Donald G Truhlar

List of Publications by Citations

1,386 papers	155,336 citations	166 h-index	355 g-index
1,522 ext. papers	169,835 ext. citations	5.9 avg, IF	9.22 L-index

#	Paper	IF	Citations
1386	The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theoretical Chemistry*	1.9	19079
1385	Universal solvation model based on solute electron density and on a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions. *Journal of Physical Chemistry B*, **2009**, 113, 6378-96	3.4	8726
1384	Density functionals with broad applicability in chemistry. *Accounts of Chemical Research*, **2008**, 41, 157-67	24.3	5345
1383	A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions. *Journal of Chemical Physics*, **2006**, 125, 194101	3.9	3551
1382	Design of Density Functionals by Combining the Method of Constraint Satisfaction with Parametrization for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions. *Journal of Chemical Theory and Computation*, **2006**, 2, 364-82	6.4	2934
1381	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
1380	Implicit Solvation Models: Equilibria, Structure, Spectra, and Dynamics. *Chemical Reviews*, **1999**, 99, 2161-2200	22.0	1976
1379	Current Status of Transition-State Theory. *The Journal of Physical Chemistry*, **1996**, 100, 12771-12800		1546
1378	Hybrid Meta Density Functional Theory Methods for Thermochemistry, Thermochemical Kinetics, and Noncovalent Interactions: The MPW1B95 and MPWB1K Models and Comparative Assessments for Hydrogen Bonding and van der Waals Interactions. *Journal of Physical Chemistry A*, **2004**, 108, 6908-6918	2.8	1410
1377	Adiabatic Connection for Kinetics. *Journal of Physical Chemistry A*, **2000**, 104, 4811-4815	2.8	1349
1376	Density functional theory for transition metals and transition metal chemistry. *Physical Chemistry Chemical Physics*, **2009**, 11, 10757-816	3.6	1248
1375	Design of density functionals that are broadly accurate for thermochemistry, thermochemical kinetics, and nonbonded interactions. *Journal of Physical Chemistry A*, **2005**, 109, 5656-67	2.8	1172
1374	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, **2016**, 37, 506-41	3.5	1047
1373	Density functional for spectroscopy: no long-range self-interaction error, good performance for Rydberg and charge-transfer states, and better performance on average than B3LYP for ground states. *Journal of Physical Chemistry A*, **2006**, 110, 13126-30	2.8	1001
1372	Consistent van der Waals radii for the whole main group. *Journal of Physical Chemistry A*, **2009**, 113, 5806-12	2.8	976
1371	How enzymes work: analysis by modern rate theory and computer simulations. *Science*, **2004**, 303, 186-95	33.3	946
1370	QM/MM: what have we learned, where are we, and where do we go from here?. *Theoretical Chemistry Accounts*, **2007**, 117, 185-199	1.9	921

1369	Computational Thermochemistry: Scale Factor Databases and Scale Factors for Vibrational Frequencies Obtained from Electronic Model Chemistries. *Journal of Chemical Theory and Computation*, **2010**, 6, 2872-87	6.4	892
1368	Exchange-correlation functional with broad accuracy for metallic and nonmetallic compounds, kinetics, and noncovalent interactions. *Journal of Chemical Physics*, **2005**, 123, 161103	3.9	877
1367	Molecular modeling of the kinetic isotope effect for the [1,5]-sigmatropic rearrangement of cis-1,3-pentadiene. *Journal of the American Chemical Society*, **1993**, 115, 2408-2415	16.4	803
1366	Benchmark Databases for Nonbonded Interactions and Their Use To Test Density Functional Theory. *Journal of Chemical Theory and Computation*, **2005**, 1, 415-32	6.4	799
1365	Exploring the Limit of Accuracy of the Global Hybrid Meta Density Functional for Main-Group Thermochemistry, Kinetics, and Noncovalent Interactions. *Journal of Chemical Theory and Computation*, **2008**, 4, 1849-68	6.4	784
1364	Variational transition-state theory. *Accounts of Chemical Research*, **1980**, 13, 440-448	24.3	761
1363	Variational Transition State Theory. *Annual Review of Physical Chemistry*, **1984**, 35, 159-189	15.7	756
1362	Parametrized Models of Aqueous Free Energies of Solvation Based on Pairwise Descreening of Solute Atomic Charges from a Dielectric Medium. *The Journal of Physical Chemistry*, **1996**, 100, 19824-19839		752
1361	Aqueous solvation free energies of ions and ion-water clusters based on an accurate value for the absolute aqueous solvation free energy of the proton. *Journal of Physical Chemistry B*, **2006**, 110, 16066-81	3.4	735
1360	Improving the Accuracy of Hybrid Meta-GGA Density Functionals by Range Separation. *Journal of Physical Chemistry Letters*, **2011**, 2, 2810-2817	6.4	716
1359	On the determination of Born□Oppenheimer nuclear motion wave functions including complications due to conical intersections and identical nuclei. *Journal of Chemical Physics*, **1979**, 70, 2284-2296	3.9	687
1358	Benchmark database of barrier heights for heavy atom transfer, nucleophilic substitution, association, and unimolecular reactions and its use to test theoretical methods. *Journal of Physical Chemistry A*, **2005**, 109, 2012-8	2.8	680
1357	Quantum mechanical methods for enzyme kinetics. *Annual Review of Physical Chemistry*, **2002**, 53, 467-505	15.7	679
1356	Current status of transition-state theory. *The Journal of Physical Chemistry*, **1983**, 87, 2664-2682		673
1355	Improved treatment of threshold contributions in variational transition-state theory. *The Journal of Physical Chemistry*, **1980**, 84, 1730-1748		637
1354	Comparative DFT study of van der Waals complexes: rare-gas dimers, alkaline-earth dimers, zinc dimer, and zinc-rare-gas dimers. *Journal of Physical Chemistry A*, **2006**, 110, 5121-9	2.8	628
1353	Effectiveness of Diffuse Basis Functions for Calculating Relative Energies by Density Functional Theory. *Journal of Physical Chemistry A*, **2003**, 107, 1384-1388	2.8	627
1352	Use of solution-phase vibrational frequencies in continuum models for the free energy of solvation. *Journal of Physical Chemistry B*, **2011**, 115, 14556-62	3.4	625

1351	Development and Assessment of a New Hybrid Density Functional Model for Thermochemical Kinetics. *Journal of Physical Chemistry A*, **2004**, 108, 2715-2719	2.8	608
1350	Conditions for the definition of a strictly diabatic electronic basis for molecular systems. *Journal of Chemical Physics*, **1982**, 77, 6090-6098	3.9	602
1349	Pairwise solute descreening of solute charges from a dielectric medium. *Chemical Physics Letters*, **1995**, 246, 122-129	2.5	599
1348	Applications and validations of the Minnesota density functionals. *Chemical Physics Letters*, **2011**, 502, 1-13	2.5	568
1347	Systematic study of basis set superposition errors in the calculated interaction energy of two HF molecules. *Journal of Chemical Physics*, **1985**, 82, 2418-2426	3.9	539
1346	Density Functionals for Noncovalent Interaction Energies of Biological Importance. *Journal of Chemical Theory and Computation*, **2007**, 3, 289-300	6.4	528
1345	How Well Can Hybrid Density Functional Methods Predict Transition State Geometries and Barrier Heights?. *Journal of Physical Chemistry A*, **2001**, 105, 2936-2941	2.8	526
1344	Basis-set extrapolation. *Chemical Physics Letters*, **1998**, 294, 45-48	2.5	524
1343	Quest for a universal density functional: the accuracy of density functionals across a broad spectrum of databases in chemistry and physics. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2014**, 372, 20120476	3	514
1342	POLYRATE 4: A new version of a computer program for the calculation of chemical reaction rates for polyatomics. *Computer Physics Communications*, **1992**, 71, 235-262	4.2	506
1341	Functional representation of Liu and Siegbahn accurate ab initio potential energy calculations for H+H2. *Journal of Chemical Physics*, **1978**, 68, 2466-2476	3.9	501
1340	MN15: A Kohn-Sham global-hybrid exchange-correlation density functional with broad accuracy for multi-reference and single-reference systems and noncovalent interactions. *Chemical Science*, **2016**, 7, 5032-5051	9.4	491
1339	A universal approach to solvation modeling. *Accounts of Chemical Research*, **2008**, 41, 760-8	24.3	475
1338	Modeling the kinetics of bimolecular reactions. *Chemical Reviews*, **2006**, 106, 4518-84	68.1	464
1337	Charge Model 5: An Extension of Hirshfeld Population Analysis for the Accurate Description of Molecular Interactions in Gaseous and Condensed Phases. *Journal of Chemical Theory and Computation*, **2012**, 8, 527-41	6.4	460
1336	M11-L: A Local Density Functional That Provides Improved Accuracy for Electronic Structure Calculations in Chemistry and Physics. *Journal of Physical Chemistry Letters*, **2012**, 3, 117-124	6.4	452
1335	Criterion of minimum state density in the transition state theory of bimolecular reactions. *Journal of Chemical Physics*, **1979**, 70, 1593-1598	3.9	443
1334	Approximations for the exchange potential in electron scattering. *Journal of Chemical Physics*, **1975**, 63, 2182-2191	3.9	427

1333	General parameterized SCF model for free energies of solvation in aqueous solution. *Journal of the American Chemical Society*, **1991**, 113, 8305-8311	16.4	425
1332	Exact tunneling calculations. *Journal of the American Chemical Society*, **1971**, 93, 1840-1851	16.4	425
1331	Ab initio effective core potentials: Reduction of all-electron molecular structure calculations to calculations involving only valence electrons. *Journal of Chemical Physics*, **1976**, 65, 3826-3853	3.9	420
1330	Density functionals for inorganometallic and organometallic chemistry. *Journal of Physical Chemistry A*, **2005**, 109, 11127-43	2.8	414
1329	The DBH24/08 Database and Its Use to Assess Electronic Structure Model Chemistries for Chemical Reaction Barrier Heights. *Journal of Chemical Theory and Computation*, **2009**, 5, 808-21	6.4	410
1328	An SCF Solvation Model for the Hydrophobic Effect and Absolute Free Energies of Aqueous Solvation. *Science*, **1992**, 256, 213-7	33.3	410
1327	Screened-exchange density functionals with broad accuracy for chemistry and solid-state physics. *Physical Chemistry Chemical Physics*, **2012**, 14, 16187-91	3.6	409
1326	Perspectives on Basis Sets Beautiful: Seasonal Plantings of Diffuse Basis Functions. *Journal of Chemical Theory and Computation*, **2011**, 7, 3027-34	6.4	393
1325	Minimally augmented Karlsruhe basis sets. *Theoretical Chemistry Accounts*, **2011**, 128, 295-305	1.9	388
1324	Self-Consistent Reaction Field Model for Aqueous and Nonaqueous Solutions Based on Accurate Polarized Partial Charges. *Journal of Chemical Theory and Computation*, **2007**, 3, 2011-33	6.4	388
1323	Generalized transition state theory. Classical mechanical theory and applications to collinear reactions of hydrogen molecules. *The Journal of Physical Chemistry*, **1979**, 83, 1052-1079		385
1322	Single-ion solvation free energies and the normal hydrogen electrode potential in methanol, acetonitrile, and dimethyl sulfoxide. *Journal of Physical Chemistry B*, **2007**, 111, 408-22	3.4	373
1321	SM6: A Density Functional Theory Continuum Solvation Model for Calculating Aqueous Solvation Free Energies of Neutrals, Ions, and Solute-Water Clusters. *Journal of Chemical Theory and Computation*, **2005**, 1, 1133-52	6.4	372
1320	Adding explicit solvent molecules to continuum solvent calculations for the calculation of aqueous acid dissociation constants. *Journal of Physical Chemistry A*, **2006**, 110, 2493-9	2.8	365
1319	Generalized transition state theory. Bond energy-bond order method for canonical variational calculations with application to hydrogen atom transfer reactions. *Journal of the American Chemical Society*, **1979**, 101, 4534-4548	16.4	361
1318	Multi-coefficient extrapolated density functional theory for thermochemistry and thermochemical kinetics. *Physical Chemistry Chemical Physics*, **2005**, 7, 43	3.6	357
1317	A double many-body expansion of the two lowest-energy potential surfaces and nonadiabatic coupling for H3. *Journal of Chemical Physics*, **1987**, 86, 6258-6269	3.9	342
1316	Performance of SM6, SM8, and SMD on the SAMPL1 test set for the prediction of small-molecule solvation free energies. *Journal of Physical Chemistry B*, **2009**, 113, 4538-43	3.4	337

1315	On the Performances of the M06 Family of Density Functionals for Electronic Excitation Energies. *Journal of Chemical Theory and Computation*, **2010**, 6, 2071-85	6.4	335
1314	Model for Aqueous Solvation Based on Class IV Atomic Charges and First Solvation Shell Effects. *The Journal of Physical Chemistry*, **1996**, 100, 16385-16398		335
1313	Oxidation of ethane to ethanol by N2O in a metal-organic framework with coordinatively unsaturated iron(II) sites. *Nature Chemistry*, **2014**, 6, 590-5	17.6	332
1312	A simple approximation for the vibrational partition function of a hindered internal rotation. *Journal of Computational Chemistry*, **1991**, 12, 266-270	3.5	324
1311	Direct dynamics calculation of the kinetic isotope effect for an organic hydrogen-transfer reaction, including corner-cutting tunneling in 21 dimensions. *Journal of the American Chemical Society*, **1993**, 115, 7806-7817	16.4	322
1310	Mechanisms and free energies of enzymatic reactions. *Chemical Reviews*, **2006**, 106, 3188-209	68.1	321
1309	Computational electrochemistry: prediction of liquid-phase reduction potentials. *Physical Chemistry Chemical Physics*, **2014**, 16, 15068-106	3.6	311
1308	OpenMolcas: From Source Code to Insight. *Journal of Chemical Theory and Computation*, **2019**, 15, 5925-5964	5.5	310
1307	Ab initio reaction paths and direct dynamics calculations. *The Journal of Physical Chemistry*, **1989**, 93, 5107-5119		309
1306	Multidimensional tunneling, recrossing, and the transmission coefficient for enzymatic reactions. *Chemical Reviews*, **2006**, 106, 3140-69	68.1	302
1305	AM1-SM2 and PM3-SM3 parameterized SCF solvation models for free energies in aqueous solution. *Journal of Computer-Aided Molecular Design*, **1992**, 6, 629-66	4.2	295
1304	A general small-curvature approximation for transition-state-theory transmission coefficients. *The Journal of Physical Chemistry*, **1981**, 85, 3019-3023		295
1303	How well can new-generation density functionals describe the energetics of bond-dissociation reactions producing radicals?. *Journal of Physical Chemistry A*, **2008**, 112, 1095-9	2.8	290
1302	Benchmark Energetic Data in a Model System for Grubbs II Metathesis Catalysis and Their Use for the Development, Assessment, and Validation of Electronic Structure Methods. *Journal of Chemical Theory and Computation*, **2009**, 5, 324-33	6.4	283
1301	Class IV charge models: a new semiempirical approach in quantum chemistry. *Journal of Computer-Aided Molecular Design*, **1995**, 9, 87-110	4.2	282
1300	An improved and broadly accurate local approximation to the exchange-correlation density functional: the MN12-L functional for electronic structure calculations in chemistry and physics. *Physical Chemistry Chemical Physics*, **2012**, 14, 13171-4	3.6	277
1299	Doubly Hybrid Meta DFT: New Multi-Coefficient Correlation and Density Functional Methods for Thermochemistry and Thermochemical Kinetics. *Journal of Physical Chemistry A*, **2004**, 108, 4786-4791	2.8	275
1298	Direct dynamics calculations with NDDO (neglect of diatomic differential overlap) molecular orbital theory with specific reaction parameters. *The Journal of Physical Chemistry*, **1991**, 95, 4618-4627		272

1297	Interpolated variational transition-state theory: Practical methods for estimating variational transition-state properties and tunneling contributions to chemical reaction rates from electronic structure calculations. *Journal of Chemical Physics*, **1991**, 95, 8875-8894	3.9	271
1296	Statistical thermodynamics of bond torsional modes. *Journal of Chemical Physics*, **2000**, 112, 1221-1228	3.9	267
1295	The MIDI! basis set for quantum mechanical calculations of molecular geometries and partial charges. *Theoretica Chimica Acta*, **1996**, 93, 281-301		266
1294	Small Representative Benchmarks for Thermochemical Calculations. *Journal of Physical Chemistry A*, **2003**, 107, 8996-8999	2.8	264
1293	Symmetry numbers and chemical reaction rates. *Theoretical Chemistry Accounts*, **2007**, 118, 813-826	1.9	259
1292	From force fields to dynamics: classical and quantal paths. *Science*, **1990**, 249, 491-8	33.3	256
1291	Polyatomic canonical variational theory for chemical reaction rates. Separable-mode formalism with application to OH+H2->H2O+H. *Journal of Chemical Physics*, **1982**, 76, 1380-1391	3.9	251
1290	Coherent switching with decay of mixing: an improved treatment of electronic coherence for non-Born-Oppenheimer trajectories. *Journal of Chemical Physics*, **2004**, 121, 7658-70	3.9	247
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1288	Multiconfiguration Pair-Density Functional Theory. *Journal of Chemical Theory and Computation*, **2014**, 10, 3669-80	6.4	246
1287	Robust and Affordable Multicoefficient Methods for Thermochemistry and Thermochemical Kinetics: The MCCM/3 Suite and SAC/3. *Journal of Physical Chemistry A*, **2003**, 107, 3898-3906	2.8	245
1286	Mapped Interpolation Scheme for Single-Point Energy Corrections in Reaction Rate Calculations and a Critical Evaluation of Dual-Level Reaction Path Dynamics Methods. *Journal of Physical Chemistry A*, **1999**, 103, 1140-1149	2.8	242
1285	New Class IV Charge Model for Extracting Accurate Partial Charges from Wave Functions. *Journal of Physical Chemistry A*, **1998**, 102, 1820-1831	2.8	241
1284	Variational Transition State Theory with Multidimensional Tunneling. *Reviews in Computational Chemistry*, **2007**, 125-232		238
1283	How well can new-generation density functional methods describe stacking interactions in biological systems?. *Physical Chemistry Chemical Physics*, **2005**, 7, 2701-5	3.6	238
1282	Reactive Scattering Cross Sections III: Quasiclassical and Semiclassical Methods **1979**, 505-566		237
1281	Factors Affecting Competitive Ion−Molecule Reactions: ClO- + C2H5Cl and C2D5Cl via E2 and SN2 Channels. *Journal of the American Chemical Society*, **1996**, 118, 860-869	16.4	235
1280	Exchange-Correlation Functional with Good Accuracy for Both Structural and Energetic Properties while Depending Only on the Density and Its Gradient. *Journal of Chemical Theory and Computation*, **2012**, 8, 2310-9	6.4	232

1279	Semiclassical tunneling calculations. *The Journal of Physical Chemistry*, **1979**, 83, 2921-2926		229
1278	Quasifree-scattering model for the imaginary part of the optical potential for electron scattering. *Physical Review A*, **1983**, 28, 2740-2751	2.6	227
1277	Electrostatically Embedded Many-Body Expansion for Large Systems, with Applications to Water Clusters. *Journal of Chemical Theory and Computation*, **2007**, 3, 46-53	6.4	226
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1272	The incorporation of quantum effects in enzyme kinetics modeling. *Accounts of Chemical Research*, **2002**, 35, 341-9	24.3	217
1271	Ab initio transition state theory calculations of the reaction rate for OH+CH4->H2O+CH3. *Journal of Chemical Physics*, **1990**, 93, 1761-1769	3.9	215
1270	Exact and Approximate Quantum Mechanical Reaction Probabilities and Rate Constants for the Collinear H + H2 Reaction. *Journal of Chemical Physics*, **1972**, 56, 2232-2252	3.9	214
1269	Vibrationally adiabatic models for reactive tunneling. *Journal of Chemical Physics*, **1982**, 77, 5955-5976	3.9	210
1268	Aqueous Mg-Ion Battery Based on Polyimide Anode and Prussian Blue Cathode. *ACS Energy Letters*, **2017**, 2, 1115-1121	20.1	207
1267	Efficient Diffuse Basis Sets: cc-pVxZ+ and maug-cc-pVxZ. *Journal of Chemical Theory and Computation*, **2009**, 5, 1197-202	6.4	206
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1265	Assessment of Model Chemistries for Noncovalent Interactions. *Journal of Chemical Theory and Computation*, **2006**, 2, 1009-18	6.4	203
1264	Incorporation of quantum effects in generalized-transition-state theory. *The Journal of Physical Chemistry*, **1982**, 86, 2252-2261		203
1263	Atmospheric Chemistry of Criegee Intermediates: Unimolecular Reactions and Reactions with Water. *Journal of the American Chemical Society*, **2016**, 138, 14409-14422	16.4	203
1262	Generalized transition state theory. Quantum effects for collinear reactions of hydrogen molecules and isotopically substituted hydrogen molecules. *The Journal of Physical Chemistry*, **1979**, 83, 1079-1112		199

1261	Quantum-Chemical Characterization of the Properties and Reactivities of Metal-Organic Frameworks. *Chemical Reviews*, **2015**, 115, 6051-111	68.1	197
1260	Representative Benchmark Suites for Barrier Heights of Diverse Reaction Types and Assessment of Electronic Structure Methods for Thermochemical Kinetics. *Journal of Chemical Theory and Computation*, **2007**, 3, 569-82	6.4	193
1259	Computation of equilibrium oxidation and reduction potentials for reversible and dissociative electron-transfer reactions in solution. *Theoretical Chemistry Accounts*, **2004**, 112, 217	1.9	189
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1257	Reaction-path energetics and kinetics of the hydride transfer reaction catalyzed by dihydrofolate reductase. *Biochemistry*, **2003**, 42, 13558-75	3.2	188
1256	NWChem: Past, present, and future. *Journal of Chemical Physics*, **2020**, 152, 184102	3.9	187
1255	Bulk Properties of Transition Metals: A Challenge for the Design of Universal Density Functionals. *Journal of Chemical Theory and Computation*, **2014**, 10, 3832-9	6.4	187
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1250	Reaction-path potential and vibrational frequencies in terms of curvilinear internal coordinates. *Journal of Chemical Physics*, **1995**, 102, 3188-3201	3.9	183
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1247	Investigation of the shape of the imaginary part of the optical-model potential for electron scattering by rare gases. *Physical Review A*, **1984**, 29, 3078-3091	2.6	180
1246	Computational characterization and modeling of buckyball tweezers: density functional study of concave-convex pi...pi interactions. *Physical Chemistry Chemical Physics*, **2008**, 10, 2813-8	3.6	179
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1241	A least-action variational method for calculating multidimensional tunneling probabilities for chemical reactions. *Journal of Chemical Physics*, **1983**, 79, 4931-4938	3.9	178
1240	Multiconfiguration Pair-Density Functional Theory: A New Way To Treat Strongly Correlated Systems. *Accounts of Chemical Research*, **2017**, 50, 66-73	24.3	175
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1236	Quantum chemical conformational analysis of glucose in aqueous solution. *Journal of the American Chemical Society*, **1993**, 115, 5745-5753	16.4	174
1235	Non-Born-Oppenheimer molecular dynamics. *Accounts of Chemical Research*, **2006**, 39, 101-8	24.3	173
1234	Optimized Parameters for Scaling Correlation Energy. *Journal of Physical Chemistry A*, **1999**, 103, 3139-3143	2.8	173
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1231	Chemical kinetics and mechanisms of complex systems: a perspective on recent theoretical advances. *Journal of the American Chemical Society*, **2014**, 136, 528-46	16.4	171
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1222	The definition of reaction coordinates for reaction-path dynamics. *Journal of Chemical Physics*, **1991**, 94, 7875-7892	3.9	166
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