

# Xiao He

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

120 papers	3,506 citations	32 h-index	56 g-index
134 ext. papers	4,393 ext. citations	5.9 avg, IF	5.97 L-index

#	Paper	IF	Citations
120	Cholesterylation of Smoothed is a calcium-accelerated autoreaction involving an intramolecular ester intermediate.. <i>Cell Research</i> , <b>2022</b> ,	24.7	2
119	Discovering inhibitors of TEAD palmitate binding pocket through virtual screening and molecular dynamics simulation.. <i>Computational Biology and Chemistry</i> , <b>2022</b> , 98, 107648	3.6	0
118	Room-temperature dynamic nuclear polarization enhanced NMR spectroscopy of small biological molecules in water. <i>Nature Communications</i> , <b>2021</b> , 12, 6880	17.4	5
117	Investigating mechanism of sweetness intensity differences through dynamic analysis of sweetener-T1R2-membrane systems.. <i>Food Chemistry</i> , <b>2021</b> , 374, 131807	8.5	2
116	Ultrasensitive Sensing of Volatile Organic Compounds Using a Cu-Doped SnO <sub>2</sub> -NiO p-n Heterostructure That Shows Significant Raman Enhancement*. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 26260-26267	16.4	5
115	Ultrasensitive Sensing of Volatile Organic Compounds Using a Cu-Doped SnO <sub>2</sub> -NiO p-n Heterostructure That Shows Significant Raman Enhancement**. <i>Angewandte Chemie</i> , <b>2021</b> , 133, 26464	3.6	2
114	Towards complete assignment of the infrared spectrum of the protonated water cluster H <sub>2</sub> (HO). <i>Nature Communications</i> , <b>2021</b> , 12, 6141	17.4	6
113	Ab initio determination of crystal stability of di-p-tolyl disulfide. <i>Scientific Reports</i> , <b>2021</b> , 11, 7076	4.9	2
112	Directional Proton Transfer in the Reaction of the Simplest Criegee Intermediate with Water Involving the Formation of Transient HO. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 3379-3386	6.4	3
111	AIE-Active Chiral [3]Rotaxanes with Switchable Circularly Polarized Luminescence. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 9507-9515	16.4	33
110	AIE-Active Chiral [3]Rotaxanes with Switchable Circularly Polarized Luminescence. <i>Angewandte Chemie</i> , <b>2021</b> , 133, 9593-9601	3.6	10
109	Atmospheric Kinetics: Bimolecular Reactions of Carbonyl Oxide by a Triple-Level Strategy. <i>Journal of the American Chemical Society</i> , <b>2021</b> , 143, 8402-8413	16.4	6
108	Analysis of the binding modes of the first- and second-generation antiandrogens with respect to F876L mutation. <i>Chemical Biology and Drug Design</i> , <b>2021</b> , 98, 60-72	2.9	
107	DeepBSP-a Machine Learning Method for Accurate Prediction of Protein-Ligand Docking Structures. <i>Journal of Chemical Information and Modeling</i> , <b>2021</b> , 61, 2231-2240	6.1	10
106	Accurate Prediction of Absorption Spectral Shifts of Proteorhodopsin Using a Fragment-Based Quantum Mechanical Method. <i>Molecules</i> , <b>2021</b> , 26,	4.8	2
105	A fixed multi-site interaction charge model for an accurate prediction of the QM/MM interactions. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 21001-21012	3.6	
104	Drug-guided screening for pancreatic lipase inhibitors in functional foods. <i>Food and Function</i> , <b>2021</b> , 12, 4644-4653	6.1	3

103	Automated fragmentation quantum mechanical calculation of C and H chemical shifts in molecular crystals. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 064502	3.9	0
102	Computational Analysis of Residue-Specific Binding Free Energies of Androgen Receptor to Ligands. <i>Frontiers in Molecular Biosciences</i> , <b>2021</b> , 8, 646524	5.6	1
101	Glucose-Lipopeptide Conjugates Reveal the Role of Glucose Modification Position in Complexation and the Potential of Malignant Melanoma Therapy. <i>Journal of Medicinal Chemistry</i> , <b>2021</b> , 64, 11483-11495	8.3	1
100	Elimination of Grain Boundary Defects in Zeolitic Imidazolate Framework ZIF-95 Membrane via Solvent-Free Secondary Growth. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 25463-25467	16.4	5
99	Fragment-Based Quantum Mechanical Calculation of Excited-State Properties of Fluorescent RNAs.. <i>Frontiers in Chemistry</i> , <b>2021</b> , 9, 801062	5	0
98	Quantitative Prediction of Aggregation-Induced Emission: A Full Quantum Mechanical Approach to the Optical Spectra. <i>Angewandte Chemie</i> , <b>2020</b> , 132, 11647-11652	3.6	3
97	Fragment-based quantum mechanical approach to biomolecules, molecular clusters, molecular crystals and liquids. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 12341-12367	3.6	16
96	Ab Initio Prediction of the Phase Transition for Solid Ammonia at High Pressures. <i>Scientific Reports</i> , <b>2020</b> , 10, 7546	4.9	3
95	Fragment Quantum Mechanical Method for Excited States of Proteins: Development and Application to the Green Fluorescent Protein. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 5174-5188	6.4	12
94	Quantitative Prediction of Aggregation-Induced Emission: A Full Quantum Mechanical Approach to the Optical Spectra. <i>Angewandte Chemie - International Edition</i> , <b>2020</b> , 59, 11550-11555	16.4	14
93	Combining the Fragmentation Approach and Neural Network Potential Energy Surfaces of Fragments for Accurate Calculation of Protein Energy. <i>Journal of Physical Chemistry B</i> , <b>2020</b> , 124, 3027-3035	3.4	15
92	M06-SX screened-exchange density functional for chemistry and solid-state physics. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2020</b> , 117, 2294-2301	11.5	16
91	Phase Transition of Ice at High Pressures and Low Temperatures. <i>Molecules</i> , <b>2020</b> , 25,	4.8	2
90	Comparative study of Minnesota functionals performance on ferroelectric BaTiO <sub>3</sub> and PbTiO <sub>3</sub> . <i>Physical Review Materials</i> , <b>2020</b> , 4,	3.2	3
89	QM Implementation in Drug Design: Does It Really Help?. <i>Methods in Molecular Biology</i> , <b>2020</b> , 2114, 19-35.	5.4	
88	Polymer-supported graphene/TiO <sub>2</sub> doped with nonmetallic elements with enhanced photocatalytic reaction under visible light. <i>Journal of Materials Science</i> , <b>2020</b> , 55, 1577-1591	4.3	13
87	Development of a New Scoring Function for Virtual Screening: APBScore. <i>Journal of Chemical Information and Modeling</i> , <b>2020</b> , 60, 6355-6365	6.1	2
86	Anisotropic Gas Separation in Oriented ZIF-95 Membranes Prepared by Vapor-Assisted In-Plane Epitaxial Growth. <i>Angewandte Chemie - International Edition</i> , <b>2020</b> , 59, 20858-20862	16.4	23

85	Anisotropic Gas Separation in Oriented ZIF-95 Membranes Prepared by Vapor-Assisted In-Plane Epitaxial Growth. <i>Angewandte Chemie</i> , <b>2020</b> , 132, 21044-21048	3.6	9
84	Low-Temperature Polymorphic Transformation of $\beta$ -Lactam Antibiotics. <i>Crystals</i> , <b>2019</b> , 9, 460	2.3	3
83	Syntheses, structures, optical properties, and electronic structures of Ba <sub>6</sub> Cu <sub>2</sub> GSn <sub>4</sub> S <sub>16</sub> (G = Fe, Ni) and Sr <sub>6</sub> D <sub>2</sub> FeSn <sub>4</sub> S <sub>16</sub> (D = Cu, Ag). <i>Journal of Solid State Chemistry</i> , <b>2019</b> , 272, 69-77	3.3	5
82	Revised M11 Exchange-Correlation Functional for Electronic Excitation Energies and Ground-State Properties. <i>Journal of Physical Chemistry A</i> , <b>2019</b> , 123, 2966-2990	2.8	45
81	Crystal Structure Optimization and Gibbs Free Energy Comparison of Five Sulfathiazole Polymorphs by the Embedded Fragment QM Method at the DFT Level. <i>Crystals</i> , <b>2019</b> , 9, 256	2.3	6
80	Prediction of Excited-State Properties of Oligoacene Crystals Using Fragment-Based Quantum Mechanical Method. <i>Journal of Physical Chemistry A</i> , <b>2019</b> , 123, 5407-5417	2.8	15
79	Stability, Vibrations, and Diffusion of Hydrogen Gas in Clathrate Hydrates: Insights from Ab Initio Calculations on Condensed-Phase Crystalline Structures. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 12052-12061	3.8	15
78	Predicting the phase diagram of solid carbon dioxide at high pressure from first principles. <i>Npj Quantum Materials</i> , <b>2019</b> , 4,	5	21
77	Rational Crystal Polymorph Design of Olanzapine. <i>Crystal Growth and Design</i> , <b>2019</b> , 19, 2388-2395	3.5	13
76	M11plus: A Range-Separated Hybrid Meta Functional with Both Local and Rung-3.5 Correlation Terms and High Across-the-Board Accuracy for Chemical Applications. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 4804-4815	6.4	11
75	A Fragment Quantum Mechanical Method for Metalloproteins. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 1430-1439	6.4	9
74	Ab initio-enabled phase transition prediction of solid carbon dioxide at ultra-high temperatures.. <i>RSC Advances</i> , <b>2019</b> , 10, 236-243	3.7	6
73	From CuFeS to BaCuFeGeS: rational band gap engineering achieves large second-harmonic-generation together with high laser damage threshold. <i>Chemical Communications</i> , <b>2019</b> , 55, 14510-14513	5.8	13
72	Exploring Protein Structures by DNP-Enhanced Methyl Solid-State NMR Spectroscopy. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 19888-19901	16.4	9
71	A Coupled Ionization-Conformational Equilibrium Is Required To Understand the Properties of Ionizable Residues in the Hydrophobic Interior of Staphylococcal Nuclease. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 1639-1648	16.4	16
70	Crius: A novel fragment-based algorithm of de novo substrate prediction for enzymes. <i>Protein Science</i> , <b>2018</b> , 27, 1526-1534	6.3	
69	Fragment-based quantum mechanical calculation of protein-protein binding affinities. <i>Journal of Computational Chemistry</i> , <b>2018</b> , 39, 1617-1628	3.5	14
68	Automated Fragmentation QM/MM Calculation of NMR Chemical Shifts for Protein-Ligand Complexes. <i>Frontiers in Chemistry</i> , <b>2018</b> , 6, 150	5	7

67	Benchmark study of ionization potentials and electron affinities of armchair single-walled carbon nanotubes using density functional theory. <i>Journal of Physics Condensed Matter</i> , <b>2018</b> , 30, 215501	1.8	7
66	Hydrogen-bond structure dynamics in bulk water: insights from simulations with coupled cluster theory. <i>Chemical Science</i> , <b>2018</b> , 9, 2065-2073	9.4	68
65	An Ab Initio QM/MM Study of the Electrostatic Contribution to Catalysis in the Active Site of Ketosteroid Isomerase. <i>Molecules</i> , <b>2018</b> , 23,	4.8	7
64	Probing the Ion-Specific Effects at the Water/Air Interface and Water-Mediated Ion Pairing in Sodium Halide Solution with Ab Initio Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 10202-10209	3.4	13
63	Revised M06 density functional for main-group and transition-metal chemistry. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2018</b> , 115, 10257-10262	11.5	67
62	Functional roles of tyrosine 185 during the bacteriorhodopsin photocycle as revealed by in situ spectroscopic studies. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , <b>2018</b> , 1859, 1006-1014	4.6	6
61	Structure of liquid water - a dynamical mixture of tetrahedral and Ring-and-chainlike structures. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 11931-11936	3.6	37
60	Fragment Quantum Mechanical Method for Large-Sized Ion-Water Clusters. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 2021-2034	6.4	39
59	Full QM Calculation of RNA Energy Using Electrostatically Embedded Generalized Molecular Fractionation with Conjugate Caps Method. <i>Journal of Physical Chemistry A</i> , <b>2017</b> , 121, 2503-2514	2.8	16
58	Reaction mechanisms of CO oxidation on cationic, neutral, and anionic X-O-Cu (X = Au, Ag) clusters. <i>Chemical Physics Letters</i> , <b>2017</b> , 686, 116-123	2.5	3
57	Revised M06-L functional for improved accuracy on chemical reaction barrier heights, noncovalent interactions, and solid-state physics. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2017</b> , 114, 8487-8492	11.5	120
56	Computational search for aflatoxin binding proteins. <i>Chemical Physics Letters</i> , <b>2017</b> , 685, 1-8	2.5	13
55	Accurate prediction of energetic properties of ionic liquid clusters using a fragment-based quantum mechanical method. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 20657-20666	3.6	28
54	MFCC-Based Fragmentation Methods for Biomolecules <b>2017</b> , 323-348		3
53	Ab initio Ice, Dry Ice, and Liquid Water <b>2017</b> , 245-296		3
52	How Well Can the M06 Suite of Functionals Describe the Electron Densities of Ne, Ne, and Ne?. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 6068-6077	6.4	19
51	Multiconfiguration Pair-Density Functional Theory Is Free From Delocalization Error. <i>Journal of Physical Chemistry Letters</i> , <b>2017</b> , 8, 5616-5620	6.4	21
50	Ab initio Quantum Mechanics/Molecular Mechanics Molecular Dynamics Simulation of CO in the Heme Distal Pocket of Myoglobin <i>Chinese Journal of Chemical Physics</i> , <b>2017</b> , 30, 705-716	0.9	5

49	A Semiautomated Structure-Based Method To Predict Substrates of Enzymes via Molecular Docking: A Case Study with Candida antarctica Lipase B. <i>Journal of Chemical Information and Modeling</i> , <b>2016</b> , 56, 1979-1994	6.1	4
48	Fragment quantum chemical approach to geometry optimization and vibrational spectrum calculation of proteins. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 1864-75	3.6	45
47	Binding mode of chitin and TLR2 via molecular docking and dynamics simulation. <i>Molecular Simulation</i> , <b>2016</b> , 42, 936-941	2	3
46	MN15-L: A New Local Exchange-Correlation Functional for Kohn-Sham Density Functional Theory with Broad Accuracy for Atoms, Molecules, and Solids. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 1280-93	6.4	246
45	Accurate Calculation of Electric Fields Inside Enzymes. <i>Methods in Enzymology</i> , <b>2016</b> , 578, 45-72	1.7	2
44	Acteoside Binds to Caspase-3 and Exerts Neuroprotection in the Rotenone Rat Model of Parkinson's Disease. <i>PLoS ONE</i> , <b>2016</b> , 11, e0162696	3.7	30
43	A systematic study on RNA NMR chemical shift calculation based on the automated fragmentation QM/MM approach. <i>RSC Advances</i> , <b>2016</b> , 6, 108590-108602	3.7	10
42	Assessing the performance of popular QM methods for calculation of conformational energies of trialanine. <i>Chemical Physics Letters</i> , <b>2016</b> , 652, 136-141	2.5	6
41	PBSA_E: A PBSA-Based Free Energy Estimator for Protein-Ligand Binding Affinity. <i>Journal of Chemical Information and Modeling</i> , <b>2016</b> , 56, 854-61	6.1	9
40	MN15: A Kohn-Sham global-hybrid exchange-correlation density functional with broad accuracy for multi-reference and single-reference systems and noncovalent interactions. <i>Chemical Science</i> , <b>2016</b> , 7, 5032-5051	9.4	491
39	Predicted PAR1 inhibitors from multiple computational methods. <i>Chemical Physics Letters</i> , <b>2016</b> , 659, 295-303	2.5	2
38	Nonseparable exchange-correlation functional for molecules, including homogeneous catalysis involving transition metals. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 12146-60	3.6	92
37	Quantum Fragment Based ab Initio Molecular Dynamics for Proteins. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 5897-905	6.4	43
36	AFNMR: automated fragmentation quantum mechanical calculation of NMR chemical shifts for biomolecules. <i>Journal of Biomolecular NMR</i> , <b>2015</b> , 63, 125-39	3	36
35	Quantum mechanical calculation of electric fields and vibrational Stark shifts at active site of human aldose reductase. <i>Journal of Chemical Physics</i> , <b>2015</b> , 143, 184111	3.9	10
34	Calculation of protein-ligand binding affinities based on a fragment quantum mechanical method. <i>RSC Advances</i> , <b>2015</b> , 5, 107020-107030	3.7	32
33	Quantum calculation of protein NMR chemical shifts based on the automated fragmentation method. <i>Advances in Experimental Medicine and Biology</i> , <b>2015</b> , 827, 49-70	3.6	3
32	Fragment quantum mechanical calculation of proteins and its applications. <i>Accounts of Chemical Research</i> , <b>2014</b> , 47, 2748-57	24.3	129

31	Second-order many-body perturbation theory: an eternal frontier. <i>Journal of Physical Chemistry A</i> , <b>2014</b> , 118, 655-72	2.8	21
30	Ab initio molecular crystal structures, spectra, and phase diagrams. <i>Accounts of Chemical Research</i> , <b>2014</b> , 47, 2721-30	24.3	65
29	Correction of erroneously packed protein's side chains in the NMR structure based on ab initio chemical shift calculations. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 18163-9	3.6	5
28	Effect of strong electric field on the conformational integrity of insulin. <i>Journal of Physical Chemistry A</i> , <b>2014</b> , 118, 8942-52	2.8	47
27	Novel theoretically designed HIV-1 non-nucleoside reverse transcriptase inhibitors derived from nevirapine. <i>Journal of Molecular Modeling</i> , <b>2014</b> , 20, 2451	2	3
26	Finite-temperature second-order many-body perturbation and Hartree-Fock theories for one-dimensional solids: an application to Peierls and charge-density-wave transitions in conjugated polymers. <i>Journal of Chemical Physics</i> , <b>2014</b> , 140, 024702	3.9	17
25	Structure, mechanism, and enantioselectivity shifting of lipase LipK107 with a simple way. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , <b>2014</b> , 1844, 1183-92	4	6
24	Quantum Mechanical Study of Vicinal J Spin-Spin Coupling Constants for the Protein Backbone. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 4653-9	6.4	12
23	A coupled two-dimensional main chain torsional potential for protein dynamics: generation and implementation. <i>Journal of Molecular Modeling</i> , <b>2013</b> , 19, 3647-57	2	9
22	Improving the scoring of protein-ligand binding affinity by including the effects of structural water and electronic polarization. <i>Journal of Chemical Information and Modeling</i> , <b>2013</b> , 53, 1306-14	6.1	34
21	On the Kohn-Luttinger conundrum. <i>Journal of Chemical Physics</i> , <b>2013</b> , 138, 204112	3.9	23
20	Predicting mutation-induced Stark shifts in the active site of a protein with a polarized force field. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 6015-23	2.8	21
19	Automated Fragmentation QM/MM Calculation of Amide Proton Chemical Shifts in Proteins with Explicit Solvent Model. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 2104-14	6.4	63
18	Electrostatically embedded generalized molecular fractionation with conjugate caps method for full quantum mechanical calculation of protein energy. <i>Journal of Physical Chemistry A</i> , <b>2013</b> , 117, 7149-61	2.8	75
17	An improved fragment-based quantum mechanical method for calculation of electrostatic solvation energy of proteins. <i>Journal of Chemical Physics</i> , <b>2013</b> , 139, 214104	3.9	27
16	COMPUTATIONAL STUDY OF HIV-1 gp41 NHR TRIMER: INHIBITION MECHANISMS OF N-SUBSTITUTED PYRROLE DERIVATIVES AND FRAGMENT-BASED VIRTUAL SCREENING. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2013</b> , 12, 1341001	1.8	1
15	Fragment density functional theory calculation of NMR chemical shifts for proteins with implicit solvation. <i>Physical Chemistry Chemical Physics</i> , <b>2012</b> , 14, 7837-45	3.6	66
14	Second-order many-body perturbation study of ice Ih. <i>Journal of Chemical Physics</i> , <b>2012</b> , 137, 204505	3.9	65

13	Formal Estimation of Errors in Computed Absolute Interaction Energies of Protein-ligand Complexes. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 790-797	6.4	116
12	The energy computation paradox and ab initio protein folding. <i>PLoS ONE</i> , <b>2011</b> , 6, e18868	3.7	41
11	Divide-and-Conquer Hartree-Fock Calculations on Proteins. <i>Journal of Chemical Theory and Computation</i> , <b>2010</b> , 6, 405-411	6.4	117
10	Further analysis and comparative study of intermolecular interactions using dimers from the S22 database. <i>Journal of Chemical Physics</i> , <b>2009</b> , 131, 065102	3.9	75
9	Protein NMR chemical shift calculations based on the automated fragmentation QM/MM approach. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 10380-8	3.4	79
8	Conformational variability of benzamidinium-based inhibitors. <i>Journal of the American Chemical Society</i> , <b>2009</b> , 131, 7742-54	16.4	28
7	Accurate benchmark calculations on the gas-phase basicities of small molecules. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 10096-103	2.8	17
6	Importance of dispersion and electron correlation in ab initio protein folding. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 5290-300	3.4	61
5	The generalized molecular fractionation with conjugate caps/molecular mechanics method for direct calculation of protein energy. <i>Journal of Chemical Physics</i> , <b>2006</b> , 124, 184703	3.9	77
4	Quantum study of mutational effect in binding of efavirenz to HIV-1 RT. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2005</b> , 59, 489-95	4.2	42
3	Quantum computational analysis for drug resistance of HIV-1 reverse transcriptase to nevirapine through point mutations. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2005</b> , 61, 423-32	4.2	49
2	A new method for direct calculation of total energy of protein. <i>Journal of Chemical Physics</i> , <b>2005</b> , 122, 31103	3.9	103
1	Comparison of quantum and mixed quantum/classical semirigid vibrating rotor target studies for isotopic reactions H(D,T)+CH <sub>4</sub> -HH(D,T)+CH <sub>3</sub> . <i>Journal of Chemical Physics</i> , <b>2003</b> , 119, 9455-9460	3.9	9