Meredith J T Jordan

List of Publications by Year
in descending order

60	2,631	172207	182168
papers	citations	29 h-index	51 g-index

62	62	62	1847
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Polyatomic molecular potential energy surfaces by interpolation in local internal coordinates. Journal of Chemical Physics, 1998, 108, 8302-8316.	1.2	226
2	Convergence of molecular potential energy surfaces by interpolation: Application to the OH+H2â†'H2O+H reaction. Journal of Chemical Physics, 1995, 102, 5647-5657.	1.2	213
3	Roaming is the dominant mechanism for molecular products in acetaldehyde photodissociation. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 12719-12724.	3.3	183
4	Classical trajectory studies of the reaction CH4+Hâ†'CH3+H2. Journal of Chemical Physics, 1995, 102, 5669-5682.	1.2	157
5	The utility of higher order derivatives in constructing molecular potential energy surfaces by interpolation. Journal of Chemical Physics, 1995, 103, 9669-9675.	1.2	99
6	Unraveling Environmental Effects on Hydrogen-Bonded Complexes:Â Matrix Effects on the Structures and Proton-Stretching Frequencies of Hydrogenâ^'Halide Complexes with Ammonia and Trimethylamine. Journal of the American Chemical Society, 2000, 122, 2101-2115.	6.6	96
7	Photo-Tautomerization of Acetaldehyde to Vinyl Alcohol: A Potential Route to Tropospheric Acids. Science, 2012, 337, 1203-1206.	6.0	93
8	Vibrational spectroscopy of the hydrogen bond: An ab initio quantum-chemical perspective. International Reviews in Physical Chemistry, 1999, 18, 119-162.	0.9	88
9	Molecular potential energy surfaces by interpolation in Cartesian coordinates. Journal of Chemical Physics, 1998, 108, 564-578.	1.2	83
10	An interpolated unrestricted Hartreeâ€"Fock potential energy surface for the OH+H2â†'H2O+H reaction. Journal of Chemical Physics, 1996, 104, 4600-4610.	1.2	69
11	CH5+:Â Chemistry's Chameleon Unmasked. Journal of the American Chemical Society, 2005, 127, 4954-4958.	6.6	68
12	A comparative study of anharmonicity and matrix effects on the complexes XH:NH3, X=F, Cl, and Br. Journal of Chemical Physics, 1998, 108, 3205-3212.	1.2	65
13	Vibrational Spectroscopic and NMR Properties of Hydrogen-Bonded Complexes:Â Do They Tell Us the Same Thing?. Journal of the American Chemical Society, 2000, 122, 4794-4797.	6.6	63
14	Ab initio potential energy surface for the reactions between H2O and H. Journal of Chemical Physics, 2000, 112, 10162-10172.	1.2	62
15	Near-threshold H/D exchange in CD3CHO photodissociation. Nature Chemistry, 2011, 3, 443-448.	6.6	60
16	Vibrational Effects on the Fâ^'F Spinâ^'Spin Coupling Constant (2hJF-F) in FHF- and FDF-. Journal of Physical Chemistry A, 2001, 105, 8399-8402.	1.1	58
17	Synthesis and Conformational Analysis of Î±,Î²â€Difluoroâ€Î³â€amino Acid Derivatives. Chemistry - A European Journal, 2011, 17, 2340-2343.	1.7	51
18	The enantiomers of syn-2,3-difluoro-4-aminobutyric acid elicit opposite responses at the GABA_Creceptor. Chemical Communications, 2012, 48, 829-831.	2.2	51

#	Article	IF	Citations
19	On the Extent of Intramolecular Hydrogen Bonding in Gas-Phase and Hydrated 1,2-Ethanediol. Journal of Physical Chemistry A, 2005, 109, 2971-2977.	1.1	49
20	Phototautomerization of Acetaldehyde to Vinyl Alcohol: A Primary Process in UV-Irradiated Acetaldehyde from 295 to 335 nm. Journal of Physical Chemistry Letters, 2012, 3, 3522-3526.	2.1	49
21	Two roaming pathways in the photolysis of CH₃CHO between 328 and 308 nm. Chemical Science, 2014, 5, 4633-4638.	3.7	49
22	Stabilization of Zwitterions in Solution:â€‰Î³-Aminobutyric Acid (GABA). Journal of Physical Chemistry A, 2004, 108, 203-211.	1.1	42
23	Photochemical formation of HCO and CH3 on the ground Sâ€˜(A1â€²) state of CH3CHO. Journal of Chemical Physics, 2009, 130, 054310.	1.2	42
24	Photo-tautomerization of acetaldehyde as a photochemical source of formic acid in the troposphere. Nature Communications, 2018, 9, 2584.	5.8	38
25	An ab initio study of anharmonicity and matrix effects on the hydrogen-bonded BrH:NH3 complex. Molecular Physics, 1997, 92, 429-439.	0.8	36
26	An ab Initio Study of Anharmonicity and Field Effects in Hydrogen-Bonded Complexes of the Deuterated Analogues of HCl and HBr with NH3and N(CH3)3. Journal of Physical Chemistry A, 2001, 105, 3371-3378.	1.1	34
27	A classical trajectory study of the photodissociation of T1 acetaldehyde: The transition from impulsive to statistical dynamics. Journal of Chemical Physics, 2006, 124, 044302.	1.2	34
28	Variational transition state theory: a simple model for dissociation and recombination reactions of small species. The Journal of Physical Chemistry, 1991, 95, 8685-8694.	2.9	31
29	Relating Environmental Effects and Structures, IR, and NMR Properties of Hydrogen-Bonded Complexes:Â ClH:Pyridine. Journal of Physical Chemistry A, 2001, 105, 5442-5449.	1.1	31
30	To What Extent Do External Fields and Vibrational and Isotopic Effects Influence NMR Coupling Constants Across Hydrogen Bonds? Two-Bond Clâ^'N Spinâ^'Spin Coupling Constants (2hJCl-N) in Model ClH:NH3Complexes. Journal of Physical Chemistry A, 2002, 106, 5385-5392.	1.1	29
31	A Phase Space Theory for Roaming Reactions. Journal of Physical Chemistry A, 2013, 117, 7631-7642.	1.1	28
32	Oxo-bridged isomers of aza-trishomocubane sigma (Ï*f*) receptor ligands: Synthesis, in vitro binding, and molecular modeling. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 145-148.	1.0	27
33	The energy dependence of CO(v,J) produced from H2CO via the transition state, roaming, and triple fragmentation channels. Journal of Chemical Physics, 2017, 147, 013935.	1.2	27
34	Rotational resonances in the H ₂ CO roaming reaction are revealed by detailed correlations. Science, 2020, 369, 1592-1596.	6.0	24
35	Enantiomers of cis-constrained and flexible 2-substituted GABA analogues exert opposite effects at recombinant GABAC receptors. Bioorganic and Medicinal Chemistry, 2006, 14, 447-455.	1.4	23
36	Roaming Reaction Pathways Along Excited States. Science, 2012, 335, 1054-1055.	6.0	22

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37	Experimental and Theoretical Investigation of Triple Fragmentation in the Photodissociation Dynamics of H₂CO. Journal of Physical Chemistry A, 2013, 117, 12091-12103.	1.1	22
38	Can Proton-Shared or Ion-Pair Nâ^Hâ^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 Nâ^Hâ^N Hydrogen Bonds. Journal of Physical Chemistry A, 2001, 105, 10906-10914.	1.1	21
39	Stabilization of Zwitterions in Solution:Â GABA Analogues. Journal of Physical Chemistry A, 2005, 109, 4195-4201.	1.1	21
40	Dynamics and quantum yields of H₂ + CH₂CO as a primary photolysis channel in CH₃CHO. Physical Chemistry Chemical Physics, 2019, 21, 14284-14295.	1.3	16
41	Infrared Spectra of Gas-Phase 1- and 2-Propenol Isomers. Journal of Physical Chemistry A, 2017, 121, 3679-3688.	1.1	15
42	Efficiency considerations in the construction of interpolated potential energy surfaces for the calculation of quantum observables by diffusion Monte Carlo. Journal of Chemical Physics, 2004, 121, 9844-9854.	1.2	14
43	Zero-point energy conservation in classical trajectory simulations: Application to H2CO. Journal of Chemical Physics, 2018, 148, 194113.	1.2	13
44	Calculation of the photodetachment spectrum for H3O-. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 747-753.	1.7	12
45	Structural Effects on the Norrish Type I Î±-Bond Cleavage of Tropospherically Important Carbonyls. Journal of Physical Chemistry A, 2019, 123, 10381-10396.	1.1	11
46	Quantum effects and anharmonicity in the H2-Li+-benzene complex: A model for hydrogen storage materials. Journal of Chemical Physics, 2013, 139, 234305.	1.2	10
47	A multi-agent quantum Monte Carlo model for charge transport: Application to organic field-effect transistors. Journal of Chemical Physics, 2015, 143, 044114.	1.2	10
48	Path integral Monte Carlo simulations of H2 adsorbed to lithium-doped benzene: A model for hydrogen storage materials. Journal of Chemical Physics, 2015, 143, 194302.	1.2	10
49	Stabilization of Zwitterions in Solution:â€‰ Phosphinic and Phosphonic Acid GABA Analogues. Journal of Physical Chemistry A, 2005, 109, 8398-8409.	1.1	8
50	Method and basis set dependence of anharmonic ground state nuclear wave functions and zero-point energies: Application to SSSH. Journal of Chemical Physics, 2010, 132, 054105.	1.2	8
51	Classical and approximate quantum investigations of vibrational energy transfer in S1 p-difluorobenzene. Journal of Chemical Physics, 1997, 106, 5439-5453.	1.2	7
52	â€œPlug-and-Playâ€•potentials: Investigating quantum effects in (H2)2â€“Li+â€“benzene. Journal of Chemical Physics, 2015, 143, 074311.	1.2	7
53	An assessment of the tropospherically accessible photo-initiated ground state chemistry of organic carbonyls. Atmospheric Chemistry and Physics, 2022, 22, 929-949.	1.9	6
54	H₂ Adsorption in a Porous Crystal: Accurate First-Principles Quantum Simulation. Journal of Physical Chemistry A, 2015, 119, 12166-12181.	1.1	5

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55	Generating accurate dipole moment surfaces using modified Shepard interpolation. Journal of Chemical Physics, 2014, 140, 204107.	1.2	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.	1.2	3
58	Path integrals with higher order actions: Application to realistic chemical systems. Journal of Chemical Physics, 2018, 148, 074106.	1.2	3
59	The proton affinity of methane and its isotopologues: A test for theory. Chemical Physics Letters, 2018, 708, 216-221.	1.2	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