

# Thomas Weiske

## List of Publications by Year in descending order

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75  
papers

3,217  
citations

126907

33  
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155660

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82  
all docs

82  
docs citations

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times ranked

1511  
citing authors

#	ARTICLE	IF	CITATIONS
1	Experiment and Theory Clarify: Sc + Receives One Oxygen Atom from SO <sub>2</sub> to Form ScO + , which Proves to be a Catalyst for the Hidden Oxygen-Exchange with SO <sub>2</sub> . ChemPhysChem, 2021, , .	2.1	2
2	Frontispiece: Counterintuitive Gas-Phase Reactivities of [V <sub>2</sub> ] <sup>+</sup> and [V <sub>2</sub> O] <sup>+</sup> towards CO <sub>2</sub> Reduction: Insight from Electronic Structure Calculations. Angewandte Chemie - International Edition, 2020, 59, .	13.8	0
3	On the Crucial Role of Isolated Electronic States in the Thermal Reaction of ReC + with Dihydrogen. Angewandte Chemie, 2020, 132, 9456-9462.	2.0	3
4	Revisiting the Intriguing Electronic Features of the BeOBeC Carbyne and Some Isomers: A Quantum-Chemical Assessment. Angewandte Chemie - International Edition, 2020, 59, 17261-17265.	13.8	2
5	Frontispiz: Counterintuitive Gas-Phase Reactivities of [V <sub>2</sub> ] <sup>+</sup> and [V <sub>2</sub> O] <sup>+</sup> towards CO <sub>2</sub> Reduction: Insight from Electronic Structure Calculations. Angewandte Chemie, 2020, 132, .	2.0	0
6	On the Crucial Role of Isolated Electronic States in the Thermal Reaction of ReC <sup>+</sup> with Dihydrogen. Angewandte Chemie - International Edition, 2020, 59, 9370-9376.	13.8	7
7	Revisiting the Intriguing Electronic Features of the BeOBeC Carbyne and Some Isomers: A Quantum-Chemical Assessment. Angewandte Chemie, 2020, 132, 17414-17418.	2.0	0
8	Counterintuitive Gas-Phase Reactivities of [V <sub>2</sub> ] <sup>+</sup> and [V <sub>2</sub> O] <sup>+</sup> towards CO <sub>2</sub> Reduction: Insight from Electronic Structure Calculations. Angewandte Chemie, 2020, 132, 12406-12412.	2.0	1
9	Counterintuitive Gas-Phase Reactivities of [V <sub>2</sub> ] <sup>+</sup> and [V <sub>2</sub> O] <sup>+</sup> towards CO <sub>2</sub> Reduction: Insight from Electronic Structure Calculations. Angewandte Chemie - International Edition, 2020, 59, 12308-12314.	13.8	10
10	A Reaction-Induced Localization of Spin Density Enables Thermal C-H Bond Activation of Methane by Pristine FeC <sub>4</sub> <sup>+</sup> . Chemistry - A European Journal, 2019, 25, 12940-12945.	3.3	22
11	Complete cleavage of the N≡N triple bond by Ta <sub>2</sub> N <sup>+</sup> via degenerate ligand exchange at ambient temperature: A perfect catalytic cycle. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 21416-21420.	7.1	60
12	Reassessment of the Mechanisms of Thermal C-H Bond Activation of Methane by Cationic Magnesium Oxides: A Critical Evaluation of the Suitability of Different Density Functionals. ChemPhysChem, 2019, 20, 1812-1821.	2.1	5
13	Intrinsic Reactivity of Diatomic 3d Transition-Metal Carbides in the Thermal Activation of Methane: Striking Electronic Structure Effects. Journal of the American Chemical Society, 2019, 141, 599-610.	13.7	39
14	Ta <sub>2</sub> <sup>+</sup> -mediated ammonia synthesis from N <sub>2</sub> and H <sub>2</sub> at ambient temperature. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 11680-11687.	7.1	84
15	Oriented external electric fields as mimics for probing the role of metal ions and ligands in the thermal gas-phase activation of methane. Dalton Transactions, 2018, 47, 15271-15277.	3.3	23
16	Thermal O-H Bond Activation of Water As Mediated by Heteronuclear [Al <sub>2</sub> Mg <sub>2</sub> O <sub>5</sub> ] <sup>+</sup> : Evidence for Oxygen-Atom Scrambling. Journal of the American Chemical Society, 2018, 140, 9275-9281.	13.7	13
17	Unexpected Mechanistic Variants in the Thermal Gas-Phase Activation of Methane. Organometallics, 2017, 36, 8-17.	2.3	91
18	Electrostatic and Charge-Induced Methane Activation by a Concerted Double C-H Bond Insertion. Journal of the American Chemical Society, 2017, 139, 1684-1689.	13.7	96

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19	Hidden Hydride Transfer as a Decisive Mechanistic Step in the Reactions of the Unligated Gold Carbide $[\text{AuC}]^+$ with Methane under Ambient Conditions. <i>Angewandte Chemie</i> , 2016, 128, 13266-13269.	2.0	22
20	On the Origin of Room-Temperature, $\text{Au}^+$ -Mediated Coupling of a Methylene Ligand with $\text{H}_2$ . Implications for the Mechanism of Methane Dehydrogenation.. <i>ChemistrySelect</i> , 2016, 1, 444-447.	1.5	10
21	Hidden Hydride Transfer as a Decisive Mechanistic Step in the Reactions of the Unligated Gold Carbide $[\text{AuC}]^+$ with Methane under Ambient Conditions. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 13072-13075.	13.8	54
22	Electronic Origins of the Variable Efficiency of Room-Temperature Methane Activation by Homo- and Heteronuclear Cluster Oxide Cations $[\text{XYO}]^+$ (X, Y = Al, Si, Mg): Competition between Proton-Coupled Electron Transfer and Hydrogen-Atom Transfer. <i>Journal of the American Chemical Society</i> , 2016, 138, 7973-7981.	13.7	90
23	Effect of Adduct Formation with Molecular Nitrogen on the Measured Collisional Cross Sections of Transition Metal-1,10-Phenanthroline Complexes in Traveling Wave Ion-Mobility Spectrometry: $\text{N}_2$ Is Not Always an "Inert" Buffer Gas. <i>Analytical Chemistry</i> , 2015, 87, 9769-9776.	6.5	14
24	Thermal Ethane Activation by Bare $[\text{V}_2\text{O}_5]^+$ and $[\text{Nb}_2\text{O}_5]^+$ Cluster Cations: on the Origin of Their Different Reactivities. <i>Chemistry - A European Journal</i> , 2014, 20, 6672-6677.	3.3	24
25	On divorcing isomers, dissecting reactivity, and resolving mechanisms of propane CH and aryl CX (X=halogen) bond activations mediated by a ligated copper(III) oxo complex. <i>Chemical Physics Letters</i> , 2014, 608, 408-424.	2.6	30
26	Thermal Methane Activation by a Binary $\text{V}^{\text{IV}}\text{Nb}$ Transition-Metal Oxide Cluster Cation: A Further Example for the Crucial Role of Oxygen-Centered Radicals. <i>Chemistry - A European Journal</i> , 2013, 19, 11496-11501.	3.3	29
27	Direct Conversion of Methane into Formaldehyde Mediated by $[\text{Al}_2\text{O}_3]^+$ at Room Temperature. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 3703-3707.	13.8	98
28	Structure of the Oxygen-Rich Cluster Cation $\text{Al}_2\text{O}_7^+$ and its Reactivity toward Methane and Water. <i>Journal of the American Chemical Society</i> , 2011, 133, 16930-16937.	13.7	73
29	Catalytic Redox Reactions in the $\text{CO}/\text{N}_2\text{O}$ System Mediated by the Bimetallic Oxide-Cluster Couple $\text{AlVO}_3^+/\text{AlVO}_4^+$ . <i>Angewandte Chemie - International Edition</i> , 2011, 50, 12351-12354.	13.8	66
30	Structural Aspects of Long-Lived $\text{C}_7\text{H}_8^+$ Dications Generated by the Electron Ionization of Toluene. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2970-2978.	2.5	34
31	Oxidative Degradation of Small Cationic Vanadium Clusters by Molecular Oxygen: On the Way from $\text{V}^n$ ( $n = 2-5$ ) to $\text{VO}^m$ ( $m = 1, 2$ ).. <i>ChemInform</i> , 2003, 34, no.	0.0	0
32	Oxidative Degradation of Small Cationic Vanadium Clusters by Molecular Oxygen: On the Way from $\text{V}^n$ ( $n = 2-5$ ) to $\text{VO}^m$ ( $m = 1, 2$ ). <i>Journal of Physical Chemistry A</i> , 2003, 107, 2855-2859.	2.5	83
33	Dissociation behavior of ionized valeramide. <i>International Journal of Mass Spectrometry</i> , 2002, 214, 155-170.	1.5	14
34	Dissociation behavior of $\text{Cu}(\text{urea})^+$ complexes generated by electrospray ionization. <i>International Journal of Mass Spectrometry</i> , 2002, 219, 729-738.	1.5	150
35	Revisiting the Mechanism of the Unimolecular Fragmentation of Protonated Fluorobenzene. <i>Journal of Physical Chemistry A</i> , 1999, 103, 4609-4620.	2.5	22
36	Gas-Phase Ion Chemistry of Dimethyl Peroxide with the Bare Transition-Metal Cations $\text{Cr}^+$ , $\text{Mn}^+$ , $\text{Fe}^+$ , and $\text{Co}^+$ . <i>Journal of the American Chemical Society</i> , 1995, 117, 7711-7718.	13.7	40

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37	High-energy collisions of Kr@C60+ with helium. Evidence for the formation of HeKr@C60+. Chemical Physics Letters, 1994, 227, 87-90.	2.6	27
38	Transfer Hydrogenation and Deuteration of Buckminsterfullerene C60 by 9,10-Dihydroanthracene and 9,10-D4-Dihydroanthracene. Angewandte Chemie International Edition in English, 1993, 32, 584-586.	4.4	136
39	Transferhydrierung und -deuterierung von Buckminsterfulleren C <sub>60</sub> durch 9,10-Dihydroanthracen bzw. 9,10-D <sub>4</sub> -Dihydroanthracen. Angewandte Chemie, 1993, 105, 609-611.	3.0	34
40	Experiments aimed at generating the long-sought-after ethylenedione (O=C=C=O) by neutralization-reionization mass spectrometry. International Journal of Mass Spectrometry and Ion Processes, 1993, 125, 75-79.	1.8	42
41	Experimental evidence for the existence of the protonitronium dication (HONO <sub>2</sub> <sup>+</sup> ) in the gas phase and ab initio molecular orbital calculations of its potential energy surface. Journal of the American Chemical Society, 1993, 115, 6312-6316.	13.7	36
42	Combined ab initio MO and experimental studies on unimolecular hydrogen fluoride loss from protonated fluorobenzene in the gas phase. Journal of the American Chemical Society, 1993, 115, 2015-2020.	13.7	63
43	High-energy collisions of carbon cluster cations with helium: experimental support for the existence of imperfect fullerene structures. The Journal of Physical Chemistry, 1993, 97, 20-22.	2.9	22
44	Application of thermal kinetics to small carbon ion clusters. The Journal of Physical Chemistry, 1993, 97, 6592-6597.	2.9	33
45	The neutralization-reionization mass spectrum of C+60. International Journal of Mass Spectrometry and Ion Processes, 1992, 113, R23-R29.	1.8	31
46	Chemical signatures of Buckminsterfullerene, C60, under chemical ionization conditions. International Journal of Mass Spectrometry and Ion Processes, 1992, 116, R13-R21.	1.8	11
47	High-energy collisions of organofullerene cations with helium. Ligand evaporation caused by encapsulation of the noble gas atom. Chemical Physics Letters, 1992, 199, 640-642.	2.6	12
48	The Neutralization of HeC60 <sup>+</sup> 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.	4.4	96
49	Sequential Insertion of <sup>3</sup> He and <sup>4</sup> He in C60 <sup>+</sup> . Angewandte Chemie International Edition in English, 1992, 31, 605-606.	4.4	19
50	Cationic and neutral nitrosamide: viable molecules in the dilute gas phase. Chemical Physics Letters, 1992, 199, 643-647.	2.6	13
51	Ab initio MO calculation on the energy barrier for the penetration of a benzene ring by a helium atom. Model studies for the formation of endohedral He@C60+ complexes by high-energy bimolecular reactions. Chemical Physics Letters, 1992, 193, 97-100.	2.6	46
52	Endohedral fullerene-noble gas clusters formed with high-energy bimolecular reactions of C <sub>x</sub> n <sup>+</sup> (x = 1-10). Journal of Physical Chemistry, 1992, 96, 1077-1081.	2.6	77
53	Beweis der Existenz einer endohedralen He@C <sub>60</sub> -Struktur durch Gasphasenneutralisation von HeC <sub>60</sub> <sup>+</sup> . Angewandte Chemie, 1992, 104, 242-244.	2.0	32
54	Sequentieller Einbau von <sup>3</sup> He und <sup>4</sup> He in C. Angewandte Chemie, 1992, 104, 639-640.	2.0	8

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55	Injection of helium atoms into doubly and triply charged carbon (C60) cations. <i>The Journal of Physical Chemistry</i> , 1991, 95, 8451-8452.	2.9	79
56	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.	1.8	134
57	Endohedral Cluster Compounds: Inclusion of Helium within C60 and C70 through Collision Experiments. <i>Angewandte Chemie International Edition in English</i> , 1991, 30, 884-886.	4.4	291
58	Formation of endohedral carbon-cluster noble-gas compounds with high-energy bimolecular reactions: C60Hen+ (n=1,2). <i>Chemical Physics Letters</i> , 1991, 186, 459-462.	2.6	86
59	Activation of carbon-hydrogen and carbon-carbon bonds of 4-octyne in the gas phase by bare transition-metal ions M+ (M = chromium, manganese, iron). <i>Organometallics</i> , 1988, 7, 898-902.	2.3	23
60	Generation of the distonic ion CH2NH3.bul.+; nucleophilic substitution of the ketene cation radical by ammonia and unimolecular decarbonylation of ionized acetamide. <i>Journal of the American Chemical Society</i> , 1987, 109, 4810-4818.	13.7	70
61	The CH2+ dication: Metastable or not? A combined theoretical and experimental investigation. <i>Chemical Physics Letters</i> , 1987, 142, 147-152.	2.6	24
62	The mechanism of methyl loss from ionized methoxypentamethylsilane: anchimeric assistance versus direct bond cleavage. <i>Journal of Organometallic Chemistry</i> , 1987, 336, 105-113.	1.8	9
63	Gas-phase dissociations of ionized methyl isopropyl ether. A case for ion / neutral complexes?. <i>International Journal of Mass Spectrometry and Ion Processes</i> , 1987, 76, 117-119.	1.8	12
64	CNH2+: Laboratory generation of a proposed interstellar species. <i>Chemical Physics Letters</i> , 1986, 132, 69-71.	2.6	7
65	Study of ion structures produced by the reaction of 2-propyl cations with water and methanol; covalently bound v. Hydrogen-bridged adducts. <i>Organic Mass Spectrometry</i> , 1986, 21, 665-671.	1.3	48
66	Hydroxyacetylene: Generation and Characterization of the Neutral Molecule, Radical Cation and Dication in the Gas Phase. <i>Angewandte Chemie International Edition in English</i> , 1986, 25, 282-284.	4.4	52
67	Aminoacetylene and Its Mono- and Dication Identification of Potentially Interstellar Molecules. <i>Angewandte Chemie International Edition in English</i> , 1986, 25, 827-828.	4.4	28
68	Massenspektrometrischer Nachweis von Aminoacetylen sowie seinem Mono- und Dikation. <i>Angewandte Chemie</i> , 1986, 98, 834-835.	2.0	3
69	The CCl4 dication revisited. <i>International Journal of Mass Spectrometry and Ion Processes</i> , 1986, 72, 313-315.	1.8	10
70	Intrinsic alkyl radical properties inferred from the study of unimolecular dissociations of gaseous carboxylic acid cation radicals. <i>Tetrahedron</i> , 1986, 42, 6245-6251.	1.9	38
71	Cl2C?Cl?Cl?, Cl2C?Cl?Br?, and Br2C?Br?Cl? by Gas-Phase Decarbonylation of CX3COY?. <i>Angewandte Chemie International Edition in English</i> , 1985, 24, 869-870.	4.4	19
72	Stereoisomeric fragment ions arising from decomposition of enol cation radicals of different internal energy content. <i>Organic Mass Spectrometry</i> , 1984, 19, 617-622.	1.3	5

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73	Reactivity of $\text{CH}_2\text{XCH}_3$ (X = Cl, Br) with Electrophiles and Nucleophiles in the Gas Phase, a Fourier Transform Ion Cyclotron Resonance Investigation. <i>Angewandte Chemie International Edition in English</i> , 1984, 23, 733-734.	4.4	22
74	On the detailed pathway of the methyl loss from ionized methyl isobutyrate in the gas phase. <i>Journal of the American Chemical Society</i> , 1984, 106, 1167-1168.	13.7	23
75	Methyl-Eliminierung aus dem metastabilen Homoadamantan-Radikalkation / Methyl Loss from Metastable Homoadamantane Cation Radical. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 1980, 35, 207-211.	0.7	5