

Alexandre Hocquet

List of Publications by Year in descending order

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759233

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docs citations

33
times ranked

728
citing authors

#	ARTICLE	IF	CITATIONS
1	Ground-State Properties of Nucleic Acid Constituents Studied by Density Functional Calculations. 3. Role of Sugar Puckering and Base Orientation on the Energetics and Geometry of 2'-Deoxyribonucleosides and Ribonucleosides. <i>Journal of Physical Chemistry B</i> , 2000, 104, 4560-4568.	2.6	97
2	An Evaluation of the MM+ Force Field. <i>Journal of Molecular Modeling</i> , 1998, 4, 94-112.	1.8	88
3	Intramolecular hydrogen bonding in 2'-deoxyribonucleosides: an AIM topological study of the electronic density. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 3192-3199.	2.8	69
4	A conceptual DFT study of hydrazino peptides: Assessment of the nucleophilicity of the nitrogen atoms by means of the dual descriptor $\bar{\rho}^b(r)$. <i>Computational and Theoretical Chemistry</i> , 2008, 849, 46-51.	1.5	54
5	The peculiar role of cytosine in nucleoside conformational behaviour: Hydrogen bond donor capacity of nucleic bases. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 5351-5353.	2.8	44
6	Interaction of sodium and potassium ions with sandwiched cytosine-, guanine-, thymine-, and uracil-base tetrads. <i>Journal of Computational Chemistry</i> , 2005, 26, 352-364.	3.3	34
7	Influence of the gelator structure and solvent on the organisation and chirality of self-assembling fibrillar networks. <i>New Journal of Chemistry</i> , 2008, 32, 1131.	2.8	33
8	Intramolecular interactions along the reaction path of keto-enol tautomerism: Fukui functions as local softnesses and charges as local hardnesses. <i>Computational and Theoretical Chemistry</i> , 2004, 686, 213-218.	1.5	32
9	Intramolecular hydrogen bonding in ribonucleosides: an AIM topological study of the electronic density. Electronic supplementary information (ESI) available: Integrated properties of atomic basins, radii characterizing hydrogen bond interactions, and properties at bond critical points of hydrogen bonds (Tables S5). See http://www.rsc.org/suppdata/cp/b2/b201339h/ . <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 3843-3848.	2.8	28
10	Are guanine tetrads stabilised by bifurcated hydrogen bonds? An AIM topological analysis of the electronic density. <i>PhysChemComm</i> , 2002, 5, 94-98.	0.8	24
11	Guanine tetrads interacting with metal ions. An AIM topological analysis of the electronic density. Electronic Supplementary Information (ESI) available: Geometric data, topologic data at the BCP and integrated properties of the hydrogen atom of every H1-O6 and H2-N7 hydrogen bond. See http://www.rsc.org/suppdata/ql/b2/b210911e/ . <i>PhysChemComm</i> , 2003, 6, 1-5.	0.8	22
12	Magnetic properties of dinuclear copper(II) complexes with a N6 pyridazine-derived ligand. <i>Journal of the Chemical Society Dalton Transactions</i> , 1997, , 3683-3690.	1.1	19
13	N-(3-Amino-1H-isoindol-1-ylidene)-R-carbohydrazides and Their Amide-Type Isomerism. <i>European Journal of Organic Chemistry</i> , 2006, 2006, 2833-2842.	2.4	11
14	Dynamic behavior of a perfunctionalized β -cyclodextrin as probed by NMR and molecular modeling. <i>Carbohydrate Research</i> , 1997, 303, 379-393.	2.3	9
15	Epistemic issues in computational reproducibility: software as the elephant in the room. <i>European Journal for Philosophy of Science</i> , 2021, 11, 1.	1.1	9
16	The hydrogen bonding network in hydrazinopeptides and aza-peptides as probed by an AIM topological analysis of the electronic density. <i>Computational and Theoretical Chemistry</i> , 2008, 869, 41-46.	1.5	8
17	L-nucleotides and 8-methylguanine of d(C1m8G2C3G4C5LG6LC7G8C9G10)2 act cooperatively to promote a left-handed helix under physiological salt conditions. <i>Nucleic Acids Research</i> , 2003, 31, 6986-6995.	14.5	7
18	DFT, ab initio, NMR, and NBO analyses of N-substituted hydrazino acetamides: Experimental vs theoretical values. <i>Tetrahedron</i> , 2010, 66, 2322-2330.	1.9	7

#	ARTICLE	IF	CITATIONS
19	Mailing list archives as useful primary sources for historians: looking for flame wars. <i>Internet Histories</i> , 2018, 2, 38-54.	1.1	6
20	“Only the Initiates Will Have the Secrets Revealed”: Computational Chemists and the Openness of Scientific Software. <i>IEEE Annals of the History of Computing</i> , 2017, 39, 40-58.	0.2	5
21	Synthesis and Spectroscopic Study of Plant Growth Regulators Phenylpyridylureas: An "Agrorganic" Undergraduate Laboratory Experiment. <i>Journal of Chemical Education</i> , 1994, 71, 1092.	2.3	4
22	Stereodynamics of Nitrogen Chiral Centers in aza ² -Cyclodipeptides. <i>Chirality</i> , 2013, 25, 341-349.	2.6	4
23	Models, Parameterization, and Software: Epistemic Opacity in Computational Chemistry. <i>Perspectives on Science</i> , 2020, 28, 610-629.	1.0	4
24	Structures of (1) N-(2-pyridyl); (2) N-(3-pyridyl)- and (3) N-(4-pyridyl)-N'-(4-chlorophenyl)urea. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 1994, 50, 1507-1511.	0.4	3
25	Alchemy 2000 Version 1.00 for Windows: A Review. <i>Journal of Chemical Information and Computer Sciences</i> , 1997, 37, 622-623.	2.8	2
26	DFT and ab initio potential energy scan and hydrogen bond analysis of N [±] -substituted hydrazino acetamides: Characterization of the “hydrazino” hydrogen bonding pattern. <i>Computational and Theoretical Chemistry</i> , 2009, 911, 92-97.	1.5	2
27	“Only the Initiates Will Have the Secrets Revealed”: Computational Chemists and the Openness of Scientific Software. <i>IEEE Annals of the History of Computing</i> , 2017, 39, 40-58.	0.2	2
28	“We were here before the Web and hype”: a brief history of and tribute to the Computational Chemistry List. <i>Journal of Cheminformatics</i> , 2018, 10, 67.	6.1	2
29	Wikipédia au prisme de l’Épistémologie sociale et des Études des sciences. <i>Cahiers Philosophiques</i> , 2015, n° 141, 68-86.	0.0	2
30	Parcours 11. Reprenez ce texte sur la science ouverte et transformez-le. , 2019, , 527-534.		2