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	Theoretical studies of the firstâ€•and secondâ€•row transitionâ€•metal monoâ€•and dicarbonyl positive ions. Journal of Chemical Physics, 1990, 93, 609-624.	1.2	190
2	The binding energies of one and two water molecules to the first transitionâ€•row metal positive ions. Journal of Chemical Physics, 1989, 90, 7264-7272.	1.2	180
3	Anab initiostudy of Fe(CO)n,n=1,5, and Cr(CO)6. Journal of Chemical Physics, 1991, 94, 2031-2039.	1.2	140
4	The binding energies of one and two water molecules to the first transitionâ€•row metal positive ions. II. Journal of Chemical Physics, 1990, 92, 1876-1878.	1.2	119
5	pKa of zinc-bound water and nucleophilicity of hydroxo-containing species. Ab initio calculations on models for zinc enzymes. Inorganic Chemistry, 1990, 29, 1460-1463.	1.9	114
6	Theoretical Study of M+â^'CO2and OM+CO Systems for First Transition Row Metal Atoms. Journal of Physical Chemistry A, 1997, 101, 7854-7859.	1.1	112
7	Methane Activation by Metalâ€Free Radical Cations: Experimental Insight into the Reaction Intermediate. Chemistry - A European Journal, 2009, 15, 4248-4252.	1.7	108
8	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
9	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
10	Theoretical study of the bonding of the first- and second-row transition-metal positive ions to methylene. The Journal of Physical Chemistry, 1992, 96, 6969-6973.	2.9	80
11	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
12	Reactions of Laser-Ablated Scandium Atoms with Dioxygen. Infrared Spectra of ScO, OScO, (O2)ScO, (ScO)2, and Sc(O2)2 in Solid Argon. Journal of Physical Chemistry A, 1997, 101, 9085-9091.	1.1	69
13	Gas-Phase Ion Chemistry of Borazine, an Inorganic Analogue of Benzene. Journal of the American Chemical Society, 1999, 121, 11204-11210.	6.6	63
14	COMPCHEM: Progress Towards GEMS a Grid Empowered Molecular Simulator and Beyond. Journal of Grid Computing, 2010, 8, 571-586.	2.5	63
15	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
16	On the binding energy of Hen+, for n = 2â€“7. Chemical Physics Letters, 1989, 159, 479-484.	1.2	51
17	A theoretical study of the lowâ€lying states of Ti2and Zr2. Journal of Chemical Physics, 1991, 95, 1057-1063.	1.2	50
18	Anabinitiostudy of the O(1D)+HCl reaction. Journal of Chemical Physics, 1996, 105, 2710-2718.	1.2	50

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19	Monocyclopentadienylchlorooxotitanium(IV) dimers, trimers and tetramers. Journal of the Chemical Society Dalton Transactions, 1992, , 1081.	1.1	49
20	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
21	Theoretical studies of the first- and second-row transition-metal dimethyls and their positive ions. The Journal of Physical Chemistry, 1990, 94, 8656-8663.	2.9	48
22	Molecular Batteries Based on Carbon-Carbon Bond Formation and Cleavage in Titanium and Vanadium Schiff Base Complexes. Chemistry - A European Journal, 1999, 5, 708-721.	1.7	48
23	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
24	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
25	Production of ions at high energy and its role in extraterrestrial environments. Rendiconti Lincei, 2013, 24, 53-65.	1.0	45
26	A highâ€level ab initio study of the N₂ + N₂ reaction channel. Journal of Computational Chemistry, 2013, 34, 2668-2676.	1.5	44
27	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
28	Dissociative double photoionization of benzene molecules in the 26â€“33 eV energy range. Physical Chemistry Chemical Physics, 2011, 13, 8245.	1.3	41
29	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
30	Combined crossed beam and theoretical studies of the C(1D) + CH4 reaction. Journal of Chemical Physics, 2013, 138, 024311.	1.2	40
31	On the bonding in Be22+. Chemical Physics Letters, 1989, 159, 485-488.	1.2	39
32	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
33	Experimental and Theoretical Approach to the Understanding of TiCl4 Interacting with Arenes. Isolation of a d0-Metal-Arene Complex and Cyclotrimerization of But-2-yne Promoted by TiCl4. Inorganic Chemistry, 1994, 33, 2018-2028.	1.9	35
34	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
35	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
36	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

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37	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
38	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
39	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
40	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
41	Modeling the Intermolecular Interactions and Characterization of the Dynamics of Collisional Autoionization Processes. Lecture Notes in Computer Science, 2013, , 69-83.	1.0	33
42	Ab initio calculations of the copper(2+)-O2- interaction as a model for the mechanism of copper/zinc superoxide dismutase. Inorganic Chemistry, 1986, 25, 1005-1008.	1.9	32
43	Dissociative Ionization of Methyl Chloride and Methyl Bromide by Collision with Metastable Neon Atoms. Journal of Physical Chemistry A, 1997, 101, 7505-7512.	1.1	32
44	Use of Norbornadiene in Solar Energy Storage:Â Theoretical Study of a Copper(I) Photosensitizer for the Norbornadieneâ"Quadricyclane Transformation. Inorganic Chemistry, 1999, 38, 1520-1522.	1.9	32
45	Metal-Metal and Carbon-Carbon Bonds as Potential Components of Molecular Batteries. Chemistry - A European Journal, 2001, 7, 3052-3061.	1.7	32
46	Nanostructure Selectivity for Molecular Adsorption and Separation: the Case of Graphyne Layers. Journal of Physical Chemistry C, 2018, 122, 16195-16208.	1.5	32
47	On the bonding of La+ and La2+ to C2H2, C2H4, and C3H6. Chemical Physics Letters, 1990, 166, 189-194.	1.2	31
48	Changes in the Interaction Mode of Bridging â€œC2â€•Units According to Transition Metal Parameters:Â A Theoretical Approach. Organometallics, 1996, 15, 4264-4273.	1.1	31
49	The vibrational frequencies of CaO 2 , ScO 2 , and TiO 2 : a comparison of theoretical methods. Theoretical Chemistry Accounts, 1998, 99, 106-112.	0.5	31
50	Experimental Detection of Theoretically Predicted N2CO. Angewandte Chemie - International Edition, 2005, 44, 462-465.	7.2	31
51	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
52	Second-Order Moeller-Plesset Perturbation Theory for Systems Involving First Transition Row Metals. The Journal of Physical Chemistry, 1994, 98, 9498-9502.	2.9	30
53	Crossed-Beam and Theoretical Studies of the S(¹D) + C₂H₂ Reaction. Journal of Physical Chemistry A, 2009, 113, 4330-4339.	1.1	28
54	On the electronic structure and bonding of the polynuclear aryl derivatives of the group IB metals Cu5(C6H5)5, Ag4(C6H5)4 and Au5(C6H5)5 by density functional theory. Chemical Physics Letters, 1996, 257, 41-48.	1.2	27

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55	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
56	The Proton Affinity and Gasâ€Phase Basicity of Sulfur Dioxide. ChemPhysChem, 2011, 12, 112-115.	1.0	27
57	The bis(methylcyclopentadienyl)titanium(IV) molybdate dimer: a titanium(IV)-molybdenum(VI) eight-membered metal-oxo ring. Inorganic Chemistry, 1991, 30, 3245-3246.	1.9	26
58	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
59	Interaction between iron(0) and heterocumulenes: "ab initio" calculations on the model compounds Fe(CO)2(PH3)2(.eta.2-OCX) and Fe(CO)2(PH3)2(.eta.2-SCX), with X = O, S, NH, CH2. Inorganic Chemistry, 1987, 26, 3805-3811.	1.9	24
60	Electron momentum spectroscopy of trisubstituted amines: The valence shell orbitals of triethylamine. Chemical Physics, 1987, 116, 399-410.	0.9	24
61	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
62	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
63	Câ^'C Bond as Shuttle of Two Electrons in Intermolecular and Intramolecular Processes: A Theoretical Approach to Molecular Batteries. Chemistry - A European Journal, 1999, 5, 2914-2920.	1.7	23
64	Mechanisms for the incorporation of a nitrogen atom into polycyclic aromatic hydrocarbon cations. Chemical Physics Letters, 2001, 347, 473-480.	1.2	23
65	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{ }	1.6	23
66	Water (H2O) m or Benzene (C6H6) n Aggregates to Solvate the Kâ€‰+â€‰?. Lecture Notes in Computer Science, 2013, , 1-15.	1.0	23
67	Orbital momentum distributions and binding energies for the complete valence shell of molecular chlorine by electron momentum spectroscopy. Chemical Physics, 1987, 113, 1-18.	0.9	21
68	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
69	Ionization of fluoromethanes: CHF3 and CF4. A Greensì€ function study and an (e, 2e) spectroscopic investigation. Chemical Physics Letters, 1982, 90, 445-452.	1.2	20
70	A novel class of hexanuclear titanoxanes: synthesis, structure and electronic configuration. Journal of Organometallic Chemistry, 1995, 488, 141-154.	0.8	20
71	Mechanisms for the growth of polycyclic aromatic hydrocarbon (PAH) cations. Chemical Physics Letters, 2002, 355, 159-163.	1.2	19
72	Reactivity of C10H7+ and C10D7+ with H2 and D2. Journal of Chemical Physics, 2004, 121, 6728-6737.	1.2	19

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73	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
74	Ionization potentials and electron momentum distributions for SiF4 valence-shell orbitals: an (e,2e) spectroscopic investigation and Green's function study. Chemical Physics Letters, 1986, 128, 67-75.	1.2	18
75	Study of the interaction between iron(0) and carbon dioxide, carbonyl sulphide and carbon disulphide: â€œab initioâ€•calculations on the model compounds Fe(CO)2(PH3)2(Î·2-CO2), Fe(CO)2(PH3)2(Î·2-COS), Fe(CO)2(PH3)2(Î·2-CS2), and Fe(PH3)4(Î·2-CO2). Journal of Organometallic Chemistry, 1987, 332, 153-164.	0.8	18
76	A Theoretical Study of Dinitrogen Activation by Vanadium(II) and Vanadium(III): Ab Initio Calculations on Various Model Compounds. Inorganic Chemistry, 1994, 33, 4390-4397.	1.9	17
77	Charged and Neutral NO3 Isomers from the Ionization of NOx and O3 Mixtures. Chemistry - A European Journal, 2002, 8, 5684-5693.	1.7	17
78	Potential energy surfaces in hyperspherical coordinates: AB initio kinetic paths for the O(3P)+H2 reaction. Chemical Physics Letters, 1989, 162, 179-184.	1.2	16
79	Gas-Phase Chemistry of NHxCly+. 1. Structure, Stability, and Reactivity of Protonated Monochloramine. Journal of Physical Chemistry A, 1998, 102, 10189-10194.	1.1	16
80	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
81	Electronic Structure, Heisenberg Coupling Constants, and Metalâ^'Metal Bond in Dimeric Iron(II) Organometallics with the Metal Centers at Variable Distances:Â A Density Functional Approach. Inorganic Chemistry, 1996, 35, 7776-7785.	1.9	15
82	Gaseous [H3Câ^'Clâ^'Cl]+ Ions from the Reaction of Methane with Cl3+, the First Example of a New Dihalogenation Process: Formation and Characterization of CH3Cl2+ Isomers by Experimental and Theoretical Methods. Chemistry - A European Journal, 1999, 5, 2750-2756.	1.7	15
83	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
84	Formation of O3+ upon Ionization of O2: The Role of Isomeric O4+ Complexes. Chemistry - A European Journal, 2002, 8, 3653.	1.7	15
85	Carbon Tetraoxide: Theoretically Predicted and Experimentally Detected. Angewandte Chemie - International Edition, 2003, 42, 2985-2990.	7.2	15
86	Reactions of phenylium ions C6(H,D)5+ with D2. Journal of Chemical Physics, 2003, 119, 8366-8372.	1.2	15
87	A theoretical investigation of the copper-super-oxide system. A model for the mechanism of copper-zinc superoxide dismutase. Inorganica Chimica Acta, 1985, 107, L21-L22.	1.2	14
88	S3O, a new sulfur oxide identified in the gas phase. Chemical Communications, 2001, , 2086-2087.	2.2	14
89	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
90	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

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91	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
92	Theoretical investigation of the energy dependence of photoionization cross-sections and angular distributions of photoemission of CH4 and CF4. Journal of Electron Spectroscopy and Related Phenomena, 1986, 41, 439-452.	0.8	13
93	Theoretical Study of Dinitrogen Activation in Dinuclear V(II) and V(III) Hexacoordinated Complexes: Ab Initio Calculations on Various Model Compounds. Inorganic Chemistry, 1995, 34, 3410-3417.	1.9	13
94	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
95	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
96	Addendum to â€œon the bonding in Be22+â€• Chemical Physics Letters, 1990, 165, 501-502.	1.2	12
97	Theoretical study of the metathesis-like reaction between ditungsten hexaalkoxides and alkynesâ€Šâ€. Journal of the Chemical Society Dalton Transactions, 1997, , 3845-3852.	1.1	12
98	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
99	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
100	The HSSS Radical and the HSSSâ¯ Anion. Journal of Physical Chemistry A, 2008, 112, 8471-8477.	1.1	12
101	An Experimental and Theoretical Investigation of 1-Butanol Pyrolysis. Frontiers in Chemistry, 2019, 7, 326.	1.8	12
102	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
103	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
104	Structure of copper(II) complexes with L-leucyl-D- or L-leucyl-L-phenylalanine and molecular orbital calculations on their stabilization. Journal of the Chemical Society Dalton Transactions, 1996, , 3449.	1.1	11
105	An â€œab initioâ€•investigation of the electronic structure of ion-pair enolates NH2COCH2Li, PH2COCH2Li, C6H5COCH2Li, C6H5SOCH2Li: the influence of the heteroatom. Computational and Theoretical Chemistry, 1998, 431, 33-46.	1.5	11
106	Elemental Chlorine and Chlorine Fluoride:â€‰ Theoretical and Experimental Proton Affinity and the Gas Phase Chemistry of Cl2H + and FClH+ Ions. Journal of Physical Chemistry A, 1998, 102, 10560-10567.	1.1	11
107	Isotope Exchange in Ionized O3/O2Mixtures:Â The Role of O5+, a Unique On+Complex. Inorganic Chemistry, 1998, 37, 1398-1400.	1.9	11
108	Ionization of Ozone/Chlorofluorocarbon Mixtures in Atmospheric Gases: Formation and Dissociation of [CHX2O3]+ Complexes (X=Cl, F). Angewandte Chemie - International Edition, 1999, 38, 2408-2410.	7.2	11

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109	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
110	Gaseous Trihalogen Cations. Formation, Structure and Reactivity of Cl3+ and Cl2F+ Ions from a Joint ab Initio and FT-ICR Study. Journal of Physical Chemistry A, 1999, 103, 2128-2133.	1.1	10
111	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
112	Gas phase protonation of trifluoromethyl sulfur pentafluoride. Physical Chemistry Chemical Physics, 2005, 7, 1181.	1.3	10
113	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
114	The Oxidation of Sulfur Dioxide by Single and Double Oxygen Transfer Paths. ChemPhysChem, 2014, 15, 2723-2731.	1.0	10
115	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
116	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
117	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
118	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
119	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
120	A theoretical study on the co-ordination of dinitrogen and related molecules to nickel(0): â€˜ab initioâ€™ calculations on the model compounds [Ni(PH3)2(N2)], [Ni(PH3)2(N2CH2)], and [Ni(PH3)2(N2H2)]. Journal of the Chemical Society Dalton Transactions, 1989, , 33-38.	1.1	9
121	On the relative stability of side-on and end-on coordination of dinitrogen to nickel (O): â€ab initioâ€œ calculations on the model compounds [NiN2] and [Ni(PH3)2N2]. Chemical Physics Letters, 1991, 185, 522-528.	1.2	9
122	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
123	Reactions of N+ ions with benzene: a theoretical study on the C6NH6+ potential energy surface. Chemical Physics, 2004, 302, 295-308.	0.9	9
124	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
125	Production and Characterization of Molecular Dications: Experimental and Theoretical Efforts. Molecules, 2020, 25, 4157.	1.7	9
126	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

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127	The Escape Probability of Some Ions from Mars and Titan Ionospheres. Lecture Notes in Computer Science, 2014, , 554-570.	1.0	9
128	Interaction between iron(0) and formaldehyde, thioformaldehyde, and acetone: ab initio calculations on the model compounds Fe(CO)2(PH3)2(.eta.2-CH2O), Fe(CO)2(PH3)2(.eta.2-CH2S), Fe(PH3)4(.eta.2-CH2O), and Fe(PH3)4(.eta.2-CMe2O). Inorganic Chemistry, 1988, 27, 69-73.	1.9	8
129	The photoelectron spectroscopy of ZnCl2. Chemical Physics, 1990, 146, 237-243.	0.9	8
130	â€˜Ab initioâ€™ calculations on methane interacting with the fourteen-electron Ni(PH3)2fragment. Journal of the Chemical Society Dalton Transactions, 1992, , 1821-1826.	1.1	8
131	Theoretical study of acetylide complexes of early transition metalsâ€Šâ€. Journal of the Chemical Society Dalton Transactions, 1997, , 3841-3844.	1.1	8
132	Differentiating between H and F or H and CN on C(111) or Si(111) Surfaces. Journal of Physical Chemistry B, 1998, 102, 2403-2405.	1.2	8
133	A theoretical analysis of the fundamental stepwise six-electron oxidation of porphyrinogen to porphyrins: the energetics of porphodimethene and artificial porphyrin intermediatesâ€Šâ€. Dalton Transactions RSC, 2001, , 1492-1497.	2.3	8
134	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
135	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
136	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
137	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
138	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
139	Ironâ€Promoted Cï£¿C Bond Formation in the Gas Phase. Angewandte Chemie - International Edition, 2015, 54, 14359-14362.	7.2	8
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