

Heat Capacity and Bond Dissociation Energy Calculations of Some Fluorinated Ethanol's and its Radicals: $\text{CH}_3\text{-}_x\text{CH}_2\text{F}_x\text{OH}$, $\text{CH}_3\text{CH}_2\text{-}_x\text{F}_x\text{OH}$

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Abstract

Structures and thermochemical properties of these species were determined by the gaussian M-062x/6-31 + g (d, p) calculation enthalpies of formation for 19 fluorinated ethanol and some radicals were calculated with a popular *Ab initio* and density functional theory methods: The gaussian M-062x/6-31 + g (d, p) via several series of isodesmic reactions. Entropies ($S_{298}^\circ\text{K}$ in $\text{Cal}\cdot\text{Mol}^{-1}\text{K}^{-1}$) were estimated using the M-062x/6-31 + g (d, p) computed frequencies and geometries. Contributions of entropy, $S_{298}^\circ\text{K}$, and heat capacities, $C_p(T)$ due to vibration, translation, and external rotation of the molecules were calculated based on the vibration frequencies and structures obtained from the M-062x/6-31 + g (d, p) Density Functional Method. Potential barriers are calculated using M-062x/6-31 + g (d, p) density functional method and are used to calculate rotor contributions to entropy and heat capacity using integration over energy levels of rotational potential. Rotational barriers were determined and hindered internal rotational contributions for $S_{298}^\circ - 1500^\circ\text{K}$, and $C_p(T)$ were calculated using the rigid rotor harmonic oscillator approximation, with direct integration over energy levels of the intramolecular rotation potential energy curves. Thermochemical properties of fluorinated alcohols are needed for understanding their stability and reactions in the environment and in thermal processes.

Keywords

Thermo-Chemistry, Enthalpy, Fluorinated Ethanol's, Thermochemical Properties

1. Introduction

Fluorinated hydrocarbons are used as refrigerants, in polymers, heat exchange fluids, and as solvents. They are present in the atmosphere, lithosphere, and hy-

drosphere. Because of their less adverse effects on the stratospheric ozone layer, they are used in place of greenhouse gases [1]. Fluorinated hydrocarbons exist as compounds ranging from pure to oxidized intermediates resulting from oxidation in the environment. In order to study their reactivity in biological systems, lifetimes, and in the environment, it's critical to understand the chemical and thermodynamic properties of fluorocarbons and their breakdown intermediates.

The thermochemistry of fluorinated alcohols with one carbon atom was studied in the past and is in the literature [2]. In 2016, Hang Wang studied thermodynamic properties of fluorinated methanol using CBS-QB3, M06, M06-2X, WB97X, W1U, B3LYP, CBS-APNO and G4 Calculations. Small standard deviation suggests good error cancellation of work reactions and accuracy. M06-2x/6-31 + g (d, p) calculation had small values for standard deviations. It is an accurate method to calculate Enthalpy of fluorinated alcohols. It shows the second smallest standard deviation after CBS-QB3 method of calculation.

Halogenated compounds are highly stable, have low reactivity and are valued chemicals in industry [3]. Due to its widespread use and their persistence in the environment, they are of concern to the environment. In order to understand the oxidation and reduction reactions involving such molecules, their thermochemical properties must be studied [3].

1.1. Isodesmic and Isogyric Reaction

The enthalpy of formation of mono and di fluorinated ethanol's and its radicals has been calculated using Gaussian M-062x/6-31 + g (d, p) method of calculation. In order to calculate the enthalpy of formation of fluorinated ethanols using this method, we use the calculated enthalpies of formation in work reactions along with reference species.

The number of each type of bond must be conserved in the isodesmic reactions in order to cancel any systematic error in the molecular orbital calculations using this method. Calculations of enthalpies of formation are allowed to accuracies close to experimental values by the careful choice of the isodesmic reactions [2]. Standard enthalpy of formation for the reference species used in the isodesmic work reactions along with their uncertainties is listed in **Table 1**. Taking 1-fluoroethanol as an example, two isodesmic reactions (**Table 2**) are selected to determine the $\Delta_f H^\circ_{(298^\circ\text{K})}$ of the target molecule, 1-fluoroethanol. Since the $\Delta_f H^\circ_{(298^\circ\text{K})}$ values of all species but 1-fluoroethanol in 1 - 2 (**Table 2**) are known, the $\Delta_f H^\circ_{(298^\circ\text{K})}$ of the target species 1-fluoroethanol is obtained from this data and the calculated $\Delta_{\text{rxn}} H^\circ_{(298^\circ\text{K})}$. $\Delta_f H^\circ_{(298^\circ\text{K})}$ calculated using two different reference molecules are within $\pm 2 \text{ Kcal}\cdot\text{mol}^{-1}$.

1.2. Reference Species

Standard enthalpy of formation for the reference species used in the isodesmic work reactions along with their uncertainties is listed in **Table 1**. **Table 2** provides one example on the method of Isodesmic Work Reactions used for the

Table 1. Reference Species in the Isodesmic Reactions Standard Enthalpy of Formation Values (kcal·mol⁻¹) [4].

Species	$\Delta_f H^\circ_{(298^\circ\text{K})}$	Species	$\Delta_f H^\circ_{(298^\circ\text{K})}$
CH ₃ F	-56.54 ± 0.07 ^a -56.62 ± 0.48 ^h	CH ₃ OOH	-30.96 ± 0.67 ^b
CH ₃ CH ₂ F	-65.42 ± 1.11 ^a	CH ₃ CH ₂ OOH	-38.94 ± 0.81 ^b
CH ₃ CH ₂ CH ₂ F	-70.24 ± 1.30 ^a	CH ₃ CH ₂ CH ₂ OOH	-44.03 ± 0.67 ^b
CH ₂ F ₂	-108.07 ± 1.46 ^a -107.67 ± 0.48 ^h	CH ₃ OO·	2.37 ± 1.24 ^b
CH ₃ CHF ₂	-120.87 ± 1.62 ^a	CH ₃ CH ₂ OO·	-6.19 ± 0.92 ^b
CH ₃ CH ₂ CHF ₂	-125.82 ± 1.65 ^a	CH ₃ CH ₂ CH ₂ OO·	-11.35 ± 1.24 ^b
CHF ₃	-166.71 ± 1.97 ^h -166.09 ± 0.48 ^h	CH ₄	-17.81 ± 0.01 ^c
CH ₃ CF ₃	-180.51 ± 2.05 ^a	CH ₃ CH ₃	-20.05 ± 0.04 ^c
CH ₃ CH ₂ CF ₃	-185.48 ± 2.15 ^a	CH ₃ CH ₂ CH ₃	-25.01 ± 0.06 ⁱ
CH ₃ ·	34.98 ± 0.02 ^c	CH ₃ CH ₂ CH ₂ CH ₃	-30.07 ± 0.08 ⁱ
CH ₃ CH ₂ ·	28.65 ± 0.07 ^c	CH ₃ O·	5.15 ± 0.08 ^c
CH ₃ CH ₂ CH ₂ ·	24.21 ± 0.24 ^g 24.18 ⁱ	CH ₃ CH ₂ O·	-3.01 ^d
H	52.10 ^c	OH	8.96 ± 0.01 ^c
O	59.57 ^c	CH ₃ OH	-47.97 ± 0.04 ^c
		CH ₃ CH ₂ OH	-56.07 ± 0.05 ⁱ
		HOO·	2.94 ^g
		HOOH	-32.39 ± 0.04 ^g -32.37 ⁱ

^aWang [2], ^bWang [4], ^cRuscic [5], ^dBurke [6], ^eChase [7], ^fLuo [8], ^gBodi [9], ^hPedley, ⁱATcT Tables [10], ^hCsontos [11]. ^jThe value we used in this study [4]

Table 2. Example for Enthalpy of Formation Calculations for 1-fluoroethanol using Isodesmic Reactions; using different reference molecules, Units in kcal·mol⁻¹.

Isodesmic Reactions	$\Delta H^\circ_{\text{Rxn}(298^\circ\text{K})}$ Hartrees	$\Delta H^\circ_{\text{Rxn}(298^\circ\text{K})}$ kcal/mol ⁻¹	$\Delta_f H^\circ_{(298^\circ\text{K})}$ CH _{3-x} CH ₂ F _x OH, CH ₃ CH _{2-x} F _x OH kcal·mol ⁻¹	Error kcal·mol ⁻¹	Equ. #
CH ₂ FCH ₂ OH + CH ₄ = CH ₃ CH ₂ OH + CH ₃ F - 254.173115 ^a - 40.447961 - 154.926666 - 139.683801 Reference Values - 17.81 - 56.21 - 56.54 Kcal·mol ⁻¹	0.010609	6.657243	-101.6	±0.2	1
CH ₂ FCH ₂ OH + CH ₃ CH ₃ = CH ₃ CH ₂ OH + CH ₃ CH ₂ F - 254.173115 - 79.717768 - 154.926666 - 178.963776 - 20.05 - 56.21 - 65.42 Reported $\Delta_f H^\circ$ (298) kcal·mol ⁻¹	0.000441	0.276731	-101.9	±1.3	2
Standard Deviation over rxns			-101.7 ± 0.7 ±0.1		

^aHartrees, kcal·mol⁻¹; *SD Standard Deviation kcal·mol⁻¹ Errors reported avg of sum of uncertainties in rxn's reference species.

calculation of the Standard Enthalpy of Formation $\Delta_f H^\circ_{(298^\circ\text{K})}$ for the fluoroethanols.

1.3. Computational Method

Composite calculations and series of Isodesmic Reactions are used to calculate

enthalpy of formation of fluorinated ethanols. All calculations are performed using the Gaussian 16 program. The DFT method M06-2x is used to initially analyze optimized structures, frequencies, thermo energies and internal rotors of the molecules studied. It's a Global-hybrid meta-GGA density functional approximation, GGA, generalized gradient approximation, in which the density functional depends on the up and down spin densities and their reduced gradient, meta GGA, in which the functional also depends on the up and down spin kinetic energy densities, hybrid GGA, a combination of GGA with Hartree-Fock exchange, hybrid meta GGA, a combination of meta GGA with Hartree-Fock exchange [12]. All reported values are for standard state of 298 K and 1 atm. We continue the calculation of fluorinated alcohols in this study with this method, because the M-062x/6-31 + g (d, p) level of calculation have been applied to fluoro hydrocarbons 6 with small reported standard deviations values.

2. Results and Discussion

2.1. Entropy and Heat Capacity Values

Internal rotor contributions to calculated entropy and heat capacity at 298 - 1500 K were determined using the molecular mass of each molecule, number of optical isomers, symmetry of the molecule, electron degeneracy, moment of inertia, and vibrational frequencies values (Table 3). The vibrational frequencies for the calculation of heat capacity and entropy at the M-062x/6-31 + g (d, p) level of calculation was scaled by a factor of 0.97 [13]. The moment of inertia values is shown in the **Supplemental Information** Table provided. To calculate the contributions of external rotor, vibration and transition to the calculated entropy and heat capacity, the "SMCPS" [14] program is used. It employs the rigid-rotor harmonic oscillator approximation using moment of inertia from optimized structure and frequencies. The "Rotator" [15] program by Lay *et al.* [16] is used to calculate internal rotor contributions from the corresponding internal rotor torsion frequencies. In this paper, a torsional potential curve presenting a ten-parameter Fourier series function is used to calculate the contribution of internal rotor. Parameters and detailed functions are shown in the **Supplemental Information** Table provided. Rotor [16] program is used to calculate thermodynamic functions from hindered rotations with arbitrary potentials.

Calculation of the Hamiltonian matrix of the internal rotor, and subsequent calculation of energy levels by direct diagonalization of the matrix are employed by this technique. Rotational barriers versus dihedral angle are presented as a potential curve. In this paper, the calculated torsional potential at discrete torsional angles.

$$V(\Phi) = a_0 + \sum a_i \cos(i\Phi) + \sum b_j \cos(j\Phi) \quad i, j = 1-10 \quad (1)$$

The coefficients a_i and b_j are calculated to present the maxima and minima of the torsional potentials with a possibility to shift from the extreme angular positions.

Table 3. Monofluoro and Difluoro-Ethanol's Ideal Gas phase Entropy and Heat Capacity obtained using M-062x/6-31 + g (d, p) level of theory (Cal·mol⁻¹·K⁻¹).

Species		S (298°K)	Cp (298°K)	Cp (400°K)	Cp (500°K)	Cp (600°K)	Cp (800°K)	Cp (1000°K)	Cp (1500°K)
CH ₂ FCH ₂ OH	TVR	64.74	13.23	17.12	20.72	23.75	28.18	31.11	35.06
	Internal Rotor	3.84	3.24	3.48	3.43	3.22	2.68	2.23	1.62
	Total	2.02	3.15	3.33	3.04	2.66	2.05	1.69	1.30
		70.60	19.62	23.94	27.20	29.62	32.91	35.03	37.98
CH ₃ CHFOH	TVR	65.17	14.06	17.90	21.37	24.26	28.51	31.32	35.15
	Internal Rotor	4.48	2.13	2.09	1.95	1.80	1.56	1.40	1.19
	Total	2.67	2.17	2.21	2.18	2.09	1.89	1.71	1.40
		72.32	18.35	22.21	25.50	28.16	31.96	34.42	37.75
C•HFCH ₂ OH	TVR	66.30	13.54	16.96	19.97	22.48	26.29	29.04	33.33
	Internal Rotor	6.19	2.31	1.91	1.69	1.54	1.36	1.25	1.13
	Total	3.09	3.16	2.52	2.04	1.74	1.41	1.25	1.11
		75.58	19.01	21.38	23.70	25.76	29.06	31.55	35.56
CH ₂ FCH•OH	TVR	66.47	13.76	17.09	20.04	22.52	26.29	29.02	33.31
	Internal Rotor	5.72	2.34	2.22	2.09	1.95	1.73	1.56	1.32
	Total	6.00	1.96	1.95	1.95	1.91	1.79	1.65	1.40
		78.19	18.06	21.27	24.07	26.38	29.81	32.24	36.03
CH ₂ FCH ₂ O•	TVR	75.30	20.44	23.66	26.27	28.39	31.55	33.79	37.16
	Internal Rotor	6.08	2.20	1.96	1.7982	1.68	1.53	1.43	1.27
	Total	81.38	22.64	25.62	28.07	30.07	33.08	35.21	38.42
CH ₂ •CHFOH	TVR	66.89	14.80	18.21	21.07	23.40	26.90	29.44	33.49
	Internal Rotor	4.94	1.42	1.25	1.17	1.12	1.06	1.04	1.01
	Total	2.84	1.95	2.12	2.12	2.04	1.83	1.64	1.35
		74.67	18.17	21.58	24.35	26.55	29.79	32.11	35.86
CH ₃ CF•OH	TVR	66.56	13.94	17.25	20.17	22.62	26.38	29.11	33.38
	Internal Rotor	4.91	1.97	1.75	1.57	1.44	1.27	1.18	1.08
	Total	1.71	2.60	3.17	3.22	3.01	2.43	1.99	1.45
		73.18	18.50	22.17	24.96	27.07	30.08	32.28	35.92
CH ₃ CHFO•	TVR	66.73	14.44	18.16	21.39	24.09	28.18	31.12	35.58
	Internal Rotor	4.55	2.12	2.05	1.90	1.75	1.51	1.36	1.18
	Total	71.27	16.56	20.21	23.29	25.84	29.69	32.48	36.75
CH ₂ FCHFOH	TVR	67.46	15.41	19.51	23.12	26.07	30.23	32.83	36.15
	Internal Rotor	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	Total	6.12	3.11	2.64	2.24	1.94	1.57	1.37	1.17
		73.58	18.52	22.15	25.35	28.00	31.79	34.20	37.31
CF ₂ HCH ₂ OH	TVR	62.94	12.00	15.54	18.95	21.90	26.43	29.57	34.06
	Internal Rotor	4.98	3.36	3.20	2.97	2.72	2.26	1.93	1.48
	Total	2.23	3.21	3.17	2.81	2.44	1.91	1.60	1.27
		70.15	18.57	21.91	24.72	27.06	30.60	33.10	36.81

Continued

CH ₃ CF ₂ OH	TVR	68.41	16.53	20.74	24.23	27.01	30.87	33.29	36.37
	Internal Rotor	4.53	2.13	2.08	1.93	1.77	1.53	1.38	1.18
	Total	1.58	2.45	3.09	3.28	3.14	2.60	2.14	1.53
		74.52	21.11	25.91	29.44	31.93	35.01	36.80	39.08
CH ₂ FC•FOH	TVR	69.58	15.15	18.76	21.84	24.36	28.05	30.59	34.38
	Internal Rotor	6.18	3.28	2.51	2.07	1.80	1.50	1.34	1.16
	Total	3.15	1.91	1.96	1.91	1.83	1.65	1.50	1.27
		78.90	20.34	23.22	25.82	27.99	31.19	33.43	36.81
C•HFCFHOH	TVR	69.60	15.48	19.22	22.30	24.76	28.32	30.75	34.41
	Internal Rotor	6.92	2.03	1.69	1.49	1.37	1.22	1.15	1.07
	Total	1.72	2.79	3.10	3.03	2.83	2.37	2.02	1.52
		78.25	20.30	24.01	26.83	28.96	31.91	33.92	37.00
CH ₂ FCHFO•	TVR	70.53	15.99	19.88	23.22	25.94	29.93	32.65	36.59
	Internal Rotor	5.48	2.92	2.79	2.58	2.37	2.01	1.76	1.40
	Total	76.01	18.91	22.67	25.80	28.31	31.94	34.41	37.99
CHF ₂ C•HOH	TVR	68.27	15.46	19.18	22.25	24.71	28.28	30.72	34.40
	Internal Rotor	6.07	2.65	2.30	2.05	1.86	1.61	1.45	1.24
	Total	1.51	2.50	3.06	3.18	3.06	2.60	2.20	1.61
		75.85	20.61	24.54	27.48	29.63	32.49	34.37	37.25
C•F ₂ CH ₂ OH	TVR	69.57	15.16	18.73	21.81	24.32	28.03	30.58	34.37
	Internal Rotor	6.18	2.68	2.38	2.11	1.89	1.5848	1.41	1.19
	Total	3.46	2.45	2.04	1.75	1.55	1.32	1.21	1.09
		79.21	20.29	23.15	25.66	27.76	30.94	33.19	36.65
CHF ₂ CH ₂ O•	TVR	70.02	15.31	18.91	22.14	24.87	29.03	31.94	36.19
	Internal Rotor	5.78	2.51	2.41	2.26	2.10	1.83	1.63	1.34
	Total	75.79	17.82	21.32	24.40	26.97	30.86	33.57	37.53
CH ₂ •CF ₂ OH	TVR	70.20	17.30	21.07	23.93	26.13	29.24	31.38	34.69
	Internal Rotor	4.97	1.37	1.23	1.16	1.11	1.06	1.04	1.01
	Total	1.78	2.81	3.33	3.25	2.9407	2.30	1.87	1.38
		76.95	21.48	25.63	28.35	27.25	32.61	34.29	37.09
CH ₃ CF ₂ O•	TVR	70.14	16.85	20.78	23.99	26.55	30.30	32.87	36.66
	Internal Rotor	4.84	2.08	1.89	1.70	1.54	1.35	1.23	1.11
	Total	5.78	2.51	2.41	2.26	2.10	1.83	1.63	1.34
		80.75	21.44	25.08	27.94	30.20	33.47	35.73	39.11

Calculations of heat capacity and standard entropy based on benchmark database and the computational chemistry comparison for the M-062x/6-31 + g (d, p) calculation method, the vibrational frequencies were scaled by a factor of 0.987 [13]. Potential Energy profiles for mono and di fluorinated ethanol and their related radicals are listed in the **Supplemental Information** Table provided., the solid lines are the fit of Fourier series expansion, rotator contribution

for barriers below 7 kcal·mol⁻¹ were added to the SMCPS calculated entropy and heat capacity. Energies are in kcal·mol⁻¹ (Table 3).

2.2. Standard Enthalpy Values

Enthalpies of formation were determined from isodesmic work reactions from M-062x/6-31 + g (d, p) method of calculation. The standard enthalpy of formation for the reference species along with their uncertainties, which are used the isodesmic work reactions, Table 4, are listed in Table 1 in kcal·mol⁻¹. The standard deviation was calculated [17] for all Enthalpies of formation values for all 19 fluorinated ethanol and is included in Table 4. Details of the method of

Table 4. Standard Enthalpy of Formation using isodesmic reactions: Monofluoro and Difluoro-Ethanols using the M06-2x/6-31 + g (d, p) Level of Theory. Errors reported as sum of avg uncertainty in rxn's reference species.

Isodesmic Reactions Target Specie				$\Delta H_{\text{Rxn}}^{\circ}(298^{\circ}\text{K})$ Hartrees	$\Delta H_{\text{Rxn}}^{\circ}(298^{\circ}\text{K})$ Kcal/mole ¹	$\Delta_f H^{\circ}(298^{\circ}\text{K})$ kcal·mol ⁻¹	Error kcal·mol ⁻¹
CH ₂ FCH ₂ OH -254.173115	+ CH ₄ = -40.447961 -17.81	CH ₃ CH ₂ OH -154.926666 -56.21 -56.54	+ CH ₃ F -139.683801	0.010609	6.657243	-101.6	±0.2
CH ₂ FCH ₂ OH -254.173115	+ CH ₃ CH ₃ = -79.717768 -20.05	CH ₃ CH ₂ OH -154.926666 -56.21	+ CH ₃ CH ₂ F -178.963776 -65.42	0.000441	0.276731	-101.9	±1.3
Reported $\Delta_f H^{\circ}(298)$ kcal·mol ⁻¹						-101.7 ± 0.7	
Standard Deviation over rxns						±0.1	
CH ₃ CHFOH -254.19203	+ CH ₃ CH ₂ CH ₃ = -118.990915 -25.02	CH ₃ CH ₂ OH -154.926666 -56.21	+ CH ₃ CH ₂ CH ₂ F -218.237381 -70.24	0.018898	11.85867	-113.3	±1.5
CH ₃ CHFOH -254.19203	+ CH ₃ CH ₃ = -79.717768 -20.05	CH ₃ CH ₂ OH -154.926666 -56.21	+ CH ₃ CH ₂ F -178.963776 -65.42	0.019356	12.14606	-113.7	±1.3
Reported $\Delta_f H^{\circ}(298)$ kcal·mol ⁻¹						-113.5 ± 1.4	
Standard Deviation over rxns						±0.2	
C•HFCH ₂ OH -253.518298	+ CH ₃ CH ₂ CH ₃ = -118.990915 -25.02	CH ₃ CH ₂ O• -154.268107 -3.01	+ CH ₃ CH ₂ CH ₂ F -218.237381 -70.24	0.003725	2.337471	-50.6	±1.4
C•HFCH ₂ OH -253.518298	+ CH ₄ = -40.447961 -17.81	CH ₃ CH ₂ O• -154.268107 -3.01	+ CH ₃ F -139.683801 -56.54	0.014351	9.005382	-50.8	±0.1
Reported $\Delta_f H^{\circ}(298)$ kcal·mol ⁻¹						-50.7 ± 0.8	
Standard Deviation over rxns						±0.1	
CH ₂ FCH•OH -253.518298	+ CH ₃ CH ₃ = -79.717768 -20.05	CH ₃ CH ₂ O• -154.268107 -3.01	+ CH ₃ CH ₂ F -178.963776 -65.42	0.012436	7.803702	-56.2	±1.2
CH ₂ FCH•OH -253.518298	+ CH ₄ = -40.447961 -17.81	CH ₃ CH ₂ O• -154.268107 -3.01	+ CH ₃ F -139.683801 -56.54	0.022604	14.18421	-55.9	±0.1
Reported $\Delta_f H^{\circ}(298)$ kcal·mol ⁻¹						-56.1 ± 0.6	

Continued

Standard Deviation over rxns							±0.1	
CH ₂ FCH ₂ O•	+ CH ₃ CH ₂ CH ₃ =	CH ₃ CHO•	+ CH ₃ CH ₂ CH ₂ F					
-253.509195	-118.990915	-154.268107	-218.237381	-0.00538	-3.37474	-44.9	±1.4	
	-25.02	-3.01	-70.24					
CH ₂ FCH ₂ O•	+ CH ₄ =	CH ₃ O•	+ CH ₃ CH ₂ F					
-253.509195	-40.447961	-114.989112	-178.963776	0.004268	2.678208	-45.1	±1.2	
	-17.81	5.15	-65.42					
Reported Δ _r H° (298) kcal·mol ⁻¹							-45.0 ± 1.3	
Standard Deviation over rxns							±0.1	
CH ₂ •CHFOH	+ CH ₄ =	CH ₃ O•	+ CH ₃ CH ₂ F					
-253.532134	-40.447961	-114.989112	-178.963776	0.027207	17.07264	-59.5	±1.2	
	-17.81	5.15	-65.42					
CH ₂ •CHFOH	+ CH ₃ CH ₃ =	CH ₃ CH ₂ O•	+ CH ₃ CH ₂ F					
-253.532134	-79.717768	-154.268107	-178.963776	0.018019	11.30708	-59.7	±1.2	
	-20.05	-3.01	-65.42					
Reported Δ _r H° (298) kcal·mol ⁻¹							-59.6 ± 1.2	
Standard Deviation over rxns							±0.1	
CH ₃ CF•OH	+ CH ₃ CH ₃ =	CH ₃ CH ₂ O•	+ CH ₃ CH ₂ F					
-253.542527	-79.717768	-154.268107	-178.963776	0.028412	17.82879	-68.2	±1.2	
	-20.05	-5.01	-65.42					
CH ₃ CF•OH	+ CH ₃ CH ₂ CH ₃ =	CH ₃ CH ₂ O•	+ CH ₃ CH ₂ CH ₂ F					
-253.542527	-118.990915	-154.268107	-218.237381	0.027954	17.54139	-67.8	±1.4	
	-25.02	-5.01	-70.24					
Reported Δ _r H° (298) kcal·mol ⁻¹							-68.0 ± 1.3	
Standard Deviation over rxns							±0.2	
CH ₃ CHFO•	+ CH ₄ =	CH ₃ O•	+ CH ₃ CH ₂ F					
-253.530783	-40.447961	-114.989112	-178.963776	0.025856	16.22487	-58.7	±1.2	
	-17.81	5.15	-65.42					
CH ₃ CHFO•	+ CH ₃ CH ₃ =	CH ₃ CH ₂ O•	+ CH ₃ CH ₂ F					
-253.530783	-79.717768	-154.268107	-178.963776	0.016668	10.45932	-58.8	±1.2	
	-20.05	-3.01	-65.42					
Reported Δ _r H° (298) kcal·mol ⁻¹							-58.8 ± 1.2	
Standard Deviation over rxns							±0.2	
CH ₂ FCHFOH	+ CH ₄ =	CH ₃ CH ₂ OH	+ CH ₂ F ₂					
-353.429924	-40.447961	-154.926666	-238.938973	0.012246	7.684475	-154.2	±1.6	
	-17.81	-56.21	-108.07					
CH ₂ FCHFOH	+ CH ₃ CH ₂ CH ₃ =	CH ₃ CH ₂ OH	+ CH ₃ CH ₂ CHF ₂					
-353.429924	-118.990915	-154.926666	-317.498882	-0.00471	-2.95494	-154.1	±1.9	
	-25.02	-56.21	-125.82					
Reported Δ _r H° (298) kcal·mol ⁻¹							-154.2 ± 1.7	
Standard Deviation over rxns							±0.6	
CF ₂ HCH ₂ OH	+ CH ₄ =	CH ₃ CH ₂ OH	+ CH ₂ F ₂					
-353.431533	40.447961	-154.926666	-238.938973	0.013855	8.694137	-155.2	±1.6	
	-17.81	-56.21	-108.07					
CF ₂ HCH ₂ OH	+ CH ₃ CH ₃ =	CH ₃ CH ₂ OH	+ CH ₃ CHF ₂					
-353.431533	-79.717768	-154.926666	-278.225303	-0.00267	-1.67419	-155.4	±1.8	
	-20.05	-56.21	-120.87					

Continued

Reported $\Delta_f H^\circ$ (298) kcal.mol ⁻¹							-155.3 ± 1.7
Standard Deviation over rxns							±0.1
CH ₃ CF ₂ OH	+ CH ₄ =	CH ₃ CH ₂ OH	+ CH ₂ F ₂				
-353.462472	-40.447961	-154.926666	-238.938973	0.044794	28.10864	-174.6	±1.6
	-17.81	-56.21	-108.07				
CH ₃ CF ₂ OH	+ CH ₃ CH ₂ CH ₃ =	CH ₃ CH ₂ OH	+ CH ₃ CH ₂ CHF ₂				
-353.462472	-118.990915	-154.926666	-317.498882	0.027839	17.46922	-174.5	±1.5
	-25.02	-56.21	-125.82				
Reported $\Delta_f H^\circ$ (298) kcal.mol ⁻¹							-174.5 ± 1.5
Standard Deviation over rxns							±0.1
CH ₂ FC•FOH	+ CH ₄ =	CH ₃ CH ₂ O•	+ CH ₂ F ₂				
-352.776406	-40.447961	-154.268107	-238.938973	0.017287	10.84775	-104.1	±1.5
	-17.81	-3.01	-108.07				
CH ₂ FC•FOH	+ CH ₃ CH ₂ CH ₃ =	CH ₃ CH ₂ O•	+ CH ₃ CH ₂ CHF ₂				
-352.776406	-118.990915	-154.268107	-317.498882	0.000332	0.208333	-104.0	±1.4
	-25.02	-3.01	-125.82				
Reported $\Delta_f H^\circ$ (298) kcal.mol ⁻¹							-104.1 ± 1.5
Standard Deviation over rxns							±0.1
C•HFCFHOH	+ CH ₄ =	CH ₃ O•	+ CH ₃ CHF ₂				
-352.778474	-40.447961	-114.989112	-278.225303	0.01202	7.542658	-105.5	±1.7
	-17.81	5.15	-120.87				
C•HFCFHOH	+ CH ₃ CH ₃ =	CH ₃ O•	+ CH ₃ CH ₂ CHF ₂				
-352.778474	-79.717768	-114.989112	-317.498882	0.008248	5.175694	-105.8	±1.8
	-20.05	5.15	-125.82				
Reported $\Delta_f H^\circ$ (298) kcal.mol ⁻¹							-105.6 ± 1.7
Standard Deviation over rxns							±0.2
CHF ₂ C•HOH	+ CH ₄ =	CH ₃ O•	+ CH ₃ CHF ₂				
-352.773245	-40.447961	-114.989112	-278.225303	0.006791	4.261414	-102.5	±1.7
	-17.81	5.15	-120.87				
CHF ₂ C•HOH	+ CH ₃ CH ₃ =	CH ₃ O•	+ CH ₃ CH ₂ CHF ₂				
-352.773245	-79.717768	-114.989112	-317.498882	0.003019	1.89445	-102.2	±1.8
	-20.05	5.15	-125.82				
Reported $\Delta_f H^\circ$ (298) kcal.mol ⁻¹							-102.3 ± 1.7
Standard Deviation over rxns							±0.2
CH ₂ FCHFO•	+ CH ₄ =	CH ₃ CH ₂ O•	+ CH ₂ F ₂				
-352.768218	-40.447961	-154.268107	-238.938973	0.009099	5.709704	-99.0	±1.5
	-17.81	-3.01	-108.07				
CH ₂ FCHFO•	+ CH ₃ CH ₃ =	CH ₃ CH ₂ O•	+ CH ₃ CHF ₂				
-352.768218	-79.717768	-154.268107	-278.225303	-0.00742	-4.65863	-99.2	±1.7
	-20.05	-3.01	-120.87				
Reported $\Delta_f H^\circ$ (298) kcal.mol ⁻¹							-99.1 ± 1.6
Standard Deviation over rxns							±0.1
C•F ₂ CH ₂ OH	+ CH ₄ =	CH ₃ CH ₂ O•	+ CH ₂ F ₂				
-352.773245	-40.447961	-154.268107	-238.938973	0.014126	8.864192	-102.1	±1.5
	-17.81	-3.01	-108.07				

Continued

C•F ₂ CH ₂ OH	+ CH ₃ CH ₃ =	CH ₃ CH ₂ O•	+ CH ₃ CHF ₂				
-352.773245	-79.717768	-154.268107	-278.225303	-0.0024	-1.50414	-102.3	±1.7
	-20.05	-3.01	-120.87				
Reported Δ _r H° (298) kcal·mol ⁻¹						-102.2 ± 1.6	
Standard Deviation over rxns						±0.2	
CHF ₂ CH ₂ O•	+ CH ₄ =	CH ₃ CH ₂ O•	+ CH ₂ F ₂				
-352.767873	-40.447961	-154.268107	-238.938973	0.008754	5.493214	-98.8	±1.5
	-17.81	-3.01	-108.07				
CHF ₂ CH ₂ O•	+ CH ₃ CH ₃ =	CH ₃ CH ₂ O•	+ CH ₃ CHF ₂				
-352.767873	-79.717768	-154.268107	-278.225303	-0.00777	-4.87512	-99.0	1.7
	-20.05	-3.01	-120.87				
Reported Δ _r H° (298) kcal·mol ⁻¹						-98.9 ± 1.6	
Standard Deviation over rxns						±0.2	
CH ₂ •CF ₂ OH	+ CH ₄ =	CH ₃ O•	+ CH ₃ CHF ₂				
-352.800434	-40.447961	-114.989112	-278.225303	0.03398	21.32276	-119.2	±1.7
	-17.81	5.15	-120.87				
CH ₂ •CF ₂ OH	+ CH ₃ CH ₃ =	CH ₃ O•	+ CH ₃ CH ₂ CHF ₂				
-352.800434	-79.717768	-114.989112	317.498882	0.030208	18.95579	-119.6	±1.8
	-20.05	5.15	-125.82				
Reported Δ _r H° (298) kcal·mol ⁻¹						-119.4 ± 1.7	
Standard Deviation over rxns						±0.2	
CH ₃ CF ₂ O•	+ CH ₄ =	CH ₃ CH ₂ O•	+ CH ₂ F ₂				
-352.786755	40.447961	-154.268107	-238.938973	0.027636	17.34184	-110.6	±1.5
	-17.81	5.15	-108.07				
CH ₃ CF ₂ O•	+ CH ₃ CH ₂ CH ₃ =	CH ₃ CH ₂ O•	+ CH ₃ CH ₂ CHF ₂				
-352.786755	-118.990915	-154.268107	-317.498882	0.010681	6.702424	-110.5	±1.8
	-25.02	5.15	-125.82				
Reported Δ _r H° (298) kcal·mol ⁻¹						-110.6 ± 1.6	
Standard Deviation over rxns						±0.1	

Hartrees, kcal·mole⁻¹ *SD Standard Deviation kcal·mol⁻¹ Errors reported avg of sum of uncertainties in rxn's reference species.

standard deviation [19] and example calculation(s) are shown in the **Supplemental Information** table provided. The bond dissociation energy (BDE's) of Monofluoro and Difluoro-Ethanol's are also calculated in **Table 5** with a small percent error, ranging from 0.2 - 0.8 Kcal/mol. A small value for percent error indicates accurate calculated values for BDB of these molecules.

2.3. Bond Energies

*Supplemental Information

Supplemental Information is available, Cartesian Coordinates; Z-matrixes, vibration frequencies, moments of inertia, the method of standard deviation, Optimized Geometries, and C-C and C-O internal rotors potential energy profile for target fluorinated ethanol and their related radicals are included.

Table 5. Bond Dissociation Energy (BDE's) of Monofluoro and Difluoro-Ethanol's.

Reactions	Bond Dissociation Energy ^a (Kcal·mol ⁻¹)		Error Kcal·mol ⁻¹
	BDE (this study)		
<u>H-CHFCH₂OH</u> H-CHFCH ₂ OH = -101.7 ± 0.1	H• 52.1	+ •CHFCH ₂ OH -50.7 ± 0.09	103.1 ± 0.1 ±0.2
<u>CH₂FC-HHOH</u> CH ₂ FC-HHOH = -101.7 ± 0.1	H• 52.1	+ CH ₂ FC•HOH -56.1 ± 0.1	97.7 ± 0.1 ±0.2
<u>CH₂FCH₂O-H</u> CH ₂ FCH ₂ O-H = -101.7 ± 0.1	H• 52.1	+ CH ₂ FCH ₂ O• -45.0 ± 0.1	108.8 ± 0.1 ±0.2
<u>H-CH₂CHFOH</u> H-CH ₂ CHFOH = -113.5 ± 0.2	H• 52.1	+ •CH ₂ CHFOH -59.6 ± 0.1	106.0 ± 0.15 ±0.3
<u>CH₃C-HFOH</u> H-CH ₂ CHFOH = -113.5 ± 0.2	H• 52.1	+ CH ₃ C•FOH -68. ±0.2	97.6 ± 0.2 ±0.4
<u>CH₃CHFO-H</u> CH ₃ CHFO-H = -113.5 ± 0.2	H• 52.1	+ CH ₃ CHFO• -58.8 ± 0.2	106.8 ± 0.2 ±0.4
<u>H-CHFCHFOH</u> H-CHFCHFOH = -154.6 ± 0.6	H• 52.1	+ •CHFCHFOH -105.6 ± 0.2	101.1 ± 0.4 ±0.8
<u>CH₂FC-HFOH</u> CH ₂ FC-HFOH = -154.6 ± 0.6	H• 52.1	+ CH ₂ FC• FOH -104.1 ± 0.1	102.6 ± 0.35 ±0.7
<u>CH₂FCHFO-H</u> CH ₂ FCHFO-H = -154.6 ± 0.6	H• 52.1	+ CH ₂ FCHFO• -99.1 ± 0.1	107.6 ± 0.35 ±0.7
<u>CF₂-HCH₂OH</u> CF ₂ -HCH ₂ OH = -155.3 ± 0.1	H• 52.1	+ •CF ₂ CH ₂ OH -102.3 ± 0.2	105.1 ± 0.15 ±0.3
<u>CF₂HCH-HOH</u> CF ₂ HCHOH-H = -155.3 ± 0.1	H• 52.1	+ CF ₂ HC•OH -102.4 ± 0.2	105.0 ± 0.15 ±0.3
<u>CF₂HCH₂O-H</u> CF ₂ HCH ₂ O-H = -155.3 ± 0.1	H• 52.1	+ CF ₂ HCH ₂ O• -98.9 ± 0.2	108.5 ± 0.15 ±0.3
<u>H-CH₂CF₂OH</u> H-CH ₂ CF ₂ OH = -174.5 ± 0.1	H• 52.1	+ •CH ₂ CF ₂ OH -119.4 ± 0.2	107.2 ± 0.15 ±0.3
<u>CH₃CF₂O-H</u> CH ₃ CF ₂ O-H = -174.5 ± 0.1	H• 52.1	CH ₃ CF ₂ O• -110.6 ± 0.1	116.0 ± 0.1 ±0.2

3. Conclusions

Thermodynamic properties of 19 mono and di-fluoro ethanols and their related

radicals are calculated using the *ab initio* and Global-hybrid meta-GGA density function methods. Isodesmic work reactions are employed for cancellation of calculation errors. Multiple work reactions are utilized to calculate standard enthalpy of formation at the Gaussian M06-2X calculation level. Optimized geometries and frequencies are used to determine entropy and heat capacity with M06-2x/6-31 + g (d, p) level of calculation. Intermolecular torsion potential curves at the M-06-2x/6-31 + g (d, p) level of calculation are used to calculate hindered internal rotation contributions to heat capacity and entropy with a correction to the calculated heat capacity and entropy. The Thermochemical properties: Entropy, Heat Capacities at (298° - 1500°K), Standard Enthalpy of formation (298K), and the C—F and C—H Bond Dissociation Energies (BDEs) for Mono and Difluorinated Ethanol and Radicals: $\text{CH}_{3-x}\text{CHF}_x\text{OH}$, $\text{CH}_3\text{CH}_{2-x}\text{F}_x\text{OH}$ have been calculated. The C-H bond energies range from 102.2 to 107.2 $\text{Kcal}\cdot\text{mol}^{-1}$ on the methyl carbons, and from 97.3 to 105.2 $\text{Kcal}\cdot\text{mol}^{-1}$ on the secondary ethyl carbons. The calculated values for C-H bond energies for fluorinated methyl carbons are higher than those of the fluorinated ethyl carbons. Calculated values for the O-H bond energies for 2-fluoroethanol are higher than those of O-H bond energies for 1-fluoroethanol and an intermediate calculated value for O-H bond energies for 1,2-difluoroethanol. Introducing a fluorine atom to either methyl or ethyl carbon increases O-H bond energy [18].

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

References

- [1] Wallington, T.J., Schneider, W.F., Worsnop, D.R., Nielsen, O.J., Sehested, J., Debruyne, W.J. and Shorter, J.A. (1994) The Environmental Impact of CFC Replacements HFCs and HCFCs. *Environmental Science & Technology*, **28**, 320A-326A. <https://doi.org/10.1021/es00056a714>
- [2] Wang, H., Castillo, A. and Bozzelli, J.W. (2015) Thermochemical Properties Enthalpy, Entropy, and Heat Capacity of C1-C4 Fluorinated Hydrocarbons: Fluorocarbon Group Additivity. *The Journal of Physical Chemistry A*, **119**, 8202-8215. <https://doi.org/10.1021/acs.jpca.5b03912>
- [3] Schneider, W.F. and Wallington, T.J. (1993) *Ab Initio* Investigation of the Heats of Formation of Several Trifluoromethyl Compounds. *The Journal of Physical Chemistry*, **97**, 12783-12788. <https://doi.org/10.1021/j100151a025>
- [4] Wang, H. and Bozzelli, J.W. (2016) Thermochemical Properties and Bond Dissociation Energies for Fluorinated Methanol, $\text{CH}_{3-x}\text{F}_x\text{OH}$, and Fluorinated Methyl Hydroperoxides, $\text{CH}_{3-x}\text{F}_x\text{OOH}$: Group Additivity. *The Journal of Physical Chemistry*

- A*, **120**, 6998-7010.
- [5] Ruscic, B. (2015) Active Thermochemical Tables: Sequential Bond Dissociation Enthalpy of Methane, Ethane, and Methanol and Related Thermochemistry. *The Journal of Physical Chemistry A*, **119**, 7810-7837. <https://doi.org/10.1021/acs.jpca.5b01346>
- [6] Burke, S.M., Simmie, J.M. and Curran, H.J. (2015) Critical Evaluation of Thermochemical Properties of C1-C4 Species: Updated Group Contributions to Estimate Thermochemical Properties. *Journal of Physical and Chemical Reference Data*, **44**, Article ID: 013101. <https://doi.org/10.1063/1.4902535>
- [7] Chase, M.W.J. (1998) NIST-JANAF Thermochemical Tables (Journal of Physical and Chemical Reference Data). Monograph No. 9, 1-1951.
- [8] Luo, X., Fleming, P.R. and Rizzo, T.R. (1992) Vibrational Overtone Spectroscopy of the $\nu_{\text{OH}} + \nu_{\text{OH}}$ Combination Level of HOOH via Sequential Local Mode-Local Mode Excitation. *The Journal of Chemical Physics*, **96**, 5659-5667. <https://doi.org/10.1063/1.462665>
- [9] Bodi, A., Kercher, J.P., Bond, C., Meteesatien, P., Sztaray, B. and Baer, T. (2006) Photoion Photoelectron Coincidence Spectroscopy of Primary Amines RCH_2NH_2 (R = H, CH_3 , C_2H_5 , C_3H_7 , $i\text{-C}_3\text{H}_7$): Alkylamine and Alkyl Radical Heats of Formation by Isodesmic Reaction Networks. *The Journal of Physical Chemistry A*, **110**, 13425-13433. <https://doi.org/10.1021/jp064739s>
- [10] Wang, H. and Bozzelli, J.W. (2016) Thermochemical Properties ($\Delta_f H^\circ(298\text{ K})$, $S^\circ(298\text{ K})$, $C_p(T)$) and Bond Dissociation Energies for C1-C4 Normal Hydroperoxides and Peroxy Radicals. *Journal of Chemical & Engineering Data*, **61**, 1836-1849. <https://doi.org/10.1021/acs.jced.5b01035>
- [11] Csontos, J., Rolik, Z., Das, S. and Kallay, M. (2010) High-Accuracy Thermochemistry of Atmospherically Important Fluorinated and Chlorinated Methane Derivatives. *The Journal of Physical Chemistry A*, **114**, 13093-13103. <https://doi.org/10.1021/jp105268m>
- [12] Expanding the Limits of Computational Chemistry, 2015-2019 (2020) Density Function Method. <https://gaussian.com/dft>
- [13] NIST Computational Chemistry Comparison and Benchmark Database, NIST Standard Reference Database Number 101, Release 16a; Johnson, R.D. III, Ed., NIST: Gaithersburg, MD. <http://cccbdb.nist.gov>
- [14] Sheng, C. (2002) Elementary, Pressure Dependent Model for Combustion of C_1 , C_2 and Nitrogen Containing Hydrocarbons: Operation of a Pilot Scale Incinerator and Model Comparison. Ph.D. Dissertation, New Jersey Institute of Technology, Newark.
- [15] Becke, A.D. (1993) Density-Functional Thermochemistry. III. The Role of Exact Exchange. *The Journal of Chemical Physics*, **98**, 5648-5652. <https://doi.org/10.1063/1.464913>
- [16] Lay, T.H., Krasnoperov, L.N., Venanzi, C.A., Bozzelli, J.W. and Shokhirev, N.V. (1996) *Ab Initio* Study of α -Chlorinated Ethyl Hydro Peroxides $\text{CH}_3\text{CH}_2\text{OOH}$, $\text{CH}_3\text{CHClOOH}$, and $\text{CH}_3\text{CCl}_2\text{OOH}$: Conformational Analysis, Internal Rotation Barriers, Vibrational Frequencies, and Thermodynamic Properties. *The Journal of Physical Chemistry*, **100**, 8240-8249. <https://doi.org/10.1021/jp952976h>
- [17] Math Is Fun Advanced, 2017. Standard Deviation and Variance. <https://www.mathsisfun.com/data/standard-deviation.html>
- [18] Myrna, H.M., Minh, T.N., David, A.D. and Minh, T.N. (2007) Theoretical Predic-

tion of the Heats of Formation of C_2H_5O Radicals Derived from Ethanol and of the Kinetics of Beta-C-C Scission in the Ethoxy Radical. *The Journal of Physical Chemistry A*, **111**, 113-126.

Supplemental Information

Table S1. Cartesian Coordinates in Angstroms for target fluorinated ethanol and their related radical's geometries at the m062x/6-31 + g (d, p) level of theory.

CH ₂ FCH ₂ OH		Cartesian Coordinates		
Center Number	Atomic Number	X	Y	Z
1	6	0.000003116	-0.000001518	0.000020526
2	9	0.000014524	-0.000002341	-0.000029060
3	1	-0.000005137	-0.000003977	0.000002345
4	1	0.000001564	0.000000767	0.000016765
5	6	-0.000021746	0.000030833	0.000003239
6	1	-0.000002396	0.000010185	0.000006184
7	1	0.000005782	-0.000006013	-0.000000243
8	8	0.000005060	-0.000028332	-0.000029361
9	1	-0.000000767	0.000000396	0.000009605

CH ₃ CHFOH		Cartesian Coordinates		
Center Number	Atomic Number	X	Y	Z
1	6	0.000021353	0.000006161	-0.000053662
2	6	-0.000117652	0.000027420	0.000072872
3	1	-0.000017542	-0.000011156	-0.000000420
4	1	0.000002761	-0.000007600	0.000015768
5	1	-0.000013646	-0.000002428	0.000033080
6	9	0.000109835	0.000008063	-0.000042913
7	1	0.000018820	-0.000022248	0.000004569
8	8	0.000000477	0.000011019	-0.000059799
9	1	-0.000004406	-0.000009231	0.000030505

C•HFCH ₂ OH		Cartesian Coordinates		
Center Number	Atomic Number	X	Y	Z
1	6	-0.000020602	0.000003182	-0.000077408
2	9	0.000008151	0.000053880	0.000000565
3	1	-0.000000850	-0.000011335	0.000020759
4	6	0.000027899	-0.000023254	0.000011757
5	1	-0.000003824	-0.000056264	-0.000008549
6	1	0.000008293	0.000001847	-0.000024269
7	8	-0.000008585	-0.000003122	0.000024031
8	1	-0.000010483	0.000035066	0.000053114

CH ₂ FCH•OH		Cartesian Coordinates		
Center Number	Atomic Number	X	Y	Z
1	6	0.000001249	-0.000000923	-0.000001559
2	9	0.000007760	0.000016425	-0.000015375
3	1	-0.000003551	0.000003238	-0.000020167
4	1	-0.000005664	0.000000417	-0.000013020
5	6	-0.000037395	0.000046885	0.000022542
6	1	0.000001277	-0.000023053	0.000004842
7	8	0.000037801	-0.000035478	-0.000015526
8	1	-0.000001476	-0.000007512	0.000038263

Continued

CH ₂ FCH ₂ O•		Cartesian Coordinates		
Center Number	Atomic Number	X	Y	Z
1	6	0.000009752	0.000030682	0.000120978
2	9	-0.000007540	0.000018428	-0.000104164
3	1	-0.000006175	-0.000009977	-0.000011573
4	1	-0.000001921	-0.000005002	-0.000038255
5	6	-0.000095473	-0.000015917	0.000025447
6	1	0.000036312	-0.000025722	0.000008467
7	1	0.000030627	0.000027608	-0.000011892
8	8	0.000034418	-0.000020100	0.000010992

CH ₂ •CHFOH		Cartesian Coordinates		
Center Number	Atomic Number	X	Y	Z
1	6	0.000014779	0.000033223	-0.000005569
2	6	-0.000030495	-0.000005099	0.000010101
3	1	0.000010354	-0.000009796	-0.000011520
4	1	-0.000018812	-0.000018702	-0.000000754
5	9	0.000041121	0.000009214	-0.000011106
6	1	0.000011136	-0.000017220	0.000008038
7	8	-0.000010627	0.000005847	0.000010223
8	1	-0.000017456	-0.000007665	0.000000588

CH ₃ CF•OH		Cartesian Coordinates		
Center Number	Atomic Number	X	Y	Z
1	6	0.000001336	0.000012708	-0.000046895
2	6	-0.000071306	0.000036407	0.000029101
3	1	-0.000014952	-0.000021374	-0.000009157
4	1	-0.000000203	0.000002487	0.000002208
5	1	-0.000029193	0.000004057	0.000022548
6	9	0.000068515	0.000006342	-0.000002103
7	8	0.000028358	-0.000032227	0.000010729
8	1	0.000017444	-0.000008399	-0.000006430

CH ₃ CHFO•		Cartesian Coordinates		
Center Number	Atomic Number	X	Y	Z
1	6	-0.000025583	0.000026726	0.000006931
2	6	-0.000004925	-0.000017774	-0.000022873
3	1	-0.000016576	0.000000727	-0.000013731
4	1	-0.000010431	0.000004336	0.000014687
5	1	-0.000006608	0.000007692	-0.000003229
6	9	0.000038154	-0.000008832	0.000013405
7	1	0.000017550	-0.000008997	-0.000000815
8	8	0.000008419	-0.000003878	0.000005626

Continued

CH ₂ FCHFOH		Cartesian Coordinates		
Center Number	Atomic Number	X	Y	Z
1	6	-0.000209387	-0.000014742	-0.000046791
2	6	-0.000078791	-0.000026117	-0.000054220
3	9	0.000055970	-0.000014001	0.000038779
4	1	0.000037582	0.000003431	0.000025080
5	1	0.000008069	-0.000003401	0.000000786
6	9	0.000213499	-0.000011196	0.000078222
7	1	-0.000002897	0.000018025	-0.000024730
8	8	-0.000003076	0.000003947	-0.000028849
9	1	-0.000020969	0.000044055	0.000011724

CF ₂ HCH ₂ OH		Cartesian Coordinates		
Center Number	Atomic Number	X	Y	Z
1	6	-0.000006264	-0.000010001	-0.000015081
2	6	0.000196771	-0.000004891	0.000062245
3	9	-0.000177152	-0.000024722	-0.000031629
4	9	0.000058924	0.000072953	-0.000005858
5	1	-0.000009820	0.000002957	-0.000026980
6	1	-0.000016810	-0.000024610	0.000029199
7	1	-0.000014380	0.000016248	-0.000024677
8	8	-0.000035113	-0.000034435	0.000010637
9	1	0.000003845	0.000006502	0.000002145

CH ₃ CF ₂ OH		Cartesian Coordinates		
Center Number	Atomic Number	X	Y	Z
1	6	0.000056837	-0.000094451	0.000110833
2	6	-0.000057651	0.000098699	0.000001478
3	1	0.000011317	-0.000004093	-0.000026345
4	1	0.000014600	-0.000025891	-0.000015228
5	1	-0.000001272	-0.000012112	-0.000025019
6	9	-0.000131047	-0.000088396	0.000020206
7	9	0.000140461	0.000063879	0.000020905
8	8	-0.000014132	0.000020314	-0.000026071
9	1	-0.000019113	0.000042051	-0.000060759

CH ₂ FC•FOH		Cartesian Coordinates		
Center Number	Atomic Number	X	Y	Z
2	6	0.000107121	0.000054590	0.000053325
3	9	-0.000086887	-0.000026092	-0.000005448
4	1	-0.000015313	-0.000013867	-0.000003160
5	1	0.000000240	-0.000001842	-0.000016239
6	9	0.000003934	0.000030284	0.000010058
7	8	0.000076030	0.000051318	-0.000056283
8	1	0.000000747	0.000022936	0.000051063

Continued

C•HFCFHOH		Cartesian Coordinates		
Center Number	Atomic Number	X	Y	Z
1	6	-0.000058756	0.000023216	0.000035904
2	6	-0.000088748	-0.000108788	-0.000099552
3	9	0.000068251	0.000068970	0.000065027
4	1	0.000023870	0.000025841	0.000034527
5	9	0.000011825	-0.000021999	-0.000019250
6	1	-0.000011611	0.000023111	-0.000006306
7	8	0.000047202	0.000013830	-0.000008891
8	1	0.000007966	-0.000024181	-0.000001459

CH ₂ FCHFO•		Cartesian Coordinates		
Center Number	Atomic Number	X	Y	Z
1	6	-0.000043639	0.000033246	0.000009821
2	6	0.000048716	-0.000026830	-0.000018036
3	9	-0.000022444	0.000006378	-0.000008784
4	1	0.000001695	0.000020117	0.000006913
5	1	0.000003424	0.000009684	0.000001110
6	9	0.000023881	0.000019171	0.000030292
7	1	0.000006948	-0.000005119	0.000004871
8	8	-0.000018580	-0.000056646	-0.000026187

CHF ₂ C•HOH		Cartesian Coordinates		
Center Number	Atomic Number	X	Y	Z
1	6	0.000004676	-0.000070251	0.000051141
2	6	0.000027275	-0.000132737	-0.000118944
3	1	-0.000013476	0.000008382	0.000015950
4	8	0.000006557	0.000005715	-0.000023257
5	1	0.000018970	-0.000003557	0.000007094
6	1	-0.000051957	-0.000006265	-0.000015262
7	9	-0.000013983	0.000033076	0.000051050
8	9	0.000021937	0.000165638	0.000032227

CF ₂ •CFOH		Cartesian Coordinates		
Center Number	Atomic Number	X	Y	Z
1	6	0.000045030	0.000052085	-0.000051151
2	6	0.000001125	0.000036125	0.000024114
3	1	-0.000002716	0.000001155	0.000006275
4	8	-0.000050429	-0.000036049	0.000025853
5	1	-0.000005831	-0.000009141	-0.000009552
6	1	-0.000015223	0.000001185	0.000012909
7	9	0.000011981	-0.000006184	0.000002242
8	9	0.000016063	-0.000039174	-0.000010691

Continued

CHF ₂ CH ₂ O•		Cartesian Coordinates		
Center Number	Atomic Number	X	Y	Z
1	6	-0.000032920	-0.000119205	0.000076072
2	6	-0.000030593	-0.000022551	-0.000053428
3	9	-0.000036099	0.000010735	0.000025263
4	9	-0.000006345	-0.000017725	-0.000018129
5	1	-0.000014790	-0.000026477	0.000021461
6	1	0.000040237	0.000019571	-0.000021746
7	1	0.000038791	0.000046905	-0.000010985
8	8	0.000041718	0.000108747	-0.000018508

CH ₂ •CF ₂ OH		Cartesian Coordinates		
Center Number	Atomic Number	X	Y	Z
2	6	-0.000001071	-0.000001757	-0.000000838
3	1	0.000004590	0.000002074	0.000000801
4	1	0.000019461	0.000007677	-0.000000682
5	9	-0.000009537	-0.000013694	-0.000009305
6	9	-0.000017948	0.000004296	0.000010263
7	8	0.000001500	0.000001265	0.000000690
8	1	-0.000006214	-0.000001754	-0.000000488

CH ₃ CF ₂ O•		Cartesian Coordinates		
Center Number	Atomic Number	X	Y	Z
1	6	-0.000049808	0.000049564	0.000101113
2	6	0.000314370	-0.000446227	-0.000322008
3	1	-0.000001882	0.000003042	0.000019595
4	1	0.000007442	0.000003265	-0.000034062
5	1	0.000007479	-0.000020681	0.000033341
6	9	-0.000225548	0.000114125	0.000063416
7	9	-0.000008257	0.000232988	0.000078418
8	8	-0.000043796	0.000063924	0.000060187

Table S2. Frequencies for target fluorinated ethanol and their related radicals at the m062x/6-31 + g (d, p) level of theory (cm⁻¹).

Target fluorinated ethanol	Frequencies (cm ⁻¹)		
CH ₂ FCH ₂ OH	153.7115	318.4318	395.2338
	526.9463	879.0892	913.6087
	1084.2017	1123.0654	1155.2746
	1227.6058	1278.1133	1382.4638
	1406.9769	1443.0414	1499.5695
	1503.3220	3040.8126	3082.2806
	3119.3826	3144.6188	3895.3665

Continued

	222.4821	381.0906	395.9003
	476.6613	591.2739	882.7961
	967.7343	1083.1639	1139.5797
CH ₃ CHFOH	1207.0636	1299.2263	1395.3640
	1408.6162	1481.8193	1491.1530
	1496.5668	3074.8833	3098.4238
	3162.1117	3168.6137	3905.4122
	117.2311	305.3799	387.2015
	487.0844	672.8813	897.2987
	1047.2118	1078.4074	1202.2847
C•HFCH ₂ OH	1230.9543	1340.0387	1397.8007
	1433.9762	1486.8167	3060.3820
	3135.9012	3227.9702	3904.1459
	136.3261	293.7121	372.9921
	469.7867	588.3163	948.2198
	976.5181	1064.6622	1237.5557
CH ₂ FCH•OH	1261.6997	1324.3255	1380.0377
	1477.7581	1517.2468	3089.0157
	3148.4826	3209.7826	3921.1700
	138.8341	326.2587	461.7143
	645.0346	900.2694	995.0829
	095.1447	1132.5555	1209.7403
CH ₂ FCH ₂ O•	287.6953	1366.6408	1397.9225
	436.1160	1499.8795	2978.3111
	021.0190	3079.4857	3141.2839
	103.9492	354.4677	378.6019
	464.4234	533.4936	615.0872
	917.9447	973.1708	1082.8162
CH ₂ •CHFOH	1204.3179	1292.9244	1375.2909
	1421.9543	1501.7259	3093.4946
	3176.3175	3301.9307	3902.4787
	183.0404	339.6091	381.8885
	446.3670	566.0359	874.2810
	992.1200	1063.5695	1140.5736
CH ₃ CF•OH	1302.2104	1363.7386	1442.6873
	1477.4645	1485.2396	3031.7545
	3128.3197	3174.6193	3874.3729
	234.8451	359.2559	443.1211
	572.8867	866.7266	929.6382
	1040.2264	1088.1878	1158.3501
CH ₃ CHFO•	1216.4848	1326.7171	1391.8028
	1484.8041	1492.1170	2997.0767
	3077.4025	3170.0581	3179.9978

Continued

	123.7297	253.3055	341.9812
	442.3530	508.5501	585.7551
	932.9529	1049.0131	1096.9489
CH ₂ FCHFOH	1132.3163	1216.5809	1244.5656
	1341.7047	1356.5333	1432.8601
	1477.0191	1509.6783	3073.3252
	3141.2603	3156.9890	3868.8911
	261.5051	333.1831	429.7499
	803.8978	905.9089	1069.3307
	1113.2025	1153.4006	1280.2493
CF ₂ HCH ₂ OH	1377.1368	1403.4215	1433.7765
	1493.5768	1500.2248	1525.4172
	3032.2176	3044.0073	3104.6932
	3125.0745	3137.9412	3910.0283
	213.0609	336.6797	378.8026
	407.4641	552.4402	575.8400
	584.5503	847.6087	959.8589
CH ₃ CF ₂ OH	1000.3581	1135.7264	1204.1092
	1301.5094	1390.3411	1483.7215
	1488.5073	1492.2192	3086.0281
	3175.9594	3186.0332	3866.1356
	109.4115	244.9232	388.6686
	436.4869	472.3557	575.6453
CH ₂ FC•FOH	917.0734	1055.3780	1102.3841
	1135.9138	1244.9454	1336.2661
	1365.0202	1448.3398	1502.9979
	3049.1641	3148.5710	3871.9507
	107.9351	257.2006	353.4210
	416.6962	546.9238	646.1233
	765.4796	916.4141	991.0405
C•HFCFHOH	1161.1762	1227.5285	1327.6897
	1356.7224	1403.4567	1473.0076
	3148.9051	3254.0619	3863.4809
	122.5173	253.1428	406.6622
	426.8055	595.6816	922.4453
CH ₂ FCHFO•	981.5646	1062.7404	1130.5318
	1159.6593	1193.8858	1264.5276
	1306.1655	1411.2155	1509.8582
	3020.9800	3106.4335	3176.7438
	102.5287	255.5062	307.6957
	498.7454	531.8669	588.6407
	776.4400	943.7162	1040.6628
CHF ₂ C•HOH	1117.9847	1203.9780	1346.8684
	1361.3396	1407.7937	1499.6505
	3165.5275	3252.1304	3846.9473

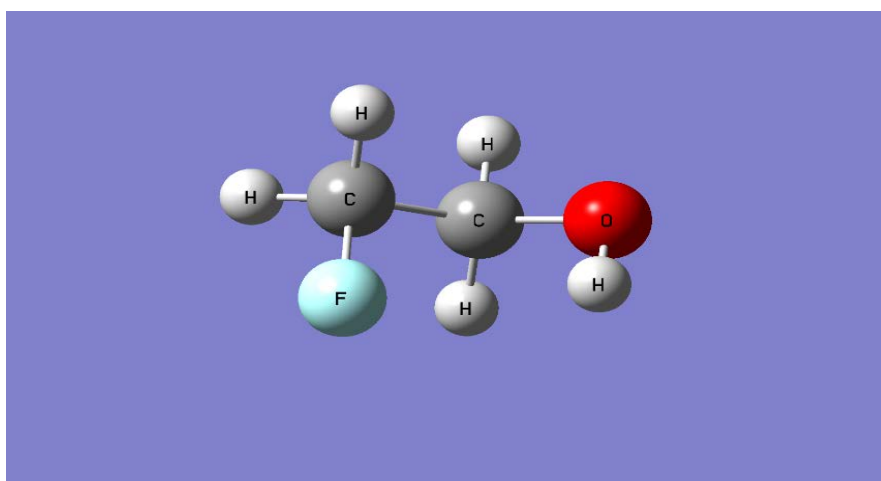
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C•F ₂ CH ₂ OH	111.2059	240.3480	355.7645
	439.8572	476.0825	590.2258
	889.8898	1035.2006	1136.6153
	1208.8861	1259.6672	1294.5087
	1380.7274	1441.8811	1496.7631
	3013.5503	3147.9499	3898.0279
CHF ₂ CH ₂ O•	128.4545	257.5539	433.4387
	494.0758	586.0455	917.5567
	1096.8914	1139.6268	1157.8405
	1232.6325	1307.2674	1385.1305
	1404.8759	1510.7673	1859.0406
	3031.4094	3120.2437	3174.3851
CH ₂ •CF ₂ OH	90.5157	313.8094	380.5941
	392.3412	492.4899	547.1101
	593.9731	597.4030	869.8795
	960.9120	1070.4557	1131.1978
	1308.1224	1403.4875	1499.7334
	3211.2694	3342.0724	3863.9788
CH ₃ CF ₂ O•	168.6127	340.9654	360.5945
	534.8395	551.7060	557.0587
	846.1077	915.5633	974.0145
	1162.5612	1220.2174	1281.3277
	1397.7811	1466.2734	1488.6608
	3077.0770	3170.5354	3190.3722

Table S3. Moment of inertia for target fluorinated ethanol and their related radicals at the m062x/6-31 + g (d, p) level of theory (GHZ).

target fluorinated ethanol	Moment of inertia(GHZ)		
CH ₂ FCH ₂ OH	15.7788859	5.5493007	4.6093694
CH ₃ CHFOH	10.0766267	8.3371985	5.1680915
C•HFCH ₂ OH	18.77997	5.13190	4.51693
CH ₂ FCH•OH	23.2409534	4.5476319	4.3485670
CH ₂ FCH ₂ O•	18.24036	5.23748	4.59279
CH ₂ •CHFOH	10.3760339	9.1250064	5.3599040
CH ₃ CF•OH	10.20355	9.05876	5.07651
CH ₃ CHFO•	10.7702750	8.5850705	5.3185779
CH ₂ FCHFOH	9.4161023	3.5112856	2.7600267
CF ₂ HCH ₂ OH	34.8864548	9.2467926	8.1783038
CH ₃ CF ₂ OH	9.4161023	3.5112856	2.7600267
CH ₂ FC•FOH	9.7798799	3.5506736	2.7289504
C•HFCFHOH	9.5295647	3.7425748	2.9008390
CH ₂ FCHFO•	10.2331738	3.5038934	2.8019184
CHF ₂ C•HOH	9.1000423	3.8971695	3.0141244
C•F ₂ CH ₂ OH	9.6401202	3.8114853	2.8520087
CHF ₂ CH ₂ O•	9.21258	3.85327	2.93914
CH ₂ •CF ₂ OH	5.7024545	5.2730634	5.1759614
CH ₃ CF ₂ O•	5.9149594	5.2219748	5.0070937

Optimized Geometries for target fluorinated ethanol and their related radicals at the m062x/6-31 + g (d, p) level of theory

**Figure S1.** Optimized Geometry for CH₂FCH₂OH at the m062x/6-31 + g (d, p) level of theory.

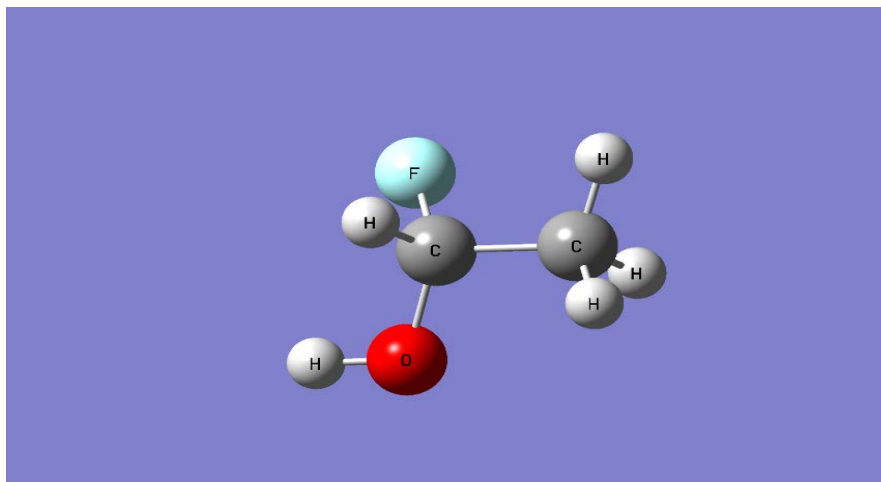


Figure S2. Optimized Geometry for CH₃CHFOH at the m062x/6-31 + g (d, p) level of theory.

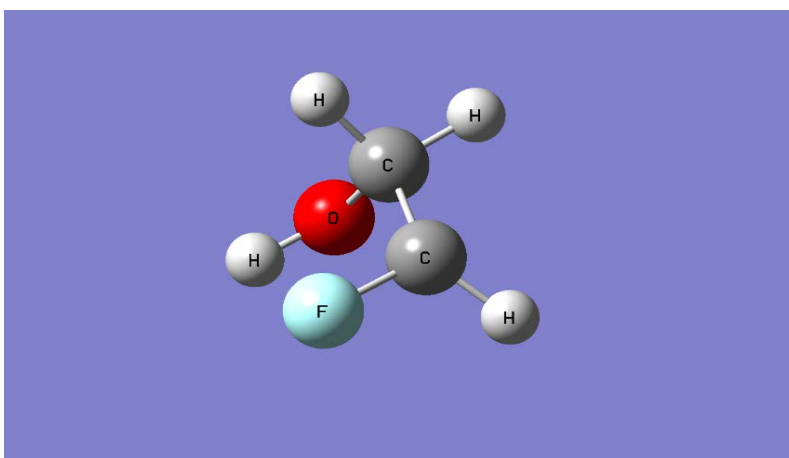


Figure S3. Optimized Geometry for C•HFCH₂OH at the m062x/6-31 + g (d, p) level of theory.

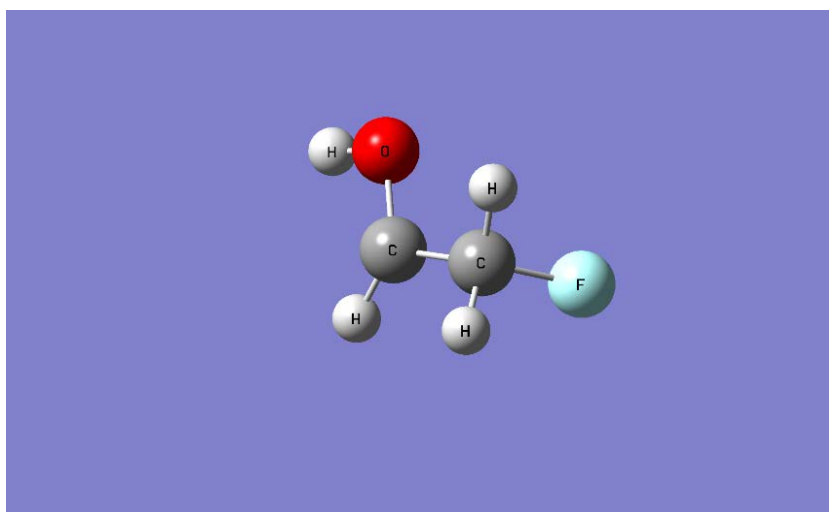


Figure S4. Optimized Geometry for CH₂FCH•OH at the m062x/6-31 + g (d, p) level of theory.

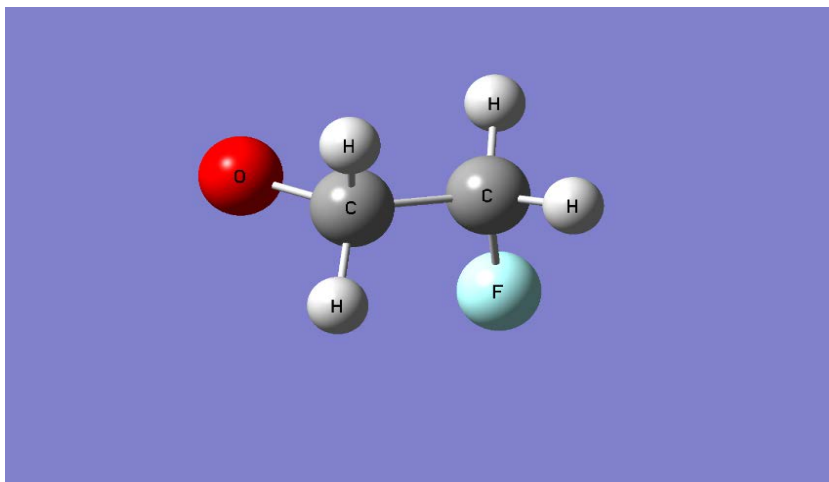


Figure S5. Optimized Geometry for $\text{CH}_2\text{FCH}_2\text{O}\cdot$ at the m062x/6-31 + g (d, p) level of theory.

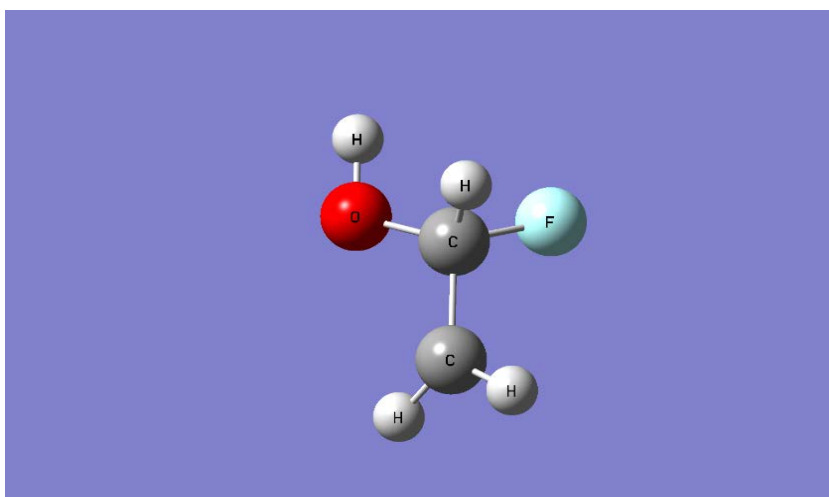


Figure S6. Optimized Geometry for $\text{CH}_2\cdot\text{CHFOH}$ at the m062x/6-31 + g (d, p) level of theory.

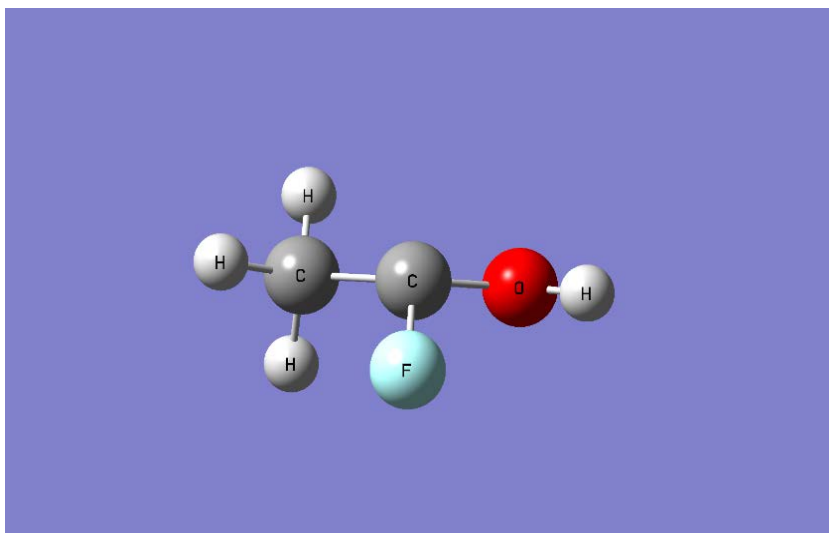


Figure S7. Optimized Geometry for $\text{CH}_3\text{CF}\cdot\text{OH}$ at the m062x/6-31 + g (d, p) level of theory.

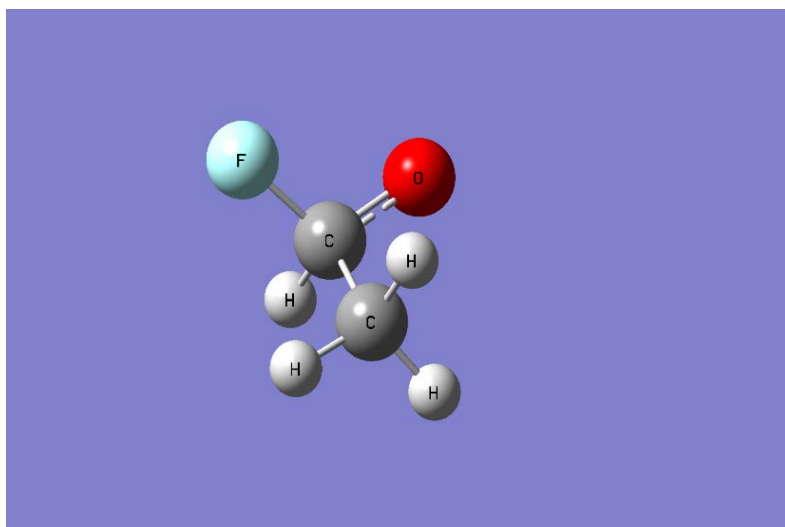


Figure S8. Optimized Geometry for CH_3CHFO at the m062x/6-31 + g (d, p) level of theory.

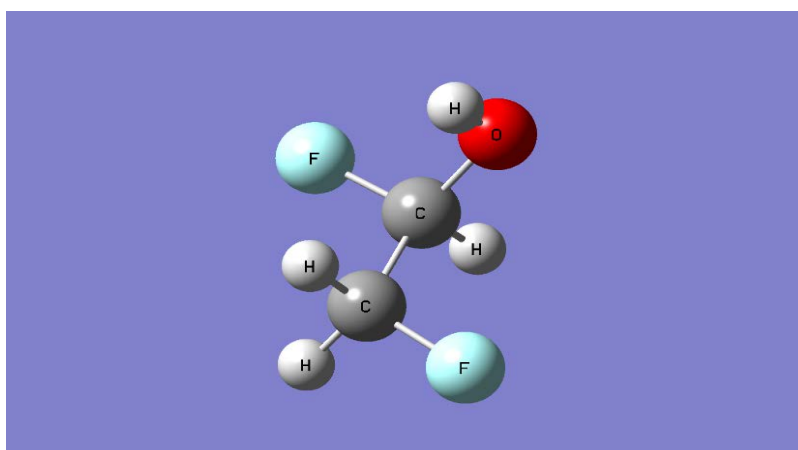


Figure S9. Optimized Geometry for CH_2FCHFOH at the m062x/6-31 + g (d, p) level of theory.

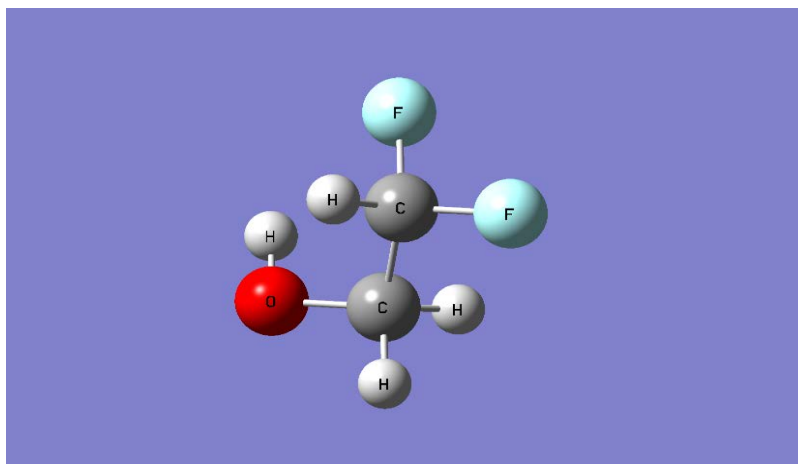


Figure S10. Optimized Geometry for $\text{CF}_2\text{HCH}_2\text{OH}$ at the m062x/6-31 + g (d, p) level of theory.

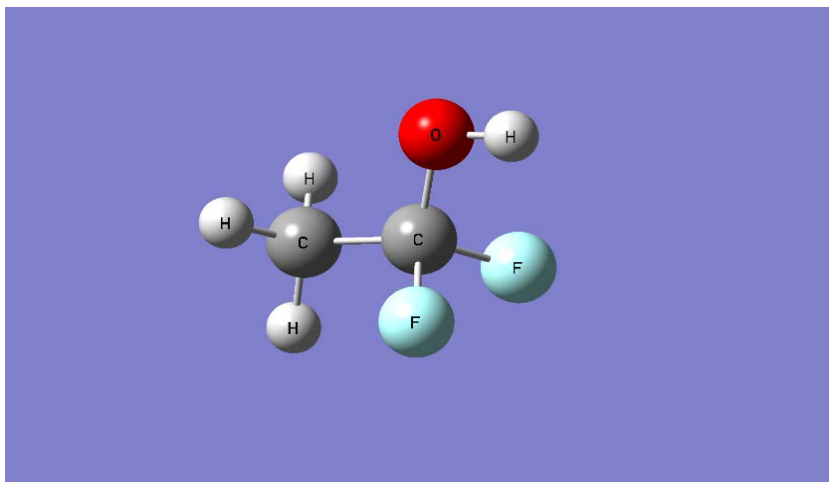


Figure S11. Optimized Geometry for CH₃CF₂OH at the m062x/6-31 + g (d, p) level of theory.

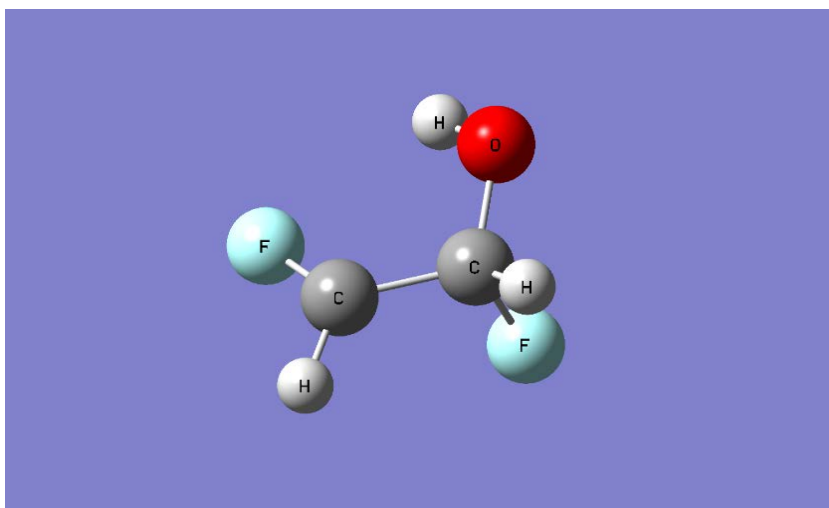


Figure S12. Optimized Geometry for C•HFCFHOH at the m062x/6-31 + g (d, p) level of theory.

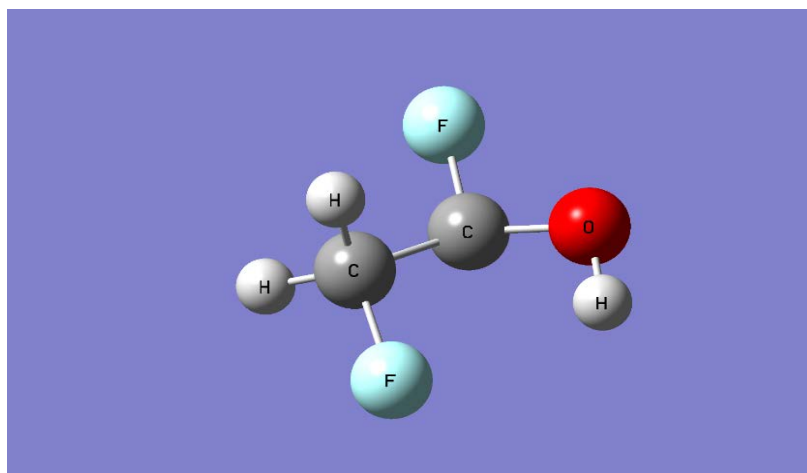


Figure S13. Optimized Geometry for CH₂FC•FOH at the m062x/6-31 + g (d, p) level of theory.

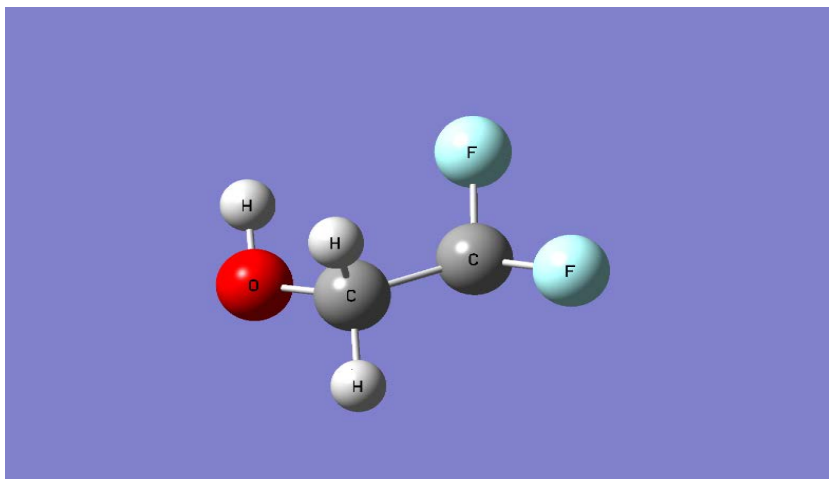


Figure S14. Optimized Geometry for $C\bullet F_2CH_2OH$ at the m062x/6-31 + g (d, p) level of theory.

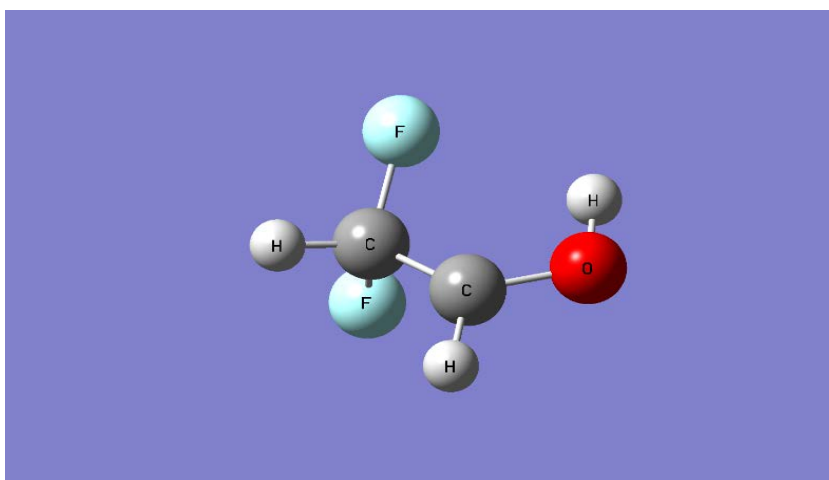


Figure S15. Optimized Geometry for $CHF_2C\bullet HOH$ at the m062x/6-31 + g (d, p) level of theory.

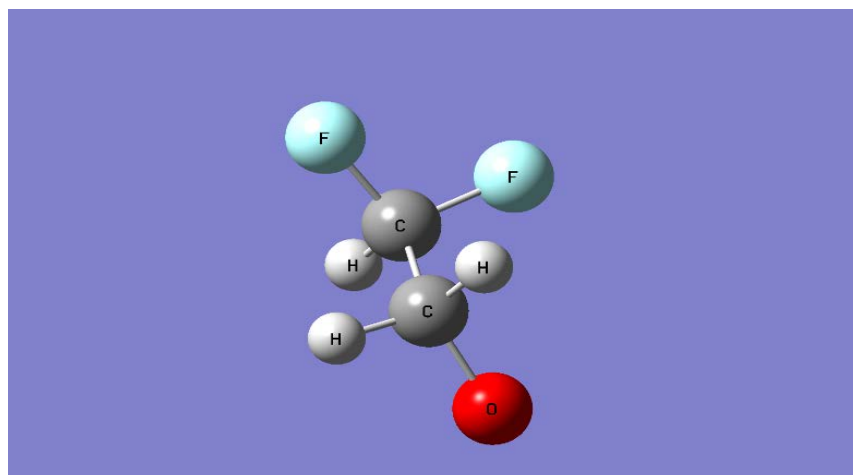


Figure S16. Optimized Geometry for $CHF_2CH_2O\bullet$ at the m062x/6-31 + g (d, p) level of theory.

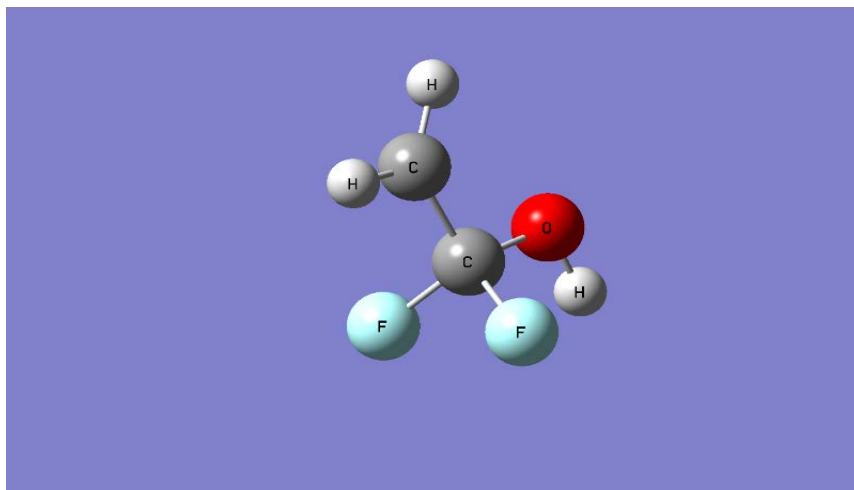


Figure S17. Optimized Geometry for CH₂•CF₂OH at the m062x/6-31 + g (d, p) level of theory.

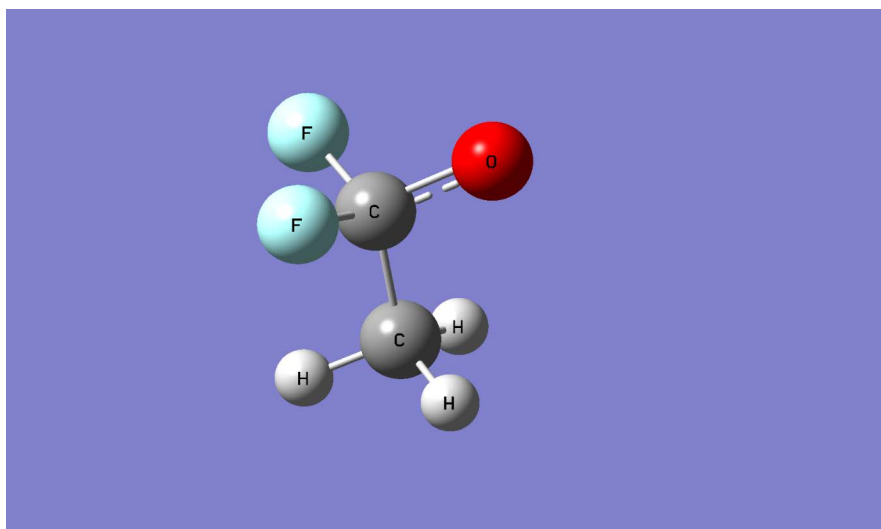
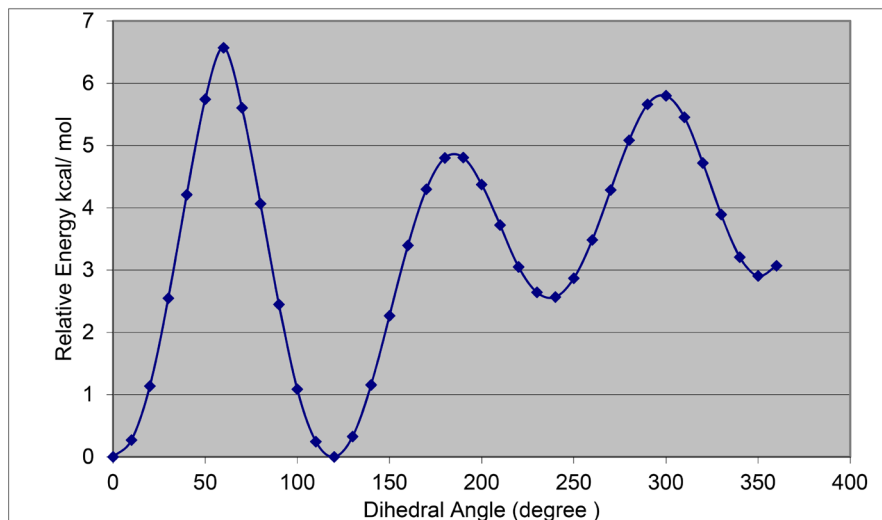


Figure S18. Optimized Geometry for CH₃CF₂O• at the m062x/6-31 + g (d, p) level of theory.

C-C Internal Rotor



C-O Internal Rotor

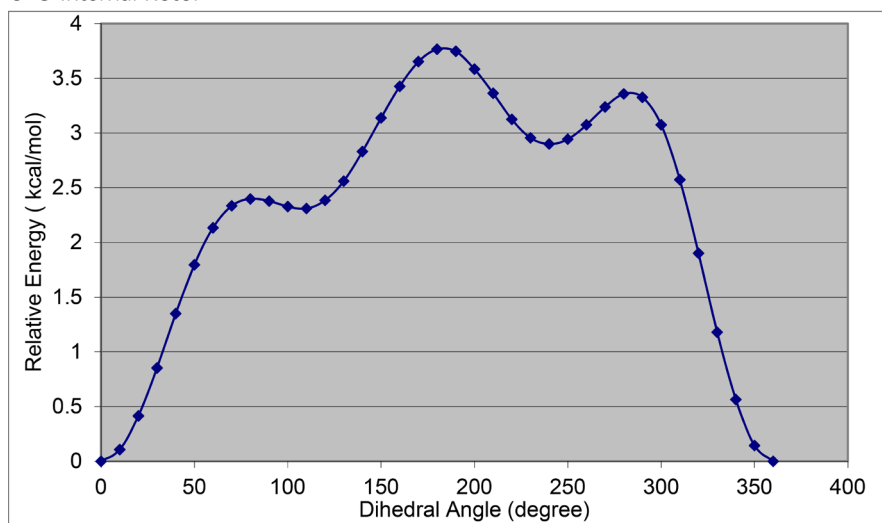
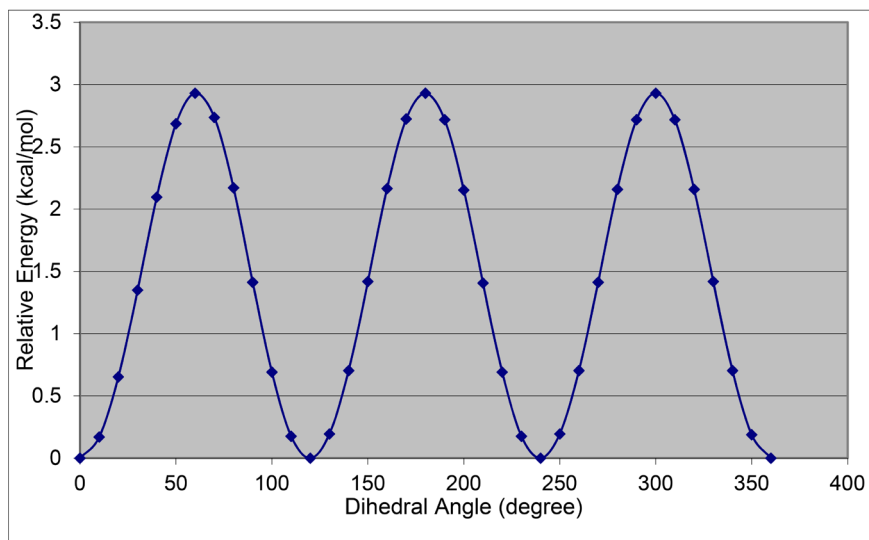


Figure S19. Potential energy profile of C-C and C-O internal rotors for $\text{CH}_2\text{FCH}_2\text{OH}$. The solid lines indicate Fourier series expansion.

C-C Internal Rotor



C-O Internal Rotor

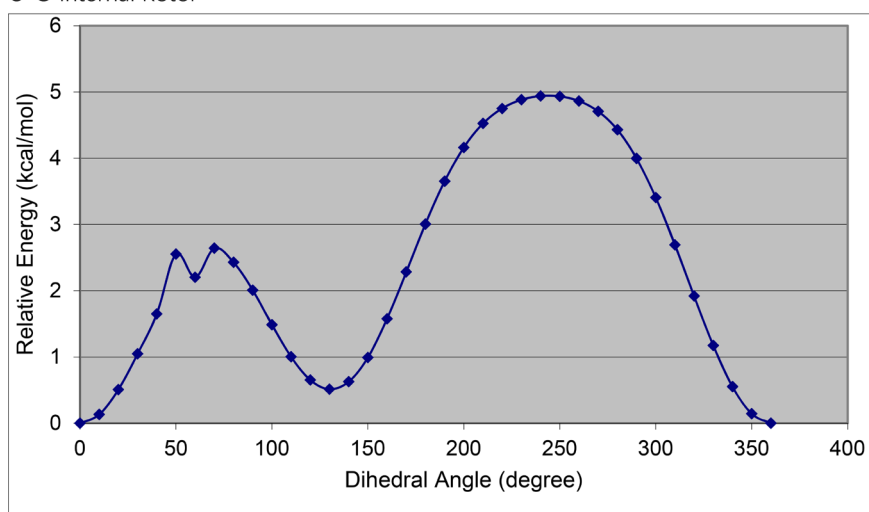
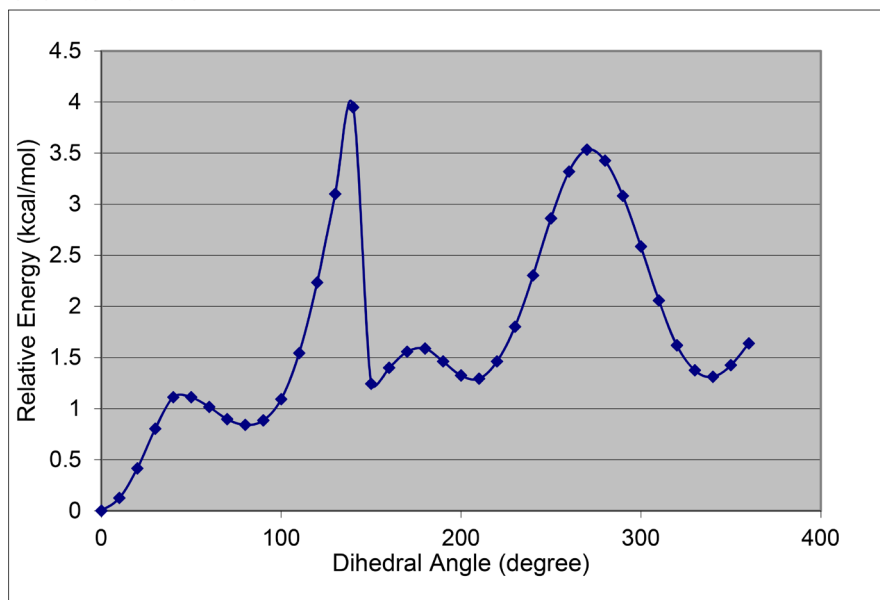


Figure S20. Potential energy profile of C-C and C-O internal rotors for CH_3CHFOH . The solid lines indicate Fourier series expansion.

C-C Internal Rotor



C-O Internal Rotor

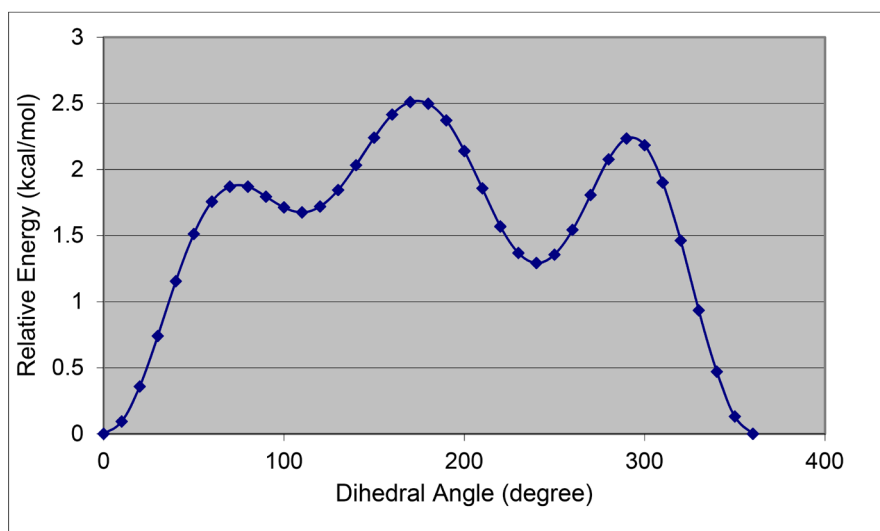
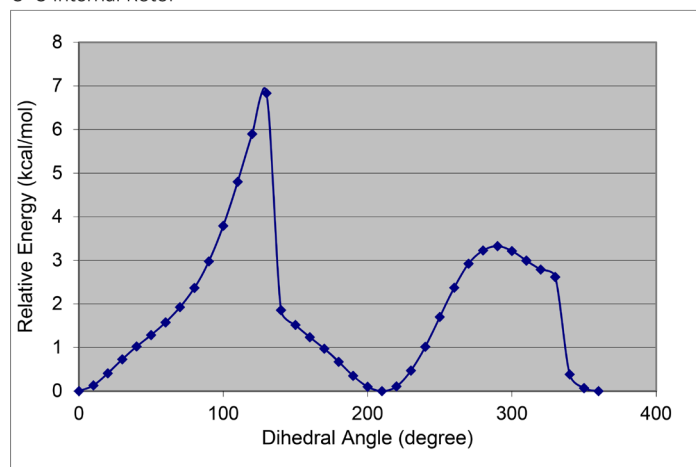


Figure S21. Potential energy profile of C-C and C-O internal rotors for C•HFCH₂OH. The solid lines indicate Fourier series expansion.

C-C Internal Rotor



C-O Internal Rotor

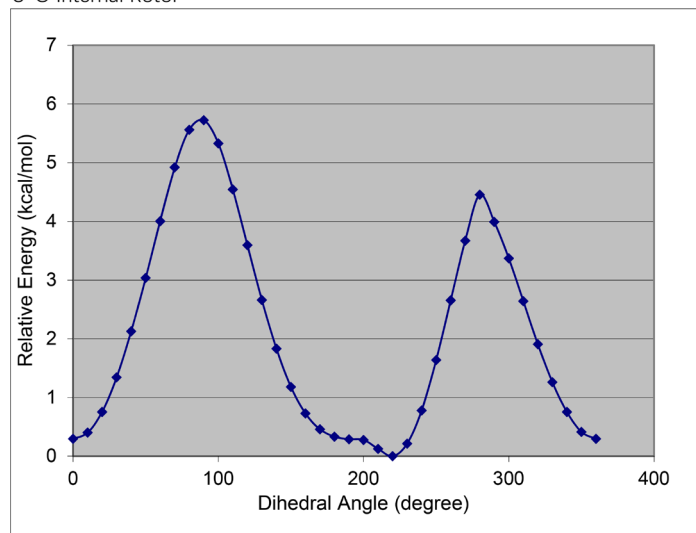


Figure S22. Potential energy profile of C-C and C-O internal rotors for $\text{CH}_2\text{FCH}\cdot\text{OH}$. The solid lines indicate Fourier series expansion.

C-C Internal Rotor

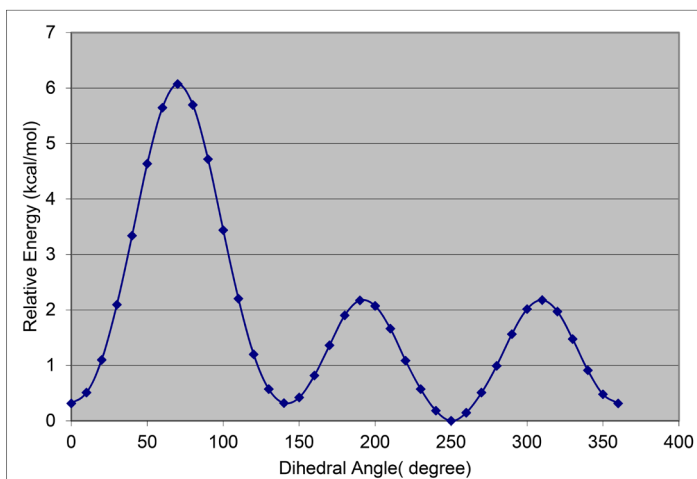
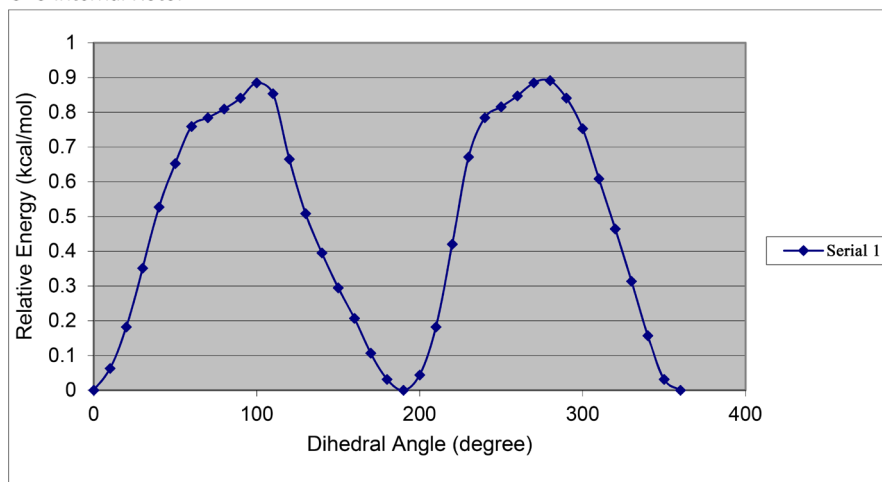


Figure S23. Potential energy profile of C-C and C-O internal rotors for $\text{CH}_2\text{FCH}_2\text{O}\cdot$. The solid lines indicate Fourier series expansion.

C-C Internal Rotor



C-O Internal Rotor

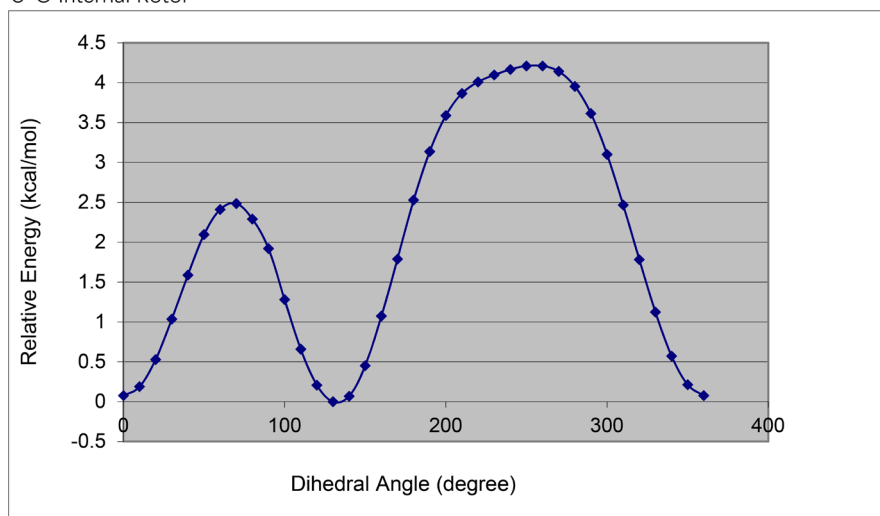
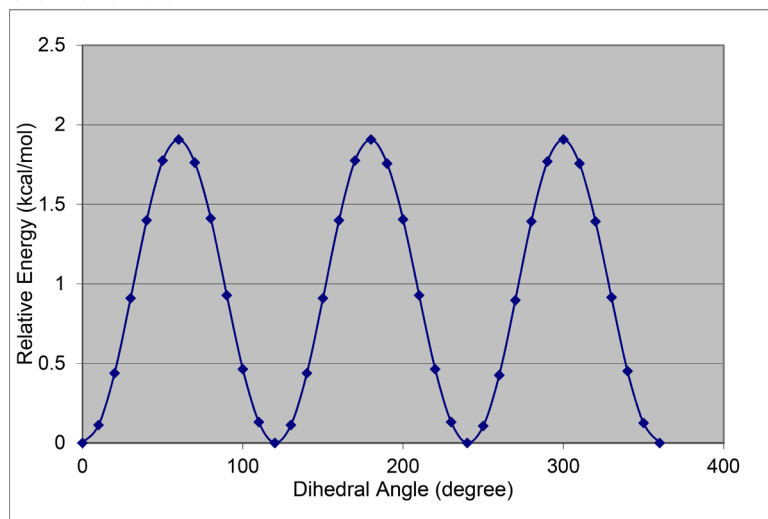


Figure S24. Potential energy profile of C-C and C-O internal rotors for $\text{CH}_2\bullet\text{CHFOH}$. The solid lines indicate Fourier series expansion.

C-C Internal Rotor



C-O Internal Rotor

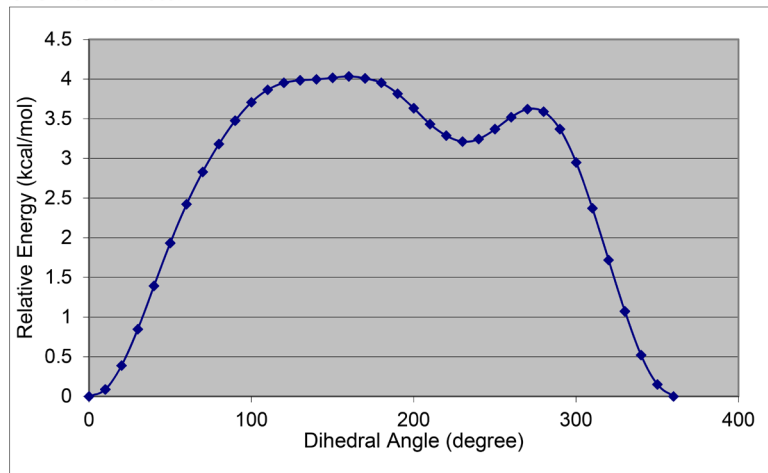


Figure S25. Potential energy profile of C-C and C-O internal rotors for $\text{CH}_3\text{CF}\cdot\text{OH}$. The solid lines indicate Fourier series expansion.

C-C Internal Rotor

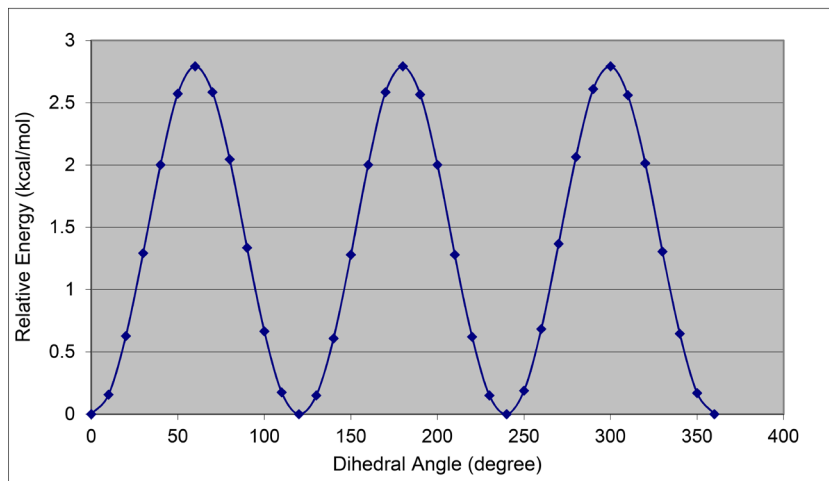


Figure S26. Potential energy profile of C-C and C-O internal rotors for $\text{CH}_3\text{CHFO}\cdot$. The solid lines indicate Fourier series expansion.

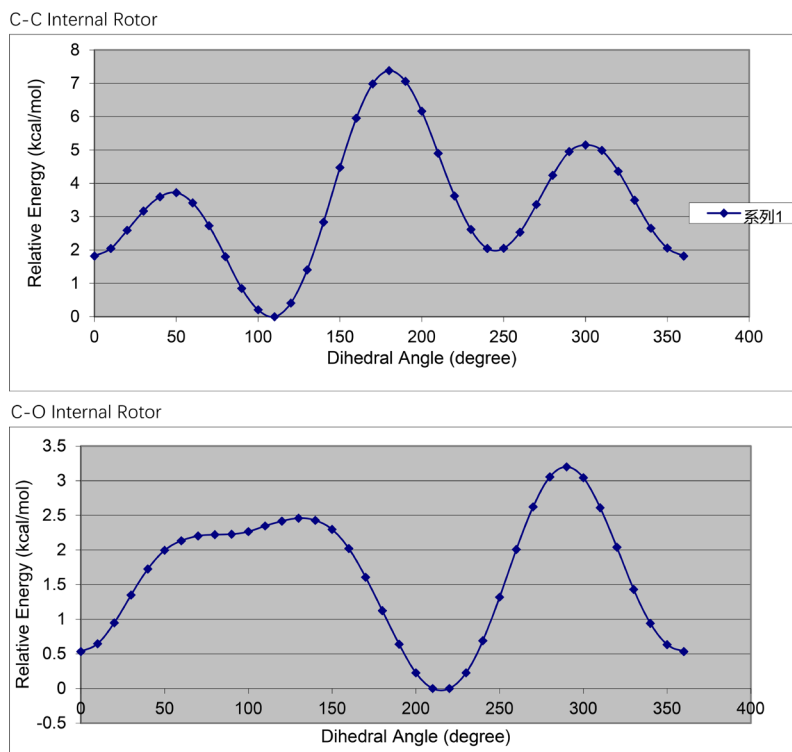


Figure S27. Potential energy profile of C-C and C-O internal rotors for CH_2FCHFOH . The solid lines indicate Fourier series expansion.

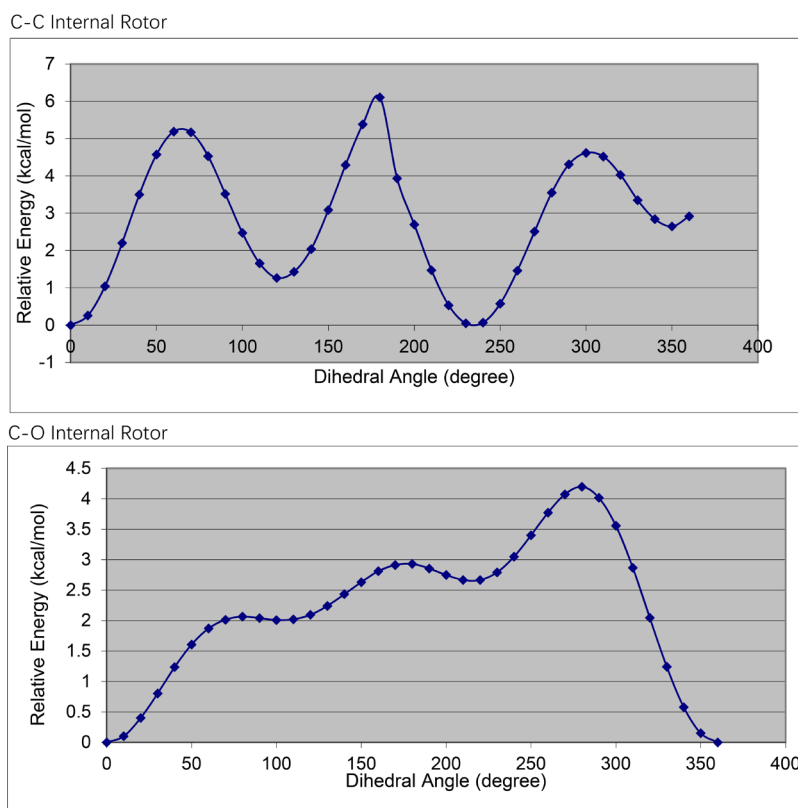


Figure S28. Potential energy profile of C-C and C-O internal rotors for $\text{CF}_2\text{HCH}_2\text{OH}$. The solid lines indicate Fourier series expansion.

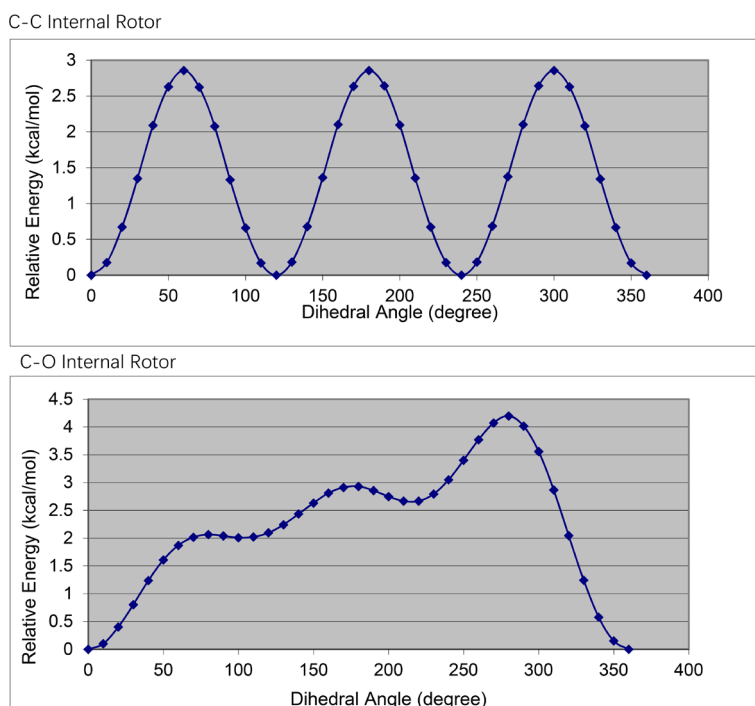


Figure S29. Potential energy profile of C-C and C-O internal rotors for $\text{CH}_3\text{CF}_2\text{OH}$. The solid lines indicate Fourier series expansion.

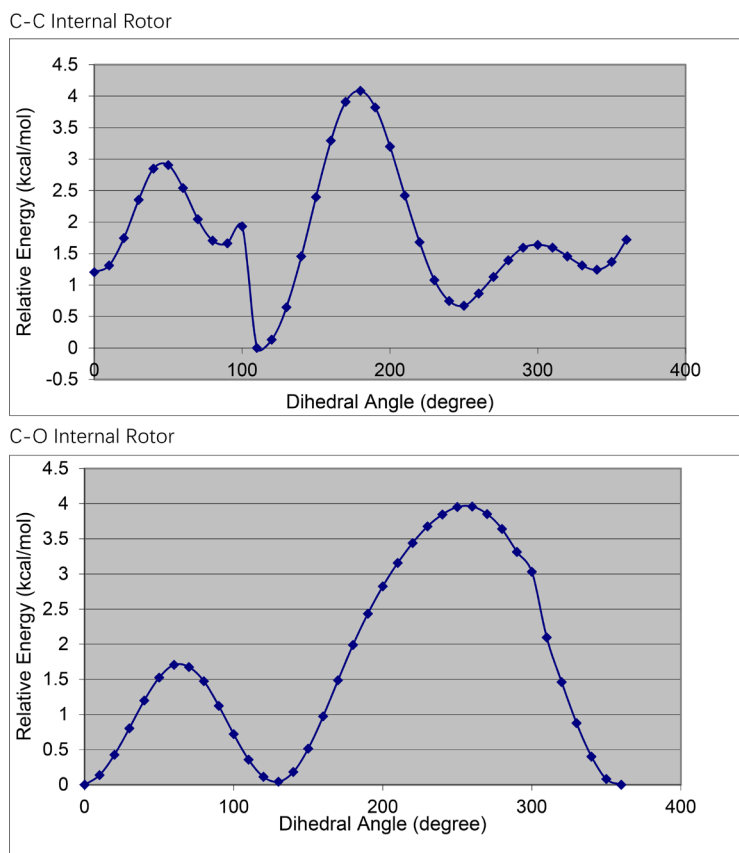
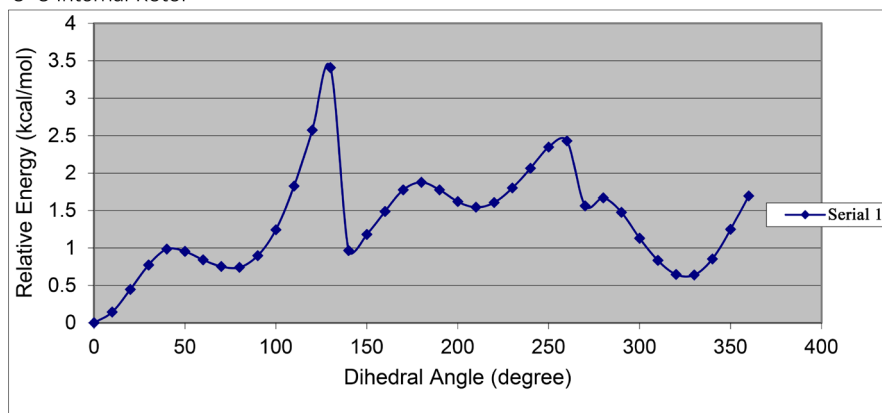


Figure S30. Potential energy profile of C-C and C-O internal rotors for $\text{CH}_2\text{FC}\cdot\text{FOH}$. The solid lines indicate Fourier series expansion.

C-C Internal Rotor



C-O Internal Rotor

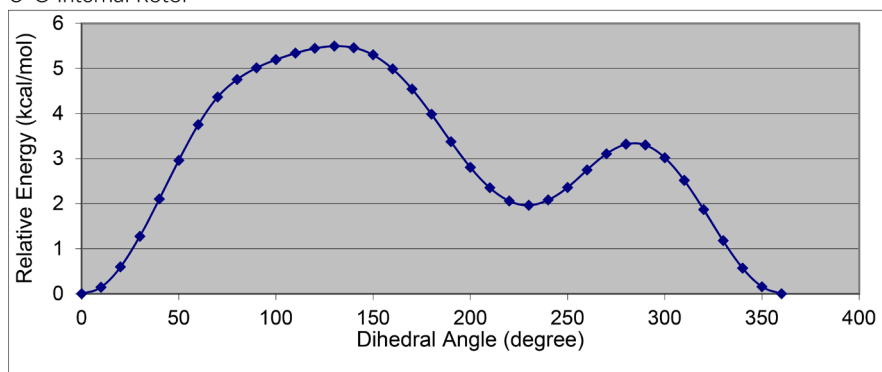


Figure S31. Potential energy profile of C-C and C-O internal rotors for C•HFCFHOH. The solid lines indicate Fourier series expansion.

C-C Internal Rotor

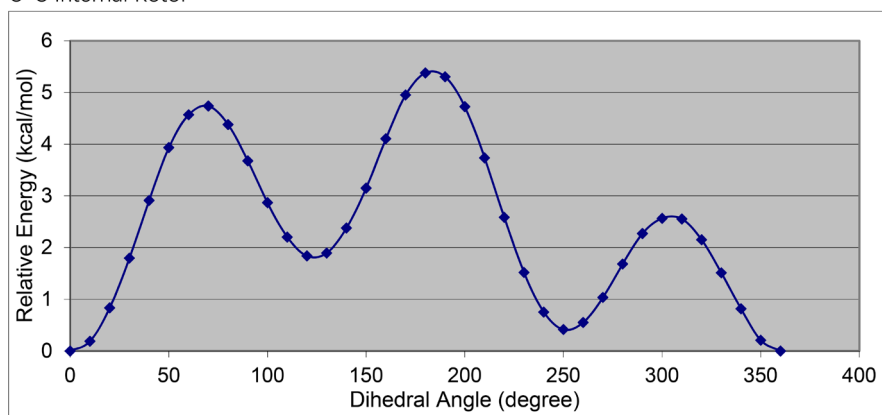


Figure S32. Potential energy profile of C-C and C-O internal rotors for CH₂FCHFO•. The solid lines indicate Fourier series expansion.

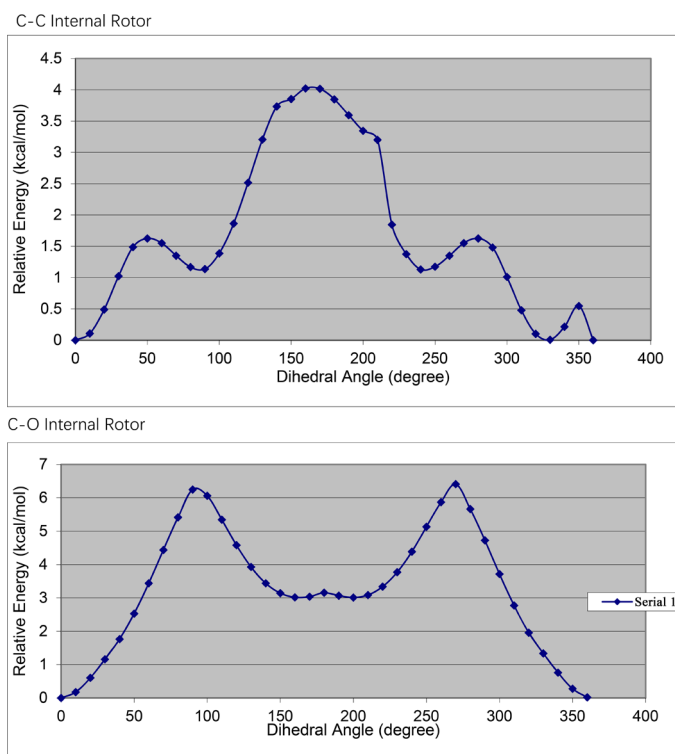


Figure S33. Potential energy profile of C-C and C-O internal rotors for $\text{CHF}_2\text{C}\cdot\text{HOH}$. The solid lines indicate Fourier series expansion.

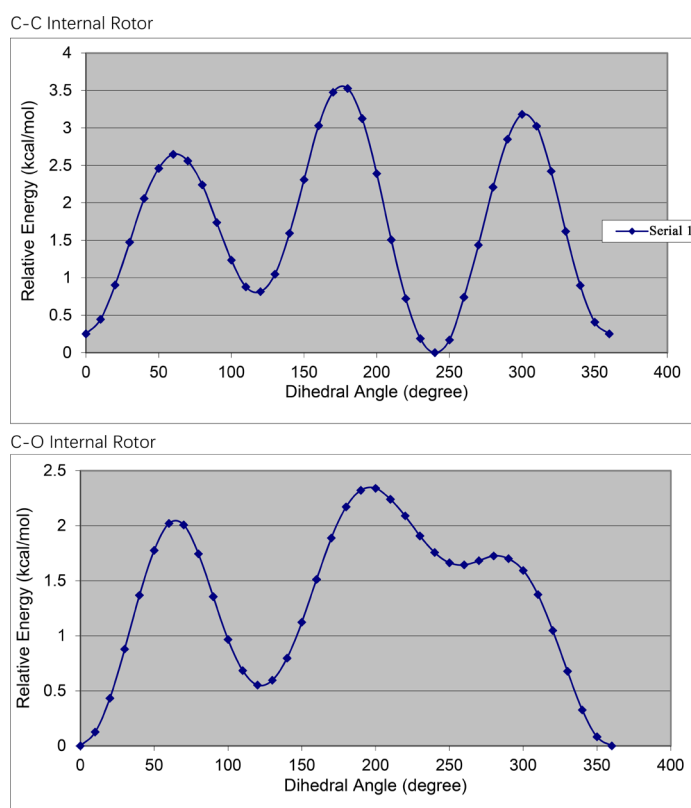


Figure S34. Potential energy profile of C-C and C-O internal rotors for $\text{C}\cdot\text{F}_2\text{CH}_2\text{OH}$. The solid lines indicate Fourier series expansion.

C-C Internal Rotor

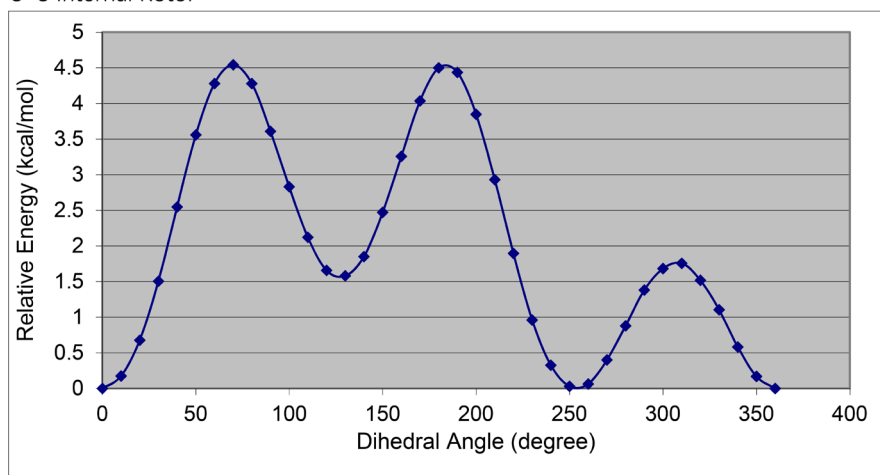
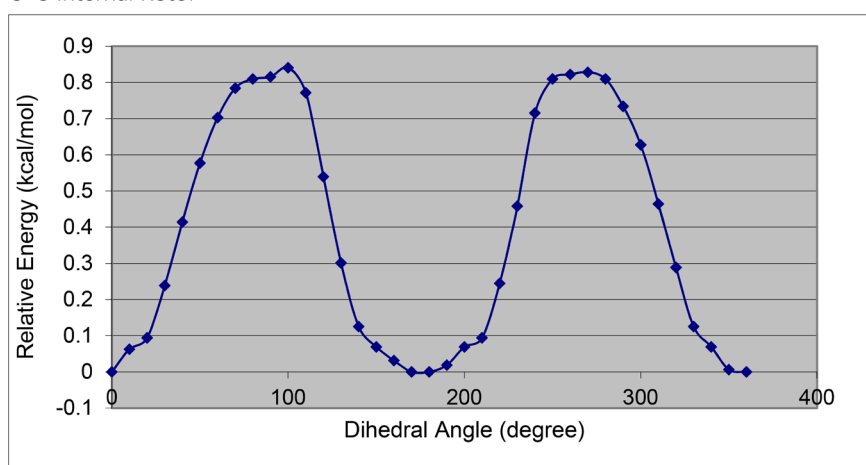


Figure S35. Potential energy profile of C-C and C-O internal rotors for $\text{CHF}_2\text{CH}_2\text{O}\cdot$. The solid lines indicate Fourier series expansion.

C-C Internal Rotor



C-O Internal Rotor

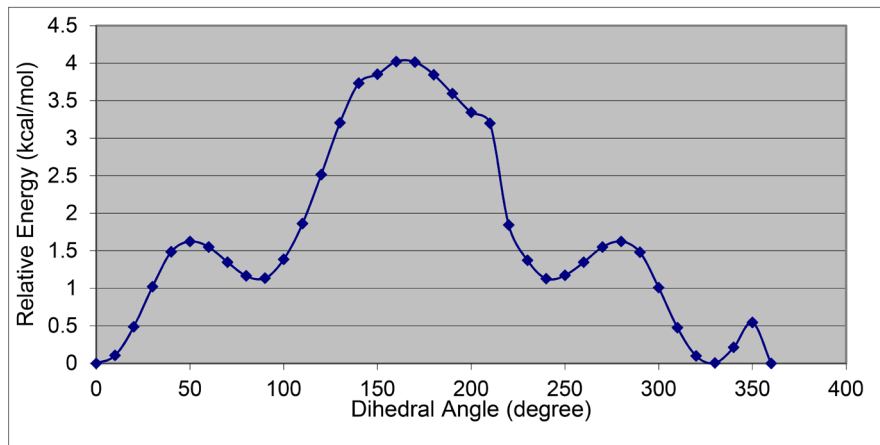


Figure S36. Potential energy profile of C-C and C-O internal rotors for $\text{CH}_2\cdot\text{CF}_2\text{OH}$. The solid lines indicate Fourier series expansion.

C-C Internal Rotor

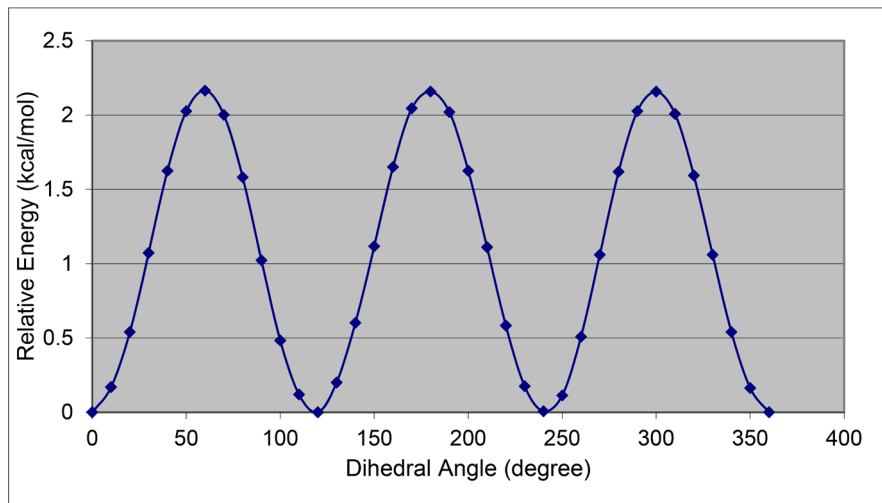


Figure S37. Potential energy profile of C-C and C-O internal rotors for $\text{CH}_3\text{CF}_2\text{O}\cdot$. The solid lines indicate Fourier series expansion.

Table S4. The method of standard deviation and example calculation.

The standard deviation is calculated using the following formula (36):

$$\sigma = \sqrt{\frac{1}{N} \sum_{i=1}^N (x_i - \mu)^2}$$

where, x_i is the mean; the average of the numbers, μ is the actual numbers to be calculated the standard deviation of, and

$$\frac{1}{N} \sum_{i=1}^N (x_i - \mu)^2$$

is the variance.

The standard deviation for standard enthalpy of formation for 1-fluoroethanol is calculated to be ± 0.1 . The calculation of standard deviation for this molecule is as follows:

$$N = 2, \mu_1 = -101.60, \mu_2 = -101.86$$

$$\text{Step 1, } X_j = (-101.60 - 101.86)/2 = -101.73$$

$$\text{Step 2, } (X_j - \mu_1) = (-101.73 + 101.60)^2 = 0.0169$$

$$(X_j - \mu_2) = (-101.73 + 101.86)^2 = 0.0169$$

$$\text{Step 3, } 1/2 (0.0169 + 0.0169) = 0.0169$$

$$\text{Step 4, square root of } 0.0169 = 0.13 = \pm 0.1$$

