

Petr BouÅ

List of Publications by Year in descending order

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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 | Measurement and Theory of Resonance Raman Optical Activity for Gases, Liquids, and Aggregates. What It Tells about Molecules. <i>Journal of Physical Chemistry B</i> , 2022, 126, 355-367. | 2.6 | 13 |
| 2 | Electronic Circular Dichroismâ€Circularly Polarized Raman (eCPâ€Raman): A New Form of Chiral Raman Spectroscopy. <i>Chemistry - A European Journal</i> , 2022, 28, . | 3.3 | 9 |
| 3 | Classical Trajectory of Molecules in Electromagnetic Field: A Handy Method to Simulate Molecular Vibrational Spectra. <i>Journal of Chemical Theory and Computation</i> , 2022, , . | 5.3 | 3 |
| 4 | New chiral ECD-Raman spectroscopy of atropisomeric naphthalenediimides. <i>Chemical Communications</i> , 2022, 58, 4524-4527. | 4.1 | 3 |
| 5 | Frontispiece: Electronic Circular Dichroismâ€Circularly Polarized Raman (eCPâ€Raman): A New Form of Chiral Raman Spectroscopy. <i>Chemistry - A European Journal</i> , 2022, 28, . | 3.3 | 0 |
| 6 | The stability of covalent dative bond significantly increases with increasing solvent polarity. <i>Nature Communications</i> , 2022, 13, 2107. | 12.8 | 13 |
| 7 | Resolving Resonant Electronic States in Chiral Metal Complexes by Raman Optical Activity Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 3873-3877. | 4.6 | 10 |
| 8 | Polymorphism of Amyloid Fibrils Induced by Catalytic Seeding: A Vibrational Circular Dichroism Study. <i>ChemPhysChem</i> , 2021, 22, 83-91. | 2.1 | 9 |
| 9 | Monitoring peptide tyrosine nitration by spectroscopic methods. <i>Amino Acids</i> , 2021, 53, 517-532. | 2.7 | 14 |
| 10 | Chiral detection by induced surface-enhanced Raman optical activity. <i>Chemical Communications</i> , 2021, 57, 6388-6391. | 4.1 | 13 |
| 11 | $\hat{\pm}$ -Synuclein conformations followed by vibrational optical activity. Simulation and understanding of the spectra. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16635-16645. | 2.8 | 10 |
| 12 | Natural and magnetic circular dichroism spectra of nucleosides: effect of the dynamics and environment. <i>RSC Advances</i> , 2021, 11, 8411-8419. | 3.6 | 4 |
| 13 | Origins of Optical Activity in an Oxo-Helicene: Experimental and Computational Studies. <i>ACS Omega</i> , 2021, 6, 2420-2428. | 3.5 | 18 |
| 14 | Influence of Lipid Membranes on $\hat{\pm}$ -Synuclein Aggregation. <i>ACS Chemical Neuroscience</i> , 2021, 12, 825-830. | 3.5 | 24 |
| 15 | Insight into the Mechanism of Action and Peptideâ€Membrane Interactions of Aibâ€Rich Peptides: Multitechnique Experimental and Theoretical Analysis. <i>ChemBioChem</i> , 2021, 22, 1656-1667. | 2.6 | 11 |
| 16 | Can One Measure Resonance Raman Optical Activity?. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 22004-22009. | 13.8 | 18 |
| 17 | Recognition of the True and False Resonance Raman Optical Activity. <i>Angewandte Chemie</i> , 2021, 133, 21375-21380. | 2.0 | 0 |
| 18 | Can One Measure Resonance Raman Optical Activity?. <i>Angewandte Chemie</i> , 2021, 133, 22175-22180. | 2.0 | 0 |

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|----|---|------|-----------|
| 19 | Recognition of the True and False Resonance Raman Optical Activity. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 21205-21210. | 13.8 | 21 |
| 20 | Chiral recognition <i>via</i> a stereodynamic vanadium probe using the electronic circular dichroism effect in differential Raman scattering. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 23336-23340. | 2.8 | 7 |
| 21 | Intense chiral signal from $\hat{\pm}$ -helical poly- <i>l</i> -alanine observed in low-frequency Raman optical activity. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 26501-26509. | 2.8 | 8 |
| 22 | Understanding CH-Stretching Raman Optical Activity in Ala-Ala Dipeptides. <i>Journal of Physical Chemistry A</i> , 2020, 124, 674-683. | 2.5 | 7 |
| 23 | Two Spectroscopies in One: Interference of Circular Dichroism and Raman Optical Activity. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 21895-21898. | 13.8 | 35 |
| 24 | Two Spectroscopies in One: Interference of Circular Dichroism and Raman Optical Activity. <i>Angewandte Chemie</i> , 2020, 132, 22079-22082. | 2.0 | 9 |
| 25 | Titelbild: Two Spectroscopies in One: Interference of Circular Dichroism and Raman Optical Activity (<i>Angew. Chem.</i> 49/2020). <i>Angewandte Chemie</i> , 2020, 132, 21973-21973. | 2.0 | 0 |
| 26 | Enantiomeric Discrimination by Surface-Enhanced Raman Scattering-Chiral Anisotropy of Chiral Nanostructured Gold Films. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 15226-15231. | 13.8 | 70 |
| 27 | Binuclear Lanthanide(III) Complexes with Chiral Ligands: Dynamic Equilibria in Solution and Binding with Nucleotides Studied by Spectroscopic Methods. <i>ChemPlusChem</i> , 2020, 85, 694-700. | 2.8 | 6 |
| 28 | Pressure dependence of vibrational optical activity of model biomolecules. A computational study. <i>Chirality</i> , 2020, 32, 710-721. | 2.6 | 0 |
| 29 | Recent Trends in Chiroptical Spectroscopy: Theory and Applications of Vibrational Circular Dichroism and Raman Optical Activity. <i>ChemPlusChem</i> , 2020, 85, 561-575. | 2.8 | 73 |
| 30 | Density Functional Computations of Vibrational Circular Dichroism Spectra beyond the Born-Oppenheimer Approximation. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2627-2634. | 5.3 | 7 |
| 31 | Interpretation of vibrational optical activity spectra of proteins. , 2020, , 219-248. | | 0 |
| 32 | Simulation of Raman and Raman optical activity of saccharides in solution. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 1983-1993. | 2.8 | 29 |
| 33 | Raman Optical Activity of Glucose and Sorbose in Extended Wavenumber Range. <i>ChemPhysChem</i> , 2020, 21, 1272-1279. | 2.1 | 9 |
| 34 | Enantiomeric Discrimination by Surface-Enhanced Raman Scattering-Chiral Anisotropy of Chiral Nanostructured Gold Films. <i>Angewandte Chemie</i> , 2020, 132, 15338-15343. | 2.0 | 22 |
| 35 | Characterization of Eight Novel Spiroleptosphols from <i>Fusarium avenaceum</i> . <i>Molecules</i> , 2019, 24, 3498. | 3.8 | 5 |
| 36 | Transfer and Amplification of Chirality Within the α -Ring of Fire-Observed in Resonance Raman Optical Activity Experiments. <i>Angewandte Chemie</i> , 2019, 131, 16647-16650. | 2.0 | 11 |

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|----|---|------|-----------|
| 37 | Transfer and Amplification of Chirality Within the "Ring of Fire" Observed in Resonance Raman Optical Activity Experiments. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 16495-16498. | 13.8 | 27 |
| 38 | Spectral counterstaining in luminescence-enhanced biological Raman microscopy. <i>Chemical Communications</i> , 2019, 55, 8329-8332. | 4.1 | 1 |
| 39 | Effects of sulfation and the environment on the structure of chondroitin sulfate studied via Raman optical activity. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7367-7377. | 2.8 | 21 |
| 40 | Europium (III) as a Circularly Polarized Luminescence Probe of DNA Structure. <i>Scientific Reports</i> , 2019, 9, 1068. | 3.3 | 30 |
| 41 | Vibrational Optical Activity of Intermolecular, Overtone, and Combination Bands: 2-Chloropropionitrile and \pm -Pinene. <i>Journal of Physical Chemistry B</i> , 2019, 123, 2147-2156. | 2.6 | 23 |
| 42 | Induced Lanthanide Circularly Polarized Luminescence as a Probe of Protein Fibrils. <i>ACS Omega</i> , 2019, 4, 1265-1271. | 3.5 | 18 |
| 43 | Binding of Lanthanide Complexes to Histidine-Containing Peptides Probed by Raman Optical Activity Spectroscopy. <i>Chemistry - A European Journal</i> , 2018, 24, 8664-8669. | 3.3 | 31 |
| 44 | Insight into vibrational circular dichroism of proteins by density functional modeling. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4926-4935. | 2.8 | 48 |
| 45 | Specific circularly polarized luminescence of Eu(III), Sm(III), and Er(III) induced by N-acetylneuraminic acid. <i>Chemical Communications</i> , 2018, 54, 1790-1792. | 4.1 | 34 |
| 46 | Gold nanoclusters with bright near-infrared photoluminescence. <i>Nanoscale</i> , 2018, 10, 3792-3798. | 5.6 | 113 |
| 47 | Transition dipole coupling modeling of optical activity enhancements in macromolecular protein systems. <i>Chirality</i> , 2018, 30, 55-64. | 2.6 | 15 |
| 48 | Calculation of Vibrational Spectra of Large Molecules from Their Fragments. , 2018, , 181-197. | | 5 |
| 49 | Recognition of Oligosaccharides by Chirality Induced in Europium (III) Compounds. <i>Chemistry - an Asian Journal</i> , 2018, 13, 3865-3870. | 3.3 | 20 |
| 50 | Optically Active Vibrational Spectroscopy of \pm -Aminoisobutyric Acid Foldamers in Organic Solvents and Phospholipid Bilayers. <i>Chemistry - A European Journal</i> , 2018, 24, 9399-9408. | 3.3 | 18 |
| 51 | Theory of Molecular Vibrational Zeeman Effects as Measured with Circular Dichroism. <i>Physical Review Letters</i> , 2018, 121, 073201. | 7.8 | 6 |
| 52 | Structure of supramolecular astaxanthin aggregates revealed by molecular dynamics and electronic circular dichroism spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 18038-18046. | 2.8 | 25 |
| 53 | Absolute Configuration Determination of a Taxol Precursor Based on Raman Optical Activity Spectra. <i>Journal of Physical Chemistry B</i> , 2017, 121, 1544-1551. | 2.6 | 13 |
| 54 | On the magnetic circular dichroism of benzene. A density-functional study. <i>Journal of Chemical Physics</i> , 2017, 146, 144301. | 3.0 | 6 |

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|----|---|------|-----------|
| 55 | Establishing the link between fibril formation and Raman optical activity spectra of insulin. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 13614-13621. | 2.8 | 19 |
| 56 | Identification of Lanthanide(III) Luminophores in Magnetic Circularly Polarized Luminescence Using Raman Optical Activity Instrumentation. <i>Analytical Chemistry</i> , 2017, 89, 5043-5049. | 6.5 | 44 |
| 57 | Reply to Comments by Pescitelli and Bruhn on "Cocaine Hydrochloride Structure in Solution Revealed by Three Chiroptical Methods". <i>ChemPhysChem</i> , 2017, 18, 2552-2552. | 2.1 | 0 |
| 58 | Quantitative Determination of Ala-Ala Conformer Ratios in Solution by Decomposition of Raman Optical Activity Spectra. <i>Journal of Physical Chemistry B</i> , 2017, 121, 8956-8964. | 2.6 | 17 |
| 59 | Cocaine Hydrochloride Structure in Solution Revealed by Three Chiroptical Methods. <i>ChemPhysChem</i> , 2017, 18, 2258-2265. | 2.1 | 15 |
| 60 | Vibrational Structure in Magnetic Circular Dichroism Spectra of Polycyclic Aromatic Hydrocarbons. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9064-9073. | 2.5 | 11 |
| 61 | Quantitative analysis of sugar composition in honey using 532 nm excitation Raman and Raman optical activity spectra. <i>Journal of Raman Spectroscopy</i> , 2016, 47, 1298-1303. | 2.5 | 24 |
| 62 | Diamagnetic Raman Optical Activity of Chlorine, Bromine, and Iodine Gases. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 3504-3508. | 13.8 | 16 |
| 63 | Circular Dichroism is Sensitive to Monovalent Cation Binding in Monensin Complexes. <i>Chirality</i> , 2016, 28, 420-428. | 2.6 | 2 |
| 64 | Resolving Electronic Transitions in Synthetic Fluorescent Protein Chromophores by Magnetic Circular Dichroism. <i>ChemPhysChem</i> , 2016, 17, 2348-2354. | 2.1 | 5 |
| 65 | Intense chirality induction in nitrile solvents by a helquat dye monitored by near resonance Raman scattering. <i>Chemical Communications</i> , 2016, 52, 6257-6260. | 4.1 | 27 |
| 66 | Chiral sensing of amino acids and proteins chelating with Eu ^{III} complexes by Raman optical activity spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 23803-23811. | 2.8 | 40 |
| 67 | Explanation of Surface-Enhanced Raman Scattering Intensities of <i>p</i> -Aminobenzenethiol by Density Functional Computations. <i>Journal of Physical Chemistry C</i> , 2016, 120, 18275-18280. | 3.1 | 13 |
| 68 | Detection of Sugars via Chirality Induced in Europium(III) Compounds. <i>Analytical Chemistry</i> , 2016, 88, 8878-8885. | 6.5 | 49 |
| 69 | Diamagnetic Raman Optical Activity of Chlorine, Bromine, and Iodine Gases. <i>Angewandte Chemie</i> , 2016, 128, 3565-3569. | 2.0 | 7 |
| 70 | Simulation of Raman optical activity of multi-component monosaccharide samples. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 2130-2142. | 2.8 | 26 |
| 71 | Magnetic circular dichroism of chlorofullerenes: Experimental and computational study. <i>Chemical Physics Letters</i> , 2016, 647, 117-121. | 2.6 | 9 |
| 72 | Detection of Circularly Polarized Luminescence of a CsEu ^{III} Complex in Raman Optical Activity Experiments. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 14933-14936. | 13.8 | 49 |

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|----|--|------|-----------|
| 73 | Detection of Circularly Polarized Luminescence of a CsEu III Complex in Raman Optical Activity Experiments. <i>Angewandte Chemie</i> , 2015, 127, 15146-15149. | 2.0 | 17 |
| 74 | Origin-independent sum over states simulations of magnetic and electronic circular dichroism spectra via the localized orbital/local origin method. <i>Journal of Computational Chemistry</i> , 2015, 36, 723-730. | 3.3 | 21 |
| 75 | First-Principles Predictions of Vibrational Raman Optical Activity of Globular Proteins. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 3314-3319. | 4.6 | 56 |
| 76 | Vibrational Properties of the Phosphate Group Investigated by Molecular Dynamics and Density Functional Theory. <i>Journal of Physical Chemistry B</i> , 2015, 119, 10682-10692. | 2.6 | 23 |
| 77 | Through-space transfer of chiral information mediated by a plasmonic nanomaterial. <i>Nature Chemistry</i> , 2015, 7, 591-596. | 13.6 | 105 |
| 78 | Transfer of Frequency-Dependent Polarizabilities: A Tool To Simulate Absorption and Circular Dichroism Molecular Spectra. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2210-2220. | 5.3 | 4 |
| 79 | Comparison of the Electronic and Vibrational Optical Activity of a Europium(III) Complex. <i>Chemistry - A European Journal</i> , 2015, 21, 5807-5813. | 3.3 | 17 |
| 80 | Determination of Absolute Configuration in Chiral Solvents with Nuclear Magnetic Resonance. A Combined Molecular Dynamics/Quantum Chemical Study. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5260-5268. | 2.5 | 4 |
| 81 | Applications of chiroptical spectroscopy to coordination compounds. <i>Coordination Chemistry Reviews</i> , 2015, 284, 1-18. | 18.8 | 74 |
| 82 | Chirality Transfer in Magnetic Coordination Complexes Monitored by Vibrational and Electronic Circular Dichroism. <i>ChemPlusChem</i> , 2014, 79, 698-707. | 2.8 | 12 |
| 83 | Inspecting chiral molecules by Raman optical activity spectroscopy. <i>RSC Advances</i> , 2014, 4, 57125-57136. | 3.6 | 68 |
| 84 | Observation of Paramagnetic Raman Optical Activity of Nitrogen Dioxide. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 9236-9239. | 13.8 | 19 |
| 85 | Solvated States of Poly-L-alanine \pm -Helix Explored by Raman Optical Activity. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3655-3662. | 2.5 | 28 |
| 86 | Arrangement of Fibril Side Chains Studied by Molecular Dynamics and Simulated Infrared and Vibrational Circular Dichroism Spectra. <i>Journal of Physical Chemistry B</i> , 2014, 118, 6937-6945. | 2.6 | 22 |
| 87 | Molecular dynamics with helical periodic boundary conditions. <i>Journal of Computational Chemistry</i> , 2014, 35, n/a-n/a. | 3.3 | 2 |
| 88 | Transition polarizability model of induced resonance Raman optical activity. <i>Journal of Computational Chemistry</i> , 2013, 34, 2152-2158. | 3.3 | 23 |
| 89 | Parallel variable selection of molecular dynamics clusters as a tool for calculation of spectroscopic properties. <i>Journal of Computational Chemistry</i> , 2013, 34, 366-371. | 3.3 | 21 |
| 90 | Communication: Fullerene resolution by the magnetic circular dichroism. <i>Journal of Chemical Physics</i> , 2013, 138, 151103. | 3.0 | 19 |

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|-----|---|------|-----------|
| 91 | Computation of magnetic circular dichroism by sum-over-states summations. <i>Journal of Computational Chemistry</i> , 2013, 34, 1531-1539. | 3.3 | 31 |
| 92 | CH Stretching Region: Computational Modeling of Vibrational Optical Activity. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3096-3108. | 5.3 | 29 |
| 93 | Experimental and theoretical study on complexation of Li ⁺ with lithium ionophore VIII. <i>Monatshefte für Chemie</i> , 2013, 144, 1607-1611. | 1.8 | 5 |
| 94 | Ramachandran Plot for Alanine Dipeptide as Determined from Raman Optical Activity. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 2763-2768. | 4.6 | 55 |
| 95 | Porphyrim Protonation Studied by Magnetic Circular Dichroism. <i>Journal of Physical Chemistry A</i> , 2012, 116, 778-783. | 2.5 | 32 |
| 96 | Ferric Complexes of 3-Hydroxy-4-pyridinones Characterized by Density Functional Theory and Raman and UV-vis Spectroscopies. <i>Inorganic Chemistry</i> , 2012, 51, 4473-4481. | 4.0 | 23 |
| 97 | Transferability of Various Molecular Property Tensors in Vibrational Spectroscopy. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 977-985. | 5.3 | 60 |
| 98 | Detection of Molecular Chirality by Induced Resonance Raman Optical Activity in Europium Complexes. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 11058-11061. | 13.8 | 37 |
| 99 | Rotationally resolved magnetic vibrational circular dichroism of the paramagnetic molecule NO. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 9586. | 2.8 | 11 |
| 100 | Structure and Vibrational Motion of Insulin from Raman Optical Activity Spectra. <i>Analytical Chemistry</i> , 2012, 84, 2440-2451. | 6.5 | 64 |
| 101 | Theoretical Modeling of the Surface-Enhanced Raman Optical Activity. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1714-1720. | 5.3 | 37 |
| 102 | Determining the Absolute Configuration of Two Marine Compounds Using Vibrational Chiroptical Spectroscopy. <i>Journal of Organic Chemistry</i> , 2012, 77, 858-869. | 3.2 | 71 |
| 103 | Correction of Vibrational Broadening in Molecular Dynamics Clusters with the Normal Mode Optimization Method. <i>Journal of Physical Chemistry B</i> , 2012, 116, 336-342. | 2.6 | 38 |
| 104 | Three Types of Induced Tryptophan Optical Activity Compared in Model Dipeptides: Theory and Experiment. <i>ChemPhysChem</i> , 2012, 13, 2748-2760. | 2.1 | 18 |
| 105 | Theoretical Modeling of Peptide α -Helical Circular Dichroism in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 2011, 115, 1734-1742. | 2.5 | 31 |
| 106 | Raman Optical Activity of Methyloxirane Gas and Liquid. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 498-502. | 4.6 | 75 |
| 107 | Tracking of the Polyproline Folding by Density Functional Computations and Raman Optical Activity Spectra. <i>Journal of Physical Chemistry B</i> , 2011, 115, 15079-15089. | 2.6 | 31 |
| 108 | Explicit versus Implicit Solvent Modeling of Raman Optical Activity Spectra. <i>Journal of Physical Chemistry B</i> , 2011, 115, 4128-4137. | 2.6 | 92 |

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|-----|---|------|-----------|
| 109 | Spectroscopic Detection of DNA Quadruplexes by Vibrational Circular Dichroism. <i>Journal of the American Chemical Society</i> , 2011, 133, 15055-15064. | 13.7 | 50 |
| 110 | Simulations of ¹²⁹ Xe NMR chemical shift of atomic xenon dissolved in liquid benzene. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 677-684. | 1.4 | 22 |
| 111 | Monitoring the Backbone Conformation of Valinomycin by Raman Optical Activity. <i>ChemPhysChem</i> , 2011, 12, 1509-1518. | 2.1 | 41 |
| 112 | On the limited precision of transfer of molecular optical activity tensors. <i>Collection of Czechoslovak Chemical Communications</i> , 2011, 76, 567-583. | 1.0 | 23 |
| 113 | Applications of the Cartesian coordinate tensor transfer technique in the simulations of vibrational circular dichroism spectra of oligonucleotides. <i>Chirality</i> , 2010, 22, E96-E114. | 2.6 | 26 |
| 114 | Transferability of anharmonic force fields in simulations of molecular vibrations. <i>Journal of Chemical Physics</i> , 2010, 133, 044117. | 3.0 | 8 |
| 115 | Structural Analysis of Valinomycin in Solution Studied by Raman Optical Activity. <i>AIP Conference Proceedings</i> , 2010, , . | 0.4 | 2 |
| 116 | Formation and structure of the potassium complex of valinomycin in solution studied by Raman optical activity spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 11021. | 2.8 | 57 |
| 117 | Theoretical Study of Vibrationally Averaged Dipole Moments for the Ground and Excited C=O Stretching States of <i>trans</i> -Formic Acid. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 817-827. | 5.3 | 8 |
| 118 | A Fourier Transform Method for Generation of Anharmonic Vibrational Molecular Spectra. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2095-2102. | 5.3 | 5 |
| 119 | Computational Analysis of Solvent Effects in NMR Spectroscopy. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 288-299. | 5.3 | 106 |
| 120 | Vibrational Raman optical activity of 1-phenylethanol and 1-phenylethylamine: Revisiting old friends. <i>Chirality</i> , 2009, 21, E4-12. | 2.6 | 30 |
| 121 | Cross-Polarization Detection Enables Fast Measurement of Vibrational Circular Dichroism. <i>ChemPhysChem</i> , 2009, 10, 1983-1985. | 2.1 | 2 |
| 122 | Simulation of Vibrational Spectra of Large Molecules by Arbitrary Time Propagation. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 200-207. | 5.3 | 8 |
| 123 | Solvent Dependence of the <i>N</i> -Methylacetamide Structure and Force Field. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9727-9736. | 2.5 | 29 |
| 124 | <i>l</i> -Alanyl- <i>l</i> -alanine Conformational Changes Induced by pH As Monitored by the Raman Optical Activity Spectra. <i>Journal of Physical Chemistry A</i> , 2009, 113, 7760-7768. | 2.5 | 29 |
| 125 | Interpretation of Raman and Raman Optical Activity Spectra of a Flexible Sugar Derivative, the Gluconic Acid Anion. <i>Journal of Physical Chemistry A</i> , 2009, 113, 3594-3601. | 2.5 | 56 |
| 126 | Tight β -turns in peptides. DFT-based study of infrared absorption and vibrational circular dichroism for various conformers including solvent effects. <i>Theoretical Chemistry Accounts</i> , 2008, 119, 81-97. | 1.4 | 29 |

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|-----|---|------|-----------|
| 127 | Vibrational circular dichroism and IR spectral analysis as a test of theoretical conformational modeling for a cyclic hexapeptide. <i>Chirality</i> , 2008, 20, 1104-1119. | 2.6 | 21 |
| 128 | Circular dichroism enhancement in large DNA aggregates simulated by a generalized oscillator model. <i>Journal of Computational Chemistry</i> , 2008, 29, 2693-2703. | 3.3 | 23 |
| 129 | Dependence of the α -Alanyl- β -Alanine Conformation on Molecular Charge Determined from Ab Initio Computations and NMR Spectra. <i>Journal of Physical Chemistry B</i> , 2008, 112, 1796-1805. | 2.6 | 22 |
| 130 | Comparison of Quantitative Conformer Analyses by Nuclear Magnetic Resonance and Raman Optical Activity Spectra for Model Dipeptides. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8633-8640. | 2.5 | 51 |
| 131 | Matrix formulation of the surface-enhanced Raman optical activity theory. <i>Journal of Chemical Physics</i> , 2007, 126, 136101. | 3.0 | 29 |
| 132 | Simulations of vibrational spectra from classical trajectories: Calibration with <i>ab initio</i> force fields. <i>Journal of Chemical Physics</i> , 2007, 127, 084502. | 3.0 | 43 |
| 133 | Anharmonic effects in IR, Raman, and Raman optical activity spectra of alanine and proline zwitterions. <i>Journal of Chemical Physics</i> , 2007, 126, 224513. | 3.0 | 61 |
| 134 | DNA Oligonucleotide α -cis-Platin Binding: Ab Initio Interpretation of the Vibrational Spectra. <i>Journal of Physical Chemistry A</i> , 2007, 111, 9714-9723. | 2.5 | 33 |
| 135 | Interpretation of Synchrotron Radiation Circular Dichroism Spectra of Anionic, Cationic, and Zwitterionic Dialanine Forms. <i>Journal of Physical Chemistry A</i> , 2007, 111, 2750-2760. | 2.5 | 33 |
| 136 | Comparison of the numerical stability of methods for anharmonic calculations of vibrational molecular energies. <i>Journal of Computational Chemistry</i> , 2007, 28, 1617-1624. | 3.3 | 48 |
| 137 | Geometry and Solvent Dependence of the Electronic Spectra of the Amide Group and Consequences for Peptide Circular Dichroism. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4702-4711. | 2.5 | 36 |
| 138 | Conformational Flexibility of α -Alanine Zwitterion Determines Shapes of Raman and Raman Optical Activity Spectral Bands. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4689-4696. | 2.5 | 90 |
| 139 | Demonstration of the Ring Conformation in Polyproline by the Raman Optical Activity. <i>Journal of the American Chemical Society</i> , 2006, 128, 2438-2443. | 13.7 | 94 |
| 140 | Proline Zwitterion Dynamics in Solution, Glass, and Crystalline State. <i>Journal of the American Chemical Society</i> , 2006, 128, 13451-13462. | 13.7 | 82 |
| 141 | Contribution of transition dipole coupling to amide coupling in IR spectra of peptide secondary structures. <i>Vibrational Spectroscopy</i> , 2006, 42, 63-73. | 2.2 | 49 |
| 142 | Empirical solvent correction for multiple amide group vibrational modes. <i>Journal of Chemical Physics</i> , 2005, 122, 144501. | 3.0 | 81 |
| 143 | Vibrational Spectral Simulation for Peptides of Mixed Secondary Structure: Method Comparisons with the Trpzip Model Hairpin. <i>Journal of Physical Chemistry B</i> , 2005, 109, 23687-23697. | 2.6 | 90 |
| 144 | A Complete Set of NMR Chemical Shifts and Spin-Spin Coupling Constants for α -Alanyl-L-alanine Zwitterion and Analysis of Its Conformational Behavior. <i>Journal of the American Chemical Society</i> , 2005, 127, 17079-17089. | 13.7 | 38 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 145 | Ab Initio Modeling of Amide I Coupling in Antiparallel β -Sheets and the Effect of ^{13}C Isotopic Labeling on Infrared Spectra. <i>Journal of Physical Chemistry B</i> , 2005, 109, 5348-5357. | 2.6 | 62 |
| 146 | Simulations of Structure and Vibrational Spectra of Deoxyoctanucleotides. <i>Journal of Physical Chemistry B</i> , 2005, 109, 20579-20587. | 2.6 | 27 |
| 147 | Convergence Properties of the Normal Mode Optimization and Its Combination with Molecular Geometry Constraints. <i>Collection of Czechoslovak Chemical Communications</i> , 2005, 70, 1315-1340. | 1.0 | 50 |
| 148 | On the influence of the water electrostatic field on the amide group vibrational frequencies. <i>Journal of Chemical Physics</i> , 2004, 121, 7545. | 3.0 | 37 |
| 149 | RNA Structural Forms Studied by Vibrational Circular Dichroism: Ab Initio Interpretation of the Spectra. <i>Journal of Physical Chemistry B</i> , 2004, 108, 3899-3911. | 2.6 | 29 |
| 150 | Calculation of NMR chemical shifts for taxol and β -pinene within the generalized gradient approximation. <i>International Journal of Quantum Chemistry</i> , 2003, 91, 277-283. | 2.0 | 3 |
| 151 | Empirical modeling of the peptide amide I band IR intensity in water solution. <i>Journal of Chemical Physics</i> , 2003, 119, 11253-11262. | 3.0 | 189 |
| 152 | Partial optimization of molecular geometry in normal coordinates and use as a tool for simulation of vibrational spectra. <i>Journal of Chemical Physics</i> , 2002, 117, 4126-4132. | 3.0 | 119 |
| 153 | Gauge-Origin Independent Density-Functional Theory Calculations of Vibrational Raman Optical Activity. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7448-7455. | 2.5 | 162 |
| 154 | Chirality in Peptide Vibrations: Ab Initio Computational Studies of Length, Solvation, Hydrogen Bond, Dipole Coupling, and Isotope Effects on Vibrational CD. <i>ACS Symposium Series</i> , 2002, , 50-64. | 0.5 | 25 |
| 155 | Ab initio quantum mechanical models of peptide helices and their vibrational spectra. <i>Biopolymers</i> , 2002, 65, 45-59. | 2.4 | 107 |
| 156 | A cluster model of liquid water and its IR spectroscopic response. <i>Chemical Physics Letters</i> , 2002, 365, 82-88. | 2.6 | 45 |
| 157 | B α Z Conformational Transition of DNA Monitored by Vibrational Circular Dichroism. Ab Initio Interpretation of the Experiment. <i>Journal of Physical Chemistry B</i> , 2002, 106, 12623-12634. | 2.6 | 53 |
| 158 | Simulation of the Raman Optical Activity of β -Alanyl-L-Alanine. <i>Journal of Physical Chemistry A</i> , 2001, 105, 6362-6368. | 2.5 | 43 |
| 159 | Vibrational circular dichroism of tetraphenylporphyrin in peptide complexes? A computational study. , 2000, 12, 191-198. | | 51 |
| 160 | Simulations of oligopeptide vibrational CD: Effects of isotopic labeling. <i>Biopolymers</i> , 2000, 53, 380-395. | 2.4 | 73 |
| 161 | Comparison of Hartree-Fock and Kohn-Sham determinants as wave functions. <i>Journal of Computational Chemistry</i> , 2000, 21, 8-16. | 3.3 | 17 |
| 162 | Measurement and Calculation of Absolute Rotational Strengths for Camphor, β -Pinene, and Borneol. <i>Journal of Physical Chemistry A</i> , 1998, 102, 102-110. | 2.5 | 54 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|------|-----------|
| 163 | Measurement and Calculation of the Raman Optical Activity of $\hat{1}\pm$ -Pinene and trans-Pinane. Collection of Czechoslovak Chemical Communications, 1997, 62, 1384-1395. | 1.0 | 51 |
| 164 | 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 |
| 165 | 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 |
| 166 | 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 |
| 167 | Observations of rotational magnetic moments in the ground and some excited vibrational $\hat{1}\Sigma$ states of C ₂ H ₂ , C ₂ HD, and C ₂ D ₂ by magnetic vibrational circular dichroism. Journal of Chemical Physics, 1996, 104, 1813-1824. | 3.0 | 5 |
| 168 | Rotationally resolved magnetic vibrational circular dichroism. Molecular Physics, 1996, 87, 299-318. | 1.7 | 6 |
| 169 | Vibrational Magnetic Dipole Moment of Acetylene in the $\hat{1}\frac{1}{2}\Sigma$ Mode. The Journal of Physical Chemistry, 1996, 100, 2062-2065. | 2.9 | 17 |
| 170 | Rotationally resolved magnetic vibrational circular dichroism Experimental spectra and theoretical simulation for diamagnetic molecules. Molecular Physics, 1996, 87, 299-318. | 1.7 | 6 |
| 171 | Ab initio simulations of the vibrational circular dichroism of coupled peptides. Journal of the American Chemical Society, 1993, 115, 9602-9607. | 13.7 | 103 |
| 172 | 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 |
| 173 | Photochemical synthesis of pink silver and its use for monitoring peptide nitration via surface enhanced Raman spectroscopy (SERS). Amino Acids, 0, , . | 2.7 | 1 |