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	Structure and dynamics of methacrylamide, a computational and free-jet rotational spectroscopic study. Journal of Molecular Structure, 2022, 1248, 131391.	1.8	3
2	Bond Length Alternation and Internal Dynamics in Model Aromatic Substituents of Lignin. ChemPhysChem, 2022, , .	1.0	3
3	The SKA as a Prebiotic Molecule Detector. Frontiers in Astronomy and Space Sciences, 2022, 9, .	1.1	1
4	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
5	The Role of Nonâ€Covalent Interactions on Cluster Formation: Pentamer, Hexamers and Heptamer of Difluoromethane. Angewandte Chemie, 2021, 133, 17031-17036.	1.6	0
6	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
7	Testing the Scalability of the HS-AUTOFIT Tool in a High-Performance Computing Environment. Electronics (Switzerland), 2021, 10, 2251.	1.8	3
8	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
9	Ïƒâ€“Hole activation and structural changes upon perfluorination of aryl halides: direct evidence from gas phase rotational spectroscopy. Physical Chemistry Chemical Physics, 2021, 23, 18093-18101.	1.3	3
10	Millimeter wave free-jet spectrum of the isotopologues of 1,2-butanediol. Journal of Molecular Structure, 2020, 1205, 127643.	1.8	7
11	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
12	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
13	Conformational impact of aliphatic side chains in local anaesthetics: benzocaine, butamben and isobutamben. Chemical Communications, 2020, 56, 6094-6097.	2.2	3
14	Observation of the Unbiased Conformers of Putative DNA-Scaffold Ribosugars. ACS Central Science, 2020, 6, 293-303.	5.3	12
15	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
16	Interactions between azines and alcohols: a rotational study of pyridineâ€“tert-butyl alcohol. Physical Chemistry Chemical Physics, 2019, 21, 3545-3549.	1.3	3
17	Non covalent interactions stabilizing the chiral dimer of CH₂ClF: a rotational study. Physical Chemistry Chemical Physics, 2019, 21, 3695-3700.	1.3	5
18	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

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19	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
20	Bond Length Alternation Observed Experimentally: The Case of 1Hâ€Indazole. Chemistry - A European Journal, 2019, 25, 10172-10178.	1.7	6
21	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
22	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
23	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
24	Investigating the Conformation of the Bridged Monosaccharide Levoglucosan. ChemPhysChem, 2018, 19, 766-773.	1.0	13
25	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
26	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
27	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
28	Rotational spectroscopy update for the newly identified atmospheric ozone depleter CF3CCl3. Journal of Molecular Spectroscopy, 2018, 352, 1-9.	0.4	5
29	Effects of Chlorination on the Tautomeric Equilibrium of 2â€Hydroxypyridine: Experiment and Theory. Chemistry - A European Journal, 2017, 23, 3501-3501.	1.7	0
30	Structural Studies of Nicotinoids: Cotinine versus Nicotine. Chemistry - A European Journal, 2017, 23, 7238-7244.	1.7	6
31	Influence of the Anomeric Conformation in the Intermolecular Interactions of Glucose. Journal of Physical Chemistry Letters, 2017, 8, 1147-1151.	2.1	14
32	Structural Studies of Nicotinoids: Cotinine versus Nicotine. Chemistry - A European Journal, 2017, 23, 7156-7156.	1.7	5
33	Regarding the torsional flexibility of the dihydrolipoic acid's pharmacophore: 1,3-propanedithiol. Physical Chemistry Chemical Physics, 2017, 19, 496-502.	1.3	11
34	High conductance values in Ï€-folded molecular junctions. Nature Communications, 2017, 8, 15195.	5.8	54
35	Comprehensive rotational spectroscopy of the newly identified atmospheric ozone depleter CF3CH2Cl. Journal of Molecular Spectroscopy, 2017, 337, 37-45.	0.4	4
36	Effects of Chlorination on the Tautomeric Equilibrium of 2â€Hydroxypyridine: Experiment and Theory. Chemistry - A European Journal, 2017, 23, 3595-3604.	1.7	14

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37	Understanding the role of tyrosine in glycogenin. Molecular BioSystems, 2017, 13, 1709-1712.	2.9	5
38	Spectroscopy and inter/intramolecular dynamics in Honor of Walther Caminati. Journal of Molecular Spectroscopy, 2017, 337, 1-2.	0.4	1
39	Nâ€Methyl Inversion and Accurate Equilibrium Structures in Alkaloids: Pseudopelletierine. Chemistry - A European Journal, 2017, 23, 16491-16496.	1.7	7
40	N -Methyl Inversion and Accurate Equilibrium Structures in Alkaloids: Pseudopelletierine. Chemistry - A European Journal, 2017, 23, 16412-16412.	1.7	2
41	Scopine Isolated in the Gas Phase. ChemPhysChem, 2016, 17, 3030-3034.	1.0	5
42	The Conformational Map of Volatile Anesthetics: Enflurane Revisited. Chemistry - A European Journal, 2016, 22, 9804-9811.	1.7	4
43	Furanosic forms of sugars: conformational equilibrium of methyl Î²-<scp>d</scp>-ribofuranoside. Chemical Communications, 2016, 52, 6241-6244.	2.2	19
44	Modeling the tyrosineâ€“sugar interactions in supersonic expansions: glucopyranoseâ€“phenol clusters. Physical Chemistry Chemical Physics, 2016, 18, 12457-12465.	1.3	23
45	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
46	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
47	Intermolecular Hydrogen Bonding in 2-Fluoropyridine-Water. ChemistrySelect, 2016, 1, 1273-1277.	0.7	10
48	Conformational Equilibrium and Internal Dynamics of E-Anethole: A Rotational Study. Journal of Physical Chemistry B, 2016, 120, 6587-6591.	1.2	10
49	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
50	On the Clâ‹¯C halogen bond: a rotational study of CF₃Clâ€“CO. Physical Chemistry Chemical Physics, 2016, 18, 17851-17855.	1.3	38
51	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
52	High-Resolution Spectroscopic Studies of Complexes Formed by Medium-Size Organic Molecules. Chemical Reviews, 2016, 116, 5014-5037.	23.0	80
53	Potential energy surface of fluoroxene: experiment and theory. Physical Chemistry Chemical Physics, 2016, 18, 3966-3974.	1.3	8
54	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

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55	Structural Distortion of the Epoxy Groups in Norbornanes: A Rotational Study of exoâ€2,3â€Epoxynorbornane. ChemPhysChem, 2015, 16, 2609-2614.	1.0	2
56	Internal Dynamics in Halogenâ€Bonded Adducts: A Rotational Study of Chlorotrifluoromethaneâ€“Formaldehyde. Chemistry - A European Journal, 2015, 21, 4148-4152.	1.7	14
57	How CO₂ Interacts with Carboxylic Acids: A Rotational Study of Formic Acidâ€“CO₂. ChemPhysChem, 2015, 16, 2961-2967.	1.0	26
58	Conformational steering in dicarboxy acids: the native structure of succinic acid. Physical Chemistry Chemical Physics, 2015, 17, 19726-19734.	1.3	9
59	N lone-pairâ‹¯Ï€ interaction: a rotational study of chlorotrifluoroethyleneâ‹¯ammonia. Physical Chemistry Chemical Physics, 2015, 17, 7694-7698.	1.3	24
60	Chiral recognition and atropisomerism in the sevoflurane dimer. Physical Chemistry Chemical Physics, 2015, 17, 18282-18287.	1.3	25
61	Stability of conformationally locked free fructose: theoretical and computational insights. New Journal of Chemistry, 2015, 39, 9006-9018.	1.4	6
62	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
63	Accurate Equilibrium Structures for Piperidine and Cyclohexane. Journal of Physical Chemistry A, 2015, 119, 1486-1493.	1.1	17
64	Carbohydrates. Topics in Current Chemistry, 2014, 364, 299-333.	4.0	19
65	Oï£¿Hâ‹¯â‹¯N and Cï£¿Hâ‹¯â‹¯O Hydrogen Bonds Control Hydration of Pivotal Tropane Alkaloids: Tropinoneâ‹¯â‹¯H₂O Complex. ChemPhysChem, 2014, 15, 918-923.	1.0	8
66	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
67	Interactions between freons and aromatic molecules: The rotational spectrum of pyridineâ€“difluoromethane. Chemical Physics Letters, 2014, 591, 216-219.	1.2	16
68	Mimicking anestheticâ€“receptor interactions in jets: the propofolâ€“isopropanol cluster. Physical Chemistry Chemical Physics, 2014, 16, 16968.	1.3	9
69	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
70	Interactions between alkanes and aromatic molecules: a rotational study of pyridineâ€“methane. Physical Chemistry Chemical Physics, 2014, 16, 13041-13046.	1.3	16
71	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
72	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

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73	Static and Dynamic Properties of 1,1â€²â€Bi2â€naphthol and Its Conjugated Acids and Bases. Chemistry - A European Journal, 2014, 20, 14816-14825.	1.7	10
74	Conformational Flexibility of Mephenesin. Journal of Physical Chemistry B, 2014, 118, 5357-5364.	1.2	3
75	Halogenâ€“Halogen Links and Internal Dynamics in Adducts of Freons. Journal of Physical Chemistry Letters, 2014, 5, 1591-1595.	2.1	25
76	Water Encapsulation by Nanomicelles. Angewandte Chemie - International Edition, 2014, 53, 12480-12483.	7.2	14
77	How Water Interacts with Halogenated Anesthetics: The Rotational Spectrum of Isofluraneâ€“Water. Chemistry - A European Journal, 2014, 20, 1980-1984.	1.7	7
78	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
79	Binding energies of micro-hydrated carbohydrates: measurements and interpretation. Chemical Science, 2013, 4, 1830.	3.7	22
80	Free Fructose Is Conformationally Locked. Journal of the American Chemical Society, 2013, 135, 2845-2852.	6.6	71
81	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
82	Unraveling the Benzocaineâ€“Receptor Interaction at Molecular Level Using Mass-Resolved Spectroscopy. Journal of Physical Chemistry B, 2013, 117, 13472-13480.	1.2	11
83	Rotational Spectra of Bicyclic Decanes: The Trans Conformation of (â^')-Lupinine. Journal of Physical Chemistry A, 2013, 117, 13673-13679.	1.1	7
84	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
85	Formation of water polyhedrons in propofolâ€“water clusters. Physical Chemistry Chemical Physics, 2013, 15, 568-575.	1.3	16
86	Rotational spectroscopy of antipyretics: Conformation, structure, and internal dynamics of phenazone. Journal of Chemical Physics, 2013, 138, 114304.	1.2	8
87	The Distorted Tropane of Scopoline. ChemPhysChem, 2013, 14, 1830-1835.	1.0	7
88	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
89	Magic Numbers in the Solvation of the Propofol Dimer. ChemPhysChem, 2013, 14, 1558-1562.	1.0	8
90	Shaping Micelles: The Interplay Between Hydrogen Bonds and Dispersive Interactions. Angewandte Chemie - International Edition, 2013, 52, 7772-7775.	7.2	31

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91	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.	1.1	3
92	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
93	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
94	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
95	Six Pyranoside Forms of Free 2â€Deoxyâ€‹<scp>D</scp>â€‹ribose. Angewandte Chemie - International Edition, 2013, 52, 11840-11845.	7.2	45
96	InnenrÃ¼cktitelbild: Shaping Micelles: The Interplay Between Hydrogen Bonds and Dispersive Interactions (Angew. Chem. 30/2013). Angewandte Chemie, 2013, 125, 8041-8041.	1.6	0
97	A combined spectroscopic and theoretical study of propofolÂ·(H2O)3. Journal of Chemical Physics, 2012, 137, 074303.	1.2	18
98	Mimicking anaestheticâ€“receptor interaction: a combined spectroscopic and computational study of propofolâ€‹phenol. Physical Chemistry Chemical Physics, 2012, 14, 8956.	1.3	25
99	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
100	Exploring microsolvation of the anesthetic propofol. Physical Chemistry Chemical Physics, 2012, 14, 4398.	1.3	40
101	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
102	Single Hydration of the Peptide Bond: The Case of the Vince Lactam. Journal of Physical Chemistry A, 2012, 116, 10099-10106.	1.1	6
103	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
104	Ribose Found in the Gas Phase. Angewandte Chemie - International Edition, 2012, 51, 3119-3124.	7.2	97
105	Inside Cover: Ribose Found in the Gas Phase (Angew. Chem. Int. Ed. 13/2012). Angewandte Chemie - International Edition, 2012, 51, 3030-3030.	7.2	0
106	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
107	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
108	Isotopic Hydration of Cellobiose: Vibrational Spectroscopy and Dynamical Simulations. Journal of Physical Chemistry A, 2011, 115, 9498-9509.	1.1	27

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109	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
110	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
111	â€œUnion is strengthâ€: how weak hydrogen bonds become stronger. Physical Chemistry Chemical Physics, 2011, 13, 13901.	1.3	62
112	Sensing the anomeric effect in a solvent-free environment. Nature, 2011, 469, 76-79.	13.7	138
113	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
114	Competing hydrogen bonding in methoxyphenols: The rotational spectrum of o-vanillin. Journal of Molecular Spectroscopy, 2011, 267, 112-117.	0.4	14
115	Discriminating the structure ofexo-2-aminonorbornane using nuclear quadrupole coupling interactions. Journal of Chemical Physics, 2011, 134, 164311.	1.2	12
116	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
117	The Conformational Landscape of Nicotinoids: Solving the Conformational Disparity of Anabasine. Chemistry - A European Journal, 2010, 16, 10214-10219.	1.7	20
118	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
119	Conformational equilibria in vanillin and ethylvanillin. Physical Chemistry Chemical Physics, 2010, 12, 12486.	1.3	44
120	N-Methyl stereochemistry in tropinone: the conformational flexibility of the tropane motif. Physical Chemistry Chemical Physics, 2010, 12, 6076.	1.3	27
121	The free jet microwave spectrum of 2-phenylethylamineâ€“water. Physical Chemistry Chemical Physics, 2010, 12, 10210.	1.3	25
122	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
123	Rotational Spectrum of the Mixed van der Waals Triad Pyridineâ€“Arâ€“Ne. ChemPhysChem, 2009, 10, 2503-2507.	1.0	11
124	Adducts of NH₃ with the Conformers of Glycidol: A Rotational Spectroscopy Study. Angewandte Chemie - International Edition, 2009, 48, 1102-1105.	7.2	22
125	Conformational change and selectivity in explicitly hydrated carbohydrates. Tetrahedron: Asymmetry, 2009, 20, 718-722.	1.8	46
126	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

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127	The intrinsic conformation of a Lewis antigen: The LewisÃ—trisaccharide. Chemical Physics Letters, 2009, 477, 365-368.	1.2	8
128	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
129	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
130	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
131	Microwave Spectrum of [1,1]-Pyridineâ‹¯Ne₂. Journal of Physical Chemistry A, 2009, 113, 14227-14230.	1.1	15
132	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
133	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
134	A rotational study of the molecular complex tert-butanolÂ·Â·Â·NH3. Chemical Physics Letters, 2008, 463, 330-333.	1.2	20
135	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
136	Probing the glycosidic linkage: secondary structures in the gas phase. Physica Scripta, 2008, 78, 058124.	1.2	10
137	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
138	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
139	Noncovalent Interactions and Internal Dynamics in Dimethoxymethaneâ€“Water. Chemistry - A European Journal, 2007, 13, 5833-5837.	1.7	7
140	The Shape of Leucine in the Gas Phase. ChemPhysChem, 2007, 8, 599-604.	1.0	76
141	Conformational equilibrium in 3-hydroxy-pyridine. Chemical Physics Letters, 2007, 435, 10-13.	1.2	9
142	The shape of neutral sarcosine in gas phase. Chemical Physics Letters, 2007, 435, 336-341.	1.2	30
143	Tautomeric equilibrium and hydroxyl group internal rotation in 4-hydroxypyridine. Chemical Physics Letters, 2006, 425, 6-9.	1.2	17
144	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

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145	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
146	The Glycineâ€“Water Complex. Angewandte Chemie - International Edition, 2006, 45, 3471-3474.	7.2	111
147	Conformations of Î±-Aminobutyric Acid in the Gas Phase. ChemPhysChem, 2006, 7, 1481-1487.	1.0	25
148	The Fourier transform rotational spectrum of difluoromethaneâ€“water: internal motion of water. Journal of Molecular Structure, 2005, 742, 87-90.	1.8	25
149	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
150	Coded Amino Acids in Gas Phase:Â The Shape of Isoleucine. Journal of the American Chemical Society, 2005, 127, 12952-12956.	6.6	90
151	Gas-Phase Structure ofN,N-Dimethylglycine. ChemPhysChem, 2005, 6, 1559-1566.	1.0	31
152	The Internuclear Potential, Electronic Structure, and Chemical Bond of Tellurium Selenide. Angewandte Chemie - International Edition, 2005, 44, 6311-6315.	7.2	27
153	Water-ketones hydrogen bonding: The rotational spectrum of cyclobutanone-water. Journal of Chemical Physics, 2005, 123, 164304.	1.2	26
154	Shape of 4(S)- and 4(R)-Hydroxyproline in Gas Phase. Journal of the American Chemical Society, 2005, 127, 2572-2579.	6.6	68
155	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
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