CÃ©lia Fonseca Guerra

List of Publications by Year
in descending order

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188 papers	20,575 citations	57681 46 h-index	11282 141 g-index
213 all docs	213 docs citations	213 times ranked	16148 citing authors

#	Article	IF	Citations
1	Ïƒâ€Electrons Responsible for Cooperativity and Ring Equalization in Hydrogenâ€Bonded Supramolecular Polymers. ChemPlusChem, 2022, 87, .	1.3	8
2	Bâ€DNA Structure and Stability: The Role of Nucleotide Composition and Order. ChemistryOpen, 2022, 11, e202100231.	0.9	9
3	Bâ€DNA Structure and Stability: The Role of Nucleotide Composition and Order. ChemistryOpen, 2022, 11, e202200013.	0.9	0
4	Polycyclic Aromatic Hydrocarbons (PAHs) in Interstellar Ices: A Computational Study into How the Ice Matrix Influences the Ionic State of PAH Photoproducts. ACS Earth and Space Chemistry, 2022, 6, 766-774.	1.2	5
5	How the Chalcogen Atom Size Dictates the Hydrogenâ€Bond Donor Capability of Carboxamides, Thioamides, and Selenoamides. Chemistry - A European Journal, 2022, 28, .	1.7	16
6	Ïƒâ€Electrons Responsible for Cooperativity and Ring Equalization in Hydrogenâ€Bonded Supramolecular Polymers. ChemPlusChem, 2022, 87, e202100541.	1.3	0
7	Probing the redox-conversion of Co(<scp>ii</scp>)-disulfide to Co(<scp>iii</scp>)-thiolate complexes: the effect of ligand-field strength. Dalton Transactions, 2022, 51, 8046-8055.	1.6	4
8	How the Chalcogen Atom Size Dictates the Hydrogenâ€Bond Donor Capability of Carboxamides, Thioamides, and Selenoamides. Chemistry - A European Journal, 2022, 28, e202201309.	1.7	6
9	Clarifying notes on the bonding analysis adopted by the energy decomposition analysis. Physical Chemistry Chemical Physics, 2022, 24, 15726-15735.	1.3	25
10	Cleaner and stronger: how 8-quinolinolate facilitates formation of Co(<scp>iii</scp>)â€“thiolate from Co(<scp>ii</scp>)â€“disulfide complexes. Dalton Transactions, 2022, 51, 11675-11684.	1.6	4
11	Lack of Cooperativity in the Triangular X₃Halogen-Bonded Synthon?. Crystal Growth and Design, 2021, 21, 597-607.	1.4	14
12	Dipolar repulsion in Î±-halocarbonyl compounds revisited. Physical Chemistry Chemical Physics, 2021, 23, 20883-20891.	1.3	4
13	The Gauche Effect in XCH₂CH₂X Revisited. ChemPhysChem, 2021, 22, 641-648.	1.0	17
14	Not Carbon sâ€“p Hybridization, but Coordination Number Determines Câˆ’H and Câˆ’C Bond Length. Chemistry - A European Journal, 2021, 27, 7074-7079.	1.7	24
15	8 Energy decomposition analysis in the context of quantitative molecular orbital theory. , 2021, , 199-212.		49
16	Cooperative Selfâ€Assembly in Linear Chains Based on Halogen Bonds. ChemPlusChem, 2021, 86, 812-819.	1.3	10
17	Boron Tunneling in the â€œWeakâ€•Bondâ€Stretch Isomerization of Nâˆ’B Lewis Adducts. ChemPhysChem, 2021, 22, 1857-1862.	1.0	4
18	A Pushâ€“Pull Mechanism Helps Design Highly Competent G-Quadruplex-DNA Catalysts. CCS Chemistry, 2021, 3, 2183-2193.	4.6	9

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19	Communicating through hydrogen bonds. CheM, 2021, 7, 2272-2274.	5.8	1
20	How Divalent Cations Interact with the Internal Channel Site of Guanine Quadruplexes. ChemPhysChem, 2021, 22, 2286-2296.	1.0	13
21	SARS-CoV spike proteins can compete for electrolytes in physiological fluids according to structure-based quantum-chemical calculations. Computational and Theoretical Chemistry, 2021, 1204, 113392.	1.1	1
22	Nature of Alkaliâ€•and Coinageâ€Metal Bonds versus Hydrogen Bonds. Chemistry - an Asian Journal, 2021, 16, 315-321.	1.7	3
23	How Divalent Cations Interact with the Internal Channel Site of Guanine Quadruplexes. ChemPhysChem, 2021, 22, 2265-2265.	1.0	5
24	Understanding chemical reactivity using the activation strain model. Nature Protocols, 2020, 15, 649-667.	5.5	188
25	Distortionâ€Controlled Redshift of Organic Dye Molecules. Chemistry - A European Journal, 2020, 26, 2080-2093.	1.7	12
26	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.	1.6	9
27	Hydrogen-Bonded Rosettes of Aminotriazines for Selective-Ion Recognition. Journal of Physical Chemistry C, 2020, 124, 3352-3363.	1.5	10
28	Tuning the Binding Strength of Even and Uneven Hydrogen-Bonded Arrays with Remote Substituents. Journal of Physical Chemistry A, 2020, 124, 9451-9463.	1.1	7
29	The Nature of Nonclassical Carbonyl Ligands Explained byâ€‰Kohnâ€“Sham Molecular Orbital Theory. Chemistry - A European Journal, 2020, 26, 15690-15699.	1.7	14
30	Nature and Strength of Lewis Acid/Base Interaction in Boron and Nitrogen Trihalides. Chemistry - an Asian Journal, 2020, 15, 4043-4054.	1.7	28
31	The Hydrogenation Problem in Cobaltâ€based Catalytic Hydroaminomethylation. ChemistrySelect, 2020, 5, 13981-13994.	0.7	5
32	Understanding alkali metal cation affinities of multi-layer guanine quadruplex DNA. Physical Chemistry Chemical Physics, 2020, 22, 21108-21118.	1.3	24
33	Performance of TDDFT Vertical Excitation Energies of Coreâ€Substituted Naphthalene Diimides. Journal of Computational Chemistry, 2020, 41, 1448-1455.	1.5	21
34	Effect of Alkali Metal Cations on Length and Strength of Hydrogen Bonds in DNA Base Pairs. ChemPhysChem, 2020, 21, 2112-2126.	1.0	15
35	Evaluation of the Alicyclic Gauche Effect in 2â€Fluorocyclohexanone Analogs: a Combined NMR and DFT Study. European Journal of Organic Chemistry, 2020, 2020, 884-890.	1.2	3
36	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.	1.2	9

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37	Halogen Bonds in Ligandâ€“Protein Systems: Molecular Orbital Theory for Drug Design. Journal of Chemical Information and Modeling, 2020, 60, 1317-1328.	2.5	27
38	New light on an old debate: does the RCNâ€“PtCl₂ bond include any back-donation? RCNâ†PtCl₂ backbonding vs. the IR Î½_{Cî€,N} blue-shift dichotomy in organonitrilesâ€“platinum(<scp>ii</scp>) complexes. A thorough density functional theory â€“ energy decomposition analysis study. Dalton Transactions, 2019, 48, 12974-12985.	1.6	7
39	Alkali Metal Cation Affinities of Neutral Maingroup-Element Hydrides across the Periodic Table. Journal of Physical Chemistry A, 2019, 123, 9137-9148.	1.1	4
40	Efficient Copper-Catalyzed Multicomponent Synthesis of N-Acyl Amidines via Acyl Nitrenes. Journal of the American Chemical Society, 2019, 141, 15240-15249.	6.6	58
41	Cation affinities throughout the periodic table. Advances in Inorganic Chemistry, 2019, 73, 123-158.	0.4	1
42	Designing Selfâ€Assembled Rosettes: Why Ammeline is a Superior Building Block to Melamine. ChemistryOpen, 2019, 8, 135-142.	0.9	15
43	Designing Selfâ€Assembled Rosettes: Why Ammeline is a Superior Building Block to Melamine. ChemistryOpen, 2019, 8, 134-134.	0.9	4
44	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.	1.7	124
45	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.	6.6	59
46	Supramolecular Selfâ€Sorting Networks using Hydrogenâ€Bonding Motifs. Chemistry - A European Journal, 2019, 25, 785-795.	1.7	24
47	How Mg²⁺ ions lower the S_N2@P barrier in enzymatic triphosphate hydrolysis. Chemical Communications, 2018, 54, 3448-3451.	2.2	16
48	Glucose-nucleobase pairs within DNA: impact of hydrophobicity, alternative linking unit and DNA polymerase nucleotide insertion studies. Chemical Science, 2018, 9, 3544-3554.	3.7	2
49	Relevance of Orbital Interactions and Pauli Repulsion in the Metalâ€“Metal Bond of Coinage Metals. Inorganic Chemistry, 2018, 57, 2603-2608.	1.9	47
50	Nature of Intramolecular Resonance Assisted Hydrogen Bonding in Malonaldehyde and Its Saturated Analogue. Journal of Physical Chemistry A, 2018, 122, 1813-1820.	1.1	51
51	Mixed guanine, adenine base quartets: possible roles of protons and metal ions in their stabilization. Journal of Biological Inorganic Chemistry, 2018, 23, 41-49.	1.1	8
52	Integrative Theory/Experimentâ€Driven Exploration of a Multicomponent Reaction towards Imidazolineâ€2â€(thi)ones. European Journal of Organic Chemistry, 2018, 2018, 104-112.	1.2	2
53	Reversible Self-Assembly of Water-Soluble Gold(I) Complexes. Inorganic Chemistry, 2018, 57, 1017-1028.	1.9	29
54	RNA versus DNA Gâ€Quadruplex: The Origin of Increased Stability. Chemistry - A European Journal, 2018, 24, 16315-16322.	1.7	42

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55	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.	1.5	26
56	NMR ¹H-Shielding Constants of Hydrogen-Bond Donor Reflect Manifestation of the Pauli Principle. Journal of Physical Chemistry Letters, 2018, 9, 3720-3724.	2.1	61
57	Oxidation of organic diselenides and ditellurides by H₂O₂for bioinspired catalyst design. Physical Chemistry Chemical Physics, 2018, 20, 20874-20885.	1.3	27
58	Redox Interconversion between Cobalt(III) Thiolate and Cobalt(II) Disulfide Compounds. Inorganic Chemistry, 2018, 57, 8796-8805.	1.9	26
59	Impact of Conformational Effects on the Ringâ€“Chain Equilibrium of Hydrogenâ€Bonded Dinucleosides. Chemistry - A European Journal, 2018, 24, 11983-11991.	1.7	21
60	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.	2.3	74
61	Asymmetric identity SN2 transition states: Nucleophilic substitution at Î±-substituted carbon and silicon centers. International Journal of Mass Spectrometry, 2017, 413, 85-91.	0.7	16
62	B-DNA model systems in non-terran bio-solvents: implications for structure, stability and replication. Physical Chemistry Chemical Physics, 2017, 19, 16969-16978.	1.3	25
63	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.	1.7	36
64	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.	1.3	11
65	Cooperativity in the Selfâ€Assembly of the Guanine Nucleobase into Quartet and Ribbon Structures on Surfaces. Chemistry - A European Journal, 2017, 23, 3042-3050.	1.7	26
66	Hydrogenâ€Bond Strength of CC and GG Pairs Determined by Steric Repulsion: Electrostatics and Charge Transfer Overruled. Chemistry - A European Journal, 2017, 23, 10234-10234.	1.7	0
67	Isohexide Dinitriles: A Versatile Family of Renewable Platform Chemicals. ChemSusChem, 2017, 10, 3202-3211.	3.6	14
68	Kekulene: Structure, stability and nature of Hâ€¢â€¢â€¢H interactions in large PAHs. Molecular Astrophysics, 2017, 8, 19-26.	1.7	17
69	The evaluation of 5-amino- and 5-hydroxyuracil derivatives as potential quadruplex-forming agents. Organic and Biomolecular Chemistry, 2017, 15, 2174-2184.	1.5	10
70	Alkali Metal Cation Affinities of Anionic Main Groupâ€Element Hydrides Across the Periodic Table. Chemistry - an Asian Journal, 2017, 12, 2604-2611.	1.7	12
71	Enhanced Ïâ€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.	1.7	17
72	A metal-mediated base pair that discriminates between the canonical pyrimidine nucleobases. Chemical Science, 2017, 8, 1337-1343.	3.7	50

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73	Effect of Intra- and Intermolecular Interactions on the Properties of para-Substituted Nitrobenzene Derivatives. Crystals, 2016, 6, 29.	1.0	19
74	Insights on selenium and tellurium diaryldichalcogenides: A benchmark DFT study. Journal of Computational Chemistry, 2016, 37, 1672-1680.	1.5	43
75	Glucoseâ€“Nucleobase Pseudo Base Pairs: Biomolecular Interactions within DNA. Angewandte Chemie, 2016, 128, 8785-8789.	1.6	2
76	Glucoseâ€“Nucleobase Pseudo Base Pairs: Biomolecular Interactions within DNA. Angewandte Chemie - International Edition, 2016, 55, 8643-8647.	7.2	6
77	Substituent effects on the optical properties of naphthalenediimides: A frontier orbital analysis across the periodic table. Journal of Computational Chemistry, 2016, 37, 304-313.	1.5	12
78	Predicting Ptâ€195 NMR chemical shift using new relativistic allâ€electron basis set. Journal of Computational Chemistry, 2016, 37, 2360-2373.	1.5	24
79	Alkali Metal Cation versus Proton and Methyl Cation Affinities: Structure and Bonding Mechanism. ChemistryOpen, 2016, 5, 247-253.	0.9	4
80	Modified Guanines as Constituents of Smart Ligands for Nucleic Acid Quadruplexes. Chemistry - A European Journal, 2016, 22, 10912-10922.	1.7	8
81	Computational understanding and experimental characterization of twice-as-smart quadruplex ligands as chemical sensors of bacterial nucleotide second messengers. Scientific Reports, 2016, 6, 33888.	1.6	11
82	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.	1.7	11
83	Source of Cooperativity in Halogenâ€Bonded Haloamine Tetramers. ChemPhysChem, 2016, 17, 474-480.	1.0	16
84	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.	1.3	80
85	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.	1.3	46
86	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.	2.3	16
87	InnenrÃ¼cktitelbild: Six-Coordinate Groupâ€…13 Complexes: The Role of dâ€…Orbitals and Electron-Rich Multi-Center Bonding (Angew. Chem. 41/2015). Angewandte Chemie, 2015, 127, 12345-12345.	1.6	1
88	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.	0.9	50
89	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, 198-198.	0.9	1
90	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.	1.7	15

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91	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.	1.7	29
92	Thermodynamic Aspects of Aurophilic Hydrogelators. Inorganic Chemistry, 2015, 54, 5195-5203.	1.9	23
93	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.	1.2	11
94	A Highly Stabilizing Silver(I)â€Mediated Base Pair in Parallelâ€Stranded DNA. Angewandte Chemie - International Edition, 2015, 54, 3603-3606.	7.2	67
95	Theoretical study of electron-attracting ability of the nitro group: classical and reverse substituent effects. Structural Chemistry, 2015, 26, 905-913.	1.0	39
96	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.	2.2	36
97	Crystallographic and Computational Study on Cationic Triply Hydrogen-Bonded Nucleobases without Direct Anionic Stabilization. Crystal Growth and Design, 2015, 15, 5873-5878.	1.4	7
98	Sixâ€Coordinate Groupâ€…13 Complexes: The Role of dâ€…Orbitals and Electronâ€Rich Multiâ€Center Bonding. Angewandte Chemie - International Edition, 2015, 54, 12034-12038.	7.2	11
99	Covalency in resonance-assisted halogen bonds demonstrated with cooperativity in N-halo-guanine quartets. Physical Chemistry Chemical Physics, 2015, 17, 1585-1592.	1.3	54
100	How the disulfide conformation determines the disulfide/thiol redox potential. Journal of Biomolecular Structure and Dynamics, 2015, 33, 93-103.	2.0	15
101	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.	1.5	64
102	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.	1.7	17
103	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)	1.1	28
104	Stabilisation of 2,6â€Diarylpyridinium Cation by Throughâ€Space Polarâ€“Ï€ Interactions. Chemistry - A European Journal, 2014, 20, 6268-6271.	1.7	18
105	Diastereoselective One-Pot Synthesis of Tetrafunctionalized 2-Imidazolines. Journal of Organic Chemistry, 2014, 79, 5219-5226.	1.7	7
106	Highly accelerated inverse electron-demand cycloaddition of electron-deficient azides with aliphatic cyclooctynes. Nature Communications, 2014, 5, 5378.	5.8	145
107	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.	1.7	18
108	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.	1.7	29

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109	Thermodynamics of the Cu^{II} Î¼-Thiolate and Cu^I Disulfide Equilibrium: A Combined Experimental and Theoretical Study. Inorganic Chemistry, 2014, 53, 8494-8504.	1.9	31
110	Bis[N,Nâ€²â€diisopropylbenzamidinato(â^')]silicon(<scp>II</scp>): Lewis Acid/Base Reactions with Triorganylboranes. Chemistry - A European Journal, 2014, 20, 12411-12415.	1.7	28
111	Effects of the protonation state in the interaction of an HIV-1 reverse transcriptase (RT) amino acid, Lys101, and a non nucleoside RT inhibitor, GW420867X. Journal of Molecular Modeling, 2014, 20, 2332.	0.8	5
112	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.	1.7	69
113	Supramolecular Ring Structures of 7-Methylguanine: A Computational Study of Its Self-assembly and Anion Binding. Molecules, 2013, 18, 225-235.	1.7	3
114	Normal-to-Abnormal Rearrangement and NHC Activation in Three-Coordinate Iron(II) Carbene Complexes. Journal of the American Chemical Society, 2013, 135, 13338-13341.	6.6	110
115	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.	1.9	39
116	Self-Assembly of N³-Substituted Xanthines in the Solid State and at the Solidâ€“Liquid Interface. Langmuir, 2013, 29, 7283-7290.	1.6	15
117	Stereodivergent S_N2@P Reactions of Borane Oxazaphospholidines: Experimental and Theoretical Studies. Journal of the American Chemical Society, 2013, 135, 4483-4491.	6.6	48
118	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.	1.3	17
119	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.	1.5	8
120	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.	0.9	32
121	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.	0.7	12
122	Solvent effects on hydrogen bonds in Watsonâ€“Crick, mismatched, and modified DNA base pairs. Computational and Theoretical Chemistry, 2012, 998, 57-63.	1.1	32
123	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.	1.6	33
124	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.	1.0	21
125	Semicrystalline Polyesters Based on a Novel Renewable Building Block. Macromolecules, 2012, 45, 5069-5080.	2.2	78
126	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.	1.4	18

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127	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.	1.1	13
128	3-Substituted xanthines as promising candidates for quadruplex formation: computational, synthetic and analytical studies. New Journal of Chemistry, 2011, 35, 476-482.	1.4	36
129	Selectivity in DNA replication. Interplay of steric shape, hydrogen bonds, Ï€-stacking and solvent effects. Chemical Communications, 2011, 47, 7326.	2.2	52
130	Chimeric GNA/DNA metal-mediated base pairs. Chemical Communications, 2011, 47, 11041.	2.2	29
131	Silver(I)-mediated Hoogsteen-type base pairs. Journal of Inorganic Biochemistry, 2011, 105, 1398-1404.	1.5	59
132	Isohexide Derivatives from Renewable Resources as Chiral Building Blocks. ChemSusChem, 2011, 4, 599-603.	3.6	76
133	Steric effects on alkyl cation affinities of maingroupâ€element hydrides. Journal of Computational Chemistry, 2011, 32, 681-688.	1.5	15
134	Contiguous Metalâ€Mediated Base Pairs Comprising Two Ag^I Ions. Chemistry - A European Journal, 2011, 17, 6533-6544.	1.7	108
135	Remote Communication in a DNAâ€Based Nanoswitch. Chemistry - A European Journal, 2011, 17, 8816-8818.	1.7	24
136	Telomere Structure and Stability: Covalency in Hydrogen Bonds, Not Resonance Assistance, Causes Cooperativity in Guanine Quartets. Chemistry - A European Journal, 2011, 17, 12612-12622.	1.7	130
137	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.	0.5	123
138	Differential stabilization of adenine quartets by anions and cations. Journal of Biological Inorganic Chemistry, 2010, 15, 387-397.	1.1	18
139	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.	1.1	27
140	C(CN)5â€“: transition state or intermediate?. Mendeleev Communications, 2010, 20, 72-73.	0.6	6
141	Scope and Limitations of an Efficient Four-Component Reaction for Dihydropyridin-2-ones. Journal of Organic Chemistry, 2010, 75, 1723-1732.	1.7	28
142	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.	1.7	30
143	Dihydrogen Bonding: Donorâ€“Acceptor Bonding (AHâ‹…â‹…â‹…HX) versus the H₂ Molecule (Aï¿½H₂ï¿½X). Chemistry - A European Journal, 2009, 15, 5814-5822.	1.7	32
144	A Ditopic Ionâ€Pair Receptor Based on Stacked Nucleobase Quartets. Angewandte Chemie - International Edition, 2009, 48, 3285-3287.	7.2	70

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145	Hypervalent Carbon Atom: â€œFreezingâ€•the S_N2 Transition State. Angewandte Chemie - International Edition, 2009, 48, 6469-6471.	7.2	49
146	Ï€â€Electronic communication through mono and multinuclear gold(I) complexes. International Journal of Quantum Chemistry, 2009, 109, 2507-2519.	1.0	5
147	A Helicoid Ferrocene. Inorganic Chemistry, 2009, 48, 2714-2716.	1.9	22
148	Suitability of III-V<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:mo>[</mml:mo><mml:mrow><mml:mi>X</mml:mi><mml:msub><mml:mtext>H</mm for hydrogen storage: A density functional study. Physical Review B, 2009, 79, .	1.1	8
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