

Jacques LiÃ©vin

List of Publications by Year in descending order

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32
papers

465
citations

759233

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713466

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g-index

32
all docs

32
docs citations

32
times ranked

415
citing authors

#	ARTICLE	IF	CITATIONS
1	The VMFCI method: A flexible tool for solving the molecular vibration problem. <i>Journal of Computational Chemistry</i> , 2006, 27, 627-640.	3.3	64
2	Alternative perturbation method for the molecular vibration-rotation problem. <i>International Journal of Quantum Chemistry</i> , 2003, 93, 245-264.	2.0	61
3	Comparison of the experimental, semi-experimental and <i>ab initio</i> equilibrium structures of acetylene: Influence of relativistic effects and of the diagonal Born-Oppenheimer corrections. <i>Journal of Chemical Physics</i> , 2011, 134, 064119.	3.0	58
4	Vinylidene-acetylene cation isomerization investigated by large scale <i>ab initio</i> calculations. <i>Journal of Chemical Physics</i> , 2006, 124, 214305.	3.0	29
5	Experimental 2CH excitation in acetylene-containing van der Waals complexes. <i>Molecular Physics</i> , 2012, 110, 2781-2796.	1.7	25
6	Potential energy surface and bound states of the NH ₃ -Ar and ND ₃ -Ar complexes. <i>Journal of Chemical Physics</i> , 2014, 141, 224303.	3.0	25
7	Ab Initio Intermolecular Potential of Ar-C ₂ H ₂ Refined Using High-Resolution Spectroscopic Data. <i>Journal of Physical Chemistry A</i> , 2013, 117, 13767-13774.	2.5	21
8	Revisiting Mulliken's Concepts about Rydberg States and Rydberg-Valence Interactions from Large-Scale Ab Initio Calculations on the Acetylene Molecule. <i>Journal of Physical Chemistry A</i> , 2009, 113, 13210-13220.	2.5	16
9	Accurate ground-state potential energy surfaces of the C ₂ H ₂ -Kr and C ₂ H ₂ -Xe van der Waals complexes. <i>Molecular Physics</i> , 2012, 110, 2751-2760.	1.7	16
10	Ab initio characterization of the state of the acetylene molecule. <i>Journal of Molecular Spectroscopy</i> , 1992, 156, 123-146.	1.2	14
11	Radiative lifetime of the $\tilde{X}^3\Sigma^+$ state of HeH ⁺ from <i>ab initio</i> calculations. <i>Journal of Chemical Physics</i> , 2010, 133, 114302.	3.0	13
12	Experimental and Theoretical Studies of the Isotope Exchange Reaction. <i>Astrophysical Journal</i> , 2019, 877, 38.	4.5	12
13	Influence of kinetic coupling in rectilinear coordinates on the vibrational spectrum of fluoroform. <i>Chemical Physics Letters</i> , 2008, 466, 16-20.	2.6	10
14	<i>Ab initio</i> study of the neutral and anionic alkali and alkaline earth hydroxides: Electronic structure and prospects for sympathetic cooling of OH ⁻ . <i>Journal of Chemical Physics</i> , 2017, 146, 194309.	3.0	10
15	Cold reactive and nonreactive collisions of Li and Rb with C ₂ : Implications for hybrid-trap experiments. <i>Physical Review A</i> , 2019, 99, ...	2.5	10
16	Rydberg states of cyanoacetylene investigated by (3+1) REMPI spectroscopy in the 77,000-90,000 cm ⁻¹ energy range. <i>Molecular Physics</i> , 2012, 110, 2829-2842.	1.7	9
17	High-resolution, near-infrared CW-CRDS, and <i>ab initio</i> investigations of N ₂ O-HDO. <i>Molecular Physics</i> , 2015, 113, 473-482.	1.7	9
18	A vibrational CASSCF study of stretch-bend interactions and their influence on infrared intensities in the water molecule. <i>Theoretica Chimica Acta</i> , 1995, 92, 211-226.	0.8	7

#	ARTICLE	IF	CITATIONS
19	Vibronic structure of the $2^1\hat{u}$ ground electronic state of dicyanoacetylene cation revisited by PFI-ZEKE photoelectron spectroscopy and <i>ab initio</i> calculations. <i>Molecular Physics</i> , 2015, 113, 3946-3954.	1.7	7
20	<i>Ab initio</i> study of reactive collisions between Rb(2^1S) or Rb(2^1P) and OH $\hat{+}$ ($1^1\Sigma^+$). <i>Journal of Chemical Physics</i> , 2016, 144, 204306.	3.0	7
21	Experimental and theoretical investigations of H ₂ O $\hat{+}$ Ar. <i>Journal of Chemical Physics</i> , 2017, 147, 014302.	3.0	7
22	Accuracy of the equilibrium structure of sulphur dioxide. <i>Molecular Physics</i> , 2022, 120, .	1.7	6
23	Experimental and <i>ab initio</i> characterization of HC ₃ N ⁺ vibronic structure. I. Synchrotron-based threshold photo-electron spectroscopy. <i>Journal of Chemical Physics</i> , 2016, 145, 234310.	3.0	5
24	Theoretical description of electronically excited vinylidene up to 10 eV: First high level <i>ab initio</i> study of singlet valence and Rydberg states. <i>Journal of Chemical Physics</i> , 2014, 141, 174317.	3.0	4
25	Experimental and <i>ab initio</i> characterization of HC ₃ N ⁺ vibronic structure. II. High-resolution VUV PFI-ZEKE spectroscopy. <i>Journal of Chemical Physics</i> , 2016, 145, 234309.	3.0	4
26	Overtone, $2NH(1^1/2_1 + 1^1/2_3)$ spectroscopy of NH ₃ $\hat{+}$ Ar and NH ₃ $\hat{+}$ Kr. <i>Molecular Physics</i> , 2015, 113, 3934-3945.	1.7	3
27	Vibronic structure of the cyanobutadiyne cation. II. Theoretical exploration of the complex energy landscape of HC ₅ N ⁺ . <i>Journal of Chemical Physics</i> , 2019, 150, 244303.	3.0	3
28	Reactivity of Hydrated Hydroxide Anion Clusters with H and Rb: An <i>ab Initio</i> Study. <i>Journal of Physical Chemistry A</i> , 2019, 123, 8893-8906.	2.5	3
29	Dynamics of the isotope exchange reaction of D with H ₃ ⁺ , H ₂ D ⁺ , and D ₂ H ⁺ . <i>Journal of Chemical Physics</i> , 2021, 154, 084307.	3.0	3
30	From atoms to biomolecules: a fruitful perspective. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	1.4	2
31	Vibronic structure of the cyanobutadiyne cation. I. VUV photoionization study of HC ₅ N. <i>Journal of Chemical Physics</i> , 2019, 150, 244304.	3.0	1
32	Cold collisions of C ₂ $\hat{+}$ with Li and Rb atoms in hybrid traps. <i>Journal of Physics: Conference Series</i> , 2020, 1412, 062003.	0.4	1