

Ibon Alkorta

List of Publications by Year in descending order

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1117
times ranked

19411
citing authors

#	ARTICLE	IF	CITATIONS
1	From weak to strong interactions: A comprehensive analysis of the topological and energetic properties of the electron density distribution involving Xâ€¦â€¦â€¦Y systems. Journal of Chemical Physics, 2002, 117, 5529-5542.	3.1	1,575
2	Definition of the hydrogen bond (IUPAC Recommendations 2011). Pure and Applied Chemistry, 2011, 83, 1637-1641.	2.0	1,516
3	Behavior of Ylides Containing N, O, and C Atoms as Hydrogen Bond Acceptors. Journal of the American Chemical Society, 2000, 122, 11154-11161.	14.6	1,391
4	Defining the hydrogen bond: An account (IUPAC Technical Report). Pure and Applied Chemistry, 2011, 83, 1619-1636.	2.0	882
5	Non-conventional hydrogen bonds. Chemical Society Reviews, 1998, 27, 163.	40.3	576
6	Interaction of Anions with Perfluoro Aromatic Compounds. Journal of the American Chemical Society, 2002, 124, 8593-8598.	14.6	502
7	About the evaluation of the local kinetic, potential and total energy densities in closed-shell interactions. Chemical Physics Letters, 2001, 336, 457-461.	2.7	388
8	Relationships between interaction energy, intermolecular distance and electron density properties in hydrogen bonded complexes under external electric fields. Chemical Physics Letters, 2011, 507, 185-189.	2.7	324
9	Not Only Hydrogen Bonds: Other Noncovalent Interactions. Crystals, 2020, 10, 180.	2.3	315
10	Cooperativity in multiple unusual weak bonds. Theoretical Chemistry Accounts, 2010, 126, 1-14.	1.5	258
11	On the Reliability of Pure and Hybrid DFT Methods for the Evaluation of Halogen, Chalcogen, and Pnicogen Bonds Involving Anionic and Neutral Electron Donors. Journal of Chemical Theory and Computation, 2013, 9, 5201-5210.	5.6	248
12	Universal Features of the Electron Density Distribution in Hydrogenâ€¦ Bonding Regions: A Comprehensive Study Involving Hâ€¦â€¦â€¦X (X=H, C, N, O, F, S, Cl, I) Interactions. Chemistry - A European Journal, 2010, 16, 2442-2452.	3.9	232
13	Bifurcated Hydrogen Bonds:â€‰ Three-Centered Interactions. Journal of Physical Chemistry A, 1998, 102, 9925-9932.	2.6	228
14	Statistical analysis of ¹³ C and ¹⁵ N NMR chemical shifts from GIAO/B3LYP/6â€‰311 + C** calculated absolute shieldings. Magnetic Resonance in Chemistry, 2007, 45, 797-800.	2.0	188
15	Charge-Transfer Complexes between Dihalogen Compounds and Electron Donors. Journal of Physical Chemistry A, 1998, 102, 9278-9285.	2.6	187
16	Molecular Complexes between Silicon Derivatives and Electron-Rich Groups. Journal of Physical Chemistry A, 2001, 105, 743-749.	2.6	185
17	Unusual Hydrogen Bonds: Hâ€¦â€¦ Interactions. Journal of Physical Chemistry A, 1997, 101, 9457-9463.	2.6	184
18	An Attractive Interaction between the I-Cloud of C6F6 and Electron-Donor Atoms. Journal of Organic Chemistry, 1997, 62, 4687-4691.	3.3	177

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19	Structures, Energies, Bonding, and NMR Properties of Pnictogen Complexes $H_2XP:NXH_2$ ($X = H, CH_3, NH_2, OH, F, Cl$). Journal of Physical Chemistry A, 2011, 115, 13724-13731.	2.6	171
20	Competition of Hydrogen Bonds and Halogen Bonds in Complexes of Hypohalous Acids with Nitrogenated Bases. Journal of Physical Chemistry A, 2008, 112, 10856-10863.	2.6	170
21	Beryllium Bonds, Do They Exist?. Journal of Chemical Theory and Computation, 2009, 5, 2763-2771.	5.6	162
22	Theoretical Study of Strong Hydrogen Bonds between Neutral Molecules: The Case of Amine Oxides and Phosphine Oxides as Hydrogen Bond Acceptors. Journal of Physical Chemistry A, 1999, 103, 272-279.	2.6	157
23	PLGA nanoparticle preparations by emulsification and nanoprecipitation techniques: effects of formulation parameters. RSC Advances, 2020, 10, 4218-4231.	3.7	153
24	Molecular polarization potential maps of the nucleic acid bases. International Journal of Quantum Chemistry, 1996, 57, 123-135.	2.1	147
25	Bond Length–Electron Density Relationships: From Covalent Bonds to Hydrogen Bond Interactions. Structural Chemistry, 1998, 9, 243-247.	2.0	146
26	Spodium Bonds: Noncovalent Interactions Involving Group 12 Elements. Angewandte Chemie - International Edition, 2020, 59, 17482-17487.	14.7	143
27	^{31}P spin coupling constants for pnictogen homodimers. Chemical Physics Letters, 2011, 512, 184-187.	2.7	132
28	Pnictogen Bonded Complexes of PO_2X ($X = F, Cl$) with Nitrogen Bases. Journal of Physical Chemistry A, 2013, 117, 10497-10503.	2.6	131
29	Intramolecular Hydrogen Bonds in ortho-Substituted Hydroxybenzenes and in 8-Substituted 1-Hydroxynaphthalenes: Can a Methyl Group Be an Acceptor of Hydrogen Bonds?. Journal of Physical Chemistry A, 2001, 105, 10462-10467.	2.6	128
30	Do coupling constants and chemical shifts provide evidence for the existence of resonance-assisted hydrogen bonds?. Molecular Physics, 2004, 102, 2563-2574.	1.7	126
31	Basicity of N-H- and N-Methyl-1,2,3-triazoles in the Gas Phase, in Solution, and in the Solid State – An Experimental and Theoretical Study. European Journal of Organic Chemistry, 2001, 2001, 3013.	2.5	124
32	Comparison of models to correlate electron density at the bond critical point and bond distance. Computational and Theoretical Chemistry, 2000, 496, 131-137.	1.5	119
33	Theoretical Study of the Influence of Electric Fields on Hydrogen-Bonded Acid–Base Complexes. Journal of Physical Chemistry A, 1997, 101, 9791-9800.	2.6	115
34	Experimental measurements and theoretical calculations of the chemical shifts and coupling constants of three azines (benzalazine, acetophenoneazine and cinnamaldazine). Magnetic Resonance in Chemistry, 2008, 46, 859-864.	2.0	111
35	Influence of Hydrogen Bonds on the $P\cdots P$ Pnictogen Bond. Journal of Chemical Theory and Computation, 2012, 8, 2320-2327.	5.6	108
36	Fluorine–Fluorine Interactions: NMR and AIM Analysis. Structural Chemistry, 2004, 15, 117-120.	2.0	106

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37	Are resonance-assisted hydrogen bonds "resonance assisted"? A theoretical NMR study. <i>Chemical Physics Letters</i> , 2005, 411, 411-415.	2.7	106
38	Cooperativity in Tetrel Bonds. <i>Journal of Physical Chemistry A</i> , 2016, 120, 648-656.	2.6	105
39	Performance assessment for EEG-based neonatal seizure detectors. <i>Clinical Neurophysiology</i> , 2011, 122, 474-482.	2.0	104
40	Intermolecular Weak Interactions in HTeXH Dimers (X=O, S, Se, Te): Hydrogen Bonds, Chalcogen-Chalcogen Contacts and Chiral Discrimination. <i>ChemPhysChem</i> , 2012, 13, 496-503.	2.3	104
41	A new avenue to the synthesis of highly substituted pyrroles: synthesis from N-propargylamines. <i>RSC Advances</i> , 2016, 6, 18619-18631.	3.7	103
42	Electrostatics at the Origin of the Stability of Phosphate-Phosphate Complexes Locked by Hydrogen Bonds. <i>ChemPhysChem</i> , 2012, 13, 1421-1424.	2.3	101
43	Inverse Hydrogen-Bonded Complexes. <i>Journal of Physical Chemistry A</i> , 1997, 101, 4236-4244.	2.6	98
44	Dihydrogen bonds (A-H...B). <i>Chemical Communications</i> , 1996, , 1633-1634.	4.2	95
45	Supramolecular structure of 1H-pyrazoles in the solid state: a crystallographic and ab initio study. <i>Acta Crystallographica Section B: Structural Science</i> , 2000, 56, 1018-1028.	2.2	95
46	Synthesis, Characterization, Molecular Structure and Theoretical Studies of Axially Fluoro-Substituted Subazaporphyrins. <i>Chemistry - A European Journal</i> , 2008, 14, 1342-1350.	3.9	95
47	The Paradox of Hydrogen-Bonded Anion-Anion Aggregates in Oxoanions: A Fundamental Electrostatic Problem Explained in Terms of Electrophilic-Nucleophilic Interactions. <i>Journal of Physical Chemistry A</i> , 2015, 119, 183-194.	2.6	95
48	Title is missing!. <i>Journal of Applied Electrochemistry</i> , 2000, 30, 1209-1222.	2.9	94
49	Pnicogen-Bonded Cyclic Trimers (PH ₂ X) ₃ with X = F, Cl, OH, NC, CN, CH ₃ , H, and BH ₂ . <i>Journal of Physical Chemistry A</i> , 2013, 117, 4981-4987.	2.6	94
50	Specific pattern of gadolinium enhancement in spondylotic myelopathy. <i>Annals of Neurology</i> , 2014, 76, 54-65.	5.9	92
51	Interplay of H ⁺ ...F Hydrogen Bonds and P ⁺ ...N Pnicogen Bonds. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9205-9213.	2.6	91
52	Ab Initio Study of the Structural, Energetic, Bonding, and IR Spectroscopic Properties of Complexes with Dihydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2002, 106, 9325-9330.	2.6	90
53	Title is missing!. <i>Structural Chemistry</i> , 1998, 9, 187-202.	2.0	89
54	Competition and Interplay between f-Hole and i-Hole Interactions: A Computational Study of 1:1 and 1:2 Complexes of Nitryl Halides (O ₂ NX) with Ammonia. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5199-5206.	2.6	89

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55	Self-Discrimination of Enantiomers in Hydrogen-Bonded Dimers. <i>Journal of the American Chemical Society</i> , 2002, 124, 1488-1493.	14.6	87
56	New page to access pyridine derivatives: synthesis from N-propargylamines. <i>RSC Advances</i> , 2016, 6, 71662-71675.	3.7	86
57	Carbenes and Silylenes as Hydrogen Bond Acceptors. <i>The Journal of Physical Chemistry</i> , 1996, 100, 19367-19370.	3.0	85
58	Theoretical Study of Dihydrogen Bonds between (XH) ₂ , X = Li, Na, BeH, and MgH, and Weak Hydrogen Bond Donors (HCN, HNC, and HCCH). <i>Journal of Physical Chemistry A</i> , 2006, 110, 10279-10286.	2.6	85
59	Atropisomerism and Axial Chirality in Heteroaromatic Compounds. <i>Advances in Heterocyclic Chemistry</i> , 2012, , 1-188.	0.8	85
60	Single Electron Pnictogen Bonded Complexes. <i>Journal of Physical Chemistry A</i> , 2014, 118, 947-953.	2.6	84
61	Personalized alignment in total knee arthroplasty: current concepts. <i>Sicot-j</i> , 2021, 7, 19.	1.9	84
62	A Solid-State NMR, X-ray Diffraction, and ab Initio Computational Study of Hydrogen-Bond Structure and Dynamics of Pyrazole-4-Carboxylic Acid Chains. <i>Journal of the American Chemical Society</i> , 2001, 123, 7898-7906.	14.6	83
63	Atom transfer radical polymerization in aqueous dispersed media. <i>Open Chemistry</i> , 2009, 7, 657-674.	2.0	83
64	Theoretical study of the HXYH dimers (X, Y = O, S, Se). Hydrogen bonding and chalcogen-chalcogen interactions. <i>Molecular Physics</i> , 2011, 109, 2543-2552.	1.7	83
65	Cooperative and Diminutive Unusual Weak Bonding In F ₃ CX ₂ ·H ₂ MgH ₂ ·Y and F ₃ CX ₂ ·Y·H ₂ MgH ₂ Trimers (X = Cl, Br; Y = HCN, and HNC). <i>Journal of Physical Chemistry A</i> , 2010, 114, 12106-12111.	2.6	82
66	Open Bis(triazolium) Structural Motifs as a Benchmark To Study Combined Hydrogen- and Halogen-Bonding Interactions in Oxoanion Recognition Processes. <i>Journal of Organic Chemistry</i> , 2014, 79, 6959-6969.	3.3	82
67	A review with comprehensive data on experimental indirect scalar NMR spin-spin coupling constants across hydrogen bonds. <i>Magnetic Resonance in Chemistry</i> , 2008, 46, 599-624.	2.0	81
68	Do Traditional, Chlorine-shared, and Ion-pair Halogen Bonds Exist? An ab Initio Investigation of FCl:CNX Complexes. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12958-12962.	2.6	81
69	Structures, Binding Energies, and Spin-Spin Coupling Constants of Geometric Isomers of Pnictogen Homodimers (PHFX) ₂ , X = F, Cl, CN, CH ₃ , NC. <i>Journal of Physical Chemistry A</i> , 2012, 116, 3056-3060.	2.6	81
70	Modulating the Strength of Hydrogen Bonds through Beryllium Bonds. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2293-2300.	5.6	81
71	Exploring (NH ₂) ₂ F ₂ , H ₂ FP:NFH ₂ , and (PH ₂) ₂ F ₂ Potential Surfaces: Hydrogen Bonds or Pnictogen Bonds?. <i>Journal of Physical Chemistry A</i> , 2013, 117, 183-191.	2.6	81
72	Review on DFT and ab initio Calculations of Scalar Coupling Constants. <i>International Journal of Molecular Sciences</i> , 2003, 4, 64-92.	4.2	80

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73	Polybrominated Diphenyl Ethers and Polychlorinated Dibenzo- <i>p</i> -dioxins and Dibenzofurans in Surface Dust at an E-Waste Processing Site in Southeast China. <i>Environmental Science & Technology</i> , 2011, 45, 5775-5782.	10.5	80
74	Charged versus Neutral Hydrogen-Bonded Complexes: Is There a Difference in the Nature of the Hydrogen Bonds?. <i>Chemistry - A European Journal</i> , 2016, 22, 9226-9234.	3.9	80
75	Nanocomposite of ZIF-67 metal-organic framework with reduced graphene oxide nanosheets for high-performance supercapacitor applications. <i>Journal of Materials Science: Materials in Electronics</i> , 2017, 28, 18040-18048.	2.2	80
76	How To Determine Whether Intramolecular H \cdots H Interactions Can Be Classified as Dihydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2008, 112, 2721-2727.	2.6	79
77	Ab initio hybrid DFT-GIAO calculations of the shielding produced by carbon-carbon bonds and aromatic rings in ¹ H NMR spectroscopy. <i>New Journal of Chemistry</i> , 1998, 22, 381-385.	2.7	78
78	Topological Properties of the Electrostatic Potential in Weak and Moderate N-H Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2007, 111, 6425-6433.	2.6	78
79	Pnictogen Bonds between XPH ₃ (X = O, S, NH, CH ₂) and Phosphorus and Nitrogen Bases. <i>Journal of Physical Chemistry A</i> , 2014, 118, 1527-1537.	2.6	77
80	Possibility of sensing, adsorbing, and destructing the Tabun-2D-skeletal (Tabun nerve agent) by C ₂₀ fullerene and its boron and nitrogen doped derivatives. <i>Synthetic Metals</i> , 2016, 220, 606-611.	4.1	77
81	Orthogonal interactions between nitril derivatives and electron donors: pnictogen bonds. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 14310.	2.9	76
82	GIAO Calculations of Chemical Shifts in Heterocyclic Compounds. <i>Structural Chemistry</i> , 2003, 14, 377-389.	2.0	75
83	Substituent Effects on the Cooperativity of Halogen Bonding. <i>Journal of Physical Chemistry A</i> , 2013, 117, 5551-5557.	2.6	75
84	Influence of Substituent Effects on the Formation of P-Cl Pnictogen Bonds or Halogen Bonds. <i>Journal of Physical Chemistry A</i> , 2014, 118, 2360-2366.	2.6	75
85	Calcined chicken eggshell electrode for battery and supercapacitor applications. <i>RSC Advances</i> , 2019, 9, 26981-26995.	3.7	75
86	P(VDF-TrFE) nanofibers: structure of the ferroelectric and paraelectric phases through IR and Raman spectroscopies. <i>RSC Advances</i> , 2020, 10, 37779-37796.	3.7	75
87	Effects of fluorine substitution on hydrogen bond interactions. <i>Journal of Fluorine Chemistry</i> , 2000, 101, 233-238.	1.8	74
88	Carbon-Carbon Weak Interactions. <i>Journal of Physical Chemistry A</i> , 2009, 113, 8387-8393.	2.6	74
89	Pnictogen and hydrogen bonds: complexes between PH ₃ X ⁺ and PH ₂ X systems. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 3261-3272.	2.9	74
90	Selective sensing of ozone and the chemically active gaseous species of the troposphere by using the C ₂₀ fullerene and graphene segment. <i>Talanta</i> , 2017, 162, 505-510.	5.7	74

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91	Novel routes to quinoline derivatives from N-propargylamines. RSC Advances, 2016, 6, 49730-49746.	3.7	73
92	Cross-Dehydrogenative C-H/S-H Coupling Reactions. Topics in Current Chemistry, 2018, 376, 39.	6.2	73
93	A computational study of the cooperativity in clusters of interhalogen derivatives. Structural Chemistry, 2009, 20, 63-71.	2.0	72
94	Effect of an external electric field on the dissociation energy and the electron density properties: The case of the hydrogen bonded dimer HF \cdots HF. Journal of Chemical Physics, 2009, 130, 044104.	3.1	72
95	N-Propargylic β^2 -enaminocarbonyls: powerful and versatile building blocks in organic synthesis. RSC Advances, 2017, 7, 13198-13211.	3.7	72
96	Discovery of 5-(4-Chlorophenyl)-1-(2,4-dichlorophenyl)-3-hexyl-1H-1,2,4-triazole, a Novel in Vivo Cannabinoid Antagonist Containing a 1,2,4-Triazole Motif. Journal of Medicinal Chemistry, 2004, 47, 2939-2942.	6.7	71
97	A DFT study on electronic and optical properties of aspirin-functionalized B12N12 fullerene-like nanocluster. Structural Chemistry, 2017, 28, 735-748.	2.0	71
98	Theoretical Study of CH $\cdots\cdots\cdots$ O Hydrogen Bonds in H ₂ O-CH ₃ F, H ₂ O-CH ₂ F ₂ , and H ₂ O-CHF ₃ . The Journal of Physical Chemistry, 1995, 99, 6457-6460.	3.0	70
99	New protocols to access imidazoles and their ring fused analogues: synthesis from N-propargylamines. RSC Advances, 2017, 7, 7079-7091.	3.7	69
100	Recent developments in decarboxylative cross-coupling reactions between carboxylic acids and N-H compounds. RSC Advances, 2019, 9, 8964-8976.	3.7	69
101	Pnictogen-Bonded Anionic Complexes. Journal of Physical Chemistry A, 2014, 118, 3386-3392.	2.6	68
102	Title is missing!. International Journal of Quantum Chemistry, 1996, 57, 123.	2.1	68
103	Large Chiral Recognition in Hydrogen-Bonded Complexes and Proton Transfer in Pyrrolo[2,3-b]pyrrole Dimers as Model Compounds. Journal of Organic Chemistry, 2003, 68, 7485-7489.	3.3	67
104	A study of the tautomerism of β^2 -dicarbonyl compounds with special emphasis on curcuminoids. Tetrahedron, 2008, 64, 8089-8094.	2.0	67
105	Properties of Complexes H ₂ \cdots (X)P:PXH ₂ , for X = F, Cl, OH, CN, NC, CCH, H, CH ₃ , and BH ₂ : P \cdots N Pnictogen Bonding at σ -Holes and π -Holes. Journal of Physical Chemistry A, 2013, 117, 11592-11604.	2.6	67
106	Synthesis and characterization of BiVO ₄ nanoparticles for environmental applications. RSC Advances, 2020, 10, 18315-18322.	3.7	67
107	Phosphorus As a Simultaneous Electron-Pair Acceptor in Intermolecular P \cdots N Pnictogen Bonds and Electron-Pair Donor to Lewis Acids. Journal of Physical Chemistry A, 2013, 117, 3133-3141.	2.6	66
108	Characterizing Complexes with Pnictogen Bonds Involving sp ² Hybridized Phosphorus Atoms: (H ₂ \cdots C \cdots PX) ₂ with X = F, Cl, OH, CN, NC, CCH, H, CH ₃ , and BH ₂ . Journal of Physical Chemistry A, 2013, 117, 6893-6903.	2.6	65

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109	Tracing environment effects that influence the stability of anion-anion complexes: The case of phosphate-phosphate interactions. <i>Chemical Physics Letters</i> , 2013, 555, 106-109.	2.7	65
110	Strategies for indirect computer-aided drug design. <i>Pharmaceutical Research</i> , 1993, 10, 475-486.	3.6	64
111	Exocyclic iminium salts as catalysts for alkene epoxidation by Oxone [®] . <i>Tetrahedron</i> , 1999, 55, 2341-2352.	2.0	64
112	Influence of Intermolecular Hydrogen Bonds on the Tautomerism of Pyridine Derivatives. <i>Journal of Organic Chemistry</i> , 2002, 67, 1515-1519.	3.3	64
113	Transition-metal-catalyzed C-N cross-coupling reactions of N-unsubstituted sulfoximines: a review. <i>Journal of Sulfur Chemistry</i> , 2018, 39, 674-698.	2.1	64
114	Discrimination of hydrogen-bonded complexes with axial chirality. <i>Journal of Chemical Physics</i> , 2002, 117, 6463-6468.	3.1	63
115	The Pnictogen Bond in Review: Structures, Binding Energies, Bonding Properties, and Spin-Spin Coupling Constants of Complexes Stabilized by Pnictogen Bonds. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2015, , 191-263.	0.0	63
116	Atropisomerism and conformational aspects of <i>meso</i> -tetraarylporphyrins and related compounds. <i>Journal of Porphyrins and Phthalocyanines</i> , 2011, 15, 1-28.	0.9	62
117	Noncovalent interactions in dimers and trimers of SO ₃ and CO. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	1.5	62
118	Intramolecular pnictogen interactions in phosphorus and arsenic analogues of proton sponges. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 15900-15909.	2.9	60
119	Recent advances in sulfur-nitrogen bond formation <i>via</i> cross-dehydrogenative coupling reactions. <i>RSC Advances</i> , 2018, 8, 18456-18469.	3.7	60
120	Hydrogen Bond vs Proton Transfer between Neutral Molecules in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2001, 105, 7481-7485.	2.6	59
121	Influence of protonation on the electron density derived properties. <i>Arkivoc</i> , 2005, 2005, 305-320.	0.6	59
122	Theoretical estimation of the annular tautomerism of indazoles. <i>Journal of Physical Organic Chemistry</i> , 2005, 18, 719-724.	1.9	58
123	Homo- and heterochiral dimers (PHFX) ₂ , X=Cl, CN, CH ₃ , NC: To what extent do they differ?. <i>Chemical Physics Letters</i> , 2012, 538, 14-18.	2.7	58
124	Chalcogen Bonds in Complexes of SOXY (X, Y = F, Cl) with Nitrogen Bases. <i>Journal of Physical Chemistry A</i> , 2015, 119, 535-541.	2.6	58
125	Cross-Dehydrogenative Coupling Reactions Between P(O)-H and X-H (X = S, N, O, P) Bonds. <i>Topics in Current Chemistry</i> , 2018, 376, 23.	0.2	58
126	Land Application of Biosolids in Europe: Possibilities, Con-Strains and Future Perspectives. <i>Water (Switzerland)</i> , 2021, 13, 103.	2.8	58

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127	The azido-tetrazole and diazo-1,2,3-triazole tautomerism in six-membered heteroaromatic rings and their relationships with aromaticity: Azines and perimidine. <i>Tetrahedron</i> , 2010, 66, 2863-2868.	2.0	57
128	Quaternized membranes bearing zwitterionic groups for vanadium redox flow battery through a green route. <i>Journal of Membrane Science</i> , 2015, 483, 60-69.	8.3	57
129	Synthesis of porous carbon material based on biomass derived from hibiscus sabdariffa fruits as active electrodes for high-performance symmetric supercapacitors. <i>RSC Advances</i> , 2021, 11, 354-363.	3.7	57
130	Can Conventional Bases and Unsaturated Hydrocarbons Be Converted into Gas-Phase Superacids That Are Stronger than Most of the Known Oxyacids? The Role of Beryllium Bonds. <i>Chemistry - A European Journal</i> , 2013, 19, 11637-11643.	3.9	56
131	Theoretical Study of HCN and HNC Neutral and Charged Clusters. <i>Journal of Physical Chemistry B</i> , 2005, 109, 18189-18194.	2.7	55
132	Simultaneous Interaction of Tetrafluoroethene with Anions and Hydrogen-Bond Donors: A Cooperativity Study. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1186-1194.	5.6	55
133	Solvent-free incorporation of CO ₂ into 2-oxazolidinones: a review. <i>RSC Advances</i> , 2019, 9, 19465-19482.	3.7	55
134	1,2-Proton shifts in pyrazole and related systems: a computational study of [1,5]-sigmatropic migrations of hydrogen and related phenomena. <i>Perkin Transactions II RSC</i> , 1998, , 2497-2504.	1.1	53
135	Cooperativity and Proton Transfer in Hydrogen-Bonded Triads. <i>ChemPhysChem</i> , 2005, 6, 1411-1418.	2.3	53
136	Energetic vs Synergetic Stability: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 3266-3273.	2.6	53
137	Interaction Energies and NMR Indirect Nuclear Spin-Spin Coupling Constants in Linear HCN and HNC Complexes. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6555-6564.	2.6	52
138	FCl:PCX Complexes: Old and New Types of Halogen Bonds. <i>Journal of Physical Chemistry A</i> , 2012, 116, 2300-2308.	2.6	52
139	New route to 1,4-oxazepane and 1,4-diazepane derivatives: synthesis from N-propargylamines. <i>RSC Advances</i> , 2016, 6, 99781-99793.	3.7	52
140	Theoretical Study of Complexes and Fluoride Cation Transfer between N ₂ F ⁺ and Electron Donors. <i>Journal of Physical Chemistry A</i> , 2007, 111, 7154-7161.	2.6	51
141	Catalysis with carbon nanoparticles. <i>RSC Advances</i> , 2019, 9, 27659-27664.	3.7	51
142	Scholl reaction as a powerful tool for the synthesis of nanographenes: a systematic review. <i>RSC Advances</i> , 2021, 11, 32158-32202.	3.7	51
143	A GIAO/DFT study of ¹ H, ¹³ C and ¹⁵ N shieldings in amines and its relevance in conformational analysis. <i>Magnetic Resonance in Chemistry</i> , 2004, 42, 955-961.	2.0	50
144	On the tautomerism of pyrazolones: the geminal 2J[pyrazole C-4,H-3(5)] spin coupling constant as a diagnostic tool. <i>Tetrahedron</i> , 2004, 60, 6791-6805.	2.0	50

#	ARTICLE	IF	CITATIONS
145	Intramolecular Pnictogen Interactions in $\text{PHFi}_2(\text{CH}_2)_n\text{PHF}$ ($n=2-6$) Systems. <i>ChemPhysChem</i> , 2013, 14, 1656-1665.	2.3	50
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