Stefan Schmatz

List of Publications by Year
in descending order

52 papers	1,091 citations	430874 18 h-index	414414 32 g-index
52 all docs	52 docs citations	52 times ranked	766 citing authors

#	Article	IF	Citations
1	Chiral Thiourea-Based Bifunctional Organocatalysts in the Asymmetric Nitro-Michael Addition: A Joint Experimental-Theoretical Study. Advanced Synthesis and Catalysis, 2006, 348, 826-832.	4.3	198
2	New highly enantioselective thiourea-based bifunctional organocatalysts for nitro-Michael addition reactions. Catalysis Today, 2007, 121, 151-157.	4.4	99
3	Theoretical study of the rovibrational energy spectrum and the numbers and densities of bound vibrational states for the system HCO+/HOC+. Journal of Chemical Physics, 1998, 109, 4456-4470.	3.0	62
4	Quantum scattering on SN2 reactions: Influence of azimuthal rotations. Journal of Chemical Physics, 1998, 109, 8200-8217.	3.0	52
5	Quantum Dynamics of Gas-Phase SN2 Reactions. ChemPhysChem, 2004, 5, 600-617.	2.1	48
6	Ultrafast Decarboxylation of Carbonyloxy Radicals:â€‰ Influence of Molecular Structure. Journal of Physical Chemistry A, 2003, 107, 9499-9510.	2.5	43
7	Origin of Syn/Anti Diastereoselectivity in Aldehyde and Ketone Crotylation Reactions:Â A Combined Theoretical and Experimental Study. Journal of the American Chemical Society, 2006, 128, 11483-11495.	13.7	39
8	Quantum scattering calculations on the SN2 reaction Clâ¯+CH3Brâ†'ClCH3+Brâ¯. Journal of Chemical Physics, 1999, 110, 9483-9491.	3.0	38
9	Quantum-mechanical study of the resonances of the SN2 reaction Cl-+CH3Clâ†'ClCH3+Cl-. Physical Chemistry Chemical Physics, 1999, 1, 1197-1203.	2.8	35
10	Coupled cluster calculations for the SN2 reaction Clâ¯ + CH3Br â†' ClCH3 + Brâ¯. International Journal of Mass Spectrometry, 2000, 201, 277-282.	1.5	34
11	Experimental and Theoretical Investigations of the Ultrafast Photoinduced Decomposition of Organic Peroxides in Solution:â€‰ Formation and Decarboxylation of Benzoyloxy Radicals. Journal of Physical Chemistry A, 2003, 107, 5157-5167.	2.5	33
12	Ultrafast Decarboxylation of Organic Peroxides in Solution: Interplay of Different Spectroscopic Techniques, Quantum Chemistry, and Theoretical Modeling. Angewandte Chemie - International Edition, 2003, 42, 299-303.	13.8	30
13	Quantum dynamics of SN2 reactions on CCSD(T) potential energy surfaces: Clâ¯+CH3Cl and Clâ¯+CH3Br. Chemical Physics Letters, 2000, 330, 188-194.	2.6	26
14	State-selected dynamics of the complex-forming bimolecular reaction Cl[sup â¯]+CH[sub 3]Cl[sup Ê¹]â†'ClCH[sub 3]+Cl[sup Ê¹â¯]: A four-dimensional quantum scattering study. Journal of Chemical Physics, 2004, 121, 220.	3.0	24
15	Structure and Rearrangement Reactions of Bis(organosilyl)(organostannyl)hydroxylamines:Â A Joint Theoretical/Experimental Study. Organometallics, 2003, 22, 490-498.	2.3	23
16	Four-dimensional quantum study on exothermic complex-forming reactions: Clâ¯+CH3Brâ†'ClCH3+Brâ¯. Journal of Chemical Physics, 2005, 122, 234307.	3.0	20
17	Secondary Kinetic Isotope Effect in Nucleophilic Substitution:â€‰ A Quantum-Mechanical Approach. Journal of Physical Chemistry A, 2006, 110, 3071-3079.	2.5	19
18	A Seemingly Well Understood Light-Induced Peroxide Decarboxylation Reaction Reinvestigated with Femtosecond Time Resolution. Journal of the American Chemical Society, 2003, 125, 13274-13278.	13.7	18

#	Article	IF	Citations
19	Resonances in SN2 reactions: Two-mode quantum calculations for Clâ¯+CH3Br on a coupled-cluster potential energy surface. Journal of Chemical Physics, 2002, 117, 9710-9718.	3.0	17
20	Four-mode calculation of resonance states of intermediate complexes in the SN2 reaction Clâ¯+CH3Clâ€²â†'ClCH3+Clâ€²â¯. Journal of Chemical Physics, 2003, 118, 4499-4516.	3.0	16
21	Intramolecular dynamics and density of states for HN. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1997, 101, 372-386.	0.9	15
22	Silyl Group Insertion into the Nâ¯N Bond:Â Experimental and Quantum Chemical Results. Journal of the American Chemical Society, 2001, 123, 378-382.	13.7	15
23	Silylhydrazine und dimere N,Nâ€²-Dilithium-N,Nâ€²-bis(silyl)hydrazide - Synthesen, Reaktionen, Isomerisierungen. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2001, 627, 2581-2588.	1.2	15
24	Spectator modes in reaction dynamics revisited: Reaction cross sections and rate constant for Clâ¯+ CH3Br â†' ClCH3+ Brâ¯ from quantum scattering. Chemical Physics Letters, 2007, 446, 250-255.	2.6	15
25	Approximate calculation of anharmonic densities of vibrational states for very large molecules. Chemical Physics, 2008, 346, 198-211.	1.9	15
26	Thermal Isomerisation of Tris(silyl)hydroxylamines to Silylaminodisiloxanes â¯ Experimental and Quantum Chemical Results. European Journal of Inorganic Chemistry, 2002, 2002, 876-885.	2.0	13
27	Reduced-dimensionality calculation of reaction cross sections and rate constant for the complex-forming gas-phase SN2 reaction Clâ¯+ CH3Clâ€² â†' ClCH3+ Clâ€²â¯. Physical Chemistry Chemical Physics, 2005, 7, 1552-1559.	2.8	12
28	Rotational effects in complex-forming bimolecular substitution reactions: A quantum-mechanical approach. Journal of Chemical Physics, 2009, 131, 224303.	3.0	12
29	Cyclization and Isomerization Reactionsin Silylhydrazine Chemistry. Monatshefte FÃ¼r Chemie, 2001, 132, 1105-1124.	1.8	11
30	Decarboxylation of carbonyloxy radicals: a density functional study. Physical Chemistry Chemical Physics, 2003, 5, 3891-3896.	2.8	10
31	Four-mode quantum calculations of resonance states in complex-forming bimolecular reactions: Clâ¯+CH3Br. Journal of Chemical Physics, 2005, 122, 234306.	3.0	10
32	Ultraschnelle Decarboxylierung organischer Peroxide in LÃ¶sung: Zusammenspiel unterschiedlicher spektroskopischer Techniken, Quantenchemie und theoretischer Modellierung. Angewandte Chemie, 2003, 115, 311-315.	2.0	9
33	Intramolecular Rearrangement of Organosilyl Groups in Silylamines:Â A Combined Experimentalâ¯Theoretical Study. Organometallics, 2007, 26, 838-845.	2.3	9
34	Differential reaction cross sections from rotationally resolved quantum scattering calculations: application to gas-phase SN2 reactions. Physical Chemistry Chemical Physics, 2012, 14, 12982.	2.8	8
35	Intramolecular rearrangement of organosilyl groups between oxygen and nitrogen in aminosiloxanes â€“ a joint experimentalâ€“theoretical study, part II. Journal of Organometallic Chemistry, 2005, 690, 1100-1119.	1.8	7
36	Mechanisms of SN2 reactions: insights from a nearside/farside analysis. Physical Chemistry Chemical Physics, 2015, 17, 26670-26676.	2.8	7

#	Article	IF	Citations
37	Quantum dynamics of the complex-forming SN2 reaction Clâ^'+ CD3Clâ€² â†' ClCD3+ Clâ€²â^'on a four-dimensional coupled-cluster potential surface. Physical Chemistry Chemical Physics, 2004, 6, 4630-4635.	2.8	6
38	Formation of (SiN2SiC) Five-Membered Rings by Intramolecular Insertion into the Siâ^'N Bond:Â A Quantum Chemical Study. Journal of Physical Chemistry A, 2001, 105, 3875-3880.	2.5	5
39	StableO,Oâ€˜-Bis(hydroxylamino)silanes R2Si(ONH2)2and IsomericN,Nâ€˜-andO,Oâ€˜-Bis(silylhydroxylamino)silanes R2Si(NHOSiR3)2and R2Si(ONHSiR3)2. Organometallics, 2003, 22, 2594-2598.	2.3	5
40	Reaction cross sections and thermal rate constant for Cl^{â^'} + CH₃Br â†' ClCH₃ + Br^{â^'} from J-dependent quantum scattering calculations. Physical Chemistry Chemical Physics, 2016, 18, 19668-19675.	2.8	5
41	Unusual Isomerization Reactions in 1,3-Diaza-2-silacyclopentanes. Organometallics, 2004, 23, 1180-1182.	2.3	4
42	(Fluorosilyl)ethylenediamines and fluorosilyl-1,3-diaza-2-silacyclopentanes. Journal of Fluorine Chemistry, 2004, 125, 1007-1017.	1.7	3
43	Rotating-Top Approximation in Reduced-Dimensionality Quantum Calculations of Rate Constants:Â Application to Complex-Forming Nucleophilic Substitutionâ€. Journal of Physical Chemistry A, 2006, 110, 1524-1533.	2.5	3
44	Intramolekulare Ringerweiterung eines 2-Lithium-anilido-2-fluoro-1,3-diaza-2-silacyclopentens zum 1,3,5-Triaza-7-bora-2-silacyclohepten - Experimentelle und Quantenchemische Ergebnisse. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2010, 636, 576-580.	1.2	3
45	Cyclic Silylhydrazinesâ€" Synthesis, Isomerizations, and Quantum Chemical Calculations. , 0, , 233-245.		0
46	Isomeric Cyclosilazanes and their Application as Precursors for Silicon-Based Ceramics. , 0, , 261-269.		0
47	Quantum Dynamics of Gas-Phase SN2 Reactions. ChemInform, 2004, 35, no.	0.0	0
48	Theoretische Chemie 2005. Nachrichten Aus Der Chemie, 2006, 54, 276-281.	0.0	0
49	Trichloroalane addition to bis(silyl)amino-silyliminoborines: a theoretical study. Journal of the Iranian Chemical Society, 2015, 12, 183-190.	2.2	0
50	Theoretical studies on chiral formamide-mediated asymmetric allylation of aldimines. Journal of the Iranian Chemical Society, 2020, 17, 623-630.	2.2	0
51	Cyclic Silylhydrazinesâ€" Synthesis, Isomerizations, and Quantum Chemical Calculations. , 0, , 233-245.		0
52	Isomeric Cyclosilazanes and their Application as Precursors for Silicon-Based Ceramics. , 0, , 261-269.		0