Marzio Rosi

List of Publications by Year
in descending order

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216	4,521	117453	149479
papers	citations	34 h-index	56 g-index

230	230	230	2712
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Combined crossed molecular beams and computational study on the N(²D)â€‰+â€‰HCCCN(X¹Î£⁺) reaction and implications for extra-terrestrial environments. Molecular Physics, 2022, 120, .	0.8	9
2	Semiempirical Potential in Kinetics Calculations on the HC3N + CN Reaction. Molecules, 2022, 27, 2297.	1.7	3
3	Unsaturated Dinitriles Formation Routes in Extraterrestrial Environments: A Combined Experimental and Theoretical Investigation of the Reaction between Cyano Radicals and Cyanoethene (C₂H₃CN). Journal of Physical Chemistry A, 2022, 126, 3569-3582.	1.1	13
4	A Computational Study on the Attack of Nitrogen and Oxygen Atoms to Toluene. Lecture Notes in Computer Science, 2021, , 620-631.	1.0	6
5	Methane Production from H2 + CO2 Reaction: An Open Molecular Science Case for Computational and Experimental Studies. Physchem, 2021, 1, 82-94.	0.5	1
6	Reactivity of transition metal dioxide anions MO2â¯ (MÂ=ÂCo, Ni, Cu, Zn) with sulfur dioxide in the gas phase: An experimental and theoretical study. Chemical Physics Letters, 2021, 776, 138555.	1.2	7
7	A crossed molecular beam investigation of the N(2D)Â+Âpyridine reaction and implications for prebiotic chemistry. Chemical Physics Letters, 2021, 779, 138852.	1.2	12
8	Long-Range Complex in the HC$$_{3}$$N + CN Potential Energy Surface: Ab Initio Calculations and Intermolecular Potential. Lecture Notes in Computer Science, 2021, , 413-425.	1.0	2
9	Free-Methane - from the Ionosphere of Mars Towards a Prototype Methanation Reactor: A Project Producing Fuels via Plasma Assisted Carbon Dioxide Hydrogenation. Lecture Notes in Computer Science, 2021, , 594-607.	1.0	0
10	Gas-Phase TiO2 Photosensitized Mineralization of Some VOCs: Mechanistic Suggestions through a Langmuirâ€“Hinshelwood Kinetic Approach. Catalysts, 2021, 11, 20.	1.6	6
11	The Reaction N(²D) + CH₃CCH (Methylacetylene): A Combined Crossed Molecular Beams and Theoretical Investigation and Implications for the Atmosphere of Titan. Journal of Physical Chemistry A, 2021, 125, 8846-8859.	1.1	12
12	Production and Characterization of Molecular Dications: Experimental and Theoretical Efforts. Molecules, 2020, 25, 4157.	1.7	9
13	The Italian National Project of Astrobiologyâ€”Life in Spaceâ€”Origin, Presence, Persistence of Life in Space, from Molecules to Extremophiles. Astrobiology, 2020, 20, 580-582.	1.5	10
14	Theoretical and Computational Analysis at a Quantum State Level of Autoionization Processes in Astrochemistry. Lecture Notes in Computer Science, 2020, , 693-706.	1.0	1
15	A Computational Study of the Reaction Cyanoacetylene and Cyano Radical Leading to 2-Butynedinitrile and Hydrogen Radical. Lecture Notes in Computer Science, 2020, , 707-716.	1.0	3
16	A Theoretical Investigation of the Reactions of N(2D) with Small Alkynes and Implications for the Prebiotic Chemistry of Titan. Lecture Notes in Computer Science, 2020, , 717-729.	1.0	3
17	A Computational Study on the Insertion of N(2D) into a Câ€”H or Câ€”C Bond: The Reactions of N(2D) with Benzene and Toluene and Their Implications on the Chemistry of Titan. Lecture Notes in Computer Science, 2020, , 744-755.	1.0	7
18	A Theoretical Investigation of the Reaction Between Glycolaldehyde and H+ and Implications for the Organic Chemistry of Star Forming Regions. Lecture Notes in Computer Science, 2020, , 730-743.	1.0	0

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19	The Fragmentation Dynamics of Simple Organic Molecules of Astrochemical Interest Interacting with VUV Photons. ACS Earth and Space Chemistry, 2019, 3, 1862-1872.	1.2	3
20	A Computational Study of the Reaction N(2D)Â+ÂC6H6 Leading to Pyridine and Phenylnitrene. Lecture Notes in Computer Science, 2019, , 316-324.	1.0	10
21	Electronic Structure and Kinetics Calculations for the Si+SH Reaction, a Possible Route of SiS Formation in Star-Forming Regions. Lecture Notes in Computer Science, 2019, , 306-315.	1.0	4
22	Analytical Potential Energy Formulation for a New Theoretical Approach in Penning Ionization. Lecture Notes in Computer Science, 2019, , 291-305.	1.0	1
23	Baseâ€Assisted Conversion of Protonated <scp>D</scp>â€Fructose to 5â€HMF: Searching for Gasâ€Phase Green Models. ChemistryOpen, 2019, 8, 1190-1198.	0.9	10
24	Angular Distribution of Ion Products in the Double Photoionization of Propylene Oxide. Frontiers in Chemistry, 2019, 7, 621.	1.8	6
25	Molecular Dynamics of CH4/N2 Mixtures on a Flexible Graphene Layer: Adsorption and Selectivity Case Study. Frontiers in Chemistry, 2019, 7, 386.	1.8	14
26	An Experimental and Theoretical Investigation of 1-Butanol Pyrolysis. Frontiers in Chemistry, 2019, 7, 326.	1.8	12
27	Editorial: Reaction Dynamics Involving Ions, Radicals, Neutral and Excited Species. Frontiers in Chemistry, 2019, 7, 859.	1.8	0
28	Effective redox reactions by chromium oxide anions: Sulfur dioxide oxidation in the gas phase. International Journal of Mass Spectrometry, 2019, 436, 18-22.	0.7	10
29	Interstellar dimethyl ether gas-phase formation: a quantum chemistry and kinetics study. Monthly Notices of the Royal Astronomical Society, 2019, 482, 3567-3575.	1.6	48
30	Possible scenarios for SiS formation in the interstellar medium: Electronic structure calculations of the potential energy surfaces for the reactions of the SiH radical with atomic sulphur and S2. Chemical Physics Letters, 2018, 695, 87-93.	1.2	33
31	Sulphur dioxide cooperation in hydrolysis reactions of vanadium oxide and hydroxide cluster dianions. New Journal of Chemistry, 2018, 42, 4008-4016.	1.4	7
32	Low temperature kinetics and theoretical studies of the reaction CN + CH₃NH₂: a potential source of cyanamide and methyl cyanamide in the interstellar medium. Physical Chemistry Chemical Physics, 2018, 20, 5478-5489.	1.3	33
33	A theoretical investigation of the reaction between the amidogen, NH, and the ethyl, C2H5, radicals: a possible gas-phase formation route of interstellar and planetary ethanimine. Molecular Astrophysics, 2018, 13, 30-37.	1.7	24
34	A Theoretical Investigation of the Reaction H+SiS2 and Implications for the Chemistry of Silicon in the Interstellar Medium. Lecture Notes in Computer Science, 2018, , 719-729.	1.0	2
35	A Theoretical Investigation of the Reaction N(2D)Â+ÂC6H6 and Implications for the Upper Atmosphere of Titan. Lecture Notes in Computer Science, 2018, , 763-772.	1.0	10
36	Nanostructure Selectivity for Molecular Adsorption and Separation: the Case of Graphyne Layers. Journal of Physical Chemistry C, 2018, 122, 16195-16208.	1.5	32

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37	Formation of Nitrogen-Bearing Organic Molecules in the Reaction NHÂ+ÂC2H5: A Theoretical Investigation and Main Implications for Prebiotic Chemistry in Space. Lecture Notes in Computer Science, 2018, , 773-782.	1.0	3
38	Double Photoionization of Simple Molecules of Astrochemical Interest. Lecture Notes in Computer Science, 2018, , 746-762.	1.0	2
39	Silicon-bearing molecules in the shock L1157-B1: first detection of SiS around a Sun-like protostar. Monthly Notices of the Royal Astronomical Society: Letters, 2017, 470, L16-L20.	1.2	44
40	Vanadium Hydroxide Cluster Ions in the Gas Phase: Bondâ€Forming Reactions of Doublyâ€Charged Negative Ions by SO₂â€Promoted Vâ‹¯O Activation. Chemistry - A European Journal, 2017, 23, 11752-11756.	1.7	21
41	A Theoretical and Computational Approach to a Semi-classical Model for Electron Spectroscopy Calculations in Collisional Autoionization Processes. Lecture Notes in Computer Science, 2016, , 258-272.	1.0	2
42	Angular and energy distributions of fragment ions in dissociative double photoionization of acetylene molecules in the 31.9-50.0 eV photon energy range. Journal of Chemical Physics, 2016, 145, 114308.	1.2	13
43	Stereoselectivity in Autoionization Reactions of Hydrogenated Molecules by Metastable Noble Gas Atoms: The Role of Electronic Couplings. Chemistry - A European Journal, 2016, 22, 12518-12526.	1.7	41
44	Isomerization Pathways of ONCNO: Unstable or Metastable?. Journal of Physical Chemistry A, 2016, 120, 4812-4817.	1.1	1
45	Measurements of Ionization Cross Sections by Molecular Beam Experiments: Information Content on the Imaginary Part of the Optical Potential. Journal of Physical Chemistry A, 2016, 120, 5169-5174.	1.1	8
46	A Theoretical Study on the Relevance of Protonated and Ionized Species of Methanimine and Methanol in Astrochemistry. Lecture Notes in Computer Science, 2016, , 296-308.	1.0	1
47	Ironâ€Promoted Cï£¿C Bond Formation in the Gas Phase. Angewandte Chemie - International Edition, 2015, 54, 14359-14362.	7.2	8
48	Dimerization of methanimine and its charged species in the atmosphere of Titan and interstellar/cometary ice analogs. Astronomy and Astrophysics, 2015, 584, A76.	2.1	48
49	Angular Distributions of Fragment Ions Produced by Coulomb Explosion of Simple Molecular Dications of Astrochemical Interest. Lecture Notes in Computer Science, 2015, , 291-307.	1.0	4
50	A Theoretical Investigation of 1-Butanol Unimolecular Decomposition. Lecture Notes in Computer Science, 2015, , 384-393.	1.0	1
51	Monocyclic and bicyclic CO₄: how stable are they?. RSC Advances, 2015, 5, 91581-91586.	1.7	1
52	The Oxidation of Sulfur Dioxide by Single and Double Oxygen Transfer Paths. ChemPhysChem, 2014, 15, 2723-2731.	1.0	10
53	Kinetic Energy Release in molecular dications fragmentation after VUV and EUV ionization and escape from planetary atmospheres. Planetary and Space Science, 2014, 99, 149-157.	0.9	49
54	All the 2p-block elements in a molecule: experimental and theoretical studies of FBNCO and FBNCO+. Chemical Communications, 2014, 50, 13900-13903.	2.2	4

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55	The Escape Probability of Some Ions from Mars and Titan Ionospheres. Lecture Notes in Computer Science, 2014, , 554-570.	1.0	9
56	Production of ions at high energy and its role in extraterrestrial environments. Rendiconti Lincei, 2013, 24, 53-65.	1.0	45
57	A Theoretical Study of Formation Routes and Dimerization of Methanimine and Implications for the Aerosols Formation in the Upper Atmosphere of Titan. Lecture Notes in Computer Science, 2013, , 47-56.	1.0	16
58	A highâ€level ab initio study of the N₂ + N₂ reaction channel. Journal of Computational Chemistry, 2013, 34, 2668-2676.	1.5	44
59	Competitive solvation of K+ by C6H6 and H2O in the K+-(C6H6)n-(H2O)m (nÂ=Â1â€“4; mÂ=Â1â€“6) aggregates. European Physical Journal D, 2013, 67, 1.	0.6	35
60	Combined crossed beam and theoretical studies of the C(1D) + CH4 reaction. Journal of Chemical Physics, 2013, 138, 024311.	1.2	40
61	The Oxidative Mechanism in Electrophilic Cï£¿H Activation: The Case of CH₂F₂ and CH₂Cl₂. Chemistry - an Asian Journal, 2013, 8, 588-595.	1.7	5
62	Selective Activation of Cï£¿Cl and Cï£¿F Bonds by SO^{.+} Radical Cations: An Experimental and Computational Study. ChemPlusChem, 2013, 78, 1065-1072.	1.3	7
63	Water (H2O) m or Benzene (C6H6) n Aggregates to Solvate the Kâ€‰+â€‰?. Lecture Notes in Computer Science, 2013, , 1-15.	1.0	23
64	Modeling the Intermolecular Interactions and Characterization of the Dynamics of Collisional Autoionization Processes. Lecture Notes in Computer Science, 2013, , 69-83.	1.0	33
65	Combined Crossed Beam and Theoretical Studies of the N(²D) + C₂H₄Reaction and Implications for Atmospheric Models of Titan. Journal of Physical Chemistry A, 2012, 116, 10467-10479.	1.1	58
66	The azido oxide N3O. Chemical Physics, 2012, 398, 129-133.	0.9	0
67	Linking Ion and Neutral Chemistry in Cï£¿H Bond Electrophilic Activation: Generation and Detection of HO₂[.] Reactive Radicals in the Gas Phase. Angewandte Chemie - International Edition, 2012, 51, 1455-1458.	7.2	6
68	Theoretical and Experimental Study of the Energy and Structure of Fragment Ions Produced by Double Photoionization of Benzene Molecules. Lecture Notes in Computer Science, 2012, , 316-330.	1.0	3
69	Theoretical Study of Reactions Relevant for Atmospheric Models of Titan: Interaction of Excited Nitrogen Atoms with Small Hydrocarbons. Lecture Notes in Computer Science, 2012, , 331-344.	1.0	19
70	A Bond-Bond Portable Approach to Intermolecular Interactions: Simulations for N-methylacetamide and Carbon Dioxide Dimers. Lecture Notes in Computer Science, 2012, , 387-400.	1.0	34
71	Low temperature kinetics, crossed beam dynamics and theoretical studies of the reaction S(1D) + CH4 and low temperature kinetics of S(1D) + C2H2. Physical Chemistry Chemical Physics, 2011, 13, 8485.	1.3	31
72	Dissociative double photoionization of benzene molecules in the 26â€“33 eV energy range. Physical Chemistry Chemical Physics, 2011, 13, 8245.	1.3	41

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73	Dissociative double photoionization of singly deuterated benzene molecules in the 26â€“33 eV energy range. Journal of Chemical Physics, 2011, 135, 144304.	1.2	34
74	The Proton Affinity and Gasâ€Phase Basicity of Sulfur Dioxide. ChemPhysChem, 2011, 12, 112-115.	1.0	27
75	COMPCHEM: Progress Towards GEMS a Grid Empowered Molecular Simulator and Beyond. Journal of Grid Computing, 2010, 8, 571-586.	2.5	63
76	Formation of nitriles and imines in the atmosphere of Titan: combined crossed-beam and theoretical studies on the reaction dynamics of excited nitrogen atoms N(2D) with ethane. Faraday Discussions, 2010, 147, 189.	1.6	79
77	Methane Activation by Metalâ€Free Radical Cations: Experimental Insight into the Reaction Intermediate. Chemistry - A European Journal, 2009, 15, 4248-4252.	1.7	108
78	Combined Crossed Molecular Beam and Theoretical Studies of the N(²D) + CH₄ Reaction and Implications for Atmospheric Models of Titan. Journal of Physical Chemistry A, 2009, 113, 11138-11152.	1.1	90
79	Observation of organosulfur products (thiovinoxy, thioketene and thioformyl) in crossed-beam experiments and low temperature rate coefficients for the reaction S(1D) + C2H4. Physical Chemistry Chemical Physics, 2009, 11, 4701.	1.3	33
80	Crossed-Beam Dynamics, Low-Temperature Kinetics, and Theoretical Studies of the Reaction S(¹D) + C₂H₄. Journal of Physical Chemistry A, 2009, 113, 15328-15345.	1.1	38
81	Crossed-Beam and Theoretical Studies of the S(¹D) + C₂H₂ Reaction. Journal of Physical Chemistry A, 2009, 113, 4330-4339.	1.1	28
82	Experimental and Theoretical Evidence for HS4. Journal of Physical Chemistry A, 2009, 113, 14420-14423.	1.1	2
83	Gas-phase ion chemistry of BF3/CH4 mixtures: Activation of methane by <mml:math altimg="si1.gif" display="inline" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/common/struct-bib/dtd"	1.2	7
84	The intermolecular potential in NOâ€“N2 and (NOâ€“N2)+ systems: implications for the neutralization of ionic molecular aggregates. Physical Chemistry Chemical Physics, 2008, 10, 5993.	1.3	34
85	The HSSS Radical and the HSSSâ^' Anion. Journal of Physical Chemistry A, 2008, 112, 8471-8477.	1.1	12
86	Quantum vs Semiclassical Dynamics Approaches from highly symmetric to asymmetric reactions. , 2007, , .		1
87	SSOH and HSSO Radicals:â€‰ An Experimental and Theoretical Study of [S2OH]0/+/- Species. Journal of Physical Chemistry A, 2007, 111, 6526-6533.	1.1	27
88	Ionization of carbonyl sulphide/disulphur monoxide mixtures in atmospheric gases: A theoretical study of the formation of S3O+ ions. Computational and Theoretical Chemistry, 2007, 822, 153-157.	1.5	0
89	The functionalization of (5, 5), (9, 0), and (10, 0) single wall carbon nanotubes by CHn fragments. Chemical Physics Letters, 2007, 437, 99-103.	1.2	10
90	S3O and S3O+ in the gas phase: ring and open-chain structures. Chemical Communications, 2006, , 4416.	2.2	6

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91	Gas-Phase Ion Chemistry of BF3/NH3Mixtures. Journal of Physical Chemistry A, 2006, 110, 12427-12433.	1.1	5
92	Gas-phase Ion Chemistry of BF3/HN3Mixtures:Â The First Observation of [BFnNxHn-1]+(n= 1, 2;x= 1, 3) Ions. Journal of Physical Chemistry B, 2006, 110, 4492-4499.	1.2	9
93	Effect of Alkali Metal Coordination on Gas-Phase Chemistry of the Diphosphate Ion: The MH2P2O7â˜ Ions. Chemistry - A European Journal, 2006, 12, 2787-2797.	1.7	5
94	Direct Experimental Observation of CS2OH. ChemPhysChem, 2006, 7, 2352-2357.	1.0	2
95	Ionization of carbon disulfide/ozone mixtures in atmospheric gases. Chemical Physics Letters, 2005, 410, 377-383.	1.2	6
96	Experimental Detection of Theoretically Predicted N2CO. Angewandte Chemie - International Edition, 2005, 44, 462-465.	7.2	31
97	CS2O+ and CS2O in the gas phase: An experimental and computational study. Journal of Chemical Physics, 2005, 123, 164307.	1.2	1
98	Theoretical Investigations of Atmospheric Species Relevant for the Search of High-Energy Density Materials. Lecture Notes in Computer Science, 2005, , 1101-1110.	1.0	0
99	Gas phase protonation of trifluoromethyl sulfur pentafluoride. Physical Chemistry Chemical Physics, 2005, 7, 1181.	1.3	10
100	C6NH6 â€‰+â€‰ Ions as Intermediates in the Reaction between Benzene and Nâ€‰+â€‰ Ions. Lecture Notes in Computer Science, 2004, , 412-421.	1.0	0
101	Reactivity of C10H7+ and C10D7+ with H2 and D2. Journal of Chemical Physics, 2004, 121, 6728-6737.	1.2	19
102	Discovery of the New Metastable HONF. Radical. ChemPhysChem, 2004, 5, 503-508.	1.0	1
103	The Diphosphate Monoanion in the Gas Phase: A Joint Mass Spectrometric and Theoretical Study. Chemistry - A European Journal, 2004, 10, 840-850.	1.7	5
104	Gaseous H5P2O8? Ions: A Theoretical and Experimental Study on the Hydrolysis and Synthesis of Diphosphate Ion. Chemistry - A European Journal, 2004, 10, 5706-5716.	1.7	8
105	Isotope Exchange in Ionised CO2/COMixtures: The Role of Asymmetrical C2O3+ Ions. Chemistry - A European Journal, 2004, 10, 6411-6421.	1.7	6
106	A theoretical approach to molecular batteries: Cî—¸C bonds functioning as electron shuttles. Future Generation Computer Systems, 2004, 20, 793-805.	4.9	0
107	Phenylium and naphtylium cations in the interstellar medium: a density functional study on their reactivity towards D2 molecules. Future Generation Computer Systems, 2004, 20, 807-819.	4.9	2
108	Reactions of N+ ions with ethylene: a theoretical study on the addition mechanism into the olefin double bond. Chemical Physics, 2004, 297, 121-131.	0.9	6

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109	Reactions of N+ ions with benzene: a theoretical study on the C6NH6+ potential energy surface. Chemical Physics, 2004, 302, 295-308.	0.9	9
110	The Stability of documentclass{aastex} usepackage{amsbsy} usepackage{amsfonts} usepackage{amssymb} usepackage{bm} usepackage{mathrsfs} usepackage{pifont} usepackage{stmaryrd} usepackage{textcomp} usepackage{portland,xspace} usepackage{amsmath,amsxtra} usepackage[OT2,OT1]{fontenc} ewcommandcyr{ enewcommandmdefault{wncyr} enewcommandsfdefault{wncyss} enewcommandencodingdefault{OT2} ormalfont selectfont} DeclareTextFontCommand{extcyr}	1.6	23
111	Carbon Tetraoxide: Theoretically Predicted and Experimentally Detected. Angewandte Chemie, 2003, 115, 3093-3098.	1.6	4
112	Carbon Tetraoxide: Theoretically Predicted and Experimentally Detected. Angewandte Chemie - International Edition, 2003, 42, 2985-2990.	7.2	15
113	Sulfur hexafluoride corona discharge decomposition: gas-phase ion chemistry of SOF+ (x=1â€“3) ions. Chemical Physics Letters, 2003, 381, 168-176.	1.2	14
114	A theoretical approach to a chemical system convertible into a storage cell: carbon_carbon bonds functioning as electron donor and electron acceptor units. Journal of Molecular Catalysis A, 2003, 204-205, 787-792.	4.8	1
115	Gas-Phase Chemistry of NHxCly+ Ions. 3. Structure, Stability, and Reactivity of Protonated Trichloramine. Journal of Physical Chemistry A, 2003, 107, 2085-2092.	1.1	8
116	Infrared Spectroscopy of Matrix-Isolated Polycyclic Aromatic Compounds and Their Ions. 6. Polycyclic Aromatic Nitrogen Heterocycles. Journal of Physical Chemistry A, 2003, 107, 1486-1498.	1.1	100
117	Reactions of phenylium ions C6(H,D)5+ with D2. Journal of Chemical Physics, 2003, 119, 8366-8372.	1.2	15
118	Experimental and theoretical investigation of the production of cations containing Câ€“N bonds in the reaction of benzene with atomic nitrogen ions. Journal of Chemical Physics, 2003, 119, 1978-1985.	1.2	14
119	Theoretical Investigations on the Reactions of C6H5 + and C10H7 + with D2. Lecture Notes in Computer Science, 2003, , 366-375.	1.0	1
120	Density Functional Investigations on the C-C Bond Formation and Cleavage in Molecular Batteries. Lecture Notes in Computer Science, 2003, , 376-385.	1.0	0
121	Thionyl Fluoride from Sulfur Hexafluoride Corona Discharge Decomposition:â€‰ Gas-Phase Chemistry of [SOF2]H+ Ions. Journal of Physical Chemistry A, 2002, 106, 9261-9266.	1.1	12
122	A density functional investigation on the structural and electronic properties of niobiumâ€“silsesquioxane and niobium-2,2â€²-thiobisphenolic frameworks as models of an oxo surface. Computational and Theoretical Chemistry, 2002, 579, 181-189.	1.5	3
123	Formation of O3+ upon Ionization of O2: The Role of Isomeric O4+ Complexes. Chemistry - A European Journal, 2002, 8, 3653.	1.7	15
124	Charged and Neutral NO3 Isomers from the Ionization of NOx and O3 Mixtures. Chemistry - A European Journal, 2002, 8, 5684-5693.	1.7	17
125	On the design of a planar oxo matrix for binding transition metals: a density functional approach. Computational and Theoretical Chemistry, 2002, 583, 73-79.	1.5	0
126	Ab initio calculation and quasi-classical dynamics study of the two lowest potential energy surfaces of the O(1D)+HBr system*. International Journal of Quantum Chemistry, 2002, 86, 79-89.	1.0	8

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127	A theoretical analysis of [M(tmtaa)] and [M(acacen)] fragments employed in the organometallic chemistry of early transition metals. Journal of Organometallic Chemistry, 2002, 648, 14-26.	0.8	4
128	Mechanisms for the growth of polycyclic aromatic hydrocarbon (PAH) cations. Chemical Physics Letters, 2002, 355, 159-163.	1.2	19
129	Mechanisms for the incorporation of a nitrogen atom into polycyclic aromatic hydrocarbon cations. Chemical Physics Letters, 2001, 347, 473-480.	1.2	23
130	A theoretical analysis of the fundamental stepwise six-electron oxidation of porphyrinogen to porphyrins: the energetics of porphodimethene and artificial porphyrin intermediatesâ€Sâ€. Dalton Transactions RSC, 2001, , 1492-1497.	2.3	8
131	A New Sulfur Oxide, OSOSO, and Its Cation, Likely Present in the Io's Atmosphere:Â Detection and Characterization by Mass Spectrometric and Theoretical Methods. Journal of the American Chemical Society, 2001, 123, 478-484.	6.6	24
132	Ionization of Atmospheric Gases Containing Ozone and Carbonyl Sulfide. Formation and Reactivity of SO+Ions. Journal of Physical Chemistry A, 2001, 105, 1144-1149.	1.1	8
133	Gas-phase electrophilic fluorination of methanol by XeF+. Formation and characterization of protonated methyl hypofluorite and hypoxenite. Journal of Mass Spectrometry, 2001, 36, 392-396.	0.7	8
134	Metal-Metal and Carbon-Carbon Bonds as Potential Components of Molecular Batteries. Chemistry - A European Journal, 2001, 7, 3052-3061.	1.7	32
135	Ionization of O3 in Excess N2: A New Route to N2O via Intermediate N2O3+ Complexes. Angewandte Chemie - International Edition, 2001, 40, 1938-1941.	7.2	12
136	Ionization of O3 in Excess N2: A New Route to N2O via Intermediate N2O3+ Complexes. Angewandte Chemie - International Edition, 2001, 40, 2947-2947.	7.2	4
137	Using hydrogen and chlorine on Si(111) to store data, an improved model. Chemical Physics Letters, 2001, 347, 291-296.	1.2	4
138	A density functional investigation on d0-Zr(IV) organometallic fragments. Chemical Physics Letters, 2001, 344, 536-542.	1.2	1
139	S3O, a new sulfur oxide identified in the gas phase. Chemical Communications, 2001, , 2086-2087.	2.2	14
140	Ionization of Ozone/Chlorofluorocarbon Mixtures in Atmospheric Gases: Formation and Remarkable Dissociation of [CHXYO3]+ Complexes (X= H, Cl, F; Y= Cl, F). Chemistry - A European Journal, 2000, 6, 2572-2581.	1.7	15
141	Anisotropy Effects in Methyl Chloride Ionization by Metastable Neon Atoms at Thermal Energies. Journal of Physical Chemistry A, 2000, 104, 1405-1415.	1.1	26
142	Reactivity of Gaseous XeF+Ions with Acetonitrile. A Joint Mass Spectrometric and Theoretical Study of Isomeric C2H3NF+and C2H3NXe+Cations. Journal of Physical Chemistry A, 2000, 104, 7574-7579.	1.1	9
143	Gas Phase Chemistry of NHxCly+Ions. II. Structure, Stability and Reactivity of Protonated Dichloramine. Journal of Physical Chemistry A, 2000, 104, 5617-5624.	1.1	10
144	Gas-phase reactions of protonated chlorine, Cl2H+, with H2(D2) and CH4. A mass spectrometric and theoretical study. Chemical Physics Letters, 1999, 304, 191-196.	1.2	10

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145	An ab initio investigation of the electronic structure of ionâ€“pair enolates NH2COCH2TiF3, PH2COCH2TiF3, C6H5COCH2TiF3, C6H5SOCH2TiF3: the influence of the heteroatom. Part II. Computational and Theoretical Chemistry, 1999, 459, 47-55.	1.5	4
146	An `ab initio' investigation of the electronic structure of ion-pair enolates NH2COCH2CuPH3, PH2COCH2CuPH3, C6H5COCH2CuPH3, C6H5SOCH2CuPH3: the influence of the heteroatom. Part III. Computational and Theoretical Chemistry, 1999, 459, 57-65.	1.5	5
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