Emilio J Cocinero

List of Publications by Year
in descending order

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171	4,918	94381	138417
papers	citations	37 h-index	58 g-index

190	190	190	3013
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The C-Fâ‹…â‹…â‹…H-C â€œAnti-Hydrogen Bondâ€•in the Gas Phase: Microwave Structure of the Difluoromethane Dimer. Angewandte Chemie - International Edition, 1999, 38, 2924-2925.	7.2	165
2	Observation of the rotational spectra of van der Waals complexes by free jet absorption millimeter wave spectroscopy: pyridine-argon. Chemical Physics Letters, 1996, 261, 267-271.	1.2	146
3	Sensing the anomeric effect in a solvent-free environment. Nature, 2011, 469, 76-79.	13.7	138
4	The Structure of Neutral Proline. Angewandte Chemie - International Edition, 2002, 41, 4673-4676.	7.2	134
5	The Building Blocks of Cellulose: The Intrinsic Conformational Structures of Cellobiose, Its Epimer, Lactose, and Their Singly Hydrated Complexes. Journal of the American Chemical Society, 2009, 131, 11117-11123.	6.6	122
6	The Glycineâ€“Water Complex. Angewandte Chemie - International Edition, 2006, 45, 3471-3474.	7.2	111
7	The Shape of Neutral Valine. Angewandte Chemie - International Edition, 2004, 43, 605-610.	7.2	103
8	Ribose Found in the Gas Phase. Angewandte Chemie - International Edition, 2012, 51, 3119-3124.	7.2	97
9	The Hydrogen Bond between Water and Aromatic Bases of Biological Interest:Â An Experimental and Theoretical Study of the 1:1 Complex of Pyrimidine with Water. Journal of the American Chemical Society, 1998, 120, 11504-11509.	6.6	92
10	The Câˆ’FÂ·Â·Â·Hâˆ’O Hydrogen Bond in the Gas Phase. Rotational Spectrum and ab Initio Calculations of Difluoromethane-Water. Journal of the American Chemical Society, 1999, 121, 10098-10101.	6.6	90
11	Coded Amino Acids in Gas Phase:Â The Shape of Isoleucine. Journal of the American Chemical Society, 2005, 127, 12952-12956.	6.6	90
12	High-Resolution Spectroscopic Studies of Complexes Formed by Medium-Size Organic Molecules. Chemical Reviews, 2016, 116, 5014-5037.	23.0	80
13	Relative Strengths of the Oï£¿Hâ‹…â‹…â‹…Cl and Oï£¿Hâ‹…â‹…â‹…F Hydrogen Bonds. Angewandte Chemie - International Edition, 2006, 45, 2438-2442.	7.2	76
14	The Shape of Leucine in the Gas Phase. ChemPhysChem, 2007, 8, 599-604.	1.0	76
15	Free Fructose Is Conformationally Locked. Journal of the American Chemical Society, 2013, 135, 2845-2852.	6.6	71
16	Shape of 4(S)- and 4(R)-Hydroxyproline in Gas Phase. Journal of the American Chemical Society, 2005, 127, 2572-2579.	6.6	68
17	Intermolecular Hydrogen Bonding between Water and Pyrazine. Angewandte Chemie - International Edition, 1998, 37, 792-795.	7.2	66
18	Toward the RNA-World in the Interstellar Mediumâ€”Detection of Urea and Search of 2-Amino-oxazole and Simple Sugars. Astrobiology, 2020, 20, 1048-1066.	1.5	65

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19	â€œUnion is strengthâ€: how weak hydrogen bonds become stronger. Physical Chemistry Chemical Physics, 2011, 13, 13901.	1.3	62
20	The Halogen Bond and Internal Dynamics in the Molecular Complex of CF₃Cl and H₂O. Angewandte Chemie - International Edition, 2011, 50, 7807-7810.	7.2	57
21	Degradation Mechanism and Relative Stability of Methylammonium Halide Based Perovskites Analyzed on the Basis of Acidâ€“Base Theory. ACS Applied Materials & Interfaces, 2019, 11, 12586-12593.	4.0	55
22	High conductance values in Ï€-folded molecular junctions. Nature Communications, 2017, 8, 15195.	5.8	54
23	Pseudorotation pathway and equilibrium structure from the rotational spectrum of jet-cooled tetrahydrofuran. Journal of Chemical Physics, 1999, 111, 7871-7880.	1.2	53
24	Free jet absorption millimeter wave spectrum of the pyrimidineâ€”argon molecular complex. Chemical Physics Letters, 1997, 268, 393-400.	1.2	52
25	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.	2.1	52
26	Shapes and Noncovalent Interactions of Oligomers:Â The Rotational Spectrum of the Difluoromethane Trimer. Journal of the American Chemical Society, 2007, 129, 2700-2703.	6.6	51
27	Carbohydrateâ€“aromatic interactions: A computational and IR spectroscopic investigation of the complex, methyl Î±-l-fucopyranosideÂ·toluene, isolated in the gas phase. Chemical Physics Letters, 2009, 471, 17-21.	1.2	51
28	Conformational Choice and Selectivity in Singly and Multiply Hydrated Monosaccharides in the Gas Phase. Chemistry - A European Journal, 2008, 14, 8947-8955.	1.7	47
29	Conformational change and selectivity in explicitly hydrated carbohydrates. Tetrahedron: Asymmetry, 2009, 20, 718-722.	1.8	46
30	Six Pyranoside Forms of Free 2â€Deoxyâ€<scp>D</scp>â€ribose. Angewandte Chemie - International Edition, 2013, 52, 11840-11845.	7.2	45
31	Conformational equilibria in vanillin and ethylvanillin. Physical Chemistry Chemical Physics, 2010, 12, 12486.	1.3	44
32	Weak hydrogen bonds Câ€“Hâ‹¯S and Câ€“Hâ‹¯Fâ€“C in the thiiraneâ€“trifluoromethane dimer. Chemical Physics Letters, 2005, 402, 4-10.	1.2	40
33	Exploring microsolvation of the anesthetic propofol. Physical Chemistry Chemical Physics, 2012, 14, 4398.	1.3	40
34	Microwave spectroscopy of hydroquinone: The rotational spectrum of the cis conformer. Journal of Chemical Physics, 1994, 100, 8569-8572.	1.2	39
35	Solvent Interactions and Conformational Choice in a Core N-Glycan Segment: Gas Phase Conformation of the Central, Branching Trimannose Unit and its Singly Hydrated Complex. Journal of the American Chemical Society, 2008, 130, 10691-10696.	6.6	39
36	Hydration of Sugars in the Gas Phase: Regioselectivity and Conformational Choice in Nâ€Acetyl Glucosamine and Glucose. Chemistry - A European Journal, 2009, 15, 13427-13434.	1.7	38

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37	On the Clâ‹¯C halogen bond: a rotational study of CF₃Clâ€“CO. Physical Chemistry Chemical Physics, 2016, 18, 17851-17855.	1.3	38
38	Conformation and Stability of Etherâ‹¯Water Adducts:â€‰ Free Jet Absorption Millimeter Wave Spectrum of 1,4-Dioxaneâ‹¯Water. Journal of the American Chemical Society, 1998, 120, 5555-5558.	6.6	37
39	Gas-Phase Tautomeric Equilibrium of 4-Hydroxypyrimidine with Its Ketonic Forms:Â A Free Jet Millimeterwave Spectroscopy Study. Journal of the American Chemical Society, 2007, 129, 6287-6290.	6.6	37
40	â€˜Nakedâ€™ and Hydrated Conformers of the Conserved Core Pentasaccharide of N-linked Glycoproteins and Its Building Blocks. Journal of the American Chemical Society, 2013, 135, 16895-16903.	6.6	37
41	Probing the Lone PairÂ·Â·Â·Ï€-Hole Interaction in Perfluorinated Heteroaromatic Rings: The Rotational Spectrum of PentafluoropyridineÂ·Water. Journal of Physical Chemistry Letters, 2016, 7, 1513-1517.	2.1	36
42	Exploring Carbohydrateâ‹¯Peptide Interactions in the Gas Phase: Structure and Selectivity in Complexes of Pyranosides with N-Acetylphenylalanine Methylamide. Journal of the American Chemical Society, 2011, 133, 4548-4557.	6.6	35
43	Unravelling Proteinâ€“DNA Interactions at Molecular Level: A DFT and NCI Study. Journal of Chemical Theory and Computation, 2016, 12, 523-534.	2.3	35
44	Features of the Cï£¿Hâ‹…â‹…â‹…N Weak Hydrogen Bond and Internal Dynamics in Pyridineâ€“CHF₃. Chemistry - A European Journal, 2010, 16, 1761-1764.	1.7	34
45	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.	7.2	33
46	Water Sculpts the Distinctive Shapes and Dynamics of the Tumor-Associated Carbohydrate Tn Antigens: Implications for Their Molecular Recognition. Journal of the American Chemical Society, 2018, 140, 9952-9960.	6.6	33
47	Gas-Phase Structure ofN,N-Dimethylglycine. ChemPhysChem, 2005, 6, 1559-1566.	1.0	31
48	Shaping Micelles: The Interplay Between Hydrogen Bonds and Dispersive Interactions. Angewandte Chemie - International Edition, 2013, 52, 7772-7775.	7.2	31
49	Conformational equilibrium in resorcinol by means of the free-jet absorption millimeter wave spectrum. Chemical Physics Letters, 1996, 256, 513-517.	1.2	30
50	The shape of neutral sarcosine in gas phase. Chemical Physics Letters, 2007, 435, 336-341.	1.2	30
51	Peptide Secondary Structures in the Gas Phase: Consensus Motif of N-Linked Glycoproteins. Journal of the American Chemical Society, 2009, 131, 1282-1287.	6.6	30
52	Carbohydrate hydration: heavy water complexes of Î± and Î² anomers of glucose, galactose, fucose and xylose. Physical Chemistry Chemical Physics, 2011, 13, 18671.	1.3	29
53	CHÂ·Â·Â·O and CHÂ·Â·Â·F Links Form the Cage Structure of Dioxaneâ‹¯Trifluoromethane. Journal of Physical Chemistry A, 2005, 109, 7402-7404.	1.1	28
54	The Internuclear Potential, Electronic Structure, and Chemical Bond of Tellurium Selenide. Angewandte Chemie - International Edition, 2005, 44, 6311-6315.	7.2	27

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55	Rotational and Core Level Spectroscopies As Complementary Techniques in Tautomeric/Conformational Studies: The Case of 2-Mercaptopyridine. Journal of the American Chemical Society, 2010, 132, 10269-10271.	6.6	27
56	N-Methyl stereochemistry in tropinone: the conformational flexibility of the tropane motif. Physical Chemistry Chemical Physics, 2010, 12, 6076.	1.3	27
57	Isotopic Hydration of Cellobiose: Vibrational Spectroscopy and Dynamical Simulations. Journal of Physical Chemistry A, 2011, 115, 9498-9509.	1.1	27
58	Ketoâ€“Enol Tautomerism and Conformational Landscape of 1,3-Cyclohexanedione from Its Free Jet Millimeter-Wave Absorption Spectrum. Journal of Physical Chemistry A, 2013, 117, 13712-13718.	1.1	27
59	Water-ketones hydrogen bonding: The rotational spectrum of cyclobutanone-water. Journal of Chemical Physics, 2005, 123, 164304.	1.2	26
60	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.	1.1	26
61	How CO₂ Interacts with Carboxylic Acids: A Rotational Study of Formic Acidâ€“CO₂. ChemPhysChem, 2015, 16, 2961-2967.	1.0	26
62	The Fourier transform rotational spectrum of difluoromethaneâ€“water: internal motion of water. Journal of Molecular Structure, 2005, 742, 87-90.	1.8	25
63	Conformations of Î±-Aminobutyric Acid in the Gas Phase. ChemPhysChem, 2006, 7, 1481-1487.	1.0	25
64	The free jet microwave spectrum of 2-phenylethylamineâ€“water. Physical Chemistry Chemical Physics, 2010, 12, 10210.	1.3	25
65	Mimicking anaestheticâ€“receptor interaction: a combined spectroscopic and computational study of propofolâ‹¯phenol. Physical Chemistry Chemical Physics, 2012, 14, 8956.	1.3	25
66	Carbohydrateâ€“Aromatic Interactions: Vibrational Spectroscopy and Structural Assignment of Isolated Monosaccharide Complexes with p-Hydroxy Toluene and N-Acetyl l-Tyrosine Methylamide. Journal of Physical Chemistry B, 2013, 117, 8135-8142.	1.2	25
67	Weak Câ€“Hâ‹¯N and Câ€“Hâ‹¯F hydrogen bonds and internal rotation in pyridineâ€“CH₃F. Physical Chemistry Chemical Physics, 2014, 16, 2149-2153.	1.3	25
68	Halogenâ€“Halogen Links and Internal Dynamics in Adducts of Freons. Journal of Physical Chemistry Letters, 2014, 5, 1591-1595.	2.1	25
69	Chiral recognition and atropisomerism in the sevoflurane dimer. Physical Chemistry Chemical Physics, 2015, 17, 18282-18287.	1.3	25
70	N lone-pairâ‹¯Ï€ interaction: a rotational study of chlorotrifluoroethyleneâ‹¯ammonia. Physical Chemistry Chemical Physics, 2015, 17, 7694-7698.	1.3	24
71	Millimeter Wave Spectrum of the Weakly Bound Complex CH₂â€¢CHCNÂ·H₂O: Structure, Dynamics, and Implications for Astronomical Search. Journal of Physical Chemistry A, 2015, 119, 11674-11682.	1.1	23
72	Modeling the tyrosineâ€“sugar interactions in supersonic expansions: glucopyranoseâ€“phenol clusters. Physical Chemistry Chemical Physics, 2016, 18, 12457-12465.	1.3	23

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73	Adducts of NH₃ with the Conformers of Glycidol: A Rotational Spectroscopy Study. Angewandte Chemie - International Edition, 2009, 48, 1102-1105.	7.2	22
74	Binding energies of micro-hydrated carbohydrates: measurements and interpretation. Chemical Science, 2013, 4, 1830.	3.7	22
75	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.	1.3	22
76	Molecular recognition in the gas phase: benzocaineâ€“phenol as a model of anaestheticâ€“receptor interaction. Physical Chemistry Chemical Physics, 2009, 11, 11608.	1.3	21
77	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.	1.3	21
78	A rotational study of the molecular complex tert-butanolÂ·Â·Â·NH3. Chemical Physics Letters, 2008, 463, 330-333.	1.2	20
79	The Conformational Landscape of Nicotinoids: Solving the Conformational Disparity of Anabasine. Chemistry - A European Journal, 2010, 16, 10214-10219.	1.7	20
80	Carbohydrates. Topics in Current Chemistry, 2014, 364, 299-333.	4.0	19
81	Furanosic forms of sugars: conformational equilibrium of methyl Î²-<scp>d</scp>-ribofuranoside. Chemical Communications, 2016, 52, 6241-6244.	2.2	19
82	A General Treatment to Study Molecular Complexes Stabilized by Hydrogenâ€, Halogenâ€, and Carbonâ€Bond Networks: Experiment and Theory of (CH 2 F 2) n â‹…â‹…â‹…(H 2 O) m. Angewandte Chemie - International Edition, 2019, 58, 8437-8442.	7.2	19
83	Rotational spectra and dynamics of the van der Waals adducts of neon and argon with 1,1-difluoroethylene. Journal of Chemical Physics, 2000, 112, 2204-2209.	1.2	18
84	A combined spectroscopic and theoretical study of propofolÂ·(H2O)3. Journal of Chemical Physics, 2012, 137, 074303.	1.2	18
85	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.	1.1	18
86	Non-bonding interactions and internal dynamics in CH2F2â‹¯H2CO: a rotational and model calculations study. Physical Chemistry Chemical Physics, 2013, 15, 6714.	1.3	18
87	Competing Dispersive Interactions: From Small Energy Differences to Large Structural Effects in Methyl Jasmonate and Zingerone. Journal of Physical Chemistry Letters, 2018, 9, 5906-5914.	2.1	18
88	Tautomeric equilibrium and hydroxyl group internal rotation in 4-hydroxypyridine. Chemical Physics Letters, 2006, 425, 6-9.	1.2	17
89	Accurate Semiexperimental Structure of 1,3,4-Oxadiazole by the Mixed Estimation Method. Journal of Physical Chemistry A, 2013, 117, 2278-2284.	1.1	17
90	Accurate Equilibrium Structures for Piperidine and Cyclohexane. Journal of Physical Chemistry A, 2015, 119, 1486-1493.	1.1	17

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91	Shapes, Dynamics, and Stability of Î²-Ionone and Its Two Mutants Evidenced by High-Resolution Spectroscopy in the Gas Phase. Journal of Physical Chemistry Letters, 2018, 9, 1497-1502.	2.1	17
92	Formation of water polyhedrons in propofolâ€“water clusters. Physical Chemistry Chemical Physics, 2013, 15, 568-575.	1.3	16
93	Interactions between freons and aromatic molecules: The rotational spectrum of pyridineâ€“difluoromethane. Chemical Physics Letters, 2014, 591, 216-219.	1.2	16
94	Interactions between alkanes and aromatic molecules: a rotational study of pyridineâ€“methane. Physical Chemistry Chemical Physics, 2014, 16, 13041-13046.	1.3	16
95	Microwave Spectrum of [1,1]-Pyridineâ‹¯Ne₂. Journal of Physical Chemistry A, 2009, 113, 14227-14230.	1.1	15
96	Structure, dipole moment and large amplitude motions of 1-benzofuran. Physical Chemistry Chemical Physics, 2005, 7, 3317.	1.3	14
97	Competing hydrogen bonding in methoxyphenols: The rotational spectrum of o-vanillin. Journal of Molecular Spectroscopy, 2011, 267, 112-117.	0.4	14
98	Water Encapsulation by Nanomicelles. Angewandte Chemie - International Edition, 2014, 53, 12480-12483.	7.2	14
99	Internal Dynamics in Halogenâ€Bonded Adducts: A Rotational Study of Chlorotrifluoromethaneâ€“Formaldehyde. Chemistry - A European Journal, 2015, 21, 4148-4152.	1.7	14
100	Influence of the Anomeric Conformation in the Intermolecular Interactions of Glucose. Journal of Physical Chemistry Letters, 2017, 8, 1147-1151.	2.1	14
101	Effects of Chlorination on the Tautomeric Equilibrium of 2â€Hydroxypyridine: Experiment and Theory. Chemistry - A European Journal, 2017, 23, 3595-3604.	1.7	14
102	Study of the conformational equilibrium of 1-chlorobutane by free-jets and conventional microwave spectroscopy. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 2183.	1.7	13
103	Conformational behaviour, hydrogen bond competition and intramolecular dynamics in vanillin derivatives: acetovanillone and 6-hydroxy-3-methoxyacetophenone. Physical Chemistry Chemical Physics, 2011, 13, 13310.	1.3	13
104	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.	1.6	13
105	Investigating the Conformation of the Bridged Monosaccharide Levoglucosan. ChemPhysChem, 2018, 19, 766-773.	1.0	13
106	Discriminating the structure ofexo-2-aminonorbornane using nuclear quadrupole coupling interactions. Journal of Chemical Physics, 2011, 134, 164311.	1.2	12
107	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.	1.7	12
108	Effects of Fluorine Substitution on the Microsolvation of Aromatic Azines: The Microwave Spectrum of 3-Fluoropyridine-Water. Journal of Physical Chemistry A, 2016, 120, 5163-5168.	1.1	12

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109	Observation of the Unbiased Conformers of Putative DNA-Scaffold Ribosugars. ACS Central Science, 2020, 6, 293-303.	5.3	12
110	The Role of Nonâ€Covalent Interactions on Cluster Formation: Pentamer, Hexamers and Heptamer of Difluoromethane. Angewandte Chemie - International Edition, 2021, 60, 16894-16899.	7.2	12
111	Rotational Spectrum of the Mixed van der Waals Triad Pyridineâ€“Arâ€“Ne. ChemPhysChem, 2009, 10, 2503-2507.	1.0	11
112	Unraveling the Benzocaineâ€“Receptor Interaction at Molecular Level Using Mass-Resolved Spectroscopy. Journal of Physical Chemistry B, 2013, 117, 13472-13480.	1.2	11
113	Regarding the torsional flexibility of the dihydrolipoic acid's pharmacophore: 1,3-propanedithiol. Physical Chemistry Chemical Physics, 2017, 19, 496-502.	1.3	11
114	Characterizing the lone pairâ‹¯Ï€â€“hole interaction in complexes of ammonia with perfluorinated arenes. Physical Chemistry Chemical Physics, 2021, 23, 9121-9129.	1.3	11
115	Interactions of Aromatic Heterocycles with Water: The Driving Force from Freeâ€Jet Rotational Spectroscopy and Model Electrostatic Calculations. ChemPhysChem, 2008, 9, 1303-1308.	1.0	10
116	Probing the glycosidic linkage: secondary structures in the gas phase. Physica Scripta, 2008, 78, 058124.	1.2	10
117	Static and Dynamic Properties of 1,1â€²â€Biâ€2â€naphthol and Its Conjugated Acids and Bases. Chemistry - A European Journal, 2014, 20, 14816-14825.	1.7	10
118	Intermolecular Hydrogen Bonding in 2-Fluoropyridine-Water. ChemistrySelect, 2016, 1, 1273-1277.	0.7	10
119	Conformational Equilibrium and Internal Dynamics of E-Anethole: A Rotational Study. Journal of Physical Chemistry B, 2016, 120, 6587-6591.	1.2	10
120	The pure rotational spectrum of TeSe: Rotational parameters, Bornâ€“Oppenheimer breakdown corrections, and hyperfine constants. Journal of Molecular Structure, 2006, 795, 163-172.	1.8	9
121	Conformational equilibrium in 3-hydroxy-pyridine. Chemical Physics Letters, 2007, 435, 10-13.	1.2	9
122	Mimicking anestheticâ€“receptor interactions in jets: the propofolâ€“isopropanol cluster. Physical Chemistry Chemical Physics, 2014, 16, 16968.	1.3	9
123	Conformational steering in dicarboxy acids: the native structure of succinic acid. Physical Chemistry Chemical Physics, 2015, 17, 19726-19734.	1.3	9
124	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.	2.1	9
125	The intrinsic conformation of a Lewis antigen: The LewisÃ—trisaccharide. Chemical Physics Letters, 2009, 477, 365-368.	1.2	8
126	Rotational spectroscopy of antipyretics: Conformation, structure, and internal dynamics of phenazone. Journal of Chemical Physics, 2013, 138, 114304.	1.2	8

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127	Magic Numbers in the Solvation of the Propofol Dimer. ChemPhysChem, 2013, 14, 1558-1562.	1.0	8
128	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.	1.0	8
129	Potential energy surface of fluoroxene: experiment and theory. Physical Chemistry Chemical Physics, 2016, 18, 3966-3974.	1.3	8
130	Phenyl-Î²-D-glucopyranoside and Phenyl-Î²-D-galactopyranoside Dimers: Small Structural Differences but Very Different Interactions. Frontiers in Physics, 2018, 6, .	1.0	8
131	Chlorination and tautomerism: a computational and UPS/XPS study of 2-hydroxypyridine â‡Œ 2-pyridone equilibrium. Physical Chemistry Chemical Physics, 2020, 22, 13440-13455.	1.3	8
132	Halogen bond and internal dynamics in the Ïƒâ€“complex of pyridine-chlorotrifluoromethane: A rotational study. Journal of Molecular Spectroscopy, 2020, 371, 111323.	0.4	8
133	Noncovalent Interactions and Internal Dynamics in Dimethoxymethaneâ€“Water. Chemistry - A European Journal, 2007, 13, 5833-5837.	1.7	7
134	Rotational Spectra of Bicyclic Decanes: The Trans Conformation of (â^')-Lupinine. Journal of Physical Chemistry A, 2013, 117, 13673-13679.	1.1	7
135	The Distorted Tropane of Scopoline. ChemPhysChem, 2013, 14, 1830-1835.	1.0	7
136	How Water Interacts with Halogenated Anesthetics: The Rotational Spectrum of Isofluraneâ€“Water. Chemistry - A European Journal, 2014, 20, 1980-1984.	1.7	7
137	Nâ€Methyl Inversion and Accurate Equilibrium Structures in Alkaloids: Pseudopelletierine. Chemistry - A European Journal, 2017, 23, 16491-16496.	1.7	7
138	Millimeter wave free-jet spectrum of the isotopologues of 1,2-butanediol. Journal of Molecular Structure, 2020, 1205, 127643.	1.8	7
139	Single Hydration of the Peptide Bond: The Case of the Vince Lactam. Journal of Physical Chemistry A, 2012, 116, 10099-10106.	1.1	6
140	Stability of conformationally locked free fructose: theoretical and computational insights. New Journal of Chemistry, 2015, 39, 9006-9018.	1.4	6
141	Structural Studies of Nicotinoids: Cotinine versus Nicotine. Chemistry - A European Journal, 2017, 23, 7238-7244.	1.7	6
142	Bond Length Alternation Observed Experimentally: The Case of 1Hâ€indazole. Chemistry - A European Journal, 2019, 25, 10172-10178.	1.7	6
143	Laboratory Observation of, Astrochemical Search for, and Structure of Elusive Erythrulose in the Interstellar Medium. Journal of Physical Chemistry Letters, 2021, 12, 1352-1359.	2.1	6
144	Scopine Isolated in the Gas Phase. ChemPhysChem, 2016, 17, 3030-3034.	1.0	5

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145	Solving the Tautomeric Equilibrium of Purine through Analysis of the Complex Hyperfine Structure of the Four ¹⁴N Nuclei. Journal of Physical Chemistry Letters, 2016, 7, 1187-1191.	2.1	5
146	Structural Studies of Nicotinoids: Cotinine versus Nicotine. Chemistry - A European Journal, 2017, 23, 7156-7156.	1.7	5
147	Understanding the role of tyrosine in glycogenin. Molecular BioSystems, 2017, 13, 1709-1712.	2.9	5
148	Rotational spectroscopy update for the newly identified atmospheric ozone depleter CF3CCl3. Journal of Molecular Spectroscopy, 2018, 352, 1-9.	0.4	5
149	Non covalent interactions stabilizing the chiral dimer of CH₂ClF: a rotational study. Physical Chemistry Chemical Physics, 2019, 21, 3695-3700.	1.3	5
150	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.	1.1	4
151	Molecular hydration of propofol dimers in supersonic expansions: formation of active centre-like structures. Physical Chemistry Chemical Physics, 2014, 16, 23301-23307.	1.3	4
152	The Conformational Map of Volatile Anesthetics: Enflurane Revisited. Chemistry - A European Journal, 2016, 22, 9804-9811.	1.7	4
153	Comprehensive rotational spectroscopy of the newly identified atmospheric ozone depleter CF3CH2Cl. Journal of Molecular Spectroscopy, 2017, 337, 37-45.	0.4	4
154	A General Treatment to Study Molecular Complexes Stabilized by Hydrogenâ€, Halogenâ€, and Carbonâ€Bond Networks: Experiment and Theory of (CH₂F₂)_nâ‹…â‹…â‹…(H₂O)_m. Angewandte Chemie, 2019, 131, 8525-8530.	1.6	4
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