

Saulo A Vazquez

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103
papers

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108
ext. papers

1,747
ext. citations

3.3
avg, IF

4.49
L-index

#	Paper	IF	Citations
103	An automated method to find reaction mechanisms and solve the kinetics in organometallic catalysis. <i>Chemical Science</i> , 2017 , 8, 3843-3851	9.4	66
102	Implementation of a fast analytic ground state potential energy surface for the N(2D)+H ₂ reaction. <i>Journal of Chemical Physics</i> , 2003 , 119, 3063-3070	3.9	59
101	Absolute configuration of secondary alcohols by ¹ H NMR: in situ complexation of alpha-methoxyphenylacetic acid esters with barium(II). <i>Journal of Organic Chemistry</i> , 2002 , 67, 4579-89	4.2	57
100	Quasiclassical trajectory study of the F + CH ₄ reaction dynamics on a dual-level interpolated potential energy surface. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 8459-70	2.8	51
99	Semiempirical Hamiltonian for simulation of azobenzene photochemistry. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 98-110	2.8	50
98	Quasi-classical trajectory calculations on a fast analytic potential energy surface for the C(1D)+H ₂ reaction. <i>Chemical Physics Letters</i> , 2003 , 374, 243-251	2.5	47
97	Quasiclassical dynamics simulation of the collision-induced dissociation of Cr(CO) ₆ + with Xe. <i>Journal of Chemical Physics</i> , 2005 , 123, 154311	3.9	44
96	Dynamics of CO ₂ scattering off a perfluorinated self-assembled monolayer. Influence of the incident collision energy, mass effects, and use of different surface models. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 3850-65	2.8	42
95	Trajectory dynamics study of the Ar + CH ₄ dissociation reaction at high temperatures: the importance of zero-point-energy effects. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 5415-23	2.8	42
94	Role of barium(II) in the determination of the absolute configuration of chiral amines by ¹ H NMR spectroscopy. <i>Journal of Organic Chemistry</i> , 2006 , 71, 1119-30	4.2	35
93	Inelastic scattering dynamics of Ar from a perfluorinated self-assembled monolayer surface. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 12785-94	2.8	32
92	Interaction and dimerization energies in methyl-blocked alpha,gamma-peptide nanotube segments. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 4973-83	3.4	31
91	The role of aromaticity in the planarity of lumiflavin. <i>Journal of Organic Chemistry</i> , 2002 , 67, 6347-52	4.2	31
90	Influence of Multiple Conformations and Paths on Rate Constants and Product Branching Ratios. Thermal Decomposition of 1-Propanol Radicals. <i>Journal of Physical Chemistry A</i> , 2018 , 122, 4790-4800	2.8	27
89	Quasiclassical trajectory study of the collision-induced dissociation of CH ₃ SH+ + Ar. <i>Journal of Chemical Physics</i> , 2004 , 121, 2571-7	3.9	26
88	Hydrogen transfer vs proton transfer in 7-hydroxy-quinoline.(NH ₃) ₃ : a CASSCF/CASPT2 study. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 5907-12	2.8	25
87	A Trajectory-Based Method to Explore Reaction Mechanisms. <i>Molecules</i> , 2018 , 23,	4.8	24

86	Dissociation of Difluoroethylenes. II. Direct Classical Trajectory Study of the HF Elimination from 1,2-Difluoroethylene. <i>Journal of Physical Chemistry A</i> , 2003 , 107, 1398-1404	2.8	23
85	Ab initio and RRKM study of the HCN/HNC elimination channels from vinyl cyanide. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 979-85	2.8	22
84	Further investigation of the HCl elimination in the photodissociation of vinyl chloride at 193 nm: a direct MP2/6-31G(d,p) trajectory study. <i>Chemical Physics Letters</i> , 2004 , 386, 225-232	2.5	22
83	A Direct Classical Trajectory Study of HCl Elimination from the 193 nm Photodissociation of Vinyl Chloride. <i>Journal of Physical Chemistry A</i> , 2003 , 107, 7611-7618	2.8	22
82	AB initio gradient optimized molecular geometry and conformational analysis of 1,2-propanediol at the 4-21G level. <i>Computational and Theoretical Chemistry</i> , 1989 , 184, 323-342		22
81	Ab initio-gradient optimized molecular geometry and conformational analysis of 1,3-propanediol at the 4-21G level. <i>Computational and Theoretical Chemistry</i> , 1988 , 181, 149-167		22
80	Direct and indirect hydrogen abstraction in Cl + alkene reactions. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 5595-607	2.8	21
79	HCN elimination from vinyl cyanide: product energy partitioning, the role of hydrogen-deuterium exchange reactions and a new pathway. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 6948-55	3.6	21
78	Collision-induced dissociation mechanisms of [Li(uracil)] ⁺ . <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 7628-37	3.6	21
77	Quasiclassical trajectory study of the collision-induced dissociation dynamics of Ar + CH ₃ SH ⁺ using an ab initio interpolated potential energy surface. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 1225-31	2.8	21
76	Dynamics calculations for the Cl+C ₂ H ₆ abstraction reaction: Thermal rate constants and kinetic isotope effects. <i>Journal of Chemical Physics</i> , 2003 , 118, 6280-6288	3.9	21
75	Recent applications of boxed molecular dynamics: a simple multiscale technique for atomistic simulations. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2014 , 372,	3	20
74	Product energy distributions for the four-center HF elimination from 1,1-difluoroethylene. A direct dynamics study. <i>Chemical Physics Letters</i> , 2001 , 348, 81-88	2.5	20
73	Three-center vs. four-center HF elimination from vinyl fluoride: a direct dynamics study. <i>Chemical Physics Letters</i> , 2000 , 332, 583-590	2.5	20
72	Photodissociation of formic acid: A trajectory surface hopping study. <i>Chemical Physics Letters</i> , 2005 , 412, 35-40	2.5	19
71	On the conformational memory in the photodissociation of formic acid. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 2836-9	2.8	18
70	Dissociation of Difluoroethylenes. I. Global Potential Energy Surface, RRKM, and VTST Calculations. <i>Journal of Physical Chemistry A</i> , 2003 , 107, 1389-1397	2.8	18
69	Unimolecular reaction dynamics of HSO. Analysis of the influence of different barrier samplings on the product energy distributions. <i>Physical Chemistry Chemical Physics</i> , 2002 , 4, 279-287	3.6	18

68	Intermolecular potential for binding of protonated peptide ions with perfluorinated hydrocarbon surfaces. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 5577-88	3.4	16
67	New lead(II) complexes with N,S-ligands, including a lead pyrazolonate with unusual packing flexibility. <i>Polyhedron</i> , 2007 , 26, 4228-4238	2.7	16
66	Ab Initio Calculations on the Vinyl Fluoride Fragmentation Reactions. <i>Structural Chemistry</i> , 2001 , 12, 95-100	10.0	16
65	Dissociation of ethylene and several deuterated derivatives at 193 and 157 nm by direct classical trajectories. <i>Chemical Physics Letters</i> , 2002 , 353, 418-425	2.5	15
64	Nonstatistical effects in the unimolecular dissociation of the acetyl radical. <i>Journal of Chemical Physics</i> , 1999 , 110, 11323-11334	3.9	15
63	Ab initio-gradient optimized molecular geometry and conformational analysis of 2-methoxyethanol at the 4-21G level. <i>Computational and Theoretical Chemistry</i> , 1989 , 188, 95-104		15
62	GAFit: A general-purpose, user-friendly program for fitting potential energy surfaces. <i>Computer Physics Communications</i> , 2017 , 217, 89-98	4.2	14
61	Theoretical and computational studies of non-equilibrium and non-statistical dynamics in the gas phase, in the condensed phase and at interfaces. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2017 , 375,	3	14
60	Direct-dynamics VTST study of the [1,7] hydrogen shift in 7-methylocta-1,3(Z),5(Z)-triene. A model system for the hydrogen transfer reaction in previtamin D3. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 719-25	2.8	14
59	Rovibrational distributions of HF in the photodissociation of vinyl fluoride at 193 nm: a direct MP2 quasiclassical trajectory study. <i>Journal of Chemical Physics</i> , 2004 , 121, 5179-82	3.9	14
58	Direct Dynamics Study of the Dissociation and Elimination Channels in the Thermal Decomposition of Methyl Nitrite. <i>Journal of the American Chemical Society</i> , 1998 , 120, 7594-7601	16.4	14
57	Molecular mechanics study of conformational trends in simple alcohols and ethers. II. Intramolecular hydrogen bonding. <i>Journal of Computational Chemistry</i> , 1992 , 13, 851-859	3.5	14
56	Is Photolytic Production a Viable Source of HCN and HNC in Astrophysical Environments? A Laboratory-based Feasibility Study of Methyl Cyanofornate. <i>Astrophysical Journal</i> , 2017 , 849, 15	4.7	12
55	Chemical Dynamics Simulations of CO ₂ in the Ground and First Excited Bend States Colliding with a Perfluorinated Self-Assembled Monolayer. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 18455-18464	3.8	12
54	Direct dynamics study of the photodissociation of triplet propanal at threshold. <i>Chemical Physics Letters</i> , 2003 , 381, 37-44	2.5	12
53	A direct DFT dynamics study of the photodissociation of triplet acetaldehyde. <i>Chemical Physics Letters</i> , 2003 , 375, 591-597	2.5	12
52	A direct classical trajectory study of the acetone photodissociation on the triplet surface. <i>Journal of Chemical Physics</i> , 2003 , 119, 10618-10625	3.9	12
51	Classical Dynamics Study of the Unimolecular Decomposition of CH ₃ SH ⁺ . <i>Journal of Physical Chemistry A</i> , 1999 , 103, 9783-9793	2.8	11

50	Quasi-classical trajectory study of H ₂ elimination in the photodissociation of difluoroethylenes at 193 nm. <i>Journal of Chemical Physics</i> , 2003 , 118, 6941-6945	3.9	10
49	Dynamical study of the dissociation and elimination channels in the decomposition of methyl nitrite. <i>Journal of Chemical Physics</i> , 1998 , 109, 8907-8919	3.9	10
48	Molecular dynamics simulations for designing biomimetic pores based on internally functionalized self-assembling peptide nanotubes. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 28586-601	3.6	9
47	Chemical Dynamics Study of NO Scattering from a Perfluorinated Self-Assembled Monolayer. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 23817-23830	3.8	9
46	Direct dynamics simulation of the methanethiol cation decomposition. <i>Chemical Physics Letters</i> , 2000 , 324, 88-94	2.5	9
45	Further dynamical studies of the dissociation and elimination reactions of methyl nitrite. <i>Journal of Chemical Physics</i> , 1999 , 111, 10501-10510	3.9	9
44	An investigation of the three oxidation forms of lumiflavin. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1992 , 889		9
43	Photodissociation of acryloyl chloride at 193 nm: interpretation of the product energy distributions, and new elimination pathways. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 5019-26	3.6	8
42	Further studies of the methyl nitrite cis-trans isomerization. <i>Journal of Chemical Physics</i> , 1997 , 107, 5393-5405	3.5	8
41	Rotational distributions of HBr in the photodissociation of vinyl bromide at 193 nm: An investigation by direct quasiclassical trajectory calculations. <i>Chemical Physics Letters</i> , 2006 , 425, 22-27	2.5	8
40	RRKM and direct MP2/6-31G(d,p) quasiclassical trajectory study of the H ₂ elimination in the photodissociation of vinyl chloride at 193 nm. <i>Chemical Physics Letters</i> , 2004 , 396, 442-447	2.5	8
39	Theoretical investigations on the vibronic coupling between the electronic states S ₀ and S ₁ of formic acid including the photodissociation at 248 nm. <i>Chemical Physics Letters</i> , 2005 , 407, 166-170	2.5	8
38	Dynamics of the cis-trans isomerization and ClO dissociation of chlorine nitrite. Classical trajectory and statistical calculations. <i>Physical Chemistry Chemical Physics</i> , 2000 , 2, 5393-5399	3.6	8
37	Intermolecular potentials for simulations of collisions of SiNCS ⁺ and (CH ₃) ₂ SiNCS ⁺ ions with fluorinated self-assembled monolayers. <i>Chemical Physics</i> , 2012 , 399, 193-204	2.3	7
36	Internal energy of HCl upon photolysis of 2-chloropropene at 193 nm investigated with time-resolved Fourier-transform spectroscopy and quasiclassical trajectories. <i>Journal of Chemical Physics</i> , 2008 , 129, 224301	3.9	7
35	Ab initio and RRKM study of the elimination of HF and HCl from chlorofluoroethylene. <i>Chemical Physics Letters</i> , 2007 , 435, 176-181	2.5	7
34	Rate constants and kinetic isotope effects for Cl+CH ₄ -ClH+CH ₃ : a comparison between LSC-IVR and statistical theories. <i>Chemical Physics Letters</i> , 2002 , 360, 59-64	2.5	7
33	Quasiclassical trajectory calculations on the photodissociation of CF ₂ CHCl at 193 nm: product energy distributions for the HF and HCl eliminations. <i>Journal of Chemical Physics</i> , 2005 , 122, 104316	3.9	7

32	Theoretical study of some nitriles: Intramolecular hydrogen bonds and anomeric effect. <i>Journal of Computational Chemistry</i> , 1992 , 13, 722-729	3.5	7
31	Ab initio gradient conformational analysis of polyazocyclohexanes: 1,4-diazocyclohexane, 1,3-diazocyclohexane and 1,3,5-triazocyclohexane. <i>Computational and Theoretical Chemistry</i> , 1990 , 205, 223-234		7
30	AutoMeKin2021: An open-source program for automated reaction discovery. <i>Journal of Computational Chemistry</i> , 2021 , 42, 2036-2048	3.5	7
29	Translational energy distributions in the photodissociation of fluorobenzene. <i>Chemical Physics</i> , 2008 , 349, 219-225	2.3	6
28	Rate constants and isotope effects for the $\text{CH}_3 + \text{H}_2 - \text{pH}_4 + \text{H}$ reaction by an approximate semiclassical initial-value representation method. <i>Chemical Physics Letters</i> , 2001 , 341, 351-357	2.5	6
27	A direct dynamics study of the H_2 elimination from 2,5-dihydrofuran. <i>Journal of Chemical Physics</i> , 2001 , 115, 7872-7880	3.9	6
26	Rotational effects in the unimolecular dissociation of the acetyl radical. <i>Chemical Physics Letters</i> , 2000 , 316, 471-476	2.5	6
25	Classical Trajectory Study of the Cis-Trans Isomerization and F ₂ O Dissociation of FONO. <i>Journal of Physical Chemistry A</i> , 1998 , 102, 8708-8715	2.8	6
24	A molecular mechanics study of conformational trends in simple alcohols and ethers. Part I: Geometric trends. <i>Journal of Computational Chemistry</i> , 1991 , 12, 872-879	3.5	6
23	Unraveling the Factors That Control Soft Landing of Small Silyl Ions on Fluorinated Self-Assembled Monolayers. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 10159-10169	3.8	5
22	Improved United-Atom Models for Perfluorinated Self-Assembled Monolayers. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 3300-3312	3.8	5
21	Anharmonic Quasiclassical Barrier Samplings in Trajectory Calculations and Their Influence on the Computed Product Energy Distributions. <i>Journal of Physical Chemistry A</i> , 2001 , 105, 4808-4813	2.8	5
20	Back to the Coordination Modes of the Thiosemicarbazone Chain: New Insights from Diorganolead(IV) and Lead(II) Derivatives of Isatin-3-thiosemicarbazone. <i>European Journal of Inorganic Chemistry</i> , 2010 , 2010, 4992-5004	2.3	4
19	Conformational analysis of model compounds of vitamin D by theoretical calculations. <i>Journal of Computational Chemistry</i> , 1997 , 18, 1647-1655	3.5	4
18	Rate constants for the $\text{CH}_3\text{O} + \text{NO} - \text{pCH}_3\text{ONO}$ reaction by classical trajectory and canonical variational transition state theory calculations. <i>Journal of Physical Organic Chemistry</i> , 2002 , 15, 123-129	2.1	4
17	Product energy distributions from ethylene photodissociation at 193 nm: a DFT direct classical trajectory study. <i>Chemical Physics Letters</i> , 2003 , 369, 1-7	2.5	4
16	A Theoretical Study of the Dynamics of the $\text{S} + \text{c-C}_3\text{H}$ Reaction. <i>Journal of Physical Chemistry A</i> , 2002 , 106, 8811-8819	2.8	4
15	Unimolecular decomposition of CH_3SH^+ : an ab initio and RRKM study. <i>Computational and Theoretical Chemistry</i> , 2000 , 505, 109-116		4

14	The unimolecular dissociation of the propionyl radical: A classical dynamics study. <i>Journal of Chemical Physics</i> , 2001 , 114, 3546-3553	3.9	4
13	An ab initio gradient study of ethylhydrazine. <i>Computational and Theoretical Chemistry</i> , 1990 , 206, 49-66		4
12	Dinámica de reacciones unimoleculares en fase gas: Desviaciones del comportamiento estadístico. <i>Química Nova</i> , 2002 , 25, 579-588	1.6	4
11	Ab initio and RRKM calculations on the dissociation of the propionyl radical. <i>Journal of Molecular Structure</i> , 2000 , 556, 123-129	3.4	3
10	Complete structural analysis of cyclic polyhalogenated monoterpenes. A force field 2-dimensional NMR study. <i>Journal of Organic Chemistry</i> , 1986 , 51, 4970-4973	4.2	3
9	New Approach for Correcting Noncovalent Interactions in Semiempirical Quantum Mechanical Methods: The Importance of Multiple-Orientation Sampling. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 5556-5567	6.4	3
8	Trajectory dynamics study of collision-induced dissociation of the Ar + CH ₄ reaction at hyperthermal conditions: vibrational excitation and isotope substitution. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 7113-21	2.8	2
7	A statistical study of the methyl nitrite isomerization reaction: inverse secondary isotope effects. <i>Chemical Physics Letters</i> , 1999 , 310, 209-214	2.5	2
6	A theoretical study of 1-amino-3-butene and 3-butene-1-thiol. <i>Structural Chemistry</i> , 1992 , 3, 225-229	1.8	1
5	An ab initio gradient study of trimethylhydrazine. <i>Computational and Theoretical Chemistry</i> , 1989 , 184, 311-322		1
4	Study of the geometric trends and rotational constants of 1-fluoro-2-propanol and 2-fluoropropanol by Ab Initio calculations. <i>Tetrahedron Computer Methodology</i> , 1989 , 2, 85-92		1
3	Relevance of weak intermolecular forces on the supramolecular structure of free or DMSO solvated 5-(4-X-benzylidene)rhodanines (X = F, Cl, Br, I). <i>Journal of Molecular Structure</i> , 2016 , 1120, 100-114	3.4	1
2	The relative position of interacting rings notably changes the nature of the substituent effect. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 12068-12081	3.6	0
1	Vibrational Energy Relaxation of Deuterium Fluoride in <i>n</i> -Dichloromethane: Insights from Different Potentials. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 1277-1289	6.4	0