Steve Scheiner

List of Publications by Year in Descending Order

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	Characterization of Type I and II Interactions between Halogen Atoms. *Crystal Growth and Design*, **2022**, 22, 2692-2702	3.5	2
303	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
302	Experimental and theoretical evidence of attractive interactions between dianions: [PdCl]?[PdCl]. *Chemical Communications*, **2021**, 57, 13305-13308	5.8	1
301	Ability of Lewis Acids with Shallow σ-Holes to Engage in Chalcogen Bonds in Different Environments. *Molecules*, **2021**, 26,	4.8	3
300	Anatomy of σ-hole bonds: Linear systems. *Journal of Chemical Physics*, **2021**, 155, 174302	3.9	1
299	Triel bonds within anionanion complexes. *Physical Chemistry Chemical Physics*, **2021**, 23, 25097-25106	3.6	1
298	Competition between a Tetrel and Halogen Bond to a Common Lewis Acid. *Journal of Physical Chemistry A*, **2021**, 125, 308-316	2.8	6
297	Noncovalent Bonds through Sigma and Pi-Hole Located on the Same Molecule. Guiding Principles and Comparisons. *Molecules*, **2021**, 26,	4.8	9
296	Competition between Inter and Intramolecular Tetrel Bonds: Theoretical Studies Complemented by CSD Survey. *ChemPhysChem*, **2021**, 22, 924-934	3.2	2
295	Crystallographic and Theoretical Evidences of Anion???Anion Interaction. *ChemPhysChem*, **2021**, 22, 818-821	3.2	10
294	Anion-Anion Interactions in Aerogen-Bonded Complexes. Influence of Solvent Environment. *Molecules*, **2021**, 26,	4.8	6
293	Fabricating Flexible Packaging Batteries in General Chemistry Laboratories. *Journal of Chemical Education*, **2021**, 98, 2471-2475	2.4	1
292	Proximity Effects of Substituents on Halogen Bond Strength. *Journal of Physical Chemistry A*, **2021**, 125, 5069-5077	2.8	5
291	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
290	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
289	Carbon as an electron donor atom. *Polyhedron*, **2021**, 193, 114905	2.7	5
288	Unusual substituent effects in the Tr□Te triel bond. *International Journal of Quantum Chemistry*, **2021**, 121, e26526	2.1	3

287	Comparison of Bifurcated Halogen with Hydrogen Bonds. *Molecules*, **2021**, 26,	4.8	8
286	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
285	Origins and properties of the tetrel bond. *Physical Chemistry Chemical Physics*, **2021**, 23, 5702-5717	3.6	24
284	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
283	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
282	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
281	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
280	Partial transfer of bridging atom in halogen-bonded complexes. *Computational and Theoretical Chemistry*, **2021**, 1204, 113398	2	0
279	Anion-anion and anion-neutral triel bonds. *Physical Chemistry Chemical Physics*, **2021**, 23, 4818-4828	3.6	11
278	Noncovalent bond between tetrel σ-hole and hydride. *Physical Chemistry Chemical Physics*, **2021**, 23, 10536-10544	3.6	4
277	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
276	Pnicogen Bonds Pairing Anionic Lewis Acid with Neutral and Anionic Bases. *Journal of Physical Chemistry A*, **2020**, 124, 4998-5006	2.8	17
275	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
274	Coordination of a Central Atom by Multiple Intramolecular Pnicogen Bonds. *Inorganic Chemistry*, **2020**, 59, 9315-9324	5.1	6
273	The ditetrel bond: noncovalent bond between neutral tetrel atoms. *Physical Chemistry Chemical Physics*, **2020**, 22, 16606-16614	3.6	16
272	How Many Pnicogen Bonds can be Formed to a Central Atom Simultaneously?. *Journal of Physical Chemistry A*, **2020**, 124, 2046-2056	2.8	19
271	Xechalcogen aerogen bond. Effect of substituents and size of chalcogen atom. *Physical Chemistry Chemical Physics*, **2020**, 22, 4115-4121	3.6	4
270	Competition between Intra and Intermolecular Triel Bonds. Complexes between Naphthalene Derivatives and Neutral or Anionic Lewis Bases. *Molecules*, **2020**, 25,	4.8	16

269	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
268	Structures and energetics of clusters surrounding diatomic anions stabilized by hydrogen, halogen, and other noncovalent bonds. *Chemical Physics*, **2020**, 530, 110590	2.3	14
267	The Hydrogen Bond: A Hundred Years and Counting. *Journal of the Indian Institute of Science*, **2020**, 100, 61-76	2.4	12
266	Tuning the Competition between Hydrogen and Tetrel Bonds by a Magnesium Bond. *ChemPhysChem*, **2020**, 21, 212-219	3.2	24
265	Coordination of anions by noncovalently bonded hole ligands. *Coordination Chemistry Reviews*, **2020**, 405, 213136	23.2	41
264	Versatility of the Cyano Group in Intermolecular Interactions. *Molecules*, **2020**, 25,	4.8	2
263	Understanding noncovalent bonds and their controlling forces. *Journal of Chemical Physics*, **2020**, 153, 140901	3.9	22
262	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
261	Noncovalent Bonds between Tetrel Atoms. *ChemPhysChem*, **2020**, 21, 1934-1944	3.2	15
260	F-Halogen Bond: Conditions for Its Existence. *Journal of Physical Chemistry A*, **2020**, 124, 7290-7299	2.8	9
259	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
258	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
257	Anion???Anion Attraction in Complexes of MCl (M=Zn, Cd, Hg) with CN. *ChemPhysChem*, **2020**, 21, 1119-1125	3.2	22
256	Chalcogen bonding of two ligands to hypervalent YF (Y = S, Se, Te, Po). *Physical Chemistry Chemical Physics*, **2019**, 21, 20829-20839	3.6	15
255	Dual Geometry Schemes in Tetrel Bonds: Complexes between TF (T = Si, Ge, Sn) and Pyridine Derivatives. *Molecules*, **2019**, 24,	4.8	21
254	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
253	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
252	Computational Insights into Mg-Cl Complex Electrolytes for Rechargeable Magnesium Batteries. *Batteries and Supercaps*, **2019**, 2, 792-800	5.6	11

251	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
250	Forty years of progress in the study of the hydrogen bond. *Structural Chemistry*, **2019**, 30, 1119-1128	1.8	26
249	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
248	Structures of clusters surrounding ions stabilized by hydrogen, halogen, chalcogen, and pnicogen bonds. *Chemical Physics*, **2019**, 524, 55-62	2.3	12
247	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
246	On the capability of metal-halogen groups to participate in halogen bonds. *CrystEngComm*, **2019**, 21, 2875-2883	3.3	14
245	Optical Stability of 1,1'-Binaphthyl Derivatives. *ACS Omega*, **2019**, 4, 6044-6049	3.9	7
244	Differential Binding of Tetrel-Bonding Bipodal Receptors to Monatomic and Polyatomic Anions. *Molecules*, **2019**, 24,	4.8	20
243	Effects of Halogen, Chalcogen, Pnicogen, and Tetrel Bonds on IR and NMR Spectra. *Molecules*, **2019**, 24,	4.8	22
242	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
241	The ability of a tetrel bond to transition a neutral amino acid into a zwitterion. *Chemical Physics Letters*, **2019**, 731, 136584	2.5	7
240	Comparison of halogen with proton transfer. Symmetric and asymmetric systems. *Chemical Physics Letters*, **2019**, 731, 136593	2.5	1
239	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
238	Structural and Functional Characterization of Sulfonium Carbon-Oxygen Hydrogen Bonding in the Deoxyamino Sugar Methyltransferase TylM1. *Biochemistry*, **2019**, 58, 2152-2159	3.2	
237	Hexacoordinated Tetrel-Bonded Complexes between TF (T=Si, Ge, Sn, Pb) and NCH: Competition between π and σ-Holes. *ChemPhysChem*, **2019**, 20, 959-966	3.2	19
236	Comparison of π-hole and σ-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
235	Definition of the chalcogen bond (IUPAC Recommendations 2019). *Pure and Applied Chemistry*, **2019**, 91, 1889-1892	2.1	183
234	Carbene triel bonds between TrR3 (Tr = B, Al) and N-heterocyclic carbenes. *International Journal of Quantum Chemistry*, **2019**, 119, e25867	2.1	24

233	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
232	Implications of monomer deformation for tetrel and pnicogen bonds. *Physical Chemistry Chemical Physics*, **2018**, 20, 8832-8841	3.6	55
231	Steric Crowding in Tetrel Bonds. *Journal of Physical Chemistry A*, **2018**, 122, 2550-2562	2.8	45
230	Halogen, Chalcogen, and Pnicogen Bonding Involving Hypervalent Atoms. *Chemistry - A European Journal*, **2018**, 24, 8167-8177	4.8	47
229	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
228	Aerogen bonds formed between AeOF (Ae = Kr, Xe) and diazines: comparisons between σhole and πhole complexes. *Physical Chemistry Chemical Physics*, **2018**, 20, 4676-4687	3.6	24
227	Comparison of Various Means of Evaluating Molecular Electrostatic Potentials for Noncovalent Interactions. *Journal of Computational Chemistry*, **2018**, 39, 500-510	3.5	20
226	Comparison between Tetrel Bonded Complexes Stabilized by σ and π Hole Interactions. *Molecules*, **2018**, 23,	4.8	36
225	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
224	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
223	The πTetrel Bond and its Influence on Hydrogen Bonding and Proton Transfer. *ChemPhysChem*, **2018**, 19, 736-743	3.2	39
222	Crystallographic and Computational Characterization of Methyl Tetrel Bonding in S-Adenosylmethionine-Dependent Methyltransferases. *Molecules*, **2018**, 23,	4.8	24
221	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
220	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
219	Tetrel Bonding as a Vehicle for Strong and Selective Anion Binding. *Molecules*, **2018**, 23,	4.8	31
218	Comparative Strengths of Tetrel, Pnicogen, Chalcogen, and Halogen Bonds and Contributing Factors. *Molecules*, **2018**, 23,	4.8	54
217	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
216	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

215	Comparison of halide receptors based on H, halogen, chalcogen, pnicogen, and tetrel bonds. *Faraday Discussions*, **2017**, 203, 213-226	3.6	47
214	The halogen bond in solution: general discussion. *Faraday Discussions*, **2017**, 203,	3.6	2
213	Computational approaches and sigma-hole interactions: general discussion. *Faraday Discussions*, **2017**,	3.6	9
212	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	
211	Systematic Elucidation of Factors That Influence the Strength of Tetrel Bonds. *Journal of Physical Chemistry A*, **2017**, 121, 5561-5568	2.8	88
210	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
209	Halogen Bonds Formed between Substituted Imidazoliums and N Bases of Varying N-Hybridization. *Molecules*, **2017**, 22,	4.8	15
208	Effects of Angular Deformation on the Energetics of the SN2 Reaction. *European Journal of Organic Chemistry*, **2016**, 2016, 3964-3968	3.2	1
207	Interactions between temozolomide and quercetin. *Structural Chemistry*, **2016**, 27, 1577-1588	1.8	6
206	Interpretation of Spectroscopic Markers of Hydrogen Bonds. *ChemPhysChem*, **2016**, 17, 2263-71	3.2	17
205	NXY halogen bonds. Comparison with NHY H-bonds and CXY halogen bonds. *Physical Chemistry Chemical Physics*, **2016**, 18, 18015-23	3.6	14
204	Building a Better Halide Receptor: Optimum Choice of Spacer, Binding Unit, and Halosubstitution. *ChemPhysChem*, **2016**, 17, 836-44	3.2	15
203	Hydrogen bonded and stacked geometries of the temozolomide dimer. *Journal of Molecular Modeling*, **2016**, 22, 77	2	10
202	Catalysis of the Aza-Diels-Alder Reaction by Hydrogen and Halogen Bonds. *Journal of Organic Chemistry*, **2016**, 81, 2589-97	4.2	28
201	Sulfur-Oxygen Chalcogen Bonding Mediates AdoMet Recognition in the Lysine Methyltransferase SET7/9. *ACS Chemical Biology*, **2016**, 11, 748-54	4.9	68
200	Comparison of σhole tetrel bonding with σhole halogen bonds in complexes of XCN (X = F, Cl, Br, I) and NH3. *Physical Chemistry Chemical Physics*, **2016**, 18, 3581-90	3.6	72
199	Assessment of the Presence and Strength of H-Bonds by Means of Corrected NMR. *Molecules*, **2016**, 21,	4.8	22
198	H-bonding and stacking interactions between chloroquine and temozolomide. *International Journal of Quantum Chemistry*, **2016**, 116, 1196-1204	2.1	6

197	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	
196	Enhancing the Reduction Potential of Quinones via Complex Formation. *Journal of Organic Chemistry*, **2016**, 81, 4316-24	4.2	9
195	Torsional and Electronic Factors Control the C-H???O Interaction. *Chemistry - A European Journal*, **2016**, 22, 16513-16521	4.8	14
194	Highly Selective Halide Receptors Based on Chalcogen, Pnicogen, and Tetrel Bonds. *Chemistry - A European Journal*, **2016**, 22, 18850-18858	4.8	80
193	Interactions of Nucleic Acid Bases with Temozolomide. Stacked, Perpendicular, and Coplanar Heterodimers. *Journal of Physical Chemistry B*, **2016**, 120, 9347-61	3.4	7
192	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
191	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
190	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
189	Structure and Properties of [8]BN-Circulenes: Inorganic Analogues of [8]Circulenes. *Journal of Physical Chemistry C*, **2015**, 119, 15541-15546	3.8	7
188	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
187	Interactions between Thiourea and Imines. Prelude to Catalysis. *Journal of Organic Chemistry*, **2015**, 80, 10334-41	4.2	4
186	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
185	Microsolvation of anions by molecules forming CH□□X□ hydrogen bonds. *Chemical Physics*, **2015**, 463, 137-144	2.3	4
184	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
183	Regioselectivity of the interaction of temozolomide with borane and boron trifluoride. *Structural Chemistry*, **2015**, 26, 1359-1365	1.8	9
182	Competitive Halide Binding by Halogen Versus Hydrogen Bonding: Bis-triazole Pyridinium. *Chemistry - A European Journal*, **2015**, 21, 13330-5	4.8	27
181	Dissection of the Factors Affecting Formation of a CH□O H-Bond. A Case Study. *Crystals*, **2015**, 5, 327-345	2.3	15
180	S□□Chalcogen Bonds between SF2 or SF4 and C-C Multiple Bonds. *Journal of Physical Chemistry A*, **2015**, 119, 5889-97	2.8	34

179	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
178	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
177	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
176	Anionic CH???X- hydrogen bonds: origin of their strength, geometry, and other properties. *Chemistry - A European Journal*, **2015**, 21, 1474-81	4.8	20
175	Chalcogen bonding between tetravalent SF4 and amines. *Journal of Physical Chemistry A*, **2014**, 118, 10849-56	2.8	90
174	Effects of charge and substituent on the S···N chalcogen bond. *Journal of Physical Chemistry A*, **2014**, 118, 3183-92	2.8	126
173	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
172	Manipulating unconventional CH-based hydrogen bonding in a methyltransferase via noncanonical amino acid mutagenesis. *ACS Chemical Biology*, **2014**, 9, 1692-7	4.9	18
171	Complexes containing CO2 and SO2. Mixed dimers, trimers and tetramers. *Physical Chemistry Chemical Physics*, **2014**, 16, 5142-9	3.6	29
170	Noncovalent interactions in dimers and trimers of SO3 and CO. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	56
169	Complexation of n SO2 molecules (n = 1, 2, 3) with formaldehyde and thioformaldehyde. *Journal of Chemical Physics*, **2014**, 140, 034302	3.9	38
168	An exploration of the ozone dimer potential energy surface. *Journal of Chemical Physics*, **2014**, 140, 244314	3.9	7
167	Strongly bound noncovalent (SO3)n:H2CO complexes (n = 1, 2). *Physical Chemistry Chemical Physics*, **2014**, 16, 18974-81	3.6	40
166	Magnitude and mechanism of charge enhancement of CH···O hydrogen bonds. *Journal of Physical Chemistry A*, **2013**, 117, 10551-62	2.8	50
165	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
164	Sensitivity of noncovalent bonds to intermolecular separation: hydrogen, halogen, chalcogen, and pnicogen bonds. *CrystEngComm*, **2013**, 15, 3119-3124	3.3	91
163	The pnicogen bond: its relation to hydrogen, halogen, and other noncovalent bonds. *Accounts of Chemical Research*, **2013**, 46, 280-8	24.3	432
162	Detailed comparison of the pnicogen bond with chalcogen, halogen, and hydrogen bonds. *International Journal of Quantum Chemistry*, **2013**, 113, 1609-1620	2.1	230

161	Sensitivity of pnicogen, chalcogen, halogen and H-bonds to angular distortions. *Chemical Physics Letters*, **2012**, 532, 31-35	2.5	165
160	Effects of carbon chain substituents on the P?N noncovalent bond. *Chemical Physics Letters*, **2012**, 536, 30-33	2.5	62
159	Can a C-H···O interaction be a determinant of conformation?. *Journal of the American Chemical Society*, **2012**, 134, 12064-71	16.4	94
158	Extrapolation to the complete basis set limit for binding energies of noncovalent interactions. *Computational and Theoretical Chemistry*, **2012**, 998, 9-13	2	31
157	Evaluation of DFT methods to study reactions of benzene with OH radical. *International Journal of Quantum Chemistry*, **2012**, 112, 1879-1886	2.1	10
156	Substituent effects on Cl···N, S···N, and P···N noncovalent bonds. *Journal of Physical Chemistry A*, **2012**, 116, 3487-97	2.8	119
155	Contributions of various noncovalent bonds to the interaction between an amide and S-containing molecules. *ChemPhysChem*, **2012**, 13, 3535-41	3.2	13
154	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
153	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
152	Definition of the hydrogen bond (IUPAC Recommendations 2011). *Pure and Applied Chemistry*, **2011**, 83, 1637-1641	2.1	1111
151	Defining the hydrogen bond: An account (IUPAC Technical Report). *Pure and Applied Chemistry*, **2011**, 83, 1619-1636	2.1	738
150	Can two trivalent N atoms engage in a direct N?N noncovalent interaction?. *Chemical Physics Letters*, **2011**, 514, 32-35	2.5	99
149	The S?N noncovalent interaction: Comparison with hydrogen and halogen bonds. *Chemical Physics Letters*, **2011**, 514, 36-39	2.5	33
148	Effects of multiple substitution upon the P?N noncovalent interaction. *Chemical Physics*, **2011**, 387, 79-84	2.3	90
147	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
146	Unconventional H-bonds: SH···N interaction. *International Journal of Quantum Chemistry*, **2011**, 111, 3196-3200	2.1	15
145	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
144	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

143	A new noncovalent force: comparison of P···N interaction with hydrogen and halogen bonds. *Journal of Chemical Physics*, **2011**, 134, 094315	3.9	189
142	Comparison of P···D (D = P,N) with other noncovalent bonds in molecular aggregates. *Journal of Chemical Physics*, **2011**, 135, 184306	3.9	80
141	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
140	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
139	Quantum chemical analysis of the energetics of the anti and gauche conformers of ethanol. *Structural Chemistry*, **2009**, 20, 43-48	1.8	20
138	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
137	Proton transfer potentials in hydrogen-bonded systems: (H5O2)+. *International Journal of Quantum Chemistry*, **2009**, 18, 199-206	2.1	
136	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	
135	Perturbations of proton transfer potentials caused by polar molecules. *International Journal of Quantum Chemistry*, **2009**, 36, 211-217	2.1	0
134	Identification of spectroscopic patterns of CH...O H-bonds in proteins. *Journal of Physical Chemistry B*, **2009**, 113, 10421-7	3.4	36
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