, 1298-1303.	2.5	24
84	Influence of Lipid Membranes on Î±-Synuclein Aggregation. ACS Chemical Neuroscience, 2021, 12, 825-830.	3.5	24
85	Circular dichroism enhancement in large DNA aggregates simulated by a generalized oscillator model. Journal of Computational Chemistry, 2008, 29, 2693-2703.	3.3	23
86	On the limited precision of transfer of molecular optical activity tensors. Collection of Czechoslovak Chemical Communications, 2011, 76, 567-583.	1.0	23
87	Ferric Complexes of 3-Hydroxy-4-pyridinones Characterized by Density Functional Theory and Raman and UVâ€“vis Spectroscopies. Inorganic Chemistry, 2012, 51, 4473-4481.	4.0	23
88	Transition polarizability model of induced resonance Raman optical activity. Journal of Computational Chemistry, 2013, 34, 2152-2158.	3.3	23
89	Vibrational Properties of the Phosphate Group Investigated by Molecular Dynamics and Density Functional Theory. Journal of Physical Chemistry B, 2015, 119, 10682-10692.	2.6	23
90	Vibrational Optical Activity of Intermolecular, Overtone, and Combination Bands: 2-Chloropropionitrile and Î±-Pinene. Journal of Physical Chemistry B, 2019, 123, 2147-2156.	2.6	23

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91	Dependence of the <scp>l</scp>-Alanyl-<scp>l</scp>-Alanine Conformation on Molecular Charge Determined from Ab Initio Computations and NMR Spectra. Journal of Physical Chemistry B, 2008, 112, 1796-1805.	2.6	22
92	Simulations of 129Xe NMR chemical shift of atomic xenon dissolved in liquid benzene. Theoretical Chemistry Accounts, 2011, 129, 677-684.	1.4	22
93	Arrangement of Fibril Side Chains Studied by Molecular Dynamics and Simulated Infrared and Vibrational Circular Dichroism Spectra. Journal of Physical Chemistry B, 2014, 118, 6937-6945.	2.6	22
94	Enantiomeric Discrimination by Surfaceâ€Enhanced Raman Scatteringâ€“Chiral Anisotropy of Chiral Nanostructured Gold Films. Angewandte Chemie, 2020, 132, 15338-15343.	2.0	22
95	Vibrational circular dichroism and IR spectral analysis as a test of theoretical conformational modeling for a cyclic hexapeptide. Chirality, 2008, 20, 1104-1119.	2.6	21
96	Parallel variable selection of molecular dynamics clusters as a tool for calculation of spectroscopic properties. Journal of Computational Chemistry, 2013, 34, 366-371.	3.3	21
97	Originâ€independent sum over states simulations of magnetic and electronic circular dichroism spectra via the localized orbital/local origin method. Journal of Computational Chemistry, 2015, 36, 723-730.	3.3	21
98	Effects of sulfation and the environment on the structure of chondroitin sulfate studiedviaRaman optical activity. Physical Chemistry Chemical Physics, 2019, 21, 7367-7377.	2.8	21
99	Recognition of the True and False Resonance Raman Optical Activity. Angewandte Chemie - International Edition, 2021, 60, 21205-21210.	13.8	21
100	Recognition of Oligosaccharides by Chirality Induced in Europium (III) Compounds. Chemistry - an Asian Journal, 2018, 13, 3865-3870.	3.3	20
101	Communication: Fullerene resolution by the magnetic circular dichroism. Journal of Chemical Physics, 2013, 138, 151103.	3.0	19
102	Observation of Paramagnetic Raman Optical Activity of Nitrogen Dioxide. Angewandte Chemie - International Edition, 2014, 53, 9236-9239.	13.8	19
103	Establishing the link between fibril formation and Raman optical activity spectra of insulin. Physical Chemistry Chemical Physics, 2017, 19, 13614-13621.	2.8	19
104	Three Types of Induced Tryptophan Optical Activity Compared in Model Dipeptides: Theory and Experiment. ChemPhysChem, 2012, 13, 2748-2760.	2.1	18
105	Optically Active Vibrational Spectroscopy of Î±â€Aminoisobutyric Acid Foldamers in Organic Solvents and Phospholipid Bilayers. Chemistry - A European Journal, 2018, 24, 9399-9408.	3.3	18
106	Induced Lanthanide Circularly Polarized Luminescence as a Probe of Protein Fibrils. ACS Omega, 2019, 4, 1265-1271.	3.5	18
107	Origins of Optical Activity in an Oxo-Helicene: Experimental and Computational Studies. ACS Omega, 2021, 6, 2420-2428.	3.5	18
108	Can One Measure Resonance Raman Optical Activity?. Angewandte Chemie - International Edition, 2021, 60, 22004-22009.	13.8	18

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109	Vibrational Magnetic Dipole Moment of Acetylene in the Î½5Mode. The Journal of Physical Chemistry, 1996, 100, 2062-2065.	2.9	17
110	Comparison of Hartree-Fock and Kohn-Sham determinants as wave functions. Journal of Computational Chemistry, 2000, 21, 8-16.	3.3	17
111	Detection of Circularly Polarized Luminescence of a Csâ€Eu III Complex in Raman Optical Activity Experiments. Angewandte Chemie, 2015, 127, 15146-15149.	2.0	17
112	Comparison of the Electronic and Vibrational Optical Activity of a Europium(III) Complex. Chemistry - A European Journal, 2015, 21, 5807-5813.	3.3	17
113	Quantitative Determination of Ala-Ala Conformer Ratios in Solution by Decomposition of Raman Optical Activity Spectra. Journal of Physical Chemistry B, 2017, 121, 8956-8964.	2.6	17
114	Diamagnetic Raman Optical Activity of Chlorine, Bromine, and Iodine Gases. Angewandte Chemie - International Edition, 2016, 55, 3504-3508.	13.8	16
115	An Experimental Comparison of Vibrational Circular Dichroism and Raman Optical Activity with 1-Amino-2-propanol and 2-Amino-1-propanol as Model Compounds. Journal of the American Chemical Society, 1997, 119, 7061-7064.	13.7	15
116	Cocaine Hydrochloride Structure in Solution Revealed by Three Chiroptical Methods. ChemPhysChem, 2017, 18, 2258-2265.	2.1	15
117	Transition dipole coupling modeling of optical activity enhancements in macromolecular protein systems. Chirality, 2018, 30, 55-64.	2.6	15
118	Monitoring peptide tyrosine nitration by spectroscopic methods. Amino Acids, 2021, 53, 517-532.	2.7	14
119	Explanation of Surface-Enhanced Raman Scattering Intensities of p-Aminobenzenethiol by Density Functional Computations. Journal of Physical Chemistry C, 2016, 120, 18275-18280.	3.1	13
120	Absolute Configuration Determination of a Taxol Precursor Based on Raman Optical Activity Spectra. Journal of Physical Chemistry B, 2017, 121, 1544-1551.	2.6	13
121	Chiral detection by induced surface-enhanced Raman optical activity. Chemical Communications, 2021, 57, 6388-6391.	4.1	13
122	Measurement and Theory of Resonance Raman Optical Activity for Gases, Liquids, and Aggregates. What It Tells about Molecules. Journal of Physical Chemistry B, 2022, 126, 355-367.	2.6	13
123	The stability of covalent dative bond significantly increases with increasing solvent polarity. Nature Communications, 2022, 13, 2107.	12.8	13
124	Chirality Transfer in Magnetic Coordination Complexes Monitored by Vibrational and Electronic Circular Dichroism. ChemPlusChem, 2014, 79, 698-707.	2.8	12
125	Rotationally resolved magnetic vibrational circular dichroism of the paramagnetic molecule NO. Physical Chemistry Chemical Physics, 2012, 14, 9586.	2.8	11
126	Vibrational Structure in Magnetic Circular Dichroism Spectra of Polycyclic Aromatic Hydrocarbons. Journal of Physical Chemistry A, 2017, 121, 9064-9073.	2.5	11

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127	Transfer and Amplification of Chirality Within the â€œRing of Fireâ€•Observed in Resonance Raman Optical Activity Experiments. Angewandte Chemie, 2019, 131, 16647-16650.	2.0	11
128	Insight into the Mechanism of Action and Peptideâ€Membrane Interactions of Aibâ€Rich Peptides: Multitechnique Experimental and Theoretical Analysis. ChemBioChem, 2021, 22, 1656-1667.	2.6	11
129	Î±-Synuclein conformations followed by vibrational optical activity. Simulation and understanding of the spectra. Physical Chemistry Chemical Physics, 2021, 23, 16635-16645.	2.8	10
130	Resolving Resonant Electronic States in Chiral Metal Complexes by Raman Optical Activity Spectroscopy. Journal of Physical Chemistry Letters, 2022, 13, 3873-3877.	4.6	10
131	Magnetic circular dichroism of chlorofullerenes: Experimental and computational study. Chemical Physics Letters, 2016, 647, 117-121.	2.6	9
132	Two Spectroscopies in One: Interference of Circular Dichroism and Raman Optical Activity. Angewandte Chemie, 2020, 132, 22079-22082.	2.0	9
133	Raman Optical Activity of Glucose and Sorbose in Extended Wavenumber Range. ChemPhysChem, 2020, 21, 1272-1279.	2.1	9
134	Polymorphism of Amyloid Fibrils Induced by Catalytic Seeding: A Vibrational Circular Dichroism Study. ChemPhysChem, 2021, 22, 83-91.	2.1	9
135	Electronic Circular Dichroismâ€Circularly Polarized Raman (eCPâ€Raman): A New Form of Chiral Raman Spectroscopy. Chemistry - A European Journal, 2022, 28, .	3.3	9
136	Simulation of Vibrational Spectra of Large Molecules by Arbitrary Time Propagation. Journal of Chemical Theory and Computation, 2009, 5, 200-207.	5.3	8
137	Transferability of anharmonic force fields in simulations of molecular vibrations. Journal of Chemical Physics, 2010, 133, 044117.	3.0	8
138	Theoretical Study of Vibrationally Averaged Dipole Moments for the Ground and Excited Câ•O Stretching States of trans-Formic Acid. Journal of Chemical Theory and Computation, 2010, 6, 817-827.	5.3	8
139	Intense chiral signal from Î±-helical poly-<scp>l</scp>-alanine observed in low-frequency Raman optical activity. Physical Chemistry Chemical Physics, 2021, 23, 26501-26509.	2.8	8
140	Diamagnetic Raman Optical Activity of Chlorine, Bromine, and Iodine Gases. Angewandte Chemie, 2016, 128, 3565-3569.	2.0	7
141	Understanding CH-Stretching Raman Optical Activity in Alaâ€“Ala Dipeptides. Journal of Physical Chemistry A, 2020, 124, 674-683.	2.5	7
142	Density Functional Computations of Vibrational Circular Dichroism Spectra beyond the Bornâ€“Oppenheimer Approximation. Journal of Chemical Theory and Computation, 2020, 16, 2627-2634.	5.3	7
143	Chiral recognition via a stereodynamic vanadium probe using the electronic circular dichroism effect in differential Raman scattering. Physical Chemistry Chemical Physics, 2021, 23, 23336-23340.	2.8	7
144	Rotationally resolved magnetic vibrational circular dichroism. Molecular Physics, 1996, 87, 299-318.	1.7	6

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145	On the magnetic circular dichroism of benzene. A density-functional study. Journal of Chemical Physics, 2017, 146, 144301.	3.0	6
146	Theory of Molecular Vibrational Zeeman Effects as Measured with Circular Dichroism. Physical Review Letters, 2018, 121, 073201.	7.8	6
147	Binuclear Lanthanide(III) Complexes with Chiral Ligands: Dynamic Equilibria in Solution and Binding with Nucleotides Studied by Spectroscopic Methods. ChemPlusChem, 2020, 85, 694-700.	2.8	6
148	Rotationally resolved magnetic vibrational circular dichroism Experimental spectra and theoretical simulation for diamagnetic molecules. Molecular Physics, 1996, 87, 299-318.	1.7	6
149	Observations of rotational magnetic moments in the ground and some excited vibrational Î£ states of C2H2, C2HD, and C2D2by magnetic vibrational circular dichroism. Journal of Chemical Physics, 1996, 104, 1813-1824.	3.0	5
150	A Fourier Transform Method for Generation of Anharmonic Vibrational Molecular Spectra. Journal of Chemical Theory and Computation, 2010, 6, 2095-2102.	5.3	5
151	Experimental and theoretical study on complexation of Li+ with lithium ionophore VIII. Monatshefte FÃ¼r Chemie, 2013, 144, 1607-1611.	1.8	5
152	Resolving Electronic Transitions in Synthetic Fluorescent Protein Chromophores by Magnetic Circular Dichroism. ChemPhysChem, 2016, 17, 2348-2354.	2.1	5
153	Calculation of Vibrational Spectra of Large Molecules from Their Fragments. , 2018, , 181-197.		5
154	Characterization of Eight Novel Spiroleptosphols from Fusarium avenaceum. Molecules, 2019, 24, 3498.	3.8	5
155	Transfer of Frequency-Dependent Polarizabilities: A Tool To Simulate Absorption and Circular Dichroism Molecular Spectra. Journal of Chemical Theory and Computation, 2015, 11, 2210-2220.	5.3	4
156	Determination of Absolute Configuration in Chiral Solvents with Nuclear Magnetic Resonance. A Combined Molecular Dynamics/Quantum Chemical Study. Journal of Physical Chemistry A, 2015, 119, 5260-5268.	2.5	4
157	Natural and magnetic circular dichroism spectra of nucleosides: effect of the dynamics and environment. RSC Advances, 2021, 11, 8411-8419.	3.6	4
158	Calculation of NMR chemical shifts for taxol and ?-pinene within the generalized gradient approximation. International Journal of Quantum Chemistry, 2003, 91, 277-283.	2.0	3
159	Classical Trajectory of Molecules in Electromagnetic Field: A Handy Method to Simulate Molecular Vibrational Spectra. Journal of Chemical Theory and Computation, 2022, , .	5.3	3
160	New chiral ECD-Raman spectroscopy of atropisomeric naphthalenediimides. Chemical Communications, 2022, 58, 4524-4527.	4.1	3
161	Crossâ€Polarization Detection Enables Fast Measurement of Vibrational Circular Dichroism. ChemPhysChem, 2009, 10, 1983-1985.	2.1	2
162	Structural Analysis of Valinomycin in Solution Studied by Raman Optical Activity. AIP Conference Proceedings, 2010, , .	0.4	2

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163	Molecular dynamics with helical periodic boundary conditions. Journal of Computational Chemistry, 2014, 35, n/a-n/a.	3.3	2
164	Circular Dichroism is Sensitive to Monovalent Cation Binding in Monensin Complexes. Chirality, 2016, 28, 420-428.	2.6	2
165	Spectral counterstaining in luminescence-enhanced biological Raman microscopy. Chemical Communications, 2019, 55, 8329-8332.	4.1	1
166	Photochemical synthesis of pink silver and its use for monitoring peptide nitration via surface enhanced Raman spectroscopy (SERS). Amino Acids, 0, , .	2.7	1
167	Reply to Comments by Pescitelli and Bruhn on â€œCocaine Hydrochloride Structure in Solution Revealed by Three Chiroptical Methodsâ€• ChemPhysChem, 2017, 18, 2552-2552.	2.1	0
168	Titelbild: Two Spectroscopies in One: Interference of Circular Dichroism and Raman Optical Activity (Angew. Chem. 49/2020). Angewandte Chemie, 2020, 132, 21973-21973.	2.0	0
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