Supporting Information (SI)

Is natural fraxin an overlooked radical scavenger?

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Table S1. Calculated BDE values of FX for all positions in the gas phase at the M06-2X/6-311++G(d,p)//M06-2X/6-31+G(d) model of chemistry.

Positions	C9–H	C10–H	C11–H	C12–H	C13–H	C14–H	C15–H	O7–H	O10–H	O11–H	O12–H	O14–H
BDE	95.6	96.6	93.9	94.6	96.4	96.1	97.3	89.4	109.6	108.3	110.4	104.0

Table S2: The Cartesian coordinates and energies of all species of the reaction between FX with HOO• radical following the FHT mechanism at the M06-2X/6-311++G(d,p) level in the studied media.

Name				**FX (gas phase)**	
Cartesian Coordinates				Frequency and Energy	
O	1.70512500	0.46282600	-0.62855800	Zero-point correction=	0.346150 (Hartree/Particle)
O	-0.24970100	-0.63780600	-0.99125700	Thermal correction to Energy=	0.370001
O	3.60611200	-3.07225600	0.21883900	Thermal correction to Enthalpy=	0.370945
O	4.85157900	-0.64073600	0.92659600	Thermal correction to Gibbs Free Energy=	0.292222
O	0.78164400	-2.94633600	0.04729400	Sum of electronic and zero-point Energies=	-1372.289879
O	4.81510100	2.00568800	0.20814300	Sum of electronic and thermal Energies=	-1372.266027
O	-0.78112500	1.99949100	-0.41570100	Sum of electronic and thermal Enthalpies=	-1372.265083
O	-2.05190000	-2.56141500	-0.27628800	Sum of electronic and thermal Free Energies=	-1372.343806
O	-4.54400400	-1.87680000	0.69666400		
O	-0.01291400	4.07532700	-0.35139900		
C	2.91886000	-1.85686200	0.43055400		
C	3.75266900	-0.64337900	0.04073100		
C	1.64183600	-1.90757000	-0.38298300		
C	2.88514100	0.62231000	0.14139000		
C	0.90011300	-0.59457900	-0.19291400		
C	3.55427200	1.85813800	-0.43942500		
C	-1.43552700	-0.25688200	-0.41768400		
C	-1.74649900	1.07925600	-0.16222900		
C	-2.35512700	-1.26366000	-0.11578800		
C	-2.99935700	1.43201600	0.34946300		
C	-3.63652300	-0.91127200	0.37081200		
C	-3.94141900	0.41761400	0.59382500		
C	-3.22877900	2.83442100	0.58993200		
C	-2.26166500	3.74449700	0.35044700		
C	-0.94929000	3.34162200	-0.15253800		
C	-5.03543400	-2.63277200	-0.40808400		
H	2.65560100	-1.75697300	1.49738900		
H	4.08809200	-0.75933600	-1.00352400		
H	1.87627900	-2.01784300	-1.45128200		
H	2.63655100	0.79728000	1.20194700		
H	0.61579300	-0.45967900	0.86516600		
H	3.68407300	1.70950400	-1.51932100		
H	2.90892700	2.72746400	-0.27441800		
H	4.45690800	-3.01391000	0.68261100		
H	5.32722800	0.20053900	0.81632600		
H	1.30361300	-3.76106600	0.12780200		
H	5.22505300	2.83820400	-0.06067300		
H	-4.92301800	0.66339800	0.98886300		
H	-4.19766600	3.14517400	0.97422100		
H	-2.39143500	4.80537600	0.52597400		
H	-1.08440700	-2.67512100	-0.39875500		
H	-5.76197300	-3.33273800	0.00562800		
H	-4.22778100	-3.18219800	-0.89849700		
H	-5.53078900	-1.96931800	-1.12717100		
Name				**FX-P (pentyl ethanoate)**	
Cartesian Coordinates				Frequency and Energy	
O	-1.64567600	0.65871500	0.31044500	Zero-point correction=	0.343820 (Hartree/Particle)

O	0.16616700	-0.52270800	1.00948900	Thermal correction to Energy= 0.368351
O	-3.94603700	-2.74915400	0.40646700	Thermal correction to Enthalpy= 0.369296
O	-4.94727100	-0.44233000	-0.89393400	Thermal correction to Gibbs Free Energy= 0.289430
O	-1.12036400	-2.89920300	0.50946900	Sum of electronic and zero-point Energies= -1372.336772
O	-4.59605500	2.27379700	-0.91790500	Sum of electronic and thermal Energies= -1372.312240
O	1.12384800	2.03224200	0.65406200	Sum of electronic and thermal Enthalpies= -1372.311296
O	1.65823600	-2.65685900	0.11794600	Sum of electronic and thermal Free Energies= -1372.391162
O	4.11611200	-2.29146000	-1.01755200	
O	0.76216500	4.19742600	0.91645800	
C	-3.13899300	-1.71134500	-0.11354500	
C	-3.82322100	-0.35449600	-0.04116400	
C	-1.85172100	-1.69879000	0.68601900	
C	-2.83258200	0.73924500	-0.47121300	
C	-0.97251500	-0.56319300	0.18644100	
C	-3.35909100	2.14427200	-0.22271000	
C	1.37197800	-0.29555200	0.39517000	
C	1.88816300	0.99199200	0.23188400	
C	2.11932700	-1.40440100	-0.01125500	
C	3.14957500	1.18607500	-0.34208700	
C	3.40067400	-1.21333000	-0.58037900	
C	3.89773300	0.06431000	-0.74018500	
C	3.60261000	2.54603300	-0.48320400	
C	2.83152400	3.57488500	-0.07302700	
C	1.52301900	3.34130700	0.52502600	
C	4.67546000	-3.08127400	0.03528700	
H	-2.89651300	-1.91489600	-1.16949000	
H	-4.13341500	-0.16159200	0.99881000	
H	-2.06778500	-1.52863700	1.75008500	
H	-2.59965300	0.60755200	-1.54066600	
H	-0.67409100	-0.73743700	-0.86165100	
H	-3.49948000	2.28190400	0.85679400	
H	-2.62584900	2.87532300	-0.58044300	
H	-4.77812500	-2.75548100	-0.08743200	
H	-5.31650400	0.44928000	-0.98851100	
H	-1.70161200	-3.65107300	0.69392200	
H	-4.97159100	3.14498500	-0.73979800	
H	4.87888000	0.19552300	-1.18724100	
H	4.57782300	2.72661200	-0.92822300	
H	3.13556700	4.61035500	-0.16372800	
H	0.73276600	-2.67337100	0.43750400	
H	5.20680200	-3.90368900	-0.44516000	
H	3.89209600	-3.48115200	0.68548100	
H	5.38004900	-2.48236900	0.62383700	

Name	**FX-W (water)**
Cartesian Coordinates	Frequency and Energy

O	1.66038800	0.65601500	-0.32082500	Zero-point correction= 0.343817 (Hartree/Particle)
O	-0.15630100	-0.51425300	-1.01344300	Thermal correction to Energy= 0.368352
O	3.97743400	-2.74174100	-0.46889500	Thermal correction to Enthalpy= 0.369296
O	4.97597600	-0.42037800	0.85008200	Thermal correction to Gibbs Free Energy= 0.289420
O	1.10246500	-2.90680300	-0.43494700	Sum of electronic and zero-point Energies= -1372.336774
O	4.55782100	2.29258700	1.02966500	Sum of electronic and thermal Energies= -1372.312240
O	-1.11916400	2.02262000	-0.66059900	Sum of electronic and thermal Enthalpies= -1372.311296
O	-1.65411200	-2.66847700	-0.09687500	Sum of electronic and thermal Free Energies= -1372.391172
O	-4.09622200	-2.30566000	1.02977800	

O	-0.75510600	4.17724900	-0.95472500
C	3.16172600	-1.72717700	0.09254500
C	3.82947200	-0.35968700	0.01644500
C	1.84700600	-1.72105500	-0.66917400
C	2.84742800	0.72941900	0.46931000
C	0.98229700	-0.56876300	-0.18116800
C	3.37587500	2.13829400	0.24925800
C	-1.36732400	-0.30313100	-0.39275400
C	-1.88903600	0.98003900	-0.23324900
C	-2.11111300	-1.40759200	0.02368400
C	-3.14821500	1.18361400	0.33831200
C	-3.38848300	-1.20831600	0.59429100
C	-3.89544100	0.06455100	0.74699900
C	-3.59848100	2.54336600	0.47029900
C	-2.82607700	3.57044200	0.05110300
C	-1.52768400	3.32603200	-0.54347100
C	-4.78086700	-2.98937300	-0.03104400
H	2.95359100	-1.95223200	1.14948100
H	4.11976900	-0.15780000	-1.02619100
H	2.03334500	-1.58617400	-1.74255400
H	2.60175500	0.57825200	1.53195200
H	0.67877600	-0.72360500	0.86570700
H	3.59522400	2.27455700	-0.81620500
H	2.61074200	2.86117200	0.55278300
H	4.77092600	-2.83116500	0.07784900
H	5.32389700	0.48296000	0.93636100
H	1.45844600	-3.62360700	-0.97853300
H	5.00422700	3.10574200	0.75882600
H	-4.87659800	0.19992000	1.19231400
H	-4.57243900	2.72785500	0.91518100
H	-3.12918200	4.60653000	0.13460300
H	-0.71247000	-2.69251600	-0.38168000
H	-5.27055900	-3.85129400	0.42196500
H	-4.07270400	-3.32412600	-0.79467700
H	-5.52869400	-2.32771100	-0.47920600

Name	**FX-O7-RAD (gas phase)**
Cartesian Coordinates	Frequency and Energy

O	1.24613900	-0.07179200	-0.69867100
O	-0.42009100	-1.34754800	0.14844300
O	4.09508100	-2.65654900	0.60950300
O	4.87201900	-0.06352900	-0.13689500
O	1.45973800	-2.84987400	1.59154000
O	3.98351300	1.99268900	-1.70452900
O	-0.37985600	1.48792000	0.75611600
O	-2.65718800	-2.42813400	-0.61322900
O	-5.12602700	-0.99339600	-0.69354500
O	0.79763500	3.32314200	1.10164900
C	3.22763300	-1.54096400	0.61000400
C	3.58696700	-0.53994300	-0.47826300
C	1.80946400	-2.07714400	0.46968700
C	2.50954700	0.55317500	-0.51660900
C	0.88033500	-0.87747000	0.39124400
C	2.64737000	1.50328500	-1.69534100
C	-1.47416000	-0.52228100	0.10277100

Zero-point correction= 0.332457 (Hartree/Particle)
Thermal correction to Energy= 0.356482
Thermal correction to Enthalpy= 0.357426
Thermal correction to Gibbs Free Energy= 0.277166
Sum of electronic and zero-point Energies= -1371.651973
Sum of electronic and thermal Energies= -1371.627948
Sum of electronic and thermal Enthalpies= -1371.627003
Sum of electronic and thermal Free Energies= -1371.707263

C	-1.52241700	0.83378700	0.37200300
C	-2.70150100	-1.23145600	-0.30501500
C	-2.74139500	1.54717700	0.25425600
C	-3.95240100	-0.45577000	-0.35215000
C	-3.93541300	0.89795600	-0.09786000
C	-2.70236000	2.96351000	0.50400500
C	-1.54558500	3.59129000	0.80417200
C	-0.29087700	2.84429000	0.89851800
C	-5.36178800	-2.40584400	-0.71349500
H	3.29855000	-1.01559800	1.57762200
H	3.60314700	-1.05332800	-1.45418900
H	1.71153000	-2.65304000	-0.46239900
H	2.52316000	1.12676100	0.42451700
H	0.91429800	-0.30749500	1.32906900
H	2.42739500	0.95194800	-2.61919700
H	1.92644400	2.32061700	-1.57922600
H	5.00310700	-2.31892400	0.66766000
H	5.07703800	0.69345500	-0.71084600
H	2.16900900	-3.49862400	1.72464500
H	4.06969200	2.70639000	-2.34942400
H	-4.86089000	1.46051900	-0.16961100
H	-3.63207300	3.52203900	0.42884800
H	-1.47674800	4.65864200	0.97576200
H	-6.44552000	-2.49532100	-0.78704200
H	-5.00084600	-2.87347600	0.20432600
H	-4.87549400	-2.86959000	-1.57114100

Name			**FX-O7-RAD-P (pentyl ethanoate)**
Cartesian Coordinates			Frequency and Energy
O	-1.11656700	-0.07639200	0.57239800
O	0.31788100	-1.28000300	-0.70110400
O	-4.28201700	-2.33712000	-0.66138300
O	-4.78263000	0.11819100	0.64754400
O	-1.84071000	-2.44713600	-2.05557200
O	-3.53758400	1.89687700	2.32497800
O	0.55455400	1.53646700	-1.05880300
O	2.31311300	-2.58647000	0.41281300
O	4.79277600	-1.33525000	1.05421100
O	-0.36454400	3.44918200	-1.66743600
C	-3.36767000	-1.25810200	-0.61557300
C	-3.49158900	-0.45838600	0.67216000
C	-1.97551200	-1.84955600	-0.78733200
C	-2.36680800	0.58562500	0.72244200
C	-0.97251800	-0.71245900	-0.67111300
C	-2.27213200	1.30047300	2.06096800
C	1.40083800	-0.55720500	-0.36105800
C	1.56981500	0.80237100	-0.50414300
C	2.48147600	-1.37605700	0.20517100
C	2.77211200	1.43076500	-0.09177100
C	3.74029600	-0.69067300	0.54605800
C	3.83892800	0.67904900	0.42355200
C	2.85730600	2.85810100	-0.24522500
C	1.82787800	3.56266200	-0.76159700
C	0.60128800	2.89712100	-1.19502800
C	5.00424000	-2.74202100	0.85935100

Zero-point correction= 0.331135 (Hartree/Particle)
Thermal correction to Energy= 0.355627
Thermal correction to Enthalpy= 0.356572
Thermal correction to Gibbs Free Energy= 0.275236
Sum of electronic and zero-point Energies= -1371.698560
Sum of electronic and thermal Energies= -1371.674067
Sum of electronic and thermal Enthalpies= -1371.673123
Sum of electronic and thermal Free Energies= -1371.754459

H	-3.55674600	-0.57063500	-1.45641300
H	-3.38064000	-1.13714100	1.53362000
H	-1.77336100	-2.57103400	0.01800100
H	-2.51274400	1.31783200	-0.08777200
H	-1.10357800	0.00339000	-1.49247800
H	-2.01509100	0.56715500	2.83610700
H	-1.48191000	2.05880600	2.01113000
H	-5.17432800	-1.97395600	-0.57345500
H	-4.83318200	0.76220900	1.37005400
H	-2.59626200	-3.03978300	-2.17515900
H	-3.51731500	2.32126800	3.19158300
H	4.75870300	1.17666400	0.71347600
H	3.76991100	3.35729500	0.06843600
H	1.85509900	4.63841100	-0.88533600
H	6.06269800	-2.89220400	1.07309300
H	4.78596000	-3.02871800	-0.17126300
H	4.39090800	-3.32658300	1.54403000

Name			**FX-O7-RAD-W (water)**
Cartesian Coordinates			Frequency and Energy
O	-1.23250600	-0.08594300	0.70352900
O	0.40379700	-1.36312200	-0.21158000
O	-4.12524100	-2.67302000	-0.52871900
O	-4.86494700	0.00015200	0.22098700
O	-1.49151500	-2.84423000	-1.60502200
O	-3.87441400	2.16466200	1.62590100
O	0.39780800	1.48191300	-0.80103800
O	2.60403500	-2.44394200	0.64007700
O	5.06083600	-1.04392400	0.83873100
O	-0.72520300	3.29910300	-1.32662500
C	-3.26693600	-1.54495400	-0.58296300
C	-3.58376200	-0.53375700	0.51425000
C	-1.83876600	-2.07007800	-0.47373800
C	-2.49828000	0.55095700	0.54298600
C	-0.90383200	-0.87485000	-0.41199900
C	-2.61504700	1.50651800	1.71786000
C	1.46315700	-0.53078600	-0.11700500
C	1.52092800	0.82472500	-0.36664500
C	2.66803000	-1.23895500	0.33238000
C	2.73085800	1.53870600	-0.17632000
C	3.91460000	-0.47180100	0.43774700
C	3.91019000	0.88457500	0.22030300
C	2.71200000	2.95504400	-0.41837300
C	1.57732800	3.57990700	-0.80099100
C	0.34714900	2.82691500	-0.99426900
C	5.37013600	-2.40929800	0.49877200
H	-3.37466600	-1.03986600	-1.55427400
H	-3.59129700	-1.04666800	1.48820300
H	-1.72425900	-2.65198900	0.45146800
H	-2.51634900	1.11474700	-0.40330300
H	-0.95832900	-0.28975100	-1.33748300
H	-2.54207900	0.93790100	2.65257100
H	-1.79151700	2.22885000	1.67064600
H	-4.99762800	-2.41412000	-0.85642500
H	-5.01444700	0.74937900	0.82089700

Zero-point correction= 0.331136 (Hartree/Particle)
Thermal correction to Energy= 0.355628
Thermal correction to Enthalpy= 0.356572
Thermal correction to Gibbs Free Energy= 0.275239
Sum of electronic and zero-point Energies= -1371.698559
Sum of electronic and thermal Energies= -1371.674067
Sum of electronic and thermal Enthalpies= -1371.673123
Sum of electronic and thermal Free Energies= -1371.754456

H	-2.12990700	-3.56895400	-1.67763100
H	-4.01473500	2.67796500	2.43262100
H	4.82502900	1.45570100	0.33841500
H	3.63360600	3.51166100	-0.27656400
H	1.52342500	4.64666600	-0.97972900
H	6.45876000	-2.45557700	0.48852900
H	4.97618000	-2.65595000	-0.48865800
H	4.97047400	-3.09040100	1.24881600

Name	**PRE-COMP- FX-O7-H-OOH (gas phase)**
Cartesian Coordinates	Frequency and Energy

O	2.24411700	-0.63393500	-1.27101200	Zero-point correction= 0.363529 (Hartree/Particle)
O	0.06029600	-0.49295200	-1.29777300	Thermal correction to Energy= 0.391057
O	2.64351200	-0.05396500	2.75029300	Thermal correction to Enthalpy= 0.392001
O	4.92509100	0.14381100	1.11199600	Thermal correction to Gibbs Free Energy= 0.304302
O	0.22620500	0.39155900	1.58849200	Sum of electronic and zero-point Energies= -1523.176236
O	5.85779200	-0.66972800	-1.40894900	Sum of electronic and thermal Energies= -1523.148709
O	-0.76931500	2.12096300	-0.62836100	Sum of electronic and thermal Enthalpies= -1523.147765
O	-1.71172500	-2.46816000	-1.30586200	Sum of electronic and thermal Free Energies= -1523.235463
O	-4.35964700	-2.06878400	-0.67188500	
O	-0.18905000	4.22411800	-0.26046700	
C	2.60143900	0.21351900	1.36470100	
C	3.74305300	-0.43744700	0.60784800	
C	1.25263100	-0.27790300	0.86110200	
C	3.53288400	-0.18276000	-0.89021100	
C	1.18717800	0.04024600	-0.63546900	
C	4.51153000	-0.96567000	-1.75828100	
C	-1.21863400	-0.17342900	-0.91600100	
C	-1.67468500	1.10649600	-0.60162700	
C	-2.12386200	-1.23561400	-0.96028000	
C	-3.01519800	1.32040400	-0.26294100	
C	-3.47906000	-1.02994800	-0.62833900	
C	-3.90828600	0.23574000	-0.28028200	
C	-3.38651000	2.66800700	0.08971300	
C	-2.47453700	3.66237400	0.10229600	
C	-1.08048700	3.41321400	-0.25355900	
C	-4.16402800	-3.03748200	0.36401500	
H	2.66158900	1.30233500	1.19385300	
H	3.72537200	-1.52415000	0.79111200	
H	1.15617500	-1.36370500	0.99600900	
H	3.63595000	0.89979000	-1.08117800	
H	1.25339300	1.12197000	-0.80716400	
H	4.36506100	-2.03481400	-1.57932800	
H	4.31201600	-0.76690800	-2.81630300	
H	3.51012800	0.22019100	3.07977500	
H	5.66885800	-0.18551300	0.58623900	
H	0.58478900	0.55305000	2.47652100	
H	6.15083200	0.11665500	-1.88258000	
H	-4.95263000	0.37765800	-0.02070600	
H	-4.42232100	2.86681900	0.35301900	
H	-2.71513200	4.68291100	0.37113900	
H	-0.75290000	-2.43746500	-1.44920400	
H	-4.93050100	-3.79716700	0.21211100	
H	-4.28989300	-2.56666000	1.34515600	
H	-3.16948900	-3.48543600	0.29964700	

H	-1.22831200	-0.54136600	1.89368200
O	-1.16675400	-2.34779300	1.62587000
O	-1.80846700	-1.31471700	2.12041900

Name	**PRE-COMP-FX-O7-H-OOH-P (pentyl ethanoate)**
Cartesian Coordinates	Frequency and Energy

O	2.28388500	-0.52873600	-1.29565500
O	0.10480000	-0.39028500	-1.35401800
O	2.61824900	-0.15201600	2.75486800
O	4.94080800	0.09607000	1.15758000
O	0.23877200	0.43857400	1.56514700
O	5.90308400	-0.59546000	-1.37806400
O	-0.86251600	2.14707300	-0.62568600
O	-1.54806900	-2.47887100	-1.35891000
O	-4.21667600	-2.22939800	-0.76146500
O	-0.41171300	4.28204800	-0.27896600
C	2.61105100	0.18975900	1.38276900
C	3.75426500	-0.44112400	0.61105100
C	1.25853900	-0.24433000	0.83533300
C	3.57472800	-0.10565200	-0.87465500
C	1.22287600	0.12252100	-0.65056500
C	4.55810900	-0.85530200	-1.76654700
C	-1.18053500	-0.16468000	-0.93681000
C	-1.70876700	1.08236900	-0.60256000
C	-2.02481600	-1.27560000	-0.99007000
C	-3.05781500	1.21736800	-0.25874000
C	-3.39229800	-1.14599600	-0.66899400
C	-3.89210400	0.08671000	-0.29876800
C	-3.50564900	2.53626600	0.11174500
C	-2.65068700	3.58111200	0.12325700
C	-1.25379600	3.41372900	-0.25319600
C	-4.03272000	-3.18773100	0.28662700
H	2.69460500	1.28391400	1.27125200
H	3.72122200	-1.53515900	0.73712000
H	1.12852700	-1.33023600	0.93961800
H	3.68595800	0.98282500	-1.01390700
H	1.28720500	1.21026300	-0.78384200
H	4.39542400	-1.93116900	-1.64961500
H	4.38657100	-0.59173100	-2.81517800
H	3.45850600	0.14370900	3.13352400
H	5.67796700	-0.19603100	0.59953600
H	0.59736400	0.60314500	2.45406500
H	6.20661200	0.21610800	-1.80599700
H	-4.94373500	0.17572200	-0.04300100
H	-4.54868300	2.67213700	0.38591100
H	-2.95138900	4.58331500	0.40273400
H	-0.59605300	-2.39140100	-1.53051200
H	-4.73954900	-3.99456500	0.08897500
H	-4.25388800	-2.73201900	1.25808100
H	-3.01223500	-3.57947700	0.28631600
H	-1.18954500	-0.41301100	1.89705700
O	-1.29234800	-2.24135600	1.85829300
O	-1.84417400	-1.10174900	2.20295000

Name	**PRE-COMP- FX-O7-H-OOH-W (water)**
Cartesian Coordinates	Frequency and Energy

Zero-point correction= 0.362235 (Hartree/Particle)
Thermal correction to Energy= 0.389888
Thermal correction to Enthalpy= 0.390833
Thermal correction to Gibbs Free Energy= 0.302871
Sum of electronic and zero-point Energies= -1523.211332
Sum of electronic and thermal Energies= -1523.183678
Sum of electronic and thermal Enthalpies= -1523.182734
Sum of electronic and thermal Free Energies= -1523.270696

O	2.16796600	-0.11067200	-1.30696400	Zero-point correction= 0.362018 (Hartree/Particle)
O	-0.01571600	0.30222600	-1.73852800	Thermal correction to Energy= 0.389521
O	2.11178600	1.91880100	2.27854900	Thermal correction to Enthalpy= 0.390465
O	4.60037800	1.22647100	1.09871000	Thermal correction to Gibbs Free Energy= 0.303375
O	-0.05484200	2.17600500	0.47662000	Sum of electronic and zero-point Energies= -1523.236790
O	5.70179100	-0.62573600	-0.68682800	Sum of electronic and thermal Energies= -1523.209287
O	-2.45463800	1.19629000	-1.16238200	Sum of electronic and thermal Enthalpies= -1523.208343
O	0.73364100	-2.33599000	-0.80522400	Sum of electronic and thermal Free Energies= -1523.295434
O	-1.06957700	-3.89091400	0.42547200	
O	-3.82228600	2.91872700	-1.30528500	
C	2.29579500	1.69164700	0.89333100	
C	3.38596900	0.65774100	0.63877000	
C	0.96868000	1.20861600	0.32774300	
C	3.45601500	0.31093300	-0.85114400	
C	1.13985200	0.84967800	-1.14720500	
C	4.37731800	-0.86902000	-1.14299700	
C	-0.85183500	-0.51735000	-1.00296400	
C	-2.15352300	-0.07137800	-0.75815700	
C	-0.48934400	-1.80586000	-0.60082100	
C	-3.10459400	-0.88069900	-0.13208100	
C	-1.44486200	-2.62014800	0.05122100	
C	-2.72689800	-2.17067600	0.27678800	
C	-4.40886000	-0.31864600	0.09200900	
C	-4.68840400	0.94777300	-0.28816200	
C	-3.68027800	1.76384700	-0.93425500	
C	-0.37783200	-3.91546800	1.68327600	
H	2.57969500	2.62902600	0.38931700	
H	3.14654900	-0.25703700	1.20350200	
H	0.64045700	0.32774300	0.89142100	
H	3.77029600	1.19899400	-1.41983100	
H	1.37611600	1.74254200	-1.73930100	
H	4.01039600	-1.74526500	-0.59948400	
H	4.36399900	-1.08630600	-2.21559500	
H	2.92432500	2.30854700	2.63165600	
H	5.31961500	0.62229500	0.84958300	
H	0.18453400	3.01280100	0.04790800	
H	6.13376200	-0.01151900	-1.29765600	
H	-3.44133300	-2.81543600	0.77986400	
H	-5.16150500	-0.93126800	0.58054400	
H	-5.65368000	1.41183600	-0.12872100	
H	1.37677400	-1.64614500	-1.08146900	
H	-0.08825700	-4.95157700	1.85839500	
H	-1.04411300	-3.57339700	2.48153900	
H	0.51353100	-3.28180300	1.64536700	
H	-1.41817600	1.95959000	1.27959900	
O	-1.89644800	0.49377300	2.30296300	
O	-2.21657900	1.67107500	1.82430100	

Name	**POST-COMP- FX-O7-H-OOH (gas phase)**
Cartesian Coordinates	Frequency and Energy

O	1.64227000	-0.01169000	-1.07356700	Zero-point correction= 0.363982 (Hartree/Particle)
O	-0.42864300	-0.88174400	-0.75962700	Thermal correction to Energy= 0.391187
O	3.50841900	-3.22024400	0.53144100	Thermal correction to Enthalpy= 0.392131
O	4.88520100	-0.71632900	0.45200300	Thermal correction to Gibbs Free Energy= 0.305551
O	0.69985800	-2.93201300	0.80473800	Sum of electronic and zero-point Energies= -1523.184180

O	4.61356600	1.98587700	-0.56899000
O	0.19556800	1.78013400	0.19571500
O	-2.93844000	-1.39792100	-1.35098300
O	-5.06932800	0.16257800	-0.36437100
O	1.72096200	3.29744300	0.67275200
C	2.88438200	-1.95442100	0.49741000
C	3.69517300	-0.92288200	-0.28009200
C	1.48611400	-2.16263800	-0.08223900
C	2.85775400	0.34855000	-0.44192900
C	0.85820500	-0.78683500	-0.21356300
C	3.52122300	1.42648000	-1.28363300
C	-1.32890800	0.07425400	-0.46312700
C	-1.09492900	1.35269500	0.00579400
C	-2.70751600	-0.34947100	-0.73577700
C	-2.17615400	2.22730400	0.29818200
C	-3.79506400	0.53242500	-0.28031000
C	-3.50822400	1.80503200	0.16537200
C	-1.84304300	3.54971100	0.75498100
C	-0.55916800	3.94986000	0.89157500
C	0.54129900	3.03711700	0.59130200
C	-5.44155600	-1.22641700	-0.28291500
H	2.76428400	-1.56857000	1.52400800
H	3.91642200	-1.32339800	-1.28300400
H	1.54233700	-2.63308900	-1.07283100
H	2.64581900	0.78317800	0.55084500
H	0.79887000	-0.32734600	0.78478600
H	3.92514600	1.00245100	-2.20821900
H	2.77404600	2.18517100	-1.53753300
H	4.39934800	-3.10385100	0.88752500
H	5.27272200	0.13236400	0.18730600
H	1.17751300	-3.74766600	1.00814600
H	4.25062800	2.59391500	0.08983100
H	-4.32245500	2.46726900	0.43905900
H	-2.65833400	4.23043700	0.98399700
H	-0.28004800	4.94200800	1.22271900
H	-2.56021300	-2.96876900	-0.34399200
H	-6.46049400	-1.21522100	0.10231700
H	-4.77908300	-1.76453500	0.39938200
H	-5.40495600	-1.68478800	-1.27003400
H	-1.08529800	-2.52399300	1.31260300
O	-2.57425700	-3.36672500	0.54629000
O	-2.03690000	-2.30938500	1.33671100

Sum of electronic and thermal Energies= -1523.156975
Sum of electronic and thermal Enthalpies= -1523.156031
Sum of electronic and thermal Free Energies= -1523.242611

Name			**POST-COMP-FX-O7-H-OOH-P (pentyl ethanoate)**
Cartesian Coordinates			Frequency and Energy
O	-1.19533400	0.27498900	0.66931800
O	0.35913700	-0.98965100	-0.38855500
O	-4.15200600	-2.35635000	-0.33334600
O	-4.86325900	0.22317900	0.60449900
O	-1.65170100	-2.48466600	-1.61689100
O	-3.80178300	2.38637600	2.04250600
O	0.37221600	1.78497500	-1.09530200
O	2.46120000	-1.98248500	0.80512000
O	4.85886000	-0.51009900	1.17902600
O	-0.72087600	3.55482300	-1.81611800

Zero-point correction= 0.362394 (Hartree/Particle)
Thermal correction to Energy= 0.390041
Thermal correction to Enthalpy= 0.390986
Thermal correction to Gibbs Free Energy= 0.302873
Sum of electronic and zero-point Energies= -1523.221243
Sum of electronic and thermal Energies= -1523.193596
Sum of electronic and thermal Enthalpies= -1523.192651
Sum of electronic and thermal Free Energies= -1523.280764

C	-3.31788700	-1.21794400	-0.41598600
C	-3.53925100	-0.25472200	0.73876300
C	-1.88467100	-1.72283200	-0.44559700
C	-2.49082400	0.86304200	0.66992200
C	-0.96618900	-0.51424200	-0.46428000
C	-2.52343700	1.78075500	1.88402200
C	1.38831900	-0.14460500	-0.18868100
C	1.44882600	1.19197800	-0.49533100
C	2.53700400	-0.80317000	0.43685300
C	2.61172400	1.94791900	-0.19640700
C	3.75194800	-0.00348100	0.64629700
C	3.74203100	1.34474600	0.36278200
C	2.58451800	3.35072500	-0.50732300
C	1.49077500	3.91877100	-1.04830900
C	0.30157800	3.12756500	-1.35276500
C	5.16987500	-1.91335100	1.13153700
H	-3.51550300	-0.67547300	-1.35219100
H	-3.41318000	-0.79425400	1.68830900
H	-1.66781700	-2.31687400	0.44977600
H	-2.63901500	1.44722100	-0.25104100
H	-1.11527300	0.06578500	-1.38039400
H	-2.33948100	1.19016400	2.78399200
H	-1.73445300	2.53311700	1.79669100
H	-5.06706400	-2.05241100	-0.32069800
H	-4.98554400	0.92830500	1.25346100
H	-2.35602600	-3.14377700	-1.67509400
H	-3.86672900	3.13652200	1.44115400
H	4.62717200	1.93690800	0.56076200
H	3.46656400	3.94199700	-0.28638700
H	1.43176700	4.97307100	-1.28277700
H	1.14690600	-3.22054300	0.36098200
H	6.24400900	-1.96162800	1.29946000
H	4.92446000	-2.33070700	0.15519700
H	4.63948400	-2.45362700	1.91216400
H	0.01193800	-3.33618200	-1.60961400
O	0.60256200	-3.96692800	0.05048000
O	0.77870300	-3.88097900	-1.36032800

Name	**POST-COMP- FX-O7-H-OOH-W (water)**
Cartesian Coordinates	Frequency and Energy

O	-1.25058900	0.21154700	0.70463800
O	0.41285000	-1.01176200	-0.23474100
O	-4.04106700	-2.58949400	-0.25648800
O	-4.89850200	0.07304400	0.40764100
O	-1.46651000	-2.66636400	-1.45930100
O	-3.96901700	2.39502900	1.70789800
O	0.22096000	1.78012100	-0.95448000
O	2.64684600	-1.87394100	0.77558200
O	4.96857000	-0.27920800	1.01737900
O	-1.02400100	3.48190800	-1.56463400
C	-3.25591900	-1.41826300	-0.40800500
C	-3.57481600	-0.37356700	0.65451500
C	-1.79756500	-1.85510800	-0.34441500
C	-2.55628700	0.76874600	0.57351300
C	-0.93178600	-0.61055800	-0.38664900

Zero-point correction= 0.361407 (Hartree/Particle)
Thermal correction to Energy= 0.389311
Thermal correction to Enthalpy= 0.390255
Thermal correction to Gibbs Free Energy= 0.301518
Sum of electronic and zero-point Energies= -1523.237414
Sum of electronic and thermal Energies= -1523.209510
Sum of electronic and thermal Enthalpies= -1523.208566
Sum of electronic and thermal Free Energies= -1523.297303

C	-2.68368600	1.78458900	1.69872000
C	1.40086000	-0.09993500	-0.12629000
C	1.36527100	1.23980700	-0.43160200
C	2.62891700	-0.68666700	0.41137000
C	2.49804400	2.05969400	-0.20130700
C	3.80429100	0.17938400	0.54491800
C	3.69978400	1.52160700	0.27782700
C	2.37037300	3.46159100	-0.48414900
C	1.20943600	3.97303400	-0.93632800
C	0.06030800	3.11288400	-1.17386600
C	5.39461100	-1.63626100	0.78567700
H	-3.43918400	-0.97106700	-1.39378600
H	-3.50272800	-0.83513900	1.64839400
H	-1.60367600	-2.38840300	0.59344300
H	-2.64772300	1.27544900	-0.39821200
H	-1.06695800	-0.07708300	-1.33155000
H	-2.56717500	1.27768700	2.65860300
H	-1.89327700	2.53344700	1.59409900
H	-4.94811200	-2.38414100	-0.51155100
H	-5.05540300	0.83936400	0.97819200
H	-2.08734800	-3.40752100	-1.48477200
H	-4.02819700	2.99433000	0.95376500
H	4.55634400	2.16835100	0.42279900
H	3.23013500	4.09900400	-0.31132200
H	1.07091500	5.02557300	-1.14244300
H	1.38642400	-3.14378100	0.52853200
H	6.48096700	-1.59812300	0.82857500
H	5.07176100	-1.97519100	-0.19795400
H	5.01013500	-2.29456600	1.56097800
H	0.18056000	-3.39812600	-1.41157400
O	0.89834000	-3.94253100	0.24279300
O	1.00981100	-3.86159100	-1.17476200

Name	**TS-FX-O7-H-OOH-FHT (gas phase)**
Cartesian Coordinates	Frequency and Energy

O	-1.64925600	-0.02632000	1.08960100
O	0.42759200	-0.88963200	0.77070600
O	-3.48684800	-3.22028300	-0.58410300
O	-4.87371800	-0.71862700	-0.48118400
O	-0.67114300	-2.90501400	-0.82519000
O	-4.60293100	1.98571000	0.55151900
O	-0.19116000	1.77146400	-0.16534900
O	2.94193600	-1.48892000	1.27055900
O	5.06305200	0.14991300	0.39849700
O	-1.73289100	3.28074100	-0.61813600
C	-2.86935600	-1.95228400	-0.52463700
C	-3.69057800	-0.93307700	0.25954500
C	-1.47837100	-2.15975300	0.06897100
C	-2.85823900	0.33828800	0.44803300
C	-0.85571900	-0.78507500	0.22513800
C	-3.53667600	1.40697300	1.28955400
C	1.34960900	0.05208400	0.44612000
C	1.10243800	1.34829900	-0.01176600
C	2.69884800	-0.36337300	0.66134200
C	2.16948900	2.21588800	-0.30324200

Zero-point correction= 0.358576 (Hartree/Particle)
Thermal correction to Energy= 0.384849
Thermal correction to Enthalpy= 0.385794
Thermal correction to Gibbs Free Energy= 0.301590
Sum of electronic and zero-point Energies= -1522.769685
Sum of electronic and thermal Energies= -1522.743411
Sum of electronic and thermal Enthalpies= -1522.742467
Sum of electronic and thermal Free Energies= -1522.826670

C	3.77311600	0.50324100	0.27426300
C	3.49534700	1.78380500	-0.16878300
C	1.82816600	3.54577100	-0.74879800
C	0.54418100	3.94370900	-0.86751000
C	-0.54913400	3.02887400	-0.55499300
C	5.44852200	-1.20783200	0.14324000
H	-2.73971200	-1.55062600	-1.54393700
H	-3.92126400	-1.34837200	1.25428000
H	-1.53793200	-2.65155000	1.04820200
H	-2.63475600	0.78547900	-0.53642200
H	-0.79780900	-0.31300300	-0.76757300
H	-3.97039700	0.97261100	2.19573800
H	-2.79059500	2.15524100	1.57512000
H	-4.37687300	-3.10210300	-0.94209800
H	-5.25356300	0.13670800	-0.22608600
H	-1.12602200	-3.72939600	-1.04491700
H	-4.21325000	2.60061400	-0.08585900
H	4.31898800	2.44327100	-0.42028800
H	2.63964000	4.22966000	-0.98287000
H	0.25898600	4.93664200	-1.19099600
H	2.69802300	-2.40328100	0.59825900
H	6.47965000	-1.15122600	-0.20587200
H	4.81422900	-1.65200500	-0.62919200
H	5.38465200	-1.80230800	1.05427900
H	1.03637500	-2.49353400	-1.15901000
O	2.55818100	-3.15293000	-0.33418600
O	2.00490800	-2.36810800	-1.29893600

Name	**TS-FX-O7-H-OOH-FHT (pentyl ethanoate)**
Cartesian Coordinates	Frequency and Energy

O	-1.75833500	0.17403200	0.97619600
O	0.28912400	-0.73502400	0.68492300
O	-3.52388800	-3.02089800	-0.87505900
O	-5.05077000	-0.67642000	-0.41294200
O	-0.75344300	-2.54413300	-1.16844600
O	-5.07089900	1.63170000	1.16950400
O	0.08653600	1.96588100	-0.27000100
O	2.65760400	-1.65243200	1.38549800
O	5.02961500	-0.32169600	0.69022400
O	-1.18444100	3.65844900	-0.89681600
C	-2.97570900	-1.72806600	-0.71507300
C	-3.79990700	-0.85774000	0.22040400
C	-1.56181000	-1.90708000	-0.19012200
C	-3.05521700	0.46205600	0.46745400
C	-0.96017100	-0.53547100	0.07261700
C	-3.72726400	1.32459100	1.52912500
C	1.34569400	0.06966700	0.42112200
C	1.30421600	1.38136100	-0.04985400
C	2.60888400	-0.51453200	0.74255300
C	2.49580800	2.09094800	-0.27591700
C	3.81273100	0.19859900	0.44095100
C	3.74084900	1.49160600	-0.04001400
C	2.37596000	3.44235500	-0.76853000
C	1.16718400	3.99668900	-0.98719500
C	-0.05890100	3.24729200	-0.73250000

Zero-point correction= 0.356959 (Hartree/Particle)
Thermal correction to Energy= 0.383565
Thermal correction to Enthalpy= 0.384510
Thermal correction to Gibbs Free Energy= 0.299757
Sum of electronic and zero-point Energies= -1522.802663
Sum of electronic and thermal Energies= -1522.776057
Sum of electronic and thermal Enthalpies= -1522.775113
Sum of electronic and thermal Free Energies= -1522.859865

C	5.26558600	-1.70172100	0.37277800
H	-2.92043900	-1.21758800	-1.69071500
H	-3.92054600	-1.37679400	1.18508100
H	-1.56644700	-2.48278500	0.74482400
H	-2.97522900	1.02220300	-0.47949800
H	-0.85064200	0.00606800	-0.87663500
H	-3.77108300	0.76590400	2.46905900
H	-3.13961000	2.23351300	1.69280600
H	-4.42906400	-2.92314100	-1.20285000
H	-5.54084100	-0.00788200	0.09055500
H	-1.15557300	-3.39492300	-1.39899400
H	-5.07080600	2.39120200	0.57148800
H	4.65575000	2.03972100	-0.23950800
H	3.28697000	4.00357700	-0.95768500
H	1.04178300	5.00770600	-1.35523100
H	2.39215200	-2.52396800	0.70657400
H	6.32283000	-1.76596200	0.11139500
H	4.65655900	-2.01130600	-0.48164500
H	5.05236300	-2.33919000	1.23125100
H	0.95618500	-2.36666100	-1.24868000
O	2.22158700	-3.28402800	-0.25246200
O	1.94582000	-2.42331000	-1.27041700

Name	**TS-FX-O7-H-OH-FHT (water)**
Cartesian Coordinates	Frequency and Energy

O	-1.81370600	0.18285700	0.97469100
O	0.27638200	-0.67153900	0.86061800
O	-3.42931600	-3.17321700	-0.69586200
O	-5.00054400	-0.78204500	-0.56054300
O	-0.62877100	-2.62427600	-0.95726900
O	-5.12207200	1.66178700	0.82116700
O	0.04270100	1.98442300	-0.11331900
O	2.69916100	-1.62639300	1.40123200
O	5.02800100	-0.29933000	0.60267900
O	-1.27774500	3.65510800	-0.66732900
C	-2.89899500	-1.85914300	-0.64720200
C	-3.78585500	-0.91928300	0.15983700
C	-1.49895600	-1.95860800	-0.05344300
C	-3.07435200	0.42452900	0.35288200
C	-0.94385600	-0.55818300	0.15773400
C	-3.81355700	1.36609400	1.29546000
C	1.33789500	0.10186300	0.51613900
C	1.27399600	1.40718100	0.03093200
C	2.61416800	-0.47833200	0.76541100
C	2.44308800	2.11330600	-0.28282400
C	3.79631000	0.23603300	0.39314500
C	3.70320900	1.51542100	-0.10815600
C	2.28832000	3.45417200	-0.79018700
C	1.06344000	4.00070600	-0.93807900
C	-0.13095700	3.25142200	-0.58389000
C	5.26672200	-1.62555300	0.09339900
H	-2.80902300	-1.45258900	-1.66574800
H	-3.97209600	-1.35989800	1.15129300
H	-1.52788500	-2.47950200	0.91155800
H	-2.92342800	0.90982000	-0.62554100

Zero-point correction= 0.356084 (Hartree/Particle)
Thermal correction to Energy= 0.383041
Thermal correction to Enthalpy= 0.383985
Thermal correction to Gibbs Free Energy= 0.298332
Sum of electronic and zero-point Energies= -1522.818821
Sum of electronic and thermal Energies= -1522.791864
Sum of electronic and thermal Enthalpies= -1522.790920
Sum of electronic and thermal Free Energies= -1522.876573

H	-0.78916200	-0.06588500	-0.81116800
H	-3.93289900	0.87844000	2.26732500
H	-3.22673900	2.28122800	1.42713900
H	-4.22675300	-3.16193100	-1.24365200
H	-5.51492000	-0.07655700	-0.13409900
H	-0.76042400	-3.58103100	-0.89052600
H	-5.05035500	2.27226000	0.07346400
H	4.60304000	2.06297600	-0.36853700
H	3.18268900	4.01390300	-1.04790200
H	0.90898100	5.00456400	-1.31396900
H	2.49890600	-2.48516200	0.69233300
H	6.32711200	-1.66118800	-0.15719400
H	4.66878100	-1.79832600	-0.80544900
H	5.03669100	-2.37681300	0.84955400
H	1.00317500	-2.24568400	-1.21349700
O	2.31051000	-3.20516800	-0.30814900
O	1.99797000	-2.29075400	-1.26570600