Bert E Holmes

List of Publications by Year
in descending order

40 papers	456 citations	623188 14 h-index	794141 19 g-index
40 all docs	40 docs citations	40 times ranked	104 citing authors

#	Article	IF	Citations
1	Threshold energies and substituent effects for unimolecular elimination of hydrogen chloride (deuterium chloride) and hydrogen fluoride (deuterium fluoride) from chemically activated 1,1-difluoro-1-chloroethane and 1,1-difluoro-1-chloro-2,2,2-trideuterioethane. The Journal of Physical Chemistry, 1990, 94, 4957-4963.	2.9	29
2	Unimolecular Reaction Kinetics of CF2ClCF2CH3and CF2ClCF2CD3:Â Experimental Evidence for a Novel 1,2-FCl Rearrangement Pathwayâ€. Journal of Physical Chemistry A, 2001, 105, 1615-1621.	1.1	27
3	1,2-FCl Rearrangement as an Intermediate Step in the Unimolecular 1,3-HCl Elimination from Chlorofluoropropanesâ€. Journal of Physical Chemistry A, 2001, 105, 1622-1625.	1.1	27
4	Comparisons between Density Functional Theory and Conventional ab Initio Methods for 1,2-Elimination of HF from 1,1,1-Trifluoroethane:â€‰ Test Case Study for HF Elimination from Fluoroalkanes. Journal of Physical Chemistry A, 2002, 106, 8471-8478.	1.1	25
5	Unimolecular HCl and HF Elimination Reactions of 1,2-Dichloroethane, 1,2-Difluoroethane, and 1,2-Chlorofluoroethane: Assignment of Threshold Energies. Journal of Physical Chemistry A, 2010, 114, 794-803.	1.1	22
6	Unimolecular rate constants for chemically activated 1,1,1-trifluoro-2-chloroethane: a competitive three-channel system. The Journal of Physical Chemistry, 1991, 95, 3968-3975.	2.9	21
7	Theoretical calculations of product percentage yields for the thermal decomposition of 2-chloro-1,1-difluoroethane. Tetrahedron Letters, 2003, 44, 7265-7268.	0.7	21
8	Unimolecular Reactions in the CF₃CH₂Cl â†” CF₂ClCH₂F System: Isomerization by Interchange of Cl and F Atoms. Journal of Physical Chemistry A, 2011, 115, 1054-1062.	1.1	18
9	Unimolecular Reactions of Chemically Activated CF₂BrCF₂CH₃ and CF₂BrCF₂CD₃:â€‰ Evidence for 1,2-FBr Interchange. Journal of Physical Chemistry A, 2008, 112, 441-447.	1.1	17
10	Substituent Effects and Threshold Energies for the Unimolecular Elimination of HCl (DCl) and HF (DF) from Chemically Activated CFCl2CH3 and CFCl2CD3. The Journal of Physical Chemistry, 1996, 100, 3044-3050.	2.9	16
11	Unimolecular Reactions Including ClF Interchange of Vibrationally Excited CF2ClCHFCH2CH3 and CF2ClCHFCD2CD3. Journal of Physical Chemistry A, 2007, 111, 8445-8455.	1.1	16
12	Undergraduate Introductory Quantitative Chemistry Laboratory Course: Interdisciplinary Group Projects in Phytoremediation. Journal of Chemical Education, 2007, 84, 128.	1.1	16
13	Unimolecular Reactions of CH₂BrCH₂Br, CH₂BrCH₂Cl, and CH₂BrCD₂Cl: Identification of the Clâ^’Br Interchange Reaction. Journal of Physical Chemistry A, 2010, 114, 4138-4147.	1.1	16
14	Unimolecular Elimination of HF and HCl from Chemically Activated CF 3CFClCH 2Cl. Journal of Physical Chemistry A, 2008, 112, 6090-6097.	1.1	14
15	Threshold Energy and Unimolecular Rate Constant for Elimination of HF from Chemically Activated CF3CF2CH3:Â Effect of the CF3Substituent on the Î±-Carbon. Journal of Physical Chemistry A, 1997, 101, 1334-1337.	1.1	13
16	Unimolecular Reactions of CF2ClCFClCH2F and CF2ClCF2CH2Cl: Observation of ClF Interchange. Journal of Physical Chemistry A, 2008, 112, 12117-12124.	1.1	13
17	Isomerisation of CF₂ClCH₂Cl and CFCl₂CH₂F by Interchange of Cl and F Atoms with Analysis of the Unimolecular Reactions of Both Molecules. ChemPhysChem, 2012, 13, 869-878.	1.0	13
18	Threshold Energies and Unimolecular Rate Constants for Elimination of HF from Chemically Activated CF3CH2CH3 and CF3CH2CF3:â€‰ Effect of CH3 and CF3 Substituents at the Î²-Carbon and Implications about the Transition State. Journal of Physical Chemistry A, 1998, 102, 5393-5397.	1.1	12

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19	Isomerization of Neopentyl Chloride and Neopentyl Bromide by a 1,2-Interchange of a Halogen Atom and a Methyl Group. Journal of Physical Chemistry A, 2010, 114, 10395-10402.	1.1	12
20	A computational study of the threshold energies of the 1,2-FCl interchange reaction of chlorofluoroethanes. Canadian Journal of Chemistry, 2010, 88, 1112-1117.	0.6	10
21	Characterization of the 1,1-HF Elimination Reaction from the Competition between the 1,1-HF and 1,2-DF Unimolecular Elimination Reactions of CD₃CD₂CHF₂. Journal of Physical Chemistry A, 2015, 119, 3887-3896.	1.1	10
22	Characterization of the 1,1-HCl Elimination Reaction of Vibrationally Excited CD₃CHFCl Molecules and Assignment of Threshold Energies for 1,1-HCl and 1,2-DCl plus 1,1-HF and 1,2-DF Elimination Reactions. Journal of Physical Chemistry A, 2015, 119, 9441-9451.	1.1	10
23	Unimolecular Isomerization of CH₂FCD₂Cl via the Interchange of Cl and F Atoms: Assignment of the Threshold Energy to the 1,2-Dyotropic Rearrangement. Journal of Physical Chemistry A, 2013, 117, 6717-6723.	1.1	8
24	Effects of CF₃ and CH₃ Groups on the Threshold Energy for the Unimolecular Interchange Reaction of Cl- and F-Atoms in CF₃CHFCH₂Cl and CH₃CHFCH₂Cl. Journal of Physical Chemistry A, 2014, 118, 2886-2896.	1.1	8
25	Unimolecular Reactions of 1,1,1-Trichloroethane, 1,1,1-Trichloropropane, and 3,3,3-Trifluoro-1,1,1-trichloropropane: Determination of Threshold Energies by Chemical Activation. Journal of Physical Chemistry A, 2014, 118, 9347-9356.	1.1	7
26	The Unimolecular Reactions of CF₃CHF₂ Studied by Chemical Activation: Assignment of Rate Constants and Threshold Energies to the 1,2-H Atom Transfer, 1,1-HF and 1,2-HF Elimination Reactions, and the Dependence of Threshold Energies on the Number of F-Atom Substituents in the Fluoroethane Molecules. Journal of Physical Chemistry A, 2017, 121, 8746-8756.	1.1	7
27	Disproportionation-combination rate constant ratios for haloalkyl radicals: Evidence for heterogeneous disproportionation. International Journal of Chemical Kinetics, 1987, 19, 401-413.	1.0	6
28	Unimolecular Rate Constant and Threshold Energy for the HF Elimination from Chemically Activated CF₃CHFCF₃. Journal of Physical Chemistry A, 2010, 114, 6996-7002.	1.1	6
29	Recent Trends in Chemistry Instrumentation Requests by Undergraduate Institutions to NSFâ€™s RUI Program. Journal of Chemical Education, 2012, 89, 4-6.	1.1	5
30	Reinvestigation of the Unimolecular Reactions of CHF₂CHF₂: Identification of the 1,1-HF Elimination Component from Addition of :CFCHF₂ to trans-2-Butene. Journal of Physical Chemistry A, 2016, 120, 9357-9362.	1.1	5
31	Substituent effects on the disproportionation-combination rate constant ratios for gas-phase halocarbon radicals. II. Reactions of ?CF3 +CF3CH2CH2? and CF3CH2CH2? + CF3CH2CH2?. International Journal of Chemical Kinetics, 1996, 28, 61-68.	1.0	4
32	Substituent effects on the disproportionation-combination rate constant ratios for gas-phase halocarbon radicals. IV. Reactions of ï¿½CF3 + CF3CH2CF2ï¿½ and CF3CH2CF2ï¿½ + CF3CH2CF2ï¿½. International Journal of Chemical Kinetics, 1999, 31, 237-243.	1.0	4
33	Chemical Activation Study of the Unimolecular Reactions of CD₃CD₂CHCl₂ and CHCl₂CHCl₂ with Analysis of the 1,1-HCl Elimination Pathway. Journal of Physical Chemistry A, 2016, 120, 8244-8253.	1.1	4
34	Experimental and Computational Studies of Unimolecular 1,1-HX (X = F, Cl) Elimination Reactions of C₂D₅CHFCl: Role of Carbene:HF and HCl Adducts in the Exit Channel of RCHFCl and RCHCl₂ Reactions. Journal of Physical Chemistry A, 2019, 123, 2621-2633.	1.1	4
35	Substituent effects on the disproportionation-combination rate constant ratios for gas-phase halocarbon radicals. Part III: Reactions of CF3 + CF3CH2 CHCF3 and CF3 CH2CHCF3 + CF3CH2 CHCF3. International Journal of Chemical Kinetics, 1996, 28, 109-114.	1.0	3
36	Analysis of the Five Unimolecular Reaction Pathways of CD₂ClCHFCl with Emphasis on CD₂Cl(F)C: and CD₂Cl(Cl)C: Formed by 1,1-HCl and 1,1-HF Elimination. Journal of Physical Chemistry A, 2018, 122, 8446-8457.	1.1	3

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37	Substituent effects on the disproportionation?combination rate constant ratios for gas-phase halocarbon radicals, Part 5: Reactions of CF3 + CF3CH2CHCH3 and CF3CH2CHCH3 + CF3CH2CHCH3. International Journal of Chemical Kinetics, 2001, 33, 549-557.	1.0	2
38	Unimolecular HBr and HF Elimination Reactions of Vibrationally Excited C₂H₅CH₂Br and C₂D₅CHFBr: Identification of the 1,1-HBr Elimination Reaction from C₂D₅CHFBr and Search for the C₂D₅(F)C:HBr Adduct. Journal of Physical Chemistry A, 2019, 123, 8776-8786.	1.1	2
39	Evolution of Undergraduate Research as a Critical Component in the Education of Chemists. ACS Symposium Series, 2015, , 219-238.	0.5	0
40	Unimolecular Rate Constants for the HF and HCl Elimination Reactions from Chemically Activated CF₂ClSH. International Journal of Chemical Kinetics, 2015, 47, 379-388.	1.0	0