Camelia MuÃ±oz-Caro

List of Publications by Year
in descending order

67	1,114	394421	414414
papers	citations	19 h-index	32 g-index

67	67	67	980
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A Survey of Parallel Programming Models and Tools in the Multi and Many-Core Era. IEEE Transactions on Parallel and Distributed Systems, 2012, 23, 1369-1386.	5.6	189
2	Modeling of Protonation Processes in Acetohydroxamic Acid. Journal of Organic Chemistry, 2000, 65, 405-410.	3.2	114
3	Deprotonation Sites of Acetohydroxamic Acid Isomers. A Theoretical and Experimental Study. Journal of Organic Chemistry, 2003, 68, 6535-6542.	3.2	47
4	Wagging and torsion vibronic structure in the T1 .rarw. S0 electronic spectrum of acetaldehyde. The Journal of Physical Chemistry, 1994, 98, 1519-1524.	2.9	44
5	Effect of Anharmonicities on the Thermodynamic Properties of the Water Dimerâ€. Journal of Physical Chemistry A, 1997, 101, 4128-4135.	2.5	41
6	Theoretical prediction of relative and absolute pKa values of aminopyridines. Biophysical Chemistry, 2006, 124, 155-160.	2.8	38
7	Computation of kinetic constants for large range internal motions in molecules. Computers & Chemistry, 1994, 18, 27-32.	1.2	35
8	Theoretical Study of the Effect of Hydrogen-Bonding on the Stability and Vibrational Spectrum of Isolated 2,2,2-Trifluoroethanol and Its Molecular Complexes. Journal of Physical Chemistry A, 2002, 106, 10673-10680.	2.5	34
9	The T1(nï€*)â†S0 laser induced phosphorescence excitation spectrum of acetaldehyde in a supersonic free jet: Torsion and wagging potentials in the lowest triplet state. Journal of Chemical Physics, 1996, 105, 2547-2552.	3.0	33
10	Mechanism of Pyridine Protonation in Water Clusters of Increasing Size. Journal of Physical Chemistry A, 2005, 109, 8341-8347.	2.5	32
11	Theoretical analysis of the molecular determinants responsible for the K+ channel blocking by aminopyridines. Biophysical Chemistry, 2001, 91, 49-60.	2.8	31
12	The nature of the receptor site for the reversible K+ channel blocking by aminopyridines. Biophysical Chemistry, 2002, 96, 1-14.	2.8	31
13	Theoretical study of the effect of torsional anharmonicity on the thermodynamic properties of methanol. Chemical Physics Letters, 1997, 273, 135-140.	2.6	30
14	Molecular docking study of the binding of aminopyridines within the K+ channel. Journal of Molecular Modeling, 2007, 13, 579-586.	1.8	26
15	The Torsionâ€“Inversion Energy Levels in theS1(n, Ï€*) Electronic State of Acetaldehyde from High-Resolution Jet-Cooled Fluorescence Excitation Spectroscopy. Journal of Molecular Spectroscopy, 1996, 175, 172-189.	1.2	21
16	Conformational population distribution of acetylcholine, nicotine and muscarine in vacuum and solution. Computational and Theoretical Chemistry, 2005, 726, 115-124.	1.5	21
17	Rational modelling of the voltage-dependent K+ channel inactivation by aminopyridines. Biophysical Chemistry, 2003, 104, 417-427.	2.8	20
18	Theoretical determination of the torsion-wagging structure of the S1 â†•S0 electronic spectrum of acetaldehyde. Chemical Physics, 1994, 186, 221-231.	1.9	19

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19	Theoretical Analysis of Pyridine Protonation in Water Clusters of Increasing Size. ChemPhysChem, 2005, 6, 139-147.	2.1	19
20	Recursive computation of Hamiltonian matrix elements using harmonic oscillator eigenfunctions: Application to the inversion of ammonia and to the methyl torsion + aldehydic hydrogen wagging of acetaldehyde. Computers & Chemistry, 1995, 19, 371-378.	1.2	18
21	Derivation of accurate kinetic and potential-energy functions for several simultaneous large-amplitude vibrations: application to acetaldehyde in the S0and T1states. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 399-403.	1.7	16
22	Derivation of self-scheduling algorithms for heterogeneous distributed computer systems: Application to internet-based grids of computers. Future Generation Computer Systems, 2009, 25, 617-626.	7.5	16
23	Three-Dimensional Vibrational Study of the Coupling between Methyl Torsion and the Molecular Frame in the S0 State of Acetaldehyde. The Journal of Physical Chemistry, 1995, 99, 8510-8515.	2.9	15
24	Suitability of different levels of theory for modelling of hydroxamic acids. Computational and Theoretical Chemistry, 2000, 530, 291-300.	1.5	15
25	On the origin of the barriers and the structures of acetaldehyde in its ground and first singlet excited state. Theoretica Chimica Acta, 1994, 88, 299-310.	0.8	13
26	Theoretical and Experimental Study of the Acetohydroxamic Acid Protonation: The Solvent Effect. Chemistry - A European Journal, 2000, 6, 2644-2652.	3.3	13
27	Analysis of B3LYP and MP2 conformational population distributions intrans-nicotine, acetylcholine, and ABT-594. International Journal of Quantum Chemistry, 2005, 103, 25-33.	2.0	13
28	Refinement of a generalized Fermatâ€™s last theorem conjecture in natural vector spaces. Journal of Mathematical Chemistry, 2017, 55, 1869-1877.	1.5	13
29	Vibrational energy levels and vibronic structure of electronic spectra in molecules with large amplitude motions. Computers & Chemistry, 1994, 18, 413-417.	1.2	12
30	The Torsionâ€“Inversionâ€“Bending Energy Levels in theS1(n, Ï€*) Electronic State of Acetaldehyde. Journal of Molecular Spectroscopy, 1998, 190, 78-90.	1.2	12
31	A study of quadratic + gaussian + cosine functions for the simultaneous description of intramolecular torsion and inversion. Journal of Molecular Structure, 1994, 318, 237-242.	3.6	11
32	Definition of a periodic methyl torsional coordinate in the S0 state of acetaldehyde. Journal of Molecular Structure, 1995, 350, 83-89.	3.6	10
33	Monitoring and steering Grid applications with GRID superscalar. Future Generation Computer Systems, 2010, 26, 645-653.	7.5	9
34	Experimental and Theoretical Study of the Secondary Equilibrium Isotope Effect (SEIE) in the Proton Transfer between the Pyridinium-d5 Cation and Pyridine. Journal of Physical Chemistry A, 2003, 107, 6160-6167.	2.5	8
35	Performance of computationally intensive parameter sweep applications on Internet-based Grids of computers: the mapping of molecular potential energy hypersurfaces. Concurrency Computation Practice and Experience, 2007, 19, 463-481.	2.2	8
36	Structural and vibrational theoretical analysis of protonated formaldehyde in its $$ilde{X}^{1} A^{prime}$$ ground electronic state. Theoretical Chemistry Accounts, 2008, 119, 343-354.	1.4	8

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37	Neural modeling of torsional potential hypersurfaces in non-rigid molecules. Computers & Chemistry, 1998, 22, 355-361.	1.2	7
38	Effect of Large-Amplitude Vibrations on the Thermodynamics of Malondialdehyde. Journal of Physical Chemistry A, 1998, 102, 1177-1180.	2.5	7
39	Effect of the Conformational Kinetic Energy and the Rotovibrational Coupling in the Conformational Population of Bioactive Compounds. Journal of Physical Chemistry A, 2003, 107, 10191-10198.	2.5	7
40	Quantum Mechanical Study and Nuclear Magnetic Resonance Measurements of Some Î±-Arylcarboxyalkyl Acids as Anti-inflammatory Agents. Journal of Pharmaceutical Sciences, 1989, 78, 764-766.	3.3	6
41	Gmat. A software tool for the computation of the rovibrational G matrix. Computer Physics Communications, 2009, 180, 1183-1187.	7.5	6
42	The accurate computation of partition functions in non-rigid molecules. Computers & Chemistry, 1997, 21, 143-151.	1.2	5
43	Customizing clustering computing for a computational chemistry environment. The case of the DBO-83 nicotinic analgesic. Computational and Theoretical Chemistry, 2005, 727, 41-48.	1.5	5
44	Ã‰tude comparative CNDO/2 des dÃ©terminants molÃ©culaires de l'activitÃ© agoniste de rÃ©cepteur-H2 dans l'histamine et le bÃ©tazol. European Journal of Medicinal Chemistry, 1989, 24, 411-414.	5.5	4
45	A structural ab initio study of the T1 triplet state of acetaldehyde. The effects of electron correlation and additional functions in the basis set. Computational and Theoretical Chemistry, 1994, 315, 9-17.	1.5	4
46	Thermodynamic conformational analysis and structural stability of the nicotinic analgesic ABT-594. Journal of Computer-Aided Molecular Design, 2003, 17, 713-724.	2.9	4
47	A Quadratic Self-Scheduling Algorithm for Heterogeneous Distributed Computing Systems. , 2006, , .		3
48	Heuristic computation of the rovibrational G matrix in optimized molecule-fixed axes. Gmat 2.1. Computer Physics Communications, 2010, 181, 1471-1475.	7.5	3
49	Quantitative modeling of degree-degree correlation in complex networks. Physical Review E, 2013, 88, 032805.	2.1	3
50	A Fault Tolerant Adaptive Method for the Scheduling of Tasks in Dynamic Grids. , 2009, , .		2
51	A metaheuristic approach to the optimal definition of molecule-fixed axes in rovibrational Hamiltonians. Computer Physics Communications, 2010, 181, 967-977.	7.5	2
52	APINetworks: A general API for the treatment of complex networks in arbitrary computational environments. Computer Physics Communications, 2015, 196, 446-454.	7.5	2
53	APINetworks Java. A Java approach to the efficient treatment of large-scale complex networks. Computer Physics Communications, 2016, 207, 549-552.	7.5	2
54	A General Approach to Fuzzy Community Detection in Social Networks. , 2019, , .		2

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55	Accurate Numerical Computation of Rovibrational G Matrices in Molecules of Arbitrary Size. Lecture Notes in Computer Science, 2008, , 1011-1025.	1.3	1
56	A Heuristic Approach to Task Scheduling in Internet-Based Grids of Computers. , 2008, , .		1
57	Analysis of the nitrile and methyl torsional vibrations of nâ€propyl cyanide in its S₀ electronic state. International Journal of Quantum Chemistry, 2011, 111, 3681-3694.	2.0	1
58	A uniform object-oriented solution to the eigenvalue problem for real symmetric and Hermitian matrices. Computer Physics Communications, 2011, 182, 2059-2064.	7.5	1
59	Structural and vibrational analysis of the OH torsional motion in difluorohydroxyborane. International Journal of Quantum Chemistry, 2011, 111, 4389-4399.	2.0	1
60	Enhanced procedure for the refinement of kinetic and potential functions for large-amplitude vibrations. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 2989-2990.	1.7	0
61	A computer simulation of the ring puckering and oxygen wagging dynamics in the S0 state of cyclobutanone. Advances in Quantum Chemistry, 2001, 40, 345-359.	0.8	0
62	A general model for the generation and scheduling of parameter sweep experiments in computational grid environments. Procedia Computer Science, 2010, 1, 565-572.	2.0	0
63	A fineâ€grained loopâ€level parallel approach to efficient fuzzy community detection in complex networks. Concurrency Computation Practice and Experience, 2020, 32, e5537.	2.2	0
64	Large Amplitude Motions in Electronically Excited States: A Study of the S1 Excited State of Formic Acid. Progress in Theoretical Chemistry and Physics, 2001, , 347-358.	0.2	0
65	A Concurrent Object-Oriented Approach to the Eigenproblem Treatment in Shared Memory Multicore Environments. Lecture Notes in Computer Science, 2011, , 630-642.	1.3	0
66	Theoretical analysis of the structural and chemical reactivity properties of the schistosomicidal drug niridazole. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1995, 92, 679-698.	0.2	0
67	MSSML: A Molecular Spectroscopic Simulations Markup Language for Rovibrational Studies. Lecture Notes in Computer Science, 2008, , 997-1010.	1.3	0