## Alberto Luna

List of Publications by Year in descending order

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all docs

25 625 15 25 g-index

25 25 25 25 376

times ranked

citing authors

docs citations

#	Article	IF	CITATIONS
1	Cu+ binding energies. Dramatic failure of the G2 method vs. good performance of the B3LYP approach. Chemical Physics Letters, 2000, 320, 129-138.	2.6	93
2	Modeling the Interactions between Peptide Functions and Cu(I): Formamideâ^'Cu+ Reactions in the Gas Phase. Journal of the American Chemical Society, 1998, 120, 5411-5426.	13.7	75
3	Reactions between Guanidine and Cu+in the Gas Phase. An Experimental and Theoretical Study. Journal of Physical Chemistry A, 1997, 101, 5931-5941.	2.5	64
4	Reactions of Urea with Cu+ in the Gas Phase:  An Experimental and Theoretical Study. Journal of Physical Chemistry A, 2000, 104, 3132-3141.	2.5	60
5	Role of Cu+Association on the Formamide → Formamidic Acid → (Aminohydroxy)carbene Isomerizations in the Gas Phase. Journal of Physical Chemistry A, 1998, 102, 4652-4659.	2.5	38
6	A theoretical analysis of the lowest excited states in HNO/NOH and HPO/POH. Chemical Physics, 1995, 196, 437-445.	1.9	33
7	Experimental and Theoretical Investigation of the Reactions between Glucose and Cu+ in the Gas Phase. Journal of Physical Chemistry A, 2002, 106, 2641-2651.	2.5	28
8	Cu+ reactivity trends in sp, sp2, and sp3 nitrogen, phosphorus, and arsenic containing bases. International Journal of Mass Spectrometry, 2000, 201, 215-231.	1.5	25
9	Unimolecular Reactivity of Strong Metal–Cation Complexes in the Gas Phase: Ethylenediamine–Cu+. Chemistry - A European Journal, 2004, 10, 2927-2934.	3.3	24
10	Exploring the Potential Energy Surface of the Association of Cu+to Oxaziridine, Nitrosomethane, and Formaldoxime. Journal of Physical Chemistry A, 1998, 102, 10120-10127.	2.5	22
11	Theoretical Survey of the Potential Energy Surface of Ethylenediamine + Cu+Reactions. Journal of Physical Chemistry A, 2004, 108, 8367-8372.	2.5	22
12	Reactions between Glycolic Acid and Cu+ in the Gas Phase. An Experimental and Theoretical Study. Journal of Physical Chemistry A, 2002, 106, 9359-9368.	2.5	19
13	Cyano substituent effects on enol and enethiol acidity and basicity: The protonation and deprotonation of 3-hydroxy-2-propenenitrile and its thio analogue. International Journal of Mass Spectrometry, 2007, 267, 125-133.	1.5	18
14	Gas-Phase Protonation and Deprotonation of Acrylonitrile Derivatives NCCHCHX (X=CH3, NH2,) Tj	ET <u>Q</u> q0 0 (	O rgBT /Overlo
15	A theoretical study of the interaction between Ni+ and small oxygen- and nitrogen-containing bases. International Journal of Mass Spectrometry, 2002, 217, 119-129.	1.5	16
16	High-level ab initio calculations on the structures and relative stabilities of [O, P, H] systems and their cations. Chemical Physics Letters, 1993, 209, 557-563.	2.6	14
17	Thermochemistry of the reactions of PH+2 (1A1) and PH+2 (3B1) with CO. A G2 molecular orbital study. Chemical Physics Letters, 1994, 223, 240-249.	2.6	12
18	A G1 ab initio MO study of the distonic ions H2Cî—,Oî—,Si+ and their isomers. Chemical Physics Letters, 1992, 197, 581-585.	2.6	10

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#	Article	IF	CITATION
19	Regio- and Stereochemistry of Alkene Expulsion from Ionized sec-Alkyl Phenyl Ethers. Journal of Physical Chemistry A, 1999, 103, 2348-2358.	2.5	9
20	PyrazoleN-methylide radical cation: ion-molecule reactions in a new hybrid tandem mass spectrometer and DFT molecular orbital calculations. Journal of Physical Organic Chemistry, 2000, 13, 13-22.	1.9	8
21	Molecular Modelling of the H <sub>2</sub> â€Adsorptive Properties of Tetrazolateâ€Based Metalâ^'Organic Frameworks: From the Cluster Approach to Periodic Simulations. ChemPhysChem, 2018, 19, 1349-1357.	2.1	6
22	Specific reactivity of 1-alkenes with transition metal cations. International Journal of Mass Spectrometry, 2003, 228, 359-371.	1.5	5
23	Perturbation of the intramolecular hydrogen bonds of glucose by Cu+association. International Journal of Quantum Chemistry, 2002, 86, 138-144.	2.0	4
24	High-Level ab Initio Calculations on the Gas-Phase Reactions between C+(2P) and Formic Acid. Journal of Physical Chemistry A, 1999, 103, 4543-4552.	2.5	2
25	High-level ab initio calculations on CH+2(2A1) + PO(2II) reactions. International Journal of Quantum Chemistry, 1996, 57, 559-566.	2.0	1