

Meredith J T Jordan

List of Publications by Year in descending order

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60
papers

2,631
citations

172457

29
h-index

182427

51
g-index

62
all docs

62
docs citations

62
times ranked

1847
citing authors

#	ARTICLE	IF	CITATIONS
1	Polyatomic molecular potential energy surfaces by interpolation in local internal coordinates. <i>Journal of Chemical Physics</i> , 1998, 108, 8302-8316.	3.0	226
2	Convergence of molecular potential energy surfaces by interpolation: Application to the OH+H ₂ →H ₂ O+H reaction. <i>Journal of Chemical Physics</i> , 1995, 102, 5647-5657.	3.0	213
3	Roaming is the dominant mechanism for molecular products in acetaldehyde photodissociation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 12719-12724.	7.1	183
4	Classical trajectory studies of the reaction CH ₄ +H→CH ₃ +H ₂ . <i>Journal of Chemical Physics</i> , 1995, 102, 5669-5682.	3.0	157
5	The utility of higher order derivatives in constructing molecular potential energy surfaces by interpolation. <i>Journal of Chemical Physics</i> , 1995, 103, 9669-9675.	3.0	99
6	Unraveling Environmental Effects on Hydrogen-Bonded Complexes: A Matrix Effects on the Structures and Proton-Stretching Frequencies of Hydrogen-Halide Complexes with Ammonia and Trimethylamine. <i>Journal of the American Chemical Society</i> , 2000, 122, 2101-2115.	13.7	96
7	Photo-Tautomerization of Acetaldehyde to Vinyl Alcohol: A Potential Route to Tropospheric Acids. <i>Science</i> , 2012, 337, 1203-1206.	12.6	93
8	Vibrational spectroscopy of the hydrogen bond: An ab initio quantum-chemical perspective. <i>International Reviews in Physical Chemistry</i> , 1999, 18, 119-162.	2.3	88
9	Molecular potential energy surfaces by interpolation in Cartesian coordinates. <i>Journal of Chemical Physics</i> , 1998, 108, 564-578.	3.0	83
10	An interpolated unrestricted Hartree-Fock potential energy surface for the OH+H ₂ →H ₂ O+H reaction. <i>Journal of Chemical Physics</i> , 1996, 104, 4600-4610.	3.0	69
11	CH ₅ ⁺ : Chemistry's Chameleon Unmasked. <i>Journal of the American Chemical Society</i> , 2005, 127, 4954-4958.	13.7	68
12	A comparative study of anharmonicity and matrix effects on the complexes XH:NH ₃ , X=F, Cl, and Br. <i>Journal of Chemical Physics</i> , 1998, 108, 3205-3212.	3.0	65
13	Vibrational Spectroscopic and NMR Properties of Hydrogen-Bonded Complexes: Do They Tell Us the Same Thing?. <i>Journal of the American Chemical Society</i> , 2000, 122, 4794-4797.	13.7	63
14	Ab initio potential energy surface for the reactions between H ₂ O and H. <i>Journal of Chemical Physics</i> , 2000, 112, 10162-10172.	3.0	62
15	Near-threshold H/D exchange in CD ₃ CHO photodissociation. <i>Nature Chemistry</i> , 2011, 3, 443-448.	13.6	60
16	Vibrational Effects on the F→F Spin-Spin Coupling Constant (2h _J -F) in FHF- and FDF-. <i>Journal of Physical Chemistry A</i> , 2001, 105, 8399-8402.	2.5	58
17	Synthesis and Conformational Analysis of β , γ -Difluoro- α -Amino Acid Derivatives. <i>Chemistry - A European Journal</i> , 2011, 17, 2340-2343.	3.3	51
18	The enantiomers of syn-2,3-difluoro-4-aminobutyric acid elicit opposite responses at the GABA _C receptor. <i>Chemical Communications</i> , 2012, 48, 829-831.	4.1	51

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19	On the Extent of Intramolecular Hydrogen Bonding in Gas-Phase and Hydrated 1,2-Ethandiol. <i>Journal of Physical Chemistry A</i> , 2005, 109, 2971-2977.	2.5	49
20	Phototautomerization of Acetaldehyde to Vinyl Alcohol: A Primary Process in UV-Irradiated Acetaldehyde from 295 to 335 nm. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 3522-3526.	4.6	49
21	Two roaming pathways in the photolysis of CH ₃ CHO between 328 and 308 nm. <i>Chemical Science</i> , 2014, 5, 4633-4638.	7.4	49
22	Stabilization of Zwitterions in Solution: γ -Aminobutyric Acid (GABA). <i>Journal of Physical Chemistry A</i> , 2004, 108, 203-211.	2.5	42
23	Photochemical formation of HCO and CH ₃ on the ground S ₁ (A ¹) state of CH ₃ CHO. <i>Journal of Chemical Physics</i> , 2009, 130, 054310.	3.0	42
24	Photo-tautomerization of acetaldehyde as a photochemical source of formic acid in the troposphere. <i>Nature Communications</i> , 2018, 9, 2584.	12.8	38
25	An ab initio study of anharmonicity and matrix effects on the hydrogen-bonded BrH:NH ₃ complex. <i>Molecular Physics</i> , 1997, 92, 429-439.	1.7	36
26	An ab Initio Study of Anharmonicity and Field Effects in Hydrogen-Bonded Complexes of the Deuterated Analogues of HCl and HBr with NH ₃ and N(CH ₃) ₃ . <i>Journal of Physical Chemistry A</i> , 2001, 105, 3371-3378.	2.5	34
27	A classical trajectory study of the photodissociation of T ₁ acetaldehyde: The transition from impulsive to statistical dynamics. <i>Journal of Chemical Physics</i> , 2006, 124, 044302.	3.0	34
28	Variational transition state theory: a simple model for dissociation and recombination reactions of small species. <i>The Journal of Physical Chemistry</i> , 1991, 95, 8685-8694.	2.9	31
29	Relating Environmental Effects and Structures, IR, and NMR Properties of Hydrogen-Bonded Complexes: A CH:Pyridine. <i>Journal of Physical Chemistry A</i> , 2001, 105, 5442-5449.	2.5	31
30	To What Extent Do External Fields and Vibrational and Isotopic Effects Influence NMR Coupling Constants Across Hydrogen Bonds? Two-Bond ¹⁵ N Spin-Spin Coupling Constants (2hJ _{Cl-N}) in Model CH:NH ₃ Complexes. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5385-5392.	2.5	29
31	A Phase Space Theory for Roaming Reactions. <i>Journal of Physical Chemistry A</i> , 2013, 117, 7631-7642.	2.5	28
32	Oxo-bridged isomers of aza-trishomocubane sigma (σ) receptor ligands: Synthesis, in vitro binding, and molecular modeling. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2010, 20, 145-148.	2.2	27
33	The energy dependence of CO(v ₁) produced from H ₂ CO via the transition state, roaming, and triple fragmentation channels. <i>Journal of Chemical Physics</i> , 2017, 147, 013935.	3.0	27
34	Rotational resonances in the H ₂ CO roaming reaction are revealed by detailed correlations. <i>Science</i> , 2020, 369, 1592-1596.	12.6	24
35	Enantiomers of cis-constrained and flexible 2-substituted GABA analogues exert opposite effects at recombinant GABAC receptors. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 447-455.	3.0	23
36	Roaming Reaction Pathways Along Excited States. <i>Science</i> , 2012, 335, 1054-1055.	12.6	22

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37	Experimental and Theoretical Investigation of Triple Fragmentation in the Photodissociation Dynamics of H_2CO . <i>Journal of Physical Chemistry A</i> , 2013, 117, 12091-12103.	2.5	22
38	Can Proton-Shared or Ion-Pair $\text{N}^+\text{H}\cdots\text{N}$ Hydrogen Bonds Be Produced in Uncharged Complexes? A Systematic ab Initio Study of the Structures and Selected NMR and IR Properties of Complexes with $\text{N}^+\text{H}\cdots\text{N}$ Hydrogen Bonds. <i>Journal of Physical Chemistry A</i> , 2001, 105, 10906-10914.	2.5	21
39	Stabilization of Zwitterions in Solution: γ -GABA Analogues. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4195-4201.	2.5	21
40	Dynamics and quantum yields of $\text{H}_2 + \text{CH}_2\text{CO}$ as a primary photolysis channel in CH_3CHO . <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 14284-14295.	2.8	16
41	Infrared Spectra of Gas-Phase 1- and 2-Propenol Isomers. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3679-3688.	2.5	15
42	Efficiency considerations in the construction of interpolated potential energy surfaces for the calculation of quantum observables by diffusion Monte Carlo. <i>Journal of Chemical Physics</i> , 2004, 121, 9844-9854.	3.0	14
43	Zero-point energy conservation in classical trajectory simulations: Application to H_2CO . <i>Journal of Chemical Physics</i> , 2018, 148, 194113.	3.0	13
44	Calculation of the photodetachment spectrum for H_3O^- . <i>Journal of the Chemical Society, Faraday Transactions</i> , 1997, 93, 747-753.	1.7	12
45	Structural Effects on the Norrish Type I $\text{C}=\text{O}$ Bond Cleavage of Tropospherically Important Carbonyls. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10381-10396.	2.5	11
46	Quantum effects and anharmonicity in the $\text{H}_2\text{-Li}^+$ -benzene complex: A model for hydrogen storage materials. <i>Journal of Chemical Physics</i> , 2013, 139, 234305.	3.0	10
47	A multi-agent quantum Monte Carlo model for charge transport: Application to organic field-effect transistors. <i>Journal of Chemical Physics</i> , 2015, 143, 044114.	3.0	10
48	Path integral Monte Carlo simulations of H_2 adsorbed to lithium-doped benzene: A model for hydrogen storage materials. <i>Journal of Chemical Physics</i> , 2015, 143, 194302.	3.0	10
49	Stabilization of Zwitterions in Solution: α -Phosphinic and Phosphonic Acid GABA Analogues. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8398-8409.	2.5	8
50	Method and basis set dependence of anharmonic ground state nuclear wave functions and zero-point energies: Application to SSSH. <i>Journal of Chemical Physics</i> , 2010, 132, 054105.	3.0	8
51	Classical and approximate quantum investigations of vibrational energy transfer in S1 p-difluorobenzene. <i>Journal of Chemical Physics</i> , 1997, 106, 5439-5453.	3.0	7
52	"Plug-and-Play" potentials: Investigating quantum effects in $(\text{H}_2)_2\text{-Li}^+$ -benzene. <i>Journal of Chemical Physics</i> , 2015, 143, 074311.	3.0	7
53	An assessment of the tropospherically accessible photo-initiated ground state chemistry of organic carbonyls. <i>Atmospheric Chemistry and Physics</i> , 2022, 22, 929-949.	4.9	6
54	H_2 Adsorption in a Porous Crystal: Accurate First-Principles Quantum Simulation. <i>Journal of Physical Chemistry A</i> , 2015, 119, 12166-12181.	2.5	5

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55	Generating accurate dipole moment surfaces using modified Shepard interpolation. Journal of Chemical Physics, 2014, 140, 204107.	3.0	4
56	Quantum Effects in Loosely Bound Complexes. ACS Symposium Series, 2006, , 101-140.	0.5	3
57	Modeling molecular response in uniform and non-uniform electric fields. Journal of Chemical Physics, 2013, 138, 054111.	3.0	3
58	Path integrals with higher order actions: Application to realistic chemical systems. Journal of Chemical Physics, 2018, 148, 074106.	3.0	3
59	The proton affinity of methane and its isotopologues: A test for theory. Chemical Physics Letters, 2018, 708, 216-221.	2.6	1
60	Chemistry at the threshold: Unexpected products, unusual mechanisms, and generally weird things that happen near the energetic threshold for a reaction. , 2011, , .		0