SÅ‚awomir J Grabowski

List of Publications by Year
in descending order

117	6,784	44069	62596
papers	citations	48 h-index	80 g-index

123	123	123	3602
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Tetrel bondâ€“Ïƒ-hole bond as a preliminary stage of the S_N2 reaction. Physical Chemistry Chemical Physics, 2014, 16, 1824-1834.	2.8	424
2	Cooperativity in Hydrogen-Bonded Interactions:â€‰ Ab Initio and â€œAtoms in Moleculesâ€•Analyses. Journal of Physical Chemistry A, 2006, 110, 6514-6521.	2.5	321
3	Properties of the Cα–HÂ·Â·Â·H Dihydrogen Bond:â€‰ An ab Initio and Topological Analysis. Journal of Physical Chemistry A, 2004, 108, 10865-10872.	2.5	257
4	High-Level Ab Initio Calculations of Dihydrogen-Bonded Complexes. Journal of Physical Chemistry A, 2000, 104, 5551-5557.	2.5	232
5	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.	2.5	224
6	Quantitative Classification of Covalent and Noncovalent H-Bonds. Journal of Physical Chemistry B, 2006, 110, 6444-6446.	2.6	224
7	How Short Can the HÂ·Â·Â·H Intermolecular Contact Be? New Findings that Reveal the Covalent Nature of Extremely Strong Interactions. Journal of Physical Chemistry A, 2005, 109, 4331-4341.	2.5	188
8	A new measure of hydrogen bonding strength â€“ ab initio and atoms in molecules studies. Chemical Physics Letters, 2001, 338, 361-366.	2.6	182
9	QTAIM Characteristics of Halogen Bond and Related Interactions. Journal of Physical Chemistry A, 2012, 116, 1838-1845.	2.5	176
10	Theoretical studies of strong hydrogen bonds. Annual Reports on the Progress of Chemistry Section C, 2006, 102, 131.	4.4	161
11	Dimers of Formic Acid, Acetic Acid, Formamide and Pyrrole-2-carboxylic Acid:â€‰ an Ab Initio Study. Journal of Physical Chemistry A, 2005, 109, 6397-6405.	2.5	157
12	CHÂ·Â·Â·N and CHÂ·Â·Â·S Hydrogen BondsInfluence of Hybridization on Their Strength. Journal of Physical Chemistry A, 2005, 109, 5683-5688.	2.5	146
13	Cooperativity halogen bonding effect â€“ Ab initio calculations on H2COâ‹¯(ClF)n complexes. Chemical Physics Letters, 2006, 427, 51-55.	2.6	142
14	Hydrogen and halogen bonds are ruled by the same mechanisms. Physical Chemistry Chemical Physics, 2013, 15, 7249.	2.8	137
15	Boron and other Triel Lewis Acid Centers: From Hypovalency to Hypervalency. ChemPhysChem, 2014, 15, 2985-2993.	2.1	133
16	Ï€â€Hole Bonds: Boron and Aluminum Lewis Acid Centers. ChemPhysChem, 2015, 16, 1470-1479.	2.1	112
17	Bond Paths Show Preferable Interactions: Ab Initio and QTAIM Studies on the Xα–HÂ·Â·Â·Ï€ Hydrogen Bond. Journal of Physical Chemistry A, 2010, 114, 7223-7229.	2.5	101
18	Triel Bonds, Ï€-Hole-Ï€-Electrons Interactions in Complexes of Boron and Aluminium Trihalides and Trihydrides with Acetylene and Ethylene. Molecules, 2015, 20, 11297-11316.	3.8	100

#	Article	IF	Citations
19	Topological reaction sites â€“ very strong chalcogen bonds. Physical Chemistry Chemical Physics, 2014, 16, 2430-2442.	2.8	97
20	Properties of a Ring Critical Pointas Measures of Intramolecular H-Bond Strength. Monatshefte FÃ¼r Chemie, 2002, 133, 1373-1380.	1.8	95
21	Properties of the Halogenâ‹¯Hydride Interaction:Â An ab Initio and â€œAtoms in Moleculesâ€•Analysis. Journal of Physical Chemistry A, 2006, 110, 10296-10302.	2.5	95
22	Halogen Bond and Its Counterparts: Bentâ€™s Rule Explains the Formation of Nonbonding Interactions. Journal of Physical Chemistry A, 2011, 115, 12340-12347.	2.5	93
23	Role of Câ‹¯HÂ·Â·Â·S and Câ‹¯HÂ·Â·Â·N Hydrogen Bonds in Organic Crystal StructuresThe Crystal and Molecular Structure of 3-Methyl-2,4-diphenyl-(1,3)-thiazolidine-5-spiro-2â€˜-adamantane and 3-Methyl-2,4,5,5-tetraphenyl-(1,3)-thiazolidine. Journal of Physical Chemistry A, 2003, 107, 2730-2736.	2.5	92
24	Red- and Blue-Shifted Hydrogen Bonds: the Bent Rule from Quantum Theory of Atoms in Molecules Perspective. Journal of Physical Chemistry A, 2011, 115, 12789-12799.	2.5	91
25	Hydrogen bonds, and Ïƒ-hole and Ï€-hole bonds â€“ mechanisms protecting doublet and octet electron structures. Physical Chemistry Chemical Physics, 2017, 19, 29742-29759.	2.8	91
26	The Possible Covalent Nature of Nâ‹¯HÂ·Â·Â·O Hydrogen Bonds in Formamide Dimer and Related Systems:Â An Ab Initio Study. Journal of Physical Chemistry A, 2006, 110, 4772-4779.	2.5	90
27	Characteristics of X-HÂ·Â·Â·Ï€ Interactions: Ab Initio and QTAIM Studies. Journal of Physical Chemistry A, 2011, 115, 4765-4773.	2.5	85
28	How To Determine Whether Intramolecular HÂ·Â·Â·H Interactions Can Be Classified as Dihydrogen Bonds. Journal of Physical Chemistry A, 2008, 112, 2721-2727.	2.5	77
29	Wide spectrum of Hâ‹¯H interactions: van der Waals contacts, dihydrogen bonds and covalency. Chemical Physics, 2007, 337, 68-76.	1.9	74
30	Non-covalent interactions â€“ QTAIM and NBO analysis. Journal of Molecular Modeling, 2013, 19, 4713-4721.	1.8	74
31	Pnicogen and hydrogen bonds: complexes between PH3X+ and PH2X systems. Physical Chemistry Chemical Physics, 2015, 17, 3261-3272.	2.8	74
32	Triel bond and coordination of triel centres â€“ Comparison with hydrogen bond interaction. Coordination Chemistry Reviews, 2020, 407, 213171.	18.8	72
33	Resonance-assisted hydrogen bonds revisited. Resonance stabilization vs. charge delocalization. Physical Chemistry Chemical Physics, 2013, 15, 2514.	2.8	71
34	Is a Ï€Â·Â·Â·H+Â·Â·Â·Ï€ Complex Hydrogen Bonded?. Journal of Physical Chemistry A, 2004, 108, 1806-1812.	2.5	68
35	Are Various Ïƒâ€Hole Bonds Steered by the Same Mechanisms?. ChemPhysChem, 2017, 18, 1569-1577.	2.1	67
36	Crystal and Molecular Structures of New Chromone Derivatives as Empirical Evidence of Intramolecular Proton Transfer Reaction; Ab Initio Studies on Intramolecular H-Bonds in Enaminones. Journal of Physical Chemistry A, 2002, 106, 11956-11962.	2.5	61

#	Article	IF	Citations
37	Ïƒâ€Hole Bond Versus Hydrogen Bond: From Tetravalent to Pentavalent N, P, and As Atoms. Chemistry - A European Journal, 2013, 19, 14600-14611.	3.3	61
38	Halogen bonding in crystal structure of 1-methylpyrrol-2-yl trichloromethyl ketone. Journal of Molecular Structure, 2007, 829, 208-211.	3.6	58
39	The enhancement of Xâ€“Hâ‹¯Ïâ€ hydrogen bond by cooperativity effects â€“ Ab initio and QTAIM calculations. Chemical Physics, 2009, 355, 169-176.	1.9	58
40	Cooperativity of hydrogen and halogen bond interactions. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	58
41	Triel bonds-complexes of boron and aluminum trihalides and trihydrides with benzene. Structural Chemistry, 2017, 28, 1163-1171.	2.0	57
42	Can Hâ€¦Ïƒ, Ïâ€¦H+â€¦Ïƒ and Ïƒâ€¦H+â€¦Ïƒ interactions be classified as H-bonded?. Chemical Physics Letters, 2006, 432, 33-39.	2.6	55
43	Blue-shifting Câ€“Hâ€¦Y intramolecular hydrogen bonds â€“ DFT and AIM analyses. Chemical Physics, 2005, 309, 183-188.	1.9	52
44	Hydride bonding â€“ Ab initio studies of BeH2â€¦Li+, BeH2â€¦Na+ and BeH2â€¦Mg2+ model systems. Chemical Physics Letters, 2006, 422, 334-339.	2.6	52
45	Do intramolecular halogen bonds exist? Ab initio calculations and crystal structuresâ€™ evidences. Structural Chemistry, 2008, 19, 5-11.	2.0	52
46	Dihydrogen bond and Xâ€“Hâ€¦Ïƒ interaction as subâ€classes of hydrogen bond. Journal of Physical Organic Chemistry, 2013, 26, 452-459.	1.9	52
47	Comparison of Hydrogen and Gold Bonding in [XHX]^{â^’}, [XAuX]^{â^’}, and Isoelectronic [NgHNg]⁺, [NgAuNg]⁺ (X=Halogen, Ng=Noble Gas). Chemistry - A European Journal, 2016, 22, 11317-11328.	3.3	50
48	Pnicogen and tetrel bondsâ€”tetrahedral Lewis acid centres. Structural Chemistry, 2019, 30, 1141-1152.	2.0	50
49	Two faces of triel bonds in boron trihalide complexes. Journal of Computational Chemistry, 2018, 39, 472-480.	3.3	49
50	Complexes between Dihydrogen and Amine, Phosphine, and Arsine Derivatives. Hydrogen Bond versus Pnictogen Interaction. Journal of Physical Chemistry A, 2013, 117, 3243-3251.	2.5	48
51	Acetylene as potential hydrogen-bond proton acceptor. Journal of Molecular Structure, 2002, 615, 209-218.	3.6	44
52	Could the lithium bond be classified as the Ïƒ-hole bond? â€“ QTAIM and NBO analysis. Chemical Physics Letters, 2014, 591, 113-118.	2.6	44
53	Hâ‹¯Ïƒ interactions â€“ an ab initio and `atoms in molecules' study. Chemical Physics Letters, 2004, 393, 81-86.	2.6	43
54	Halogen bond with the multivalent halogen acting as the Lewis acid center. Chemical Physics Letters, 2014, 605-606, 131-136.	2.6	41

#	Article	IF	Citations
55	Ab initio and AIM studies on measures of hydrogen bonding strengthâ€”Râ€“C˜†N‹¯HF and Râ€“C˜†N‹¯HCl complexes. Journal of Molecular Structure, 2002, 615, 239-245.	3.6	37
56	Tetrel Bonds with Ï€-Electrons Acting as Lewis Basesâ€”Theoretical Results and Experimental Evidences. Molecules, 2018, 23, 1183.	3.8	37
57	Attractive halogenâ€“halogen interactions: F3CCl‹¯FH and F3CCl‹¯FCH3 dimers. Chemical Physics, 2006, 327, 151-158.	1.9	34
58	Do intramolecular halogen bonds exist? Ab initio calculations and crystal structuresâ€™ evidences. Structural Chemistry, 2007, 18, 859-865.	2.0	34
59	The Nature of Triel Bonds, a Case of B and Al Centres Bonded with Electron Rich Sites. Molecules, 2020, 25, 2703.	3.8	32
60	Lewis Acid Properties of Tetrel Tetrafluoridesâ€”The Coincidence of the Ïƒ-Hole Concept with the QTAIM Approach. Crystals, 2017, 7, 43.	2.2	31
61	Dihydrogen Bonding vs Metalâ˜Ïƒ Interaction in Complexes between H₂ and Metal Hydride. Journal of Physical Chemistry A, 2011, 115, 201-210.	2.5	30
62	Xâ€“H‹¯Ï€ and Xâ€“H‹¯N hydrogen bonds â€“ Acetylene and hydrogen cyanide as proton acceptors. Chemical Physics, 2009, 363, 42-48.	1.9	29
63	Analysis of Hydrogen Bonds in Crystals. Crystals, 2016, 6, 59.	2.2	29
64	Tetrel bonds, pentaâ€•and hexaâ€coordinated tin and lead centres. Applied Organometallic Chemistry, 2017, 31, e3727.	3.5	29
65	[FHF]â˜â€”The Strongest Hydrogen Bond under the Influence of External Interactions. Crystals, 2016, 6, 3.	2.2	28
66	Heteronuclear Intermolecular Resonance-Assisted Hydrogen Bonds. The Structure of Pyrrole-2-Carboxamide (PyCa). Journal of Physical Chemistry B, 2006, 110, 5875-5882.	2.6	27
67	An analysis of bifurcated H-bonds: crystal and molecular structures ofO,O-diphenyl 1-(3-phenylthioureido)Âpentanephosphonate andO,O-diphenyl 1-(3-phenylthioureido)butanephosphonate. Journal of Physical Organic Chemistry, 2003, 16, 213-219.	1.9	26
68	Dihydrogen bond interactions as a result of H₂cleavage at Cu, Ag and Au centres. Physical Chemistry Chemical Physics, 2016, 18, 12810-12818.	2.8	26
69	Intramolecular Hydrogen Bond Energy and Its Decompositionâ€”Oâ€“Hâ^™â^™Oâ^™â^™O Interactions. Crystals, 2021, 11, 5.	2.2	26
70	New Type of Halogen Bond: Multivalent Halogen Interacting with Ï€- and Ïƒ-Electrons. Molecules, 2017, 22, 2150.	3.8	25
71	High-level ab initio calculations on low barrier hydrogen bonds and proton bound homodimers. Chemical Physics Letters, 2010, 493, 37-44.	2.6	23
72	Hydrogen Bonds with BF4â^’ Anion as a Proton Acceptor. Crystals, 2020, 10, 460.	2.2	23

#	Article	IF	Citations
73	Spectroscopic and theoretical studies on the monomeric and dimeric forms of methyl pyrrole-2-carboxylate. New Journal of Chemistry, 2002, 26, 165-169.	2.8	22
74	Hydrocarbons as proton donors in Câ€“Hâ‹¯N and Câ€“Hâ‹¯S hydrogen bonds. Chemical Physics, 2010, 367, 1-6.	1.9	22
75	Structural, energetic, spectroscopic and QTAIM analyses of cationâ€“Ï€ interactions involving mono- and bi-cyclic ring fused benzene systems. Physical Chemistry Chemical Physics, 2013, 15, 20839.	2.8	21
76	Hydrogen Bond and Other Lewis Acidâ€“Lewis Base Interactions as Preliminary Stages of Chemical Reactions. Molecules, 2020, 25, 4668.	3.8	21
77	Clusters of Ammonium Cationâ”Hydrogen Bond versus Ïƒâ€Hole Bond. ChemPhysChem, 2014, 15, 876-884.	2.1	19
78	Where the two carbon atoms touch in the triple bond in disubstituted acetylenes: the AIM analysis. Chemical Physics Letters, 2004, 389, 51-57.	2.6	17
79	Aâ”Hâ€¦Ïƒ Hydrogen Bonds: Dihydrogen and Cycloalkanes as Proton Acceptors. ChemPhysChem, 2019, 20, 565-574.	2.1	17
80	Ï€-Hole Tetrel Bondsâ€”Lewis Acid Properties of Metallylenes. Crystals, 2022, 12, 112.	2.2	17
81	Covalent character of three-center, two-electron systems â€“C2H3+ and C2H5+. Chemical Physics Letters, 2007, 436, 63-67.	2.6	16
82	Bifurcated Triel Bondsâ”Hydrides and Halides of 1,2-Bis(Dichloroboryl)Benzene and 1,8-Bis(Dichloroboryl)Naphthalene. Crystals, 2019, 9, 503.	2.2	16
83	Classification of So-Called Non-Covalent Interactions Based on VSEPR Model. Molecules, 2021, 26, 4939.	3.8	16
84	Spectroscopic and theoretical studies on some new pyrrol-2-yl-chloromethyl ketones. New Journal of Chemistry, 2010, 34, 556.	2.8	15
85	Ï€â‹…â‹…â‹…H⁺â‹…â‹…â‹…Ï€ Hydrogen Bonds and Their Lithium and Gold Analogues: MP2 and CASPT2 Calculations. ChemPhysChem, 2017, 18, 2409-2417.	2.1	14
86	The substituent effect in ethylenes and acetylenes â€“ AIM analysis. Chemical Physics Letters, 2004, 400, 362-367.	2.6	13
87	Coordination of Be and Mg Centres by HCN Ligands â€“ Beâ€¦N and Mgâ€¦N Interactions. ChemPhysChem, 2018, 19, 1830-1840.	2.1	13
88	Thieno[3,4â€c]pyroleâ€4,6â€dione Oligothiophenes Have Two Crossed Paths for Electron Delocalization. Chemistry - A European Journal, 2018, 24, 13523-13534.	3.3	13
89	Partial Hydrogen Bonds:Â Structural Studies on Thioureidoalkylphosphonates. Journal of Physical Chemistry A, 2005, 109, 2942-2947.	2.5	12
90	Reaction pathway of proton transfer from the neutral to zwitterionic forms of amino acids. Support for a water molecule-mediated mechanism. Journal of Physical Organic Chemistry, 2000, 13, 740-744.	1.9	11

#	Article	IF	Citations
91	Hydrogen bonds assisted by Ï€â€•electron delocalization â€“ the influence of external intermolecular interactions on dimer of formic acid. Journal of Physical Organic Chemistry, 2008, 21, 694-702.	1.9	11
92	Non-covalent interactions in ammonium cationâ€“acetylene clusters. Computational and Theoretical Chemistry, 2012, 992, 70-77.	2.5	11
93	Coexistence of Intra- and Intermolecular Hydrogen Bonds: Salicylic Acid and Salicylamide and Their Thiol Counterparts. Journal of Physical Chemistry A, 2021, 125, 1526-1539.	2.5	11
94	Sâˆ’Hâ€¦O and Oâˆ’Hâ€¦O Hydrogen Bondsâ€•Comparison of Dimers of Thiocarboxylic and Carboxylic Acids. ChemPhysChem, 2020, 21, 1653-1664.	2.1	10
95	Hydrogen bonds and other interactions as a response to protect doublet/octet electron structure. Journal of Molecular Modeling, 2018, 24, 38.	1.8	9
96	Angular group-induced bond alternation (AGIBA). Part 5?Conformation dependence and additivity of the effect: structural studies of 3,5-dimethoxybenzaldehyde ï¿½derivatives and related systems. Journal of Physical Organic Chemistry, 2001, 14, 349-354.	1.9	8
97	Ab initio calculations onÂC₆H₆Â·Â·Â·(HF)_nclustersÂâ€”ÂXâ€“HÂ·Â·Â·Ï€ÂhydrogenÂbond. Canadian Journal of Chemistry, 2010, 88, 769-778.	1.1	8
98	Stabilizing H₃⁺: Or Are We Stabilizing a Proton?. ChemPhysChem, 2012, 13, 2286-2288.	2.1	8
99	Magnesium Bonds: From Divalent Mg Centres to Trigonal and Tetrahedral Coordination. ChemistrySelect, 2018, 3, 3147-3154.	1.5	8
100	Tetravalent Oxygen and Sulphur Centres Mediated by Carborane Superacid: Theoretical Analysis. ChemPhysChem, 2019, 20, 2443-2450.	2.1	8
101	Complexes of carborane acids linked by strong hydrogen bonds: acidity scales. Physical Chemistry Chemical Physics, 2016, 18, 16152-16160.	2.8	7
102	Hydrogen and Lithium Bondsâ€”Lewis Acid Units Possessing Multi-Center Covalent Bonds. Molecules, 2021, 26, 6939.	3.8	7
103	Cleavage of hydrogen by activation at a single non-metal centre â€“ towards new hydrogen storage materials. Physical Chemistry Chemical Physics, 2015, 17, 13539-13546.	2.8	6
104	Molecular Hydrogen as a Lewis Base in Hydrogen Bonds and Other Interactions. Molecules, 2020, 25, 3294.	3.8	6
105	Cooperativity of hydrogen and halogen bond interactions. Highlights in Theoretical Chemistry, 2014, , 59-68.	0.0	5
106	What is Common for Dihydrogen Bond and Hâ€¦Ïƒ Interactionâ€”Theoretical Analysis and Experimental Evidences. Challenges and Advances in Computational Chemistry and Physics, 2015, , 159-187.	0.6	3
107	Aâ€“Xâ‹¯Ïƒ Interactionsâ€”Halogen Bonds with Ïƒ-Electrons as the Lewis Base Centre. Molecules, 2021, 26, 5175.	3.8	3
108	Hydrogen Bonding Properties of the Complexes of Formaldehyde and its Derivatives with HF and HCl. Monatshefte FÃ¼r Chemie, 2002, 133, 305-312.	1.8	2

#	Article	IF	Citations
109	Lewis acidâ€“Lewis base interactions: From NFH3+â‹¯NCH and NF4+â‹¯NCH complexes to NFH3+â‹¯(NCH)n and NF4+â‹¯(NCH)n clusters. Computational and Theoretical Chemistry, 2015, 1053, 289-297.	2.5	2
110	What Can Be Learnt from a Location of Bond Paths and from Electron Density Distribution. Challenges and Advances in Computational Chemistry and Physics, 2016, , 399-433.	0.6	2
111	Ïƒ-Hole Bonds and the VSEPR Modelâ€”From the Tetrahedral Structure to the Trigonal Bipyramid. Sci, 2022, 4, 17.	3.0	2
112	Crystal Structure of Two Dimethyl 1,3-Thiazolidinedicarboxylates Obtained in Thermal [2 + 3]Cycloaddition of an Azomethine Ylide with 2,2,4,4-Tetramethyl-3-Thioxocyclobutanone. Structural Chemistry, 2005, 16, 55-59.	2.0	1
113	Professor Tadeusz Marek Krygowski. Structural Chemistry, 2007, 18, 755-756.	2.0	1
114	Interactions Steering Arrangement of Molecules in Crystals. Crystals, 2020, 10, 130.	2.2	1
115	The coordination of beryllium and magnesium centres in half-sandwich and sandwich compounds. Journal of Organometallic Chemistry, 2021, 948, 121906.	1.8	1
116	Xâ€“Hâ€¦Ï€ and Xâ€“Hâ€¦Ïƒ Interactions â€“ Hydrogen Bonds with Multicenter Proton Acceptors. , 2011, , 497-516.		0
117	Hydrogen Bond and Other Lewis Acidâ€“Lewis Base Interactionsâ€”Mechanisms of Formation. , 2016, , 245-277.		0