# James J P Stewart

## List of Publications by Year in Descending Order



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|---|---|---|---|
| 30 papers | 28,323 citations | 21 h-index | 30 g-index |
| 30 ext. papers | 29,460 ext. citations | 3.4 avg, IF | 7.64 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 30 | An examination of the nature of localized molecular orbitals and their value in understanding various phenomena that occur in organic chemistry. *Journal of Molecular Modeling*, **2018**, 25, 7 | 2 | 8 |
| 29 | An investigation into the applicability of the semiempirical method PM7 for modeling the catalytic mechanism in the enzyme chymotrypsin. *Journal of Molecular Modeling*, **2017**, 23, 154 | 2 | 22 |
| 28 | A comparison of X-ray and calculated structures of the enzyme MTH1. *Journal of Molecular Modeling*, **2016**, 22, 168 | 2 | 10 |
| 27 | A method for predicting individual residue contributions to enzyme specificity and binding-site energies, and its application to MTH1. *Journal of Molecular Modeling*, **2016**, 22, 259 | 2 | 8 |
| 26 | Insights into colour-tuning of chlorophyll optical response in green plants. *Physical Chemistry Chemical Physics*, **2015**, 17, 26599-606 | 3.6 | 37 |
| 25 | Accuracy issues involved in modeling in vivo protein structures using PM7. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 1427-35 | 4.2 | 15 |
| 24 | Standards-based curation of a decade-old digital repository dataset of molecular information. *Journal of Cheminformatics*, **2015**, 7, 43 | 8.6 | 6 |
| 23 | An approach to creating a more realistic working model from a protein data bank entry. *Journal of Molecular Modeling*, **2015**, 21, 3 | 2 | 16 |
| 22 | Self-consistent field convergence for proteins: a comparison of full and localized-molecular-orbital schemes. *Journal of Molecular Modeling*, **2014**, 20, 2159 | 2 | 12 |
| 21 | High-Throughput Calculations of Molecular Properties in the MedeA Environment: Accuracy of PM7 in Predicting Vibrational Frequencies, Ideal Gas Entropies, Heat Capacities, and Gibbs Free Energies of Organic Molecules. *Journal of Chemical & Engineering Data*, **2014**, 59, 3136-3143 | 2.8 | 21 |
| 20 | Sparkle/PM7 Lanthanide Parameters for the Modeling of Complexes and Materials. *Journal of Chemical Theory and Computation*, **2013**, 9, 3333-3341 | 6.4 | 86 |
| 19 | Optimization of parameters for semiempirical methods VI: more modifications to the NDDO approximations and re-optimization of parameters. *Journal of Molecular Modeling*, **2013**, 19, 1-32 | 2 | 1126 |
| 18 | MNDO-Like Semiempirical Molecular Orbital Theory and Its Application to Large Systems **2011**, 259-286 | | 18 |
| 17 | Application of the PM6 method to modeling proteins. *Journal of Molecular Modeling*, **2009**, 15, 765-805 | 2 | 235 |
| 16 | Application of the PM6 method to modeling the solid state. *Journal of Molecular Modeling*, **2008**, 14, 499-535 | 2 | 125 |
| 15 | Optimization of parameters for semiempirical methods V: modification of NDDO approximations and application to 70 elements. *Journal of Molecular Modeling*, **2007**, 13, 1173-213 | 2 | 2577 |
| 14 | RM1: a reparameterization of AM1 for H, C, N, O, P, S, F, Cl, Br, and I. *Journal of Computational Chemistry*, **2006**, 27, 1101-11 | 3.5 | 571 |

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| 13 | Use of Semiempirical Methods for Detecting Anomalies in Reported Enthalpies of Formation of Organic Compounds. *Journal of Physical and Chemical Reference Data*, **2004**, 33, 713-724 | 4.3 | 24 |
| 12 | Comparison of the accuracy of semiempirical and some DFT methods for predicting heats of formation. *Journal of Molecular Modeling*, **2004**, 10, 6-12 | 2 | 95 |
| 11 | Optimization of parameters for semiempirical methods IV: extension of MNDO, AM1, and PM3 to more main group elements. *Journal of Molecular Modeling*, **2004**, 10, 155-64 | 2 | 213 |
| 10 | Application of localized molecular orbitals to the solution of semiempirical self-consistent field equations. *International Journal of Quantum Chemistry*, **1996**, 58, 133-146 | 2.1 | 303 |
| 9 | Optimization of parameters for semiempirical methods. III Extension of PM3 to Be, Mg, Zn, Ga, Ge, As, Se, Cd, In, Sn, Sb, Te, Hg, Tl, Pb, and Bi. *Journal of Computational Chemistry*, **1991**, 12, 320-341 | 3.5 | 553 |
| 8 | Optimization of parameters for semiempirical methods I. Method. *Journal of Computational Chemistry*, **1989**, 10, 209-220 | 3.5 | 6553 |
| 7 | Optimization of parameters for semiempirical methods II. Applications. *Journal of Computational Chemistry*, **1989**, 10, 221-264 | 3.5 | 3335 |
| 6 | X-Ray crystallographic and NMR evidence for a uniquely strong OH ? N hydrogen bond in the solid state and solution. *Journal of the Chemical Society Chemical Communications*, **1989**, 1722 | | 21 |
| 5 | Calculation of polymer elastic moduli using semiempirical methods. *International Journal of Quantum Chemistry*, **1986**, 30, 529-540 | 2.1 | 19 |
| 4 | Development and use of quantum mechanical molecular models. 76. AM1: a new general purpose quantum mechanical molecular model. *Journal of the American Chemical Society*, **1985**, 107, 3902-3909 | 16.4 | 12010 |
| 3 | Location of transition states in reaction mechanisms. *Journal of the Chemical Society, Faraday Transactions 2*, **1984**, 80, 227 | | 237 |
| 2 | A new rapid method for orbital localisation. *Journal of the Chemical Society, Faraday Transactions 2*, **1982**, 78, 285 | | 35 |
| 1 | Cluster model for solids. *Journal of the Chemical Society, Faraday Transactions 2*, **1980**, 76, 520 | | 32 |