Steve Scheiner

List of Publications by Year
in descending order

316 papers	18,242 citations	12303 69 h-index	17055 122 g-index
327 all docs	327 docs citations	327 times ranked	10900 citing authors

#	Article	IF	Citations
1	Definition of the hydrogen bond (IUPAC Recommendations 2011). Pure and Applied Chemistry, 2011, 83, 1637-1641.	0.9	1,449
2	Fundamental Properties of the CHÂ·Â·Â·O Interaction:Â Is It a True Hydrogen Bond?. Journal of the American Chemical Society, 1999, 121, 9411-9422.	6.6	940
3	Defining the hydrogen bond: An account (IUPAC Technical Report). Pure and Applied Chemistry, 2011, 83, 1619-1636.	0.9	856
4	Electronic structure and bonding in metal phthalocyanines, Metal=Fe, Co, Ni, Cu, Zn, Mg. Journal of Chemical Physics, 2001, 114, 9780-9791.	1.2	553
5	The Pnicogen Bond: Its Relation to Hydrogen, Halogen, and Other Noncovalent Bonds. Accounts of Chemical Research, 2013, 46, 280-288.	7.6	524
6	Electronic structure and bonding in metal porphyrins, metal=Fe, Co, Ni, Cu, Zn. Journal of Chemical Physics, 2002, 117, 205-219.	1.2	384
7	Red- versus Blue-Shifting Hydrogen Bonds:Â Are There Fundamental Distinctions?. Journal of Physical Chemistry A, 2002, 106, 1784-1789.	1.1	331
8	Comparison of Various Types of Hydrogen Bonds Involving Aromatic Amino Acids. Journal of the American Chemical Society, 2002, 124, 13257-13264.	6.6	328
9	Definition of the chalcogen bond (IUPAC Recommendations 2019). Pure and Applied Chemistry, 2019, 91, 1889-1892.	0.9	322
10	Strength of the CÎ±HÂ·Â·O Hydrogen Bond of Amino Acid Residues. Journal of Biological Chemistry, 2001, 276, 9832-9837.	1.6	267
11	Detailed comparison of the pnicogen bond with chalcogen, halogen, and hydrogen bonds. International Journal of Quantum Chemistry, 2013, 113, 1609-1620.	1.0	256
12	Influence of Hybridization and Substitution on the Properties of the CHÂ·Â·Â·O Hydrogen Bond. Journal of Physical Chemistry A, 2001, 105, 10607-10612.	1.1	224
13	Theoretical studies of proton transfers. Accounts of Chemical Research, 1985, 18, 174-180.	7.6	219
14	A new noncovalent force: Comparison of PÂ·Â·Â·N interaction with hydrogen and halogen bonds. Journal of Chemical Physics, 2011, 134, 094315.	1.2	205
15	Comparison of Cooperativity in CHÂ·Â·Â·O and OHÂ·Â·Â·O Hydrogen Bonds. Journal of Physical Chemistry A, 2004, 108, 9161-9168.	1.1	183
16	Sensitivity of pnicogen, chalcogen, halogen and H-bonds to angular distortions. Chemical Physics Letters, 2012, 532, 31-35.	1.2	181
17	Effects of Substituents upon the PÂ·Â·Â·N Noncovalent Interaction: The Limits of Its Strength. Journal of Physical Chemistry A, 2011, 115, 11202-11209.	1.1	172
18	Theoretical Studies of Excited State Proton Transfer in Small Model Systems. Journal of Physical Chemistry A, 2000, 104, 5898-5909.	1.1	171

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19	Weak H-bonds. Comparisons of CHâ‹¯O to NHâ‹¯O in proteins and PHâ‹¯N to direct Pâ‹¯N interactions. Physical Chemistry Chemical Physics, 2011, 13, 13860.	1.3	163
20	Proton transfers in hydrogen-bonded systems. Cationic oligomers of water. Journal of the American Chemical Society, 1981, 103, 315-320.	6.6	151
21	Effects of Charge and Substituent on the SÂ·Â·Â·N Chalcogen Bond. Journal of Physical Chemistry A, 2014, 118, 3183-3192.	1.1	144
22	The Nonexistence of Specially Stabilized Hydrogen Bonds in Enzymes. Journal of the American Chemical Society, 1995, 117, 6970-6975.	6.6	142
23	Correction of the basis set superposition error in SCF and MP2 interaction energies. The water dimer. Journal of Chemical Physics, 1986, 84, 6328-6335.	1.2	128
24	Substituent Effects on ClÂ·Â·Â·N, SÂ·Â·Â·N, and PÂ·Â·Â·N Noncovalent Bonds. Journal of Physical Chemistry A, 2012, 116, 3487-3497.	1.1	127
25	SHÂ·Â·Â·N and SHÂ·Â·Â·P blue-shifting H-bonds and NÂ·Â·Â·P interactions in complexes pairing HSN with amines and phosphines. Journal of Chemical Physics, 2011, 134, 024312.	1.2	126
26	Contributions of NHÂ·Â·Â·O and CHÂ·Â·Â·O Hydrogen Bonds to the Stability of Î²-Sheets in Proteins. Journal of Physical Chemistry B, 2006, 110, 18670-18679.	1.2	112
27	Can a Câ€“HÂ·Â·Â·O Interaction Be a Determinant of Conformation?. Journal of the American Chemical Society, 2012, 134, 12064-12071.	6.6	110
28	Sensitivity of noncovalent bonds to intermolecular separation: hydrogen, halogen, chalcogen, and pnicogen bonds. CrystEngComm, 2013, 15, 3119-3124.	1.3	109
29	Systematic Elucidation of Factors That Influence the Strength of Tetrel Bonds. Journal of Physical Chemistry A, 2017, 121, 5561-5568.	1.1	108
30	Can two trivalent N atoms engage in a direct Nâ‹¯N noncovalent interaction?. Chemical Physics Letters, 2011, 514, 32-35.	1.2	105
31	Abilities of Different Electron Donors (D) to Engage in a PÂ·Â·Â·D Noncovalent Interaction. Journal of Physical Chemistry A, 2011, 115, 11101-11110.	1.1	103
32	On the properties of Xâ‹…â‹…â‹…â‹…N noncovalent interactions for first-, second-, and third-row X atoms. Journal of Chemical Physics, 2011, 134, 164313.	1.2	100
33	Comparison of Ï€-hole tetrel bonding with Ïƒ-hole halogen bonds in complexes of XCN (X = F, Cl, Br, I) and NH₃. Physical Chemistry Chemical Physics, 2016, 18, 3581-3590.	1.3	99
34	Insertion of Lithium Ions into Carbon Nanotubes:Â An ab Initio Study. Journal of Physical Chemistry A, 2001, 105, 10397-10403.	1.1	98
35	Highly Selective Halide Receptors Based on Chalcogen, Pnicogen, and Tetrel Bonds. Chemistry - A European Journal, 2016, 22, 18850-18858.	1.7	98
36	Comparison of tetrel bonds in neutral and protonated complexes of pyridineTF₃and furanTF₃(T = C, Si, and Ge) with NH₃. Physical Chemistry Chemical Physics, 2017, 19, 5550-5559.	1.3	98

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37	Chalcogen Bonding between Tetravalent SF₄ and Amines. Journal of Physical Chemistry A, 2014, 118, 10849-10856.	1.1	97
38	Comparison between hydrogen and dihydrogen bonds among H3BNH3, H2BNH2, and NH3. Journal of Chemical Physics, 2003, 119, 1473-1482.	1.2	95
39	Proton Transfer Properties of Imidazole. The Journal of Physical Chemistry, 1996, 100, 9235-9241.	2.9	94
40	Sulfurâ€“Oxygen Chalcogen Bonding Mediates AdoMet Recognition in the Lysine Methyltransferase SET7/9. ACS Chemical Biology, 2016, 11, 748-754.	1.6	93
41	Relative Strengths of NHÂ·Â·O and CHÂ·Â·O Hydrogen Bonds between Polypeptide Chain Segments. Journal of Physical Chemistry B, 2005, 109, 16132-16141.	1.2	92
42	Effect of Solvent upon CHÂ·Â·Â·O Hydrogen Bonds with Implications for Protein Folding. Journal of Physical Chemistry B, 2005, 109, 3681-3689.	1.2	92
43	Effects of multiple substitution upon the Pâ‹¯N noncovalent interaction. Chemical Physics, 2011, 387, 79-84.	0.9	92
44	Conservation and Functional Importance of Carbonâ€“Oxygen Hydrogen Bonding in AdoMet-Dependent Methyltransferases. Journal of the American Chemical Society, 2013, 135, 15536-15548.	6.6	92
45	Comparison of CHÂ·Â·Â·O, SHÂ·Â·Â·O, Chalcogen, and Tetrel Bonds Formed by Neutral and Cationic Sulfur-Containing Compounds. Journal of Physical Chemistry A, 2015, 119, 9189-9199.	1.1	92
46	Theoretical study of hydrogen bonding and proton transfer in the ground and lowest excited singlet states of tropolone. Journal of Chemical Physics, 1994, 101, 9755-9765.	1.2	91
47	Electronic structure and bonding in unligated and ligated FeII porphyrins. Journal of Chemical Physics, 2002, 116, 3635-3645.	1.2	88
48	Origins and properties of the tetrel bond. Physical Chemistry Chemical Physics, 2021, 23, 5702-5717.	1.3	88
49	Noncovalent Ï€â‹¯Ï€ Stacking and CH⋯Ï€ Interactions of Aromatics on the Surface of Single-Wall Carbon Nanotubes: An MP2 Study. Journal of Physical Chemistry C, 2008, 112, 20070-20075.	1.5	87
50	Excited-State Energetics and Proton-Transfer Barriers in Malonaldehyde. The Journal of Physical Chemistry, 1994, 98, 3582-3587.	2.9	86
51	Hydrogen Bonding and Proton Transfer in the Ground and Lowest Excited Singlet States of o-Hydroxyacetophenone. The Journal of Physical Chemistry, 1995, 99, 642-649.	2.9	86
52	Boronâ‹¯Nitrogen (BN) Substitution of Fullerenes:Â C60to C12B24N24CBN Ball. Journal of Physical Chemistry A, 2002, 106, 2970-2978.	1.1	86
53	Comparison of Pâ‹¯D (D = P,N) with other noncovalent bonds in molecular aggregates. Journal of Chemical Physics, 2011, 135, 184306.	1.2	85
54	Critical assessment of density functional methods for study of proton transfer processes. (FHF)â‹¯. Chemical Physics Letters, 1995, 234, 159-164.	1.2	82

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55	Comparison of proton transfers in heterodimers and homodimers of NH3 and OH2. Journal of Chemical Physics, 1982, 77, 4039-4050.	1.2	81
56	Primary and secondary basis set superposition error at the SCF and MP2 levels. H3Nâ€â€Li+ and H2Oâ€â€Li+. Journal of Chemical Physics, 1987, 87, 1194-1204.	1.2	81
57	Tetrel, chalcogen, and CHâ‹…â‹…O hydrogen bonds in complexes pairing carbonyl-containing molecules with 1, 2, and 3 molecules of CO2. Journal of Chemical Physics, 2015, 142, 034307.	1.2	81
58	Ab initio comparison of H bonds and Li bonds. Complexes of LiF, LiCl, HF, and HCl with NH3. Journal of Chemical Physics, 1984, 81, 4014-4017.	1.2	80
59	Performance assessment of density-functional methods for study of charge-transfer complexes. Journal of Computational Chemistry, 2003, 24, 623-631.	1.5	79
60	Comparison of Morokuma and perturbation theory approaches to decomposition of interaction energy. (NH4)+â€¦NH3. Chemical Physics Letters, 1990, 166, 57-64.	1.2	77
61	The potential energy surface of (NH3)2. Journal of Chemical Physics, 1986, 84, 341-347.	1.2	76
62	Hydrogen bonding and proton transfers involving triply bonded atoms. Acetylene and hydrocyanic acid. Journal of the American Chemical Society, 1987, 109, 4199-4206.	6.6	76
63	Hydrogen bonding and proton transfers of the amide group. Journal of the American Chemical Society, 1993, 115, 1958-1963.	6.6	76
64	Intermolecular HÂ·Â·Â·H Bonding and Proton Transfer in Semisandwich Re and Ru Complexes. Journal of Physical Chemistry A, 1998, 102, 4813-4818.	1.1	76
65	Effect of adjoining aromatic ring upon excited state proton transfer, o-hydroxybenzaldehyde. Computational and Theoretical Chemistry, 1999, 467, 37-49.	1.5	76
66	Proton transfers in hydrogen-bonded systems. 2. Electron correlation effects in diamminehydrogen(1+). Journal of the American Chemical Society, 1981, 103, 2169-2173.	6.6	75
67	Effects of basis set and electron correlation on the calculated properties of the ammonia dimer. Journal of Chemical Physics, 1984, 81, 407-409.	1.2	74
68	Intermolecular MHÂ·Â·Â·HR Bonding in Monohydride Mo and W Complexes. Journal of Physical Chemistry A, 1998, 102, 260-269.	1.1	74
69	Mo/llerâ€“Plesset treatment of electron correlation effects in (HOHOH)â¯. Journal of Chemical Physics, 1982, 77, 4586-4593.	1.2	72
70	Hydrogen bonding and proton transfers involving the carboxylate group. Journal of the American Chemical Society, 1989, 111, 23-31.	6.6	71
71	Basis sets for molecular interactions. 2. Application to H3N?HF, H3N?HOH, H2O?HF, (NH3)2, and H3CH?OH2. Journal of Computational Chemistry, 1987, 8, 674-682.	1.5	70
72	Effects of carbon chain substituents on the Pâ‹¯N noncovalent bond. Chemical Physics Letters, 2012, 536, 30-33.	1.2	69

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73	Comparative Strengths of Tetrel, Pnicogen, Chalcogen, and Halogen Bonds and Contributing Factors. Molecules, 2018, 23, 1681.	1.7	69
74	Halogen, Chalcogen, and Pnicogen Bonding Involving Hypervalent Atoms. Chemistry - A European Journal, 2018, 24, 8167-8177.	1.7	68
75	Implications of monomer deformation for tetrel and pnicogen bonds. Physical Chemistry Chemical Physics, 2018, 20, 8832-8841.	1.3	67
76	Structure, energetics, and vibrational spectrum of H2Oâ€“HCl. Journal of Chemical Physics, 1987, 87, 5928-5936.	1.2	66
77	DFT Calculations and Spectral Measurements of Charge-Transfer Complexes Formed by Aromatic Amines and Nitrogen Heterocycles with Tetracyanoethylene and Chloranil. Journal of Physical Chemistry A, 2003, 107, 8939-8948.	1.1	66
78	Coordination of anions by noncovalently bonded Ïƒ-hole ligands. Coordination Chemistry Reviews, 2020, 405, 213136.	9.5	66
79	Ab initio study of proton transfers including effects of electron correlation. International Journal of Quantum Chemistry, 1983, 23, 739-751.	1.0	61
80	Intramolecular SÂ·Â·Â·O Chalcogen Bond as Stabilizing Factor in Geometry of Substituted Phenyl-SF3 Molecules. Journal of Organic Chemistry, 2015, 80, 2356-2363.	1.7	61
81	Ab initio molecular orbital estimates of charge partitioning between Bjerrum and ionic defects in ice. The Journal of Physical Chemistry, 1983, 87, 4267-4272.	2.9	60
82	Noncovalent interactions in dimers and trimers of SO3 and CO. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	60
83	Proton transfer between phenol and ammonia in ground and excited electronic states. Chemical Physics Letters, 1996, 262, 567-572.	1.2	59
84	Spectroscopic and Structural Signature of the CHâ‹¯O Hydrogen Bond. Journal of Physical Chemistry A, 2008, 112, 11854-11860.	1.1	59
85	Effects of molecular charge and methyl substitution on proton transfer between oxygen atoms. Journal of the American Chemical Society, 1984, 106, 6266-6273.	6.6	58
86	Chalcogen Bonds in Complexes of SOXY (X, Y = F, Cl) with Nitrogen Bases. Journal of Physical Chemistry A, 2015, 119, 535-541.	1.1	58
87	Magnitude and Mechanism of Charge Enhancement of CHÂ·Â·O Hydrogen Bonds. Journal of Physical Chemistry A, 2013, 117, 10551-10562.	1.1	57
88	Comparison of halide receptors based on H, halogen, chalcogen, pnicogen, and tetrel bonds. Faraday Discussions, 2017, 203, 213-226.	1.6	57
89	Assembly of Effective Halide Receptors from Components. Comparing Hydrogen, Halogen, and Tetrel Bonds. Journal of Physical Chemistry A, 2017, 121, 3606-3615.	1.1	56
90	Steric Crowding in Tetrel Bonds. Journal of Physical Chemistry A, 2018, 122, 2550-2562.	1.1	55

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91	Effects of external ions on the energetics of proton transfers across hydrogen bonds. The Journal of Physical Chemistry, 1985, 89, 262-266.	2.9	53
92	Activation and Cleavage of Hâ^'R Bonds through Intermolecular H...H Bonding upon Reaction of Proton Donors HR with 18-Electron Transition Metal Hydrides. Journal of Physical Chemistry A, 1999, 103, 514-520.	1.1	52
93	Substituent Effects in the Noncovalent Bonding of SO₂ to Molecules Containing a Carbonyl Group. The Dominating Role of the Chalcogen Bond. Journal of Physical Chemistry A, 2014, 118, 3835-3845.	1.1	51
94	Boronâ^'Nitrogen (BN) Substitution Patterns in C/BN Hybrid Fullerenes:â€‰ C60-2x(BN)x (x = 1â^'7). Journal of Physical Chemistry A, 2001, 105, 8376-8384.	1.1	49
95	Proton transfer in the ground and first excited triplet states of malonaldehyde. The Journal of Physical Chemistry, 1992, 96, 9764-9767.	2.9	48
96	Energetics, proton transfer rates, and kinetic isotope effects in bent hydrogen bonds. Journal of the American Chemical Society, 1992, 114, 5849-5856.	6.6	48
97	Quantum mechanical test of Marcus theory. Effects of alkylation upon proton transfer. The Journal of Physical Chemistry, 1986, 90, 2969-2974.	2.9	47
98	Effects of Peripheral Substituents on the Electronic Structure and Properties of Unligated and Ligated Metal Phthalocyanines, Metal = Fe, Co, Zn. Journal of Chemical Theory and Computation, 2005, 1, 1201-1210.	2.3	46
99	The Ïâ€Tetrel Bond and its Influence on Hydrogen Bonding and Proton Transfer. ChemPhysChem, 2018, 19, 736-743.	1.0	46
100	Regium bonds between M_n clusters (M = Cu, Ag, Au and n = 2â€“6) and nucleophiles NH₃ and HCN. Physical Chemistry Chemical Physics, 2018, 20, 22498-22509.	1.3	46
101	Understanding noncovalent bonds and their controlling forces. Journal of Chemical Physics, 2020, 153, 140901.	1.2	46
102	Comparison between Tetrel Bonded Complexes Stabilized by Ïƒ and Ïâ€ Hole Interactions. Molecules, 2018, 23, 1416.	1.7	45
103	Strongly bound noncovalent (SO3)n:H2CO complexes (n = 1, 2). Physical Chemistry Chemical Physics, 2014, 16, 18974-18981.	1.3	43
104	Vibrational frequencies and intensities of Hâ€bonded and Liâ€bonded complexes. H3Nâ‹…â‹…HCl and H3Nâ‹…â‹…LiCl. Journal of Chemical Physics, 1988, 89, 3131-3138.	1.2	42
105	Proton Conduction by a Chain of Water Molecules in Carbonic Anhydrase. Journal of Physical Chemistry B, 2001, 105, 6420-6426.	1.2	42
106	Effects of Halogen, Chalcogen, Pnicogen, and Tetrel Bonds on IR and NMR Spectra. Molecules, 2019, 24, 2822.	1.7	41
107	Ab Initio investigation of the structure of hydrogen halide-amine complexes in the gas phase and in a polarizable medium. International Journal of Quantum Chemistry, 1987, 32, 47-56.	1.0	40
108	Complexation ofnSO2molecules (n= 1, 2, 3) with formaldehyde and thioformaldehyde. Journal of Chemical Physics, 2014, 140, 034302.	1.2	40

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109	SÂ·Â·Â·Ï€ Chalcogen Bonds between SF₂ or SF₄ and Câ€“C Multiple Bonds. Journal of Physical Chemistry A, 2015, 119, 5889-5897.	1.1	40
110	Analysis of the principles governing proton-transfer reactions. Carboxyl group. Journal of the American Chemical Society, 1986, 108, 7178-7186.	6.6	39
111	Cooperativity of conventional and unconventional hydrogen bonds involving imidazole. International Journal of Quantum Chemistry, 2006, 106, 843-851.	1.0	39
112	Tetrel Bonding as a Vehicle for Strong and Selective Anion Binding. Molecules, 2018, 23, 1147.	1.7	39
113	Forty years of progress in the study of the hydrogen bond. Structural Chemistry, 2019, 30, 1119-1128.	1.0	39
114	Identification of Spectroscopic Patterns of CHÂ·Â·Â·O H-Bonds in Proteins. Journal of Physical Chemistry B, 2009, 113, 10421-10427.	1.2	38
115	Analysis of the Reactivities of Protein Câˆ’H Bonds to H Atom Abstraction by OH Radical. Journal of the American Chemical Society, 2010, 132, 16450-16459.	6.6	38
116	Catalysis of the Aza-Dielsâ€“Alder Reaction by Hydrogen and Halogen Bonds. Journal of Organic Chemistry, 2016, 81, 2589-2597.	1.7	38
117	Complexing of the Ammonium Ion by Polyethers. Comparative Complexing Thermochemistry of Ammonium, Hydronium, and Alkali Cations. The Journal of Physical Chemistry, 1996, 100, 6445-6450.	2.9	37
118	The Sâ‹¯N noncovalent interaction: Comparison with hydrogen and halogen bonds. Chemical Physics Letters, 2011, 514, 36-39.	1.2	37
119	Calculating the Properties of Hydrogen Bonds by ab Initio Methods. Reviews in Computational Chemistry, 0, , 165-218.	1.5	37
120	Effects of external ions on the dynamics of proton transfer across a hydrogen bond. The Journal of Physical Chemistry, 1985, 89, 1835-1840.	2.9	36
121	Ab initiostudy of He(1S)+Cl2(Xâ€‰1Î£g,3Îu) potential energy surfaces. Journal of Chemical Physics, 1994, 101, 6800-6809.	1.2	36
122	Effects of chemical substitution upon excited state proton transfer. Fluoroderivatives of salicylaldimine. Chemical Physics, 1999, 246, 65-74.	0.9	36
123	Aerogen bonds formed between AeOF₂ (Ae = Kr, Xe) and diazines: comparisons between Ïƒ-hole and Ï€-hole complexes. Physical Chemistry Chemical Physics, 2018, 20, 4676-4687.	1.3	36
124	Studies of dispersion energy in hydrogenâ€bonded systems. H2Oâ€“HOH, H2Oâ€“HF, H3Nâ€“HF, HFâ€“HF. Journal of Chemical Physics, 1984, 80, 1535-1542.	1.2	35
125	Rules for BN-Substitution in BCNâˆ’Fullerenes. Separation of BN and C Domains. Journal of Physical Chemistry A, 2003, 107, 8630-8637.	1.1	35
126	Complexes containing CO₂and SO₂. Mixed dimers, trimers and tetramers. Physical Chemistry Chemical Physics, 2014, 16, 5142-5149.	1.3	35

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127	Substituent Effects on the Binding of Halides by Neutral and Dicationic Bis(triazolium) Receptors. Journal of Physical Chemistry A, 2015, 119, 13064-13073.	1.1	35
128	Theoretical Studies of IR and NMR Spectral Changes Induced by Sigma-Hole Hydrogen, Halogen, Chalcogen, Pnicogen, and Tetrel Bonds in a Model Protein Environment. Molecules, 2019, 24, 3329.	1.7	35
129	Excited State Intramolecular Proton Transfer in Anionic Analogues of Malonaldehyde. Journal of Physical Chemistry A, 1997, 101, 5901-5909.	1.1	34
130	The Hydrogen Bond: A Hundred Years and Counting. Journal of the Indian Institute of Science, 2020, 100, 61-76.	0.9	34
131	Ab initiostudy of the structure of guanine-cytosine base pair conformers in gas phase and polar solvents. Molecular Physics, 1995, 84, 469-480.	0.8	33
132	Competitive Halide Binding by Halogen Versus Hydrogen Bonding: Bisâ€triazole Pyridinium. Chemistry - A European Journal, 2015, 21, 13330-13335.	1.7	33
133	Factors contributing to distortion energies of bent hydrogen bonds. Implications for proton-transfer potentials. The Journal of Physical Chemistry, 1989, 93, 6565-6574.	2.9	32
134	Theoretical Investigation of the Dihydrogen Bond Linking MH2 with HCCRgF (M = Zn, Cd; Rg = Ar, Kr). Journal of Physical Chemistry A, 2005, 109, 11933-11935.	1.1	32
135	Extrapolation to the complete basis set limit for binding energies of noncovalent interactions. Computational and Theoretical Chemistry, 2012, 998, 9-13.	1.1	32
136	Noncovalent Bonds through Sigma and Pi-Hole Located on the Same Molecule. Guiding Principles and Comparisons. Molecules, 2021, 26, 1740.	1.7	32
137	Ability of IR and NMR Spectral Data to Distinguish between a Tetrel Bond and a Hydrogen Bond. Journal of Physical Chemistry A, 2018, 122, 7852-7862.	1.1	31
138	Anionâ‹…â‹…â‹…Anion Attraction in Complexes of MCl₃^{â^’} (M=Zn, Cd, Hg) with CN^{â^’}. ChemPhysChem, 2020, 21, 1119-1125.	1.0	31
139	Proton transfers in hydrogenâ€bonded systems. VI. Electronic redistributions in (N2H7)+ and (O2H5)+. Journal of Chemical Physics, 1981, 75, 5791-5801.	1.2	30
140	Calculation of barriers to proton transfer using multiconfiguration selfâ€consistentâ€field methods. I. Effects of localization. Journal of Chemical Physics, 1992, 97, 7507-7518.	1.2	30
141	Assessment of the Presence and Strength of H-Bonds by Means of Corrected NMR. Molecules, 2016, 21, 1426.	1.7	30
142	Molecular orbital study of proton transfer in (H3NHOH2)+. The Journal of Physical Chemistry, 1983, 87, 1145-1153.	2.9	29
143	Crystallographic and Computational Characterization of Methyl Tetrel Bonding in S-Adenosylmethionine-Dependent Methyltransferases. Molecules, 2018, 23, 2965.	1.7	29
144	On the ability of pnicogen atoms to engage in both Ïƒ and Ï€-hole complexes. Heterodimers of ZF2C6H5 (Zâ€‰=â€‰P, As, Sb, Bi) and NH3. Journal of Molecular Modeling, 2019, 25, 152.	0.8	29

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145	The ditetrel bond: noncovalent bond between neutral tetrel atoms. Physical Chemistry Chemical Physics, 2020, 22, 16606-16614.	1.3	29
146	How Many Pnicogen Bonds can be Formed to a Central Atom Simultaneously?. Journal of Physical Chemistry A, 2020, 124, 2046-2056.	1.1	29
147	Participation of S and Se in hydrogen and chalcogen bonds. CrystEngComm, 2021, 23, 6821-6837.	1.3	29
148	Vibrational frequencies and intensities of Hâ€bonded systems. 1:1 and 1:2 complexes of NH3 and PH3 with HF. Journal of Chemical Physics, 1987, 87, 2214-2224.	1.2	28
149	Hardness and Chemical Potential Profiles for Some Open-Shell HAB â†' HBA Type Reactions. Ab Initio and Density Functional Study. Journal of Physical Chemistry A, 1998, 102, 5967-5973.	1.1	28
150	Dual Geometry Schemes in Tetrel Bonds: Complexes between TF4 (T = Si, Ge, Sn) and Pyridine Derivatives. Molecules, 2019, 24, 376.	1.7	28
151	Switchable Aromaticity in an Isostructural Mn Phthalocyanine Series Isolated in Five Separate Redox States. Journal of the American Chemical Society, 2019, 141, 2604-2613.	6.6	28
152	Tuning the Competition between Hydrogen and Tetrel Bonds by a Magnesium Bond. ChemPhysChem, 2020, 21, 212-219.	1.0	28
153	Structure, Stability, and Bonding of BC2N:Â An ab Initio Study. Journal of Physical Chemistry A, 1998, 102, 10134-10141.	1.1	27
154	Inter- and Intramolecular Hydrogen Bonds with Transition Metal Atoms in Metallocenes of the Iron Subgroup. Organometallics, 1998, 17, 4362-4367.	1.1	27
155	Substitution Patterns in Mono-BN-Fullerenes:Â Cn(n= 20, 24, 28, 32, 36, and 40). Journal of Physical Chemistry A, 2004, 108, 7681-7685.	1.1	27
156	The Strength with Which a Peptide Group Can Form a Hydrogen Bond Varies with the Internal Conformation of the Polypeptide Chain. Journal of Physical Chemistry B, 2007, 111, 11312-11317.	1.2	27
157	Comparison of Various Means of Evaluating Molecular Electrostatic Potentials for Noncovalent Interactions. Journal of Computational Chemistry, 2018, 39, 500-510.	1.5	27
158	Chalcogen bonding of two ligands to hypervalent YF₄(Y = S, Se, Te, Po). Physical Chemistry Chemical Physics, 2019, 21, 20829-20839.	1.3	27
159	Carbene triel bonds between TrR 3 (Trâ€‰=â€‰B, Al) and Nâ€heterocyclic carbenes. International Journal of Quantum Chemistry, 2019, 119, e25867.	1.0	27
160	Comparison between proton transfers involving carbonyl and hydroxyl oxygens. The Journal of Physical Chemistry, 1985, 89, 3053-3060.	2.9	26
161	Factors influencing proton positions in biomolecules. International Journal of Quantum Chemistry, 1986, 29, 817-827.	1.0	26
162	Correlation between interaction energy and shift of the carbonyl stretching frequency. Chemical Physics Letters, 1990, 174, 179-184.	1.2	26

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