# Ryan P A Bettens

List of Publications by Year
in descending order



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|---|---|---|---|
| 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 | 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 |
| 2 | When are Many-Body Effects Significant?. Journal of Chemical Theory and Computation, 2016, 12, 5860-5867. | 2.3 | 28 |
| 3 | 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 |
| 4 | Energy-Based Molecular Fragmentation Methods. Chemical Reviews, 2015, 115, 5607-5642. | 23.0 | 240 |
| 5 | Many-Body Basis Set Superposition Effect. Journal of Chemical Theory and Computation, 2015, 11, 5132-5143. | 2.3 | 38 |
| 6 | Modelling Water: A Lifetime Enigma. Chimia, 2015, 69, 104. | 0.3 | 57 |
| 7 | Trouble with the Many-Body Expansion. Journal of Chemical Theory and Computation, 2014, 10, 3699-3707. | 2.3 | 48 |
| 8 | The Combined Fragmentation and Systematic Molecular Fragmentation Methods. Accounts of Chemical Research, 2014, 47, 2776-2785. | 7.6 | 69 |
| 9 | 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 |
| 10 | Ab initio NMR chemical-shift calculations based on the combined fragmentation method. Physical Chemistry Chemical Physics, 2013, 15, 7541. | 1.3 | 30 |
| 11 | 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 |
| 12 | Combined Fragmentation Method: A Simple Method for Fragmentation of Large Molecules. Journal of Chemical Theory and Computation, 2012, 8, 469-478. | 2.3 | 81 |
| 13 | Monte Carlo simulation of several biologically relevant molecules and zwitterions in water. Chemical Physics Letters, 2012, 524, 90-95. | 1.2 | 0 |
| 14 | Distributed Multipoles and Energies of Flexible Molecules. Journal of Chemical Theory and Computation, 2011, 7, 921-930. | 2.3 | 8 |
| 15 | Accurately Reproducing Ab Initio Electrostatic Potentials with Multipoles and Fragmentation. Journal of Physical Chemistry A, 2009, 113, 10527-10533. | 1.1 | 34 |
| 16 | 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 |
| 17 | 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 |
| 18 | First Principles NMR Calculations by Fragmentation. Journal of Physical Chemistry A, 2007, 111, 5111-5115. | 1.1 | 43 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | The Conformers of Hydroxyacetaldehyde. Journal of Physical Chemistry A, 2007, 111, 5081-5085. | 1.1 | 6 |
| 20 | On the accurate reproduction of ab initio interaction energies between an enzyme and substrate. Chemical Physics Letters, 2007, 449, 341-346. | 1.2 | 25 |
| 21 | Approximating Coupled Cluster Level Vibrational Frequencies with Composite Methods. Journal of Physical Chemistry A, 2006, 110, 2796-2800. | 1.1 | 6 |
| 22 | A New Algorithm for Molecular Fragmentation in Quantum Chemical Calculations. Journal of Physical Chemistry A, 2006, 110, 8777-8785. | 1.1 | 111 |
| 23 | Millimeter wave measurement and assignment of the rotational spectrum of aniline. Journal of Molecular Spectroscopy, 2005, 229, 54-56. | 0.4 | 7 |
| 24 | 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 |
| 25 | Modeling the Maillard Reaction: Schiff Base Formation. Annals of the New York Academy of Sciences, 2005, 1043, 890-890. | 1.8 | 0 |
| 26 | Prevalence of the thioamide {â‹¯Hâ€“Nâ€“Cî€¶}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 |
| 27 | Millimeter wave measurement and assignment of the rotational spectrum of 2-aminopyridine. Journal of Molecular Spectroscopy, 2004, 223, 73-79. | 0.4 | 5 |
| 28 | 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 |
| 29 | 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 |
| 30 | The Millimeterâ€•and Submillimeterâ€Wave Spectrum of the transâ€trans Conformer of Diethyl Ether (C 2 H) Tj ETQq0 0 0 rgBT /Overlo | 3.0 | 19 |
| 31 | 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 |
| 32 | Capture rates for collisions of C (3Pj) and Ge (1S0) with unsaturated hydrocarbons. Journal of Chemical Physics, 2001, 114, 10342-10354. | 1.2 | 3 |
| 33 | Interpolated potential-energy surface and reaction dynamics for BH++H2. Journal of Chemical Physics, 2001, 114, 10711-10716. | 1.2 | 14 |
| 34 | Ab initio potential energy surface for the reactions between H2O and H. Journal of Chemical Physics, 2000, 112, 10162-10172. | 1.2 | 62 |
| 35 | 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 |
| 36 | Learning to interpolate molecular potential energy surfaces with confidence: A Bayesian approach. Journal of Chemical Physics, 1999, 111, 816-826. | 1.2 | 212 |

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|---|---|---|---|
| 37 | 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 |
| 38 | Potential energy surface for the reactions BeH2+HBeH+H2. Physical Chemistry Chemical Physics, 1999, 1, 939-945. | 1.3 | 17 |
| 39 | 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 |
| 40 | 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 |
| 41 | A fast scan submillimeter spectroscopic technique. Review of Scientific Instruments, 1997, 68, 1675-1683. | 0.6 | 146 |
| 42 | A Microwave Study and Centrifugal Distortion Analysis of the Pyrrole-CO Complex. The Journal of Physical Chemistry, 1994, 98, 4551-4563. | 2.9 | 27 |
| 43 | 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 |
| 44 | Ion-molecule chemistry of HnC3O+, C3O2+, and C3O+. The Journal of Physical Chemistry, 1993, 97, 13673-13676. | 2.9 | 18 |
| 45 | The dipole moment of C3H2. Monthly Notices of the Royal Astronomical Society, 1987, 227, 19P-20P. | 1.6 | 20 |