(1) Wu, J. Y.; Liu, J. Y.; Li, Z. S.; Sun, C. C., Theoretical Study of The Reactions of CF_3OCHF_2 with The Hydroxyl Radical and the Chlorine Atom. *Chemphyschem* **2004,***5*, 1336−1344.

(2) Chandra, A. K., Theoretical Studies on the Kinetics and Mechanism of the Gas-phase Reactions of CHF_2OCHF_2 with OH Radicals. *J. Mol. Model.* **2012,***18*, 4239−4247.

(3) Jogeshwari Devi, K.; Chandra, A. K., Theoretical Study of the Gas-phase Reactions of CHF_2OCHF_2 (HFE-134) with Cl Atoms. *Curr. Sci.* **2012,***102*, 470-477.

(4) Gour, N. K.; Deka, R. C.; Singh, H. J.; Mishra, B. K., Theoretical Study on the Gas-phase Reactions of Ethyl Butyrate with OH Radicals at 298 K. *Monatsh. Chem.* **2014,***145*, 1759−1767.

(5) Lily, M.; Sutradhar, D.; Chandra, A. K., Theoretical Investigations on Kinetics, Mechanism and Thermochemistry of the Gas Phase Reactions of $CHF_2OCF_2CHF_2$ with OH Radicals. *Comput. Theor. Chem.* **2013,***1022*, 50−58.

(6) Deka, R. C.; Mishra, B. K., Theoretical Studies on Kinetics, Mechanism and Thermochemistry of Gas-phase Reactions of HFE-449mec-f with OH Radicals and Cl Atom. *J. Mol. Graphics Modell.* **2014,***53*, 23−30.

(7) Deka, R. C.; Mishra, B. K., A Theoretical Investigation on the Kinetics, Mechanism and Thermochemistry of Gas-phase Reactions of Methyl Acetate with Chlorine Atoms at 298 K. *Chem. Phys. Lett.* **2014,***595−596*, 43−47.

(8) Srinivasulu, G.; Rajakumar, B., Theoretical Investigations on the Kinetics of H-abstraction Reactions from $CF_3CH(OH)CF_3$ by OH Radicals. *J. Phys. Chem. A* **2013,***117*, 4534−4544.

(9) Mishra, B. K., Computational Study on Kinetics and Mechanism of Cl-initiated Hydrogen Abstraction of Methyl Fluoroacetate. *J. Fluor. Chem.* **2015,***172*, 74-79.

(10) Mishra, B. K.; Chakrabartty, A. K.; Deka, R. C., Theoretical Investigation of the Gas-phase Reactions of $CF_2ClC(O)OCH_3$ with the Hydroxyl Radical and the Chlorine Atom at 298 K. *J. Mol. Model.* **2013,***19*, 3263−3270.

(11) Mishra, B. K.; Chakrabartty, A. K.; Deka, R. C., A Theoretical Investigation on the Kinetics and Reactivity of the Gas-phase Reactions of Ethyl Chlorodifluoroacetate with OH Radical and Cl Atom at 298 K. *Struct. Chem.* **2014,***25*, 463−470.

(12) Deka, R. C.; Mishra, B. K., Theoretical Investigation of the Atmospheric Chemistry of Methyl Difluoroacetate: Reaction with Cl Atoms and Fate of Alkoxy Radical at 298 K. *Struct. Chem.* **2014,***25*, 1475−1482.

(13) Singh, H. J.; Gour, N. K.; Rao, P. K.; Tiwari, L., Theoretical Investigation on the Kinetics and Branching Ratio of the Gas Phase Reaction of Sevoflurane with Cl atom. *J. Mol. Model.* **2013,***19*, 4815−4822.

(14) Mishra, B. K.; Singh, H. J.; Tiwari, L., Theoretical Investigation on Mechanism and Kinetics of the Cl-initiated Hydrogen Abstraction Reactions of Ethyl Trifluoroacetate at 298 K. *J. Mol. Model.* **2014,***20*, 2475.

(15) Lily, M.; Chandra, A. K., Theoretical Studies on Atmospheric Chemistry of $(CF_3)_2C(OH)CH_3$: Kinetics, Mechanism and Thermochemistry of Gas Phase Reactions with OH Radicals. *J. Fluor. Chem.* **2015,***175*, 185−192.

(16) Lily, M.; Chandra, A. K., Theoretical Investigation on Kinetics and Thermochemistry of Reaction of $CHF_2CF_2OCH_2CF_3$ with OH Radicals and Global Warming Potentials. *Mol. Phys.* **2015,***113*, 508−520.

(17) Mishra, B. K.; Chakrabartty, A. K.; Bhattacharjee, D.; Deka, R. C., Theoretical Study on the Kinetics and Branching Ratios of the Gas Phase Reactions of 1, 1-Dichlorodimethylether

(DCDME) with Cl Atom. *Struct. Chem.***2013,***24*, 1621−1626.
(18) Liu, F. Y.; Long, Z. W.; Tan, X. F.; Long, B., The Reaction Mechanisms and Kinetics of $CF_3CHFOCH_3$ and $CHF_2CHFOCF_3$ with Atomic Chlorine: A Computational Study. *J. Mol. Model.* **2014,***20*, 2435.
(19) Singh, H. J.; Rao, P. K.; Tiwari, L., Theoretical Studies on OH and Cl Initiated Hydrogen Atom Abstraction of HFE-227pc ($CF_3OCF_2CHF_2$). *J. Atmos. Chem.* **2013,***70*, 257−268.
(20) Zhu, P.; Ai, L. L.; Wang, H.; Liu, J. Y., Theoretical Studies on Mechanism and Kinetics of the Hydrogen-Abstraction Reaction of $CF_2HCOOCH_3$ with OH Radicals. *Comput. Theor. Chem.* **2014,***1029*, 91−98.
(21) Zhang, H.; Liu, Y.; Liu, J.-Y.; Li, Z.-S., Theoretical Study and Rate Constants Calculation for the Reactions X + $CF_3CH_2OCF_3$ (X = F, Cl, Br). *J. Comput. Chem.***2012,***33*, 685−690.
(22) Singh, H. J.; Mishra, B. K.; Rao, P. K., Hydrogen-Atom Abstraction Reaction of $CF_3CH_2OCF_3$ by Hydroxyl Radical. *Bull. Kor. Chem. Soc.* **2010,***31*, 3718−3722.
(23) Yang, L.; Liu, J. Y.; and Li, Z. S., Theoretical Studies of the Reaction of Hydroxyl Radical with $CH_3C(O)OCH_3$. *J. Phys. Chem. A***2008**, *112*, 6364−6372.
(24) Ren, H.; Yang, X.; Li, X.; Liu, Y.; Wei, X., The Hydrogen Abstraction Reaction Mechanism and Rate Constants from 200K to 2000 K Between Sevoflurane and Chlorine Atom: A Theoretical Investigation. *Chem. Phys. Lett.* **2014,***605−606*, 28−34.
(25) Mishra, B. K.; Deka, R. C., A Theoretical Investigation on Kinetics, Mechanism, and Thermochemistry of the Gas-Phase Reactions of Methyl Fluoroacetate with OH Radicals and Fate of Alkoxy Radical. *J. Phys. Chem. A* **2014,***118*, 8779−8786.
(26) Singh, H. J.; Tiwari, L.; Rao, P. K., Computational Study on the Kinetics of OH Initiated Oxidation of Methyl Difluoroacetate ($CF_2HCOOCH_3$). *Mol. Phys.* **2013,***112*, 1892−1898.
(27) Chakrabartty, A. K.; Mishra, B. K.; Bhattacharjee, D.; Deka, R. C., Mechanistic and Kinetics Study of the Gas Phase Reactions of Methyltrifluoroacetate with OH Radical and Cl Atom. *Mol. Phys.* **2013,***111*, 860−867.
(28) Wang, L.; Wen, J.; He, H.; Zhang, J., The Mechanism and Dynamic Studies for the Reactions of OH Radical with $CH_{3-n}F_nOCF_2CHFCl$ (n=0, 1, and 2). *J. Fluor. Chem.* **2014,***164*, 1−9.
(29) Rao, P. K.; Singh, H. J., Kinetics and Mechanism of Gas-Phase Reaction of $CF_3OCH_2CH_3$ (HFE-263) with the OH Radical-A Theoretical Study. *Can. J. Chem.* **2015,***93*, 303−310.
(30) Yang, L.; He, H.-Q.; Ji, Y.-M.; Liu, J.-Y.; Li, Z.-S., Direct Ab Initio Dynamics Calculations of the Rate Constants for the Reaction of $CHF_2CF_2OCH_3$ with Cl. *Int. J. Chem. Kinet.* **2007,***39*, 221−230.
(31) Zierkiewicz, W., Reaction of Volatile Anaesthetic Desflurane with Chlorine Atom. Theoretical Investigation. *Chem. Phys. Lett.* **2013,***555*, 72−78.
(32) Singh, H. J.; Tiwari, L.; Rao, P. K., Computational Study on OH and Cl Initiated Oxidation of 2,2,2-Trifluoroethyl Trifluoroacetate ($CF_3C(O)OCH_2CF_3$). *Bull. Kor. Chem. Soc.* **2014,***35*, 1385−1390.
(33) Gour, N. K.; Deka, R. C.; Singh, H. J.; Mishra, B. K., Theoretical Studies on Kinetics, Mechanism and Thermochemistry of Gas-Phase Reactions of $CF_3CHFCF_2OCF_3$ with OH Radicals and Cl Atoms and Fate of Alkoxy Radical at 298 K. *J. Fluor. Chem.* **2014,***166*, 110−116.
(34) Espinosa-Garcıa, J., Ab Initio and Variational Transition-State Theory Study of the $CF_3CF_2OCH_3$ + OH Reaction Using Integrated Methods: Mechanism and Kinetics. *J. Phys. Chem. A* **2003,***107,* 1618−1626.

(35) Wang, L.; Zhang, T.; Wen, J.; He, H.; Zhang, J., Theoretical Study on Dynamics of the Gas Phase Reactions of $CF_3CF_2CH_2OCHF_2$ with OH Radicals. *J. Fluor. Chem.* **2014,***168*, 25−33.
(36) Mishra, B. K.; Lily, M.; Chakrabartty, A. K.; Deka, R. C.; Chandra, A. K., A DFT Study on Kinetics of the Gas Phase Reactions of $CH_3CH_2OCF_3$ with OH Radicals and Cl Atoms. *J. Fluor. Chem.* **2014,***159*, 57−64.
(37) Gour, N. K.; Deka, R. C.; Singh, H. J.; Mishra, B. K., A Computational Perspective on Mechanism and Kinetics of the Reactions of $CF_3C(O)OCH_2CF_3$ with OH Radicals and Cl Atoms at 298K. *J. Fluor. Chem.* **2014,***160*, 64−71.
(38) Lily, M.; Mishra, B. K.; Chandra, A. K., Kinetics, Mechanism and Thermochemistry of the Gas Phase Reactions of $CF_3CH_2OCH_2CF_3$ with OH Radicals: A Theoretical Study. *J. Fluor. Chem.* **2014,***161*, 51−59.
(39) Zhang, H.; Liu, C. Y.; Zhang, G. L; Hou, W. J.; Sun, M.; Liu, B.; Li, Z. S., Theoretical studies of the reactions of Cl atoms with $CF_3CH_2OCH_nF_{(3-n)}$ (n = 1, 2, 3). *Theor. Chem. Acc.* **2010,***127*, 551−560.
(40) Zhu, P.; Duan, X. M.; Liu, J. Y., Theoretical Studies on Mechanism and Kinetics of the Hydrogen-Abstraction Reaction of $CF_3C(O)OCH_2CH_3$ with OH Radicals. *J. Fluor. Chem.* **2015,***176*, 61−70.

Table S1a. Comparison of the k_{OH} and k_{Cl} at 298 ± 2 K, methods, and lifetime (τ_{OH}, τ_{Cl}, τ_{eff}) for the existing ethers in theory. (Blue font is obtained from this paper. Black font is obtained from the reference)

Ethers	k_{OH}	Methods	k_{Cl}	Methods	τ_{OH} (years)	τ_{Cl} (years)	τ_{eff} (years)
CH_3OCH_3	2.15×10^{-12}	CVT/SCT MP2			0.015		
CH_3OCF_3	1.22×10^{-14}	CVT/SCT MP2			2.60		
CF_3OCHF_2	3.38×10^{-16}	CVT/SCT B3LYP	2.80×10^{-17}	CVT/SCT B3LYP	93.82	1.13×10^{5}	93.74
CHF_2OCHF_2	2.40×10^{-15}	CTST MPWB1K	6.1×10^{-16}	CTST MPWBK	12	5198.33	15
CH_2FOCH_2F	6.06×10^{-16}	CVT/SCT B3LYP			52.33		
CH_3OCHCl_2	2.03×10^{-13}	CVT/SCT BH&HLYP	1.20×10^{-12}	CVT/SCT BH&HLYP	0.156	2.642	0.147
$CH_3OCH_2CH_3$	5.00×10^{-12}	CVT/SCT B3LYP			0.0063		
$CH_3OCHFCF_3$	9.01×10^{-14}	CVT/SCT MP2	1.39×10^{-10}	CVT BH&HLYP	0.352	0.023	0.021
$CH_3OCH_2CF_3$	2.17×10^{-12}	CTST MPWB1K	2.55×10^{-11}	CVT/SCT MP2	0.066	0.124	0.043
$CH_3OCF_2CHF_2$			2.41×10^{-13}	CVT/SCT B3LYP		13.16	
$CH_2FOCH_2CF_3$			5.85×10^{-9}	CVT/SCT MP2		5.42×10^{-4}	
CH_2FOCF_2CHFCl	1.20×10^{-14}	CVT/SCT BMK			2.64		
CH_3OCF_2CHFCl	2.00×10^{-14}	CVT/SCT BMK			1.58		
$CH_3OCF_2CF_3$			6.84×10^{-15}	CVT/SCT MP2		4.8	
CHF_2OCF_2CHFCl	9.08×10^{-15}	CVT/SCT BMK	2.90×10^{-15}	CVT/SCT B3LYP	3.49	1093.44	3.48
$CHF_2OCF_2CHF_2$	1.01×10^{-15}	CTST MPWB1K			35		
$CHF_2OCHClCF_3$	2.51×10^{-14}	CVT/SCT B3LYP	6.67×10^{-15}	CVT/SCT B3LYP	1.26	475.41	1.256
$CHF_2OCHFCF_3$	7.06×10^{-15}	CVT/SCT B3LYP	1.45×10^{-15}	CVT/SCT B3LYP	4.49	2186.89	4.48
			0.11×10^{-15}	CTST wB97XD		2.88×10^{4}	
$CHF_2OCF_2CH_2F$	6.74×10^{-15}	CVT/SCT B3LYP			4.7		
$CHF_2OCH_2CF_3$	2.38×10^{-13}	CVT/SCT B3LYP	2.38×10^{-14}	CVT/SCT B3LYP	0.133	133.23	0.1328
			3.99×10^{-14}	CVT/SCT MP2		79.47	
$CF_3OCH_2CH_3$	5.30×10^{-14}	CTST MPWB1K	7.78×10^{-13}	CTST MPWB1K	0.598	4.075	0.521
	7.6×10^{-14}	CTST M06-2X			0.417		
$CF_3OCHFCHF_2$	6.64×10^{-15}	CVT/SCT B3LYP	4.27×10^{-15}	CVT/SCT BH&HLYP	4.77	742.61	4.74
$CF_3OCHFCF_3$	1.30×10^{-15}	ICVT/SCT BH&HLYP	3.06×10^{-17}	ICVT/SCT BH&HLYP	24.39	1.04×10^{5}	24.38
$CF_3OCH_2CHF_2$	2.74×10^{-14}	CVT/SCT B3LYP			1.16		
$CF_3OCH_2CF_3$	5.47×10^{-12}	CTST B3LYP	7.19×10^{-15}	CVT/SCT MP2	0.0058	441.03	0.0057
$CF_3OCF_2CHF_2$	1.50×10^{-15}	CTST MPWB1K	5.30×10^{-17}	CTST MPWB1K	21.14		
$CF_3OCF_2CHFCF_3$	1.22×10^{-15}	CTST M06-2X	3.40×10^{-17}	CTST M06-2X	25.99	9.33×10^{4}	38.5
$CH_3OCH_2CF_2CF_3$	3.59×10^{-13}	CTST M06-2X			0.115		
$CH_3OCF_2CF_2CF_3$	7.76×10^{-15}	CTST M06-2X	4.67×10^{-14}	CTST M06-2X	4.09	67.90	4.4
$CF_3CH_2OCH_2CF_3$	1.32×10^{-13}	CTST M06-2X			0.272		
$(CF_3)_2CHOCH_2F$	3.68×10^{-14}	CTST M06-2X	1.10×10^{-13}	CTST BH&HLYP	5.99	28.83	4.96
			2.60×10^{-13}	CTST wB97XD		12.20	
$(CF_3)_2CHOCH_3$	1.88×10^{-13}	CTST MPWB1K			0.189		
$(CF_3)_2CFOCH_3$	1.25×10^{-14}	CVT/SCT B3LYP	1.34×10^{-14}	CVT/SCT B3LYP	2.54	236.64	2.51
$CHF_2OCH_2CF_2CF_3$	9.05×10^{-15}	CVT/SCT BMK			3.50		
$CHF_2CF_2OCH_2CF_3$	1.01×10^{-14}	CTST M06-2X			4.50		
$CF_3CH_2OCF_2CHFCF_3$	9.10×10^{-15}	CTST M06-2X	4.77×10^{-17}	CTST M06-2X	3.48	6.65×10^{4}	3.479

Table S1b. Comparison of the k_{OH} and k_{Cl} at 298 ± 2 K, methods, and lifetime (τ_{OH}, τ_{Cl}, τ_{eff}) for the existing esters in theory. (Blue font is obtained from this paper. Black font is obtained from the reference)

Esters	k_{OH}	Methods	k_{Cl}	Methods	τ_{OH} (days)	τ_{Cl} (years)	τ_{eff} (years)
CH_3COOCH_3	3.26×10^{-13}	CVT/SCT MP2	2.61×10^{-12}	CTST MPWB1K	35.50	0.121	0.054
$CF_2HCOOCH_3$	6.06×10^{-14}	ICVT/SCT M06-2X	1.18×10^{-13}	CVT/SCT B3LYP	190.99	26.87	0.513
	1.38×10^{-14}	CTST MPWB1K	1.95×10^{-13}	CTST MPWB1K	42	16	0.114
$CH_2FCOOCH_3$	2.44×10^{-13}	CTST MPWB1K	2.62×10^{-13}	CTST MPWB1K	24	12.10	1.21
CF_3COOCH_3	4.05×10^{-14}	CVT/SCT B3LYP	8.75×10^{-14}	CVT/SCT B3LYP	285.78	36.24	0.766
	5.50×10^{-14}	CTST MPWB1K	5.90×10^{-14}	CTST MPWB1K	210.44	53.75	0.570
$CF_2ClCOOCH_3$	9.10×10^{-14}	CTST MPWB1K	1.20×10^{-12}	CTST MPWB1K	127.19	2.64	0.389
$CF_3COOCH_2CH_3$	7.00×10^{-13}	ICVT/SCT M06-2X	9.96×10^{-13}	CVT/SCT B3LYP	16.53	3.18	0.045
			1.60×10^{-12}	CTST MPWB1K		1.98	0.044
$CF_2ClCOOCH_2CH_3$	5.09×10^{-13}	CTST MPWB1K	1.86×10^{-12}	CTST MPWB1K	22.74	1.70	0.066
$CF_3COOCH_2CF_3$	5.30×10^{-13}	CTST MPWB1K	2.00×10^{-14}	CTST MPWB1K	21.84	158.55	0.060
	1.20×10^{-13}	CTST M06-2X	9.80×10^{-16}	CTST M06-2X	96.45	3235.69	0.15
$CH_3(CH_2)_2COOCH_2CH_3$	4.87×10^{-12}	CTST M06-2X			2.37		

Table S1c. Comparison of the k_{OH} and k_{Cl} at 298 ± 2 K, methods, and lifetime (τ_{OH}, τ_{Cl}, τ_{eff}) for the existing alcohols in theory. (Blue font is obtained from this paper. Black font is obtained from the reference)

alcohols	k_{OH}	Methods	k_{Cl}	Methods	τ_{OH} (days)	τ_{Cl} (years)	τ_{eff} (years)
CH_3OH	6.82×10^{-13}	CTST BH&HLYP			16.97		
	7.97×10^{-13}	VTST MP2			14.52		
CF_3OH	9.7×10^{-18}	CTST MP2			1.19×10^{6}		
CH_3CH_2OH	2.40×10^{-12}	CTST BH&HLYP			4.82		
	2.71×10^{-12}	VTST MP2			4.27		
CH_2FCH_2OH			2.51×10^{-11}	CVT/SCT MP2		0.126	
CF_2HCH_2OH			2.83×10^{-12}	CVT/SCT MP2		1.12	
CF_3CH_2OH	9.89×10^{-14}	CVT/SCT B3LYP	6.05×10^{-13}	CVT/SCT MP2	117.03	5.24	0.302
$CF_3CH(OH)CF_3$	3.54×10^{-14}	CVT/SCT M06-2X			441.65		
	2.01×10^{-14}	CVT/SCT B3LYP			575.82		
n-$CH_3CH_2CH_2OH$	4.04×10^{-12}	CTST BH&HLYP			2.86		
i-$CH_3CH_2CH_2OH$	4.19×10^{-12}	CTST BH&HLYP			2.76		
$CF_3CH_2CH_2OH$	4.70×10^{-13}	CVT/SCT M06-2X			24.62		
$CF_3CF_2CH_2OH$	8.44×10^{-14}	CVT/SCT B3LYP	3.19×10^{-13}	CVT/SCT BH&HLYP	137.13	9.94	0.362
			7.14×10^{-13}	CTST MP2		4.44	
$CH_3(CH_2)_3OH$	6.88×10^{-12}	CTST BH&HLYP			1.68		
	5.51×10^{-12}	MS-CVT/SCT MG3S			2.10		
$CF_3(CH_2)_3OH$	3.93×10^{-12}	CVT/SCT MP2			2.94		
$(CF_3)_2C(OH)CH_3$	7.46×10^{-15}	CTST M06-2X			1825		