# Emilio Martinez-Nunez

## List of Publications by Year in Descending Order



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| 129 papers | 28,115 citations | 28 h-index | 137 g-index |
| 137 ext. papers | 29,393 ext. citations | 3.6 avg, IF | 7.66 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 129 | Photoisomerization of Linear and Stacked Isomers of a Charged Styryl Dye: A Tandem Ion Mobility Study. *Journal of the American Society for Mass Spectrometry*, **2021**, 32, 2842-2851 | 3.5 | |
| 128 | ChemDyME: Kinetically Steered, Automated Mechanism Generation through Combined Molecular Dynamics and Master Equation Calculations. *Journal of Chemical Theory and Computation*, **2021**, 17, 4901-4912 | 6.4 | 5 |
| 127 | New Approach for Correcting Noncovalent Interactions in Semiempirical Quantum Mechanical Methods: The Importance of Multiple-Orientation Sampling. *Journal of Chemical Theory and Computation*, **2021**, 17, 5556-5567 | 6.4 | 3 |
| 126 | AutoMeKin2021: An open-source program for automated reaction discovery. *Journal of Computational Chemistry*, **2021**, 42, 2036-2048 | 3.5 | 7 |
| 125 | Femtochemistry under scrutiny: Clocking state-resolved channels in the photodissociation of CHI in the A-band. *Journal of Chemical Physics*, **2020**, 152, 014304 | 3.9 | 10 |
| 124 | Enhancing Automated Reaction Discovery with Boxed Molecular Dynamics in Energy Space. *ChemSystemsChem*, **2020**, 2, e1900024 | 3.1 | 9 |
| 123 | l-Cysteine Modified by S-Sulfation: Consequence on Fragmentation Processes Elucidated by Tandem Mass Spectrometry and Chemical Dynamics Simulations. *Journal of Physical Chemistry A*, **2019**, 123, 3685-3696 | 2.8 | 16 |
| 122 | Specific Reaction Parameter Multigrid POTFIT (SRP-MGPF): Automatic Generation of Sum-of-Products Form Potential Energy Surfaces for Quantum Dynamical Calculations. *Frontiers in Chemistry*, **2019**, 7, 576 | 5 | 4 |
| 121 | Reply to the Comment on "Methanol dimer formation drastically enhances hydrogen abstraction from methanol by OH at low temperature" by D. Heard, R. Shannon, J. Gomez Martin, R. Caravan, M. Blitz, J. Plane, M. Antiñolo, M. Agundez, E. Jimenez, B. Ballesteros, A. Canosa, G. El Dib, J. Albaladejo and J. Cernicharo, Phys. Chem. Chem. Phys., 2018, 20, DOI: 10.1039/C7CP04561A. | 3.6 | 5 |
| 120 | Quasi-Classical Trajectory Dynamics Study of the Cl(P) + CH -nHCl(v,j) + CH Reaction. Comparison with Experiment. *Journal of Physical Chemistry A*, **2018**, 122, 2626-2633 | 2.8 | 9 |
| 119 | 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 |
| 118 | A Trajectory-Based Method to Explore Reaction Mechanisms. *Molecules*, **2018**, 23, | 4.8 | 24 |
| 117 | Influence of Multiple Conformations and Paths on Rate Constants and Product Branching Ratios. Thermal Decomposition of 1-Propanol Radicals. *Journal of Physical Chemistry A*, **2018**, 122, 4790-4800 | 2.8 | 27 |
| 116 | Effect of the Metal Ion on the Enantioselectivity and Linkage Isomerization of Thiosemicarbazone Helicates. *Chemistry - A European Journal*, **2017**, 23, 4884-4892 | 4.8 | 2 |
| 115 | An automated method to find reaction mechanisms and solve the kinetics in organometallic catalysis. *Chemical Science*, **2017**, 8, 3843-3851 | 9.4 | 66 |
| 114 | GAFit: A general-purpose, user-friendly program for fitting potential energy surfaces. *Computer Physics Communications*, **2017**, 217, 89-98 | 4.2 | 14 |
| 113 | Theoretical and computational studies of non-equilibrium and non-statistical dynamics in the gas phase, in the condensed phase and at interfaces. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2017**, 375, | 3 | 14 |

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| 112 | Is Photolytic Production a Viable Source of HCN and HNC in Astrophysical Environments? A Laboratory-based Feasibility Study of Methyl Cyanoformate. *Astrophysical Journal*, **2017**, 849, 15 | 4.7 | 12 |
| 111 | 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 |
| 110 | A comparison of X-ray and calculated structures of the enzyme MTH1. *Journal of Molecular Modeling*, **2016**, 22, 168 | 2 | 10 |
| 109 | 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 |
| 108 | Methanol dimer formation drastically enhances hydrogen abstraction from methanol by OH at low temperature. *Physical Chemistry Chemical Physics*, **2016**, 18, 22712-8 | 3.6 | 21 |
| 107 | Photodissociation of acryloyl chloride at 193 nm: interpretation of the product energy distributions, and new elimination pathways. *Physical Chemistry Chemical Physics*, **2016**, 18, 5019-26 | 3.6 | 8 |
| 106 | On the gas phase fragmentation of protonated uracil: a statistical perspective. *Physical Chemistry Chemical Physics*, **2016**, 18, 14980-90 | 3.6 | 28 |
| 105 | An automated transition state search using classical trajectories initialized at multiple minima. *Physical Chemistry Chemical Physics*, **2015**, 17, 14912-21 | 3.6 | 72 |
| 104 | DFT and Kinetic Monte Carlo Study of TMS-Substituted Ruthenium Vinyl Carbenes: Key Intermediates for Stereoselective Cyclizations. *ACS Catalysis*, **2015**, 5, 6255-6262 | 13.1 | 10 |
| 103 | Standards-based curation of a decade-old digital repository dataset of molecular information. *Journal of Cheminformatics*, **2015**, 7, 43 | 8.6 | 6 |
| 102 | HCN elimination from vinyl cyanide: product energy partitioning, the role of hydrogen-deuterium exchange reactions and a new pathway. *Physical Chemistry Chemical Physics*, **2015**, 17, 6948-55 | 3.6 | 21 |
| 101 | An automated method to find transition states using chemical dynamics simulations. *Journal of Computational Chemistry*, **2015**, 36, 222-34 | 3.5 | 111 |
| 100 | Understanding Energy Transfer in Gas–Surface Collisions from Gas-Phase Models. *Journal of Physical Chemistry C*, **2014**, 118, 2609-2621 | 3.8 | 10 |
| 99 | Unraveling the Factors That Control Soft Landing of Small Silyl Ions on Fluorinated Self-Assembled Monolayers. *Journal of Physical Chemistry C*, **2014**, 118, 10159-10169 | 3.8 | 5 |
| 98 | Recent applications of boxed molecular dynamics: a simple multiscale technique for atomistic simulations. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2014**, 372, | 3 | 20 |
| 97 | 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 |
| 96 | Collision-induced dissociation mechanisms of [Li(uracil)]+. *Physical Chemistry Chemical Physics*, **2013**, 15, 7628-37 | 3.6 | 21 |
| 95 | Energy Transfer and Thermal Accommodation in Ozone Scattering from a Perfluorinated Self-Assembled Monolayer. *Journal of Physical Chemistry C*, **2012**, 116, 25454-25464 | 3.8 | 8 |

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| 94 | Semiempirical Hamiltonian for simulation of azobenzene photochemistry. *Journal of Physical Chemistry A*, **2012**, 116, 98-110 | 2.8 | 50 |
| 93 | Intermolecular potentials for simulations of collisions of SiNCS+ and (CH3)2SiNCS+ ions with fluorinated self-assembled monolayers. *Chemical Physics*, **2012**, 399, 193-204 | 2.3 | 7 |
| 92 | Ab initio and RRKM study of the HCN/HNC elimination channels from vinyl cyanide. *Journal of Physical Chemistry A*, **2011**, 115, 979-85 | 2.8 | 22 |
| 91 | Chemical Dynamics Study of NO Scattering from a Perfluorinated Self-Assembled Monolayer. *Journal of Physical Chemistry C*, **2011**, 115, 23817-23830 | 3.8 | 9 |
| 90 | Chemical Dynamics Simulations of CO2in the Ground and First Excited Bend States Colliding with a Perfluorinated Self-Assembled Monolayer. *Journal of Physical Chemistry C*, **2010**, 114, 18455-18464 | 3.8 | 12 |
| 89 | Dynamics of Mg+ + H2O + He: capture, collisional stabilization and collision-induced dissociation. *Journal of Physical Chemistry A*, **2010**, 114, 6472-9 | 2.8 | 9 |
| 88 | Application of the PM6 method to modeling proteins. *Journal of Molecular Modeling*, **2009**, 15, 765-805 | 2 | 235 |
| 87 | Improved United-Atom Models for Perfluorinated Self-Assembled Monolayers. *Journal of Physical Chemistry C*, **2009**, 113, 3300-3312 | 3.8 | 5 |
| 86 | Classical, quantum and statistical simulations of vibrationally excited HOSO(2): IVR, dissociation, and implications for OH + SO(2) kinetics at high pressures. *Physical Chemistry Chemical Physics*, **2009**, 11, 963-74 | 3.6 | 21 |
| 85 | Dynamics of CO2 scattering off a perfluorinated self-assembled monolayer. Influence of the incident collision energy, mass effects, and use of different surface models. *Journal of Physical Chemistry A*, **2009**, 113, 3850-65 | 2.8 | 42 |
| 84 | Chemical Dynamics Simulations of Energy Transfer in Collisions of Protonated Peptide Ions with a Perfluorinated Alkylthiol Self-Assembled Monolayer Surface. *Journal of Physical Chemistry C*, **2008**, 112, 9377-9386 | 3.8 | 35 |
| 83 | Internal energy of HCl upon photolysis of 2-chloropropene at 193 nm investigated with time-resolved Fourier-transform spectroscopy and quasiclassical trajectories. *Journal of Chemical Physics*, **2008**, 129, 224301 | 3.9 | 7 |
| 82 | Application of the PM6 method to modeling the solid state. *Journal of Molecular Modeling*, **2008**, 14, 499-535 | 2 | 125 |
| 81 | Translational energy distributions in the photodissociation of fluorobenzene. *Chemical Physics*, **2008**, 349, 219-225 | 2.3 | 6 |
| 80 | Inelastic scattering dynamics of Ar from a perfluorinated self-assembled monolayer surface. *Journal of Physical Chemistry A*, **2007**, 111, 12785-94 | 2.8 | 32 |
| 79 | Hydrogen transfer vs proton transfer in 7-hydroxy-quinoline.(NH3)3: a CASSCF/CASPT2 study. *Journal of Physical Chemistry A*, **2007**, 111, 5907-12 | 2.8 | 25 |
| 78 | Direct-dynamics VTST study of the [1,7] hydrogen shift in 7-methylocta-1,3(Z),5(Z)-triene. A model system for the hydrogen transfer reaction in previtamin D3. *Journal of Physical Chemistry A*, **2007**, 111, 719-25 | 2.8 | 14 |
| 77 | Representing and selecting vibrational angular momentum states for quasiclassical trajectory chemical dynamics simulations. *Journal of Physical Chemistry A*, **2007**, 111, 10292-301 | 2.8 | 3 |

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| 76 | Chemical Dynamics Simulations of CO2Scattering off a Fluorinated Self-Assembled Monolayer Surface. *Journal of Physical Chemistry C*, **2007**, 111, 354-364 | 3.8 | 66 |
| 75 | Ab initio and RRKM study of the elimination of HF and HCl from chlorofluoroethylene. *Chemical Physics Letters*, **2007**, 435, 176-181 | 2.5 | 7 |
| 74 | 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 |
| 73 | 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 |
| 72 | Acceleration of Classical Mechanics by Phase Space Constraints. *Journal of Chemical Theory and Computation*, **2006**, 2, 912-9 | 6.4 | 23 |
| 71 | Quasiclassical trajectory study of the collision-induced dissociation dynamics of Ar + CH3SH+ using an ab initio interpolated potential energy surface. *Journal of Physical Chemistry A*, **2006**, 110, 1225-31 | 2.8 | 21 |
| 70 | Trajectory dynamics study of collision-induced dissociation of the Ar + CH4 reaction at hyperthermal conditions: vibrational excitation and isotope substitution. *Journal of Physical Chemistry A*, **2006**, 110, 7113-21 | 2.8 | 2 |
| 69 | Rotational distributions of HBr in the photodissociation of vinyl bromide at 193 nm: An investigation by direct quasiclassical trajectory calculations. *Chemical Physics Letters*, **2006**, 425, 22-27 | 2.5 | 8 |
| 68 | On the conformational memory in the photodissociation of formic acid. *Journal of Physical Chemistry A*, **2005**, 109, 2836-9 | 2.8 | 18 |
| 67 | Trajectory dynamics study of the Ar + CH4 dissociation reaction at high temperatures: the importance of zero-point-energy effects. *Journal of Physical Chemistry A*, **2005**, 109, 5415-23 | 2.8 | 42 |
| 66 | Quasiclassical trajectory study of the F + CH4 reaction dynamics on a dual-level interpolated potential energy surface. *Journal of Physical Chemistry A*, **2005**, 109, 8459-70 | 2.8 | 51 |
| 65 | Theoretical investigations on the vibronic coupling between the electronic states S0 and S1 of formic acid including the photodissociation at 248 nm. *Chemical Physics Letters*, **2005**, 407, 166-170 | 2.5 | 8 |
| 64 | Photodissociation of formic acid: A trajectory surface hopping study. *Chemical Physics Letters*, **2005**, 412, 35-40 | 2.5 | 19 |
| 63 | Quasiclassical trajectory calculations on the photodissociation of CF2CHCl at 193 nm: product energy distributions for the HF and HCl eliminations. *Journal of Chemical Physics*, **2005**, 122, 104316 | 3.9 | 7 |
| 62 | Quasiclassical dynamics simulation of the collision-induced dissociation of Cr(CO)6 + with Xe. *Journal of Chemical Physics*, **2005**, 123, 154311 | 3.9 | 44 |
| 61 | 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 |
| 60 | Quasiclassical trajectory study of the collision-induced dissociation of CH3SH+ + Ar. *Journal of Chemical Physics*, **2004**, 121, 2571-7 | 3.9 | 26 |
| 59 | Rovibrational distributions of HF in the photodissociation of vinyl fluoride at 193 nm: a direct MP2 quasiclassical trajectory study. *Journal of Chemical Physics*, **2004**, 121, 5179-82 | 3.9 | 14 |

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| 58 | 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 |
| 57 | 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 |
| 56 | New interpretation of ground- and excited-state tunneling splitting in 2-pyridone/2-hydroxypyridine. *Chemical Physics Letters*, **2004**, 386, 396-402 | 2.5 | 15 |
| 55 | Further investigation of the HCl elimination in the photodissociation of vinyl chloride at 193 nm: a direct MP2/6-31G(d,p) trajectory study. *Chemical Physics Letters*, **2004**, 386, 225-232 | 2.5 | 22 |
| 54 | RRKM and direct MP2/6-31G(d,p) quasiclassical trajectory study of the H2 elimination in the photodissociation of vinyl chloride at 193 nm. *Chemical Physics Letters*, **2004**, 396, 442-447 | 2.5 | 8 |
| 53 | Direct dynamics study of the photodissociation of triplet propanal at threshold. *Chemical Physics Letters*, **2003**, 381, 37-44 | 2.5 | 12 |
| 52 | Product energy distributions from ethylene photodissociation at 193 nm: a DFT direct classical trajectory study. *Chemical Physics Letters*, **2003**, 369, 1-7 | 2.5 | 4 |
| 51 | A direct DFT dynamics study of the photodissociation of triplet acetaldehyde. *Chemical Physics Letters*, **2003**, 375, 591-597 | 2.5 | 12 |
| 50 | Dissociation of Difluoroethylenes. I. Global Potential Energy Surface, RRKM, and VTST Calculations. *Journal of Physical Chemistry A*, **2003**, 107, 1389-1397 | 2.8 | 18 |
| 49 | A Direct Classical Trajectory Study of HCl Elimination from the 193 nm Photodissociation of Vinyl Chloride. *Journal of Physical Chemistry A*, **2003**, 107, 7611-7618 | 2.8 | 22 |
| 48 | Dissociation of Difluoroethylenes. II. Direct Classical Trajectory Study of the HF Elimination from 1,2-Difluoroethylene. *Journal of Physical Chemistry A*, **2003**, 107, 1398-1404 | 2.8 | 23 |
| 47 | Dynamics calculations for the Cl+C2H6 abstraction reaction: Thermal rate constants and kinetic isotope effects. *Journal of Chemical Physics*, **2003**, 118, 6280-6288 | 3.9 | 21 |
| 46 | Quasi-classical trajectory study of H2 elimination in the photodissociation of difluoroethylenes at 193 nm. *Journal of Chemical Physics*, **2003**, 118, 6941-6945 | 3.9 | 10 |
| 45 | A direct classical trajectory study of the acetone photodissociation on the triplet surface. *Journal of Chemical Physics*, **2003**, 119, 10618-10625 | 3.9 | 12 |
| 44 | Rate constants for the CH3O + NO -rCH3ONO reaction by classical trajectory and canonical variational transition state theory calculations. *Journal of Physical Organic Chemistry*, **2002**, 15, 123-129 | 2.1 | 4 |
| 43 | Dissociation of ethylene and several deuterated derivatives at 193 and 157 nm by direct classical trajectories. *Chemical Physics Letters*, **2002**, 353, 418-425 | 2.5 | 15 |
| 42 | Rate constants and kinetic isotope effects for Cl+CH4-6lH+CH3: a comparison between LSC-IVR and statistical theories. *Chemical Physics Letters*, **2002**, 360, 59-64 | 2.5 | 7 |
| 41 | The role of aromaticity in the planarity of lumiflavin. *Journal of Organic Chemistry*, **2002**, 67, 6347-52 | 4.2 | 31 |

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|---|---|---|---|
| 40 | A Theoretical Study of the Dynamics of the S + c-C3H Reaction. *Journal of Physical Chemistry A*, **2002**, 106, 8811-8819 | 2.8 | 4 |
| 39 | Unimolecular reaction dynamics of HSO. Analysis of the influence of different barrier samplings on the product energy distributions. *Physical Chemistry Chemical Physics*, **2002**, 4, 279-287 | 3.6 | 18 |
| 38 | Dinâmica de reacciones unimoleculares en fase gas: Desviaciones del comportamiento estadístico. *Quimica Nova*, **2002**, 25, 579-588 | 1.6 | 4 |
| 37 | Rate constants and isotope effects for the CH3+H2-CH4+H reaction by an approximate semiclassical initial-value representation method. *Chemical Physics Letters*, **2001**, 341, 351-357 | 2.5 | 6 |
| 36 | Product energy distributions for the four-center HF elimination from 1,1-difluoroethylene. A direct dynamics study. *Chemical Physics Letters*, **2001**, 348, 81-88 | 2.5 | 20 |
| 35 | Ab Initio Calculations on the Vinyl Fluoride Fragmentation Reactions. *Structural Chemistry*, **2001**, 12, 95-108 | 1.8 | 16 |
| 34 | A direct dynamics study of the H2 elimination from 2,5-dihydrofuran. *Journal of Chemical Physics*, **2001**, 115, 7872-7880 | 3.9 | 6 |
| 33 | The unimolecular dissociation of the propionyl radical: A classical dynamics study. *Journal of Chemical Physics*, **2001**, 114, 3546-3553 | 3.9 | 4 |
| 32 | Anharmonic Quasiclassical Barrier Samplings in Trajectory Calculations and Their Influence on the Computed Product Energy Distributions. *Journal of Physical Chemistry A*, **2001**, 105, 4808-4813 | 2.8 | 5 |
| 31 | Single-Valued DMBE Potential Energy Surface for HSO:´A Distributedn-Body Polynomial Approach. *Journal of Physical Chemistry A*, **2001**, 105, 5923-5932 | 2.8 | 60 |
| 30 | Guidelines for preservation of methodological choices in the publication of computational results: B. Semiempirical electronic structure calculations(Technical report). *Pure and Applied Chemistry*, **2000**, 72, 1449-1452 | 2.1 | 2 |
| 29 | Direct dynamics simulation of the methanethiol cation decomposition. *Chemical Physics Letters*, **2000**, 324, 88-94 | 2.5 | 9 |
| 28 | Three-center vs. four-center HF elimination from vinyl fluoride: a direct dynamics study. *Chemical Physics Letters*, **2000**, 332, 583-590 | 2.5 | 20 |
| 27 | Rotational effects in the unimolecular dissociation of the acetyl radical. *Chemical Physics Letters*, **2000**, 316, 471-476 | 2.5 | 6 |
| 26 | Ab initio and RRKM calculations on the dissociation of the propionyl radical. *Journal of Molecular Structure*, **2000**, 556, 123-129 | 3.4 | 3 |
| 25 | A quantum chemical study of aniline/ammonia clusters. Thermodynamic properties and frequency analysis. *Computational and Theoretical Chemistry*, **2000**, 497, 105-113 | | 8 |
| 24 | Intermolecular interactions and cooperative effects in acetonitrile clusters. An ab initio molecular orbital study. *Computational and Theoretical Chemistry*, **2000**, 498, 21-28 | | 43 |
| 23 | DFT conformational study of cysteine in gas phase and aqueous solution. *Computational and Theoretical Chemistry*, **2000**, 498, 191-200 | | 60 |

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| 22 | Unimolecular decomposition of CH3SH+: an ab initio and RRKM study. *Computational and Theoretical Chemistry*, **2000**, 505, 109-116 | | 4 |
| 21 | Dynamics of the cis□trans isomerization and Cl□O dissociation of chlorine nitrite. Classical trajectory and statistical calculations. *Physical Chemistry Chemical Physics*, **2000**, 2, 5393-5399 | 3.6 | 8 |
| 20 | Further dynamical studies of the dissociation and elimination reactions of methyl nitrite. *Journal of Chemical Physics*, **1999**, 111, 10501-10510 | 3.9 | 9 |
| 19 | A statistical study of the methyl nitrite isomerization reaction: inverse secondary isotope effects. *Chemical Physics Letters*, **1999**, 310, 209-214 | 2.5 | 2 |
| 18 | An ab initio study of a model compound of penicillins. *Computational and Theoretical Chemistry*, **1999**, 491, 177-185 | | 10 |
| 17 | A DFT study of a model compound of vitamin D. *Computational and Theoretical Chemistry*, **1999**, 492, 143-150 | | 2 |
| 16 | Nonstatistical effects in the unimolecular dissociation of the acetyl radical. *Journal of Chemical Physics*, **1999**, 110, 11323-11334 | 3.9 | 15 |
| 15 | Classical Dynamics Study of the Unimolecular Decomposition of CH3SH+. *Journal of Physical Chemistry A*, **1999**, 103, 9783-9793 | 2.8 | 11 |
| 14 | Symmetry groups for unit cells in solids. *Journal of Computational Chemistry*, **1998**, 19, 168-180 | 3.5 | 8 |
| 13 | Direct Dynamics Study of the Dissociation and Elimination Channels in the Thermal Decomposition of Methyl Nitrite. *Journal of the American Chemical Society*, **1998**, 120, 7594-7601 | 16.4 | 14 |
| 12 | Classical Trajectory Study of the Cis□Trans Isomerization and F□O Dissociation of FONO. *Journal of Physical Chemistry A*, **1998**, 102, 8708-8715 | 2.8 | 6 |
| 11 | Dynamical study of the dissociation and elimination channels in the decomposition of methyl nitrite. *Journal of Chemical Physics*, **1998**, 109, 8907-8919 | 3.9 | 10 |
| 10 | Symmetry groups for unit cells in solids **1998**, 19, 168 | | 1 |
| 9 | Further studies of the methyl nitrite cis-trans isomerization. *Journal of Chemical Physics*, **1997**, 107, 5393-5405 | 3.9 | 8 |
| 8 | Conformational analysis of model compounds of vitamin D by theoretical calculations. *Journal of Computational Chemistry*, **1997**, 18, 1647-1655 | 3.5 | 4 |
| 7 | 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 |
| 6 | Application of localized molecular orbitals to the solution of semiempirical self-consistent field equations **1996**, 58, 133 | | 3 |
| 5 | Development and use of quantum mechanical molecular models. 76. AM1: a new general purpose quantum mechanical molecular model. [Erratum to document cited in CA103(2):11627f]. *Journal of the American Chemical Society*, **1993**, 115, 5348-5348 | 16.4 | 59 |

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| 4 | MOPAC: a semiempirical molecular orbital program. *Journal of Computer-Aided Molecular Design*, **1990**, 4, 1-105 | 4.2 | 2256 |
| 3 | Optimization of parameters for semiempirical methods I. Method. *Journal of Computational Chemistry*, **1989**, 10, 209-220 | 3.5 | 6553 |
| 2 | 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 |
| 1 | New Tools for Taming Complex Reaction Networks: The Unimolecular Decomposition of Indole Revisited. *ACS Physical Chemistry Au*, | | 2 |