Sergio Abbate

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/2088065/publications.pdf

Version: 2024-02-01

		109321	168389
152	3,976	35	53
papers	citations	h-index	g-index
156	156	156	3384
all docs	docs citations	times ranked	citing authors

#	Article	IF	CITATIONS
1	Enantiopure Double <i>ortho</i> â€Oligophenylethynyleneâ€Based Helical Structures with Circularly Polarized Luminescence Activity. ChemPhotoChem, 2022, 6, .	3.0	5
2	Circularly Polarized Luminescence of Some [2]Paracyclo[2](5,8)quinoliphane Derivatives with Planar and Central Chirality. ChemPhotoChem, 2022, 6, .	3.0	9
3	Helicity control of a perfluorinated carbon chain within a chiral supramolecular cage monitored by VCD. Chemical Communications, 2022, 58, 2152-2155.	4.1	8
4	Spectroscopic investigation on 1,2-substituted ferrocenes with only planar chirality: how chiroptical data are related to absolute configuration and to substituents. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 272, 121010.	3.9	2
5	Resolution of a Configurationally Stable Hetero[4]helicene. Molecules, 2022, 27, 1160.	3.8	3
6	Synthesis, Stereochemical and Photophysical Properties of Functionalized Thiahelicenes. Catalysts, 2022, 12, 366.	3.5	5
7	MCD and Induced CD of a Tetraphenoxyperylene-Based Dye in Chiral Solvents: An Experimental and Computational Study. Symmetry, 2022, 14, 1108.	2.2	2
8	Vibrational and Electronic Circular Dichroism Study of Chiral Seleno Compounds Prepared from a Naphthol Based Diselenide. European Journal of Organic Chemistry, 2022, 2022, .	2.4	2
9	Chiral bis(benzo[1,2-b:4,3-b′]dithiophene) atropisomers: experimental and theoretical investigations of the stereochemical and chiroptical properties. New Journal of Chemistry, 2021, 45, 16442-16451.	2.8	O
10	1,2-Disubstituted Planar Chiral Ferrocene Derivatives from Sulfonamide-Directed <i>ortho</i> -Lithiation: Synthesis, Absolute Configuration, and Chiroptical Properties. Organometallics, 2021, 40, 578-590.	2.3	14
11	MCD and MCPL Characterization of Luminescent Si(IV) and P(V) Tritolylcorroles: The Role of Coordination Number. ACS Omega, 2021, 6, 26659-26671.	3.5	12
12	Biliverdin chiral derivatives as chiroptical switches for pH and metal cation sensing. Physical Chemistry Chemical Physics, 2021, 23, 20138-20151.	2.8	8
13	Extended enantiopure <i>ortho</i> -phenylene ethylene (<i>o</i> -OPE)-based helical systems as scaffolds for supramolecular architectures: a study of chiroptical response and its connection to the CISS effect. Organic Chemistry Frontiers, 2021, 8, 5071-5086.	4.5	16
14	Characterization of "Free Base―and Metal Complex Thioalkyl Porphyrazines by Magnetic Circular Dichroism and TDDFT Calculations. Journal of Physical Chemistry B, 2021, 125, 264-280.	2.6	5
15	Magnetic Circular Dichroism of Naphthalene Derivatives: A Coupled Cluster Singles and Approximate Doubles and Time-Dependent Density Functional Theory Study. Journal of Physical Chemistry A, 2021, 125, 243-250.	2.5	7
16	The Assignment of the Absolute Configuration of Non-Cyclic Sesquiterpenes by Vibrational and Electronic Circular Dichroism: The Example of Chiliadenus lopadusanus Metabolites. Biomolecules, 2021, 11, 1902.	4.0	1
17	Plasmonic Superchiral Lattice Resonances in the Mid-Infrared. ACS Photonics, 2020, 7, 2676-2681.	6.6	26
18	Vibrational Circular Dichroism Detects Symmetry Breaking due to Conformational Mobility in C2-Symmetry Chiral Molecules and Provides Further Insight into Inter-Chromophoric Interactions. Symmetry, 2020, 12, 1752.	2.2	3

#	Article	IF	Citations
19	Solvent Effects and Aggregation Phenomena Studied by Vibrational Optical Activity and Molecular Dynamics: The Case of Pantolactone. Journal of Physical Chemistry B, 2020, 124, 4512-4526.	2.6	24
20	Testing the vibrational exciton and the local mode models on the instructive cases of dicarvone, dipinocarvone, and dimenthol vibrational circular dichroism spectra. Chirality, 2020, 32, 907-921.	2.6	5
21	Characterization of tetrakis(thiadiazole)porphyrazine metal complexes by magnetic circular dichroism and magnetic circularly polarized luminescence. Chirality, 2020, 32, 808-816.	2.6	16
22	Toward Fully Unsupervised Anharmonic Computations Complementing Experiment for Robust and Reliable Assignment and Interpretation of IR and VCD Spectra from Mid-IR to NIR: The Case of 2,3-Butanediol and <i>trans</i> -1,2-Cyclohexanediol. Journal of Physical Chemistry A, 2020, 124, 1011-1024.	2,5	26
23	Structural and Electronic Information Drawn from the Circularly Polarized Luminescence Spectra: Many Questions and Some Answers for Simple Organic Molecules, Polymers, and Molecular Aggregates., 2020,, 219-248.		O
24	Chiral double stapled <i>o</i> -OPEs with intense circularly polarized luminescence. Chemical Communications, 2019, 55, 10685-10688.	4.1	41
25	Four-Fold Alkyne Benzannulation: Synthesis, Properties, and Structure of Pyreno[<i>a</i>]pyrene-Based Helicene Hybrids. Organic Letters, 2019, 21, 8652-8656.	4.6	32
26	Assignment Through Chiroptical Methods of The Absolute Configuration of Fungal Dihydropyranpyran-4-5-Diones Phytotoxins, Potential Herbicides for Buffelgrass (Cenchrus ciliaris) Biocontrol. Molecules, 2019, 24, 3022.	3.8	13
27	Optically active Ag(<scp>i</scp>): <i>o</i> -OPE helicates using a single homochiral sulfoxide as chiral inducer. Organic and Biomolecular Chemistry, 2019, 17, 8425-8434.	2.8	8
28	Unbiased Determination of Absolute Configurations by vis-Ã-vis Comparison of Experimental and Simulated Spectra: The Challenging Case of Diplopyrone. Journal of Physical Chemistry B, 2019, 123, 9230-9237.	2.6	29
29	Highly enantioselective "inherently chiral―electroactive materials based on a 2,2′-biindole atropisomeric scaffold. Chemical Science, 2019, 10, 2708-2717.	7.4	22
30	Bilirubin and its congeners: conformational analysis and chirality from metadynamics and related computational methods. Monatshefte Für Chemie, 2019, 150, 801-812.	1.8	4
31	CF ₃ : an overlooked chromophore in VCD spectra. A review of recent applications in structural determination. RSC Advances, 2019, 9, 11781-11796.	3.6	7
32	Ferrocenes with simple chiral substituents: an in-depth theoretical and experimental VCD and ECD study. Physical Chemistry Chemical Physics, 2019, 21, 9419-9432.	2.8	19
33	Evaluation of Molecular Polarizability and of Intensity Carrying Modes Contributions in Circular Dichroism Spectroscopies. Applied Sciences (Switzerland), 2019, 9, 4691.	2.5	5
34	Toward a general mixed quantum/classical method for the calculation of the vibronic ECD of a flexible dye molecule with different stable conformers: Revisiting the case of 2,2,2â€trifluoroâ€anthrylethanol. Chirality, 2018, 30, 730-743.	2.6	10
35	Searching for Models Exhibiting High Circularly Polarized Luminescence: Electroactive Inherently Chiral Oligothiophenes. Chemistry - A European Journal, 2018, 24, 11082-11093.	3.3	23
36	Pyrene-Containing <i>ortho</i> -Oligo(phenylene)ethynylene Foldamer as a Ratiometric Probe Based on Circularly Polarized Luminescence. Journal of Organic Chemistry, 2018, 83, 4455-4463.	3.2	75

#	Article	IF	CITATIONS
37	Exploring potentialities and limitations of stapled <i>o</i> â€oligo(phenyleneethynylene)s (<i>o</i> â€∢scp>OPEs) as efficient circularly polarized luminescence emitters. Chirality, 2018, 30, 43-54.	2.6	6
38	Sulfoxideâ€Induced Homochiral Folding of <i>ortho</i> â€Phenylene Ethynylenes (<i>o</i> â€OPEs) by Silver(I) Templating: Structure and Chiroptical Properties. Chemistry - A European Journal, 2018, 24, 2653-2662.	3.3	38
39	On the aggregation of bilirubinoids in solution as evidenced by <scp>VCD</scp> and <scp>ECD</scp> spectroscopy and <scp>DFT</scp> calculations. Chirality, 2018, 30, 19-28.	2.6	6
40	A stereodynamic fluorescent probe for amino acids. Circular dichroism and circularly polarized luminescence analysis. Chirality, 2018, 30, 65-73.	2.6	19
41	OFF/ON switching of circularly polarized luminescence by oxophilic interaction of homochiral sulfoxide-containing <i>o</i> -OPEs with metal cations. Chemical Communications, 2018, 54, 13985-13988.	4.1	53
42	Mannich-type addition of 1,3-dicarbonyl compounds to chiral <i>tert</i> -butanesulfinyltrifluoroacetaldimines. Mechanistic aspects and chiroptical studies. Organic and Biomolecular Chemistry, 2018, 16, 8742-8750.	2.8	11
43	<i>I</i> -Stercobilin-HCl and <i>d</i> -Urobilin-HCl. Analysis of Their Chiroptical and Conformational Properties by VCD, ECD, and CPL Experiments and MD and DFT Calculations. Journal of Physical Chemistry B, 2018, 122, 12351-12362.	2.6	17
44	Absolute configuration assignment to anticancer Amaryllidaceae alkaloid jonquailine. Fìtoterapìâ, 2018, 129, 78-84.	2.2	25
45	Asymmetric Synthesis of Spirooxindoles via Nucleophilic Epoxidation Promoted by Bifunctional Organocatalysts. Molecules, 2018, 23, 438.	3.8	8
46	Azabora[5]helicene Chargeâ€Transfer Dyes Show Efficient and Spectrally Variable Circularly Polarized Luminescence. Chemistry - A European Journal, 2018, 24, 12660-12668.	3.3	71
47	Luminescent water-soluble cycloplatinated complexes: Structural, photophysical, electrochemical and chiroptical properties. Inorganica Chimica Acta, 2017, 461, 267-274.	2.4	17
48	Solvent-free, uncatalyzed asymmetric "ene―reactions of N-tert-butylsulfinyl-3,3,3-trifluoroacetaldimines: a general approach to enantiomerically pure α-(trifluoromethyl)tryptamines. Organic and Biomolecular Chemistry, 2017, 15, 3930-3937.	2.8	10
49	Chiral-at-Metal Phosphorescent Square-Planar Pt(II)-Complexes from an Achiral Organometallic Ligand. Journal of the American Chemical Society, 2017, 139, 6863-6866.	13.7	99
50	The role of chirality in a set of key intermediates of pharmaceutical interest, 3-aryl-substituted-13-butyrolactones, evidenced by chiral HPLC separation and by chiroptical spectroscopies. Journal of Pharmaceutical and Biomedical Analysis, 2017, 144, 41-51.	2.8	28
51	Vibrational Optical Activity of BODIPY Dimers: The Role of Magnetic–Electric Coupling in Vibrational Excitons. Journal of Physical Chemistry A, 2017, 121, 394-400.	2.5	27
52	Circularly polarized luminescence of syndiotactic polystyrene. Optical Materials, 2017, 73, 595-601.	3.6	23
53	Chiral Peropyrene: Synthesis, Structure, and Properties. Journal of the American Chemical Society, 2017, 139, 13102-13109.	13.7	99
54	Synthesis of Intrinsically Blue-Colored <i>bis</i> -Nitronyl Nitroxide Peptidomimetic Templates and Their Conformational Preferences as Revealed by a Combined Spectroscopic Analysis. Journal of Organic Chemistry, 2017, 82, 10033-10042.	3.2	6

#	Article	IF	CITATIONS
55	Importance and Difficulties in the Use of Chiroptical Methods to Assign the Absolute Configuration of Natural Products: The Case of Phytotoxic Pyrones and Furanones Produced by <i>Diplodia corticola</i> . Journal of Natural Products, 2017, 80, 2406-2415.	3.0	33
56	Vibrational Circular Dichroism Unveils Chiroptical, Electrical, and Magnetic Properties of Borylated Isocyanides and Aldehydes. European Journal of Organic Chemistry, 2017, 2017, 5262-5268.	2.4	1
57	(R)-(â^')-Aloesaponol III 8-Methyl Ether from Eremurus persicus: A Novel Compound against Leishmaniosis. Molecules, 2017, 22, 519.	3.8	21
58	Analytical and preparative enantioseparation and main chiroptical properties of Iridium(III) bis(4,6-difluorophenylpyridinato)picolinato. Journal of Chromatography A, 2016, 1467, 335-346.	3.7	30
59	Vibronic Coupling Explains the Different Shape of Electronic Circular Dichroism and of Circularly Polarized Luminescence Spectra of Hexahelicenes. Journal of Chemical Theory and Computation, 2016, 12, 2799-2819.	5.3	59
60	Discrimination of Axial and Central Stereogenic Elements in Chiral Bis(oxazolines) Based on Atropisomeric 3,3′â€Bithiophene Scaffolds Through Chiroptical Spectroscopies. Chirality, 2016, 28, 686-695.	2.6	7
61	Circularly Polarized Luminescence: A Review of Experimental and Theoretical Aspects. Chirality, 2016, 28, 696-707.	2.6	339
62	Enantiomeric 4â€Acylaminoâ€6â€alkyloxyâ€2 Alkylthiopyrimidines As Potential A ₃ Adenosine Receptor Antagonists: HPLC Chiral Resolution and Absolute Configuration Assignment by a Full Set of Chiroptical Spectroscopy. Chirality, 2016, 28, 434-440.	2.6	13
63	Stapled helical o-OPE foldamers as new circularly polarized luminescence emitters based on carbophilic interactions with Ag(<scp>i</scp>)-sensitivity. Chemical Science, 2016, 7, 5663-5670.	7.4	84
64	Thioflavinâ€T: Electronic Circular Dichroism and Circularly Polarized Luminescence Induced by Amyloid Fibrils. ChemPhysChem, 2016, 17, 2931-2937.	2.1	33
65	Quantum-Classical Calculation of Vibronic Spectra along a Reaction Path: The Case of the ECD of Easily Interconvertible Conformers with Opposite Chiral Responses. Journal of Physical Chemistry Letters, 2016, 7, 4891-4897.	4.6	19
66	Chiroptical properties of the ground and excited states of two thia-bridged triarylamine heterohelicenes. Journal of Photochemistry and Photobiology A: Chemistry, 2016, 331, 138-145.	3.9	39
67	Vibrational circular dichroism and chiroptical properties of chiral Ir(<scp>iii</scp>) luminescent complexes. Dalton Transactions, 2016, 45, 992-999.	3.3	40
68	pH Dependent Chiroptical Properties of $(1 < i > R < i > , 2 < i > R < i >)$ - and $(1 < i > S < i > , 2 < i > S < i >)$ - $< i > trans < i >$ - Cyclohexane Diesters and Diamides from VCD, ECD, and CPL Spectroscopy. Journal of Physical Chemistry B, 2016, 120, 2380-2387.	2.6	21
69	The connection between robustness angles and dissymmetry factors in vibrational circular dichroism spectra. Chemical Physics Letters, 2015, 639, 320-325.	2.6	24
70	Vibrational Circular Dichroism (VCD) Reveals Subtle Conformational Aspects and Intermolecular Interactions in the Carnitine Family. Chirality, 2015, 27, 907-913.	2.6	7
71	Circularly polarized luminescence under near-UV excitation and structural elucidation of a Eu complex. Chemical Communications, 2015, 51, 11903-11906.	4.1	42
72	On the handedness of helical aggregates of C ₃ tricarboxamides: a multichiroptical characterization. Chemical Communications, 2015, 51, 9781-9784.	4.1	26

#	Article	IF	Citations
73	VCD spectroscopy as an excellent probe of chiral metal complexes containing a carbon monoxide vibrational chromophore. Chemical Communications, 2015, 51, 9385-9387.	4.1	10
74	Bicamphor: A Prototypic Molecular System to Investigate Vibrational Excitons. Journal of Physical Chemistry A, 2015, 119, 4261-4267.	2.5	37
75	Chiroptical Phenomena in Reverse Micelles: The Case of (1 <i>R</i> ,2 <i>S</i>)â€Dodecyl (2â€hydroxyâ€1â€methylâ€2â€phenylethyl)dimethylammonium Bromide (DMEB). Chirality, 2014, 26, 532-538.	2.6	11
76	Mode Robustness in Raman Optical Activity. Journal of Chemical Theory and Computation, 2014, 10, 5520-5527.	5.3	23
77	Chiroptical spectroscopic techniques based on fluorescence. Methods and Applications in Fluorescence, 2014, 2, 024006.	2.3	35
78	Helical Sense-Responsive and Substituent-Sensitive Features in Vibrational and Electronic Circular Dichroism, in Circularly Polarized Luminescence, and in Raman Spectra of Some Simple Optically Active Hexahelicenes. Journal of Physical Chemistry C, 2014, 118, 1682-1695.	3.1	135
79	Chiroptical Signatures of Planar and Central Chirality in [2]Paracyclo[2](5,8)quinolinophane Derivatives. European Journal of Organic Chemistry, 2014, 2014, 7353-7363.	2.4	15
80	Structural and Optical Properties of Inherently Chiral Polythiophenes: A Combined CD-Electrochemistry, Circularly Polarized Luminescence, and TD-DFT Investigation. Journal of Physical Chemistry C, 2014, 118, 16019-16027.	3.1	32
81	Inherently Chiral Macrocyclic Oligothiophenes: Easily Accessible Electrosensitive Cavities with Outstanding Enantioselection Performances. Chemistry - A European Journal, 2014, 20, 15298-15302.	3.3	57
82	Importance of C*â€"H Based Modes and Large Amplitude Motion Effects in Vibrational Circular Dichroism Spectra: The Case of the Chiral Adduct of Dimethyl Fumarate and Anthracene. Journal of Physical Chemistry A, 2014, 118, 4339-4350.	2.5	30
83	Looking at Human Cytosolic Sialidase NEU2 Structural Features with an Interdisciplinary Approach. Biochemistry, 2014, 53, 5343-5355.	2.5	3
84	Inherently Chiral Macrocyclic Oligothiophenes: Easily Accessible Electrosensitive Cavities with Outstanding Enantioselection Performances. Chemistry - A European Journal, 2014, 20, 15261-15261.	3.3	5
85	Experimental and Calculated CPL Spectra and Related Spectroscopic Data of Camphor and Other Simple Chiral Bicyclic Ketones. Chirality, 2013, 25, 589-599.	2.6	72
86	Combined use of three forms of chiroptical spectroscopies in the study of the absolute configuration and conformational properties of 3-phenylcyclopentanone, 3-phenylcyclohexanone, and 3-phenylcycloheptanone. Tetrahedron, 2013, 69, 10752-10762.	1.9	15
87	Raman and ROA Spectra of (â^')- and (+)-2-Br-Hexahelicene: Experimental and DFT Studies of a Ï€-Conjugated Chiral System. Journal of Physical Chemistry B, 2013, 117, 2221-2230.	2.6	42
88	Conformational Studies of Phe-Rich Foldamers by VCD Spectroscopy and ab Initio Calculations. Journal of Organic Chemistry, 2012, 77, 6033-6042.	3.2	17
89	Electronic and vibrational circular dichroism spectra of (R)-(â^')-apomorphine. Chemical Physics, 2012, 405, 197-205.	1.9	6
90	Vibrational and Electronic Circular Dichroism of Dimethyl Mesobilirubins-XIIIα. Journal of Physical Chemistry B, 2012, 116, 5628-5636.	2.6	11

#	Article	IF	CITATIONS
91	Vibrational and electronic circular dichroism spectroscopies and DFT calculations for the assignment of the absolute configuration of hydroxy-substituted 2-tetralols. RSC Advances, 2012, 2, 10200.	3.6	8
92	Ultraviolet, Circular Dichroism, Fluorescence, and Circularly Polarized Luminescence Spectra of Regioregular Polyâ€[3â€((<i>S</i>)â€2â€Methylbutyl)â€7hiophene] in Solution. Chirality, 2012, 24, 725-730.	2.6	40
93	Investigations of methyl lactate in the presence of reverse micelles by vibrational spectroscopy and circular dichroism. Vibrational Spectroscopy, 2012, 60, 54-62.	2.2	11
94	Experimental methods for measuring optical rotatory dispersion: Survey and outlook. Chirality, 2011, 23, 711-716.	2.6	31
95	Vibrational Circular Dichroism: A Valuable Tool for Conformational Analysis and Absolute Configuration Assignment of Chiral 1â€Arylâ€2,2,2â€₹rifluoroethanols. ChemPhysChem, 2011, 12, 3519-3523.	2.1	10
96	Triggering dissymmetry in achiral dye molecules by chiral solvents: Circular dichroism experiments and DFT calculations. Chirality, 2011, 23, 910-915.	2.6	9
97	Electrical and mechanical anharmonicities from NIRâ€VCD spectra of compounds exhibiting axial and planar chirality: The cases of (<i>S</i>)â€2,3â€pentadiene and methylâ€ <i>d₃</i> (<i>R</i>)―and (<i>S</i>)â€{2.2]paracyclophaneâ€4â€carboxylate. Chirality, 2011, 23, 841-849.	2.6	8
98	Solving the Puzzling Absolute Configuration Determination of a Flexible Molecule by Vibrational and Electronic Circular Dichroism Spectroscopies and DFT Calculations: The Case Study of a Chiral 2,2′-Dinitro-2,2′-biaziridine. European Journal of Organic Chemistry, 2010, 2010, 6193-6199.	2.4	11
99	Evaluation of instrumental errors built in circular dichroism spectrometers. Chirality, 2010, 22, E142-8.	2.6	10
100	Revisiting with Updated Hardware an Old Spectroscopic Technique: Circularly Polarized Luminescence. Applied Spectroscopy, 2010, 64, 1416-1419.	2.2	48
101	A vibrational circular dichroism approach to the determination of the absolute configuration of flexible and transparent molecules: fluorenone ketals of 1,n-diols. Physical Chemistry Chemical Physics, 2010, 12, 4725.	2.8	12
102	Assessment of configurational and conformational properties of naringenin by vibrational circular dichroism. Chirality, 2009, 21, 436-441.	2.6	53
103	Determination of the absolute configuration of aromatase and dual aromataseâ€sulfatase inhibitors by vibrational and electronic circular dichroism spectra analysis. Chirality, 2009, 21, 802-808.	2.6	14
104	Experimental aspects of solid state circular dichroism. Chirality, 2009, 21, E28-36.	2.6	77
105	NIRâ€VCD, vibrational circular dichroism in the nearâ€infrared: Experiments, theory and calculations. Chirality, 2009, 21, E242-52.	2.6	26
106	Calculations of overtone NIR and NIR-VCD spectra in the local mode approximation: Camphor and Camphorquinone. Vibrational Spectroscopy, 2009, 50, 257-267.	2.2	21
107	Comparative Analysis of IR and Vibrational Circular Dichroism Spectra for a Series of Camphor-Related Molecules. Journal of Physical Chemistry A, 2009, 113, 11390-11405.	2.5	37
108	Experimental and ab-initio calculated vcd spectra of the first OH-stretching overtone of (1R)-(\hat{a}^{-1}) and (1S)-(+)-endo-BORNEOL. Physical Chemistry Chemical Physics, 2009, 11, 2683.	2.8	19

#	Article	IF	CITATIONS
109	Experimental and calculated vibrational and electronic circular dichroism spectra of 2-Br-hexahelicene. Physical Chemistry Chemical Physics, 2009, 11, 9039.	2.8	31
110	Spectroscopic and Structural Investigation of the Confinement of <scp>d</scp> and <scp>l</scp> Dimethyl Tartrate in Lecithin Reverse Micelles. Journal of Physical Chemistry B, 2009, 113, 3024-3033.	2.6	28
111	An operative approach to correct CD spectra distortions due to absorption flattening. Chirality, 2008, 20, 1047-1052.	2.6	12
112	Confinement of chiral molecules in reverse micelles: FT-IR, polarimetric and VCD investigation on the state of dimethyl tartrate in sodium bis(2-ethylhexyl) sulfosuccinate reverse micelles dispersed in carbon tetrachloride. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2008, 327, 44-50.	4.7	19
113	Chiral Aromatase and Dual Aromataseâ 'Steroid Sulfatase Inhibitors from the Letrozole Template: Synthesis, Absolute Configuration, and In Vitro Activity. Journal of Medicinal Chemistry, 2008, 51, 4226-4238.	6.4	80
114	Molecular Dynamics Simulation of Aqueous Solutions of 26-Unit Segments of p(NIPAAm) and of p(NIPAAm) "Doped―with Amino Acid Based Comonomers. Journal of Physical Chemistry B, 2008, 112, 11896-11906.	2.6	35
115	Harmonic and Anharmonic Features of IR and NIR Absorption and VCD Spectra of Chiral 4-X-[2.2]Paracyclophanes. Journal of Physical Chemistry A, 2007, 111, 7031-7040.	2.5	26
116	Wavelength shifts in solid-state circular dichroism spectra: A possible explanation. Chirality, 2007, 19, 491-496.	2.6	39
117	Absorption flattening as one cause of distortion of circular dichroism spectra of Δ-RuPhen3 · H2TPPS complex. Chirality, 2007, 19, 642-646.	2.6	22
118	Study of conformational properties of a biologically active peptide of fibronectin by circular dichroism, NMR and molecular dynamics simulation. Physical Chemistry Chemical Physics, 2006, 8, 4668.	2.8	8
119	Fenchone, Camphor, 2-Methylenefenchone and 2-Methylenecamphor:Â A Vibrational Circular Dichroism Study. Journal of Physical Chemistry A, 2006, 110, 4958-4968.	2.5	41
120	Monoaza[5]helicenes. Part 2: Synthesis, characterisation and theoretical calculations. Tetrahedron, 2006, 62, 139-148.	1.9	66
121	Calculated absorption and vibrational circular dichroism spectra of fundamental and overtone transitions for a chiral HCCH molecular fragment in the hypothesis of coupled dipoles. Chirality, 2005, 17, 530-539.	2.6	6
122	Vibrational Excitons in CH-Stretching Fundamental and Overtone Vibrational Circular Dichroism Spectra. Monatshefte FÃ $\frac{1}{4}$ r Chemie, 2005, 136, 325-345.	1.8	9
123	Molecular dynamics simulation of a model oligomer for poly(N-isopropylamide) in water. Chemical Physics Letters, 2004, 386, 123-127.	2.6	46
124	Chiroptical Properties of Some Monoazapentahelicenes. Journal of Physical Chemistry A, 2004, 108, 11752-11761.	2.5	29
125	A Comparative Study of Overtone CH-Stretching Vibrational Circular Dichroism Spectra of Fenchone and Camphorâ€. Journal of Physical Chemistry A, 2004, 108, 5338-5352.	2.5	29
126	Detection by circular dichroism of conformational transitions in pH and thermosensitive copolymers based on N-isopropylacrylamide and N-methacryloyl-L-leucine. Chirality, 2003, 15, 251-255.	2.6	7

#	Article	IF	CITATIONS
127	Dipole and rotational strengths for overtone transitions of a C2-symmetry HCCH molecular fragment using Van Vleck perturbation theory. Journal of Chemical Physics, 2002, 117, 7575-7586.	3.0	11
128	Vibrational Circular Dichroism in the Near Infrared: Instrumental Developments and Applications. Enantiomer, 2002, 7, 161-173.	0.5	36
129	Solid-State Optical and Structural Modifications Induced by Temperature in a Chiral Poly-3-alkylthiophene. Chemistry of Materials, 2002, 14, 4819-4826.	6.7	38
130	Conformational Analysis of (S)-(+)-1-Bromo-2-methylbutane and the Influence of Bromine on Conformational Stability. Journal of Physical Chemistry A, 2002, 106, 12365-12369.	2.5	26
131	Theoretical and experimental studies for the interpretation of vibrational circular dichroism spectra in the CH-stretching overtone region., 2000, 12, 180-190.		19
132	Investigations on the mobility of the glycosidic linkage in sucrose by study of the phase space structure of a two-degrees of freedom model. Journal of Molecular Graphics and Modelling, 2000, 18, 153-162.	2.4	0
133	The use of cross-correlation functions in the analysis of circular dichroism spectra. Journal of Chemical Physics, 1998, 108, 50-62.	3.0	49
134	Study of the phase space structure for a two-degrees of freedom model of a symmetric glycosidic linkage. Carbohydrate Research, 1997, 300, 59-66.	2.3	1
135	Observation of Vibrational Circular Dichroism for Overtone Transitions with Commercially Available CD Spectrometers. Applied Spectroscopy, 1996, 50, 642-643.	2.2	18
136	Characterization of vibrational transition modes by use of normal forms. Theoretica Chimica Acta, 1993, 87, 215-232.	0.8	5
137	Analysis of the transition from normal modes to local modes in a system of two harmonically coupled Morse oscillators. Theoretica Chimica Acta, 1992, 82, 321-337.	0.8	16
138	Characterisation of the glycosidic linkage by infrared and Raman spectroscopy in the C-H stretching region: $\hat{l}_{\pm},\hat{l}_{\pm}$ -trehalose and $\hat{l}_{\pm},\hat{l}_{\pm}$ -trehalose-2,3,4,6,6-d10. Carbohydrate Research, 1991, 210, 1-12.	2.3	10
139	Vibrational circular dichroism as a criterion for local-mode versus normal-mode behavior. Near-infrared circular dichroism spectra of some monoterpenes. Journal of the American Chemical Society, 1989, 111, 836-840.	13.7	32
140	Assessment of the values of the Cî—,H-stretching force constants in sugar molecules. Carbohydrate Research, 1988, 184, 1-11.	2.3	39
141	Vibrational optical activity in deuteriated phenylethanes. The Journal of Physical Chemistry, 1988, 92, 3302-3311.	2.9	10
142	Conformational dependence of CH(CD)-strechings in D-glucose and some deuterated derivatives as revealed by infrared and raman spectroscopy. Carbohydrate Research, 1987, 161, 1-22.	2.3	34
143	The charge flow model applied to the vibrational circular dichroism of oriented species. Chemical Physics Letters, 1985, 113, 202-206.	2.6	1
144	Conformationally dependent Fermi resonances and long-range interactions between .sigma. bonds in polymethylene systems derived from their Raman spectra. The Journal of Physical Chemistry, 1985, 89, 4793-4799.	2.9	45

#	Article	IF	CITATIONS
145	Anharmonic vibrational averages for formaldehyde. Spectrochimica Acta Part A: Molecular Spectroscopy, 1984, 40, 591-596.	0.1	0
146	Vibrational circular dichroism of (R)-(-)-neopentyl-1-d chloride and (R)-(-)-neopentyl-1-d bromide. The Journal of Physical Chemistry, 1984, 88, 505-507.	2.9	5
147	Infrared intensities of methane and ethane. A starting set of electrooptical parameters for n-hydrocarbons. Computational and Theoretical Chemistry, 1982, 87, 87-96.	1.5	18
148	Least squares calculations of electroâ€optical parameters from infrared intensities of CH4 and C2H6 and their deuterated derivatives. Journal of Chemical Physics, 1979, 71, 3428-3439.	3.0	30
149	Raman intensities of methanes from electrooptical parameters. Journal of Molecular Spectroscopy, 1978, 73, 415-429.	1.2	15
150	Infrared and Raman intensities of polyethylene and perdeuteropolyethylene by electroâ€optical parameters. Single chain. Journal of Chemical Physics, 1977, 67, 1519-1531.	3.0	51
151	Raman intensities: Transferability of electrooptical parameters. Journal of Raman Spectroscopy, 1977, 6, 289-298.	2.5	32
152	Ï€â€Extended Helical Nanographenes: Synthesis and Photophysical Properties of Naphtho[1,2―a]pyrenes**. European Journal of Organic Chemistry, 0, , .	2.4	2