CÃ©lia Fonseca Guerra

List of Publications by Year
in descending order

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Version: 2024-02-01

188 papers	20,575 citations	50273 46 h-index	9860 141 g-index
213 all docs	213 docs citations	213 times ranked	14448 citing authors

#	Article	IF	Citations
1	Chemistry with ADF. Journal of Computational Chemistry, 2001, 22, 931-967.	3.3	8,854
2	Towards an order-. Theoretical Chemistry Accounts, 1998, 99, 391.	1.4	2,434
3	Towards an order- N DFT method. Theoretical Chemistry Accounts, 1998, 99, 391-403.	1.4	1,283
4	Voronoi deformation density (VDD) charges: Assessment of the Mulliken, Bader, Hirshfeld, Weinhold, and VDD methods for charge analysis. Journal of Computational Chemistry, 2004, 25, 189-210.	3.3	956
5	Hydrogen Bonding in DNA Base Pairs:â€‰ Reconciliation of Theory and Experiment. Journal of the American Chemical Society, 2000, 122, 4117-4128.	13.7	418
6	The Nature of the Hydrogen Bond in DNA Base Pairs: The Role of Charge Transfer and Resonance Assistance. Chemistry - A European Journal, 1999, 5, 3581-3594.	3.3	340
7	Absolute Rates of Hole Transfer in DNA. Journal of the American Chemical Society, 2005, 127, 14894-14903.	13.7	325
8	The Carbonâ^'Lithium Electron Pair Bond in (CH3Li)n(n= 1, 2, 4). Organometallics, 1996, 15, 2923-2931.	2.3	286
9	Understanding chemical reactivity using the activation strain model. Nature Protocols, 2020, 15, 649-667.	12.0	188
10	Performance of various density functionals for the hydrogen bonds in DNA base pairs. Chemical Physics Letters, 2006, 426, 415-421.	2.6	149
11	Highly accelerated inverse electron-demand cycloaddition of electron-deficient azides with aliphatic cyclooctynes. Nature Communications, 2014, 5, 5378.	12.8	145
12	Telomere Structure and Stability: Covalency in Hydrogen Bonds, Not Resonance Assistance, Causes Cooperativity in Guanine Quartets. Chemistry - A European Journal, 2011, 17, 12612-12622.	3.3	130
13	Ï€-Ï€ stacking tackled with density functional theory. Journal of Molecular Modeling, 2007, 13, 1245-1257.	1.8	126
14	The Nature of Hydrogen Bonds: A Delineation of the Role of Different Energy Components on Hydrogen Bond Strengths and Lengths. Chemistry - an Asian Journal, 2019, 14, 2760-2769.	3.3	124
15	Adenine versus guanine quartets in aqueous solution: dispersion-corrected DFT study on the differences in Ï€-stacking and hydrogen-bonding behavior. Theoretical Chemistry Accounts, 2010, 125, 245-252.	1.4	123
16	Adenine Tautomers:â€‰ Relative Stabilities, Ionization Energies, and Mismatch with Cytosine. Journal of Physical Chemistry A, 2006, 110, 4012-4020.	2.5	115
17	Charge Transfer and Environment Effects Responsible for Characteristics of DNA Base Pairing. Angewandte Chemie - International Edition, 1999, 38, 2942-2945.	13.8	114
18	Normal-to-Abnormal Rearrangement and NHC Activation in Three-Coordinate Iron(II) Carbene Complexes. Journal of the American Chemical Society, 2013, 135, 13338-13341.	13.7	110

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19	Contiguous Metalâ€Mediated Base Pairs Comprising Two Ag^I Ions. Chemistry - A European Journal, 2011, 17, 6533-6544.	3.3	108
20	Mapping the Sites for Selective Oxidation of Guanines in DNA. Journal of the American Chemical Society, 2003, 125, 13658-13659.	13.7	97
21	Hypervalent Silicon versus Carbon: Ballâ€inâ€aâ€Box Model. Chemistry - A European Journal, 2008, 14, 819-828.	3.3	90
22	Hydrogen Bonds of RNA Are Stronger than Those of DNA, but NMR Monitors Only Presence of Methyl Substituent in Uracil/Thymine. Journal of the American Chemical Society, 2004, 126, 16718-16719.	13.7	87
23	Orbital Interactions in Strong and Weak Hydrogen Bonds are Essential for DNA Replication We thank the National Research School Combinationâ€"Catalysis (NRSCC) for a postdoctoral fellowship for C.F.G. and the National Computer Facilities (NCF) foundation of the Netherlands Organization for Scientific Research (NWO) for financial support.. Angewandte Chemie - International Edition, 2002, 41, 2092.	13.8	82
24	The role of alkali metal cations in the stabilization of guanine quadruplexes: why K⁺ is the best. Physical Chemistry Chemical Physics, 2016, 18, 20895-20904.	2.8	80
25	Semicrystalline Polyesters Based on a Novel Renewable Building Block. Macromolecules, 2012, 45, 5069-5080.	4.8	78
26	Isohexide Derivatives from Renewable Resources as Chiral Building Blocks. ChemSusChem, 2011, 4, 599-603.	6.8	76
27	Comparison of the DFT-SAPT and Canonical EDA Schemes for the Energy Decomposition of Various Types of Noncovalent Interactions. Journal of Chemical Theory and Computation, 2018, 14, 3440-3450.	5.3	74
28	A Ditopic Ionâ€Pair Receptor Based on Stacked Nucleobase Quartets. Angewandte Chemie - International Edition, 2009, 48, 3285-3287.	13.8	70
29	The Donorâ€Stabilized Silylene Bis[N,Nâ€²â€diisopropylbenzamidinato(â^')]silicon(II): Synthesis, Electronic Structure, and Reactivity. Chemistry - A European Journal, 2014, 20, 9319-9329.	3.3	69
30	Towards excitation energies and (hyper)polarizability calculations of large molecules. Application of parallelization and linear scaling techniques to time-dependent density functional response theory. Journal of Computational Chemistry, 2000, 21, 1511-1523.	3.3	68
31	A Highly Stabilizing Silver(I)â€Mediated Base Pair in Parallelâ€Stranded DNA. Angewandte Chemie - International Edition, 2015, 54, 3603-3606.	13.8	67
32	B-DNA structure and stability: the role of hydrogen bonding, Ï€â€“Ï€ stacking interactions, twist-angle, and solvation. Organic and Biomolecular Chemistry, 2014, 12, 4691-4700.	2.8	64
33	NMR ¹H-Shielding Constants of Hydrogen-Bond Donor Reflect Manifestation of the Pauli Principle. Journal of Physical Chemistry Letters, 2018, 9, 3720-3724.	4.6	61
34	Silver(I)-mediated Hoogsteen-type base pairs. Journal of Inorganic Biochemistry, 2011, 105, 1398-1404.	3.5	59
35	Secondary Electrostatic Interaction Model Revised: Prediction Comes Mainly from Measuring Charge Accumulation in Hydrogen-Bonded Monomers. Journal of the American Chemical Society, 2019, 141, 4878-4885.	13.7	59
36	Efficient Copper-Catalyzed Multicomponent Synthesis of N-Acyl Amidines via Acyl Nitrenes. Journal of the American Chemical Society, 2019, 141, 15240-15249.	13.7	58

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37	Covalency in resonance-assisted halogen bonds demonstrated with cooperativity in N-halo-guanine quartets. Physical Chemistry Chemical Physics, 2015, 17, 1585-1592.	2.8	54
38	Selectivity in DNA replication. Interplay of steric shape, hydrogen bonds, Ï€-stacking and solvent effects. Chemical Communications, 2011, 47, 7326.	4.1	52
39	Nature of Intramolecular Resonance Assisted Hydrogen Bonding in Malonaldehyde and Its Saturated Analogue. Journal of Physical Chemistry A, 2018, 122, 1813-1820.	2.5	51
40	Orbital Interactions in Hydrogen Bonds Important for Cohesion in Molecular Crystals and Mismatched Pairs of DNA Bases. Crystal Growth and Design, 2002, 2, 239-245.	3.0	50
41	The Role of Aromaticity, Hybridization, Electrostatics, and Covalency in Resonance-Assisted Hydrogen Bonds of Adenine-Thymine (AT) Base Pairs and Their Mimics. ChemistryOpen, 2015, 4, 318-327.	1.9	50
42	A metal-mediated base pair that discriminates between the canonical pyrimidine nucleobases. Chemical Science, 2017, 8, 1337-1343.	7.4	50
43	Hypervalent Carbon Atom: â€œFreezingâ€•the S_N2 Transition State. Angewandte Chemie - International Edition, 2009, 48, 6469-6471.	13.8	49
44	8 Energy decomposition analysis in the context of quantitative molecular orbital theory. , 2021, , 199-212.		49
45	Covalency in Highly Polar Bonds. Structure and Bonding of Methylalkalimetal Oligomers (CH3M)n (M) Tj ETQq1 1 0.784314 rgBT /Ov	5.3	48
46	Stereodivergent S_N2@P Reactions of Borane Oxazaphospholidines: Experimental and Theoretical Studies. Journal of the American Chemical Society, 2013, 135, 4483-4491.	13.7	48
47	Supramolecular Switches Based on the Guanineâ€“Cytosine (GC) Watsonâ€“Crick Pair: Effect of Neutral and Ionic Substituents. Chemistry - A European Journal, 2006, 12, 3032-3042.	3.3	47
48	Intercalation of Daunomycin into Stacked DNA Base Pairs. DFT Study of an Anticancer Drug. Journal of Biomolecular Structure and Dynamics, 2008, 26, 115-129.	3.5	47
49	Relevance of Orbital Interactions and Pauli Repulsion in the Metalâ€“Metal Bond of Coinage Metals. Inorganic Chemistry, 2018, 57, 2603-2608.	4.0	47
50	How amino and nitro substituents direct electrophilic aromatic substitution in benzene: an explanation with Kohnâ€“Sham molecular orbital theory and Voronoi deformation density analysis. Physical Chemistry Chemical Physics, 2016, 18, 11624-11633.	2.8	46
51	PyFragâ€”Streamlining your reaction path analysis. Journal of Computational Chemistry, 2008, 29, 312-315.	3.3	44
52	Insights on selenium and tellurium diaryldichalcogenides: A benchmark DFT study. Journal of Computational Chemistry, 2016, 37, 1672-1680.	3.3	43
53	RNA versus DNA Gâ€Quadruplex: The Origin of Increased Stability. Chemistry - A European Journal, 2018, 24, 16315-16322.	3.3	42
54	Hydrogen Bonding in Mimics of Watsonâ€“Crick Base Pairs Involving Cï£¿H Proton Donor and F Proton Acceptor Groups: A Theoretical Study. ChemPhysChem, 2004, 5, 481-487.	2.1	41

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55	Neutral Six-Coordinate and Cationic Five-Coordinate Silicon(IV) Complexes with Two Bidentate Monoanionic N,S-Pyridine-2-thiolato(â^') Ligands. Inorganic Chemistry, 2013, 52, 10664-10676.	4.0	39
56	Theoretical study of electron-attracting ability of the nitro group: classical and reverse substituent effects. Structural Chemistry, 2015, 26, 905-913.	2.0	39
57	Orbital interactions and charge redistribution in weak hydrogen bonds: The Watsonâ€“Crick AT mimic adenine-2,4-difluorotoluene. Journal of Chemical Physics, 2003, 119, 4262-4273.	3.0	38
58	3-Substituted xanthines as promising candidates for quadruplex formation: computational, synthetic and analytical studies. New Journal of Chemistry, 2011, 35, 476-482.	2.8	36
59	Direct detection of the mercuryâ€“nitrogen bond in the thymineâ€“Hg^{II}â€“thymine base-pair with ¹⁹⁹Hg NMR spectroscopy. Chemical Communications, 2015, 51, 8488-8491.	4.1	36
60	Hydrogenâ€Bond Strength of CC and GG Pairs Determined by Steric Repulsion: Electrostatics and Charge Transfer Overruled. Chemistry - A European Journal, 2017, 23, 10249-10253.	3.3	36
61	Synthesis and structural characterisation of neutral pentacoordinate silicon(iv) complexes with a tridentate dianionic N,N,S chelate ligand. Dalton Transactions, 2012, 41, 2148-2162.	3.3	33
62	Dihydrogen Bonding: Donorâ€“Acceptor Bonding (AHâ‹…â‹…â‹…HX) versus the H₂ Molecule (Aï£¿H₂ï£¿X). Chemistry - A European Journal, 2009, 15, 5814-5822.	3.3	32
63	Solvent effects on hydrogen bonds in Watsonâ€“Crick, mismatched, and modified DNA base pairs. Computational and Theoretical Chemistry, 2012, 998, 57-63.	2.5	32
64	Bâ€DNA Structure and Stability as Function of Nucleic Acid Composition: Dispersionâ€Corrected DFT Study of Dinucleoside Monophosphate Single and Double Strands. ChemistryOpen, 2013, 2, 186-193.	1.9	32
65	Thermodynamics of the Cu^{II} Î¼-Thiolate and Cu^I Disulfide Equilibrium: A Combined Experimental and Theoretical Study. Inorganic Chemistry, 2014, 53, 8494-8504.	4.0	31
66	Substituent Effects on Hydrogen Bonding in Watsonâ€“Crick Base Pairs. A Theoretical Study. Structural Chemistry, 2005, 16, 211-221.	2.0	30
67	Rare Tautomers of 1â€Methyluracil and 1â€Methylthymine: Tuning Relative Stabilities through Coordination to Pt^{II} Complexes. Chemistry - A European Journal, 2009, 15, 209-218.	3.3	30
68	Chimeric GNA/DNA metal-mediated base pairs. Chemical Communications, 2011, 47, 11041.	4.1	29
69	Rationalizing the Structural Variability of the Exocyclic Amino Groups in Nucleobases and Their Metal Complexes: Cytosine and Adenine. Chemistry - A European Journal, 2014, 20, 9494-9499.	3.3	29
70	Stable Fourâ€Coordinate Guanidinatosilicon(IV) Complexes with SiN 3 El Skeletons (El=S, Se, Te) and Sïï£¾El Double Bonds. Chemistry - A European Journal, 2015, 21, 14011-14021.	3.3	29
71	Reversible Self-Assembly of Water-Soluble Gold(I) Complexes. Inorganic Chemistry, 2018, 57, 1017-1028.	4.0	29
72	Scope and Limitations of an Efficient Four-Component Reaction for Dihydropyridin-2-ones. Journal of Organic Chemistry, 2010, 75, 1723-1732.	3.2	28

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73	Silicon Î±-Effect: A Systematic Experimental and Computational Study of the Hydrolysis of C_{Î±}- and C_{Î³}-Functionalized Alkoxytriorganylsilanes of the Formula Type ROSiMe₂(CH₂)_nX (R = Me, Et; n = 1, 3; X = Functional) Tj ETQq1 1 0.784314 rg	2.3	28
74	Bis[N,Nâ€²â€diisopropylbenzamidinato(â^')]silicon(<scp>II</scp>): Lewis Acid/Base Reactions with Triorganylboranes. Chemistry - A European Journal, 2014, 20, 12411-12415.	3.3	28
75	Nature and Strength of Lewis Acid/Base Interaction in Boron and Nitrogen Trihalides. Chemistry - an Asian Journal, 2020, 15, 4043-4054.	3.3	28
76	Methyl Cation Affinities of Neutral and Anionic Maingroup-Element Hydrides: Trends Across the Periodic Table and Correlation with Proton Affinities. Journal of Physical Chemistry A, 2010, 114, 7604-7608.	2.5	27
77	Oxidation of organic diselenides and ditellurides by H₂O₂for bioinspired catalyst design. Physical Chemistry Chemical Physics, 2018, 20, 20874-20885.	2.8	27
78	Halogen Bonds in Ligandâ€“Protein Systems: Molecular Orbital Theory for Drug Design. Journal of Chemical Information and Modeling, 2020, 60, 1317-1328.	5.4	27
79	Extension of a predictive substrate model for human cytochrome P4502D6. Xenobiotica, 1997, 27, 357-368.	1.1	26
80	Cooperativity in the Selfâ€Assembly of the Guanine Nucleobase into Quartet and Ribbon Structures on Surfaces. Chemistry - A European Journal, 2017, 23, 3042-3050.	3.3	26
81	Rational design of nearâ€infrared absorbing organic dyes: Controlling the HOMOâ€“LUMO gap using quantitative molecular orbital theory. Journal of Computational Chemistry, 2018, 39, 2690-2696.	3.3	26
82	Redox Interconversion between Cobalt(III) Thiolate and Cobalt(II) Disulfide Compounds. Inorganic Chemistry, 2018, 57, 8796-8805.	4.0	26
83	B-DNA model systems in non-terran bio-solvents: implications for structure, stability and replication. Physical Chemistry Chemical Physics, 2017, 19, 16969-16978.	2.8	25
84	Clarifying notes on the bonding analysis adopted by the energy decomposition analysis. Physical Chemistry Chemical Physics, 2022, 24, 15726-15735.	2.8	25
85	Remote Communication in a DNAâ€Based Nanoswitch. Chemistry - A European Journal, 2011, 17, 8816-8818.	3.3	24
86	Predicting Ptâ€195 NMR chemical shift using new relativistic allâ€electron basis set. Journal of Computational Chemistry, 2016, 37, 2360-2373.	3.3	24
87	Supramolecular Selfâ€Sorting Networks using Hydrogenâ€Bonding Motifs. Chemistry - A European Journal, 2019, 25, 785-795.	3.3	24
88	Understanding alkali metal cation affinities of multi-layer guanine quadruplex DNA. Physical Chemistry Chemical Physics, 2020, 22, 21108-21118.	2.8	24
89	Not Carbon sâ€“p Hybridization, but Coordination Number Determines Câ^'H and Câ^'C Bond Length. Chemistry - A European Journal, 2021, 27, 7074-7079.	3.3	24
90	Thermodynamic Aspects of Aurophilic Hydrogelators. Inorganic Chemistry, 2015, 54, 5195-5203.	4.0	23

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91	A Helicoid Ferrocene. Inorganic Chemistry, 2009, 48, 2714-2716.	4.0	22
92	Neutral Pentacoordinate Halogeno- and Pseudohalogenosilicon(IV) Complexes with a Tridentate Dianionic O,N,O or N,N,O Ligand: Synthesis and Structural Characterization in the Solid State and in Solution. European Journal of Inorganic Chemistry, 2012, 2012, 3216-3228.	2.0	21
93	Impact of Conformational Effects on the Ringâ€“Chain Equilibrium of Hydrogenâ€Bonded Dinucleosides. Chemistry - A European Journal, 2018, 24, 11983-11991.	3.3	21
94	Performance of TDDFT Vertical Excitation Energies of Coreâ€Substituted Naphthalene Diimides. Journal of Computational Chemistry, 2020, 41, 1448-1455.	3.3	21
95	Orbitalwechselwirkungen in starken und schwachen WasserstoffbrÃ¼cken sind essentiell fÃ¼r die DNA-Replikation Wir danken der Stiftung Nationale Computerfaciliteiten (NCF) der Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO) fÃ¼r finanzielle UnterstÃ¼tzung. C.F.G. dankt der National Research School Combination-Catalysis (NRSCC) fÃ¼r ein Stipendium.. Angewandte Chemie, 2002, 114, 2194.	2.0	20
96	Highly polar bonds and the meaning of covalency and ionicityâ€”structure and bonding of alkali metal hydride oligomers. Faraday Discussions, 2007, 135, 451-468.	3.2	19
97	Effect of Intra- and Intermolecular Interactions on the Properties of para-Substituted Nitrobenzene Derivatives. Crystals, 2016, 6, 29.	2.2	19
98	Nanoswitches Based on DNA Base Pairs: Why Adeninâ€“Thymine is Less Suitable than Guanineâ€“Cytosine. ChemPhysChem, 2006, 7, 1971-1979.	2.1	18
99	Covalentversus ionic bonding in alkalimetal fluoride oligomers. Journal of Computational Chemistry, 2007, 28, 238-250.	3.3	18
100	Differential stabilization of adenine quartets by anions and cations. Journal of Biological Inorganic Chemistry, 2010, 15, 387-397.	2.6	18
101	Neutral and positively charged new purine tetramer structures: a computational study of xanthine and uric acid derivatives. New Journal of Chemistry, 2011, 35, 119-126.	2.8	18
102	Stabilisation of 2,6â€Diarylpyridinium Cation by Throughâ€Space Polarâ€“Ï€ Interactions. Chemistry - A European Journal, 2014, 20, 6268-6271.	3.3	18
103	Reactions of the Donor-Stabilized Silylene Bis[N,Nâ€²-diisopropyl-benzamidinato(â¯)]silicon(II) with BrÃ¸nsted Acids. Chemistry - A European Journal, 2014, 20, 16462-16466.	3.3	18
104	Table Salt and Other Alkali Metal Chloride Oligomers:â€‰ Structure, Stability, and Bonding. Inorganic Chemistry, 2007, 46, 5411-5418.	4.0	17
105	Supramolecular H-bonded porous networks at surfaces: exploiting primary and secondary interactions in a bi-component melamineâ€“xanthine system. Physical Chemistry Chemical Physics, 2013, 15, 12442.	2.8	17
106	Protonation of a Biologically Relevant Cu^{II} Î¼â€Thiolate Complex: Ligand Dissociation or Formation of a Protonated Cu^I Disulfide Species?. Chemistry - A European Journal, 2014, 20, 16913-16921.	3.3	17
107	Kekulene: Structure, stability and nature of Hâ€¢â€¢â€¢H interactions in large PAHs. Molecular Astrophysics, 2017, 8, 19-26.	1.6	17
108	Enhanced Ï€â€Backâ€Donation as a Way to Higher Coordination Numbers in d¹⁰ [M(NHC)_n] Complexes: A DFT Study. Chemistry - A European Journal, 2017, 23, 614-622.	3.3	17

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109	The Gauche Effect in XCH₂CH₂X Revisited. ChemPhysChem, 2021, 22, 641-648.	2.1	17
110	Source of Cooperativity in Halogenâ€Bonded Haloamine Tetramers. ChemPhysChem, 2016, 17, 474-480.	2.1	16
111	New Insight into the Nature of Bonding in the Dimers of Lappertâ€™s Stannylene and Its Ge Analogs: A Quantum Mechanical Study. Journal of Chemical Theory and Computation, 2016, 12, 1696-1704.	5.3	16
112	Asymmetric identity SN2 transition states: Nucleophilic substitution at Î±-substituted carbon and silicon centers. International Journal of Mass Spectrometry, 2017, 413, 85-91.	1.5	16
113	How Mg²⁺ ions lower the S_N2@P barrier in enzymatic triphosphate hydrolysis. Chemical Communications, 2018, 54, 3448-3451.	4.1	16
114	How the Chalcogen Atom Size Dictates the Hydrogenâ€Bond Donor Capability of Carboxamides, Thioamides, and Selenoamides. Chemistry - A European Journal, 2022, 28, .	3.3	16
115	Steric effects on alkyl cation affinities of maingroupâ€element hydrides. Journal of Computational Chemistry, 2011, 32, 681-688.	3.3	15
116	Self-Assembly of N³-Substituted Xanthines in the Solid State and at the Solidâ€“Liquid Interface. Langmuir, 2013, 29, 7283-7290.	3.5	15
117	Computational (DFT) and Experimental (EXAFS) Study of the Interaction of [Ir(IMes)(H)₂(L)₃] with Substrates and Coâ€substrates Relevant for SABRE in Dilute Systems. Chemistry - A European Journal, 2015, 21, 10482-10489.	3.3	15
118	How the disulfide conformation determines the disulfide/thiol redox potential. Journal of Biomolecular Structure and Dynamics, 2015, 33, 93-103.	3.5	15
119	Designing Selfâ€Assembled Rosettes: Why Ammeline is a Superior Building Block to Melamine. ChemistryOpen, 2019, 8, 135-142.	1.9	15
120	Effect of Alkali Metal Cations on Length and Strength of Hydrogen Bonds in DNA Base Pairs. ChemPhysChem, 2020, 21, 2112-2126.	2.1	15
121	Isohexide Dinitriles: A Versatile Family of Renewable Platform Chemicals. ChemSusChem, 2017, 10, 3202-3211.	6.8	14
122	The Nature of Nonclassical Carbonyl Ligands Explained byâ€‰Kohnâ€“Sham Molecular Orbital Theory. Chemistry - A European Journal, 2020, 26, 15690-15699.	3.3	14
123	Lack of Cooperativity in the Triangular X₃Halogen-Bonded Synthon?. Crystal Growth and Design, 2021, 21, 597-607.	3.0	14
124	Hydrogen bonding of 3- and 5-methyl-6-aminouracil with natural DNA bases. New Journal of Chemistry, 2008, 32, 1981.	2.8	13
125	tert-Butyl Cation Affinities of Maingroup-Element Hydrides: Effect of Methyl Substituents at the Protophilic Center. Journal of Physical Chemistry A, 2011, 115, 8310-8315.	2.5	13
126	How Divalent Cations Interact with the Internal Channel Site of Guanine Quadruplexes. ChemPhysChem, 2021, 22, 2286-2296.	2.1	13

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127	The Role of Protein Plasticity in Computational Rationalization Studies on Regioselectivity in Testosterone Hydroxylation by Cytochrome P450 BM3 Mutants. Current Drug Metabolism, 2012, 13, 155-166.	1.2	12
128	Substituent effects on the optical properties of naphthalenediimides: A frontier orbital analysis across the periodic table. Journal of Computational Chemistry, 2016, 37, 304-313.	3.3	12
129	Alkali Metal Cation Affinities of Anionic Main Groupâ€Element Hydrides Across the Periodic Table. Chemistry - an Asian Journal, 2017, 12, 2604-2611.	3.3	12
130	Distortionâ€Controlled Redshift of Organic Dye Molecules. Chemistry - A European Journal, 2020, 26, 2080-2093.	3.3	12
131	Structure and bonding of methyl alkali metal molecules. Journal of Molecular Modeling, 2006, 12, 563-568.	1.8	11
132	Insights into the Structure of Intrastrand Cross-Link DNA Lesion-Containing Oligonucleotides: G[8â€“5m]T and G[8â€“5]C from Molecular Dynamics Simulations. Biochemistry, 2015, 54, 1259-1267.	2.5	11
133	Sixâ€Coordinate Groupâ€…13 Complexes: The Role of dâ€…Orbitals and Electronâ€Rich Multiâ€Center Bonding. Angewandte Chemie - International Edition, 2015, 54, 12034-12038.	13.8	11
134	Computational understanding and experimental characterization of twice-as-smart quadruplex ligands as chemical sensors of bacterial nucleotide second messengers. Scientific Reports, 2016, 6, 33888.	3.3	11
135	Predicting Multicomponent Adsorption Isotherms in Openâ€Metal Site Materials Using Force Field Calculations Based on Energy Decomposed Density Functional Theory. Chemistry - A European Journal, 2016, 22, 18045-18050.	3.3	11
136	The influence of substituents and the environment on the NMR shielding constants of supramolecular complexes based on Aâ€“T and Aâ€“U base pairs. Physical Chemistry Chemical Physics, 2017, 19, 13496-13502.	2.8	11
137	The evaluation of 5-amino- and 5-hydroxyuracil derivatives as potential quadruplex-forming agents. Organic and Biomolecular Chemistry, 2017, 15, 2174-2184.	2.8	10
138	Hydrogen-Bonded Rosettes of Aminotriazines for Selective-Ion Recognition. Journal of Physical Chemistry C, 2020, 124, 3352-3363.	3.1	10
139	Cooperative Selfâ€Assembly in Linear Chains Based on Halogen Bonds. ChemPlusChem, 2021, 86, 812-819.	2.8	10
140	Watson-crick base pairs with thiocarbonyl groups: How sulfur changes the hydrogen bonds in DNA. Open Chemistry, 2008, 6, 15-21.	1.9	9
141	Aggregation induced emission of a new naphthyridine-ethynylâ€“gold(<scp>i</scp>) complex as a potential tool for sensing guanosine nucleotides in aqueous media. Dalton Transactions, 2020, 49, 171-178.	3.3	9
142	Nonrelativistic protocol for calculating the 1J(195Pt-15N) coupling constant in Pt(II)-complexes using all-electron Gaussian basis-set. Chemical Physics Letters, 2020, 745, 137279.	2.6	9
143	A Pushâ€“Pull Mechanism Helps Design Highly Competent G-Quadruplex-DNA Catalysts. CCS Chemistry, 2021, 3, 2183-2193.	7.8	9
144	Bâ€DNA Structure and Stability: The Role of Nucleotide Composition and Order. ChemistryOpen, 2022, 11, e202100231.	1.9	9

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145	Orbital interactions and charge redistribution in weak hydrogen bonds: Watson-Crick GC mimic involving Cï¿¿H proton donor and F proton acceptor groups. International Journal of Quantum Chemistry, 2006, 106, 2428-2443.	2.0	8
146	Complexes of 4â€substituted phenolates with HF and HCN: Energy decomposition and electronic structure analyses of hydrogen bonding. Journal of Computational Chemistry, 2013, 34, 696-705.	3.3	8
147	Modified Guanines as Constituents of Smart Ligands for Nucleic Acid Quadruplexes. Chemistry - A European Journal, 2016, 22, 10912-10922.	3.3	8
148	Mixed guanine, adenine base quartets: possible roles of protons and metal ions in their stabilization. Journal of Biological Inorganic Chemistry, 2018, 23, 41-49.	2.6	8
149	Charge Transfer and Environment Effects Responsible for Characteristics of DNA Base Pairing. Angewandte Chemie - International Edition, 1999, 38, 2942-2945.	13.8	8
150	Ïƒâ€Electrons Responsible for Cooperativity and Ring Equalization in Hydrogenâ€Bonded Supramolecular Polymers. ChemPlusChem, 2022, 87, .	2.8	8
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