Tadeusz Marek Krygowski

List of Publications by Year
in descending order

117	6,495	147566 31	64668 79
papers	citations	h-index	g-index

118	118	118	3724
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Energetic and Geometric Characteristics of Substituents, Part 3: The Case of NO2 and NH2 Groups in Their Mono-Substituted Derivatives of Six-Membered Heterocycles. Symmetry, 2022, 14, 145.	1.1	1
2	Aromaticity Concepts Derived from Experiments. Sci, 2022, 4, 24.	1.8	2
3	On differences in substituent effects in substituted ethene and acetylene derivatives and their boranyl analogs. Structural Chemistry, 2021, 32, 285-296.	1.0	3
4	Aromaticity of nucleic acid bases. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1509.	6.2	7
5	Energetic and geometric characteristics of the substituents. Part 1. The case of NO2 and NH2 groups in their mono-substituted derivatives of simple benzenoid hydrocarbons. Structural Chemistry, 2021, 32, 915-923.	1.0	4
6	Energetic characteristics of the substituents in para- and meta-substituted derivatives of benzoic acids. Chemical Physics Letters, 2021, 771, 138464.	1.2	2
7	Solvent Effect on the Stability and Reverse Substituent Effect in Nitropurine Tautomers. Symmetry, 2021, 13, 1223.	1.1	3
8	Effect of the Solvent and Substituent on Tautomeric Preferences of Amine-Adenine Tautomers. ACS Omega, 2021, 6, 18890-18903.	1.6	5
9	Dependence of the substituent energy on the level of theory. Journal of Computational Chemistry, 2021, 42, 2079-2088.	1.5	6
10	Energetic and Geometric Characteristics of the Substituents: Part 2: The Case of NO2, Cl, and NH2 Groups in Their Mono-Substituted Derivatives of Simple Nitrogen Heterocycles. Molecules, 2021, 26, 6543.	1.7	4
11	Mutual Relations between Substituent Effect, Hydrogen Bonding, and Aromaticity in Adenine-Uracil and Adenine-Adenine Base Pairs. Molecules, 2020, 25, 3688.	1.7	5
12	Solvent influence on intramolecular interactions and aromaticity in meta and para nitroanilines. Structural Chemistry, 2020, 31, 1717-1728.	1.0	6
13	How amino and nitro substituents affect the aromaticity of benzene ring. Chemical Physics Letters, 2020, 753, 137567.	1.2	7
14	Study of the influence of intermolecular interaction on classical and reverse substituent effects in para-substituted phenylboranes. New Journal of Chemistry, 2020, 44, 9656-9670.	1.4	13
15	Impact of the Substituents on the Electronic Structure of the Four Most Stable Tautomers of Purine and Their Adenine Analogues. ACS Omega, 2020, 5, 11570-11577.	1.6	3
16	Substituted adenine quartets: interplay between substituent effect, hydrogen bonding, and aromaticity. RSC Advances, 2020, 10, 23350-23358.	1.7	6
17	Changes in Electron Structure of the Triple Bond in Substituted Acetylene and Diacetylene Derivatives. ChemPhysChem, 2020, 21, 1847-1857.	1.0	6
18	Effect of Alkali Metal Cations on Length and Strength of Hydrogen Bonds in DNA Base Pairs. ChemPhysChem, 2020, 21, 2112-2126.	1.0	15

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19	On the relations between aromaticity and substituent effect. Structural Chemistry, 2019, 30, 1529-1548.	1.0	23
20	Aromaticity of the most stable adenine and purine tautomers in terms of HÃ¼ckel's 4N+2 principle. Tetrahedron, 2019, 75, 130474.	1.0	8
21	Classical and Reverse Substituent Effects in Substituted Anthrol Derivatives. ChemistryOpen, 2019, 8, 64-73.	0.9	9
22	Most of the field/inductive substituent effect works through the bonds. Journal of Molecular Modeling, 2019, 25, 350.	0.8	4
23	Substituent effects on the stability of the four most stable tautomers of adenine and purine. RSC Advances, 2019, 9, 31343-31356.	1.7	8
24	Stacking of nucleic acid bases: optimization of the computational approachâ€"the case of adenine dimers. Structural Chemistry, 2019, 30, 351-359.	1.0	20
25	Dependence of the Substituent Effect on Solvent Properties. Journal of Physical Chemistry A, 2018, 122, 1896-1904.	1.1	12
26	Aromaticity of acenes: the model of migrating Ï€-circuits. Physical Chemistry Chemical Physics, 2018, 20, 13430-13436.	1.3	36
27	How far the substituent effects in disubstituted cyclohexa-1,3-diene derivatives differ from those in bicyclo[2.2.2]octane and benzene?. Structural Chemistry, 2018, 29, 1201-1212.	1.0	9
28	Classical and reverse substituent effects in meta- and para-substituted nitrobenzene derivatives. Structural Chemistry, 2017, 28, 1125-1132.	1.0	22
29	Towards a physical interpretation of substituent effect: Quantum chemical interpretation of Hammett substituent constants. Journal of Molecular Structure, 2017, 1137, 581-588.	1.8	23
30	Towards physical interpretation of substituent effects: the case of N- and C3-substituted pyrrole derivatives. Structural Chemistry, 2017, 28, 1223-1227.	1.0	3
31	Olefinic vs aromatic way of substituent effects: The case of 3- and 4-substituted cyclohexa-1,3-dienamine derivatives. Journal of Physical Organic Chemistry, 2017, 30, e3694.	0.9	8
32	The role of the longâ€range exchange corrections in the description of electron delocalization in aromatic species. Journal of Computational Chemistry, 2017, 38, 1640-1654.	1.5	69
33	Inductive or Field Substituent Effect? Quantum Chemical Modeling of Interactions in 1-Monosubstituted Bicyclooctane Derivatives. ACS Omega, 2017, 2, 1746-1749.	1.6	10
34	Toward the Physical Interpretation of Inductive and Resonance Substituent Effects and Reexamination Based on Quantum Chemical Modeling. ACS Omega, 2017, 2, 7163-7171.	1.6	32
35	The electron density of delocalized bonds (EDDB) applied for quantifying aromaticity. Physical Chemistry Chemical Physics, 2017, 19, 28970-28981.	1.3	114
36	How OH and Oâ€“ groups affect electronic structure of meta-substituted and para-substituted phenols and phenolates. Structural Chemistry, 2017, 28, 1563-1572.	1.0	20

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37	Substituent Effect on the Ïƒ- and Ï€-Electron Structure of the Nitro Group and the Ring in Meta- and Para-Substituted Nitrobenzenes. Journal of Physical Chemistry A, 2017, 121, 5196-5203.	1.1	18
38	Effect of Intra- and Intermolecular Interactions on the Properties of para-Substituted Nitrobenzene Derivatives. Crystals, 2016, 6, 29.	1.0	19
39	Calculating the Aromaticity of Heterocycles. Advances in Heterocyclic Chemistry, 2016, , 301-327.	0.9	16
40	Introduction: Special issue devoted in memory of Professor Oleg V. Shishkin. Structural Chemistry, 2016, 27, 1-1.	1.0	4
41	Towards physical interpretation of substituent effects: the case of meta- and para-substituted anilines. Physical Chemistry Chemical Physics, 2016, 18, 11711-11721.	1.3	43
42	Aromaticity of H-bonded and metal complexes of guanine tautomers. Structural Chemistry, 2016, 27, 111-118.	1.0	10
43	Theoretical study of electron-attracting ability of the nitro group: classical and reverse substituent effects. Structural Chemistry, 2015, 26, 905-913.	1.0	39
44	Why 1,2-quinone derivatives are more stable than their 2,3-analogues?. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	16
45	Aromaticity Induced by Electric Field: The Case of Polycalicenes. Journal of Organic Chemistry, 2015, 80, 9091-9101.	1.7	4
46	Metal Complexation and H-bonding Effects on Electronic Structure of Cytosine Studied in the Gas Phase. Croatica Chemica Acta, 2014, 87, 335-342.	0.1	7
47	Aromaticity from the Viewpoint of Molecular Geometry: Application to Planar Systems. Chemical Reviews, 2014, 114, 6383-6422.	23.0	439
48	Substituent effects in 1-nitro-4-substituted bicyclo[2.2.2]octane derivatives: inductive or field effects?. Journal of Molecular Modeling, 2014, 20, 2352.	0.8	16
49	Tautomerisation of thymine acts against the HÃ¼ckel 4N + 2 rule. The effect of metal ions and H-bond complexations on the electronic structure of thymine. Organic and Biomolecular Chemistry, 2014, 12, 6476-6483.	1.5	22
50	Toward a Physical Interpretation of Substituent Effects: The Case of Fluorine and Trifluoromethyl Groups. Journal of Organic Chemistry, 2014, 79, 7321-7331.	1.7	69
51	Effect of H-bonding and complexation with metal ions on the Ï€-electron structure of adenine tautomers. Organic and Biomolecular Chemistry, 2014, 12, 456-466.	1.5	21
52	Comparative studies on CHâ‹¯F^{â‹¯} hydrogen bond formation in benzene and exocyclically substituted pentafulvene derivatives. Journal of Physical Organic Chemistry, 2013, 26, 575-582.	0.9	4
53	Effect of the H-Bonding on Aromaticity of Purine Tautomers. Journal of Organic Chemistry, 2012, 77, 4035-4045.	1.7	32
54	Application of graph theory and topological models for the determination of fundamentals of the aromatic character of pi-conjugated hydrocarbons. Pure and Applied Chemistry, 2012, 84, 1069-1088.	0.9	3

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55	Modeling the electronic structure of formamide: an acid/base amphoteric solvent. Structural Chemistry, 2012, 23, 1711-1721.	1.0	11
56	Aromaticity of pentafulveneâ€™s complexes with alkaline metal atoms. Structural Chemistry, 2012, 23, 931-938.	1.0	17
57	Aromatic character of heptafulvene and its complexes with halogen atoms. Journal of Molecular Modeling, 2012, 18, 2453-2460.	0.8	22
58	The effect of benzoannulation on the transition state and the proton transfer equilibrium in di(2-pyridyl)methane derivatives. New Journal of Chemistry, 2011, 35, 1433.	1.4	7
59	Sigma- and pi- electron structure of aza-azoles. Journal of Molecular Modeling, 2011, 17, 1427-1433.	0.8	19
60	Natural bond orbital (NBO) analysis of the angular group induced bond alternation (AGIBA) substituent effect. Journal of Physical Organic Chemistry, 2010, 23, 551-556.	0.9	12
61	How to Find the Fries Structures for Benzenoid Hydrocarbons. Symmetry, 2010, 2, 1390-1400.	1.1	18
62	H-Bonding-Assisted Substituent Effect. Journal of Organic Chemistry, 2010, 75, 4944-4949.	1.7	45
63	Aromaticity of substituted fulvene derivatives: substituent-dependent ring currents. Physical Chemistry Chemical Physics, 2010, 12, 10740.	1.3	44
64	Long distance structural consequences of Hâ€bonding: the case of complexes ofparaâ€substituted phenol derivatives. Journal of Physical Organic Chemistry, 2009, 22, 740-746.	0.9	4
65	Substituent effects in mono- and disubstituted 1,3,5,7-cyclooctatetraene derivatives in natural and planar conformations. New Journal of Chemistry, 2009, 33, 1753.	1.4	22
66	An explicit solvent quantum chemistry study on the water environment influence on the interactions of fluoride with phenol. New Journal of Chemistry, 2009, 33, 831.	1.4	5
67	Relation between Ï€-Electron Localization/Delocalization and H-Bond Strength in Derivatives ofo-Hydroxy-Schiff Bases. Journal of Organic Chemistry, 2008, 73, 2138-2145.	1.7	44
68	Investigation of induced currents in cyclic forms of ortho-acylphenols and lithium analogues: does the lithium cation contribute to aromatic Ï€-electron delocalisation?. Physical Chemistry Chemical Physics, 2008, 10, 6979.	1.3	9
69	Long-Distance Structural Consequences of H-Bonding. How H-Bonding Affects Aromaticity of the Ring in Variously Substituted Aniline/Anilinium/Anilide Complexes with Bases and Acids. Journal of Chemical Information and Modeling, 2007, 47, 875-886.	2.5	30
70	Aromaticityâ€"What Does It Mean?. AIP Conference Proceedings, 2007, , .	0.3	3
71	Relationship between substituent effect and aromaticity â€“ Part III: naphthalene as a transmitting moiety for substituent effect. Journal of Physical Organic Chemistry, 2007, 20, 297-306.	0.9	61
72	Geometry-based analysis of azulene and azulene-like systems with H- or Li-bonding. Journal of Physical Organic Chemistry, 2007, 20, 594-599.	0.9	6

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73	Varying Electronegativity of OH/O-Groups Depending on the Nature and Strength of H-Bonding in Phenol/Phenolate Involved in H-Bond Complexation. Journal of Physical Chemistry A, 2006, 110, 7232-7236.	1.1	19
74	Relation between the substituent effect and aromaticity. Part II. The case ofmeta-andpara-homodisubstituted benzene derivatives. Journal of Physical Organic Chemistry, 2006, 19, 889-895.	0.9	33
75	Molecular geometry as a source of chemical information. Part 2?An attempt to estimate the H-bond strength: the case ofp-nitrophenol complexes with bases. Journal of Physical Organic Chemistry, 2005, 18, 110-114.	0.9	26
76	Relation between resonance energy and substituent resonance effect inP-phenols. Journal of Physical Organic Chemistry, 2005, 18, 886-891.	0.9	31
77	Tautomeric equilibria, H-bonding and Ï€-electron delocalization ino-nitrosophenol. A B3LYP/6-311â€‰+â€‰G(2df,2p) study. Journal of Physical Organic Chemistry, 2005, 18, 892-897.	0.9	34
78	Sigma- and Pi-Electron Delocalization:Â Focus on Substituent Effects. Chemical Reviews, 2005, 105, 3482-3512.	23.0	303
79	Molecular Geometry as a Source of Chemical Information. 5. Substituent Effect on Proton Transfer in Para-Substituted Phenol Complexes with Fluoridea B3LYP/6-311+G** Study. Journal of Chemical Information and Modeling, 2005, 45, 652-656.	2.5	18
80	How H-bonding Modifies Molecular Structure and Ï€-Electron Delocalization in the Ring of Pyridine/Pyridinium Derivatives Involved in H-Bond Complexationâ€. Journal of Organic Chemistry, 2005, 70, 8859-8865.	1.7	54
81	Theoretical Study of Changes in Ï€-Electron Delocalization in the Analogues of anortho-Hydroxy Schiff Base When the Proton Is Replaced with Li+or BeH+. Journal of Chemical Information and Modeling, 2005, 45, 1837-1841.	2.5	24
82	Relation between the Substituent Effect and Aromaticity. Journal of Organic Chemistry, 2004, 69, 6634-6640.	1.7	177
83	Solvolysis of aromatic benzoyl chlorides: how is the Ï€-electron stabilization of the aromatic acyl chlorides and acylium cations related to the Ï€-electron delocalization?. Journal of Physical Organic Chemistry, 2004, 17, 699-706.	0.9	15
84	Where the two carbon atoms touch in the triple bond in disubstituted acetylenes: the AIM analysis. Chemical Physics Letters, 2004, 389, 51-57.	1.2	17
85	How H-Bonding Affects Aromaticity of the Ring in Variously Substituted Phenol Complexes with Bases. 4. Molecular Geometry as a Source of Chemical Information. Journal of Chemical Information and Computer Sciences, 2004, 44, 2077-2082.	2.8	29
86	Molecular Geometry as a Source of Chemical Information. 3. How H-Bonding Affects Aromaticity of the Ring in the Case of Phenol and p-Nitrophenol Complexes:â€‰ A B3LYP/6-311+G** Study. Journal of Organic Chemistry, 2004, 69, 7038-7043.	1.7	41
87	Two faces of the structural aspects of aromaticity. Physical Chemistry Chemical Physics, 2004, 6, 249-255.	1.3	64
88	Variation of the ?-electron delocalization in exocyclically substituted heptafulvene derivatives. Journal of Physical Organic Chemistry, 2003, 16, 426-430.	0.9	21
89	On the Aromatic Character of the Heterocyclic Bases of DNA and RNA#. Journal of Organic Chemistry, 2003, 68, 8607-8613.	1.7	70
90	To What Extent Can Aromaticity Be Defined Uniquely?â€‰â€. Journal of Organic Chemistry, 2002, 67, 1333-1338.	1.7	678

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91	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.	0.9	8
92	Angular group induced bond alternation (AGIBA). Part VI ? Competition between the AGIBA and through resonance effects. Journal of Physical Organic Chemistry, 2001, 14, 764-769.	0.9	1
93	Structural Aspects of Aromaticity. Chemical Reviews, 2001, 101, 1385-1420.	23.0	1,189
94	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.	0.9	11
95	Substituent and temperature controlled tautomerism: multinuclear magnetic resonance, X-ray, and theoretical studies on 2-phenacylquinolines. Perkin Transactions II RSC, 2000, , 1259-1266.	1.1	68
96	Global and Local Aromaticity in Porphyrins: An Analysis Based on Molecular Geometries and Nucleus-Independent Chemical Shifts. Angewandte Chemie - International Edition, 1998, 37, 177-180.	7.2	220
97	Separation of the energetic and geometric contributions to aromaticity. Part VI. Changes of the aromatic character of the rings in naphthalene, anthracene, phenanthrene and pyrene derivatives induced by the charged substituent CH2+. Tetrahedron, 1997, 53, 11383-11398.	1.0	23
98	IMBALANCE OF THE KEKULï¿½ STRUCTURES IN 2,4,6-TRIMETHOXY-S-TRIAZINE. Journal of Physical Organic Chemistry, 1997, 10, 125-127.	0.9	16
99	Solid-state NMR and x-ray diffraction studies of ionic complex of 1,8-bis(dimethylamino)naphthalene (DMAN) with picrolonic acid. Journal of Physical Organic Chemistry, 1997, 10, 814-824.	0.9	12
100	Conformational Aspects of the p-Nitrosophenolate Anion and Related Compounds: NMR Study and ab initio 6-31G Optimizations of Molecular Structures. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 1997, 52, 263-280.	0.3	1
101	Separation of the Energetic and Geometric Contributions to Aromaticity. 3. Analysis of the Aromatic Character of Benzene Rings in Their Various Topological and Chemical Environments in the Substituted Benzene Derivatives. Journal of Chemical Information and Computer Sciences, 1996, 36, 1142-1145.	2.8	39
102	The nitro group as substituent. Chemical Society Reviews, 1996, 25, 71.	18.7	90
103	Aromatic Character of the Benzene Ring Present in Various Topological Environments in Benzenoid Hydrocarbons. Nonequivalence of Indices of Aromaticity. Journal of Chemical Information and Computer Sciences, 1995, 35, 203-210.	2.8	130
104	Crystal and moecular structure ofN-nitro-N-methyl-p-nitroaniline: Analysis of substituent effects on the ring geometry and estimation of the Hammett substituent constant for theN-methylnitramino group. Journal of Physical Organic Chemistry, 1993, 6, 257-260.	0.9	17
105	Crystallographic studies of inter- and intramolecular interactions reflected in aromatic character of .pi.-electron systems. Journal of Chemical Information and Computer Sciences, 1993, 33, 70-78.	2.8	1,139
106	Ab initio 3-21 G Calculations of Push-Pull Interactions of Substituents at Imino-Nitrogen in Formamidines. Non-Equivalence of NO-Bonds of the Nitro-Substituent. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 1992, 47, 1480-1490.	0.3	3
107	Low temperature crystal and molecular structure of nitrobenzene. Structural Chemistry, 1992, 3, 363-368.	1.0	74
108	Crystallographic studies of intra- and inter-molecular interactions Part III. Refinement of the crystal and molecular structure of N,N-dimethyl-m-nitroaniline: additivity of substituent effects on geometrical parameters of the ring. Journal of Molecular Structure, 1991, 246, 113-122.	1.8	3

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109	Crystal and molecular structure of pyrylium salts. IV. Crystal and molecular structure of 2,6-diphenyl-4-(4-carboxyphenyl)pyrylium perchlorate. Interrelations between structural parameters due to substituent effects. Journal of Physical Organic Chemistry, 1991, 4, 121-124.	0.9	10
110	Crystallographic studies of intra- and inter- molecular interactions. Part VI. Crystal and molecular structure ofN,N?-dimethyl-N?-phenylsulphonylformamidine. Equalization of CN bond lengths in the amidine fragment as a result of substituent effects due to push-pull. Journal of Physical Organic Chemistry, 1991, 4, 331-335.	0.9	5
111	Correlations between empirical lewis acid-base solvent parameters and the thermodynamic parameters of ion solvation. Part II. Acidity parameters of cations and basicity parameters of anions. Journal of Physical Organic Chemistry, 1991, 4, 439-448.	0.9	7
112	Structural studies of 1,3-di(N,N-dimethylformamidyl)-2-cyanoguanidine. The case of a strongly lewis basic nitrogen atom in the cyano group VIII. Crystallographic studies of intra- and inter-molecular interactions. Journal of Physical Organic Chemistry, 1991, 4, 689-692.	0.9	3
113	Empirical Parameters of Lewis Basicity of Binary Solvent Mixtures, Part II Mixtures with Water. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 1989, 44, 673-678.	0.3	6
114	Basis set dependence, precision, and accuracy of fullab initiogradient optimizations of molecular structures of nonstrained hydrocarbons. I. CC bond lengths. Journal of Computational Chemistry, 1989, 10, 329-343.	1.5	24
115	Crystallographic studies of intra- and inter-molecular interactions. Crystal and molecular structure of N,N-dimethyl-4-nitro-3,5-xylidine. Structural evidence against the classical through-resonance concept in p-nitroaniline and derivatives. Journal of the Chemical Society Perkin Transactions II, 1989, , 695.	0.9	22
116	Interpretation of Substituent Angular Parameters of Monosubstituted Benzenes by Means of ab initio STO-3G Fully Optimized Molecular Structures and Charges Densities. Part VI of the Series: â€œCrystallographic Studies and Physicochemical Properties of Ï€-Electron Systemsâ€• Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 1986, 41, 895-903.	0.3	23
117	Correlation Analysis in Organic Crystal Chemistry. Progress in Physical Organic Chemistry, 0, , 239-291.	1.2	7