Ryan P A Bettens

List of Publications by Year
in descending order

45 papers	1,772 citations	279701 23 h-index	265120 42 g-index
47 all docs	47 docs citations	47 times ranked	1456 citing authors

#	Article	IF	Citations
1	Energy-Based Molecular Fragmentation Methods. Chemical Reviews, 2015, 115, 5607-5642.	23.0	240
2	Learning to interpolate molecular potential energy surfaces with confidence: A Bayesian approach. Journal of Chemical Physics, 1999, 111, 816-826.	1.2	212
3	A fast scan submillimeter spectroscopic technique. Review of Scientific Instruments, 1997, 68, 1675-1683.	0.6	146
4	A New Algorithm for Molecular Fragmentation in Quantum Chemical Calculations. Journal of Physical Chemistry A, 2006, 110, 8777-8785.	1.1	111
5	Combined Fragmentation Method: A Simple Method for Fragmentation of Large Molecules. Journal of Chemical Theory and Computation, 2012, 8, 469-478.	2.3	81
6	The Combined Fragmentation and Systematic Molecular Fragmentation Methods. Accounts of Chemical Research, 2014, 47, 2776-2785.	7.6	69
7	Ab initio potential energy surface for the reactions between H2O and H. Journal of Chemical Physics, 2000, 112, 10162-10172.	1.2	62
8	Modelling Water: A Lifetime Enigma. Chimia, 2015, 69, 104.	0.3	57
9	Prevalence of the thioamide {â‹¯Hâ€“Nâ€“C=S}2 synthonâ€”solid-state (X-ray crystallography), solution (NMR) and gas-phase (theoretical) structures of O-methyl-N-aryl-thiocarbamides. CrystEngComm, 2005, 7, 682.	1.3	56
10	Co-crystallisation of 2,2â€²-dithiodibenzoic acid with the isomeric n-pyridinealdazines, n = 2, 3 and 4: supramolecular polymers and the influence of steric factors upon aggregation patterns. CrystEngComm, 2008, 10, 879.	1.3	48
11	Trouble with the Many-Body Expansion. Journal of Chemical Theory and Computation, 2014, 10, 3699-3707.	2.3	48
12	Interpolated potential energy surface and reaction dynamics for O(3P)+H3+(1A1â€²) and OH+(3Î£â¯)+H2(1Î£g+). Journal of Chemical Physics, 1999, 111, 6322-6332.	1.2	43
13	First Principles NMR Calculations by Fragmentation. Journal of Physical Chemistry A, 2007, 111, 5111-5115.	1.1	43
14	Potential energy surfaces and dynamics for the reactions between C(3P) and H3+(1A1â€²). Journal of Chemical Physics, 1998, 108, 2424-2433.	1.2	42
15	The Microwave Spectrum, Structure, and Ring-Puckering of the Cyclic Dipeptide Diketopiperazine. Journal of the American Chemical Society, 2000, 122, 5856-5860.	6.6	42
16	Interpolated potential energy surface and dynamics for the reactions between N(4S) and H3+(1A1â€²). Journal of Chemical Physics, 1998, 109, 9728-9736.	1.2	41
17	Many-Body Basis Set Superposition Effect. Journal of Chemical Theory and Computation, 2015, 11, 5132-5143.	2.3	38
18	Aryl-substituents moderate the nature of hydrogen bonds, Nâ€“Hâ‹¯N versus Nâ€“Hâ‹¯O, leading to supramolecular chains in the crystal structures of N-arylamino 1,2,3-triazole esters. CrystEngComm, 2013, 15, 4917.	1.3	37

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19	Accurately Reproducing Ab Initio Electrostatic Potentials with Multipoles and Fragmentation. Journal of Physical Chemistry A, 2009, 113, 10527-10533.	1.1	34
20	Ab initio NMR chemical-shift calculations based on the combined fragmentation method. Physical Chemistry Chemical Physics, 2013, 15, 7541.	1.3	30
21	When are Many-Body Effects Significant?. Journal of Chemical Theory and Computation, 2016, 12, 5860-5867.	2.3	28
22	A Microwave Study and Centrifugal Distortion Analysis of the Pyrrole-CO Complex. The Journal of Physical Chemistry, 1994, 98, 4551-4563.	2.9	27
23	The influence of crystal packing effects upon the molecular structures of Ph3Sn(CH2)nSnPh3, n = 1 to 8, as determined by X-ray crystallography and DFT molecular orbital calculations. Supramolecular aggregation patterns sustained by Câ€“Hâ‹Ï€ interactions. CrystEngComm, 2009, 11, 1362.	1.3	26
24	On the accurate reproduction of ab initio interaction energies between an enzyme and substrate. Chemical Physics Letters, 2007, 449, 341-346.	1.2	25
25	Millimeter and submillimeter wave rotational spectrum of pyridine in the ground and excited vibrational states. Journal of Molecular Spectroscopy, 2005, 232, 61-65.	0.4	21
26	The dipole moment of C3H2. Monthly Notices of the Royal Astronomical Society, 1987, 227, 19P-20P.	1.6	20
27	The Millimeterâ€•and Submillimeterâ€Wave Spectrum of the transâ€trans Conformer of Diethyl Ether (C 2 H) Tj ETQq1 1 0.784314 rgBT	3.0	19
28	Ion-molecule chemistry of HnC3O+, C3O2+, and C3O+. The Journal of Physical Chemistry, 1993, 97, 13673-13676.	2.9	18
29	Potential energy surface for the reactions BeH2+HBeH+H2. Physical Chemistry Chemical Physics, 1999, 1, 939-945.	1.3	17
30	Interpolated potential-energy surface and reaction dynamics for BH++H2. Journal of Chemical Physics, 2001, 114, 10711-10716.	1.2	14
31	Bound State Potential Energy Surface Construction:Â Ab Initio Zero-Point Energies and Vibrationally Averaged Rotational Constants. Journal of the American Chemical Society, 2003, 125, 584-587.	6.6	14
32	The ion chemistry of Formula in dense interstellar clouds: an experimental study. Monthly Notices of the Royal Astronomical Society, 1993, 264, 862-864.	1.6	11
33	Distributed Multipoles and Energies of Flexible Molecules. Journal of Chemical Theory and Computation, 2011, 7, 921-930.	2.3	8
34	Millimeter wave measurement and assignment of the rotational spectrum of aniline. Journal of Molecular Spectroscopy, 2005, 229, 54-56.	0.4	7
35	Approximating Coupled Cluster Level Vibrational Frequencies with Composite Methods. Journal of Physical Chemistry A, 2006, 110, 2796-2800.	1.1	6
36	The Conformers of Hydroxyacetaldehyde. Journal of Physical Chemistry A, 2007, 111, 5081-5085.	1.1	6

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37	Millimeter wave measurement and assignment of the rotational spectrum of 2-aminopyridine. Journal of Molecular Spectroscopy, 2004, 223, 73-79.	0.4	5
38	Multiple surface long-range interaction potentials between C ([sup 3]P[sub j]) and closed-shell molecules. Journal of Chemical Physics, 2002, 116, 101.	1.2	4
39	Capture rates for collisions of C (3Pj) and Ge (1S0) with unsaturated hydrocarbons. Journal of Chemical Physics, 2001, 114, 10342-10354.	1.2	3
40	Rate coefficient for the important interstellar radiative association between and H2 from classical reaction dynamics. Chemical Physics Letters, 2013, 555, 247-251.	1.2	3
41	Modelling potential energy surfaces for small clusters using Shepard interpolation with Gaussian-form nodal functions. Physical Chemistry Chemical Physics, 2019, 21, 4513-4522.	1.3	3
42	Comparison of Fundamental and Harmonic Frequencies of First-Row Closed-Shell Diatomics Calculated Using Full ab Initio Methods and Composite Methods. Journal of Physical Chemistry A, 2004, 108, 1826-1829.	1.1	2
43	Comparing Vibrationally Averaged Nuclear Shielding Constants by Quantum Diffusion Monte Carlo and Second-Order Perturbation Theory. Journal of Physical Chemistry A, 2016, 120, 1297-1306.	1.1	1
44	Modeling the Maillard Reaction: Schiff Base Formation. Annals of the New York Academy of Sciences, 2005, 1043, 890-890.	1.8	0
45	Monte Carlo simulation of several biologically relevant molecules and zwitterions in water. Chemical Physics Letters, 2012, 524, 90-95.	1.2	0