Ibon Alkorta

List of Publications by Year
in descending order

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957 papers	31,716 citations	9264 74 h-index	11308 136 g-index
993 all docs	993 docs citations	993 times ranked	16587 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€“Hâ‹¯Fâ€“Y systems. Journal of Chemical Physics, 2002, 117, 5529-5542.	3.0	1,510
2	Definition of the hydrogen bond (IUPAC Recommendations 2011). Pure and Applied Chemistry, 2011, 83, 1637-1641.	1.9	1,449
3	Behavior of Ylides Containing N, O, and C Atoms as Hydrogen Bond Acceptors. Journal of the American Chemical Society, 2000, 122, 11154-11161.	13.7	1,334
4	Defining the hydrogen bond: An account (IUPAC Technical Report). Pure and Applied Chemistry, 2011, 83, 1619-1636.	1.9	856
5	Non-conventional hydrogen bonds. Chemical Society Reviews, 1998, 27, 163.	38.1	564
6	Interaction of Anions with Perfluoro Aromatic Compounds. Journal of the American Chemical Society, 2002, 124, 8593-8598.	13.7	496
7	About the evaluation of the local kinetic, potential and total energy densities in closed-shell interactions. Chemical Physics Letters, 2001, 336, 457-461.	2.6	385
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.	2.6	312
9	Not Only Hydrogen Bonds: Other Noncovalent Interactions. Crystals, 2020, 10, 180.	2.2	289
10	Cooperativity in multiple unusual weak bonds. Theoretical Chemistry Accounts, 2010, 126, 1-14.	1.4	254
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.	5.3	243
12	Water Clusters: Towards an Understanding Based on First Principles of Their Static and Dynamic Properties. Angewandte Chemie - International Edition, 2000, 39, 717-721.	13.8	229
13	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, Ï€) Interactions. Chemistry - A European Journal, 2010, 16, 2442-2452.	3.3	228
14	Bifurcated Hydrogen Bonds:â€‰ Three-Centered Interactions. Journal of Physical Chemistry A, 1998, 102, 9925-9932.	2.5	225
15	Charge-Transfer Complexes between Dihalogen Compounds and Electron Donors. Journal of Physical Chemistry A, 1998, 102, 9278-9285.	2.5	187
16	Statistical analysis of ¹³C and ¹⁵N NMR chemical shifts from GIAO/B3LYP/6â€311 + + G** calculated absolute shieldings. Magnetic Resonance in Chemistry, 2007, 45, 797-800.	1.9	186
17	Molecular Complexes between Silicon Derivatives and Electron-Rich Groups. Journal of Physical Chemistry A, 2001, 105, 743-749.	2.5	182
18	Unusual Hydrogen Bonds:Â HÂ·Â·Â·Ï€ Interactions. Journal of Physical Chemistry A, 1997, 101, 9457-9463.	2.5	180

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19	An Attractive Interaction between the Ï€-Cloud of C6F6 and Electron-Donor Atoms. Journal of Organic Chemistry, 1997, 62, 4687-4691.	3.2	176
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.	2.5	170
21	Structures, Energies, Bonding, and NMR Properties of Pnicogen Complexes H₂XP:NXH₂(X â••H, CH₃, NH₂, OH, F, Cl). Journal of Physical Chemistry A, 2011, 115, 13724-13731.	2.5	170
22	Beryllium Bonds, Do They Exist?. Journal of Chemical Theory and Computation, 2009, 5, 2763-2771.	5.3	158
23	Theoretical Study of Strong Hydrogen Bonds between Neutral Molecules:â€‰ The Case of Amine Oxides and Phosphine Oxides as Hydrogen Bond Acceptors. Journal of Physical Chemistry A, 1999, 103, 272-279.	2.5	154
24	Molecular polarization potential maps of the nucleic acid bases. International Journal of Quantum Chemistry, 1996, 57, 123-135.	2.0	144
25	Bond Lengthâ€“Electron Density Relationships: From Covalent Bonds to Hydrogen Bond Interactions. Structural Chemistry, 1998, 9, 243-247.	2.0	143
26	Spodium Bonds: Noncovalent Interactions Involving Groupâ€…12 Elements. Angewandte Chemie - International Edition, 2020, 59, 17482-17487.	13.8	136
27	31Pâ€“31P spinâ€“spin coupling constants for pnicogen homodimers. Chemical Physics Letters, 2011, 512, 184-187.	2.6	132
28	Pnicogen Bonded Complexes of PO₂X (X = F, Cl) with Nitrogen Bases. Journal of Physical Chemistry A, 2013, 117, 10497-10503.	2.5	129
29	Intramolecular Hydrogen Bonds inortho-Substituted Hydroxybenzenes and in 8-Susbtituted 1-Hydroxynaphthalenes:Â Can a Methyl Group Be an Acceptor of Hydrogen Bonds?. Journal of Physical Chemistry A, 2001, 105, 10462-10467.	2.5	126
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 â^' An Experimental and Theoretical Study. European Journal of Organic Chemistry, 2001, 2001, 3013.	2.4	121
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	116
33	Theoretical Study of the Influence of Electric Fields on Hydrogen-Bonded Acidâ^'Base Complexes. Journal of Physical Chemistry A, 1997, 101, 9791-9800.	2.5	114
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.	1.9	109
35	Are resonance-assisted hydrogen bonds â€˜resonance assistedâ€™? A theoretical NMR study. Chemical Physics Letters, 2005, 411, 411-415.	2.6	106
36	Influence of Hydrogen Bonds on the PÂ·Â·Â·P Pnicogen Bond. Journal of Chemical Theory and Computation, 2012, 8, 2320-2327.	5.3	106

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37	Fluorineâ€“Fluorine Interactions: NMR and AIM Analysis. Structural Chemistry, 2004, 15, 117-120.	2.0	103
38	Cooperativity in Tetrel Bonds. Journal of Physical Chemistry A, 2016, 120, 648-656.	2.5	103
39	Intermolecular Weak Interactions in HTeXH Dimers (X=O, S, Se, Te): Hydrogen Bonds, Chalcogenâ€“Chalcogen Contacts and Chiral Discrimination. ChemPhysChem, 2012, 13, 496-503.	2.1	101
40	A new avenue to the synthesis of highly substituted pyrroles: synthesis from N-propargylamines. RSC Advances, 2016, 6, 18619-18631.	3.6	99
41	Electrostatics at the Origin of the Stability of Phosphateâ€Phosphate Complexes Locked by Hydrogen Bonds. ChemPhysChem, 2012, 13, 1421-1424.	2.1	97
42	Inverse Hydrogen-Bonded Complexes. Journal of Physical Chemistry A, 1997, 101, 4236-4244.	2.5	95
43	Dihydrogen bonds (Aâ€“Hâ‹¯Hâ€“B). Chemical Communications, 1996, , 1633-1634.	4.1	94
44	Pnicogen-Bonded Cyclic Trimers (PH₂X)₃ with X = F, Cl, OH, NC, CN, CH₃, H, and BH₂. Journal of Physical Chemistry A, 2013, 117, 4981-4987.	2.5	94
45	The Paradox of Hydrogen-Bonded Anionâ€“Anion Aggregates in Oxoanions: A Fundamental Electrostatic Problem Explained in Terms of ElectrophilicÂ·Â·Â·Nucleophilic Interactions. Journal of Physical Chemistry A, 2015, 119, 183-194.	2.5	94
46	Supramolecular structure of 1H-pyrazoles in the solid state: a crystallographic and ab initio study. Acta Crystallographica Section B: Structural Science, 2000, 56, 1018-1028.	1.8	93
47	Synthesis, Characterization, Molecular Structure and Theoretical Studies of Axially Fluoroâ€Substituted Subazaporphyrins. Chemistry - A European Journal, 2008, 14, 1342-1350.	3.3	93
48	Ab Initio Study of the Structural, Energetic, Bonding, and IR Spectroscopic Properties of Complexes with Dihydrogen Bonds. Journal of Physical Chemistry A, 2002, 106, 9325-9330.	2.5	90
49	Interplay of Fâ€“H^{...}F Hydrogen Bonds and P^{...}N Pnicogen Bonds. Journal of Physical Chemistry A, 2012, 116, 9205-9213.	2.5	90
50	Title is missing!. Structural Chemistry, 1998, 9, 187-202.	2.0	89
51	Self-Discrimination of Enantiomers in Hydrogen-Bonded Dimers. Journal of the American Chemical Society, 2002, 124, 1488-1493.	13.7	86
52	Competition and Interplay between Ïƒ-Hole and Ï€-Hole Interactions: A Computational Study of 1:1 and 1:2 Complexes of Nitryl Halides (O₂NX) with Ammonia. Journal of Physical Chemistry A, 2012, 116, 5199-5206.	2.5	86
53	Theoretical Study of Dihydrogen Bonds between (XH)2, X = Li, Na, BeH, and MgH, and Weak Hydrogen Bond Donors (HCN, HNC, and HCCH). Journal of Physical Chemistry A, 2006, 110, 10279-10286.	2.5	85
54	Carbenes and Silylenes as Hydrogen Bond Acceptors. The Journal of Physical Chemistry, 1996, 100, 19367-19370.	2.9	84

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55	Atropisomerism and Axial Chirality in Heteroaromatic Compounds. Advances in Heterocyclic Chemistry, 2012, , 1-188.	1.7	84
56	Single Electron Pnicogen Bonded Complexes. Journal of Physical Chemistry A, 2014, 118, 947-953.	2.5	84
57	A Solid-State NMR, X-ray Diffraction, and ab Initio Computational Study of Hydrogen-Bond Structure and Dynamics of Pyrazole-4-Carboxylic Acid Chains. Journal of the American Chemical Society, 2001, 123, 7898-7906.	13.7	83
58	Do Traditional, Chlorine-shared, and Ion-pair Halogen Bonds Exist? An ab Initio Investigation of FCl:CNX Complexes. Journal of Physical Chemistry A, 2010, 114, 12958-12962.	2.5	81
59	Modulating the Strength of Hydrogen Bonds through Beryllium Bonds. Journal of Chemical Theory and Computation, 2012, 8, 2293-2300.	5.3	81
60	Exploring (NH₂F)₂, H₂FP:NFH₂, and (PH₂F)₂ Potential Surfaces: Hydrogen Bonds or Pnicogen Bonds?. Journal of Physical Chemistry A, 2013, 117, 183-191.	2.5	81
61	New page to access pyridine derivatives: synthesis from N-propargylamines. RSC Advances, 2016, 6, 71662-71675.	3.6	81
62	Cooperative and Diminutive Unusual Weak Bonding In F₃CXÂ·Â·Â·HMgHÂ·Â·Â·Y and F₃CXÂ·Â·Â·YÂ·Â·Â·HMgH Trimers (X = Cl, Br; Y = HCN, and HNC). Journal of Physical Chemistry A, 2010, 114, 12106-12111.	2.5	80
63	Theoretical study of the HXYH dimers (X,â€‰Yâ€‰=â€‰O, S, Se). Hydrogen bonding and chalcogenâ€“chalcogen interactions. Molecular Physics, 2011, 109, 2543-2552.	1.7	80
64	Open Bis(triazolium) Structural Motifs as a Benchmark To Study Combined Hydrogen- and Halogen-Bonding Interactions in Oxoanion Recognition Processes. Journal of Organic Chemistry, 2014, 79, 6959-6969.	3.2	80
65	Structures, Binding Energies, and Spinâ€“Spin Coupling Constants of Geometric Isomers of Pnicogen Homodimers (PHFX)₂, X = F, Cl, CN, CH₃, NC. Journal of Physical Chemistry A, 2012, 116, 3056-3060.	2.5	79
66	Review on DFT and ab initio Calculations of Scalar Coupling Constants. International Journal of Molecular Sciences, 2003, 4, 64-92.	4.1	78
67	A review with comprehensive data on experimental indirect scalar NMR spinâ€“spin coupling constants across hydrogen bonds. Magnetic Resonance in Chemistry, 2008, 46, 599-624.	1.9	78
68	How To Determine Whether Intramolecular HÂ·Â·Â·H Interactions Can Be Classified as Dihydrogen Bonds. Journal of Physical Chemistry A, 2008, 112, 2721-2727.	2.5	77
69	Pnicogen Bonds between Xâ•PH₃ (X = O, S, NH, CH₂) and Phosphorus and Nitrogen Bases. Journal of Physical Chemistry A, 2014, 118, 1527-1537.	2.5	77
70	Charged versus Neutral Hydrogenâ€Bonded Complexes: Is There a Difference in the Nature of the Hydrogen Bonds?. Chemistry - A European Journal, 2016, 22, 9226-9234.	3.3	77
71	Ab initio hybrid DFTâ€“GIAO calculations of the shielding produced by carbonâ€“carbon bonds and aromatic rings in 1H NMR spectroscopy. New Journal of Chemistry, 1998, 22, 381-385.	2.8	76
72	Study of the reaction of chalcone analogs of dehydroacetic acid and o-aminothiophenol: synthesis and structure of 1,5-benzothiazepines and 1,4-benzothiazines. Tetrahedron, 2005, 61, 6642-6651.	1.9	76

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73	Topological Properties of the Electrostatic Potential in Weak and Moderate NÂ·Â·Â·H Hydrogen Bonds. Journal of Physical Chemistry A, 2007, 111, 6425-6433.	2.5	75
74	Orthogonal interactions between nitryl derivatives and electron donors: pnictogen bonds. Physical Chemistry Chemical Physics, 2013, 15, 14310.	2.8	75
75	Influence of Substituent Effects on the Formation of PÂ·Â·Â·Cl Pnicogen Bonds or Halogen Bonds. Journal of Physical Chemistry A, 2014, 118, 2360-2366.	2.5	75
76	GIAO Calculations of Chemical Shifts in Heterocyclic Compounds. Structural Chemistry, 2003, 14, 377-389.	2.0	74
77	Pnicogen and hydrogen bonds: complexes between PH3X+ and PH2X systems. Physical Chemistry Chemical Physics, 2015, 17, 3261-3272.	2.8	74
78	Effects of fluorine substitution on hydrogen bond interactions. Journal of Fluorine Chemistry, 2000, 101, 233-238.	1.7	73
79	CarbonÂ·Â·Â·Carbon Weak Interactions. Journal of Physical Chemistry A, 2009, 113, 8387-8393.	2.5	73
80	Substituent Effects on the Cooperativity of Halogen Bonding. Journal of Physical Chemistry A, 2013, 117, 5551-5557.	2.5	73
81	Novel routes to quinoline derivatives from N-propargylamines. RSC Advances, 2016, 6, 49730-49746.	3.6	73
82	Possibility of sensing, adsorbing, and destructing the Tabun-2D-skeletal (Tabun nerve agent) by C20 fullerene and its boron and nitrogen doped derivatives. Synthetic Metals, 2016, 220, 606-611.	3.9	73
83	Cross-Dehydrogenative Câ€“H/Sâ€“H Coupling Reactions. Topics in Current Chemistry, 2018, 376, 39.	5.8	72
84	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.	6.4	71
85	Theoretical Study of CH.cntdot..cntdot..cntdot.O Hydrogen Bonds in H2O-CH3F, H2O-CH2F2, and H2O-CHF3. The Journal of Physical Chemistry, 1995, 99, 6457-6460.	2.9	70
86	A computational study of the cooperativity in clusters of interhalogen derivatives. Structural Chemistry, 2009, 20, 63-71.	2.0	70
87	Effect of an external electric field on the dissociation energy and the electron density properties: The case of the hydrogen bonded dimer HFâ‹¯HF. Journal of Chemical Physics, 2009, 130, 044104.	3.0	70
88	N-Propargylic Î²-enaminocarbonyls: powerful and versatile building blocks in organic synthesis. RSC Advances, 2017, 7, 13198-13211.	3.6	70
89	Nanocomposite of ZIF-67 metalâ€“organic framework with reduced graphene oxide nanosheets for high-performance supercapacitor applications. Journal of Materials Science: Materials in Electronics, 2017, 28, 18040-18048.	2.2	69
90	Selective sensing of ozone and the chemically active gaseous species of the troposphere by using the C20 fullerene and graphene segment. Talanta, 2017, 162, 505-510.	5.5	69

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91	Field effects on dihydrogen bonded systems. Chemical Physics Letters, 1997, 275, 423-428.	2.6	68
92	Pnicogen-Bonded Anionic Complexes. Journal of Physical Chemistry A, 2014, 118, 3386-3392.	2.5	68
93	A DFT study on electronic and optical properties of aspirin-functionalized B12N12 fullerene-like nanocluster. Structural Chemistry, 2017, 28, 735-748.	2.0	68
94	Recent developments in decarboxylative cross-coupling reactions between carboxylic acids and Nâ€“H compounds. RSC Advances, 2019, 9, 8964-8976.	3.6	68
95	Title is missing!. International Journal of Quantum Chemistry, 1996, 57, 123.	2.0	68
96	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.	3.2	67
97	Periodic Trends in Bond Dissociation Energies. A Theoretical Study. Journal of Physical Chemistry A, 2005, 109, 4359-4365.	2.5	67
98	Properties of Complexes H₂Câ•(X)P:PXH₂, for X = F, Cl, OH, CN, NC, CCH, H, CH₃, and BH₂: PÂ·Â·Â·P Pnicogen Bonding at Ïƒ-Holes and Ï€-Holes. Journal of Physical Chemistry A, 2013, 117, 11592-11604.	2.5	67
99	Phosphorus As a Simultaneous Electron-Pair Acceptor in Intermolecular PÂ·Â·Â·N Pnicogen Bonds and Electron-Pair Donor to Lewis Acids. Journal of Physical Chemistry A, 2013, 117, 3133-3141.	2.5	66
100	A study of the tautomerism of Î²-dicarbonyl compounds with special emphasis on curcuminoids. Tetrahedron, 2008, 64, 8089-8094.	1.9	65
101	Characterizing Complexes with Pnicogen Bonds Involving sp² Hybridized Phosphorus Atoms: (H₂Câ•PX)₂ with X = F, Cl, OH, CN, NC, CCH, H, CH₃, and BH₂. Journal of Physical Chemistry A, 2013, 117, 6893-6903.	2.5	65
102	Tracing environment effects that influence the stability of anionâ€“anion complexes: The case of phosphateâ€“phosphate interactions. Chemical Physics Letters, 2013, 555, 106-109.	2.6	64
103	Borophene as an electronic sensor for metronidazole drug: A computational study. Journal of Molecular Graphics and Modelling, 2020, 96, 107539.	2.4	64
104	Strategies for indirect computer-aided drug design. Pharmaceutical Research, 1993, 10, 475-486.	3.5	63
105	Discrimination of hydrogen-bonded complexes with axial chirality. Journal of Chemical Physics, 2002, 117, 6463-6468.	3.0	63
106	Influence of Intermolecular Hydrogen Bonds on the Tautomerism of Pyridine Derivatives. Journal of Organic Chemistry, 2002, 67, 1515-1519.	3.2	63
107	A theoretical study of the tautomerism and ionization of 5-substituted NH-tetrazoles. Computational and Theoretical Chemistry, 2004, 668, 123-132.	1.5	63
108	On the Existence of Î±-Agostic Bonds:â€‰ Bonding Analyses of Titanium Alkyl Complexes. Organometallics, 2006, 25, 5638-5647.	2.3	63

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109	New protocols to access imidazoles and their ring fused analogues: synthesis from N-propargylamines. RSC Advances, 2017, 7, 7079-7091.	3.6	63
110	Transition-metal-catalyzed Câ€“N cross-coupling reactions of N-unsubstituted sulfoximines: a review. Journal of Sulfur Chemistry, 2018, 39, 674-698.	2.0	61
111	The structure of halogeno-1,2,4-triazoles in the solid state and in solution. New Journal of Chemistry, 2001, 25, 1061-1068.	2.8	60
112	Noncovalent interactions in dimers and trimers of SO3 and CO. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	60
113	Intramolecular pnicogen interactions in phosphorus and arsenic analogues of proton sponges. Physical Chemistry Chemical Physics, 2014, 16, 15900-15909.	2.8	60
114	Atropisomerism and conformational aspects of meso-tetraarylporphyrins and related compounds. Journal of Porphyrins and Phthalocyanines, 2011, 15, 1-28.	0.8	59
115	The Pnicogen Bond in Review: Structures, Binding Energies, Bonding Properties, and Spin-Spin Coupling Constants of Complexes Stabilized by Pnicogen Bonds. Challenges and Advances in Computational Chemistry and Physics, 2015, , 191-263.	0.6	59
116	Influence of protonation on the electron density derived properties. Arkivoc, 2005, 2005, 305-320.	0.5	59
117	The tautomerism of Omeprazole in solution: a1H and13C NMR study. Magnetic Resonance in Chemistry, 2004, 42, 712-714.	1.9	58
118	Homo- and heterochiral dimers (PHFX)2, X=Cl, CN, CH3, NC: To what extent do they differ?. Chemical Physics Letters, 2012, 538, 14-18.	2.6	58
119	Chalcogen Bonds in Complexes of SOXY (X, Y = F, Cl) with Nitrogen Bases. Journal of Physical Chemistry A, 2015, 119, 535-541.	2.5	58
120	Cross-Dehydrogenative Coupling Reactions Between P(O)â€“H and Xâ€“H (Xâ€‰=â€‰S, N, O, P) Bonds. Topics in Current Chemistry, 2018, 376, 23.	5.8	58
121	Recent advances in sulfurâ€“nitrogen bond formation via cross-dehydrogenative coupling reactions. RSC Advances, 2018, 8, 18456-18469.	3.6	58
122	Hydrogen Bond vs Proton Transfer between Neutral Molecules in the Gas Phase. Journal of Physical Chemistry A, 2001, 105, 7481-7485.	2.5	57
123	The azido-tetrazole and diazo-1,2,3-triazole tautomerism in six-membered heteroaromatic rings and their relationships with aromaticity: Azines and perimidine. Tetrahedron, 2010, 66, 2863-2868.	1.9	57
124	Theoretical estimation of the annular tautomerism of indazoles. Journal of Physical Organic Chemistry, 2005, 18, 719-724.	1.9	56
125	Theoretical Study of HCN and HNC Neutral and Charged Clusters. Journal of Physical Chemistry B, 2005, 109, 18189-18194.	2.6	55
126	Can Conventional Bases and Unsaturated Hydrocarbons Be Converted into Gasâ€Phase Superacids That Are Stronger than Most of the Known Oxyacids? The Role of Beryllium Bonds. Chemistry - A European Journal, 2013, 19, 11637-11643.	3.3	55

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127	1,2-Proton shifts in pyrazole and related systems: a computational study of [1,5]-sigmatropic migrations of hydrogen and related phenomenaâ€Šâ€. Journal of the Chemical Society Perkin Transactions II, 1998, , 2497-2504.	0.9	53
128	Aromatic Systems as Charge Insulators:Â Their Simultaneous Interaction with Anions and Cations. Journal of Physical Chemistry A, 2003, 107, 9428-9433.	2.5	52
129	Interaction Energies and NMR Indirect Nuclear Spinâ^'Spin Coupling Constants in Linear HCN and HNC Complexes. Journal of Physical Chemistry A, 2005, 109, 6555-6564.	2.5	52
130	Simultaneous Interaction of Tetrafluoroethene with Anions and Hydrogen-Bond Donors: A Cooperativity Study. Journal of Chemical Theory and Computation, 2009, 5, 1186-1194.	5.3	52
131	Energetic vs Synergetic Stability: A Theoretical Study. Journal of Physical Chemistry A, 2009, 113, 3266-3273.	2.5	52
132	FCl:PCX Complexes: Old and New Types of Halogen Bonds. Journal of Physical Chemistry A, 2012, 116, 2300-2308.	2.5	51
133	A GIAO/DFT study of1H,13C and15N shieldings in amines and its relevance in conformational analysis. Magnetic Resonance in Chemistry, 2004, 42, 955-961.	1.9	50
134	Cooperativity and Proton Transfer in Hydrogen-Bonded Triads. ChemPhysChem, 2005, 6, 1411-1418.	2.1	50
135	Atropisomerism in the 2-Arylimino-N-(2-hydroxyphenyl)thiazoline Series:â€‰ Influence of Hydrogen Bonding on the Racemization Process. Journal of Organic Chemistry, 2008, 73, 403-411.	3.2	50
136	Intramolecular Pnicogen Interactions in PHFï£¿(CH₂)_nï£¿PHF (n=2â€“6) Systems. ChemPhysChem, 2013, 14, 1656-1665.	2.1	50
137	On the tautomerism of pyrazolones: the geminal 2J[pyrazole C-4,H-3(5)] spin coupling constant as a diagnostic tool. Tetrahedron, 2004, 60, 6791-6805.	1.9	49
138	An ab Initio Study of15Nâ^'11B Spinâ^'Spin Coupling Constants for Borazine and Selected Derivatives. Journal of Physical Chemistry A, 2006, 110, 9959-9966.	2.5	49
139	Theoretical Study of Complexes and Fluoride Cation Transfer between N2F+and Electron Donors. Journal of Physical Chemistry A, 2007, 111, 7154-7161.	2.5	49
140	Using beryllium bonds to change halogen bonds from traditional to chlorine-shared to ion-pair bonds. Physical Chemistry Chemical Physics, 2015, 17, 2259-2267.	2.8	49
141	An experimental (NMR) and theoretical (GIAO) study of the tautomerism of benzotriazole in solution. Tetrahedron, 2002, 58, 9089-9094.	1.9	48
142	A Systematic Comparison of Second-Order Polarization Propagator Approximation (SOPPA) and Equation-of-Motion Coupled Cluster Singles and Doubles (EOMâ^'CCSD) Spinâ^'Spin Coupling Constants for Selected Singly Bonded Molecules, and the Hydrides NH₃, H₂O, and HF and Their Protonated and Deprotonated Ions and Hydrogen-Bonded Complexes. Journal of Chemical Theory and Computation, 2008, 4, 967-973.	5.3	48
143	Complexes between Dihydrogen and Amine, Phosphine, and Arsine Derivatives. Hydrogen Bond versus Pnictogen Interaction. Journal of Physical Chemistry A, 2013, 117, 3243-3251.	2.5	48
144	New route to 1,4-oxazepane and 1,4-diazepane derivatives: synthesis from N-propargylamines. RSC Advances, 2016, 6, 99781-99793.	3.6	48

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145	Carbenes as Electron-Pair Donors To CO₂ for CÂ·Â·Â·C Tetrel Bonds and Câ€“C Covalent Bonds. Journal of Physical Chemistry A, 2017, 121, 4039-4047.	2.5	48
146	Solvent-free incorporation of CO₂ into 2-oxazolidinones: a review. RSC Advances, 2019, 9, 19465-19482.	3.6	48
147	Theoretical Study of the 1:1 Complexes between Carbon Monoxide and Hypohalous Acids. Journal of Physical Chemistry A, 2009, 113, 3237-3244.	2.5	47
148	Halogen, chalcogen and pnictogen interactions in (XNO₂)₂homodimers (X = F,) Tj ETQq0 0 0 rgBT /Overlock	2.8	47
149	Radicals as hydrogen bond acceptors. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1998, 102, 429-435.	0.9	46
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