Steve Scheiner

List of Publications by Citations

304 papers	15,491 citations	66 h-index	113 g-index
327 ext. papers	16,833 ext. citations	4.1 avg, IF	7.62 L-index

#	Paper	IF	Citations
304	Definition of the hydrogen bond (IUPAC Recommendations 2011). *Pure and Applied Chemistry*, **2011**, 83, 1637-1641	2.1	1111
303	Fundamental Properties of the CH□□O Interaction: Is It a True Hydrogen Bond?. *Journal of the American Chemical Society*, **1999**, 121, 9411-9422	16.4	845
302	Defining the hydrogen bond: An account (IUPAC Technical Report). *Pure and Applied Chemistry*, **2011**, 83, 1619-1636	2.1	738
301	Electronic structure and bonding in metal phthalocyanines, Metal=Fe, Co, Ni, Cu, Zn, Mg. *Journal of Chemical Physics*, **2001**, 114, 9780-9791	3.9	508
300	The pnicogen bond: its relation to hydrogen, halogen, and other noncovalent bonds. *Accounts of Chemical Research*, **2013**, 46, 280-8	24.3	432
299	Electronic structure and bonding in metal porphyrins, metal=Fe, Co, Ni, Cu, Zn. *Journal of Chemical Physics*, **2002**, 117, 205-219	3.9	330
298	Red- versus Blue-Shifting Hydrogen Bonds: Are There Fundamental Distinctions?. *Journal of Physical Chemistry A*, **2002**, 106, 1784-1789	2.8	310
297	Comparison of various types of hydrogen bonds involving aromatic amino acids. *Journal of the American Chemical Society*, **2002**, 124, 13257-64	16.4	274
296	Strength of the Calpha H..O hydrogen bond of amino acid residues. *Journal of Biological Chemistry*, **2001**, 276, 9832-7	5.4	243
295	Detailed comparison of the pnicogen bond with chalcogen, halogen, and hydrogen bonds. *International Journal of Quantum Chemistry*, **2013**, 113, 1609-1620	2.1	230
294	Theoretical studies of proton transfers. *Accounts of Chemical Research*, **1985**, 18, 174-180	24.3	211
293	Influence of Hybridization and Substitution on the Properties of the CH□□O Hydrogen Bond. *Journal of Physical Chemistry A*, **2001**, 105, 10607-10612	2.8	210
292	A new noncovalent force: comparison of P□□N interaction with hydrogen and halogen bonds. *Journal of Chemical Physics*, **2011**, 134, 094315	3.9	189
291	Definition of the chalcogen bond (IUPAC Recommendations 2019). *Pure and Applied Chemistry*, **2019**, 91, 1889-1892	2.1	183
290	Comparison of Cooperativity in CH□□D and OH□□D Hydrogen Bonds. *Journal of Physical Chemistry A*, **2004**, 108, 9161-9168	2.8	171
289	Sensitivity of pnicogen, chalcogen, halogen and H-bonds to angular distortions. *Chemical Physics Letters*, **2012**, 532, 31-35	2.5	165
288	Theoretical Studies of Excited State Proton Transfer in Small Model Systems. *Journal of Physical Chemistry A*, **2000**, 104, 5898-5909	2.8	164

287	Effects of substituents upon the P⋯N noncovalent interaction: the limits of its strength. *Journal of Physical Chemistry A*, **2011**, 115, 11202-9	2.8	161
286	Weak H-bonds. Comparisons of CH⋯O to NH⋯O in proteins and PH⋯N to direct P⋯N interactions. *Physical Chemistry Chemical Physics*, **2011**, 13, 13860-72	3.6	153
285	Proton transfers in hydrogen-bonded systems. Cationic oligomers of water. *Journal of the American Chemical Society*, **1981**, 103, 315-320	16.4	139
284	The Nonexistence of Specially Stabilized Hydrogen Bonds in Enzymes. *Journal of the American Chemical Society*, **1995**, 117, 6970-6975	16.4	130
283	Effects of charge and substituent on the S⋯N chalcogen bond. *Journal of Physical Chemistry A*, **2014**, 118, 3183-92	2.8	126
282	Correction of the basis set superposition error in SCF and MP2 interaction energies. The water dimer. *Journal of Chemical Physics*, **1986**, 84, 6328-6335	3.9	124
281	Substituent effects on Cl⋯N, S⋯N, and P⋯N noncovalent bonds. *Journal of Physical Chemistry A*, **2012**, 116, 3487-97	2.8	119
280	SH⋯N and SH⋯P blue-shifting H-bonds and N⋯P interactions in complexes pairing HSN with amines and phosphines. *Journal of Chemical Physics*, **2011**, 134, 024312	3.9	116
279	Contributions of NH...O and CH...O hydrogen bonds to the stability of beta-sheets in proteins. *Journal of Physical Chemistry B*, **2006**, 110, 18670-9	3.4	104
278	Can two trivalent N atoms engage in a direct N?N noncovalent interaction?. *Chemical Physics Letters*, **2011**, 514, 32-35	2.5	99
277	Abilities of different electron donors (D) to engage in a P⋯D noncovalent interaction. *Journal of Physical Chemistry A*, **2011**, 115, 11101-10	2.8	97
276	Can a C-H⋯O interaction be a determinant of conformation?. *Journal of the American Chemical Society*, **2012**, 134, 12064-71	16.4	94
275	On the properties of X⋯N noncovalent interactions for first-, second-, and third-row X atoms. *Journal of Chemical Physics*, **2011**, 134, 164313	3.9	94
274	Insertion of Lithium Ions into Carbon Nanotubes: An ab Initio Study. *Journal of Physical Chemistry A*, **2001**, 105, 10397-10403	2.8	92
273	Sensitivity of noncovalent bonds to intermolecular separation: hydrogen, halogen, chalcogen, and pnicogen bonds. *CrystEngComm*, **2013**, 15, 3119-3124	3.3	91
272	Comparison between hydrogen and dihydrogen bonds among H3BNH3, H2BNH2, and NH3. *Journal of Chemical Physics*, **2003**, 119, 1473-1482	3.9	91
271	Comparison of tetrel bonds in neutral and protonated complexes of pyridineTF and furanTF (T = C, Si, and Ge) with NH. *Physical Chemistry Chemical Physics*, **2017**, 19, 5550-5559	3.6	90
270	Chalcogen bonding between tetravalent SF4 and amines. *Journal of Physical Chemistry A*, **2014**, 118, 10849-56	2.8	90

269	Effects of multiple substitution upon the P?N noncovalent interaction. *Chemical Physics*, **2011**, 387, 79-84	1.3	90
268	Systematic Elucidation of Factors That Influence the Strength of Tetrel Bonds. *Journal of Physical Chemistry A*, **2017**, 121, 5561-5568	2.8	88
267	Boron□Nitrogen (BN) Substitution of Fullerenes: C60 to C12B24N24 CBN Ball. *Journal of Physical Chemistry A*, **2002**, 106, 2970-2978	2.8	85
266	Comparison of CH□□O, SH□□O, Chalcogen, and Tetrel Bonds Formed by Neutral and Cationic Sulfur-Containing Compounds. *Journal of Physical Chemistry A*, **2015**, 119, 9189-99	2.8	81
265	Electronic structure and bonding in unligated and ligated FeII porphyrins. *Journal of Chemical Physics*, **2002**, 116, 3635-3645	3.9	81
264	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	3.9	81
263	Comparison of P□□D (D = P,N) with other noncovalent bonds in molecular aggregates. *Journal of Chemical Physics*, **2011**, 135, 184306	3.9	80
262	Relative strengths of NH..O and CH..O hydrogen bonds between polypeptide chain segments. *Journal of Physical Chemistry B*, **2005**, 109, 16132-41	3.4	80
261	Effect of solvent upon CH...O hydrogen bonds with implications for protein folding. *Journal of Physical Chemistry B*, **2005**, 109, 3681-9	3.4	80
260	Proton Transfer Properties of Imidazole. *The Journal of Physical Chemistry*, **1996**, 100, 9235-9241		80
259	Highly Selective Halide Receptors Based on Chalcogen, Pnicogen, and Tetrel Bonds. *Chemistry - A European Journal*, **2016**, 22, 18850-18858	4.8	80
258	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		78
257	Noncovalent □Stacking and CH---□Interactions of Aromatics on the Surface of Single-Wall Carbon Nanotubes: An MP2 Study. *Journal of Physical Chemistry C*, **2008**, 112, 20070-20075	3.8	77
256	Critical assessment of density functional methods for study of proton transfer processes. (FHF)□ *Chemical Physics Letters*, **1995**, 234, 159-164	2.5	77
255	Primary and secondary basis set superposition error at the SCF and MP2 levels. H3N--Li+ and H2O--Li+. *Journal of Chemical Physics*, **1987**, 87, 1194-1204	3.9	77
254	Comparison of proton transfers in heterodimers and homodimers of NH3 and OH2. *Journal of Chemical Physics*, **1982**, 77, 4039-4050	3.9	75
253	Conservation and functional importance of carbon-oxygen hydrogen bonding in AdoMet-dependent methyltransferases. *Journal of the American Chemical Society*, **2013**, 135, 15536-48	16.4	73
252	Comparison of □hole tetrel bonding with □hole halogen bonds in complexes of XCN (X = F, Cl, Br, I) and NH3. *Physical Chemistry Chemical Physics*, **2016**, 18, 3581-90	3.6	72

251	Performance assessment of density-functional methods for study of charge-transfer complexes. *Journal of Computational Chemistry*, **2003**, 24, 623-31	3.5	72
250	Intermolecular MH□□HR Bonding in Monohydride Mo and W Complexes. *Journal of Physical Chemistry A*, **1998**, 102, 260-269	2.8	72
249	Excited-State Energetics and Proton-Transfer Barriers in Malonaldehyde. *The Journal of Physical Chemistry*, **1994**, 98, 3582-3587		72
248	Effects of basis set and electron correlation on the calculated properties of the ammonia dimer. *Journal of Chemical Physics*, **1984**, 81, 407-409	3.9	72
247	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	3.9	72
246	Intermolecular H□□H Bonding and Proton Transfer in Semisandwich Re and Ru Complexes. *Journal of Physical Chemistry A*, **1998**, 102, 4813-4818	2.8	71
245	Proton transfers in hydrogen-bonded systems. 2. Electron correlation effects in diamminehydrogen(1+). *Journal of the American Chemical Society*, **1981**, 103, 2169-2173	16.4	70
244	The potential energy surface of (NH3)2. *Journal of Chemical Physics*, **1986**, 84, 341-347	3.9	69
243	Sulfur-Oxygen Chalcogen Bonding Mediates AdoMet Recognition in the Lysine Methyltransferase SET7/9. *ACS Chemical Biology*, **2016**, 11, 748-54	4.9	68
242	Tetrel, chalcogen, and CH??O hydrogen bonds in complexes pairing carbonyl-containing molecules with 1, 2, and 3 molecules of CO2. *Journal of Chemical Physics*, **2015**, 142, 034307	3.9	67
241	Effect of adjoining aromatic ring upon excited state proton transfer, o-hydroxybenzaldehyde. *Computational and Theoretical Chemistry*, **1999**, 467, 37-49		67
240	Hydrogen bonding and proton transfers of the amide group. *Journal of the American Chemical Society*, **1993**, 115, 1958-1963	16.4	66
239	Comparison of Morokuma and perturbation theory approaches to decomposition of interaction energy. (NH4)+□NH3. *Chemical Physics Letters*, **1990**, 166, 57-64	2.5	66
238	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	3.5	66
237	Hydrogen bonding and proton transfers involving triply bonded atoms. Acetylene and hydrocyanic acid. *Journal of the American Chemical Society*, **1987**, 109, 4199-4206	16.4	63
236	Effects of carbon chain substituents on the P?N noncovalent bond. *Chemical Physics Letters*, **2012**, 536, 30-33	2.5	62
235	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	2.8	62
234	Structure, energetics, and vibrational spectrum of H2O□HCl. *Journal of Chemical Physics*, **1987**, 87, 5928-5936	3.9	62

233	Hydrogen bonding and proton transfers involving the carboxylate group. *Journal of the American Chemical Society*, **1989**, 111, 23-31	16.4	60
232	Mo/llerPlesset treatment of electron correlation effects in (HOHOH)□*Journal of Chemical Physics*, **1982**, 77, 4586-4593	3.9	58
231	Ab initio molecular orbital estimates of charge partitioning between Bjerrum and ionic defects in ice. *The Journal of Physical Chemistry*, **1983**, 87, 4267-4272		57
230	Noncovalent interactions in dimers and trimers of SO3 and CO. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	56
229	Spectroscopic and structural signature of the CH-O hydrogen bond. *Journal of Physical Chemistry A*, **2008**, 112, 11854-60	2.8	56
228	Ab initio study of proton transfers including effects of electron correlation. *International Journal of Quantum Chemistry*, **1983**, 23, 739-751	2.1	56
227	Implications of monomer deformation for tetrel and pnicogen bonds. *Physical Chemistry Chemical Physics*, **2018**, 20, 8832-8841	3.6	55
226	Proton transfer between phenol and ammonia in ground and excited electronic states. *Chemical Physics Letters*, **1996**, 262, 567-572	2.5	55
225	Intramolecular S□□O chalcogen bond as stabilizing factor in geometry of substituted phenyl-SF3 molecules. *Journal of Organic Chemistry*, **2015**, 80, 2356-63	4.2	54
224	Comparative Strengths of Tetrel, Pnicogen, Chalcogen, and Halogen Bonds and Contributing Factors. *Molecules*, **2018**, 23,	4.8	54
223	Effects of molecular charge and methyl substitution on proton transfer between oxygen atoms. *Journal of the American Chemical Society*, **1984**, 106, 6266-6273	16.4	53
222	Chalcogen bonds in complexes of SOXY (X, Y = F, Cl) with nitrogen bases. *Journal of Physical Chemistry A*, **2015**, 119, 535-41	2.8	52
221	Assembly of Effective Halide Receptors from Components. Comparing Hydrogen, Halogen, and Tetrel Bonds. *Journal of Physical Chemistry A*, **2017**, 121, 3606-3615	2.8	50
220	Magnitude and mechanism of charge enhancement of CH□□O hydrogen bonds. *Journal of Physical Chemistry A*, **2013**, 117, 10551-62	2.8	50
219	Effects of external ions on the energetics of proton transfers across hydrogen bonds. *The Journal of Physical Chemistry*, **1985**, 89, 262-266		49
218	BoronNitrogen (BN) Substitution Patterns in C/BN Hybrid Fullerenes: C60-2x(BN)x (x = 1□). *Journal of Physical Chemistry A*, **2001**, 105, 8376-8384	2.8	48
217	Comparison of halide receptors based on H, halogen, chalcogen, pnicogen, and tetrel bonds. *Faraday Discussions*, **2017**, 203, 213-226	3.6	47
216	Halogen, Chalcogen, and Pnicogen Bonding Involving Hypervalent Atoms. *Chemistry - A European Journal*, **2018**, 24, 8167-8177	4.8	47

215	Activation and Cleavage of HR 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	2.8	47
214	Steric Crowding in Tetrel Bonds. *Journal of Physical Chemistry A*, **2018**, 122, 2550-2562	2.8	45
213	Substituent Effects in the Noncovalent Bonding of SO to Molecules Containing a Carbonyl Group. The Dominating Role of the Chalcogen Bond. *Journal of Physical Chemistry A*, **2014**, 118, 3835-3845	2.8	44
212	Proton transfer in the ground and first excited triplet states of malonaldehyde. *The Journal of Physical Chemistry*, **1992**, 96, 9764-9767		44
211	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, 1201-10	6.4	43
210	Quantum mechanical test of Marcus theory. Effects of alkylation upon proton transfer. *The Journal of Physical Chemistry*, **1986**, 90, 2969-2974		43
209	Proton Conduction by a Chain of Water Molecules in Carbonic Anhydrase. *Journal of Physical Chemistry B*, **2001**, 105, 6420-6426	3.4	41
208	Coordination of anions by noncovalently bonded hole ligands. *Coordination Chemistry Reviews*, **2020**, 405, 213136	23.2	41
207	Strongly bound noncovalent (SO3)n:H2CO complexes (n = 1, 2). *Physical Chemistry Chemical Physics*, **2014**, 16, 18974-81	3.6	40
206	Vibrational frequencies and intensities of H-bonded and Li-bonded complexes. H3N??HCl and H3N??LiCl. *Journal of Chemical Physics*, **1988**, 89, 3131-3138	3.9	39
205	The Tetrel Bond and its Influence on Hydrogen Bonding and Proton Transfer. *ChemPhysChem*, **2018**, 19, 736-743	3.2	39
204	Complexation of n SO2 molecules (n = 1, 2, 3) with formaldehyde and thioformaldehyde. *Journal of Chemical Physics*, **2014**, 140, 034302	3.9	38
203	Cooperativity of conventional and unconventional hydrogen bonds involving imidazole. *International Journal of Quantum Chemistry*, **2006**, 106, 843-851	2.1	38
202	Energetics, proton transfer rates, and kinetic isotope effects in bent hydrogen bonds. *Journal of the American Chemical Society*, **1992**, 114, 5849-5856	16.4	38
201	Comparison between Tetrel Bonded Complexes Stabilized by and Hole Interactions. *Molecules*, **2018**, 23,	4.8	36
200	Regium bonds between M clusters (M = Cu, Ag, Au and n = 2-6) and nucleophiles NH and HCN. *Physical Chemistry Chemical Physics*, **2018**, 20, 22498-22509	3.6	36
199	Identification of spectroscopic patterns of CH...O H-bonds in proteins. *Journal of Physical Chemistry B*, **2009**, 113, 10421-7	3.4	36
198	Analysis of the reactivities of protein C-H bonds to H atom abstraction by OH radical. *Journal of the American Chemical Society*, **2010**, 132, 16450-9	16.4	35

197	S□□□Chalcogen Bonds between SF2 or SF4 and C-C Multiple Bonds. *Journal of Physical Chemistry A*, **2015**, 119, 5889-97	2.8	34
196	Excited State Intramolecular Proton Transfer in Anionic Analogues of Malonaldehyde. *Journal of Physical Chemistry A*, **1997**, 101, 5901-5909	2.8	34
195	Analysis of the principles governing proton-transfer reactions. Carboxyl group. *Journal of the American Chemical Society*, **1986**, 108, 7178-7186	16.4	34
194	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	2.1	34
193	Studies of dispersion energy in hydrogen-bonded systems. H2O□HOH, H2O□HF, H3N□HF, HF□HF. *Journal of Chemical Physics*, **1984**, 80, 1535-1542	3.9	34
192	The S?N noncovalent interaction: Comparison with hydrogen and halogen bonds. *Chemical Physics Letters*, **2011**, 514, 36-39	2.5	33
191	Rules for BN-Substitution in BCN□ullerenes. Separation of BN and C Domains. *Journal of Physical Chemistry A*, **2003**, 107, 8630-8637	2.8	33
190	Effects of chemical substitution upon excited state proton transfer. Fluoroderivatives of salicylaldimine. *Chemical Physics*, **1999**, 246, 65-74	2.3	33
189	Ab initio study of He(1S)+Cl2(X 1□g,3□u) potential energy surfaces. *Journal of Chemical Physics*, **1994**, 101, 6800-6809	3.9	33
188	Effects of external ions on the dynamics of proton transfer across a hydrogen bond. *The Journal of Physical Chemistry*, **1985**, 89, 1835-1840		33
187	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		32
186	Extrapolation to the complete basis set limit for binding energies of noncovalent interactions. *Computational and Theoretical Chemistry*, **2012**, 998, 9-13	2	31
185	Tetrel Bonding as a Vehicle for Strong and Selective Anion Binding. *Molecules*, **2018**, 23,	4.8	31
184	Substituent Effects on the Binding of Halides by Neutral and Dicationic Bis(triazolium) Receptors. *Journal of Physical Chemistry A*, **2015**, 119, 13064-73	2.8	30
183	Theoretical investigation of the dihydrogen bond linking MH2 with HCCRgF (M = Zn, Cd; Rg = Ar, Kr). *Journal of Physical Chemistry A*, **2005**, 109, 11933-5	2.8	30
182	Calculation of barriers to proton transfer using multiconfiguration self-consistent-field methods. I. Effects of localization. *Journal of Chemical Physics*, **1992**, 97, 7507-7518	3.9	30
181	Complexes containing CO2 and SO2. Mixed dimers, trimers and tetramers. *Physical Chemistry Chemical Physics*, **2014**, 16, 5142-9	3.6	29
180	Ab initio study of the structure of guanine-cytosine base pair conformers in gas phase and polar solvents. *Molecular Physics*, **1995**, 84, 469-480	1.7	29

179	Catalysis of the Aza-Diels-Alder Reaction by Hydrogen and Halogen Bonds. *Journal of Organic Chemistry*, **2016**, 81, 2589-97	4.2	28
178	Factors contributing to distortion energies of bent hydrogen bonds. Implications for proton-transfer potentials. *The Journal of Physical Chemistry*, **1989**, 93, 6565-6574		28
177	Vibrational frequencies and intensities of H-bonded systems. 1:1 and 1:2 complexes of NH3 and PH3 with HF. *Journal of Chemical Physics*, **1987**, 87, 2214-2224	3.9	28
176	Molecular orbital study of proton transfer in (H3NHOH2)+. *The Journal of Physical Chemistry*, **1983**, 87, 1145-1153		28
175	Proton transfers in hydrogen-bonded systems. VI. Electronic redistributions in (N2H7)+ and (O2H5)+. *Journal of Chemical Physics*, **1981**, 75, 5791-5801	3.9	28
174	Competitive Halide Binding by Halogen Versus Hydrogen Bonding: Bis-triazole Pyridinium. *Chemistry - A European Journal*, **2015**, 21, 13330-5	4.8	27
173	Structure, Stability, and Bonding of BC2N: An ab Initio Study. *Journal of Physical Chemistry A*, **1998**, 102, 10134-10141	2.8	27
172	Hardness and Chemical Potential Profiles for Some Open-Shell HAB -lHBA Type Reactions. Ab Initio and Density Functional Study. *Journal of Physical Chemistry A*, **1998**, 102, 5967-5973	2.8	27
171	Calculating the Properties of Hydrogen Bonds by ab Initio Methods. *Reviews in Computational Chemistry*,165-218		27
170	Forty years of progress in the study of the hydrogen bond. *Structural Chemistry*, **2019**, 30, 1119-1128	1.8	26
169	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, 11312-7	3.4	26
168	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	2.8	26
167	Inter- and Intramolecular Hydrogen Bonds with Transition Metal Atoms in Metallocenes of the Iron Subgroup. *Organometallics*, **1998**, 17, 4362-4367	3.8	25
166	Variational transition state theory calculation of proton transfer dynamics in (H3CH...CH3)-. *The Journal of Physical Chemistry*, **1993**, 97, 1765-1769		25
165	Correlation between interaction energy and shift of the carbonyl stretching frequency. *Chemical Physics Letters*, **1990**, 174, 179-184	2.5	25
164	Factors influencing proton positions in biomolecules. *International Journal of Quantum Chemistry*, **1986**, 29, 817-827	2.1	25
163	Kinetics of proton transfer in (H3CH..CH3)-. *The Journal of Physical Chemistry*, **1987**, 91, 724-730		25
162	Aerogen bonds formed between AeOF (Ae = Kr, Xe) and diazines: comparisons between ⊟hole and ⊟hole complexes. *Physical Chemistry Chemical Physics*, **2018**, 20, 4676-4687	3.6	24

161	Substitution Patterns in Mono-BN-Fullerenes:Cn(n= 20, 24, 28, 32, 36, and 40). *Journal of Physical Chemistry A*, **2004**, 108, 7681-7685	2.8	24
160	Comparison of proton transfers in (S2H5)+ and (O2H5)+. *Journal of Chemical Physics*, **1985**, 82, 3316-3321	3.9	24
159	Tuning the Competition between Hydrogen and Tetrel Bonds by a Magnesium Bond. *ChemPhysChem*, **2020**, 21, 212-219	3.2	24
158	Carbene triel bonds between TrR3 (Tr = B, Al) and N-heterocyclic carbenes. *International Journal of Quantum Chemistry*, **2019**, 119, e25867	2.1	24
157	Origins and properties of the tetrel bond. *Physical Chemistry Chemical Physics*, **2021**, 23, 5702-5717	3.6	24
156	Crystallographic and Computational Characterization of Methyl Tetrel Bonding in S-Adenosylmethionine-Dependent Methyltransferases. *Molecules*, **2018**, 23,	4.8	24
155	On the ability of pnicogen atoms to engage in both and hole complexes. Heterodimers of ZFCH (Z = P, As, Sb, Bi) and NH. *Journal of Molecular Modeling*, **2019**, 25, 152	2	23
154	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,	4.8	23
153	Comparison between proton transfers involving carbonyl and hydroxyl oxygens. *The Journal of Physical Chemistry*, **1985**, 89, 3053-3060		23
152	Effects of Halogen, Chalcogen, Pnicogen, and Tetrel Bonds on IR and NMR Spectra. *Molecules*, **2019**, 24,	4.8	22
151	Actinyls in Expanded Porphyrin: A Relativistic Density-Functional Study *Journal of Physical Chemistry A*, **2004**, 108, 3056-3063	2.8	22
150	Transfer of a Proton between N Atoms in Excited Electronic States of 1,5-Diaza-1,3-pentadiene. *The Journal of Physical Chemistry*, **1995**, 99, 9854-9861		22
149	Ground and excited state intramolecular proton transfer in OCCNN ring. *Chemical Physics Letters*, **1993**, 204, 36-44	2.5	22
148	Energetics of proton transfer between carbon atoms (H3CH ? CH3) *International Journal of Quantum Chemistry*, **1986**, 29, 285-292	2.1	22
147	Understanding noncovalent bonds and their controlling forces. *Journal of Chemical Physics*, **2020**, 153, 140901	3.9	22
146	Assessment of the Presence and Strength of H-Bonds by Means of Corrected NMR. *Molecules*, **2016**, 21,	4.8	22
145	Anion???Anion Attraction in Complexes of MCl (M=Zn, Cd, Hg) with CN. *ChemPhysChem*, **2020**, 21, 1119-1125	3.2	22
144	Dual Geometry Schemes in Tetrel Bonds: Complexes between TF (T = Si, Ge, Sn) and Pyridine Derivatives. *Molecules*, **2019**, 24,	4.8	21

143	Comparison of methods for calculating the properties of intramolecular hydrogen bonds. Excited state proton transfer. *Journal of Chemical Physics*, **1999**, 111, 849-858	3.9	21
142	Switchable Aromaticity in an Isostructural Mn Phthalocyanine Series Isolated in Five Separate Redox States. *Journal of the American Chemical Society*, **2019**, 141, 2604-2613	16.4	20
141	Differential Binding of Tetrel-Bonding Bipodal Receptors to Monatomic and Polyatomic Anions. *Molecules*, **2019**, 24,	4.8	20
140	Comparison of Various Means of Evaluating Molecular Electrostatic Potentials for Noncovalent Interactions. *Journal of Computational Chemistry*, **2018**, 39, 500-510	3.5	20
139	Anionic CH???X- hydrogen bonds: origin of their strength, geometry, and other properties. *Chemistry - A European Journal*, **2015**, 21, 1474-81	4.8	20
138	Quantum chemical analysis of the energetics of the anti and gauche conformers of ethanol. *Structural Chemistry*, **2009**, 20, 43-48	1.8	20
137	Proton transfers between first- and second-row atoms: (H2OHSH2)+ and (H3NHSH2)+. *Journal of Chemical Physics*, **1984**, 80, 1982-1987	3.9	20
136	How Many Pnicogen Bonds can be Formed to a Central Atom Simultaneously?. *Journal of Physical Chemistry A*, **2020**, 124, 2046-2056	2.8	19
135	Comparison of BN and AlN Substitution on the Structure and Electronic and Chemical Properties of C60 Fullerene. *Journal of Physical Chemistry A*, **2003**, 107, 4056-4065	2.8	19
134	Ab initio study of FH□PH3 and ClH□PH3 including the effects of electron correlation. *Journal of Chemical Physics*, **1984**, 81, 2713-2716	3.9	19
133	Proton transfers in hydrogen bonded systems. Electron correlation effects in (H3NHOH2)+. *Chemical Physics Letters*, **1981**, 79, 39-42	2.5	19
132	Hexacoordinated Tetrel-Bonded Complexes between TF (T=Si, Ge, Sn, Pb) and NCH: Competition between □and □Holes. *ChemPhysChem*, **2019**, 20, 959-966	3.2	19
131	Site and chirality selective chemical modifications of boron nitride nanotubes (BNNTs) via Lewis acid-base interactions. *Physical Chemistry Chemical Physics*, **2015**, 17, 3850-66	3.6	18
130	Long-range behavior of noncovalent bonds. Neutral and charged H-bonds, pnicogen, chalcogen, and halogen bonds. *Chemical Physics*, **2015**, 456, 34-40	2.3	18
129	On the Stability of Interactions between Pairs of Anions - Complexes of MCl (M=Be, Mg, Ca, Sr, Ba) with Pyridine and CN. *ChemPhysChem*, **2020**, 21, 870-877	3.2	18
128	Manipulating unconventional CH-based hydrogen bonding in a methyltransferase via noncanonical amino acid mutagenesis. *ACS Chemical Biology*, **2014**, 9, 1692-7	4.9	18
127	Variation of atomic charges during proton transfer in hydrogen bonds. *Journal of Computational Chemistry*, **1994**, 15, 553-560	3.5	18
126	Effect of bond multiplicity upon hydrogen bonding and proton transfers. Double bonded atoms. *Journal of the American Chemical Society*, **1992**, 114, 3650-3655	16.4	18

125	Triel-Bonded Complexes between TrR (Tr=B, Al, Ga; R=H, F, Cl, Br, CH) and Pyrazine. *ChemPhysChem*, **2018**, 19, 3122-3133	3.2	18
124	Influence of monomer deformation on the competition between two types of σ-holes in tetrel bonds. *Physical Chemistry Chemical Physics*, **2019**, 21, 10336-10346	3.6	17
123	Pnicogen Bonds Pairing Anionic Lewis Acid with Neutral and Anionic Bases. *Journal of Physical Chemistry A*, **2020**, 124, 4998-5006	2.8	17
122	Interpretation of Spectroscopic Markers of Hydrogen Bonds. *ChemPhysChem*, **2016**, 17, 2263-71	3.2	17
121	Proton Transfer in Ground and Excited Electronic States of Glyoxal Monohydrazone. *The Journal of Physical Chemistry*, **1995**, 99, 7352-7359		17
120	Influence of basis set on the calculated properties of (H3N-HCl). *Journal of Chemical Physics*, **1985**, 82, 4131-4134	3.9	17
119	Contribution of dispersion to the properties of H2S--HF and H2S--HCl. *Journal of Chemical Physics*, **1985**, 83, 1778-1783	3.9	17
118	Analysis of the principles governing proton-transfer reactions. Comparison of the imine and amine groups. *Journal of the American Chemical Society*, **1985**, 107, 7690-7696	16.4	17
117	The ditetrel bond: noncovalent bond between neutral tetrel atoms. *Physical Chemistry Chemical Physics*, **2020**, 22, 16606-16614	3.6	16
116	Competition between Intra and Intermolecular Triel Bonds. Complexes between Naphthalene Derivatives and Neutral or Anionic Lewis Bases. *Molecules*, **2020**, 25,	4.8	16
115	Effect of CH···O hydrogen bond length on the geometric and spectroscopic features of the peptide unit of proteins. *International Journal of Quantum Chemistry*, **2010**, 110, 2775-2783	2.1	16
114	Effect of nonproximate atomic substitution on excited state intramolecular proton transfer. *Journal of Computational Chemistry*, **1998**, 19, 129-138	3.5	16
113	Calculation of barriers to proton transfer using variations of multiconfiguration self-consistent-field methods. II. Configuration interaction. *Journal of Chemical Physics*, **1992**, 97, 7519-7527	3.9	16
112	Chalcogen bonding of two ligands to hypervalent YF (Y = S, Se, Te, Po). *Physical Chemistry Chemical Physics*, **2019**, 21, 20829-20839	3.6	15
111	The interplay between charge transfer, rehybridization, and atomic charges in the internal geometry of subunits in noncovalent interactions. *International Journal of Quantum Chemistry*, **2015**, 115, 28-33	2.1	15
110	Building a Better Halide Receptor: Optimum Choice of Spacer, Binding Unit, and Halosubstitution. *ChemPhysChem*, **2016**, 17, 836-44	3.2	15
109	Halogen Bonds Formed between Substituted Imidazoliums and N Bases of Varying N-Hybridization. *Molecules*, **2017**, 22,	4.8	15
108	Dissection of the Factors Affecting Formation of a CHO H-Bond. A Case Study. *Crystals*, **2015**, 5, 327-345	2.3	15

107	Unconventional H-bonds: SH□□N interaction. *International Journal of Quantum Chemistry*, **2011**, 111, 3196-3200	2.1	15
106	Analysis of catalytic mechanism of serine proteases. Viability of the ring-flip hypothesis. *Journal of Physical Chemistry B*, **2008**, 112, 6837-46	3.4	15
105	Noncovalent Bonds between Tetrel Atoms. *ChemPhysChem*, **2020**, 21, 1934-1944	3.2	15
104	On the capability of metal□halogen groups to participate in halogen bonds. *CrystEngComm*, **2019**, 21, 2875-2883	3.3	14
103	NXY halogen bonds. Comparison with NHY H-bonds and CXY halogen bonds. *Physical Chemistry Chemical Physics*, **2016**, 18, 18015-23	3.6	14
102	Three-dimensional spatial characteristics of primary and secondary basis set superposition error. *Chemical Physics Letters*, **1987**, 140, 338-344	2.5	14
101	Relationship between the angular characteristics of a hydrogen bond and the energetics of proton transfer occurring within. *Journal of Molecular Structure*, **1988**, 177, 79-91	3.4	14
100	Hydrogen bonding of the carbonyl groups of uridine nucleosides. *Biopolymers*, **1983**, 22, 731-745	2.2	14
99	Structures and energetics of clusters surrounding diatomic anions stabilized by hydrogen, halogen, and other noncovalent bonds. *Chemical Physics*, **2020**, 530, 110590	2.3	14
98	Torsional and Electronic Factors Control the C-H???O Interaction. *Chemistry - A European Journal*, **2016**, 22, 16513-16521	4.8	14
97	Comparison of □hole and □hole tetrel bonds in complexes of borazine with TH3F and F2TO/H2TO (T = C, Si, Ge). *International Journal of Quantum Chemistry*, **2019**, 119, e25910	2.1	14
96	Dependence of NMR chemical shifts upon CH bond lengths of a methyl group involved in a tetrel bond. *Chemical Physics Letters*, **2019**, 714, 61-64	2.5	14
95	B?N Bond Cleavage and BN Ring Expansion at the Surface of Boron Nitride Nanotubes by Iminoborane. *Journal of Physical Chemistry C*, **2015**, 119, 3253-3259	3.8	13
94	Contributions of various noncovalent bonds to the interaction between an amide and S-containing molecules. *ChemPhysChem*, **2012**, 13, 3535-41	3.2	13
93	Nature of interactions in open-shell complexes pairing H2X with HXX, X=S,O. *Molecular Physics*, **2009**, 107, 713-719	1.7	13
92	Comparison between Hydrogen and Halogen Bonds in Complexes of 6-OX-Fulvene with Pnicogen and Chalcogen Electron Donors. *ChemPhysChem*, **2019**, 20, 1978-1984	3.2	12
91	Structures of clusters surrounding ions stabilized by hydrogen, halogen, chalcogen, and pnicogen bonds. *Chemical Physics*, **2019**, 524, 55-62	2.3	12
90	Substituent Effects upon Protonation-Induced Red Shift of Phenyl□Pyridine Copolymers. *Journal of Physical Chemistry B*, **2002**, 106, 534-539	3.4	12

89	Modeling of coupled proton transfers by analytic functions. *International Journal of Quantum Chemistry*, **1992**, 44, 109-124	2.1	12
88	Role of d functions in ab initio calculation of the equilibrium structure of H2SHF. *Journal of Chemical Physics*, **1983**, 78, 599-600	3.9	12
87	The Hydrogen Bond: A Hundred Years and Counting. *Journal of the Indian Institute of Science*, **2020**, 100, 61-76	2.4	12
86	Computational Insights into Mg-Cl Complex Electrolytes for Rechargeable Magnesium Batteries. *Batteries and Supercaps*, **2019**, 2, 792-800	5.6	11
85	Anion-anion and anion-neutral triel bonds. *Physical Chemistry Chemical Physics*, **2021**, 23, 4818-4828	3.6	11
84	Hydrogen bonded and stacked geometries of the temozolomide dimer. *Journal of Molecular Modeling*, **2016**, 22, 77	2	10
83	Violation of Electrostatic Rules: Shifting the Balance between Pnicogen Bonds and Lone Pair-π Interactions Tuned by Substituents. *Journal of Physical Chemistry A*, **2019**, 123, 7288-7295	2.8	10
82	Evaluation of DFT methods to study reactions of benzene with OH radical. *International Journal of Quantum Chemistry*, **2012**, 112, 1879-1886	2.1	10
81	INFLUENCE OF ISOTOPIC SUBSTITUTION ON STRENGTH OF HYDROGEN BONDS OF COMMON ORGANIC GROUPS. *Journal of Physical Organic Chemistry*, **1997**, 10, 383-395	2.1	10
80	The basis set dependence of structures and energies of various states of cyclodisiloxane. *International Journal of Quantum Chemistry*, **1986**, 29, 1191-1208	2.1	10
79	Relationships between Bond Strength and Spectroscopic Quantities in H-Bonds and Related Halogen, Chalcogen, and Pnicogen Bonds. *Journal of Physical Chemistry A*, **2020**, 124, 7716-7725	2.8	10
78	Crystallographic and Theoretical Evidences of Anion???Anion Interaction. *ChemPhysChem*, **2021**, 22, 818-821	3.2	10
77	Computational approaches and sigma-hole interactions: general discussion. *Faraday Discussions*, **2017**,	3.6	9
76	Water-Mediated Carbon-Oxygen Hydrogen Bonding Facilitates S-Adenosylmethionine Recognition in the Reactivation Domain of Cobalamin-Dependent Methionine Synthase. *Biochemistry*, **2018**, 57, 3733-3740	3.2	9
75	Regioselectivity of the interaction of temozolomide with borane and boron trifluoride. *Structural Chemistry*, **2015**, 26, 1359-1365	1.8	9
74	Search for Analytical Functions To Simulate Proton Transfers in Hydrogen Bonds. *ACS Symposium Series*, **1994**, 125-138	0.4	9
73	Calculation of barriers to proton transfer using a variety of electron correlation methods. *International Journal of Quantum Chemistry*, **1992**, 44, 817-835	2.1	9
72	Effects of alkylation upon the proton affinities of nitrogen and oxygen bases. *Journal of Computational Chemistry*, **1985**, 6, 168-172	3.5	9

71	F-Halogen Bond: Conditions for Its Existence. *Journal of Physical Chemistry A*, **2020**, 124, 7290-7299	2.8	9
70	Noncovalent Bonds through Sigma and Pi-Hole Located on the Same Molecule. Guiding Principles and Comparisons. *Molecules*, **2021**, 26,	4.8	9
69	Enhancing the Reduction Potential of Quinones via Complex Formation. *Journal of Organic Chemistry*, **2016**, 81, 4316-24	4.2	9
68	STRUCTURE AND PROPERTIES OF PERFLUOROALKYLATED PHTHALOCYANINES: A THEORETICAL STUDY. *Journal of Theoretical and Computational Chemistry*, **2008**, 07, 541-563	1.8	8
67	A DFT/TDDFT study of Group 4A metal porphyrins. *Molecular Physics*, **2003**, 101, 1227-1238	1.7	8
66	Effects of external ions upon proton transfer reactions: H-bonded systems containing HCOOH. *International Journal of Quantum Chemistry*, **1988**, 34, 137-147	2.1	8
65	Energetics and electronic rearrangements of proton transfer in (H3NHOH2)+. *International Journal of Quantum Chemistry*, **1983**, 23, 753-764	2.1	8
64	Comparison of Bifurcated Halogen with Hydrogen Bonds. *Molecules*, **2021**, 26,	4.8	8
63	Optical Stability of 1,1Q-Binaphthyl Derivatives. *ACS Omega*, **2019**, 4, 6044-6049	3.9	7
62	Structure and Properties of [8]BN-Circulenes: Inorganic Analogues of [8]Circulenes. *Journal of Physical Chemistry C*, **2015**, 119, 15541-15546	3.8	7
61	Effect of Magnesium Bond on the Competition Between Hydrogen and Halogen Bonds and the Induction of Proton and Halogen Transfer. *ChemPhysChem*, **2018**, 19, 1456-1464	3.2	7
60	The ability of a tetrel bond to transition a neutral amino acid into a zwitterion. *Chemical Physics Letters*, **2019**, 731, 136584	2.5	7
59	An exploration of the ozone dimer potential energy surface. *Journal of Chemical Physics*, **2014**, 140, 2443[illegible]	3.1	7
58	Behavior of interaction energy and intramolecular bond stretch in linear and bifurcated hydrogen bonds. *International Journal of Quantum Chemistry*, **1993**, 48, 181-190	2.1	7
57	Comparison of ground and triplet state geometries of malonaldehyde. *International Journal of Quantum Chemistry*, **1993**, 48, 419-429	2.1	7
56	Interactions of Nucleic Acid Bases with Temozolomide. Stacked, Perpendicular, and Coplanar Heterodimers. *Journal of Physical Chemistry B*, **2016**, 120, 9347-61	3.4	7
55	Experimental and Theoretical Studies of Dimers Stabilized by Two Chalcogen Bonds in the Presence of a N⋯N Pnicogen Bond. *Journal of Physical Chemistry A*, **2021**, 125, 657-668	2.8	7
54	Weak σ-Hole Triel Bond between C H Tr (Tr=B, Al, Ga) and Haloethyne: Substituent and Cooperativity Effects. *ChemPhysChem*, **2021**, 22, 481-487	3.2	7

53	Coordination of a Central Atom by Multiple Intramolecular Pnicogen Bonds. *Inorganic Chemistry*, **2020**, 59, 9315-9324	5.1	6
52	Interactions between temozolomide and quercetin. *Structural Chemistry*, **2016**, 27, 1577-1588	1.8	6
51	Modeling proton transfer potentials in angularly deformed hydrogen bonds. *International Journal of Quantum Chemistry*, **1993**, 48, 77-87	2.1	6
50	Competition between a Tetrel and Halogen Bond to a Common Lewis Acid. *Journal of Physical Chemistry A*, **2021**, 125, 308-316	2.8	6
49	Anion-Anion Interactions in Aerogen-Bonded Complexes. Influence of Solvent Environment. *Molecules*, **2021**, 26,	4.8	6
48	H-bonding and stacking interactions between chloroquine and temozolomide. *International Journal of Quantum Chemistry*, **2016**, 116, 1196-1204	2.1	6
47	Relative Strengths of a Pnicogen and a Tetrel Bond and Their Mutual Effects upon One Another. *Journal of Physical Chemistry A*, **2021**, 125, 2631-2641	2.8	6
46	Anionanion (MX) dimers (M = Zn, Cd, Hg; X = Cl, Br, I) in different environments. *Physical Chemistry Chemical Physics*, **2021**, 23, 13853-13861	3.6	6
45	Does Thermochemical Mimicry Extend to Gibbs Energies? The Differences of K+ and NH4 +, and of Na+ and H3O+. *Structural Chemistry*, **1999**, 10, 391-392	1.8	5
44	Characterization of ground and excited electronic state deprotonation energies of systems containing double bonds using natural bond orbital analysis. *Journal of Chemical Physics*, **1996**, 105, 4675-4691	3.0	5
43	Dissection of basis set superposition error at SCF and correlated levels: HF dimer. *Computational and Theoretical Chemistry*, **1989**, 199, 9-22		5
42	Proximity Effects of Substituents on Halogen Bond Strength. *Journal of Physical Chemistry A*, **2021**, 125, 5069-5077	2.8	5
41	Carbon as an electron donor atom. *Polyhedron*, **2021**, 193, 114905	2.7	5
40	Dissection of the Origin of σ-Holes and the Noncovalent Bonds in Which They Engage. *Journal of Physical Chemistry A*, **2021**, 125, 6514-6528	2.8	5
39	Interactions between Thiourea and Imines. Prelude to Catalysis. *Journal of Organic Chemistry*, **2015**, 80, 10334-41	4.2	4
38	Microsolvation of anions by molecules forming CH···X hydrogen bonds. *Chemical Physics*, **2015**, 463, 137-144	1.9	4
37	Complexes of HArF and AuX (X = F, Cl, Br, I). Comparison of H-bonds, halogen bonds, F-shared bonds and covalent bonds. *Applied Organometallic Chemistry*, **2020**, 34, e5891	3.1	4
36	Xechalcogen aerogen bond. Effect of substituents and size of chalcogen atom. *Physical Chemistry Chemical Physics*, **2020**, 22, 4115-4121	3.6	4

35	Proton transfer in H5O and H3O with an external restraining force. *International Journal of Quantum Chemistry*, **1995**, 56, 567-575	2.1	4
34	On the Ability of Nitrogen to Serve as an Electron Acceptor in a Pnicogen Bond. *Journal of Physical Chemistry A*, **2021**, 125, 10419-10427	2.8	4
33	Effect of carbon hybridization in C-F bond as an electron donor in triel bonds. *Journal of Chemical Physics*, **2020**, 153, 074304	3.9	4
32	Diboron Bonds Between BX (X=H, F, CH) and BYZ (Y=H, F; Z=CO, N , CNH). *ChemPhysChem*, **2021**, 22, 1461-1469	3.2	4
31	The heat capacities and standard entropies of corresponding potassium and ammonium ion species: is there a constant difference?. *Structural Chemistry*, **2009**, 20, 31-35	1.8	3
30	Proton transfers in hydrogen-bonded systems V. Analysis of electronic redistributions in (N2H7)+. *International Journal of Quantum Chemistry*, **1981**, 20, 221-229	2.1	3
29	Ability of Lewis Acids with Shallow σ-Holes to Engage in Chalcogen Bonds in Different Environments. *Molecules*, **2021**, 26,	4.8	3
28	Unusual substituent effects in the Tr···Te triel bond. *International Journal of Quantum Chemistry*, **2021**, 121, e26526	2.1	3
27	Enhancement of the Tetrel Bond by the Effects of Substituents, Cooperativity, and Electric Field: Transition from Noncovalent to Covalent Bond. *ChemPhysChem*, **2021**, 22, 2305-2312	3.2	3
26	The halogen bond in solution: general discussion. *Faraday Discussions*, **2017**, 203,	3.6	2
25	Applicability of the Marcus equation to proton transfer in symmetric and unsymmetric systems. *Computational and Theoretical Chemistry*, **1993**, 285, 27-32		2
24	Versatility of the Cyano Group in Intermolecular Interactions. *Molecules*, **2020**, 25,	4.8	2
23	Competition between Inter and Intramolecular Tetrel Bonds: Theoretical Studies Complemented by CSD Survey. *ChemPhysChem*, **2021**, 22, 924-934	3.2	2
22	Probing the Hydrogen-Bonding Environment of Individual Bases in DNA Duplexes with Isotope-Edited Infrared Spectroscopy. *Journal of Physical Chemistry B*, **2021**, 125, 7613-7627	3.4	2
21	Participation of S and Se in hydrogen and chalcogen bonds. *CrystEngComm*,	3.3	2
20	Noncovalent bond between tetrel σ-hole and hydride. *Physical Chemistry Chemical Physics*, **2021**, 23, 10536-10544	3.6	2
19	Characterization of Type I and II Interactions between Halogen Atoms. *Crystal Growth and Design*, **2022**, 22, 2692-2702	3.5	2
18	Effects of Angular Deformation on the Energetics of the SN2 Reaction. *European Journal of Organic Chemistry*, **2016**, 2016, 3964-3968	3.2	1

17	Comparison of halogen with proton transfer. Symmetric and asymmetric systems. *Chemical Physics Letters*, **2019**, 731, 136593	2.5	1
16	Monitoring the Charge Distribution during Proton and Sodium Ion Conduction along Chains of Water Molecules and Protein Residues. *Israel Journal of Chemistry*, **2017**, 57, 385-392	3.4	1
15	Ingredients Necessary for Proton Transfer in Enzymes. *Israel Journal of Chemistry*, **2009**, 49, 139-147	3.4	1
14	Experimental and theoretical evidence of attractive interactions between dianions: [PdCl]?[PdCl]. *Chemical Communications*, **2021**, 57, 13305-13308	5.8	1
13	Anatomy of □hole bonds: Linear systems. *Journal of Chemical Physics*, **2021**, 155, 174302	3.9	1
12	Triel bonds within anionanion complexes. *Physical Chemistry Chemical Physics*, **2021**, 23, 25097-25106	3.6	1
11	The balance between side-chain and backbone-driven association in folding of the □helical influenza A transmembrane peptide. *Journal of Computational Chemistry*, **2020**, 41, 2177-2188	3.5	1
10	Fabricating Flexible Packaging Batteries in General Chemistry Laboratories. *Journal of Chemical Education*, **2021**, 98, 2471-2475	2.4	1
9	Interactions of (MY)6 (M = Zn, Cd; Y = O, S, Se) quantum dots with N-bases. *Structural Chemistry*, **2019**, 30, 1003-1014	1.8	0
8	Perturbations of proton transfer potentials caused by polar molecules. *International Journal of Quantum Chemistry*, **2009**, 36, 211-217	2.1	0
7	Partial transfer of bridging atom in halogen-bonded complexes. *Computational and Theoretical Chemistry*, **2021**, 1204, 113398	2	0
6	Can HCCH/HBNH Break B?N/C?C Bonds of Single-Wall BN/Carbon Nanotubes at Their Surface?. *Journal of Physical Chemistry C*, **2017**, 121, 26044-26053	3.8	
5	Proton transfer potentials in hydrogen-bonded systems: (H5O2)+. *International Journal of Quantum Chemistry*, **2009**, 18, 199-206	2.1	
4	Additivity of the effects of external ions and dipoles upon the energetics of proton transfer. *International Journal of Quantum Chemistry*, **2009**, 30, 71-79	2.1	
3	Effect of proton transfer on neighboring hydrogen-bond strength. *International Journal of Quantum Chemistry*, **1991**, 40, 37-48	2.1	
2	Segmentation and additive approach: A reliable technique to study noncovalent interactions of large molecules at the surface of single-wall carbon nanotubes. *Journal of Computational Chemistry*, **2016**, 37, 1953-61	3.5	
1	Structural and Functional Characterization of Sulfonium Carbon-Oxygen Hydrogen Bonding in the Deoxyamino Sugar Methyltransferase TylM1. *Biochemistry*, **2019**, 58, 2152-2159	3.2	