

Josep Anglada

List of Publications by Year in descending order

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135
all docs

135
docs citations

135
times ranked

3657
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#	ARTICLE	IF	CITATIONS
1	Effects of the substituents on the reactivity of carbonyl oxides. A theoretical study on the reaction of substituted carbonyl oxides with water. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 13034.	1.3	173
2	Molecular reactions at aqueous interfaces. <i>Nature Reviews Chemistry</i> , 2020, 4, 459-475.	13.8	149
3	Unimolecular Isomerizations and Oxygen Atom Loss in Formaldehyde and Acetaldehyde Carbonyl Oxides. A Theoretical Investigation. <i>Journal of the American Chemical Society</i> , 1996, 118, 4636-4647.	6.6	137
4	The Ozonolysis of Ethylene: A Theoretical Study of the Gas-Phase Reaction Mechanism. <i>Chemistry - A European Journal</i> , 1999, 5, 1809-1822.	1.7	134
5	Sulfuric Acid as Autocatalyst in the Formation of Sulfuric Acid. <i>Journal of the American Chemical Society</i> , 2012, 134, 20632-20644.	6.6	126
6	Water effects on atmospheric reactions. <i>International Reviews in Physical Chemistry</i> , 2011, 30, 335-369.	0.9	119
7	The reactions of SO ₃ with HO ₂ radical and H ₂ O⋅HO ₂ radical complex. Theoretical study on the atmospheric formation of HSO ₅ and H ₂ SO ₄ . <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 2116.	1.3	106
8	Atmospheric Significance of Water Clusters and Ozone⋅Water Complexes. <i>Journal of Physical Chemistry A</i> , 2013, 117, 10381-10396.	1.1	101
9	Atmospheric Formation of OH Radicals and H ₂ O ₂ from Alkene Ozonolysis under Humid Conditions. <i>ChemPhysChem</i> , 2002, 3, 215-221.	1.0	100
10	Tropospheric Formation of Hydroxymethyl Hydroperoxide, Formic Acid, H ₂ O ₂ , and OH from Carbonyl Oxide in the Presence of Water Vapor: A Theoretical Study of the Reaction Mechanism. <i>Chemistry - A European Journal</i> , 2001, 7, 2227-2235.	1.7	92
11	Impact of Water on the OH + HOCl Reaction. <i>Journal of the American Chemical Society</i> , 2011, 133, 3345-3353.	6.6	92
12	A reduced-restricted-quasi-Newton-Raphson method for locating and optimizing energy crossing points between two potential energy surfaces. <i>Journal of Computational Chemistry</i> , 1997, 18, 992-1003.	1.5	91
13	Effects of a Single Water Molecule on the OH + H ₂ O ₂ Reaction. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5821-5829.	1.1	91
14	Interconnection of Reactive Oxygen Species Chemistry across the Interfaces of Atmospheric, Environmental, and Biological Processes. <i>Accounts of Chemical Research</i> , 2015, 48, 575-583.	7.6	90
15	Complex Mechanism of the Gas Phase Reaction between Formic Acid and Hydroxyl Radical. Proton Coupled Electron Transfer versus Radical Hydrogen Abstraction Mechanisms. <i>Journal of the American Chemical Society</i> , 2004, 126, 9809-9820.	6.6	86
16	Evaluation of the Nonlinear Optical Properties for Annulenes with Hückel and Möbius Topologies. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3935-3943.	2.3	86
17	Finding transition states using reduced potential-energy surfaces. <i>Theoretical Chemistry Accounts</i> , 2001, 105, 463-472.	0.5	81
18	Impact of the water dimer on the atmospheric reactivity of carbonyl oxides. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17698-17712.	1.3	78

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19	The Mechanism of Methoxy Radical Oxidation by O ₂ in the Gas Phase. Computational Evidence for Direct H Atom Transfer Assisted by an Intermolecular Noncovalent O ^{δ-} ⋯O Bonding Interaction. <i>Journal of the American Chemical Society</i> , 1999, 121, 1337-1347.	6.6	77
20	Gas Phase Reaction of Nitric Acid with Hydroxyl Radical without and with Water. A Theoretical Investigation. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9151-9162.	1.1	74
21	Cysteinyflavan-3-ol Conjugates from Grape Procyanidins. Antioxidant and Antiproliferative Properties. <i>Bioorganic and Medicinal Chemistry</i> , 2002, 10, 2497-2509.	1.4	72
22	Inductive Effects in Neutral Pentacoordinated Silicon Compounds Containing a Si δ ⁺ ⋯N Dative Bond. A Theoretical Study. <i>Organometallics</i> , 1999, 18, 5584-5593.	1.1	69
23	Different Catalytic Effects of a Single Water Molecule: The Gas-Phase Reaction of Formic Acid with Hydroxyl Radical in Water Vapor. <i>ChemPhysChem</i> , 2009, 10, 3034-3045.	1.0	69
24	Correlation between Photophysical Parameters and Gold-Gold Distances in Gold(I) (4-Pyridyl)ethynyl Complexes. <i>Inorganic Chemistry</i> , 2012, 51, 7636-7641.	1.9	69
25	Reactivity of Atmospherically Relevant Small Radicals at the Air-Water Interface. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 5413-5417.	7.2	69
26	Theoretical investigation of the eight low-lying electronic states of the cis- and trans-nitric oxide dimers and its isomerization using multiconfigurational second-order perturbation theory (CASPT2). <i>Journal of Chemical Physics</i> , 2000, 112, 6608-6624.	1.2	67
27	Reactivity of Volatile Organic Compounds at the Surface of a Water Droplet. <i>Journal of the American Chemical Society</i> , 2012, 134, 11821-11827.	6.6	65
28	m-Benzyne and bicyclo[3.1.0]hexatriene – which isomer is more stable? – a quantum chemical investigation. <i>Chemical Physics Letters</i> , 2001, 348, 115-125.	1.2	64
29	Relevance of the DFT method to study expanded porphyrins with different topologies. <i>Journal of Computational Chemistry</i> , 2017, 38, 2819-2828.	1.5	64
30	A new look at the reduced-gradient-following path. <i>Theoretical Chemistry Accounts</i> , 2002, 107, 130-139.	0.5	63
31	Mechanism of the Hydrogen Transfer from the OH Group to Oxygen-Centered Radicals: Proton-Coupled Electron-Transfer versus Radical Hydrogen Abstraction. <i>Chemistry - A European Journal</i> , 2004, 10, 3404-3410.	1.7	63
32	Mechanism for the Gas-Phase Reaction between Formaldehyde and Hydroperoxyl Radical. A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 10786-10794.	1.1	60
33	Theoretical Studies of the Isoprene Ozonolysis under Tropospheric Conditions. 2. Unimolecular and Water-Assisted Decomposition of the $\dot{\text{I}}\pm$ -Hydroxy Hydroperoxides. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5812-5820.	1.1	58
34	Mechanistic Study of the CH ₃ O ₂ + HO ₂ → CH ₃ O ₂ H + O ₂ Reaction in the Gas Phase. Computational Evidence for the Formation of a Hydrogen-Bonded Diradical Complex. <i>Journal of Physical Chemistry A</i> , 2006, 110, 6073-6082.	1.1	58
35	Spectroscopic signatures of ozone at the air-water interface and photochemistry implications. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 11618-11623.	3.3	58
36	Reaction Modes of Carbonyl Oxide, Dioxirane, and Methylenebis(oxy) with Ethylene: A New Reaction Mechanism. <i>Journal of Physical Chemistry A</i> , 2002, 106, 3917-3929.	1.1	57

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37	On the quadratic reaction path evaluated in a reduced potential energy surface model and the problem to locate transition states. <i>Journal of Computational Chemistry</i> , 2001, 22, 387-406.	1.5	52
38	The Ozonolysis of Acetylene: A Quantum Chemical Investigation. <i>Journal of the American Chemical Society</i> , 2001, 123, 6127-6141.	6.6	51
39	On the nature of the unusually long OO bond in HO ₃ and HO ₄ radicals. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 5865.	1.3	51
40	The Reaction of CH ₂ (X ₃ B ₁) with O ₂ (X ₃): A Theoretical CASSCF/CASPT2 Investigation. <i>Journal of Physical Chemistry A</i> , 2002, 106, 1877-1884.	1.1	46
41	New Insight into the Gas-Phase Bimolecular Self-Reaction of the HOO Radical. <i>Journal of Physical Chemistry A</i> , 2007, 111, 1695-1704.	1.1	46
42	Unconventional Biradical Character of Titanium Enolates. <i>Journal of the American Chemical Society</i> , 2008, 130, 3242-3243.	6.6	46
43	Practical remarks on the selection of the active space in the CAS-SCF wavefunction. <i>Chemical Physics Letters</i> , 1995, 243, 151-157.	1.2	44
44	How good is a Broyden-Fletcher-Goldfarb-Shanno-like update Hessian formula to locate transition structures? Specific reformulation of Broyden-Fletcher-Goldfarb-Shanno for optimizing saddle points. <i>Journal of Computational Chemistry</i> , 1998, 19, 349-362.	1.5	43
45	Theoretical Studies on Isoprene Ozonolysis under Tropospheric Conditions. 1. Reaction of Substituted Carbonyl Oxides with Water. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5798-5811.	1.1	43
46	On the Dissociation of Ground State trans-HOOO Radical: A Theoretical Study. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2743-2750.	2.3	42
47	Photochemistry of SO ₂ at the Air-Water Interface: A Source of OH and HOSO Radicals. <i>Journal of the American Chemical Society</i> , 2018, 140, 12341-12344.	6.6	42
48	A New Mechanism of Acid Rain Generation from HOSO at the Air-Water Interface. <i>Journal of the American Chemical Society</i> , 2019, 141, 16564-16568.	6.6	39
49	Atmospheric Spectroscopy and Photochemistry at Environmental Water Interfaces. <i>Annual Review of Physical Chemistry</i> , 2019, 70, 45-69.	4.8	38
50	Photoinduced Oxidation Reactions at the Air-Water Interface. <i>Journal of the American Chemical Society</i> , 2020, 142, 16140-16155.	6.6	38
51	The Gas-Phase Hydrogen Bond Complexes between Formic Acid with Hydroxyl Radical: A Theoretical Study. <i>ChemPhysChem</i> , 2004, 5, 183-191.	1.0	37
52	The reaction between HO and (H ₂ O) _n (n=1, 3) clusters: reaction mechanisms and tunneling effects. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 579-592.	0.5	37
53	Theoretical Investigation of the Low-Lying Electronic States of Dioxirane: Ring Opening to Dioxymethane and Dissociation into CO ₂ and H ₂ . <i>Journal of Physical Chemistry A</i> , 1998, 102, 3398-3406.	1.1	36
54	Evaluation of the nonlinear optical properties for an expanded porphyrin Hückel-Möbius aromaticity switch. <i>Journal of Chemical Physics</i> , 2012, 137, 184306.	1.2	35

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55	Design of H _{1/4} ckelâ€“MÃ¶bius Topological Switches with High Nonlinear Optical Properties. <i>Journal of Physical Chemistry C</i> , 2017, 121, 19348-19357.	1.5	34
56	Hydrogen Transfer between Sulfuric Acid and Hydroxyl Radical in the Gas Phase:â€‰% Competition among Hydrogen Atom Transfer, Proton-Coupled Electron-Transfer, and Double Proton Transfer. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1982-1990.	1.1	33
57	Theoretical investigation of the low-lying electronic states of TiH. <i>Molecular Physics</i> , 1990, 69, 281-303.	0.8	30
58	Reaction Mechanism between Carbonyl Oxide and Hydroxyl Radical:â€‰% A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4001-4011.	1.1	29
59	The Gas-Phase Reaction between O ₃ and HO Radical: A Theoretical Study. <i>ChemPhysChem</i> , 2007, 8, 1534-1539.	1.0	29
60	Anharmonicity and the Eigen-Zundel Dilemma in the IR Spectrum of the Protonated 21 Water Cluster. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 467-472.	2.3	29
61	Prediction of approximate transition states by Bell-Evans-Polanyi principle: I. <i>Journal of Computational Chemistry</i> , 1999, 20, 1112-1129.	1.5	28
62	Theoretical Study of the Switching between H _{1/4} ckel and MÃ¶bius Topologies for Expanded Porphyrins. <i>Journal of Physical Chemistry C</i> , 2012, 116, 24358-24366.	1.5	28
63	The atmospheric oxidation of CH ₃ OOH by the OH radical: the effect of water vapor. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 12331-12342.	1.3	28
64	Effect of the Meso-Substituent in the H _{1/4} ckel-to-MÃ¶bius Topological Switches. <i>Journal of Organic Chemistry</i> , 2014, 79, 5036-5046.	1.7	27
65	Triplet state promoted reaction of SO ₂ with H ₂ O by competition between proton coupled electron transfer (pcet) and hydrogen atom transfer (hat) processes. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9779-9784.	1.3	27
66	Low-lying electronic states of CSi and electron affinity of CSi according to ab initio MRD-CI calculations. <i>Journal of Physics B: Atomic and Molecular Physics</i> , 1983, 16, 2469-2484.	1.6	26
67	The gas-phase reaction of methane sulfonic acid with the hydroxyl radical without and with water vapor. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 5140.	1.3	26
68	The reaction of formaldehyde carbonyl oxide with the methyl peroxy radical and its relevance in the chemistry of the atmosphere. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 18921.	1.3	26
69	The ozoneâ€“acetylene reaction: concerted or non-concerted reaction mechanism? A quantum chemical investigation. <i>Chemical Physics Letters</i> , 2001, 347, 268-276.	1.2	25
70	The Gas-Phase Hydrogen-Bonded Complex between Ozone and Hydroperoxyl Radical. A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2007, 111, 976-981.	1.1	25
71	The Stability of $\hat{1}\pm$ â€“Hydroperoxyalkyl Radicals. <i>Chemistry - A European Journal</i> , 2016, 22, 18092-18100.	1.7	24
72	The electronic spectrum of SçH. <i>Molecular Physics</i> , 1989, 66, 541-563.	0.8	23

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73	A geometry optimization benchmark using highly correlated wavefunctions (FCI and MRD-CI). <i>Theoretica Chimica Acta</i> , 1995, 92, 369-381.	0.9	23
74	On the Gas Phase Hydrogen Bond Complexes between Formic Acid and Hydroperoxyl Radical. A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9718-9726.	1.1	23
75	Electronic Structure and Unimolecular Reactions of Cyclopropanone Carbonyl Oxide. A Theoretical Study. <i>Journal of Organic Chemistry</i> , 1997, 62, 2720-2726.	1.7	21
76	On the restricted step method coupled with the augmented Hessian for the search of stationary points of any continuous function. <i>International Journal of Quantum Chemistry</i> , 1997, 62, 153-165.	1.0	21
77	Ab initio \hat{A}^2 ground potential energy surface and transition state theory kinetics study of the $O(1D)+N_2O \rightarrow 2NO$, N_2+O_2 (singlet) reactions. <i>Journal of Chemical Physics</i> , 2001, 115, 7015-7031.	1.2	21
78	Inductive and External Electric Field Effects in Pentacoordinated Phosphorus Compounds. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 49-63.	2.3	21
79	Hyperconjugation in adjacent OO bonds: Remarkable odd/even effects. <i>Chemical Physics Letters</i> , 2009, 481, 180-182.	1.2	20
80	Bipyridyl Derivatives as Photomemory Devices: A Comparative Electronic Structure Study. <i>Chemistry - A European Journal</i> , 2010, 16, 6693-6703.	1.7	20
81	Theoretical Study of the Low-Lying Electronic States of 4-Oxo-2,5-cyclohexadienylidene and Their Formation from 1H-Bicyclo[3.1.0]hexa-3,5-dien-2-one. <i>The Journal of Physical Chemistry</i> , 1995, 99, 5934-5944.	2.9	19
82	Structure, stability, and dynamics of hydrogen polyoxides. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 1543-1554.	1.0	19
83	Atmospheric formation of the NO_3 radical from gas-phase reaction of HNO_3 acid with the NH_2 radical: proton-coupled electron-transfer versus hydrogen atom transfer mechanisms. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 19437-19445.	1.3	17
84	Two-step reaction mechanism reveals new antioxidant capability of cysteine disulfides against hydroxyl radical attack. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 18216-18223.	3.3	17
85	The Aqueous Surface as an Efficient Transient Stop for the Reactivity of Gaseous NO_2 in Liquid Water. <i>Journal of the American Chemical Society</i> , 2020, 142, 20937-20941.	6.6	17
86	Photosensitization mechanisms at the air-water interface of aqueous aerosols. <i>Chemical Science</i> , 2022, 13, 2624-2631.	3.7	17
87	The search for stationary points on a quantum mechanical/molecular mechanical potential-energy surface. <i>Theoretical Chemistry Accounts</i> , 2002, 107, 147-153.	0.5	16
88	Title is missing!. <i>Journal of Mathematical Chemistry</i> , 1999, 25, 85-92.	0.7	15
89	Description of pentacoordinated phosphorus under an external electric field: which basis sets and semi-empirical methods are needed?. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 2442.	1.3	15
90	The gas phase reaction of carbonyl oxide with hydroxyl radical in presence of water vapor. A theoretical study on the reaction mechanism. <i>Computational and Theoretical Chemistry</i> , 2011, 965, 313-320.	1.1	15

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91	Unexpected Reactivity of Amidogen Radical in the Gas Phase Degradation of Nitric Acid. <i>Journal of the American Chemical Society</i> , 2014, 136, 6834-6837.	6.6	15
92	The Atmospheric Oxidation of HONO by OH, Cl, and ClO Radicals. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9698-9707.	1.1	15
93	Studies on the Intramolecular C ^α -H ^β -X (X = O, S) Interactions in (S)-N-Acyl-4-isopropyl-1,3-thiazolidine-2-thiones and Related 1,3-Oxazolidin-2-ones. <i>Organic Letters</i> , 2003, 5, 2809-2812.	2.4	14
94	Protonation of Water Clusters Induced by Hydroperoxyl Radical Surface Adsorption. <i>Chemistry - A European Journal</i> , 2011, 17, 5076-5085.	1.7	14
95	Theoretical Investigation of the Photoexcited NO ₂ +H ₂ O reaction at the Air-Water Interface and Its Atmospheric Implications. <i>Chemistry - A European Journal</i> , 2019, 25, 13899-13904.	1.7	14
96	Reactivity of Undissociated Molecular Nitric Acid at the Air-Water Interface. <i>Journal of the American Chemical Society</i> , 2021, 143, 453-462.	6.6	14
97	Theoretical study of low-lying electronic states of CoH ⁺ . <i>Journal of Chemical Physics</i> , 1990, 92, 6732-6741.	1.2	13
98	On the Regio- and Stereoselective Synthesis of Aminocyclitols from Cyclitol Epoxides: The Effect of Li as a Chelating Agent. <i>Chemistry - A European Journal</i> , 2005, 11, 4465-4472.	1.7	13
99	Role of Proton Tunneling and Metal-Free Organocatalysis in the Decomposition of Methanediol: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4318-4325.	1.1	13
100	Photochemistry of HOSO radical in the gas phase. <i>Journal of Chemical Physics</i> , 2019, 151, 111103.	1.2	13
101	Remarks on large-scale matrix diagonalization using a Lagrange-Newton-Raphson minimization in a subspace. <i>Theoretical Chemistry Accounts</i> , 1999, 103, 163-166.	0.5	12
102	Theoretical Characterization of the Gas-Phase O ₃ ...HO Hydrogen-Bonded Complex. <i>ChemPhysChem</i> , 2006, 7, 1488-1493.	1.0	12
103	Role of vibrational anharmonicity in atmospheric radical hydrogen-bonded complexes. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 6377.	1.3	12
104	The Gas Phase HO-Initiated Oxidation of Furan: A Theoretical Investigation on the Reaction Mechanism. <i>The Open Chemical Physics Journal</i> , 2008, 1, 80-93.	0.7	12
105	Cyclization of carbodiimides with 2-(bromomethyl)acrylic acid. A direct entry to the system 5-methylene-6-hydroxypyrimidine-2,4-dione, a new class of thymine analogues. <i>Journal of Heterocyclic Chemistry</i> , 1996, 33, 1259-1270.	1.4	11
106	Is the HO ₄ [•] Anion a Key Species in the Aqueous Phase Decomposition of Ozone?. <i>Chemistry - A European Journal</i> , 2012, 18, 13435-13445.	1.7	11
107	Impacts of cloud water droplets on the OH production rate from peroxide photolysis. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 31621-31627.	1.3	11
108	Twisted intramolecular charge transfer in a carbazole-based chromophore: the stable [(4-N-carbazolyl)-2,3,5,6-tetrachlorophenyl]bis(2,3,5,6-tetrachlorophenyl)methyl radical. <i>New Journal of Chemistry</i> , 2017, 41, 8422-8430.	1.4	10

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109	MRD-CI calculations for the low-lying electronic states of scandiumhydride and titaniumhydride. Computational and Theoretical Chemistry, 1983, 93, 299-308.	1.5	9
110	Comparison between isoelectronic transition metal hydrides. MRD-CI results for ScH ⁺ and TiH ⁺ . Computational and Theoretical Chemistry, 1984, 107, 163-168.	1.5	9
111	Accurate and efficient determination of higher roots in diagonalization of large matrices based in function restricted optimization algorithms. Journal of Computational Chemistry, 2000, 21, 1375-1386.	1.5	9
112	Reactivity of hydropersulfides toward the hydroxyl radical unraveled: disulfide bond cleavage, hydrogen atom transfer, and proton-coupled electron transfer. Physical Chemistry Chemical Physics, 2018, 20, 4793-4804.	1.3	9
113	Tight electrostatic regulation of the OH production rate from the photolysis of hydrogen peroxide adsorbed on surfaces. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	9
114	Structure of hydrogen tetroxide in gas phase and in aqueous environments: relationship to the hydroperoxyl radical self-reaction. Structural Chemistry, 2016, 27, 231-242.	1.0	8
115	Tropospheric oxidation of methyl hydrotrioxide (CH ₃ OOOH) by hydroxyl radical. Physical Chemistry Chemical Physics, 2018, 20, 27406-27417.	1.3	7
116	The gas phase oxidation of HCOOH by Cl and NH ₂ radicals. Proton coupled electron transfer versus hydrogen atom transfer. Molecular Physics, 2019, 117, 1430-1441.	0.8	6
117	Prediction of approximate transition states by Bell-Evans-Polanyi principle: II. Gas phase unimolecular decomposition of methyldioxirane. Journal of Computational Chemistry, 1999, 20, 1130-1137.	1.5	5
118	Ab initio CI calculations on ScC ₂ H ₄ ⁺ ions. Chemical Physics Letters, 1990, 167, 421-428.	1.2	4
119	Computational Insights into the CH ₃ Cl+OH Chemical Reaction Dynamics at the Air-Water Interface. ChemPhysChem, 2017, 18, 2747-2755.	1.0	4
120	A Bohmian total potential view to quantum effects. II: decay of temporarily trapped states. Theoretical Chemistry Accounts, 2009, 123, 51-58.	0.5	3
121	Formation of a stable biradical triplet state cation <i>versus</i> a closed shell singlet state cation by oxidation of adducts of 3,6-dimethoxycarbazole and polychlorotriphenylmethyl radicals. Physical Chemistry Chemical Physics, 2019, 21, 20225-20231.	1.3	3
122	Large-scale matrix diagonalization methods by direct optimization of Taylor expansion of Rayleigh-Ritz quotient up to third order. Chemical Physics Letters, 2000, 329, 160-167.	1.2	2
123	A symmetric orthogonal transformation applied to molecular geometry optimizations constrained on a hypersphere. Chemical Physics Letters, 1997, 269, 469-474.	1.2	1
124	Quantum Chemical Reactivity: Beyond the Study of Small Molecules. Mathematical and Computational Chemistry, 2001, , 125-141.	0.3	1
125	On the Regio- and Stereoselective Synthesis of Aminocyclitols from Cyclitol Epoxides: The Effect of Li as a Chelating Agent. Chemistry - A European Journal, 2006, 12, 349-349.	1.7	0
126	The 65th birthday of Professor Santiago Olivella Nello. Theoretical Chemistry Accounts, 2009, 123, 1-2.	0.5	0

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127	Mechanistic Studies on the Intramolecular Cyclization of <i>O</i> -Tosyl Phytosphingosines to Jaspines. Natural Product Communications, 2014, 9, 1934578X1400900.	0.2	0
128	Spectroscopic characterization of the ethyl radical-water complex. Journal of Chemical Physics, 2016, 145, 144301.	1.2	0