

Helmut Schwarz

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89
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39,623
ext. citations

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7.62
L-index

#	Paper	IF	Citations
1054	Two-state reactivity as a new concept in organometallic chemistry. <i>Accounts of Chemical Research</i> , 2000 , 33, 139-45	24.3	981
1053	Organometallic chemistry in the gas phase. <i>Chemical Reviews</i> , 1991 , 91, 1121-1177	68.1	750
1052	Gas-phase catalysis by atomic and cluster metal ions: the ultimate single-site catalysts. <i>Angewandte Chemie - International Edition</i> , 2005 , 44, 2336-54	16.4	720
1051	The singlet and triplet states of phenyl cation. A hybrid approach for locating minimum energy crossing points between non-interacting potential energy surfaces. <i>Theoretical Chemistry Accounts</i> , 1998 , 99, 95-99	1.9	693
1050	Chemistry with methane: concepts rather than recipes. <i>Angewandte Chemie - International Edition</i> , 2011 , 50, 10096-115	16.4	534
1049	C-H and C-C Bond Activation by Bare Transition-Metal Oxide Cations in the Gas Phase. <i>Angewandte Chemie International Edition in English</i> , 1995 , 34, 1973-1995		416
1048	Thermal hydrogen-atom transfer from methane: the role of radicals and spin states in oxo-cluster chemistry. <i>Angewandte Chemie - International Edition</i> , 2012 , 51, 5544-55	16.4	338
1047	On the Question of Stability, Conjugation, and Aromaticity in Imidazol-2-ylidenes and Their Silicon Analogs. <i>Journal of the American Chemical Society</i> , 1996 , 118, 2023-2038	16.4	337
1046	Electronic Structure Makes a Difference: Cytochrome P-450 Mediated Hydroxylations of Hydrocarbons as a Two-State Reactivity Paradigm. <i>Chemistry - A European Journal</i> , 1998 , 4, 193-199	4.8	303
1045	Relativistic effects in gas-phase ion chemistry: an experimentalist's view. <i>Angewandte Chemie - International Edition</i> , 2003 , 42, 4442-54	16.4	300
1044	Two-state reactivity mechanisms of hydroxylation and epoxidation by cytochrome P-450 revealed by theory. <i>Current Opinion in Chemical Biology</i> , 2002 , 6, 556-67	9.7	299
1043	On the spin-forbiddenness of gas-phase ion-molecule reactions: a fruitful intersection of experimental and computational studies. <i>International Journal of Mass Spectrometry</i> , 2004 , 237, 75-105	1.9	288
1042	Activation of hydrogen and methane by thermalized FeO ⁺ in the gas phase as studied by multiple mass spectrometric techniques. <i>International Journal of Mass Spectrometry and Ion Processes</i> , 1997 , 161, 175-191		274
1041	Generation, Stability, and Reactivity of Small, Multiply Charged Ions in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 1999 , 103, 7385-7394	2.8	274
1040	Two-State Reactivity in Organometallic Gas-Phase Ion Chemistry. <i>Helvetica Chimica Acta</i> , 1995 , 78, 1393-1407		270
1039	Electronic Structures and Gas-Phase Reactivities of Cationic Late-Transition-Metal Oxides. <i>Journal of the American Chemical Society</i> , 1994 , 116, 10734-10741	16.4	261
1038	Gas-phase chemistry of collisionally activated ions. <i>Mass Spectrometry Reviews</i> , 1983 , 2, 77-148	11	254

1037	Endohedral Cluster Compounds: Inclusion of Helium within C and C through Collision Experiments. <i>Angewandte Chemie International Edition in English</i> , 1991 , 30, 884-886		246
1036	Cationic Gold(I) Complexes of Xenon and of Ligands Containing the Donor Atoms Oxygen, Nitrogen, Phosphorus, and Sulfur <i>Inorganic Chemistry</i> , 1998 , 37, 624-632	5.1	228
1035	Thermal activation of methane by tetranuclear [V ₄ O ₁₀] ⁺ . <i>Angewandte Chemie - International Edition</i> , 2006 , 45, 4681-5	16.4	227
1034	Gas-phase activation of methane by ligated transition-metal cations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008 , 105, 18114-9	11.5	216
1033	Collisional Activation Mass Spectrometry: A New Probe for Determining the Structure of Ions in the Gas Phase. <i>Angewandte Chemie International Edition in English</i> , 1976 , 15, 509-519		213
1032	The Generation and Characterization of Molecules by Neutralization-Reionization Mass Spectrometry (NRMS). <i>New Analytical Methods (33)</i> . <i>Angewandte Chemie International Edition in English</i> , 1987 , 26, 805-815		196
1031	FeO ⁺ Activates Methane. <i>Angewandte Chemie International Edition in English</i> , 1990 , 29, 1433-1434		190
1030	Experimental and theoretical studies toward a characterization of conceivable intermediates involved in the gas-phase oxidation of methane by bare FeO ⁺ . Generation of four distinguishable [Fe,C,H ₄ ,O] ⁺ isomers. <i>Journal of the American Chemical Society</i> , 1992 , 114, 1215-1222	16.4	185
1029	A Comparative Computational Study of Cationic Coinage Metal Ethylene Complexes (C ₂ H ₄)M ⁺ (M = Cu, Ag, and Au). <i>The Journal of Physical Chemistry</i> , 1996 , 100, 12253-12260		184
1028	Neutralization-reionization mass spectrometry: a powerful "laboratory" to generate and probe elusive neutral molecules. <i>Accounts of Chemical Research</i> , 1994 , 27, 347-352	24.3	175
1027	Mass spectrometric approaches to the reactivity of transient neutrals. <i>Chemical Society Reviews</i> , 1998 , 27, 91	58.5	166
1026	Gasphasenkatalyse mit atomaren und Cluster-Metall-Ionen: ultimative Single-Site-Katalysatoren. <i>Angewandte Chemie</i> , 2005 , 117, 2388-2406	3.6	166
1025	Chemie mit Methan: Studieren geht über Probieren!. <i>Angewandte Chemie</i> , 2011 , 123, 10276-10297	3.6	164
1024	Activation of methane by oligomeric (Al ₂ O ₃) _x ⁺ (x = 3,4,5): the role of oxygen-centered radicals in thermal hydrogen-atom abstraction. <i>Angewandte Chemie - International Edition</i> , 2008 , 47, 1946-50	16.4	164
1023	Remote functionalization of C-H and C-C bonds by "naked" transition-metal ions (Cosi Fan Tutte). <i>Accounts of Chemical Research</i> , 1989 , 22, 282-287	24.3	163
1022	How and Why Do Cluster Size, Charge State, and Ligands Affect the Course of Metal-Mediated Gas-Phase Activation of Methane?. <i>Israel Journal of Chemistry</i> , 2014 , 54, 1413-1431	3.4	162
1021	How Does Fe ⁺ Activate C-C and C-H Bonds in Ethane? A Theoretical Investigation Using Density Functional Theory <i>The Journal of Physical Chemistry</i> , 1996 , 100, 6236-6242		157
1020	Gas-phase chemistry of bare transition-metal ions in comparison. <i>Journal of the American Chemical Society</i> , 1990 , 112, 621-627	16.4	155

1019	Organometallic chemistry in the gas phase. A comparative fourier transform-ion cyclotron resonance/tandem mass spectrometry study. <i>International Journal of Mass Spectrometry and Ion Processes</i> , 1989 , 93, 243-257		151
1018	Diatomic [CuO] ⁺ and its role in the spin-selective hydrogen- and oxygen-atom transfers in the thermal activation of methane. <i>Angewandte Chemie - International Edition</i> , 2011 , 50, 4966-9	16.4	145
1017	Dissociation behavior of Cu(urea) ⁺ complexes generated by electrospray ionization. <i>International Journal of Mass Spectrometry</i> , 2002 , 219, 729-738	1.9	145
1016	Pt ⁺ -Catalyzed Oxidation of Methane: Theory and Experiment. <i>Journal of Physical Chemistry A</i> , 1997 , 101, 1567-1579	2.8	143
1015	The performance of density-functional/Hartree-Fock hybrid methods: Cationic transition-metal methyl complexes MCH ₃ ⁺ (M=Sc, Cu, La, Hf, Au). <i>Journal of Chemical Physics</i> , 1995 , 102, 4931-4941	3.9	141
1014	Radical-like Behavior of Manganese Oxide Cation in Its Gas-Phase Reactions with Dihydrogen and Alkanes. <i>Journal of the American Chemical Society</i> , 1995 , 117, 2033-2040	16.4	136
1013	Relativistic Effects on Bonding in Cationic Transition-Metal-Carbene Complexes: A Density-Functional Study. <i>Journal of the American Chemical Society</i> , 1995 , 117, 495-500	16.4	134
1012	Effects of Sequential Ligation of Molybdenum Cation by Chalcogenides on Electronic Structure and Gas-Phase Reactivity. <i>Journal of Physical Chemistry A</i> , 1997 , 101, 6252-6264	2.8	131
1011	Radical-Like Activation of Alkanes by the Ligated Copper Oxide Cation (Phenanthroline)CuO ⁺ . <i>Journal of Physical Chemistry B</i> , 2004 , 108, 14407-14416	3.4	129
1010	Carbon-fluorine bond activation: looking at and learning from unsolvated systems. <i>Chemical Communications</i> , 2003 , 1321-1326	5.8	128
1009	Roller-coaster: cyclometalation. Early history, recent developments, mechanistic insights and application aspects. <i>Chemical Science</i> , 2012 , 3, 308-326	9.4	127
1008	Aktivierung von C-H- und C-C-Bindungen durch fackelbergangsmetalloxid-Kationen in der Gasphase. <i>Angewandte Chemie</i> , 1995 , 107, 2126-2150	3.6	127
1007	SiOH ⁺ /HSiO ⁺ and SiOH./HSiO.: gas-phase generation and characterization. A combined neutralization-reionization mass spectrometry and ab initio molecular orbital study. <i>Journal of the American Chemical Society</i> , 1991 , 113, 5970-5975	16.4	125
1006	Doping Effects in Cluster-Mediated Bond Activation. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 10090-100	16.4	123
1005	Gas-Phase Reactivity of Lanthanide Cations with Hydrocarbons. <i>Organometallics</i> , 1995 , 14, 992-999	3.8	123
1004	Organic Dications: Gas Phase Experiments and Theory in Concert. <i>Angewandte Chemie International Edition in English</i> , 1989 , 28, 1321-1341		123
1003	Platinum dioxide cation: easy to generate experimentally but difficult to describe theoretically. <i>Journal of the American Chemical Society</i> , 2001 , 123, 142-7	16.4	122
1002	Room-temperature C-H bond activation of methane by bare [P(4)O(10)] ^{(*)+} . <i>Angewandte Chemie - International Edition</i> , 2009 , 48, 4861-3	16.4	120

1001	Generation and characterization of neutral and cationic 3-sila-cyclopropenylidene in the gas phase. <i>International Journal of Mass Spectrometry and Ion Processes</i> , 1991 , 107, 369-376		119
1000	Effects of Ligands, Cluster Size, and Charge State in Gas-Phase Catalysis: A Happy Marriage of Experimental and Computational Studies. <i>Catalysis Letters</i> , 2012 , 142, 1265-1278	2.8	117
999	Stoßaktivierungsmassenspektrometrie - eine neue Sonde zur Strukturbestimmung von Ionen in der Gasphase. <i>Angewandte Chemie</i> , 1976 , 88, 589-599	3.6	116
998	Transfer Hydrogenation and Deuteration of Buckminsterfullerene C60 by 9,10-Dihydroanthracene and 9,9',10,10'-[D4]Dihydroanthracene. <i>Angewandte Chemie International Edition in English</i> , 1993 , 32, 584-586		115
997	Electronic Effects on Room-Temperature, Gas-Phase C-H Bond Activations by Cluster Oxides and Metal Carbides: The Methane Challenge. <i>Journal of the American Chemical Society</i> , 2017 , 139, 17201-17212	16.4	114
996	Oxidation properties of the early transition-metal dioxide cations MO ₂ ⁺ (M = Ti, V, Zr, Nb) in the gas-phase. <i>International Journal of Mass Spectrometry</i> , 1999 , 182-183, 85-97	1.9	114
995	Thermische Wasserstoffabstraktion aus Methan - zur Rolle von Radikalen und Spinzuständen in der Chemie von Oxoclustern. <i>Angewandte Chemie</i> , 2012 , 124, 5638-5650	3.6	111
994	Additivity effects in the reactivities of bimetallic cluster ions Pt _m Au _n ⁺ . <i>ChemPhysChem</i> , 2003 , 4, 1233-7	3.2	110
993	Chromium Dioxide Cation OCrO ⁺ in the Gas Phase: Structure, Electronic States, and the Reactivity with Hydrogen and Hydrocarbons ¹ . <i>Journal of the American Chemical Society</i> , 1996 , 118, 9941-9952	16.4	110
992	Concepts of metal-mediated methane functionalization. An intersection of experiment and theory. <i>Pure and Applied Chemistry</i> , 2000 , 72, 2319-2332	2.1	109
991	Gas-phase oxidation of propane and 1-butene with [V ₃ O ₇] ⁺ : experiment and theory in concert. <i>Angewandte Chemie - International Edition</i> , 2006 , 45, 4677-81	16.4	108
990	Reactivity of Small Cationic Platinum Clusters. <i>Journal of Physical Chemistry A</i> , 2003 , 107, 4999-5006	2.8	108
989	Kinetic-energy dependence of competitive spin-allowed and spin-forbidden reactions: V ⁺⁺ CS ₂ . <i>Journal of Chemical Physics</i> , 1999 , 110, 7858-7870	3.9	108
988	Métagéométries: single-atom catalysis, mass spectrometry, and computational chemistry. <i>Catalysis Science and Technology</i> , 2017 , 7, 4302-4314	5.5	107
987	Amino acid sequence of Manduca sexta adipokinetic hormone elucidated by combined fast atom bombardment (FAB)/tandem mass spectrometry. <i>Biochemical and Biophysical Research Communications</i> , 1985 , 133, 337-42	3.4	107
986	Surprisingly low reactivity of bare iron monoxide ion (FeO ⁺) in its spin-allowed, highly exothermic reaction with molecular hydrogen to generate iron(1+) and water. <i>The Journal of Physical Chemistry</i> , 1994 , 98, 68-70		105
985	Ethylenedione: An Intrinsically Short-Lived Molecule. <i>Chemistry - A European Journal</i> , 1998 , 4, 2550-2557	4.8	104
984	Probing cooperative effects in bimetallic clusters: indications of C-N coupling of CH ₄ and NH ₃ mediated by the cluster ion PtAu ⁺ in the gas phase. <i>Journal of the American Chemical Society</i> , 2003 , 125, 3676-7	16.4	103

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- 982 Gas-phase oxidation of isomeric butenes and small alkanes by vanadium-oxide and -hydroxide cluster cations. *Journal of Physical Chemistry A*, **2006**, 110, 2647-54 2.8 102
- 981 Characterization, Orbital Description, and Reactivity Patterns of Transition-Metal Oxo Species in the Gas Phase **2000**, 91-123 101
- 980 Experimental and Theoretical Studies of Gold(I) Complexes Au(L)⁺ (L = H₂O, CO, NH₃, C₂H₄, C₃H₆, C₄H₆, C₆H₆, C₆F₆). *Organometallics*, **1995**, 14, 312-316 3.8 101
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- 971 The Bare⁺Uranyl(2+) Ion, UO. *Angewandte Chemie International Edition in English*, **1996**, 35, 891-894 95
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- 969 Some newer aspects of mass spectrometric ortho effects **1978**, 231-263 93
- 968 Competing reactions of the acetone cation radical: RRKM-QET calculations on an ab initio potential-energy surface. *Journal of the American Chemical Society*, **1988**, 110, 8183-8192 16.4 92
- 967 Metal-mediated activation of carbon dioxide in the gas phase: Mechanistic insight derived from a combined experimental/computational approach. *Coordination Chemistry Reviews*, **2017**, 334, 112-123 23.2 91
- 966 Direct conversion of methane into formaldehyde mediated by [Al₂O₃]⁺ at room temperature. *Angewandte Chemie - International Edition*, **2012**, 51, 3703-7 16.4 89

965	A gas-phase reaction as a functional model for the activation of carbon dioxide by carbonic anhydrase. <i>Angewandte Chemie - International Edition</i> , 2003 , 42, 5087-90	16.4	87
964	Long-lived dications of Cu(H ₂ O) ₂ ²⁺ and Cu(NH ₃) ₂ ²⁺ do exist!. <i>Chemical Physics Letters</i> , 2001 , 343, 258-264	2.5	87
963	Ligand and electronic-structure effects in metal-mediated gas-phase activation of methane: a cold approach to a hot problem. <i>Dalton Transactions</i> , 2009 , 10155-65	4.3	86
962	Raumtemperaturaktivierung von Methan durch das vierkernige Oxidclusterion [V ₄ O ₁₀] ⁺ . <i>Angewandte Chemie</i> , 2006 , 118, 4797-4801	3.6	86
961	Relativistische Effekte in der Gasphasenchemie von Ionen aus experimenteller Sicht. <i>Angewandte Chemie</i> , 2003 , 115, 4580-4593	3.6	86
960	Innocent and less-innocent solvent ligands: a systematic investigation of cationic iron chloride/alcohol complexes by electrospray ionization mass spectrometry complemented by DFT calculations. <i>Chemistry - A European Journal</i> , 2006 , 12, 2454-64	4.8	82
959	Unexpected Mechanistic Variants in the Thermal Gas-Phase Activation of Methane. <i>Organometallics</i> , 2017 , 36, 8-17	3.8	80
958	Mass spectrometry as a tool to probe the gas-phase reactivity of neutral molecules. <i>International Journal of Mass Spectrometry and Ion Processes</i> , 1998 , 172, 181-208		80
957	Activation of methane by gaseous platinum(II) ions PtX ⁺ (X = H, Cl, Br, CHO). <i>Canadian Journal of Chemistry</i> , 2005 , 83, 1936-1940	0.9	80
956	Stoichiometric Gas-Phase Oxidation Reactions of CoO ⁺ with Molecular Hydrogen, Methane, and Small Alkanes. <i>Organometallics</i> , 1994 , 13, 4072-4081	3.8	80
955	Gas-phase C-H and N-H bond activation by a high valent nitrido-iron dication and NH-transfer to activated olefins. <i>Journal of the American Chemical Society</i> , 2008 , 130, 4285-94	16.4	79
954	Coordination of iron(III) cations to beta-keto esters as studied by electrospray mass spectrometry: implications for iron-catalyzed Michael addition reactions. <i>Chemistry - A European Journal</i> , 2005 , 11, 619-27	4.8	78
953	Hydrocarbon activation by Bare Uranium cations: formation of a cationic uranium-benzene complex from three ethylene units. <i>Journal of Organometallic Chemistry</i> , 1995 , 501, 201-209	2.3	77
952	Observation of the Hammick Intermediate: Reduction of the Pyridine-2-ylid Ion in the Gas Phase. <i>Journal of the American Chemical Society</i> , 1996 , 118, 11898-11904	16.4	77
951	Neutralization/ionization mass spectrometry as a novel probe to structurally characterize organic ligands generated in the Fe(I)-mediated oligomerization of acetylene in the gas phase. <i>International Journal of Mass Spectrometry and Ion Processes</i> , 1991 , 110, 145-156		77
950	Conversion of methane to methanol: nickel, palladium, and platinum (d ₉) cations as catalysts for the oxidation of methane by ozone at room temperature. <i>Chemistry - A European Journal</i> , 2010 , 16, 11605-10	4.8	76
949	Thermochemistry and Reactivity of Cationic Scandium and Titanium Sulfide in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2000 , 104, 5046-5058	2.8	76
948	Generation and Characterization of the Anionic, Neutral, and Cationic Iron-Dioxygen Adducts [FeO ₂] in the Gas Phase. <i>Inorganic Chemistry</i> , 1994 , 33, 5094-5100	5.1	76

- 947 The Neutralization of HeC in the Gas Phase: Compelling Evidence for the Existence of an Endohedral Structure for He@C60. *Angewandte Chemie International Edition in English*, **1992**, 31, 183-185 76
- 946 Electrostatic and Charge-Induced Methane Activation by a Concerted Double C-H Bond Insertion. *Journal of the American Chemical Society*, **2017**, 139, 1684-1689 16.4 75
- 945 Oxidative Degradation of Small Cationic Vanadium Clusters by Molecular Oxygen: On the Way from V_n^+ ($n = 2\text{B}$) to VO_m^+ ($m = 1, 2$). *Journal of Physical Chemistry A*, **2003**, 107, 2855-2859 2.8 75
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- 941 Gas-phase ion/molecule reactions of corannulene, a fullerene subunit. *Journal of the American Chemical Society*, **1993**, 115, 11636-11637 16.4 73
- 940 Tantalum-Mediated Coupling of Methane and Carbon Dioxide in the Gas Phase. *Angewandte Chemie International Edition in English*, **1995**, 34, 2033-2035 73
- 939 Thermolysis of NH_4HCO_3 : A Simple Route to the Formation of Free Carbonic Acid (H_2CO_3) in the Gas Phase. *Angewandte Chemie International Edition in English*, **1987**, 26, 354-355 73
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- 932 Methanaktivierung durch $(Al_2O_3)_x$ ($x=3,4,5$): die Rolle von Sauerstoff-zentrierten Radikalen bei thermischer Abstraktion eines Wasserstoffatoms von Methan. *Angewandte Chemie*, **2008**, 120, 1972-1976 3.6 70
- 931 Gas-Phase Chemistry of Bare V^+ Cation with Oxygen and Water at Room Temperature: Formation and Hydration of Vanadium Oxide Cations. *Journal of Physical Chemistry A*, **2001**, 105, 4259-4271 2.8 70
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- 922 NUO⁺, a New Species Isoelectronic to the Uranyl Dication UO. *Chemistry - A European Journal*, **1995**, 1, 7-11 4.8 67
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