Alberto Lesarri

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/2704322/publications.pdf

Version: 2024-02-01

194	4,957	117625	133252
papers	citations	34 h-index	59 g-index

207	207	207	2332
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The Gas-Phase Structure of Alanine. Journal of the American Chemical Society, 2004, 126, 11675-11683.	13.7	183
2	Noble Gasâ^'Metal Chemical Bonds. Microwave Spectra, Geometries, and Nuclear Quadrupole Coupling Constants of Arâ^'AuCl and Krâ^'AuCl. Journal of the American Chemical Society, 2000, 122, 6100-6105.	13.7	182
3	Molecular beam Fourier transform microwave spectrum of the dimethyletherâ€“xenon complex: tunnelling splitting and 131Xe quadrupole coupling constants. Chemical Physics Letters, 2004, 392, 1-6.	2.6	139
4	Weak Câ^'HÂ·Â·Â·O and Câ^'HÂ·Â·Â·Fâ^'C Hydrogen Bonds in the Oxiraneâ^'Trifluoromethane Dimer. Journal of the American Chemical Society, 2004, 126, 3244-3249.	13.7	139
5	The Structure of Neutral Proline. Angewandte Chemie - International Edition, 2002, 41, 4673-4676.	13.8	134
6	The Glycineâ€“Water Complex. Angewandte Chemie - International Edition, 2006, 45, 3471-3474.	13.8	111
7	Microsolvation of Formamide:Â A Rotational Study. Journal of the American Chemical Society, 2006, 128, 12111-12121.	13.7	108
8	The Shape of Neutral Valine. Angewandte Chemie - International Edition, 2004, 43, 605-610.	13.8	103
9	A laser-ablation molecular-beam Fourier-transform microwave spectrometer: The rotational spectrum of organic solids. Review of Scientific Instruments, 2003, 74, 4799-4804.	1.3	100
10	Ribose Found in the Gas Phase. Angewandte Chemie - International Edition, 2012, 51, 3119-3124.	13.8	97
11	Construction of a molecular beam Fourier transform microwave spectrometer used to study the 2,5-dihydrofuran-argon van der Waals complex. Chemical Physics, 1997, 218, 267-275.	1.9	93
12	Coded Amino Acids in Gas Phase:Â The Shape of Isoleucine. Journal of the American Chemical Society, 2005, 127, 12952-12956.	13.7	90
13	The Shape of Î²-Alanine. Journal of the American Chemical Society, 2006, 128, 3812-3817.	13.7	84
14	AUTOFIT, an automated fitting tool for broadband rotational spectra, and applications to 1-hexanal. Journal of Molecular Spectroscopy, 2015, 312, 13-21.	1.2	82
15	The Hydrogen Bond and Beyond: Perspectives for Rotational Investigations of Nonâ€Covalent Interactions. Chemistry - A European Journal, 2019, 25, 11402-11411.	3.3	82
16	The Shape of Leucine in the Gas Phase. ChemPhysChem, 2007, 8, 599-604.	2.1	76
17	Fourier Transform Microwave Spectrum and ab Initio Study of Dimethyl Methylphosphonate. Journal of Molecular Spectroscopy, 2002, 211, 110-118.	1.2	74
18	Free Fructose Is Conformationally Locked. Journal of the American Chemical Society, 2013, 135, 2845-2852.	13.7	71

#	Article	IF	Citations
19	Shape of 4(S)- and 4(R)-Hydroxyproline in Gas Phase. Journal of the American Chemical Society, 2005, 127, 2572-2579.	13.7	68
20	The interplay of hydrogen bonding and dispersion in phenol dimer and trimer: structures from broadband rotational spectroscopy. Physical Chemistry Chemical Physics, 2013, 15, 11468.	2.8	64
21	Rotational spectroscopy of iodobenzene and iodobenzeneâ€“neon with a direct digital 2â€“8GHz chirped-pulse Fourier transform microwave spectrometer. Journal of Molecular Spectroscopy, 2011, 269, 21-29.	1.2	58
22	Submillimeter-Wave Spectrum and Structure of Acrylonitrile. Journal of Molecular Spectroscopy, 1994, 167, 400-418.	1.2	55
23	Rotational Spectrum of 1,1-Difluoroethane: Internal Rotation Analysis and Structure. Journal of Molecular Spectroscopy, 1995, 171, 223-247.	1.2	54
24	Proton Tunneling in Heterodimers of Carboxylic Acids: A Rotational Study of the Benzoic Acidâ€“Formic Acid Bimolecule. Journal of Physical Chemistry Letters, 2012, 3, 3770-3775.	4.6	52
25	Rotational spectrum of jet-cooled HfO2 and HfO. Journal of Chemical Physics, 2002, 117, 9651-9662.	3.0	45
26	Six Pyranoside Forms of Free 2â€Deoxyâ€‹scp›D‹/scp›â€‹ribose. Angewandte Chemie - International Edition, 2013, 52, 11840-11845.	13.8	45
27	Conformational equilibria in vanillin and ethylvanillin. Physical Chemistry Chemical Physics, 2010, 12, 12486.	2.8	44
28	A molecular-beam Fourier transform microwave study of difluoromethane dimer. Journal of Molecular Structure, 2002, 612, 255-260.	3.6	43
29	A rotational study of laser ablated thiourea. Journal of Chemical Physics, 2004, 120, 6191-6196.	3.0	43
30	Weak hydrogen bonds Câ€“Hâ‹¯S and Câ€“Hâ‹¯Fâ€“C in the thiiraneâ€“trifluoromethane dimer. Chemical Physics Letters, 2005, 402, 4-10.	2.6	40
31	Exploring microsolvation of the anesthetic propofol. Physical Chemistry Chemical Physics, 2012, 14, 4398.	2.8	40
32	The Millimeter-Wave Spectra of 1-Chloro-1-fluoroethylene and cis-1-Chloro-2-fluoroethylene. Journal of Molecular Spectroscopy, 1993, 162, 4-19.	1.2	39
33	The Rotational Spectrum of Chlorofluoromethane. Journal of Molecular Spectroscopy, 1995, 174, 397-416.	1.2	38
34	Hydrogen Bond in Molecules with Large-Amplitude Motions: A Rotational Study of Trimethylene Sulfideâ‹…â‹…â‹…HCl. Angewandte Chemie - International Edition, 2001, 40, 935-938.	13.8	36
35	Jet-cooled rotational spectrum of laser-ablated 1,3,5-trithiane. Journal of Molecular Structure, 2002, 612, 125-131.	3.6	36
36	The centimeter and millimeter microwave spectra of butadiene sulfone and Î±,Î±â€²-D4 butadiene sulfone. Journal of Molecular Spectroscopy, 1991, 149, 317-328.	1.2	35

#	Article	IF	Citations
37	Unravelling Proteinâ€“DNA Interactions at Molecular Level: A DFT and NCI Study. Journal of Chemical Theory and Computation, 2016, 12, 523-534.	5.3	35
38	Probing the Cï£¿Hâ‹…â‹…â‹…Ï€ Weak Hydrogen Bond in Anesthetic Binding: The Sevofluraneâ€“Benzene Cluster. Angewandte Chemie - International Edition, 2014, 53, 3210-3213.	13.8	33
39	Simultaneous Analysis of Rovibrational and Rotational Spectra of thev5= 1 andv8= 1 Vibrational Levels of Propyne. Journal of Molecular Spectroscopy, 1996, 177, 124-133.	1.2	31
40	Gas-Phase Structure ofN,N-Dimethylglycine. ChemPhysChem, 2005, 6, 1559-1566.	2.1	31
41	Structural evidence of anomeric effects in the anesthetic isoflurane. Physical Chemistry Chemical Physics, 2011, 13, 6610.	2.8	31
42	Structural studies of biomolecules in the gas phase by chirped-pulse Fourier transform microwave spectroscopy. Faraday Discussions, 2011, 150, 227.	3.2	31
43	Shaping Micelles: The Interplay Between Hydrogen Bonds and Dispersive Interactions. Angewandte Chemie - International Edition, 2013, 52, 7772-7775.	13.8	31
44	Bifurcated CH2â‹…â‹…â‹…â‹…O and (Cï£¿H)2â‹…â‹…â‹…Fï£¿C Weak Hydrogen Bonds: The Oxirane-Difluoromethane Complex. ChemPhysChem, 2004, 5, 1779-1782.	2.1	30
45	The shape of neutral sarcosine in gas phase. Chemical Physics Letters, 2007, 435, 336-341.	2.6	30
46	Interplay of Phenol and Isopropyl Isomerism in Propofol from Broadband Chirped-Pulse Microwave Spectroscopy. Journal of the American Chemical Society, 2010, 132, 13417-13424.	13.7	30
47	The conformational landscape of the volatile anesthetic sevoflurane. Physical Chemistry Chemical Physics, 2010, 12, 9624.	2.8	30
48	Switching Hydrogen Bonding to Ï€-Stacking: The Thiophenol Dimer and Trimer. Journal of Physical Chemistry Letters, 2021, 12, 1367-1373.	4.6	29
49	The Internuclear Potential, Electronic Structure, and Chemical Bond of Tellurium Selenide. Angewandte Chemie - International Edition, 2005, 44, 6311-6315.	13.8	27
50	N-Methyl stereochemistry in tropinone: the conformational flexibility of the tropane motif. Physical Chemistry Chemical Physics, 2010, 12, 6076.	2.8	27
51	Sulfur Hydrogen Bonding in Isolated Monohydrates: Furfuryl Mercaptan versus Furfuryl Alcohol. Chemistry - A European Journal, 2018, 24, 6564-6571.	3.3	27
52	Semiexperimental Equilibrium Structures for the Equatorial Conformers of N-Methylpiperidone and Tropinone by the Mixed Estimation Method. Journal of Physical Chemistry A, 2012, 116, 8684-8692.	2.5	26
53	Six-fold-symmetry internal rotation in toluenes: the low barrier challenge of 2,6- and 3,5-difluorotoluene. Physical Chemistry Chemical Physics, 2015, 17, 26463-26470.	2.8	26
54	Conformations of Î±-Aminobutyric Acid in the Gas Phase. ChemPhysChem, 2006, 7, 1481-1487.	2.1	25

#	Article	IF	Citations
55	Mimicking anaestheticâ€“receptor interaction: a combined spectroscopic and computational study of propofolâ‹¯phenol. Physical Chemistry Chemical Physics, 2012, 14, 8956.	2.8	25
56	Weak Câ€“Hâ‹¯N and Câ€“Hâ‹¯F hydrogen bonds and internal rotation in pyridineâ€“CH₃F. Physical Chemistry Chemical Physics, 2014, 16, 2149-2153.	2.8	25
57	Chiral recognition and atropisomerism in the sevoflurane dimer. Physical Chemistry Chemical Physics, 2015, 17, 18282-18287.	2.8	25
58	Internal dynamics of cyclohexanol and the cyclohexanolâ€“water adduct. Physical Chemistry Chemical Physics, 2019, 21, 3676-3682.	2.8	25
59	Rotational spectrum of trifluoroacetone. Journal of Molecular Spectroscopy, 2010, 259, 65-69.	1.2	24
60	Rotational spectrum, H, F nuclear spinâ€“nuclear spin coupling and structure of the furanâ€“HF dimer. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 729-733.	1.7	22
61	The equilibrium molecular structures of 2-deoxyribose and fructose by the semiexperimental mixed estimation method and coupled-cluster computations. Physical Chemistry Chemical Physics, 2016, 18, 15555-15563.	2.8	22
62	The Rotational Spectrum and Nuclear Quadrupole Coupling of CH³⁵C1F₂. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1996, 51, 129-132.	1.5	21
63	Molecular recognition in the gas phase: benzocaineâ€“phenol as a model of anaestheticâ€“receptor interaction. Physical Chemistry Chemical Physics, 2009, 11, 11608.	2.8	21
64	Competition between weak hydrogen bonds: Câ€“Hâ‹¯Cl is preferred to Câ€“Hâ‹¯F in CH₂ClFâ€“H₂CO, as revealed by rotational spectroscopy. Physical Chemistry Chemical Physics, 2014, 16, 12261-12265.	2.8	21
65	Sulfur hydrogen bonding and internal dynamics in the monohydrates of thenyl mercaptan and thenyl alcohol. Physical Chemistry Chemical Physics, 2020, 22, 12412-12421.	2.8	21
66	The millimetre-wave spectrum of oxetane. Journal of Molecular Structure, 1995, 354, 237-243.	3.6	20
67	The Conformational Landscape of Nicotinoids: Solving the Conformational Disparity of Anabasine. Chemistry - A European Journal, 2010, 16, 10214-10219.	3.3	20
68	The microwave spectrum and ring-puckering vibration of 3-methyloxetane. Chemical Physics, 1990, 148, 21-31.	1.9	19
69	Furanosic forms of sugars: conformational equilibrium of methyl Î²-<scp>d</scp>-ribofuranoside. Chemical Communications, 2016, 52, 6241-6244.	4.1	19
70	Isomerism of the Aniline Trimer. Angewandte Chemie - International Edition, 2018, 57, 15112-15116.	13.8	19
71	New insights on the reaction mechanisms for CO oxidation on Au catalysts. Chemical Physics Letters, 2009, 468, 201-204.	2.6	18
72	A combined spectroscopic and theoretical study of propofolÂ·(H2O)3. Journal of Chemical Physics, 2012, 137, 074303.	3.0	18

#	Article	IF	Citations
73	A Spectroscopic Approach to the Solvation of Anesthetics in Jets: Propofol(H2O)n, n = 4â€“6. Journal of Physical Chemistry A, 2012, 116, 8934-8941.	2.5	18
74	Non-bonding interactions and internal dynamics in CH2F2â‹¯H2CO: a rotational and model calculations study. Physical Chemistry Chemical Physics, 2013, 15, 6714.	2.8	18
75	Axialâ€“equatorial isomerism and semiexperimental equilibrium structures of fluorocyclohexane. Physical Chemistry Chemical Physics, 2017, 19, 29162-29169.	2.8	18
76	The millimetre-wave spectrum of trimethylene sulphide Vibration-rotation coupling between thev=2 andv=3 ring-puckering excited states. Molecular Physics, 1994, 82, 283-302.	1.7	17
77	Conformational equilibrium of formanilide: detection of the pure rotational spectrum of the tunnellingcisconformer. Molecular Physics, 2005, 103, 1473-1479.	1.7	17
78	Accurate Semiexperimental Structure of 1,3,4-Oxadiazole by the Mixed Estimation Method. Journal of Physical Chemistry A, 2013, 117, 2278-2284.	2.5	17
79	Accurate Equilibrium Structures for Piperidine and Cyclohexane. Journal of Physical Chemistry A, 2015, 119, 1486-1493.	2.5	17
80	Pseudorotation in tetrahydrofuranâ‹¯HF heterodimer. Journal of Chemical Physics, 2000, 113, 2760-2767.	3.0	16
81	Axial and Equatorial Hydrogen Bonds: Jet-Cooled Rotational Spectrum of the Pentamethylene Sulfideâ‹…â‹…â‹…Hydrogen Fluoride Complex. Chemistry - A European Journal, 2002, 8, 1603-1613.	3.3	16
82	Investigation of the quadrupole coupling hyperfine structure due to two nuclei by molecular beam Fourier transform microwave spectroscopy: spectra of dichlorofluoromethane and pyridazine. Journal of Molecular Structure, 2002, 612, 287-303.	3.6	16
83	Formation of water polyhedrons in propofolâ€“water clusters. Physical Chemistry Chemical Physics, 2013, 15, 568-575.	2.8	16
84	Interactions between freons and aromatic molecules: The rotational spectrum of pyridineâ€“difluoromethane. Chemical Physics Letters, 2014, 591, 216-219.	2.6	16
85	Interactions between alkanes and aromatic molecules: a rotational study of pyridineâ€“methane. Physical Chemistry Chemical Physics, 2014, 16, 13041-13046.	2.8	16
86	A butterfly motion of formic acid and cyclobutanone in the 1â€‰:â€‰1 hydrogen bonded molecular cluster. Physical Chemistry Chemical Physics, 2017, 19, 204-209.	2.8	16
87	Semiexperimental and mass-dependent structures by the mixed regression method: Accurate equilibrium structure and failure of the Kraitchman method for ethynylcyclohexane. Journal of Chemical Physics, 2018, 148, 064306.	3.0	16
88	The low internal rotation barriers of halogenated toluenes: Rotational spectrum of 2,4-difluorotoluene. Journal of Molecular Spectroscopy, 2018, 344, 21-26.	1.2	16
89	Rotational Spectrum, Molecular Constants, and Dipole Moment of theSynForm of Vinylphosphine. Journal of Molecular Spectroscopy, 1996, 176, 180-184.	1.2	15
90	Rotational spectrum, internal rotation barrier andabinitiocalculations on 1â€chloroâ€1â€fluoroethane. Journal of Chemical Physics, 1996, 104, 9729-9734.	3.0	15

#	Article	IF	Citations
91	Internal rotation in halogenated toluenes: Rotational spectrum of 2,5-difluorotoluene. Journal of Molecular Spectroscopy, 2017, 337, 46-50.	1.2	15
92	Molecular systems with nearly-free internal rotation and nuclear quadrupole coupling: Meta-chlorotoluene. Journal of Molecular Spectroscopy, 2019, 361, 1-7.	1.2	15
93	The centimeter and millimeter microwave spectrum of cyclobutanone. Journal of Molecular Spectroscopy, 1992, 156, 341-359.	1.2	14
94	Rotational Spectra of cis and trans Crotononitriles: Centrifugal Distortion, Hyperfine Structure, Internal Rotation and Structure. Journal of Molecular Spectroscopy, 1995, 172, 520-535.	1.2	14
95	Fermi Resonance and Coriolis Coupling between Î½25and 2Î½26in CH235ClF. Journal of Molecular Spectroscopy, 1996, 175, 267-276.	1.2	14
96	Fourier transform microwave study on 2-methyloxetane and 3-methyloxetane. Chemical Physics, 1996, 208, 391-401.	1.9	14
97	Tunnelling Motion of HF Between the Two Oxygen Lone Pairs in the Dimethyl Etherâ€“Hydrogen Fluoride Complex: A Pure Rotational Study. ChemPhysChem, 2004, 5, 336-341.	2.1	14
98	Competing hydrogen bonding in methoxyphenols: The rotational spectrum of o-vanillin. Journal of Molecular Spectroscopy, 2011, 267, 112-117.	1.2	14
99	Water Encapsulation by Nanomicelles. Angewandte Chemie - International Edition, 2014, 53, 12480-12483.	13.8	14
100	Internal Dynamics in Halogenâ€Bonded Adducts: A Rotational Study of Chlorotrifluoromethaneâ€“Formaldehyde. Chemistry - A European Journal, 2015, 21, 4148-4152.	3.3	14
101	Internal rotation in halogenated toluenes: Rotational spectrum of 2,3-difluorotoluene. Journal of Molecular Spectroscopy, 2018, 349, 37-42.	1.2	14
102	The Six Isomers of the Cyclohexanol Dimer: A Delicate Test for Dispersion Models. Angewandte Chemie - International Edition, 2020, 59, 14081-14085.	13.8	14
103	The microwave spectrum of 2(5H)-thiophenone. Journal of Molecular Structure, 1992, 273, 123-131.	3.6	13
104	Conformational behaviour, hydrogen bond competition and intramolecular dynamics in vanillin derivatives: acetovanillone and 6-hydroxy-3-methoxyacetophenone. Physical Chemistry Chemical Physics, 2011, 13, 13310.	2.8	13
105	THE CM-, MM-, AND SUB-MM-WAVE SPECTRUM OF ALLYL ISOCYANIDE AND RADIOASTRONOMICAL OBSERVATIONS IN ORION KL AND THE SgrB2 LINE SURVEYS. Astrophysical Journal, 2013, 777, 120.	4.5	13
106	How flexible is the disulfide linker? A combined rotationalâ€“computational investigation of diallyl disulfide. Physical Chemistry Chemical Physics, 2019, 21, 19732-19736.	2.8	13
107	An Efficient Microkinetic Modeling Protocol: Start with Only the Dominant Mechanisms, Adjust All Parameters, and Build the Complete Model Incrementally. ACS Catalysis, 2019, 9, 4804-4809.	11.2	13
108	The Sâˆ’S Bridge: A Mixed Experimentalâ€Computational Estimation of the Equilibrium Structure of Diphenyl Disulfide. ChemPhysChem, 2019, 20, 366-373.	2.1	13

#	Article	IF	Citations
109	Rovibronic signatures of molecular aggregation in the gas phase: subtle homochirality trends in the dimer, trimer and tetramer of benzyl alcohol. Physical Chemistry Chemical Physics, 2021, 23, 23610-23624.	2.8	13
110	Vibration-rotation interactions and ring-puckering in 3,3-dimethyl oxetane by microwave spectroscopy. Journal of Molecular Spectroscopy, 1990, 141, 231-242.	1.2	12
111	The Millimeter-Wave Spectrum of cis-1,2-Dichloroethylene. Journal of Molecular Spectroscopy, 1994, 165, 368-376.	1.2	12
112	Internal dynamics in azetidine: A microwave and ab initio study. Journal of Chemical Physics, 2001, 114, 2237-2250.	3.0	12
113	Line assignments and global analysis of the tunnelingâ€“rotational microwave absorption spectrum of dimethyl methylphosphonate. Journal of Molecular Spectroscopy, 2003, 218, 114-126.	1.2	12
114	Free internal rotation in CH3â€“CCâ€“CF3. Chemical Physics Letters, 2004, 397, 379-381.	2.6	12
115	Structure and properties of the (HCl)2H2O cluster observed by chirped-pulse Fourier transform microwave spectroscopy. Physical Chemistry Chemical Physics, 2011, 13, 13912.	2.8	12
116	Discriminating the structure ofexo-2-aminonorbornane using nuclear quadrupole coupling interactions. Journal of Chemical Physics, 2011, 134, 164311.	3.0	12
117	Pseudorotational Landscape of Sevenâ€Membered Rings: The Most Stable Chair and Twistâ€Boat Conformers of Îµâ€Caprolactone. Chemistry - A European Journal, 2014, 20, 14084-14089.	3.3	12
118	A DFT-Based Computational-Experimental Methodology for Synthetic Chemistry: Example of Application to the Catalytic Opening of Epoxides by Titanocene. Journal of Organic Chemistry, 2017, 82, 3760-3766.	3.2	12
119	Stepwise Nucleation of Aniline: Emergence of Spectroscopic Fingerprints of the Liquid Phase. Chemistry - A European Journal, 2018, 24, 10291-10295.	3.3	12
120	Rotational spectrum, ring-puckering vibration and ab initio calculations on 1,1-difluorocyclobutane. Journal of Chemical Physics, 1999, 111, 6375-6384.	3.0	11
121	Conformation and Stability of the Hydrogen-Bonded Complex 6-Oxabicyclo[3.1.0]hexaneâ‹…â‹…â‹…HCl. Chemistry - A European Journal, 2000, 6, 3345-3350.	3.3	11
122	HF inversion in the 2,5-dihydrofuranâ‹¯HF complex. Journal of Chemical Physics, 2001, 114, 9421-9429.	3.0	11
123	Molecular beam pulsed-discharge Fourier transform microwave spectra of CH3â€“C˜†Câ€“F, CH3â€“(C˜†C)2â€“F, and CH3â€“(C˜†C)3â€“F. Chemical Physics Letters, 2003, 375, 355-363.	2.6	11
124	Combined Experimental and Theoretical Study of the Benzocaine/Ar van der Waals System in Supersonic Expansions. Journal of Physical Chemistry A, 2009, 113, 982-988.	2.5	11
125	How Trifluoroacetone Interacts with Water. Journal of Physical Chemistry A, 2011, 115, 9493-9497.	2.5	11
126	Unraveling the Benzocaineâ€“Receptor Interaction at Molecular Level Using Mass-Resolved Spectroscopy. Journal of Physical Chemistry B, 2013, 117, 13472-13480.	2.6	11

#	Article	IF	Citations
127	Molecular Recognition, Transient Chirality and Sulfur Hydrogen Bonding in the Benzyl Mercaptan Dimer. Symmetry, 2021, 13, 2022.	2.2	11
128	Rotational spectrum and structure of the oxetaneâ€“argon Van der Waals complex. Chemical Physics Letters, 1998, 286, 272-276.	2.6	10
129	Detection of SiCCO in the Laboratory. Astrophysical Journal, 2005, 621, L157-L159.	4.5	10
130	Static and Dynamic Properties of 1,1â€²â€Bi2â€naphthol and Its Conjugated Acids and Bases. Chemistry - A European Journal, 2014, 20, 14816-14825.	3.3	10
131	Intermolecular Hydrogen Bonding in 2-Fluoropyridine-Water. ChemistrySelect, 2016, 1, 1273-1277.	1.5	10
132	Rotational spectrum, internal rotation barrier and structure of 3,3,3-trifluoropropene. Molecular Physics, 1997, 91, 731-750.	1.7	10
133	The hydrogen-bonded heterodimer between methylene cyclobutane and hydrogen chloride: Observation of an endo conformer. Journal of Chemical Physics, 2002, 116, 4116-4123.	3.0	9
134	Intermolecular hydrogen bond in molecules with large amplitude motions: rotational spectrum of the complex 3,3-dimethyloxetaneâ‹¯hydrogen fluoride. Physical Chemistry Chemical Physics, 2005, 7, 1157-1163.	2.8	9
135	The pure rotational spectrum of TeSe: Rotational parameters, Bornâ€“Oppenheimer breakdown corrections, and hyperfine constants. Journal of Molecular Structure, 2006, 795, 163-172.	3.6	9
136	Semiexperimental Equilibrium Structure for the C₆ Backbone of cis-1,3,5-Hexatriene; Structural Evidence for Greater Ï€-Electron Delocalization with Increasing Chain Length in Polyenes. Journal of Physical Chemistry A, 2009, 113, 1864-1868.	2.5	9
137	Mimicking anestheticâ€“receptor interactions in jets: the propofolâ€“isopropanol cluster. Physical Chemistry Chemical Physics, 2014, 16, 16968.	2.8	9
138	Conformational Behavior of <scp>d</scp>-Lyxose in Gas and Solution Phases by Rotational and NMR Spectroscopies. Journal of Physical Chemistry Letters, 2019, 10, 3339-3345.	4.6	9
139	Internal rotation and chlorine nuclear quadrupole coupling in 2-chloro-4-fluorotoluene explored by microwave spectroscopy and quantum chemistry. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 247, 119120.	3.9	9
140	The rotational spectrum of fluorotetraacetylene produced by electric discharge. Journal of Molecular Spectroscopy, 2004, 227, 202-205.	1.2	8
141	Rotational spectroscopy of antipyretics: Conformation, structure, and internal dynamics of phenazone. Journal of Chemical Physics, 2013, 138, 114304.	3.0	8
142	Magic Numbers in the Solvation of the Propofol Dimer. ChemPhysChem, 2013, 14, 1558-1562.	2.1	8
143	Oï£¿Hâ‹…â‹…â‹…N and Cï£¿Hâ‹…â‹…â‹…O Hydrogen Bonds Control Hydration of Pivotal Tropane Alkaloids: Tropinoneâ‹…â‹…â‹…H₂O Complex. ChemPhysChem, 2014, 15, 918-923.	2.1	8
144	Potential energy surface of fluoroxene: experiment and theory. Physical Chemistry Chemical Physics, 2016, 18, 3966-3974.	2.8	8

#	Article	IF	Citations
145	Halogen bond and internal dynamics in the Ïƒâ€“complex of pyridine-chlorotrifluoromethane: A rotational study. Journal of Molecular Spectroscopy, 2020, 371, 111323.	1.2	8
146	Rotational spectrum and intramolecular hydrogen bonding in 1,2-butanedithiol. Journal of Molecular Structure, 2020, 1211, 128080.	3.6	8
147	Interaction topologies of the Sâ‹¯O chalcogen bond: the conformational equilibrium of the cyclohexanolâ‹¯SO‹sub›2‹/sub› cluster. Physical Chemistry Chemical Physics, 2021, 23, 10799-10806.	2.8	8
148	The microwave spectrum of pentafluoroethane. Journal of Molecular Structure, 2001, 599, 219-223.	3.6	7
149	On the Trimerization of Cyanoacetylene: Mechanism of Formation of Tricyanobenzene Isomers and Laboratory Detection of Their Radio Spectra. Chemistry - A European Journal, 2010, 16, 14115-14123.	3.3	7
150	Rotational Spectra of Bicyclic Decanes: The Trans Conformation of (â^')-Lupinine. Journal of Physical Chemistry A, 2013, 117, 13673-13679.	2.5	7
151	The Distorted Tropane of Scopoline. ChemPhysChem, 2013, 14, 1830-1835.	2.1	7
152	How Water Interacts with Halogenated Anesthetics: The Rotational Spectrum of Isofluraneâ€“Water. Chemistry - A European Journal, 2014, 20, 1980-1984.	3.3	7
153	‹i›N‹/i›â€Methyl Inversion and Accurate Equilibrium Structures in Alkaloids: Pseudopelletierine. Chemistry - A European Journal, 2017, 23, 16491-16496.	3.3	7
154	Rotational spectra, nuclear quadrupole hyperfine tensors, and conformational structures of the mustard gas simulent 2-chloroethyl ethyl sulfide. Journal of Molecular Spectroscopy, 2005, 233, 180-188.	1.2	6
155	Single Hydration of the Peptide Bond: The Case of the Vince Lactam. Journal of Physical Chemistry A, 2012, 116, 10099-10106.	2.5	6
156	Structural Studies of Nicotinoids: Cotinine versus Nicotine. Chemistry - A European Journal, 2017, 23, 7238-7244.	3.3	6
157	Isomerism of the Aniline Trimer. Angewandte Chemie, 2018, 130, 15332-15336.	2.0	6
158	Rotational Spectrum, Tunneling Motions, and Intramolecular Potential Barriers in Benzyl Mercaptan. Journal of Physical Chemistry A, 2019, 123, 8435-8440.	2.5	6
159	Rotational Spectra of Fluorodiacetylene and Fluorotriacetylene Produced by Electrical Discharge. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2002, 57, 76-78.	1.5	5
160	Scopine Isolated in the Gas Phase. ChemPhysChem, 2016, 17, 3030-3034.	2.1	5
161	Structural Studies of Nicotinoids: Cotinine versus Nicotine. Chemistry - A European Journal, 2017, 23, 7156-7156.	3.3	5
162	How accurate is the determination of equilibrium structures for van der Waals complexes? The dimer N2Oâ‹¯CO as an example. Journal of Chemical Physics, 2021, 154, 194302.	3.0	5

#	Article	IF	Citations
163	The rotational spectrum of the 3,3-dimethyloxetaneâ¯hydrogen chloride complex. Chemical Physics Letters, 2005, 401, 259-265.	2.6	4
164	N-Methyl Inversion and Structure of Six-Membered Heterocyclic Rings: Rotational Spectrum of 1-Methyl-4-piperidone. Journal of Physical Chemistry A, 2011, 115, 9545-9551.	2.5	4
165	Molecular hydration of propofol dimers in supersonic expansions: formation of active centre-like structures. Physical Chemistry Chemical Physics, 2014, 16, 23301-23307.	2.8	4
166	The Conformational Map of Volatile Anesthetics: Enflurane Revisited. Chemistry - A European Journal, 2016, 22, 9804-9811.	3.3	4
167	Rotational spectra of tetracyclic quinolizidine alkaloids: does a water molecule flip sparteine?. Physical Chemistry Chemical Physics, 2017, 19, 17553-17559.	2.8	4
168	Torsional chirality and molecular recognition: the homo and heterochiral dimers of thenyl and furfuryl alcohol. Physical Chemistry Chemical Physics, 2022, 24, 8999-9006.	2.8	4
169	Conformation of chiral molecules: The rotational spectrum of 2-chloropropionic acid. Chemical Physics Letters, 2009, 468, 18-22.	2.6	3
170	Transition from Planar to Nonplanar Hydrogen Bond Networks in the Solvation of Aromatic Dimers: Propofol2-(H2O)2â€“4. Journal of Physical Chemistry A, 2013, 117, 3396-3404.	2.5	3
171	Conformational Flexibility of Mephenesin. Journal of Physical Chemistry B, 2014, 118, 5357-5364.	2.6	3
172	Inversion of Bicyclic Decanes: Rotational Spectra of the Trans and Double Cis Conformations of 2â€Decalone. ChemPhysChem, 2017, 18, 3620-3624.	2.1	3
173	Conformational impact of aliphatic side chains in local anaesthetics: benzocaine, butamben and isobutamben. Chemical Communications, 2020, 56, 6094-6097.	4.1	3
174	Hydrogen Bonding in the Dimer and Monohydrate of 2-Adamantanol: A Test Case for Dispersion-Corrected Density Functional Methods. Molecules, 2022, 27, 2584.	3.8	3
175	The First Stages of Nanomicelle Formation Captured in the Sevoflurane Trimer. Journal of Physical Chemistry Letters, 2022, 13, 3770-3775.	4.6	3
176	Structural Distortion of the Epoxy Groups in Norbornanes: A Rotational Study of exoâ€2,3â€Epoxynorbornane. ChemPhysChem, 2015, 16, 2609-2614.	2.1	2
177	N -Methyl Inversion and Accurate Equilibrium Structures in Alkaloids: Pseudopelletierine. Chemistry - A European Journal, 2017, 23, 16412-16412.	3.3	2
178	Exploring Epigenetic Marks by Analysis of Noncovalent Interactions. ChemBioChem, 2021, 22, 408-415.	2.6	2
179	Water binding to the atmospheric oxidation product methyl vinyl ketone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 270, 120846.	3.9	2
180	Spectroscopy and inter/intramolecular dynamics in Honor of Walther Caminati. Journal of Molecular Spectroscopy, 2017, 337, 1-2.	1.2	1

#	Article	IF	Citations
181	Frontispiece: The Hydrogen Bond and Beyond: Perspectives for Rotational Investigations of Nonâ€Covalent Interactions. Chemistry - A European Journal, 2019, 25, .	3.3	1
182	Chirality, structure and hydrogen bonding in dithiols: Rotational spectrum of the chiral and meso 2,3-butanedithiol. Journal of Molecular Structure, 2021, 1246, 131221.	3.6	1
183	Rotational spectrum, internal rotation barrier and structure of 3,3,3-trifluoropropene. Molecular Physics, 1997, 91, 731-750.	1.7	1
184	Chirality-Puckering correlation and intermolecular interactions in Sphingosines: Rotational spectroscopy of jaspine B3 and its monohydrate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 267, 120531.	3.9	1
185	Rotational spectroscopy of the large saturated dinitriles hexanedinitrile and heptanedinitrile. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 270, 120844.	3.9	1
186	Call for papers for special issue of Journal of Molecular Spectroscopy focusing on â€Spectroscopy and Inter/Intramolecular Dynamics in Honor of Walther Caminatiâ€. Journal of Molecular Spectroscopy, 2016, 330, 248.	1.2	0
187	Spectroscopy and inter/intramolecular dynamics in honor of Walther Caminati. Journal of Molecular Spectroscopy, 2017, 335, 1-2.	1.2	0
188	Frontispiece: Stepwise Nucleation of Aniline: Emergence of Spectroscopic Fingerprints of the Liquid Phase. Chemistry - A European Journal, 2018, 24, .	3.3	0
189	Evaluation of the aggregation process in a mixture of propofol and benzocaine. Physical Chemistry Chemical Physics, 2019, 21, 3537-3544.	2.8	0
190	Rotational spectroscopy of organophosphorous chemical agents: cresyl and phenyl saligenin phosphates. Physical Chemistry Chemical Physics, 2019, 21, 16418-16422.	2.8	0
191	Noncovalent interactions in isolated molecular aggregates: From single molecules to nanostructures. , 2021, , 143-188.		0
192	Molecular Rotation Spectrum of Tetracyclic Quinolizidines: Observation of trans-Matrine and the Elusive cis-Matrine. Journal of Organic Chemistry, 2021, 86, 1861-1867.	3.2	0
193	The Six Isomers of the Cyclohexanol Dimer: A Delicate Test for Dispersion Models. Angewandte Chemie, 2020, 132, 14185-14189.	2.0	0
194	Hydrogen Bond in Molecules with Large-Amplitude Motions: A Rotational Study of Trimethylene Sulfideâ‹…â‹…â‹…HCl. Angewandte Chemie - International Edition, 2001, 40, 935-938.	13.8	0