

Marcin Palusiak

List of Publications by Year in descending order

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docs citations

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2457
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#	ARTICLE	IF	CITATIONS
1	Aromaticity from the Viewpoint of Molecular Geometry: Application to Planar Systems. <i>Chemical Reviews</i> , 2014, 114, 6383-6422.	23.0	439
2	Application of AIM Parameters at Ring Critical Points for Estimation of π -Electron Delocalization in Six-Membered Aromatic and Quasi-Aromatic Rings. <i>Chemistry - A European Journal</i> , 2007, 13, 7996-8006.	1.7	159
3	On the nature of halogen bond π -The Kohn-Sham molecular orbital approach. <i>Computational and Theoretical Chemistry</i> , 2010, 945, 89-92.	1.5	122
4	Interplay between Intramolecular Resonance-Assisted Hydrogen Bonding and Aromaticity in o-Hydroxyaryl Aldehydes. <i>Journal of Organic Chemistry</i> , 2006, 71, 5241-5248.	1.7	110
5	Electron Density Characteristics in Bond Critical Point (QTAIM) versus Interaction Energy Components (SAPT): The Case of Charge-Assisted Hydrogen Bonding. <i>Journal of Physical Chemistry A</i> , 2012, 116, 452-459.	1.1	109
6	Nature of a Hydride-Halogen Bond. A SAPT-, QTAIM-, and NBO-Based Study. <i>Journal of Physical Chemistry A</i> , 2012, 116, 2322-2332.	1.1	96
7	Basis Set and Method Dependence in Atoms in Molecules Calculations. <i>Journal of Physical Chemistry A</i> , 2010, 114, 2240-2244.	1.1	93
8	Intramolecular H \cdots H Interactions for the Crystal Structures of [4-((E)-But-1-enyl)-2,6-dimethoxyphenyl]pyridine-3-carboxylate and [4-((E)-Pent-1-enyl)-2,6-dimethoxyphenyl]pyridine-3-carboxylate; DFT Calculations on Modeled Styrene Derivatives. <i>Journal of Physical Chemistry B</i> , 2004, 108, 1831-1837.	1.2	71
9	Interplay between Intramolecular Resonance-Assisted Hydrogen Bonding and Local Aromaticity. II. 1,3-Dihydroxyaryl-2-aldehydes. <i>Journal of Organic Chemistry</i> , 2009, 74, 2059-2066.	1.7	68
10	Basis Set and Method Dependence in Quantum Theory of Atoms in Molecules Calculations for Covalent Bonds. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12498-12505.	1.1	65
11	Methoxy group as an acceptor of proton in hydrogen bonds. <i>Journal of Molecular Structure</i> , 2002, 642, 97-104.	1.8	63
12	Relationship between substituent effect and aromaticity π -Part III: naphthalene as a transmitting moiety for substituent effect. <i>Journal of Physical Organic Chemistry</i> , 2007, 20, 297-306.	0.9	61
13	Substituent effect in para substituted Cr(CO) $_5$ -pyridine complexes. <i>Journal of Organometallic Chemistry</i> , 2007, 692, 3866-3873.	0.8	53
14	Do intramolecular halogen bonds exist? Ab initio calculations and crystal structures π evidences. <i>Structural Chemistry</i> , 2008, 19, 5-11.	1.0	52
15	H-Bonding-Assisted Substituent Effect. <i>Journal of Organic Chemistry</i> , 2010, 75, 4944-4949.	1.7	45
16	The nature of NO-bonding in N-oxide group. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 16375-16387.	1.3	45
17	Relation between π -Electron Localization/Delocalization and H-Bond Strength in Derivatives of <i>o</i> -Hydroxy-Schiff Bases. <i>Journal of Organic Chemistry</i> , 2008, 73, 2138-2145.	1.7	44
18	Aromaticity of substituted fulvene derivatives: substituent-dependent ring currents. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 10740.	1.3	44

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19	The proton transfer reaction in malonaldehyde derivatives: Substituent effects and quasi-aromaticity of the proton bridge. <i>Chemical Physics</i> , 2007, 342, 43-54.	0.9	43
20	Divalent carbon atom as the proton acceptor in hydrogen bonding. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 5711.	1.3	43
21	EL: the new aromaticity measure based on one-electron density function. <i>Structural Chemistry</i> , 2012, 23, 1173-1183.	1.0	42
22	Halogen bond, hydrogen bond and N π -C interaction – On interrelation among these three noncovalent interactions. <i>Computational and Theoretical Chemistry</i> , 2012, 998, 26-33.	1.1	40
23	Ferrocenyl D- π -A chromophores containing 3-dicyanomethylidene-1-indanone and 1,3-bis(dicyanomethylidene)indane acceptor groups. <i>Journal of Organometallic Chemistry</i> , 2003, 675, 35-41.	0.8	35
24	Crystal and Molecular Structure of Pyrrole-2-carboxylic Acid; π -Electron Delocalization of Its Dimers – DFT and MP2 Calculations. <i>Journal of Physical Chemistry A</i> , 2004, 108, 5815-5822.	1.1	35
25	Quasi-aromaticity – what does it mean?. <i>Tetrahedron</i> , 2015, 71, 4895-4908.	1.0	35
26	Ferrocenyl D- π -A conjugated polyenes with 3-dicyanomethylidene-1-indanone and 1,3-bis(dicyanomethylidene)indane acceptor groups: Synthesis, linear and second-order nonlinear optical properties and electrochemistry. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 323-330.	0.8	34
27	Do intramolecular halogen bonds exist? Ab initio calculations and crystal structures – evidences. <i>Structural Chemistry</i> , 2007, 18, 859-865.	1.0	34
28	The halogen π - π oxygen interaction in 3-halogenopropenal revisited – The dimer model vs. QTAIM indications. <i>Chemical Physics</i> , 2013, 415, 207-213.	0.9	33
29	Does electron density in bond critical point reflect the formal charge distribution in H-bridges? The case of charge-assisted hydrogen bonds (CAHBs). <i>Computational and Theoretical Chemistry</i> , 2011, 966, 113-119.	1.1	31
30	The influence of substituent effect on noncovalent interactions in ternary complexes stabilized by hydrogen-bonding and halogen-bonding. <i>Computational and Theoretical Chemistry</i> , 2014, 1027, 173-178.	1.1	28
31	Tuning the Strength of the Resonance-Assisted Hydrogen Bond in <i>o</i> -Hydroxybenzaldehyde by Substitution in the Aromatic Ring ^{>1</sup>. <i>Journal of Physical Chemistry A</i>, 2018, 122, 2279-2287.}	1.1	28
32	Heteronuclear Intermolecular Resonance-Assisted Hydrogen Bonds. The Structure of Pyrrole-2-Carboxamide (PyCa). <i>Journal of Physical Chemistry B</i> , 2006, 110, 5875-5882.	1.2	27
33	Halogen – halogen interaction in view of many-body approach. <i>Chemical Physics Letters</i> , 2013, 583, 8-13.	1.2	26
34	Extremely Strong Halogen Bond. The Case of a Double-Charge-Assisted Halogen Bridge. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5484-5492.	1.1	26
35	Sulfhydryl-Selective, Covalent Labeling of Biomolecules with Transition Metallocarbonyl Complexes. Synthesis of (1-5-C5H5)M(CO)3(1-1-N-Maleimidato) (M = Mo, W), X-ray Structure, and Reactivity Studies. <i>Bioconjugate Chemistry</i> , 2005, 16, 1218-1224.	1.8	25
36	Does the concept of Clar's aromatic sextet work for dicationic forms of polycyclic aromatic hydrocarbons? – testing the model against charged systems in singlet and triplet states. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 11976-11984.	1.3	25

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37	Substituent effects in mono- and disubstituted 1,3,5,7-cyclooctatetraene derivatives in natural and planar conformations. <i>New Journal of Chemistry</i> , 2009, 33, 1753.	1.4	22
38	The shape of the halogen atom's anisotropy of electron distribution and its dependence on basis set and method used. <i>Structural Chemistry</i> , 2013, 24, 1297-1306.	1.0	22
39	<i>N</i> -Oxide as a Proton Accepting Group in Multicomponent Crystals: X-ray and Theoretical Studies on New <i>p</i> -Nitropyridine- <i>N</i> -oxide Co-Crystals. <i>Crystal Growth and Design</i> , 2015, 15, 5802-5815.	1.4	22
40	Halogen bond versus hydrogen bond: The many-body interactions approach. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25348.	1.0	21
41	Intramolecular carbonyl-carbonyl interactions in W, Mo and Fe complexes containing the $\hat{1}$ -N-maleimidato ligand: X-ray, DFT and AIM studies. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 3232-3238.	0.8	19
42	Cyclooctatetraene in metal complexes' planar does not mean aromatic. <i>New Journal of Chemistry</i> , 2010, 34, 1855.	1.4	17
43	Cyclooctatetraene dianion' an artifact?. <i>Journal of Computational Chemistry</i> , 2011, 32, 1441-1448.	1.5	17
44	The substituent effect on benzene dications. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 4752-4763.	1.3	17
45	Why 1,2-quinone derivatives are more stable than their 2,3-analogues?. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	16
46	Source of Cooperativity in Halogen-Bonded Haloamine Tetramers. <i>ChemPhysChem</i> , 2016, 17, 474-480.	1.0	16
47	Routes of π -Electron Delocalization in 4-Substituted-1,2-benzoquinones. <i>Journal of Organic Chemistry</i> , 2011, 76, 550-556.	1.7	15
48	Temperature-dependent polymorphism of N-(4-fluorophenyl)-1,5-dimethyl-1H-imidazole-4-carboxamide 3-oxide: experimental and theoretical studies on intermolecular interactions in the crystal state. <i>Structural Chemistry</i> , 2014, 25, 979-989.	1.0	14
49	The role of sulfur interactions in crystal architecture: experimental and quantum theoretical studies on hydrogen, halogen, and chalcogen bonds in trithiocyanuric acid' pyridine <i>N</i> -oxide co-crystals. <i>CrystEngComm</i> , 2021, 23, 324-334.	1.3	13
50	The phospho-Michael addition of dimethyl- and diphenylphosphites to the $\hat{1}$ -N-maleimidato ligand: Inhibition of serine hydrolases by half-sandwich metallocarbonyl azaphosphonates. <i>Journal of Organometallic Chemistry</i> , 2009, 694, 908-915.	0.8	12
51	<i>N</i> -Oxide' <i>N</i> -oxide interactions and Cl...Cl halogen bonds in pentachloropyridine <i>N</i> -oxide: the many-body approach to interactions in the crystal state. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2018, 74, 113-119.	0.2	12
52	Tuning Aromaticity of <i>para</i> -Substituted Benzene Derivatives with an External Electric Field. <i>ChemPhysChem</i> , 2018, 19, 590-595.	1.0	12
53	Are the O=C-H-C intramolecular systems of 2-cyclopropyl ethenol and its derivatives classified as dihydrogen bonds? Ab initio and DFT study. <i>Computational and Theoretical Chemistry</i> , 2004, 674, 147-152.	1.5	11
54	Aryl (ferrocenyl)-capped ethenylzazaferrocenes: synthesis, structure and electrochemistry. <i>New Journal of Chemistry</i> , 2006, 30, 901-907.	1.4	11

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55	Inter- and intramolecular hydrogen bonds – Structures of 1-methylpyrrole-2-carboxamide and 1-hydroxypyrrole-2-carboxamide. <i>Journal of Molecular Structure</i> , 2007, 844-845, 173-180.	1.8	11
56	Modeling the electronic structure of formamide: an acid/base amphoteric solvent. <i>Structural Chemistry</i> , 2012, 23, 1711-1721.	1.0	11
57	Synthesis and characterization of new M(II) carbonyl complexes (M=Fe or Ru) including an η^1 -N-maleimidato ligand. Reactivity studies with biological thiols. <i>Journal of Organometallic Chemistry</i> , 2016, 801, 101-110.	0.8	11
58	Unusual electron density topology and intramolecular steric – interaction in 1,3,5,7-cyclooctatetraene. <i>Chemical Physics Letters</i> , 2009, 481, 34-38.	1.2	10
59	Feynman force components: basis for a solution to the covalent vs. ionic dilemma. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 25022-25026.	1.3	10
60	Non-covalent interactions of N-phenyl-1,5-dimethyl-1H-imidazole-4-carboxamide 3-oxide derivatives – a case of intramolecular N-oxide hydrogen bonds. <i>Structural Chemistry</i> , 2017, 28, 1229-1241.	1.0	9
61	Metallobarbonyl complexes: (η^5 -C ₅ H ₅)M(CO) _n (η^1 -N-imidato) (M = Fe, Ru, Mo, W; n = 2, 3) as new photoactive CO-releasing molecules (CORMs). <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 351, 115-123.	2.0	9
62	Does Proton Transfer Always Take Place in Molecules of 2-Substituted Pyridine-N-oxides? The Case of 2-Aminopyridine-N-oxide Crystal Structure and Its 3,5-Dinitrobenzoic Acid Co-crystal. <i>Crystal Growth and Design</i> , 2018, 18, 7373-7382.	1.4	9
63	Characteristics of ring critical point as descriptors of H-bond strength. <i>Journal of Chemical Research</i> , 2004, 2004, 492-493.	0.6	8
64	Reaction of ferrocenecarbothioamide and N-(ethoxycarbonyl)ferrocenecarbothioamide with alkyl halides. <i>Journal of Organometallic Chemistry</i> , 2008, 693, 263-268.	0.8	8
65	Use of Quantum Theory of Atoms in Molecules in the Search for Appropriate Hydrogen Atom Locations in X-ray Diffraction Based Studies. <i>Crystal Growth and Design</i> , 2016, 16, 6841-6848.	1.4	8
66	η^1 -N-succinimidato complexes of iron, molybdenum and tungsten as reversible inhibitors of papain. <i>Journal of Inorganic Biochemistry</i> , 2009, 103, 1162-1168.	1.5	7
67	Diels-Alder reaction with cyclopentadiene and electronic structures of (η^5 -cyclopentadienyl)M(CO) _x (η^1 -N-maleimidato) (M=Fe, Mo, W, x=2 or 3). <i>Journal of Organometallic Chemistry</i> , 2009, 694, 1354-1358.	0.8	7
68	The effect of benzoannulation on the transition state and the proton transfer equilibrium in di(2-pyridyl)methane derivatives. <i>New Journal of Chemistry</i> , 2011, 35, 1433.	1.4	7
69	–Br...S halogen bonds in novel thiourea-N-oxide cocrystals: analysis of energetic and QTAIM parameters. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 170-176.	0.2	7
70	Bonding in η^2 -diketiminato boron and its analogues. <i>Structural Chemistry</i> , 2009, 20, 919-923.	1.0	6
71	UV-vis spectra of singlet state cationic polycyclic aromatic hydrocarbons: Time-dependent density functional theory study. <i>Journal of Chemical Physics</i> , 2014, 140, 044324.	1.2	6
72	Interactions of polar hydrogen bond donor solvents with ions: a theoretical study. <i>Structural Chemistry</i> , 2016, 27, 1279-1289.	1.0	6

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73	Cooperation/Competition between Halogen Bonds and Hydrogen Bonds in Complexes of 2,6-Diaminopyridines and X-CY3 (X = Cl, Br; Y = H, F). <i>Symmetry</i> , 2021, 13, 766.	1.1	6
74	A straightforward conversion of 1,4-quinones into polycyclic pyrazoles via [3 + 2]-cycloaddition with fluorinated nitrile imines. <i>Beilstein Journal of Organic Chemistry</i> , 2021, 17, 1509-1517.	1.3	6
75	Cytotoxicity of piano-stool ruthenium cyclopentadienyl complexes bearing different imidato ligands. <i>Applied Organometallic Chemistry</i> , 2022, 36, .	1.7	6
76	Resonance-Assisted Hydrogen Bond—Revisiting the Original Concept in the Context of Its Criticism in the Literature. <i>International Journal of Molecular Sciences</i> , 2022, 23, 233.	1.8	6
77	—Electronic communication through mono and multinuclear gold(I) complexes. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 2507-2519.	1.0	5
78	Aromaticity Induced by Electric Field: The Case of Polycalicenes. <i>Journal of Organic Chemistry</i> , 2015, 80, 9091-9101.	1.7	4
79	A Useful Synthetic Route to <i>N</i> -Nonsubstituted Succinimides via Light-Induced Degradation of Metallocarbonyl Complexes. <i>Organometallics</i> , 2021, 40, 663-673.	1.1	4
80	Trithiocyanuric acid: novel cocrystals and analysis of its tautomeric forms. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 49-55.	0.2	4
81	Co-crystals synthesis of 2- and 4-mercaptopyridine with thiourea and its analogue, trithiocyanuric acid. <i>CrystEngComm</i> , 0, , .	1.3	4
82	Charge-assisted N—H...I and C—H...I hydrogen bonding in (1 <i>R</i> ,2 <i>S</i>)-1-(ferrocenylmethyl)-2-(methoxymethyl)pyrrolidinium iodide. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2005, 61, m55-m57.	0.4	3
83	Ionic cocrystals of dithiobispyridines: the role of I...I halogen bonds in the building of iodine frameworks and the stabilization of crystal structures. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 458-466.	0.2	3
84	Inverse electron-demand Diels-Alder (iEDDA) bioorthogonal conjugation of half-sandwich transition metallocarbonyl entities to a model protein. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5507.	1.7	2
85	A rare case of a 2:2:1 ternary cocrystal of pyridine sulfides and trithiocyanuric acid. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 479-484.	0.2	2
86	2-[3-Dicyanomethylene-2-(3-methoxybenzylidene)indan-1-ylidene]malononitrile. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2006, 62, o3052-o3053.	0.2	1
87	Professor Tadeusz Marek Krygowski. <i>Structural Chemistry</i> , 2007, 18, 755-756.	1.0	1
88	A novel hydrogen-bonding <i>N</i> -oxide—sulfonamide—nitro N—H...O synthon determining the architecture of benzenesulfonamide cocrystals. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2022, 78, 7-13.	0.2	1
89	Novel melamine — salicylic salt solvates and co-crystals; an analysis of the energetic parameters of the intermolecular hydrogen bonds stabilizing the crystal structure. <i>CrystEngComm</i> , 2022, 24, 5688-5696.	1.3	1
90	5-Methoxy-4-(4-methoxyphenyl)isochroman-3-ol. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2003, 59, o11-o13.	0.2	0

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91	4-(E)-But-1-enyl-2,6-dimethoxyphenyl nicotinate. Acta Crystallographica Section E: Structure Reports Online, 2003, 59, o854-o856.	0.2	0
92	8-Methoxy-4-(4-methoxyphenyl)isochroman-3-ol. Acta Crystallographica Section E: Structure Reports Online, 2003, 59, o2000-o2002.	0.2	0
93	Isochroman derivatives and their tendency to crystallize in chiral space groups. Acta Crystallographica Section C: Crystal Structure Communications, 2004, 60, o239-o241.	0.4	0
94	Dimethyl 3,4,5,5-tetraphenyl-1,3-thiazolidine-2,2-dicarboxylate and 3,3-dichloro-2,2,4,4,3 λ^2 -pentamethyl-r-2 α^2 ,t-4 λ^2 -diphenylcyclobutane-1-spiro-5 α^2 -1,3-thiazolidine. Acta Crystallographica Section C: Crystal Structure Communications, 2004, 60, o595-o599.	0.4	0
95	Crystal structure of 3,6-bis(pyridin-2-yl)-1,4-dihydro-1,2,4,5-tetrazine. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 86-88.	0.2	0