Massimiliano Aschi

List of Publications by Citations

169 papers	4,263 citations	30 h-index	57 g-index
174 ext. papers	4,610 ext. citations	4.2 avg, IF	5.26 L-index

#	Paper	IF	Citations
169	The singlet and triplet states of phenyl cation. A hybrid approach for locating minimum energy crossing points between non-interacting potential energy surfaces. *Theoretical Chemistry Accounts*, **1998**, 99, 95-99	1.9	693
168	Spin-forbidden dehydrogenation of methoxy cation: a statistical view. *Physical Chemistry Chemical Physics*, **1999**, 1, 5555-5563	3.6	257
167	Gold-catalyzed reactions of 2-alkynyl-phenylamines with alpha,beta-enones. *Journal of Organic Chemistry*, **2005**, 70, 2265-73	4.2	168
166	Modelling spin-forbidden reactions: recombination of carbon monoxide with iron tetracarbonyl. *Faraday Discussions*, **2003**, 124, 129-43; discussion 145-53, 453-5	3.6	140
165	Antimicrobial peptides: natural templates for synthetic membrane-active compounds. *Cellular and Molecular Life Sciences*, **2008**, 65, 2450-60	10.3	137
164	A first-principles method to model perturbed electronic wavefunctions: the effect of an external homogeneous electric field. *Chemical Physics Letters*, **2001**, 344, 374-380	2.5	98
163	HCN Synthesis from Methane and Ammonia: Mechanisms of Pt+-Mediated C□N Coupling. *Journal of the American Chemical Society*, **1999**, 121, 10614-10625	16.4	98
162	Crystal structure of the peroxisome proliferator-activated receptor gamma (PPARgamma) ligand binding domain complexed with a novel partial agonist: a new region of the hydrophobic pocket could be exploited for drug design. *Journal of Medicinal Chemistry*, **2008**, 51, 7768-76	8.3	80
161	A Gas-Phase Model for the Pt -Catalyzed Coupling of Methane and Ammonia. *Angewandte Chemie - International Edition*, **1998**, 37, 829-832	16.4	64
160	Pd-catalyzed regioselective hydroarylation of □(2-aminoaryl)-□ynones with organoboron derivatives as a tool for the synthesis of quinolines: experimental evidence and quantum-chemical calculations. *Tetrahedron*, **2008**, 64, 5354-5361	2.4	63
159	The reversible opening of water channels in cytochrome c modulates the heme iron reduction potential. *Journal of the American Chemical Society*, **2012**, 134, 13670-8	16.4	62
158	Experimental and computational study of neutral xenon halides (XeX) in the gas phase for X=F, Cl, Br, and I. *Journal of Chemical Physics*, **1998**, 108, 8446-8455	3.9	58
157	Theoretical characterization of electronic states in interacting chemical systems. *Journal of Chemical Physics*, **2009**, 130, 084109	3.9	53
156	Does adsorption at hydroxyapatite surfaces induce peptide folding? Insights from large-scale B3LYP calculations. *Journal of the American Chemical Society*, **2012**, 134, 10899-910	16.4	47
155	Extension of the perturbed matrix method: application to a water molecule. *Chemical Physics Letters*, **2002**, 365, 450-456	2.5	46
154	Electronic properties of formaldehyde in water: a theoretical study. *Chemical Physics Letters*, **2003**, 381, 187-193	2.5	45
153	Rhodium- and Palladium-Catalyzed Hydroarylation of Propargylic Amines with Arylboronic Acids. *Advanced Synthesis and Catalysis*, **2010**, 352, 493-498	5.6	44

152	Quantitative structure-retention relationships of pesticides in reversed-phase high-performance liquid chromatography. *Analytica Chimica Acta*, **2007**, 582, 235-42	6.6	44
151	Cation□Interactions between ammonium ion and aromatic rings: an energy decomposition study. *Computational and Theoretical Chemistry*, **2002**, 587, 177-188		43
150	Structural insight into peroxisome proliferator-activated receptor gamma binding of two ureidofibrate-like enantiomers by molecular dynamics, cofactor interaction analysis, and site-directed mutagenesis. *Journal of Medicinal Chemistry*, **2010**, 53, 4354-66	8.3	39
149	Theoretical modeling of the valence UV spectra of 1,2,3-triazine and uracil in solution. *Physical Chemistry Chemical Physics*, **2006**, 8, 1385-93	3.6	36
148	Role of the amino sugar in the DNA binding of disaccharide anthracyclines: crystal structure of the complex MAR70/d(CGATCG). *Bioorganic and Medicinal Chemistry*, **2005**, 13, 1673-9	3.4	36
147	Theoretical modeling of UV-Vis absorption and emission spectra in liquid state systems including vibrational and conformational effects: explicit treatment of the vibronic transitions. *Journal of Chemical Physics*, **2014**, 140, 164104	3.9	35
146	Conformational fluctuations and electronic properties in myoglobin. *Journal of Computational Chemistry*, **2004**, 25, 974-84	3.5	34
145	Extending the perturbed matrix method beyond the dipolar approximation: comparison of different levels of theory. *Physical Chemistry Chemical Physics*, **2018**, 20, 24369-24378	3.6	32
144	Theoretical-computational modelling of infrared spectra in peptides and proteins: a new frontier for combined theoretical-experimental investigations. *Current Opinion in Structural Biology*, **2010**, 20, 155-61	8.1	31
143	Theoretical modeling of vibroelectronic quantum states in complex molecular systems: solvated carbon monoxide, a test case. *Journal of Chemical Physics*, **2005**, 122, 124506	3.9	30
142	Design, modelling, synthesis and biological evaluation of peptidomimetic phosphinates as inhibitors of matrix metalloproteinases MMP-2 and MMP-8. *Bioorganic and Medicinal Chemistry*, **2005**, 13, 4740-9	3.4	30
141	Theoretical characterisation of the electronic excitation in liquid water. *ChemPhysChem*, **2005**, 6, 53-8	3.2	30
140	Synthesis of 2-Acylindoles via Ag- and Cu-Catalyzed anti-Michael Hydroamination of □(2-Aminophenyl)-□ynones: Experimental Results and DFT Calculations. *Journal of Organic Chemistry*, **2018**, 83, 6354-6362	4.2	30
139	Visualizing Excited-State Dynamics of a Diaryl Thiophene: Femtosecond Stimulated Raman Scattering as a Probe of Conjugated Molecules. *Journal of Physical Chemistry Letters*, **2016**, 7, 2981-8	6.4	29
138	The effect of protein conformational flexibility on the electronic properties of a chromophore. *Biophysical Journal*, **2003**, 84, 2805-13	2.9	29
137	Computational study of the reaction of N(2D) atoms with CH2F radicals: an example of a barrier-free reaction involving very high internal energies. *Journal of Chemical Physics*, **2005**, 123, 114312	3.9	29
136	Theoretical modeling of the absorption spectrum of aqueous riboflavin. *Chemical Physics Letters*, **2017**, 669, 119-124	2.5	28
135	A few key residues determine the high redox potential shift in azurin mutants. *Organic and Biomolecular Chemistry*, **2015**, 13, 11003-13	3.9	28

134	Theoretical modeling of UV-Vis absorption and emission spectra in liquid state systems including vibrational and conformational effects: the vertical transition approximation. *Journal of Chemical Physics*, **2013**, 139, 114102	3.9	28
133	Structural modifications of ionic liquid surfactants for improving the water dispersibility of carbon nanotubes: an experimental and theoretical study. *Physical Chemistry Chemical Physics*, **2011**, 13, 11373-83	3.6	28
132	New insight into the IR-spectra/structure relationship in amyloid fibrils: a theoretical study on a prion peptide. *Journal of the American Chemical Society*, **2011**, 133, 11414-7	16.4	28
131	On the origin of IR spectral changes upon protein folding. *Chemical Physics Letters*, **2010**, 488, 213-218	2.5	28
130	Theoretical Modeling of Enzyme Reaction Chemistry: The Electron Transfer of the Reduction Mechanism in CuZn Superoxide Dismutase. *Journal of Physical Chemistry B*, **2004**, 108, 16255-16260	3.4	28
129	A general theoretical model for electron transfer reactions in complex systems. *Physical Chemistry Chemical Physics*, **2012**, 14, 1360-70	3.6	27
128	Reappraisal of the spin-forbidden unimolecular decay of the methoxy cation *Chemical Communications*, **1998**, 531-533	5.8	27
127	Mixed Quantum-Classical Methods for Molecular Simulations of Biochemical Reactions With Microwave Fields: The Case Study of Myoglobin. *IEEE Transactions on Microwave Theory and Techniques*, **2008**, 56, 2511-2519	4.1	27
126	Statistical mechanical modelling of chemical reactions in complex systems: the kinetics of the Haem carbon monoxide binding nbinding reaction in Myoglobin. *Theoretical Chemistry Accounts*, **2007**, 117, 637-647	1.9	26
125	Gaseous Protonated Nitrosyl Fluoride. Experimental and Theoretical Characterization of Two Distinguishable Isomers, HONF+ and ONFH+, and Evaluation of the Barrier for Their Interconversion. *The Journal of Physical Chemistry*, **1994**, 98, 2713-2718		26
124	Chirality transfer from a single chiral molecule to 2D superstructures in alaninol on the Cu(100) surface. *Langmuir*, **2011**, 27, 7410-8	4	25
123	Physicochemical properties of fluorescent probes: experimental and computational determination of the overlapping pKa values of carboxyfluorescein. *Journal of Organic Chemistry*, **2008**, 73, 3411-7	4.2	25
122	Theoretical modeling of chemical reactions in complex environments: the intramolecular proton transfer in aqueous malonaldehyde. *Journal of Physical Organic Chemistry*, **2006**, 19, 518-530	2.1	25
121	Computational study on the kinetics of the reaction of N(4S) with CH2F. *Chemical Physics Letters*, **2003**, 374, 594-600	2.5	25
120	Dynamical aspects of TEM-1 beta-lactamase probed by molecular dynamics. *Journal of Computer-Aided Molecular Design*, **2005**, 19, 329-40	4.2	25
119	Toward a Better Understanding of Steric Stabilization When Using Block Copolymers as Stabilizers of Single-Walled Carbon Nanotubes (SWCNTs) Aqueous Dispersions. *Macromolecules*, **2012**, 45, 8043-8050	5.5	24
118	Theoretical modeling of enzyme reactions: the thermodynamics of formation of compound 0 in horseradish peroxidase. *Journal of Physical Chemistry B*, **2008**, 112, 3184-92	3.4	24
117	Theoretical characterization of carbon monoxide vibrational spectrum in sperm whale myoglobin distal pocket. *Biophysical Journal*, **2007**, 92, 3442-7	2.9	22

116	Folding propensity and biological activity of peptides: the effect of a single stereochemical isomerization on the conformational properties of bombinins in aqueous solution. *Biopolymers*, **2008**, 89, 769-78	2.2	22
115	Cyclochiral resorcin[4]arenes as effective enantioselectors in the gas phase. *Journal of Mass Spectrometry*, **2012**, 47, 72-8	2.2	20
114	Modeling quantum vibrational excitations in condensed-phase molecular systems. *Theoretical Chemistry Accounts*, **2011**, 129, 31-43	1.9	20
113	Theoretical characterization of temperature and density dependence of liquid water electronic excitation energy: comparison with recent experimental data. *Journal of Chemical Physics*, **2008**, 128, 021103	3.9	20
112	A DFT Study of the Low-Lying Singlet Excited States of the All-Trans Peridinin in vacuo. *Journal of Physical Chemistry A*, **2004**, 108, 6763-6770	2.8	20
111	Modeling of chemical reactions in micelle: water-mediated keto-enol interconversion as a case study. *Journal of Physical Chemistry B*, **2011**, 115, 8102-11	3.4	19
110	Conformational analysis and UV/Vis spectroscopic properties of a rotaxane-based molecular machine in acetonitrile dilute solution: when simulations meet experiments. *Physical Chemistry Chemical Physics*, **2011**, 13, 2342-9	3.6	19
109	Peptide backbone folding induced by the C(alpha)-tetrasubstituted cyclic alpha-amino acids 4-amino-1,2-dithiolane-4-carboxylic acid (Adt) and 1-aminocyclopentane-1-carboxylic acid (Ac5c). A joint computational and experimental study. *Organic and Biomolecular Chemistry*, **2003**, 1, 1980-8	3.9	19
108	Experimental and Theoretical Characterization of Long-Lived Triplet State CH3CH2S+Cations. *Journal of the American Chemical Society*, **2000**, 122, 10133-10142	16.4	19
107	An Alternative Route To Electrophilic Substitution. 2. Aromatic Alkylation in the Ion Neutral Complexes Formed Upon Addition of Gaseous Arenium Ions to Olefins. *Journal of the American Chemical Society*, **1995**, 117, 12832-12839	16.4	19
106	The Crafts□Friedel Reaction: Aromatic Alkylation within the Complex Formed upon Addition of a Gaseous Arenium Ion to an Olefin. *Angewandte Chemie International Edition in English*, **1995**, 34, 1589-1591		19
105	Theoretical modeling of the spectroscopic absorption properties of luciferin and oxyluciferin: A critical comparison with recent experimental studies. *Chemical Physics*, **2012**, 392, 205-214	2.3	18
104	Insights on the mechanistic features of catalytic oxidations of simple and conjugated olefins promoted by VO(acac)2/H2O2 system, in acetonitrile: A computational study. *Catalysis Today*, **2012**, 192, 56-62	5.3	17
103	The role of arginine 38 in horseradish peroxidase enzyme revisited: a computational investigation. *Biophysical Chemistry*, **2009**, 141, 87-93	3.5	17
102	Natural D240G Toho-1 mutant conferring resistance to ceftazidime: biochemical characterization of CTX-M-43. *Journal of Antimicrobial Chemotherapy*, **2008**, 62, 991-7	5.1	17
101	Unimolecular decay of the thiomethoxy cation, CH3S+: A computational study on the detailed mechanistic aspects. *Journal of Chemical Physics*, **1999**, 111, 6759-6768	3.9	17
100	Simulation of the amide I infrared spectrum in photoinduced peptide folding/unfolding transitions. *Journal of Physical Chemistry B*, **2013**, 117, 12383-90	3.4	16
99	Alternative Electron-Transfer Channels Ensure Ultrafast Deactivation of Light-Induced Excited States in Riboflavin Binding Protein. *Journal of Physical Chemistry Letters*, **2017**, 8, 3321-3327	6.4	16

98	Characterization of electronic properties in complex molecular systems: modeling of a micropolarity probe. *Journal of Physical Chemistry B*, **2010**, 114, 1915-24	3.4	16
97	Mechanistic Aspects of F+ Transfer Reactions: A Model Study in the Gas Phase. *Chemistry - A European Journal*, **1998**, 4, 2366-2374	4.8	16
96	On the effect of a point mutation on the reactivity of CuZn superoxide dismutase: a theoretical study. *Journal of Physical Chemistry B*, **2006**, 110, 7538-44	3.4	16
95	The ionization potential of NF 3 : a G3 computational study on the thermochemical properties of NF x and NF x + (x =1□). *Computational and Theoretical Chemistry*, **2000**, 497, 205-209		16
94	Experimental Study on the Mechanism of Gas-Phase Aromatic Nitration by Protonated Methyl Nitrate. *Journal of the American Chemical Society*, **1994**, 116, 9535-9542	16.4	16
93	The role of disulfide bonds and N-terminus in the structural properties of hepcidins: insights from molecular dynamics simulations. *Biopolymers*, **2010**, 93, 917-26	2.2	15
92	Gaseous protonated nitrosamide. A G2 theoretical study on the structure, stability, and interconversion of (H2N?NO) H+ isomers. *Chemical Physics Letters*, **1997**, 267, 98-104	2.5	15
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90	The addition of NF+2 to H2O as a route to gaseous protonated F2NOH. *International Journal of Mass Spectrometry and Ion Processes*, **1994**, 130, 117-125		15
89	Photoexcitation and relaxation kinetics of molecular systems in solution: towards a complete in silico model. *Physical Chemistry Chemical Physics*, **2016**, 18, 28919-28931	3.6	15
88	Liposome destabilization by a 2,7-diazapyrenium derivative through formation of transient pores in the lipid bilayer. *Small*, **2010**, 6, 952-9	11	14
87	Reaction of N(2D) atoms with bromomethyl radicals: A theoretical study. *Chemical Physics*, **2006**, 328, 45-52	2.3	14
86	Essential dynamics for the study of microstructures in liquids. *Journal of Computational Chemistry*, **2015**, 36, 399-407	3.5	13
85	Computational study of the catalytic domain of human neutrophil collagenase. specific role of the S3 and S□ subsites in the interaction with a phosphonate inhibitor. *Journal of Computer-Aided Molecular Design*, **2002**, 16, 213-25	4.2	13
84	Flexible and Comprehensive Implementation of MD-PMM Approach in a General and Robust Code. *Journal of Chemical Theory and Computation*, **2017**, 13, 5506-5514	6.4	12
83	Peptides containing 4-amino-1,2-dithiolane-4-carboxylic acid (Adt): conformation of Boc-Adt-Adt-NHMe and NH...S interactions. *Journal of Peptide Science*, **2005**, 11, 104-12	2.1	12
82	Theoretical-computational modeling of photo-induced charge separation spectra and charge recombination kinetics in solution. *Physical Chemistry Chemical Physics*, **2014**, 16, 20624-38	3.6	11
81	Modeling triplet flavin-indole electron transfer and interradical dipolar interaction: a perturbative approach. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	11

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79	Can a synthetic thread act as an electrochemically switchable molecular device?. *Chemical Communications*, **2008**, 3399-401	5.8	11
78	Theoretical study of intramolecular charge transfer in conjugated oligomers. *Chemical Physics Letters*, **2007**, 434, 194-199	2.5	11
77	Computational study of the thermal reaction rate between S+(4S) and acetylene. *Chemical Physics*, **2001**, 265, 251-261	2.3	11
76	FBeNg(+) (Ng=He, Ne, Ar): Suitable Cations for Salts of the Lightest Noble Gases? This work was supported by the Italian Ministero dell'Universita e della Ricerca Scientifica e Tecnologica (MURST) and the Consiglio Nazionale delle Ricerche (CNR). *Angewandte Chemie - International Edition*, **2000**, 39, 1690-1692	16.4	11
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74	Toward a Realistic Modeling of the Photophysics of Molecular Building Blocks for Energy Harvesting: The Charge-Transfer State in 4,7-Dithien-2-yl-2,1,3-benzothiadiazole As a Case Study. *Journal of Physical Chemistry C*, **2013**, 117, 13785-13797	3.8	10
73	Lifetimes of Gaseous Ion–Neutral Complexes: The Rate of Isotopic Scrambling within Ethyl Ions as an Internal Clock. *Chemistry - A European Journal*, **1998**, 4, 1535-1541	4.8	10
72	Molecular dynamics simulation of Leishmania major surface metalloprotease GP63 (leishmanolysin). *Proteins: Structure, Function and Bioinformatics*, **2006**, 64, 385-90	4.2	10
71	Photoinduced electron transfer in a dichromophoric peptide: a numerical experiment. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	10
70	Exploring the role of L209 residue in the active site of NDM-1 a metallo-lactamase. *PLoS ONE*, **2018**, 13, e0189686	3.7	9
69	Structural basis of the transactivation deficiency of the human PPARF360L mutant associated with familial partial lipodystrophy. *Acta Crystallographica Section D: Biological Crystallography*, **2014**, 70, 1965-76		9
68	Theoretical study of alpha-84 phycocyanobilin chromophore from the thermophilic cyanobacterium Synechococcus elongatus. *Journal of Physical Chemistry B*, **2007**, 111, 5596-601	3.4	9
67	Stereoselectivity by enantiomeric inhibitors of matrix metalloproteinase-8: new insights from molecular dynamics simulations. *Journal of Medicinal Chemistry*, **2007**, 50, 211-8	8.3	9
66	Modelling of the effect of solute structure and mobile phase pH and composition on the retention of phenoxy acid herbicides in reversed-phase high-performance liquid chromatography. *Analytica Chimica Acta*, **2008**, 616, 123-37	6.6	9
65	On the formation of Horseradish Peroxidase Compound I at high pH: New insights from ab initio molecular dynamics. *Chemical Physics Letters*, **2006**, 428, 152-156	2.5	9
64	Aromatic substitution in the complexes formed upon addition of gaseous arenium ions to proelectrophiles. A FT-ICR study. *Research on Chemical Intermediates*, **1996**, 22, 645-658	2.8	9
63	Kinetic Profile and Molecular Dynamic Studies Show that Y229W Substitution in an NDM-1/L209F Variant Restores the Hydrolytic Activity of the Enzyme toward Penicillins, Cephalosporins, and Carbapenems. *Antimicrobial Agents and Chemotherapy*, **2019**, 63,	5.9	8

62	Ionic liquids vs conventional solvents: A comparative study in the selective catalytic oxidations promoted by oxovanadium(IV) complexes. *Applied Catalysis A: General*, **2020**, 599, 117622	5.1	8
61	Reaction of (2-aminophenyl)-Ynones with Tosyl Isocyanate: Experimental and Computational Investigations. *Advanced Synthesis and Catalysis*, **2018**, 360, 3672-3676	5.6	8
60	Structure and solvation properties of aqueous sulfobetaine micelles in the presence of organic spin probes: a Molecular Dynamics simulation study. *Structural Chemistry*, **2013**, 24, 945-953	1.8	8
59	Evaluation of the Lifetime of Gaseous Ion–Neutral Complexes. 1. A Chemical Activation Study. *Journal of the American Chemical Society*, **1998**, 120, 3982-3987	16.4	8
58	Statistical Mechanical Modeling of Chemical Reactions in Condensed Phase Systems. *Challenges and Advances in Computational Chemistry and Physics*, **2008**, 191-213	0.7	8
57	Effect of the Incorporation of Functionalized Cyclodextrins in the Liposomal Bilayer. *Molecules*, **2019**, 24,	4.8	7
56	Folding propensity of anoplin: A molecular dynamics study of the native peptide and four mutated isoforms. *Biopolymers*, **2015**, 103, 692-701	2.2	7
55	Thermal and environmental effects on Oligothiophene low-energy singlet electronic excitations in dilute solution: a theoretical and experimental study. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	7
54	Entropy–energy balance in base catalyzed keto-enol interconversion: A joint theoretical and experimental investigation. *International Journal of Quantum Chemistry*, **2011**, 111, 1293-1305	2.1	7
53	Molecular dynamics simulation of the interaction between the complex iron-sulfur flavoprotein glutamate synthase and its substrates. *Protein Science*, **2004**, 13, 2979-91	6.3	7
52	Intramolecular charge transfer in π-conjugated oligomers: a theoretical study on the effect of temperature and oxidation state. *Theoretical Chemistry Accounts*, **2008**, 119, 469-476	1.9	7
51	On the performance of time-dependent density functional theory and polarizable continuum model in the study of aqueous formaldehyde. *Computational and Theoretical Chemistry*, **2004**, 680, 117-120		7
50	Crabrolin, a natural antimicrobial peptide: structural properties. *Journal of Peptide Science*, **2017**, 23, 693-700	2.1	6
49	Theoretical calculation of the pyrene emission properties in different solvents. *Chemical Physics Letters*, **2015**, 639, 17-22	2.5	6
48	P-113 peptide: New experimental evidences on its biological activity and conformational insights from molecular dynamics simulations. *Biopolymers*, **2014**, 102, 159-67	2.2	6
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43	Supramolecular organization of chiral molecules on metallic surfaces: D-alaninol on Cu(100) as a case study. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2010**, 7, 2616-2619		6
42	Gas-phase positive and negative ion chemistry of methyl hydroperoxide. *Inorganica Chimica Acta*, **1998**, 275-276, 192-202	2.7	6
41	Conformational properties of -residue-containing oligopeptides in apolar solvent. *Journal of Molecular Structure*, **2006**, 785, 176-181	3.4	6
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27	Embedding calix[4]resorcinarenes in liposomes: Experimental and computational investigation of the effect of resorcinarene inclusion on liposome properties and stability. *Biochimica Et Biophysica Acta - Biomembranes*, **2019**, 1861, 1252-1259	3.8	4

26	Experimental results and computational insight into sequential reactions of ‡(2-aminophenyl)-‡ynones with aryl isocyanates/benzoyl isothiocyanate. *Organic and Biomolecular Chemistry*, **2020**, 18, 3177-3189	3.9	4
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20	Reactivity of gaseous protonated ozone: a computational investigation on the carbon monoxide oxidation reaction. *International Journal of Mass Spectrometry*, **2003**, 228, 613-627	1.9	4
19	The Unimolecular Loss of HF by Simple Inorganic Ions: A Computational Dynamic Reaction Path Study. *European Journal of Mass Spectrometry*, **2000**, 6, 31-37	1.1	4
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