Rajakumar Balla

List of Publications by Year
in descending order

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		516215	642321
91	836	16	23
papers	citations	h-index	g-index

91	91	91	686
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Temperature dependent kinetics for the reaction between OH radicals and (E)- and (Z)- CHFÂ=ÂCHCl: A dual-level computational study. Computational and Theoretical Chemistry, 2022, 1208, 113558.	1.1	1
2	Kinetic investigation of the reaction of ethylperoxy radicals with ethanol. International Journal of Chemical Kinetics, 2021, 53, 274-286.	1.0	1
3	Reaction kinetics of a series of alkenes with ClO and BrO radicals: A theoretical study. International Journal of Chemical Kinetics, 2021, 53, 250-264.	1.0	2
4	Reaction kinetics of a series of alkanes with ClO and BrO radicals: A theoretical study. International Journal of Chemical Kinetics, 2021, 53, 189-206.	1.0	3
5	Absorption cross-section measurements of ortho-xylyl radical in the 460.1â€“475.1Ânm region and investigation of its temperature and pressure dependence using cavity ringdown spectroscopy. Chemical Physics Letters, 2021, 765, 138314.	1.2	0
6	Temperature-dependent kinetic study of the photo-oxidation reaction of vinyl butyrate with Cl atoms and fate of the formation of alkoxy radicals. Chemical Physics Letters, 2021, 771, 138500.	1.2	2
7	Thermal Decomposition of 2-Methyltetrahydrofuran behind Reflected Shock Waves over the Temperature Range of 1179â€“1361 K. Journal of Physical Chemistry A, 2021, 125, 5406-5422.	1.1	2
8	Investigation of kinetics of phenyl radicals with ethyl formate in the gas phase using cavity ring-down spectroscopy and theoretical methodologies. Photochemical and Photobiological Sciences, 2021, 20, 859-873.	1.6	1
9	A Combined Experimental and Theoretical Study to Determine the Kinetics of 2-Ethoxy Ethanol with OH Radical in the Gas Phase. Journal of Physical Chemistry A, 2021, 125, 8869-8881.	1.1	4
10	Theoretical investigations on the OH radical mediated kinetics of cis- and trans-CH3CF=CHF and CH3CH=CF2 over temperature range of 200-400K. Journal of Fluorine Chemistry, 2021, 250, 109884.	0.9	1
11	Experimental and Computational Investigations of the Tropospheric Photooxidation Reactions of 1,1,1,3,3,3-Hexafluoro-2-Methyl-2-Propanol Initiated by OH Radicals and Cl Atoms. Journal of Physical Chemistry A, 2021, 125, 523-535.	1.1	4
12	Kinetics of IO radicals with ethyl formate and ethyl acetate: a study using cavity ring-down spectroscopy and theoretical methods. Physical Chemistry Chemical Physics, 2021, 23, 25974-25993.	1.3	2
13	Oxidative Degradation Kinetics and Mechanism of Two Biodiesel Constituents (Ethyl-2-Methyl) Tj ETQq1 1 0.784314 rgBT /Overlock 1 Space Chemistry, 2020, 4, 142-156.	1.2	3
14	Temperature-Dependent Kinetics of the Reactions of Methyl-2-methyl Propionate and Methyl-2-methyl Butanoate with Cl Atoms under Tropospheric Conditions. ACS Earth and Space Chemistry, 2020, 4, 1448-1460.	1.2	1
15	Reaction of phenyl radicals towards propionaldehyde and butyraldehyde over the temperature range of 200â€“2000ÂK. Chemical Physics Letters, 2020, 758, 137915.	1.2	1
16	Kinetic Studies on the Photo-oxidation Reactions of Methyl-2-methyl Butanoate and Methyl-3-methyl Butanoate with OH Radicals. Journal of Physical Chemistry A, 2020, 124, 10923-10936.	1.1	1
17	Tropospheric Photo-oxidation of Ethyl Methacrylate Initiated by Cl Atoms in the Gas Phase: Kinetic and Mechanistic Investigations. ACS Earth and Space Chemistry, 2020, 4, 831-842.	1.2	1
18	Kinetic Investigations of the Reaction of Phenyl Radicals with Ethyl Acetate in the Gas Phase: An Experimental and Computational Study. Journal of Physical Chemistry A, 2020, 124, 5503-5512.	1.1	7

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19	Kinetic and Mechanistic Investigation for the Gas-Phase Tropospheric Photo-oxidation Reactions of 2,2,2-Trifluoroethyl Acrylate with OH Radicals and Cl Atoms. Journal of Physical Chemistry A, 2020, 124, 2335-2351.	1.1	1
20	Cl-Initiated Photo-oxidation Studies of Methyl Valerate and Methyl Isovalerate under Tropospherically Relevant Conditions. Journal of Physical Chemistry A, 2020, 124, 2515-2529.	1.1	0
21	Dissociative nature of C(sp²)â€“N(sp³) bonds of carbazole based materials via conical intersection: simple method to predict the exciton stability of host materials for blue OLEDs: a computational study. Physical Chemistry Chemical Physics, 2020, 22, 7995-8005.	1.3	4
22	Photooxidation Reactions of Ethyl 2-Methylpropionate (E2MP) and Ethyl 2,2-Dimethylpropionate (E22DMP) Initiated by OH Radicals: An Experimental and Computational Study. Journal of Physical Chemistry A, 2020, 124, 2768-2784.	1.1	1
23	Cl Atom-Initiated Photo-Oxidation Reactions of Vinyl Trifluoroacetate and Allyl Trifluoroacetate in Tropospheric Conditions. Journal of Physical Chemistry A, 2020, 124, 2123-2139.	1.1	0
24	Reaction kinetics of CH2OO with 1,3-butadiene: Mechanistic investigation with RRKM calculations. Chemical Physics Letters, 2020, 742, 137157.	1.2	1
25	Tropospheric chemistry of ethyl tiglate initiated by Cl atoms. Chemical Physics Letters, 2020, 748, 137371.	1.2	0
26	Cl-Atom-Initiated Atmospheric Degradation of Saturated Cyclic Hydrocarbons: Kinetic and Mechanistic Investigation. Journal of Physical Chemistry A, 2019, 123, 7361-7373.	1.1	3
27	Cl atom initiated tropospheric chemistry of ethyl butyrate. Chemical Physics Letters, 2019, 731, 136594.	1.2	1
28	Investigation of the Absorption Cross Section of Phenyl Radical and Its Kinetics with Methanol in the Gas Phase Using Cavity Ring-Down Spectroscopy and Theoretical Methodologies. Journal of Physical Chemistry A, 2019, 123, 9682-9692.	1.1	11
29	Gas Phase Kinetics and Mechanistic Insights for the Reactions of Cl atoms with Isopropyl Formate and Isobutyl Formate. Journal of Physical Chemistry A, 2019, 123, 9978-9994.	1.1	2
30	Excited state Câ€“N bond dissociation and cyclization of tri-aryl amine-based OLED materials: a theoretical investigation. Physical Chemistry Chemical Physics, 2019, 21, 438-447.	1.3	15
31	A theoretical insight on the kinetics for the reaction of (E)-/(Z)-CHF=CF(CF2)x=1,2CF3 with OH radicals under tropospheric conditions. Journal of Fluorine Chemistry, 2019, 222-223, 31-45.	0.9	6
32	A Dual Level Direct Dynamics Study for the Reaction of CF₂=CHCF₃ (HFCâ€1225â€‰zc) and CF₂=CHCF₂CF₃ (HFCâ€1327â€‰cz) towards OH Radicals. ChemistrySelect, 2019, 4, 4827-4838.	0.7	4
33	Photo-Oxidation Reaction Kinetics and Mechanistics of 4-Hydroxy-2-butanone with Cl Atoms and OH Radicals in the Gas Phase. Journal of Physical Chemistry A, 2019, 123, 4342-4353.	1.1	7
34	Kinetics and Mechanistic Study for Gas Phase Tropospheric Photo-oxidation Reactions of 2,2,2-Trifluoroethyl Methacrylate with OH Radicals and Cl Atoms: An Experimental and Computational Approach. Journal of Physical Chemistry A, 2019, 123, 10868-10884.	1.1	2
35	Cl Atoms and OH Radicals Initiated Kinetic and Mechanistic Study on the Degradation of Propyl Butanoate under Tropospheric Conditions. Journal of Physical Chemistry A, 2019, 123, 10976-10989.	1.1	5
36	Cl Atom Initiated Photo-oxidation of Mono-chlorinated Propanes To Form Carbonyl Compounds: A Kinetic and Mechanistic Approach. Journal of Physical Chemistry A, 2019, 123, 723-741.	1.1	18

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37	Kinetic Investigations on the Gas Phase Reaction of 2,2,2â€Trifluoroethylbutyrate with OH Radicals: An Experimental and Theoretical Study. ChemistrySelect, 2018, 3, 4480-4489.	0.7	2
38	Theoretical investigations on the kinetics of Cl atom initiated reactions of series of 1-alkenes. Environmental Science and Pollution Research, 2018, 25, 4387-4405.	2.7	4
39	Temperature-Dependent Kinetics of the Reaction of a Criegee Intermediate with Propionaldehyde: A Computational Investigation. Journal of Physical Chemistry A, 2018, 122, 8433-8445.	1.1	14
40	Photo Oxidation Reaction Kinetics of Ethyl Propionate with Cl Atom and Formation of Propionic Acid. Journal of Physical Chemistry A, 2018, 122, 8274-8285.	1.1	14
41	Cl-initiated photo-oxidation reactions of methyl propionate in atmospheric condition. Environmental Science and Pollution Research, 2018, 25, 20999-21010.	2.7	13
42	Thermochemistry and Kinetic Studies on the Autoignition of 2-Butanone: A Computational Study. Journal of Physical Chemistry A, 2018, 122, 6134-6146.	1.1	5
43	Experimental and Theoretical Investigations on the Reaction of 1,3-Butadiene with Cl Atom in the Gas Phase. Journal of Physical Chemistry A, 2017, 121, 1976-1984.	1.1	7
44	Addition and abstraction kinetics of H atom with propylene and isobutylene between 200 and 2500 K: A DFT study. Chemical Physics, 2017, 491, 82-94.	0.9	1
45	Experimental and computational kinetic investigations for the reactions of Cl atoms with unsaturated ketones in the gas phase. New Journal of Chemistry, 2017, 41, 14299-14314.	1.4	3
46	Shock tube study and RRKM calculations on thermal decomposition of 2-chloroethyl methyl ether. Combustion and Flame, 2017, 186, 263-276.	2.8	3
47	Kinetic investigations of Cl atom initiated photo-oxidation reactions of cyclic unsaturated hydrocarbons in the gas phase: an experimental and theoretical study. New Journal of Chemistry, 2017, 41, 7491-7505.	1.4	14
48	An Exprimental and Computational Study on the Cl Atom Initiated Photo-Oxidization Reactions of Butenes in the Gas Phase. Journal of Physical Chemistry A, 2017, 121, 5487-5499.	1.1	7
49	Experimental and RRKM Investigations on the Degradation of Ethyl Formate. ChemistrySelect, 2017, 2, 11603-11614.	0.7	2
50	Thermal Decomposition of 2-Pentanol: A Shock Tube Study and RRKM Calculations. Journal of Physical Chemistry A, 2016, 120, 8024-8036.	1.1	5
51	Kinetic investigations of chlorine atom initiated photo oxidation reactions of 2,3-dimethyl-1,3-butadiene in the gas phase: an experimental and theoretical study. RSC Advances, 2016, 6, 67739-67750.	1.7	11
52	Kinetics of the thermal decomposition of tetramethylsilane behind the reflected shock waves between 1058 and 1194 K. Journal of Chemical Sciences, 2016, 128, 573-588.	0.7	6
53	Metal-free bipolar/octupolar organic dyes for DSSC application: A combined experimental and theoretical approach. Organic Electronics, 2016, 36, 177-184.	1.4	24
54	Is H Atom Abstraction Important in the Reaction of Cl with 1-Alkenes?. Journal of Physical Chemistry A, 2016, 120, 4096-4107.	1.1	7

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55	Rate coefficients for hydrogen abstraction reaction of pinonaldehyde (C10H16O2) with Cl atoms between 200 and 400 K: A DFT study. Journal of Chemical Sciences, 2016, 128, 977-989.	0.7	1
56	Theoretical investigations of the gas phase reaction of limonene (C₁₀H₁₆) with OH radical. Molecular Physics, 2015, 113, 3202-3215.	0.8	17
57	Experimental and Computational Investigation on the Gas Phase Reaction of p-Cymene with Cl Atoms. Journal of Physical Chemistry A, 2015, 119, 559-570.	1.1	9
58	Abstraction and addition kinetics of C₂H radicals with CH₄, C₂H₆, C₃H₈, C₂H₄, and C₃H₆: CVT/SCT/ISPE and hybrid meta-DFT methods. Physical Chemistry Chemical Physics, 2015, 17, 3142-3156.	1.3	22
59	Experimental and theoretical study on thermal decomposition of methyl butanoate behind reflected shock waves. RSC Advances, 2015, 5, 86536-86550.	1.7	9
60	Kinetic parameters for the reaction of OH radical with cis-CHFCHCHF2, trans-CHFCHCHF2, CF2CHCHF2 and CF2CCHF: Hybrid meta DFT and CVT/SCT/ISPE calculations. Journal of Fluorine Chemistry, 2015, 178, 266-278.	0.9	5
61	Gas Phase Kinetics of 2,2,2-Trifluoroethylbutyrate with the Cl Atom: An Experimental and Theoretical Study. Journal of Physical Chemistry A, 2015, 119, 9294-9306.	1.1	13
62	Rate coefficients for the gas-phase reaction of OH radical with Î±-pinene: an experimental and computational study. Molecular Physics, 2014, 112, 1495-1511.	0.8	14
63	Mechanism, kinetics and atmospheric fate of CF3CHCH2, CF3CFCH2, and CF3CFCF2 by its reaction with OH-radicals: CVT/SCT/ISPE and hybrid meta-DFT methods. Journal of Molecular Graphics and Modelling, 2014, 48, 60-69.	1.3	28
64	Theoretical investigations on the kinetics of p-cymene+OH reaction. Chemical Physics Letters, 2014, 597, 75-85.	1.2	12
65	Experimental and Computational Investigation on the Gas Phase Reaction of Ethyl Formate with Cl Atoms. Journal of Physical Chemistry A, 2014, 118, 5272-5278.	1.1	23
66	Thermal decomposition of 1-chloropropane behind the reflected shock waves in the temperature range of 1015â€“1220 K: Single pulse shock tube and computational studies. Journal of Chemical Sciences, 2014, 126, 897-909.	0.7	7
67	Reaction kinetics of Cl atoms with limonene: An experimental and theoretical study. Atmospheric Environment, 2014, 99, 183-195.	1.9	15
68	Experimental and theoretical rate coefficients for the gas phase reaction of Î²-Pinene with OH radical. Atmospheric Environment, 2013, 79, 161-171.	1.9	27
69	Theoretical Investigations on the Kinetics of H-Abstraction Reactions from CF₃CH(OH)CF₃ by OH Radicals. Journal of Physical Chemistry A, 2013, 117, 4534-4544.	1.1	31
70	Abstraction Kinetics of H-Atom by OH Radical from Pinonaldehyde (C10H16O2): Ab Initio and Transition-State Theory Calculations. Journal of Physical Chemistry A, 2012, 116, 5856-5866.	1.1	16
71	Rate Coefficients and Reaction Mechanism for the Reaction of OH Radicals with (E)-CF₃CHâ•CHF, (Z)-CF₃CHâ•CHF, (E)-CF₃CFâ•CHF, and (Z)-CF₃CFâ•CHF between 200 and 400 K: Hybrid Density Functional Theory and Canonical Variational Transition State Theory Calculations. Journal of Physical Chemistry A, 2012, 116, 9832-9842.	1.1	26
72	Kinetic parameters for the reaction of hydroxyl radical with CH₃OCH₂F (HFEâ€161) in the temperature range of 200â€“400 K: Transition state theory and Ab initio calculations. International Journal of Quantum Chemistry, 2012, 112, 1066-1077.	1.0	12

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73	Kinetic parameters of abstraction reactions of OH radical with ethylene, fluoroethylene, cis- and trans-1,2-difluoroethylene and 1,1-difluoroethylene, in the temperature range of 200â€“400K: Gaussian-3/B3LYP theory. Chemical Physics Letters, 2011, 511, 440-446.	1.2	11
74	Computational study on OH radical reaction with CHF₂CHFCHF₂(HFCâ€245ea) between 200 and 400 K. International Journal of Chemical Kinetics, 2011, 43, 418-430.	1.0	15
75	Thermodynamic and kinetic studies of hydroxyl radical reaction with bromine oxide using density functional theory. Computational and Theoretical Chemistry, 2011, 964, 283-290.	1.1	3
76	Rate coefficients for the reaction of OH with CF₃CH₂CH₃ (HFCâ€263fb) between 200 and 400 K: Ab initio, DFT, and transition state theory calculations. Journal of Computational Chemistry, 2010, 31, 500-509.	1.5	9
77	Kinetic study of the reaction of the acetyl radical, CH3CO, with O3 using cavity ring-down spectroscopy. Chemical Physics Letters, 2010, 484, 160-164.	1.2	3
78	Rate coefficients for the reactions of OH with nâ€propanol and isoâ€propanol between 237 and 376 K. International Journal of Chemical Kinetics, 2010, 42, 10-24.	1.0	15
79	Kinetics of OH radical reaction with CF3CHFCH2F (HFC-245eb) between 200 and 400K: G3MP2, G3B3 and transition state theory calculations. Computational and Theoretical Chemistry, 2010, 949, 73-81.	1.5	11
80	Rate coefficients for the reaction of the acetyl radical, CH₃CO, with Cl₂ between 253 and 384 K. International Journal of Chemical Kinetics, 2009, 41, 543-553.	1.0	8
81	The CH3CO quantum yield in the 248nm photolysis of acetone, methyl ethyl ketone, and biacetyl. Journal of Photochemistry and Photobiology A: Chemistry, 2008, 199, 336-344.	2.0	36
82	Visible Absorption Spectrum of the CH₃CO Radical. Journal of Physical Chemistry A, 2007, 111, 8950-8958.	1.1	21
83	The relaxation of OH (v = 1) and OD (v = 1) by H2O and D2O at temperatures from 251 to 390 K. Physical Chemistry Chemical Physics, 2006, 8, 4563.	1.3	18
84	Rate Coefficients for the Reactions of OH with CF3CH2CH3(HFC-263fb), CF3CHFCH2F (HFC-245eb), and CHF2CHFCHF2(HFC-245ea) between 238 and 375 Kâ€. Journal of Physical Chemistry A, 2006, 110, 6724-6731.	1.1	22
85	Rate coefficients for the relaxation of OH (v=1) by O2 at temperatures from 204â€“371K and by N2O from 243â€“372K. Chemical Physics Letters, 2006, 421, 111-117.	1.2	17
86	Rate coefficients for the OH + CFH2CH2OH reaction between 238 and 355 K. Physical Chemistry Chemical Physics, 2005, 7, 2498.	1.3	21
87	Thermal decomposition of haloethanols: single pulse shock tube and ab initio studies. , 2005, , 621-626.		2
88	Thermal Decomposition of 2-Fluoroethanol:â€‰ Single Pulse Shock Tube and ab Initio Studies. Journal of Physical Chemistry A, 2003, 107, 9782-9793.	1.1	18
89	Ab initio, DFT and transition state theory calculations on 1,2-HF, HCl and ClF elimination reactions from CH2Fâ€“CH2Cl. Physical Chemistry Chemical Physics, 2003, 5, 3897-3904.	1.3	34
90	Unimolecular HCl Elimination from 1,2-Dichloroethane:â€‰ A Single Pulse Shock Tube and ab Initio Study. Journal of Physical Chemistry A, 2002, 106, 8366-8373.	1.1	24

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91	Kinetics for the photo-chemical degradation of Methyl butyrate in presence of Cl atoms and OH radicals. Journal of Atmospheric Chemistry, 0, , 1.	1.4	1