Supporting Information (SI)

The Antioxidant Activity of Natural Diterpenes: Theoretical Insights

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Table S1. BDE and PA values of the X-H (X = O, C) bonds of the studied compounds in the gas phase at the B3LYP/3-21g level of theory

Compounds	BDE		PA	
	B3LYP/3-21G	**(RO)B3LYP/6-311++G(2df,2p)//B3LYP/6-311G(d,p)**	**B3LYP/3-21G**	**(RO)B3LYP/6-311++G(2df,2p)//B3LYP/6-311G(d,p)**
1				
1-C1-H	97.4		317.7	
1-C2-H	96.5		287.6	
1-C3-H	95.5		293.8	
1-C6-H	107.9		317.7	
1-C11-H	111.5		318.6	
1-C12-OH-H	**77.6**	85.3	**265.0**	307.2
1-C14-H	113.0		322.0	
1-C15-H	89.2		294.6	
1-C18-H	100.2		326.9	
1-C19-H	97.8		293.7	
1-C20-H	97.6		293.0	
2				
2-C1-H	97.1		318.4	
2-C2-H	96.4		322.8	
2-C3-H	97.3		321.2	
2-C6-H	103.8		309.3	
2-C11-H	111.8		316.6	
2-C12-OH-H	**77.7**	85.4	**262.2**	305.1
2-C14-H	112.6		318.2	
2-C15-H	89.1		293.1	
2-C18-H	100.0		326.9	
2-C19-H	98.0		322.1	
2-C20-H	97.7		288.9	
3				
3-C1-H	97.7		323	
3-C2-H	96.3		328.9	
3-C3-H	97.3		326.7	
3-C5-H	92.3		306.9	
3-C6-H	87.4		288.3	
3-C11-H	111.4		317.1	
3-C12-OH-H	**85.3**	87.6	**259.2**	293.6

3-C14-H	110.5		317.7	
3-C15-H	87.9		293.6	
3-C16-H	97.4		311.6	
3-C16-OH-H	93.7		269.2	
3-C17-H	100.9		312.4	
3-C18-H	100.1		329.7	
3-C19-H	98.0		328	
3-C20-H	99.0		290.2	
4				
4-C1-H	89.9		275.9	
4-C2-H	95.8		273.8	
4-C3-H	96.4		274.7	
4-C5-H	90.1		268.9	
4-C6-H	95.6		273.9	
4-C7-H	83.5		266.8	
4-C11-OH-H	**71.1**	84.4	**263.9**	306.0
4-C14-H	103.8		298.7	
4-C16-H	**67.5**	74.6	270.2	
4-C18-H	100.0		281.8	
4-C19-H	97.3		281	
4-C20-H	93.4		281.2	
5			307.8	
5-C1-H	97.8		324.3	
5-C2-H	96.4		329.9	
5-C3-H	97.4		327.6	
5-C5-H	92.4		313.7	
5-C6-H	87.0		290.1	
5-C11-H	111.8		319.9	
5-C12-OH-H	**77.3**	85.6	**264.9**	304.5
5-C14-H	112.7		322.1	
5-C15-H	89.3		295.3	
5-C18-H	100.2		330.6	
5-C19-H	98.1		329	
5-C20-H	97.8		294.2	
6				
6-C1-H	97.5		330.5	
6-C2-H	95.2		335.4	
6-C3-H	97.0		332.3	
6-C5-H	91.1		321.2	
6-C6-H	94.7		329.5	

6-C7-H	81.9		294.1	
6-C11-H	111.4		324.8	
6-C12-OH-H	**68.1**	74.7	**272.4**	311.0
6-13-OH-H	**68.4**	75.2	**271.2**	310.7
6-C14-H	110.7		318.7	
6-C18-H	100.0		334.9	
6-C19-H	98.0		334.2	
6-C20-H	97.2		310.6	
7				
7-C1-H	94.4		327.4	
7-C1'-H	92.4		321	
7-C2-H	92.7		332.9	
7-C2'-H	93.7		328.1	
7-C3'-H	93.9		325.2	
7-C3-H	93.9		330.7	
7-C5'-H	90.2		274.7	
7-C5-H	91.2		318.7	
7-C6'-H	100.9		315.9	
7-C6-H	92.1		327.3	
7-C7'-H	103.7		307.5	
7-C7-H	84.3		290.9	
7-C11'-H	118.4		313.3	
7-C11-H	110.4		318.5	
7-C12'-OH-H	81.6		259.2	
7-C12-OH-H	**79.4**	83.0	**254.1**	273.5
7-C14'-H	99.0		309	
7-C14-H	98.2		265.3	
7-C18'-H	89.1		329.9	
7-C18-H	98.5		334	
7-C19'-H	80.9		326	
7-C19-H	80.6		332.6	
7-C20'-H	90.1		291.7	
7-C20-H	90.9		299.4	
8				
8-C2-H	85.6		277.7	
8-C3-H	**63.0**	74.7	267.5	
8-C3-OH-H	98.8		291.5	
8-C7-H	101.0		303.2	
8-C8-H	73.9		264.8	
8-C9-H	74.3		**256.9**	351.6

8-C12-H	85.1		297	
8-C13-H	97.1		314.1	
8-C14-H	81.2		287.5	
8-C16-H	107.3		266.9	
8-C17-H	86.8		302.3	
8-C18-H	110.0		275.2	
8-C19-H	100.7		133.3	
8-C20-H	88.0		296.1	
9				
9-C1-H	112.8		294.9	
9-C5-H	103.6		298.9	
9-C6-OH-H	103.0		293.2	
9-C7-H	96.4		275.6	
9-C8-H	92.3		307	
9-C9-H	97.2		261.7	
9-C11-H	99.3		275.3	
9-C12-H	92.4		289.4	
9-C13-H	**86.8**	88.7	261.5	
9-C15-OH-H	92.6		276.8	
9-C16-H	99.6		**256.7**	356.2
9-C17-H	89.2		276.5	
9-C18-H	89.4		322.9	
9-C19-H	98.3		326.5	
9-C20-H	112.8		286.6	

Table S2. The Calculated Free Energy (ΔG°, in kcal/mol at 298.15 k) of the Reaction Between the Selected Compounds with HOO• Radical via the Formal Hydrogen Transfer (FHT), Sequential Proton (SA) and SET Processes in the Gas Phase Using the (RO)B3LYP/6-311++g(2df,2p)//B3LYP/6-311g(d,p) Method.

	ΔG		
Compounds	**FHT**	**PA**	**SET**
1	-0.1	158.2	157.2
2	-0.1	156.1	158.1
3	2.1	145.2	150.8
4	-11.1	157.4	151.9
5	0.3	155.7	158.5
6	-9.9	162.5	143.9
7	-3.4	127.2	138.0
8	-24.6	153.5	189.5
9	3.0	159.5	160.0

Table S3. The Calculated Free Energy (ΔG°, in kcal/mol at 298.15 k) of the Reaction Between the neutral Compounds with HOO• Radical via the SET Processes in the water and pentyl ethanoate solvents

	ΔG	
Compounds	water	pentyl ethanoate
1	48.3	70.8
2	49.2	71.6
3	44.7	66.6
4	41.4	64.5
5	48.8	71.5
6	33.1	55.8
7	33.7	55.5
8	57.0	92.1
9	46.8	70.7

Table S4: The cartesian coordinates and energies of TS of the reaction between selected compounds with HOO• at the M06-2x/6-311++G(d,p) calculating method following the FHT mechanism

Name				**1-O12-H-OOH (gas phase)**	
Cartesian Coordinates				Frequency and Energy	
C	2.12261800	0.42586600	0.10753400	Zero-point correction=	0.375059 (Hartree/Particle)
C	1.04260900	-0.66241100	0.07659900	Thermal correction to Energy=	0.396544
C	-0.35178000	-0.10738400	-0.22146200	Thermal correction to Enthalpy=	0.397488
C	-0.65922700	1.26027000	-0.10997100	Thermal correction to Gibbs Free Energy=	0.324463
C	0.41423200	2.23596400	0.20576500	Sum of electronic and zero-point Energies=	-999.767032
C	1.79083500	1.72638400	0.20214400	Sum of electronic and thermal Energies=	-999.745547
H	-1.26597600	-2.04567600	-0.59006000	Sum of electronic and thermal Enthalpies=	-999.744603
C	-1.39914800	-0.97149700	-0.51902900	Sum of electronic and thermal Free Energies=	-999.817628
C	-1.96249400	1.74523500	-0.30396800		
H	2.53964200	2.50702000	0.27129100		
C	-3.00584000	0.89776400	-0.62341600		
C	-2.71065500	-0.49614700	-0.73923600		
H	-2.12057300	2.81520200	-0.19888200		
O	-3.66784200	-1.34107700	-1.05087500		
H	-4.28780800	-1.55287900	-0.11063500		
C	-4.41282400	1.36561400	-0.84858400		
H	-4.73496300	1.12860500	-1.86718000		
H	-5.11373900	0.84898400	-0.18191100		
H	-4.49566600	2.44207800	-0.68911600		
O	0.16865300	3.41505900	0.41519900		
C	1.40239600	-1.73199800	-0.98521500		
H	1.24998600	-1.29587700	-1.98127100		
H	0.71028900	-2.57445400	-0.89655300		
C	2.83718100	-2.23614000	-0.87453800		
H	2.98498600	-2.77035100	0.07157600		
H	3.02387200	-2.96646100	-1.66864300		
C	3.81725200	-1.07762600	-0.99733400		
H	3.70616500	-0.62548700	-1.99299700		
H	4.85242400	-1.43323700	-0.92420000		
C	3.60702800	0.02233600	0.06438200		
C	4.50362700	1.20839000	-0.32530800		
H	4.56288800	1.96004700	0.46733000		
H	5.51901400	0.83843500	-0.49903100		
H	4.15530000	1.69339200	-1.24196800		
C	4.10084400	-0.47039000	1.44356200		
H	5.19521600	-0.51164500	1.43203000		
H	3.79440400	0.22008800	2.23548200		
H	3.74352400	-1.46783200	1.70117400		
C	0.92873700	-1.32471300	1.47755000		
H	0.74108700	-0.56600600	2.24302000		
H	0.09051900	-2.02723500	1.47979200		
H	1.82867800	-1.87428200	1.75004500		
O	-3.67135600	-0.99397100	1.73282700		
H	-3.92296700	-0.06797500	1.89585200		
O	-4.72303600	-1.52145600	1.04260000		
Name				**1-O12-H-OOH (water)**	
Cartesian Coordinates				Frequency and Energy	
C	2.13772300	0.41722900	0.11245500	Zero-point correction=	0.374533 (Hartree/Particle)
C	1.06442100	-0.67123700	0.09947700	Thermal correction to Energy=	0.395741
C	-0.33142900	-0.12399000	-0.18972800	Thermal correction to Enthalpy=	0.396685

C	-0.64144300	1.24888700	-0.10949300
C	0.43407800	2.21678200	0.19999700
C	1.80286900	1.72221800	0.19861900
H	-1.23261500	-2.07100200	-0.50622700
C	-1.37716600	-0.99639300	-0.46456400
C	-1.94119700	1.72967000	-0.33115400
H	2.55544900	2.50024100	0.26301600
C	-2.98154600	0.87572500	-0.64703000
C	-2.68207500	-0.52002100	-0.71249300
H	-2.12169900	2.79821500	-0.26228300
O	-3.63832500	-1.37941000	-1.03399900
H	-4.32472700	-1.51035000	-0.14248200
C	-4.37360700	1.35077100	-0.92278800
H	-4.65625600	1.12730000	-1.95706500
H	-5.09900800	0.83920900	-0.27981100
H	-4.45131100	2.42689600	-0.76007800
O	0.18409200	3.41019300	0.40804700
C	1.41806400	-1.75104700	-0.95552600
H	1.26184300	-1.32375500	-1.95465300
H	0.72634100	-2.59088000	-0.84725100
C	2.85432400	-2.24825300	-0.84474900
H	3.00764300	-2.76634200	0.10908100
H	3.03712700	-2.98566800	-1.63304100
C	3.82828500	-1.08828700	-0.98938800
H	3.70816300	-0.64813900	-1.98920600
H	4.86575900	-1.43484900	-0.91248600
C	3.62165500	0.02376800	0.06060700
C	4.50670300	1.21035100	-0.34908700
H	4.56675800	1.97216500	0.43413800
H	5.52138000	0.83883200	-0.52336900
H	4.15140600	1.68133700	-1.27095600
C	4.12642000	-0.45038300	1.44216100
H	5.22129900	-0.46631100	1.42104500
H	3.81056800	0.23874800	2.23222400
H	3.79147400	-1.45481900	1.70348700
C	0.96988000	-1.32000500	1.50830400
H	0.76962500	-0.55768100	2.26749300
H	0.14834500	-2.04200400	1.51211900
H	1.88219700	-1.85005900	1.77743700
O	-3.90993800	-0.82310700	1.73325000
H	-4.26539100	0.08568700	1.77974800
O	-4.82209500	-1.52786000	1.00587800

Thermal correction to Gibbs Free Energy= 0.324666
Sum of electronic and zero-point Energies= -999.790578
Sum of electronic and thermal Energies= -999.769371
Sum of electronic and thermal Enthalpies= -999.768427
Sum of electronic and thermal Free Energies= -999.840446

Name			**1-O12-H-OOH (pentyl ethanoate)**
Cartesian Coordinates			Frequency and Energy
C	2.12261800	0.42586600	0.10753400
C	1.04260900	-0.66241100	0.07659900
C	-0.35178000	-0.10738400	-0.22146200
C	-0.65922700	1.26027000	-0.10997100
C	0.41423200	2.23596400	0.20576500
C	1.79083500	1.72638400	0.20214400
H	-1.26597600	-2.04567600	-0.59006000
C	-1.39914800	-0.97149700	-0.51902900
C	-1.96249400	1.74523500	-0.30396800

Zero-point correction= 0.375059 (Hartree/Particle)
Thermal correction to Energy= 0.396544
Thermal correction to Enthalpy= 0.397488
Thermal correction to Gibbs Free Energy= 0.324463
Sum of electronic and zero-point Energies= -999.767032
Sum of electronic and thermal Energies= -999.745547
Sum of electronic and thermal Enthalpies= -999.744603
Sum of electronic and thermal Free Energies= -999.817628

H	2.53964200	2.50702000	0.27129100
C	-3.00584000	0.89776400	-0.62341600
C	-2.71065500	-0.49614700	-0.73923600
H	-2.12057300	2.81520200	-0.19888200
O	-3.66784200	-1.34107700	-1.05087500
H	-4.28780800	-1.55287900	-0.11063500
C	-4.41282400	1.36561400	-0.84858400
H	-4.73496300	1.12860500	-1.86718000
H	-5.11373900	0.84898400	-0.18191100
H	-4.49566600	2.44207800	-0.68911600
O	0.16865300	3.41505900	0.41519900
C	1.40239600	-1.73199800	-0.98521500
H	1.24998600	-1.29587700	-1.98127100
H	0.71028900	-2.57445400	-0.89655300
C	2.83718100	-2.23614000	-0.87453800
H	2.98498600	-2.77035100	0.07157600
H	3.02387200	-2.96646100	-1.66864300
C	3.81725200	-1.07762600	-0.99733400
H	3.70616500	-0.62548700	-1.99299700
H	4.85242400	-1.43323700	-0.92420000
C	3.60702800	0.02233600	0.06438200
C	4.50362700	1.20839000	-0.32530800
H	4.56288800	1.96004700	0.46733000
H	5.51901400	0.83843500	-0.49903100
H	4.15530000	1.69339200	-1.24196800
C	4.10084400	-0.47039000	1.44356200
H	5.19521600	-0.51164500	1.43203000
H	3.79440400	0.22008800	2.23548200
H	3.74352400	-1.46783200	1.70117400
C	0.92873700	-1.32471300	1.47755000
H	0.74108700	-0.56600600	2.24302000
H	0.09051900	-2.02723500	1.47979200
H	1.82867800	-1.87428200	1.75004500
O	-3.67135600	-0.99397100	1.73282700
H	-3.92296700	-0.06797500	1.89585200
O	-4.72303600	-1.52145600	1.04260000

Name			**2-O12-H-OOH (gas phase)**
Cartesian Coordinates			Frequency and Energy
C	2.08211500	0.31067400	-0.12537600
C	0.98083000	-0.70553700	0.25277600
C	-0.39804400	-0.16249300	-0.13885400
C	-0.70657700	1.20805700	0.03637900
C	0.37541900	2.16427800	0.37924800
C	1.74248000	1.75307000	-0.06490100
H	-1.29095900	-2.05977000	-0.68899100
C	-1.42964500	-0.99647800	-0.52854500
C	-1.99725500	1.70587700	-0.15608400
C	-3.03859900	0.88204700	-0.55707200
C	-2.73696700	-0.49802500	-0.76065700
H	-2.16239600	2.76881200	-0.00103500
O	-3.66387700	-1.32593400	-1.18678700
H	-4.47125400	-1.43735800	-0.40255300
C	-4.42977600	1.38135200	-0.79603400
H	-4.79184100	1.05103000	-1.77393200

Zero-point correction= 0.379806 (Hartree/Particle)
Thermal correction to Energy= 0.401884
Thermal correction to Enthalpy= 0.402828
Thermal correction to Gibbs Free Energy= 0.329396
Sum of electronic and zero-point Energies= -1074.943661
Sum of electronic and thermal Energies= -1074.921584
Sum of electronic and thermal Enthalpies= -1074.920639
Sum of electronic and thermal Free Energies= -1074.994072

H	-5.11695800	0.97870600	-0.04417100
H	-4.46258300	2.47118200	-0.74915400
O	0.18510800	3.22200400	0.94748800
C	1.27869000	-2.03514600	-0.47095100
H	1.09148100	-1.89544400	-1.54391200
H	0.58455600	-2.80500500	-0.11738000
C	2.71508100	-2.51889700	-0.27205800
H	2.88922600	-2.77886800	0.77898000
H	2.86104800	-3.44367900	-0.83954700
C	3.71997200	-1.46832500	-0.73612900
H	3.58961200	-1.30455000	-1.81490900
H	4.74670100	-1.82582200	-0.58997300
C	3.56509200	-0.11103100	-0.02140300
C	4.47188900	0.90442300	-0.73458600
H	4.54931600	1.84532500	-0.18088300
H	5.48088500	0.48492500	-0.79632500
H	4.12130200	1.11851900	-1.74580200
H	2.51390600	2.50544300	0.07605200
O	1.77402000	1.04194300	-1.30212100
C	0.91426000	-0.92646400	1.78199500
H	1.77085400	-1.48089100	2.16371900
H	0.85669600	0.02807500	2.31598200
H	0.01409500	-1.50084500	2.01977700
C	4.03918600	-0.19629000	1.44021500
H	3.72117600	0.68481500	2.00832800
H	3.68622000	-1.08476800	1.96438500
H	5.13344800	-0.22738000	1.45656500
O	-4.29261500	-0.75351100	1.50995300
H	-3.77173000	-1.38578100	2.03296600
O	-5.05660000	-1.54115400	0.69447200

Name	**2-O12-H-OOH (water)**
Cartesian Coordinates	Frequency and Energy

C	2.04748300	0.31747700	-0.13483500
C	0.93501600	-0.69611900	0.20965800
C	-0.43135000	-0.12791900	-0.18008000
C	-0.73019000	1.24070300	0.03419900
C	0.36285300	2.16103100	0.41873700
C	1.72463200	1.76305300	-0.03435900
H	-1.33189700	-2.00349500	-0.77750300
C	-1.46734000	-0.94232300	-0.59957900
C	-2.01743100	1.75789600	-0.13897100
C	-3.06536400	0.94878100	-0.55331200
C	-2.76812400	-0.42287700	-0.80516200
H	-2.18816600	2.81561800	0.04256800
O	-3.72536100	-1.23070100	-1.23821700
H	-4.36013000	-1.52802300	-0.35160200
C	-4.46057800	1.45273800	-0.73869800
H	-4.78515000	1.32206000	-1.77611300
H	-5.15743600	0.88616400	-0.11085000
H	-4.52611100	2.50991300	-0.47687400
O	0.18127900	3.19516000	1.04885300
C	1.22540300	-2.01444900	-0.53707100
H	1.05609300	-1.85539800	-1.61058800
H	0.51711300	-2.77913100	-0.20320600

Zero-point correction= 0.378701 (Hartree/Particle)
Thermal correction to Energy= 0.400640
Thermal correction to Enthalpy= 0.401584
Thermal correction to Gibbs Free Energy= 0.328428
Sum of electronic and zero-point Energies= -1074.968715
Sum of electronic and thermal Energies= -1074.946776
Sum of electronic and thermal Enthalpies= -1074.945832
Sum of electronic and thermal Free Energies= -1075.018988

C	2.65347900	-2.51466600	-0.32526800
H	2.80952900	-2.78978000	0.72423400
H	2.79710900	-3.42993400	-0.90828900
C	3.67425600	-1.46759000	-0.75922800
H	3.56153200	-1.28865100	-1.83786900
H	4.69577900	-1.83274100	-0.59906300
C	3.52410500	-0.11860300	-0.02810400
C	4.45195100	0.89593400	-0.71140900
H	4.49585600	1.84567500	-0.16929200
H	5.46401000	0.47945400	-0.71869700
H	4.15724400	1.09118300	-1.74491300
H	2.50505000	2.50018100	0.13082900
O	1.74928100	1.08951400	-1.29765300
C	0.84460400	-0.94948900	1.73306800
H	1.67670500	-1.54546500	2.10621900
H	0.81627900	-0.00674800	2.29062700
H	-0.07829000	-1.49840500	1.94440800
C	3.97170100	-0.22673300	1.43941700
H	3.65918400	0.65521700	2.00966400
H	3.59481200	-1.11596600	1.94540400
H	5.06508500	-0.27661000	1.46836200
O	-3.93865500	-0.94713200	1.55393300
H	-3.20459100	-1.53561600	1.81908200
O	-4.77782300	-1.72691200	0.81676400

Name	**2-O12-H-OOH (pentyl ethanoate)**
Cartesian Coordinates	Frequency and Energy

C	2.07396000	0.31099300	-0.12972600
C	0.97003500	-0.70433100	0.24308900
C	-0.40541800	-0.15291200	-0.14589000
C	-0.70895100	1.21856700	0.03827900
C	0.37900200	2.16113900	0.39964500
C	1.74191300	1.75537800	-0.05365300
H	-1.30032000	-2.04397000	-0.70572800
C	-1.43979400	-0.98060100	-0.54405000
C	-1.99694900	1.72457200	-0.15463100
C	-3.04081600	0.90618900	-0.56161000
C	-2.74328300	-0.47331900	-0.77287400
H	-2.16599700	2.78665000	0.00208600
O	-3.67965900	-1.29218200	-1.20660900
H	-4.44438100	-1.45000500	-0.39867000
C	-4.42858200	1.41365200	-0.79603900
H	-4.75681400	1.18531900	-1.81515500
H	-5.13834600	0.93278500	-0.11397200
H	-4.47562800	2.49315300	-0.64109700
O	0.19193400	3.20632600	0.99725300
C	1.26357800	-2.03273400	-0.48507700
H	1.07993900	-1.89297500	-1.55887300
H	0.56604200	-2.79979900	-0.13286000
C	2.69767200	-2.52079500	-0.28306700
H	2.86789100	-2.78144300	0.76837600
H	2.84114400	-3.44414300	-0.85391600
C	3.70766500	-1.47357500	-0.74260100
H	3.58426700	-1.31143900	-1.82275300
H	4.73261600	-1.83312200	-0.58906500

Zero-point correction= 0.379168 (Hartree/Particle)
Thermal correction to Energy= 0.401204
Thermal correction to Enthalpy= 0.402148
Thermal correction to Gibbs Free Energy= 0.328934
Sum of electronic and zero-point Energies= -1074.971109
Sum of electronic and thermal Energies= -1074.949074
Sum of electronic and thermal Enthalpies= -1074.948129
Sum of electronic and thermal Free Energies= -1075.021343

C	3.55572500	-0.11544900	-0.02829000
C	4.46716000	0.89749800	-0.73698700
H	4.53529600	1.84366000	-0.19026800
H	5.47785000	0.47922800	-0.78292800
H	4.13361300	1.10333900	-1.75635100
H	2.51941300	2.50057300	0.09286800
O	1.76440900	1.05702000	-1.30025300
C	0.90085500	-0.93374500	1.77071500
H	1.75270700	-1.49889800	2.14771800
H	0.85067200	0.01663400	2.31392700
H	-0.00329300	-1.50427200	2.00515000
C	4.02582500	-0.20294800	1.43389500
H	3.71259700	0.68010300	2.00246800
H	3.66774900	-1.09066100	1.95642200
H	5.12036300	-0.23965700	1.45094300
O	-4.22991300	-0.81031400	1.52920700
H	-3.63417600	-1.43540900	1.98298200
O	-5.00186800	-1.59598900	0.72189300

Name	**3-O12-H-OOH (gas phase)**
Cartesian Coordinates	Frequency and Energy

C	-2.62816700	0.52388400	0.14851300
C	-1.74494200	-0.72188500	-0.17125100
C	-0.29297500	-0.34170800	0.13891200
C	0.18267300	0.96924700	-0.09969600
C	-0.73365400	2.04879700	-0.58080000
C	-2.20330600	1.71577600	-0.71210300
H	0.35220300	-2.30125500	0.80393000
C	0.62681600	-1.27331900	0.59264300
C	1.52439100	1.31139200	0.11851000
C	2.45041300	0.39377800	0.58131000
C	1.98132000	-0.93038700	0.82698900
H	1.81319300	2.33787100	-0.09241600
O	2.79376800	-1.86027800	1.29168700
H	3.49986200	-2.14425500	0.47958400
C	3.88855800	0.76845500	0.84994300
H	4.42484000	-0.14235300	1.13867400
O	-0.31225200	3.15745400	-0.84997600
C	-2.19804900	-1.90244400	0.71043500
H	-1.93074200	-1.68728500	1.75464300
H	-1.65673800	-2.81074100	0.42272600
C	-3.70163900	-2.16146700	0.63114400
H	-3.98326200	-2.47386000	-0.38185600
H	-3.95824200	-2.99846600	1.28902400
C	-4.48543500	-0.91948700	1.04335100
H	-4.24254400	-0.68369000	2.09009800
H	-5.56483600	-1.11382900	1.00803400
C	-4.17172100	0.31541500	0.17937200
C	-4.82283600	1.53294000	0.85857800
H	-4.79104800	2.42641800	0.22811600
H	-5.87706700	1.31968500	1.06598400
H	-4.33398200	1.76651200	1.81090900
H	-2.39405100	1.52377100	-1.77539500
C	-1.76081200	-1.15798200	-1.65378900
H	-2.74068900	-1.51356400	-1.97443100

Zero-point correction= 0.461674 (Hartree/Particle)
Thermal correction to Energy= 0.486899
Thermal correction to Enthalpy= 0.487843
Thermal correction to Gibbs Free Energy= 0.407152
Sum of electronic and zero-point Energies= -1154.683234
Sum of electronic and thermal Energies= -1154.658008
Sum of electronic and thermal Enthalpies= -1154.657064
Sum of electronic and thermal Free Energies= -1154.737755

H	-1.45255200	-0.35217200	-2.32547000
H	-1.04805700	-1.97832100	-1.78792300
C	-4.82143000	0.16794200	-1.20628500
H	-4.55823500	0.99971600	-1.86715200
H	-4.55773600	-0.76176000	-1.71283700
H	-5.91107200	0.17665400	-1.09283800
H	-2.36791100	0.77613900	1.19048500
H	-2.75095600	2.62716600	-0.45973200
C	4.57504700	1.34132100	-0.39659000
H	4.11608500	2.29816700	-0.67126800
H	5.62743600	1.54328300	-0.14435900
O	4.46838300	0.51439800	-1.52951900
H	4.67059900	-0.40081400	-1.28843800
C	3.98837400	1.76469800	2.01367100
H	3.45470400	2.69164400	1.77907600
H	3.55475400	1.34390300	2.92425400
H	5.03466400	2.01440800	2.21460800
O	2.95639700	-1.99706100	-1.50318700
H	2.50485500	-2.83655100	-1.69638400
O	3.98755000	-2.35404100	-0.67985300

Name			**3-O12-H-OOH (water)**
Cartesian Coordinates			Frequency and Energy
C	-2.62704400	0.50190000	0.21834800
C	-1.78047800	-0.71512100	-0.26239000
C	-0.31754900	-0.40233600	0.06060900
C	0.18590900	0.92189600	-0.03719800
C	-0.71751800	2.04950100	-0.40186700
C	-2.19268200	1.77880300	-0.50247600
H	0.28352200	-2.43680600	0.47953700
C	0.58465000	-1.39846800	0.39214400
C	1.53481800	1.21162900	0.19754100
C	2.44690600	0.22332400	0.53794600
C	1.94454400	-1.10857200	0.65065300
H	1.85852100	2.24371100	0.10270900
O	2.74748200	-2.09690000	1.02040700
H	3.42359300	-2.36941000	0.16060700
C	3.89852500	0.50999100	0.83171200
H	4.47514800	-0.39178800	0.59375200
O	-0.26599400	3.17022900	-0.62007600
C	-2.24187300	-1.97983500	0.48825800
H	-1.95499000	-1.88778200	1.54525200
H	-1.72398100	-2.85757700	0.08705000
C	-3.75197600	-2.19564100	0.40813500
H	-4.05585400	-2.38375300	-0.62879200
H	-4.01467100	-3.09541400	0.97472100
C	-4.50117400	-0.99259700	0.97202600
H	-4.23380500	-0.87907700	2.03305700
H	-5.58543600	-1.15723700	0.93196700
C	-4.17347900	0.32344800	0.24503500
C	-4.78754500	1.47212700	1.06189100
H	-4.74058600	2.42802600	0.53069300
H	-5.84427500	1.25825800	1.25799900
H	-4.28021100	1.58804500	2.02651400
H	-2.42462800	1.73226000	-1.57459700

Zero-point correction= 0.459741 (Hartree/Particle)
Thermal correction to Energy= 0.485166
Thermal correction to Enthalpy= 0.486110
Thermal correction to Gibbs Free Energy= 0.405252
Sum of electronic and zero-point Energies= -1154.715024
Sum of electronic and thermal Energies= -1154.689599
Sum of electronic and thermal Enthalpies= -1154.688655
Sum of electronic and thermal Free Energies= -1154.769512

C	-1.82828100	-0.97699700	-1.78408600
H	-2.81841000	-1.29021100	-2.11709300
H	-1.53320300	-0.09761400	-2.36432800
H	-1.12589200	-1.78194700	-2.02503700
C	-4.84283900	0.34086800	-1.13823300
H	-4.56025700	1.22798200	-1.71450100
H	-4.61625200	-0.54109400	-1.73989600
H	-5.93025500	0.37178300	-1.00378100
H	-2.34976900	0.62495500	1.27813200
H	-2.70271100	2.66428600	-0.11319000
C	4.46631300	1.64989500	-0.01040900
H	3.99878200	2.60450700	0.25077200
H	5.53810600	1.73400600	0.20906000
O	4.26069700	1.46868300	-1.40801500
H	4.42869700	0.53949700	-1.62523500
C	4.08854200	0.82176300	2.32292600
H	3.52044000	1.71600400	2.59996600
H	3.74310800	-0.01165200	2.94053100
H	5.14585900	0.99974800	2.54192600
O	3.44550000	-1.42134500	-1.64412200
H	2.65901300	-1.75379100	-2.11924100
O	3.94903700	-2.49709000	-0.97593800

Name	**3-O12-H-OOH (pentyl ethanoate)**
Cartesian Coordinates	Frequency and Energy

C	-2.62702500	0.52706000	0.14735900
C	-1.74087400	-0.71985900	-0.15627200
C	-0.29063700	-0.33104400	0.14860400
C	0.18166100	0.98030200	-0.09543800
C	-0.73909000	2.04861800	-0.59319200
C	-2.20293600	1.71001200	-0.72560100
H	0.35883000	-2.28904700	0.80906800
C	0.63353700	-1.25988900	0.60308100
C	1.52344000	1.32745900	0.12373400
C	2.45239800	0.41325700	0.58729300
C	1.98644900	-0.91184500	0.83432500
H	1.81786900	2.35280000	-0.08505200
O	2.80549600	-1.83760900	1.30226200
H	3.48630200	-2.14717600	0.48329500
C	3.89175800	0.79335300	0.84548500
H	4.43148500	-0.10901500	1.15356500
O	-0.31555700	3.15573100	-0.88115800
C	-2.19071400	-1.88999400	0.74117000
H	-1.92838500	-1.65895800	1.78339900
H	-1.64623300	-2.80032300	0.46650300
C	-3.69347300	-2.15321600	0.66019700
H	-3.96969500	-2.47798900	-0.35047000
H	-3.94909800	-2.98174300	1.32970500
C	-4.48349200	-0.90872000	1.05188600
H	-4.24657000	-0.65689000	2.09635100
H	-5.56217600	-1.10719900	1.01135000
C	-4.16989600	0.31450800	0.17156200
C	-4.82768300	1.53982900	0.82838500
H	-4.79918000	2.42310800	0.18246700
H	-5.88177100	1.32468100	1.03750400

Zero-point correction= 0.460695 (Hartree/Particle)
Thermal correction to Energy= 0.485917
Thermal correction to Enthalpy= 0.486861
Thermal correction to Gibbs Free Energy= 0.406371
Sum of electronic and zero-point Energies= -1154.713265
Sum of electronic and thermal Energies= -1154.688044
Sum of electronic and thermal Enthalpies= -1154.687099
Sum of electronic and thermal Free Energies= -1154.767590

H	-4.34164400	1.79291700	1.77783800
H	-2.38386900	1.50319300	-1.78823800
C	-1.75305600	-1.17362500	-1.63274300
H	-2.72868200	-1.54959600	-1.94396000
H	-1.46244800	-0.36891900	-2.31448400
H	-1.02808700	-1.98495300	-1.76122900
C	-4.81057000	0.14337900	-1.21489900
H	-4.53842900	0.95990400	-1.89184600
H	-4.54970800	-0.79883200	-1.70048400
H	-5.90143900	0.16112700	-1.10823400
H	-2.37389300	0.79250900	1.18726900
H	-2.75942400	2.62005900	-0.48648600
C	4.57440400	1.33717800	-0.41358500
H	4.11023600	2.28336500	-0.71479200
H	5.62609500	1.54712000	-0.16883800
O	4.47871500	0.47303500	-1.52794300
H	4.61903500	-0.44145100	-1.24152700
C	3.99795400	1.81875100	1.98188000
H	3.47064000	2.74339100	1.72390600
H	3.56264300	1.42379500	2.90394100
H	5.04655800	2.06534900	2.17626400
O	2.91923700	-2.06720700	-1.49949200
H	2.43937800	-2.90719600	-1.62907900
O	3.96320200	-2.39234000	-0.68080600

Name	**4-C16-H-OOH (gas phase)**
Cartesian Coordinates	Frequency and Energy

C	-2.81541900	0.63864300	0.21887100
C	-1.92550000	-0.52622200	-0.31418500
C	-0.45281200	-0.06272100	-0.30050700
C	-0.08592800	1.30187100	-0.19876500
C	-1.12558200	2.40335300	-0.12797400
C	-2.51368800	1.93300800	-0.53591700
C	0.58601200	-1.01099600	-0.46172800
C	1.25404500	1.71046200	-0.17479900
H	-3.24245800	2.71325200	-0.30142600
C	2.26022200	0.75973500	-0.26959500
C	1.89234300	-0.56993900	-0.41814900
H	1.49055800	2.76765700	-0.08943300
O	2.97646700	-1.41470100	-0.58513600
C	3.72675900	0.79025100	-0.28500500
C	-2.13966700	-1.72405100	0.64680300
H	-1.73849800	-1.44903300	1.63298000
H	-1.57916100	-2.59316700	0.30468200
C	-3.61641300	-2.09866700	0.79558000
H	-4.00822700	-2.47319300	-0.15796500
H	-3.70105400	-2.93310700	1.50048000
C	-4.45774000	-0.92625000	1.28847800
H	-4.13649100	-0.67057400	2.30923400
H	-5.51633000	-1.21018200	1.35500300
C	-4.32758300	0.33616300	0.41648100
C	-4.96897900	1.49589100	1.20052400
H	-5.11724700	2.38598900	0.58202000
H	-5.95477800	1.18889400	1.56707600
H	-4.36018900	1.77620800	2.06792000

Zero-point correction= 0.439857 (Hartree/Particle)
Thermal correction to Energy= 0.463952
Thermal correction to Enthalpy= 0.464896
Thermal correction to Gibbs Free Energy= 0.387461
Sum of electronic and zero-point Energies= -1153.510109
Sum of electronic and thermal Energies= -1153.486015
Sum of electronic and thermal Enthalpies= -1153.485071
Sum of electronic and thermal Free Energies= -1153.562506

C	-5.12101200	0.18223000	-0.89172000
H	-6.19313500	0.25299300	-0.67652600
H	-4.87418400	0.97799000	-1.60342700
H	-4.95411400	-0.77538600	-1.38647400
C	-2.23133200	-0.95932100	-1.76672300
H	-2.27218000	-0.10342300	-2.44593000
H	-1.44511000	-1.63042300	-2.12052900
H	-3.17510100	-1.49818400	-1.84603800
H	-1.16997300	2.78251800	0.90235700
H	-0.79225500	3.23898600	-0.75283300
H	-2.55712700	1.77607700	-1.61969300
H	-2.44812000	0.80074700	1.24804400
C	4.11213300	-0.63459700	-0.56610500
O	5.21066300	-1.10905600	-0.68202100
O	0.33450700	-2.33052200	-0.69191200
H	1.17519500	-2.80137500	-0.77681900
C	4.52864200	1.88609800	-0.94730700
H	5.59594900	1.67303500	-0.85789100
H	4.27024400	1.96094600	-2.00853700
H	4.32175400	2.84919700	-0.47441100
H	4.15672200	0.81402300	0.93022100
O	4.96799200	-0.64727300	2.16561200
H	5.73365100	-0.93183900	1.63380800
O	4.88795200	0.69676900	1.94777700

Name	**4-C16-H-OOH (water)**
Cartesian Coordinates	Frequency and Energy

C	2.65080000	-0.66193000	0.02679300
C	1.78304800	0.59399600	-0.29899500
C	0.29796400	0.16685000	-0.33270200
C	-0.09525600	-1.19153100	-0.44273500
C	0.91815500	-2.31131300	-0.56837000
C	2.30979000	-1.81144300	-0.91996400
C	-0.72412600	1.15169200	-0.32026700
C	-1.44300500	-1.57544600	-0.45802000
H	3.02228900	-2.63429400	-0.82201600
C	-2.42843200	-0.60039500	-0.38808000
C	-2.03780800	0.73105700	-0.32263600
H	-1.70463500	-2.62725200	-0.53557400
O	-3.12578300	1.60037300	-0.32238500
C	-3.89148900	-0.61996800	-0.32391700
C	2.04443500	1.61694400	0.83695300
H	1.64786100	1.19903300	1.77354200
H	1.51189300	2.54787700	0.64713000
C	3.53236900	1.92630500	1.02044600
H	3.92245300	2.43572800	0.13097800
H	3.64497800	2.63434000	1.84921000
C	4.34713800	0.67033200	1.30470700
H	4.02911400	0.25820000	2.27395300
H	5.41376300	0.91387600	1.39754700
C	4.17203000	-0.42700300	0.24023500
C	4.79863800	-1.71194500	0.80927000
H	4.91118100	-2.49217500	0.05042700
H	5.79901700	-1.48855400	1.19764500
H	4.19807500	-2.11622700	1.63280400

Zero-point correction= 0.437748 (Hartree/Particle)
Thermal correction to Energy= 0.462118
Thermal correction to Enthalpy= 0.463062
Thermal correction to Gibbs Free Energy= 0.384826
Sum of electronic and zero-point Energies= -1153.530847
Sum of electronic and thermal Energies= -1153.506477
Sum of electronic and thermal Enthalpies= -1153.505533
Sum of electronic and thermal Free Energies= -1153.583769

C	4.94354500	-0.07594900	-1.04123800
H	6.01883200	-0.18449800	-0.85692600
H	4.67854900	-0.75339800	-1.86125400
H	4.77404500	0.94765300	-1.37950300
C	2.08521500	1.24184400	-1.67057900
H	2.17323200	0.49279000	-2.46255300
H	1.27608000	1.92239600	-1.94849500
H	3.00532600	1.82691000	-1.65458500
H	0.96665700	-2.84966700	0.38776500
H	0.55176100	-3.02765300	-1.31086300
H	2.34381400	-1.48492600	-1.96557300
H	2.29622800	-0.97878900	1.02338500
C	-4.26385900	0.82786300	-0.42731400
O	-5.35030300	1.34127500	-0.53994100
O	-0.44187500	2.48841700	-0.33442800
H	-1.26832200	2.99420100	-0.37124400
C	-4.74979500	-1.63705500	-1.03254900
H	-5.80046900	-1.50162200	-0.76681000
H	-4.64445900	-1.52912100	-2.11688400
H	-4.44180000	-2.64627100	-0.75083700
H	-4.10403200	-0.78429200	0.91072200
O	-2.82769400	-0.70590300	2.57339700
H	-2.71466600	0.25678000	2.68600300
O	-4.12970900	-0.86772300	2.21032900

Name	**4-C16-H-OOH (pentyl ethanoate)**
Cartesian Coordinates	Frequency and Energy

C	-2.80889900	0.64010800	0.21722200
C	-1.91935800	-0.52837800	-0.31019100
C	-0.44427400	-0.06892100	-0.29416500
C	-0.07634100	1.29673900	-0.19841600
C	-1.11405200	2.39991700	-0.13157300
C	-2.50254900	1.93192800	-0.53958300
C	0.59445500	-1.02047200	-0.45152600
C	1.26470700	1.70504200	-0.17850900
H	-3.22828600	2.71507500	-0.30498100
C	2.26864700	0.75185700	-0.27178900
C	1.90112500	-0.57908500	-0.41126100
H	1.50330300	2.76248800	-0.10083800
O	2.98798500	-1.42088200	-0.57999900
C	3.73653900	0.78732500	-0.29508400
C	-2.14204300	-1.72418900	0.65150700
H	-1.74467200	-1.44985400	1.63954700
H	-1.58496700	-2.59695300	0.31225500
C	-3.62036100	-2.09485300	0.79461600
H	-4.00860000	-2.46934500	-0.16058600
H	-3.70862600	-2.92732500	1.50211200
C	-4.46105900	-0.91975400	1.28146900
H	-4.14434700	-0.66295600	2.30347600
H	-5.52084400	-1.20153400	1.34133500
C	-4.32304200	0.34054100	0.40781900
C	-4.96461600	1.50336600	1.18598800
H	-5.10940000	2.39241800	0.56442200
H	-5.95264800	1.19939500	1.55083800
H	-4.35783400	1.78651500	2.05446400

Zero-point correction= 0.438737 (Hartree/Particle)
Thermal correction to Energy= 0.462945
Thermal correction to Enthalpy= 0.463889
Thermal correction to Gibbs Free Energy= 0.386121
Sum of electronic and zero-point Energies= -1153.535316
Sum of electronic and thermal Energies= -1153.511108
Sum of electronic and thermal Enthalpies= -1153.510164
Sum of electronic and thermal Free Energies= -1153.587932

C	-5.11113200	0.18577700	-0.90308800
H	-6.18441000	0.26379400	-0.69276800
H	-4.85797200	0.97767100	-1.61758000
H	-4.94929100	-0.77553300	-1.39375500
C	-2.22323600	-0.96046300	-1.76280600
H	-2.26379800	-0.10390300	-2.44186400
H	-1.43683300	-1.63070600	-2.12004000
H	-3.16629700	-1.50101100	-1.84385700
H	-1.15749500	2.78100000	0.89800100
H	-0.77702500	3.23295800	-0.75776500
H	-2.54653200	1.77379600	-1.62332900
H	-2.44721200	0.80360700	1.24771400
C	4.11912200	-0.63846500	-0.58167200
O	5.21346100	-1.11493900	-0.73161600
O	0.33830200	-2.33901700	-0.67552300
H	1.17375900	-2.82019100	-0.76828700
C	4.52155600	1.88451600	-0.97368500
H	5.59450900	1.70603500	-0.87133100
H	4.27168300	1.92467900	-2.03925800
H	4.28295700	2.85281400	-0.52668900
H	4.15125200	0.81897900	0.91136100
O	4.92738100	-0.63079800	2.20766600
H	5.76353800	-0.87435500	1.76821600
O	4.81224100	0.71403800	1.99916600

Name			**5-O12-H-OOH (gas phase)**
Cartesian Coordinates			Frequency and Energy
C	-1.96874300	0.30555300	0.35252400
C	-1.12247500	-0.50806400	-0.67521500
C	0.33632600	-0.06583300	-0.51452200
C	0.65739200	1.27940000	-0.20500200
C	-0.41358300	2.29132800	0.04321900
C	-1.84612000	1.80557500	0.07814400
H	1.23845000	-1.98244400	-0.97485900
C	1.39189800	-0.93818400	-0.72570900
C	1.98762300	1.71069900	-0.11932400
H	-2.35885700	2.40895300	0.83147800
C	3.05110100	0.85014500	-0.33404400
C	2.73931500	-0.50711100	-0.65137300
H	2.16344300	2.75564300	0.12038100
O	3.69707900	-1.36809200	-0.90958000
H	4.31222300	-1.55260700	0.02457200
C	4.48265000	1.28184200	-0.25142300
H	4.97615200	0.81329900	0.60698300
H	5.02899600	0.97083000	-1.14657300
H	4.55318100	2.36563600	-0.14482500
O	-0.14405200	3.46545600	0.21377000
C	-1.27079800	-2.01282700	-0.37422700
H	-0.76375300	-2.23523900	0.57563700
H	-0.76657300	-2.59865600	-1.15061300
C	-2.72825200	-2.45814700	-0.26708500
H	-3.23672000	-2.33780400	-1.23133400
H	-2.76223100	-3.52852000	-0.03816700
C	-3.45375900	-1.67222000	0.82033500
H	-2.96900800	-1.88085200	1.78577200

Zero-point correction= 0.398400 (Hartree/Particle)
Thermal correction to Energy= 0.420218
Thermal correction to Enthalpy= 0.421162
Thermal correction to Gibbs Free Energy= 0.347954
Sum of electronic and zero-point Energies= -1000.962147
Sum of electronic and thermal Energies= -1000.940329
Sum of electronic and thermal Enthalpies= -1000.939385
Sum of electronic and thermal Free Energies= -1001.012593

H	-4.49401500	-2.00901900	0.91294500
C	-3.44009100	-0.15079000	0.58614800
C	-3.97017100	0.51944700	1.86574400
H	-4.14816200	1.59032800	1.73038600
H	-4.92509200	0.06535700	2.15180000
H	-3.27323000	0.38971200	2.70123300
C	-4.40750600	0.21501200	-0.55152100
H	-5.43145700	-0.01652800	-0.23817300
H	-4.37415900	1.28414700	-0.78305600
H	-4.22034700	-0.33587100	-1.47446500
C	-1.48330900	-0.24879200	-2.15545100
H	-1.41186800	0.81009500	-2.41890700
H	-0.77478800	-0.78807000	-2.79205900
H	-2.48665700	-0.59472700	-2.40641500
H	-2.29588900	2.06886600	-0.88726400
H	-1.47021900	0.11797400	1.31880300
O	3.74986700	-0.92694200	1.87864000
H	3.09354000	-1.54939400	2.23434700
O	4.64061400	-1.72208500	1.21280400

Name			**5-O12-H-OOH (water)**
Cartesian Coordinates			Frequency and Energy
C	-1.93757000	0.30110700	0.35365700
C	-1.09167000	-0.48021800	-0.69685200
C	0.36203500	-0.02985700	-0.52906600
C	0.67742500	1.30871900	-0.18019100
C	-0.40573000	2.29814300	0.07840000
C	-1.82594800	1.80741100	0.11590000
H	1.26734600	-1.92781900	-1.04355200
C	1.42266800	-0.89110500	-0.76467300
C	2.00595000	1.74200200	-0.06207800
H	-2.33972900	2.38732400	0.88734600
C	3.07247600	0.88929900	-0.29082400
C	2.76329300	-0.45342100	-0.66330300
H	2.19588100	2.77306400	0.22097300
O	3.74470900	-1.30076700	-0.93603200
H	4.23354400	-1.60751300	0.03413900
C	4.50019000	1.31434000	-0.15938500
H	5.01598600	0.70230500	0.58914600
H	5.03303900	1.17837400	-1.10608300
H	4.56373300	2.36271200	0.13645100
O	-0.14430100	3.48561800	0.25143900
C	-1.22424600	-1.99239500	-0.42884700
H	-0.71579300	-2.23026000	0.51622800
H	-0.71679000	-2.55398100	-1.22051200
C	-2.67884000	-2.44835600	-0.33069600
H	-3.18798800	-2.30729900	-1.29185400
H	-2.70307500	-3.52353800	-0.12325200
C	-3.40901000	-1.69208000	0.77439300
H	-2.92034700	-1.91637300	1.73412300
H	-4.44821900	-2.03476000	0.85793500
C	-3.40623800	-0.16645900	0.57280600
C	-3.94079300	0.47350400	1.86465100
H	-4.12720600	1.54595000	1.74959400
H	-4.89232300	0.00419900	2.13900400

Zero-point correction= 0.397225 (Hartree/Particle)
Thermal correction to Energy= 0.418966
Thermal correction to Enthalpy= 0.419910
Thermal correction to Gibbs Free Energy= 0.347009
Sum of electronic and zero-point Energies= -1000.983719
Sum of electronic and thermal Energies= -1000.961978
Sum of electronic and thermal Enthalpies= -1000.961034
Sum of electronic and thermal Free Energies= -1001.033935

H	-3.24103000	0.33203200	2.69630000
C	-4.37275500	0.21677700	-0.55865000
H	-5.39631000	-0.01652100	-0.24333500
H	-4.33546800	1.28898000	-0.77745800
H	-4.18830700	-0.32585300	-1.48750200
C	-1.45691000	-0.18904600	-2.16911200
H	-1.40133400	0.87746900	-2.40691100
H	-0.74374000	-0.70860200	-2.81778700
H	-2.45630200	-0.54424100	-2.42320700
H	-2.27722400	2.09366200	-0.84315100
H	-1.43940900	0.09189900	1.31449500
O	3.47115100	-1.12002100	1.85913500
H	2.71851400	-1.73576500	1.95327300
O	4.45051500	-1.84678200	1.25030800

Name	**5-O12-H-OOH (pentyl ethanoate)**
Cartesian Coordinates	Frequency and Energy

C	-1.95885200	0.30195600	0.35460700	Zero-point correction= 0.397760 (Hartree/Particle)
C	-1.11337000	-0.49580400	-0.68560500	Thermal correction to Energy= 0.419625
C	0.34311600	-0.04769900	-0.52417700	Thermal correction to Enthalpy= 0.420569
C	0.66098100	1.29467800	-0.19635300	Thermal correction to Gibbs Free Energy= 0.346753
C	-0.41677000	2.29675700	0.06274500	Sum of electronic and zero-point Energies= -1000.988134
C	-1.84312100	1.80561100	0.09820600	Sum of electronic and thermal Energies= -1000.966270
H	1.24541700	-1.95535100	-1.01007100	Sum of electronic and thermal Enthalpies= -1000.965326
C	1.40202500	-0.91452000	-0.74727300	Sum of electronic and thermal Free Energies= -1001.039141
C	1.99068800	1.72744600	-0.09906500	
H	-2.35795500	2.39513500	0.86142600	
C	3.05647500	0.87122100	-0.32066500	
C	2.74658000	-0.48091000	-0.65991400	
H	2.17264000	2.76702400	0.15826300	
O	3.71316700	-1.33505100	-0.92618700	
H	4.28107500	-1.56696800	0.01684800	
C	4.48553800	1.30428500	-0.22153900	
H	5.00159400	0.76083600	0.57774800	
H	5.02067600	1.09040400	-1.15230300	
H	4.55063200	2.37360900	-0.01194200	
O	-0.14924500	3.47418900	0.23869200	
C	-1.25168500	-2.00468500	-0.40007500	
H	-0.74144400	-2.23515800	0.54621500	
H	-0.74777200	-2.57842400	-1.18565800	
C	-2.70682600	-2.45721600	-0.29308300	
H	-3.21778400	-2.32951000	-1.25526600	
H	-2.73314000	-3.52992300	-0.07231300	
C	-3.43435500	-1.68551300	0.80309600	
H	-2.94722300	-1.90072000	1.76597900	
H	-4.47367600	-2.02694400	0.89176700	
C	-3.42862900	-0.16185400	0.58329700	
C	-3.96151600	0.49442900	1.86825800	
H	-4.15432600	1.56429800	1.74025000	
H	-4.91008400	0.02626700	2.15499600	
H	-3.26003900	0.36914000	2.70137700	
C	-4.39695700	0.20884800	-0.55111800	
H	-5.42118100	-0.02071200	-0.23494400	
H	-4.36199800	1.27857900	-0.78217000	
H	-4.21379900	-0.34255300	-1.47502700	

C	-1.48012400	-0.22249700	-2.16119900
H	-1.42774200	0.84102800	-2.41301200
H	-0.76634600	-0.74498300	-2.80697500
H	-2.47861600	-0.58247800	-2.41300100
H	-2.29484200	2.07931700	-0.86390200
H	-1.45973700	0.10424600	1.31794400
O	3.67931400	-1.00313300	1.88364700
H	2.97367900	-1.61726000	2.16003000
O	4.57711400	-1.78926600	1.21920700

Name	**6-O12-H-OOH (gas phase)**
Cartesian Coordinates	Frequency and Energy

C	-2.00911100	0.48262700	0.29681900
C	-1.10513600	-0.44292000	-0.57236600
C	0.34673200	0.04642000	-0.44447200
C	0.65403900	1.39741300	-0.13041200
C	-0.41995100	2.40658500	0.20850100
C	-1.83245800	1.94120300	-0.13226000
H	1.22935300	-1.86606500	-0.95491200
C	1.39786600	-0.82451700	-0.70363500
C	1.98140900	1.83108100	-0.08651700
H	-2.55015000	2.59110500	0.37584800
C	3.01854400	0.95386600	-0.35680000
C	2.73519600	-0.40155200	-0.67292100
H	2.21550600	2.86401100	0.15616300
O	3.75485900	-1.20352100	-0.94792600
H	4.27156700	-1.46478000	-0.00201200
C	-1.24062600	-1.88772300	-0.04476200
H	-0.78659800	-1.94184500	0.95458000
H	-0.68239000	-2.57821900	-0.68556500
C	-2.69533300	-2.35120200	0.03901200
H	-3.13573100	-2.40255900	-0.96420600
H	-2.72617800	-3.37201800	0.43479600
C	-3.51663300	-1.42785100	0.93363100
H	-3.11618700	-1.48690300	1.95664000
H	-4.55926100	-1.76745200	0.98526200
C	-3.49041700	0.04641700	0.48908100
C	-4.10867800	0.87669000	1.62845300
H	-4.30522500	1.91099200	1.33090100
H	-5.06747800	0.43771700	1.92552400
H	-3.45793600	0.88964300	2.51017400
C	-4.37677100	0.24949300	-0.75116000
H	-5.42960500	0.15467800	-0.46274300
H	-4.24252200	1.24794100	-1.18082100
H	-4.19230800	-0.48344100	-1.53801600
C	-1.42555500	-0.42920400	-2.08432900
H	-1.36018600	0.57537800	-2.51004600
H	-0.68875500	-1.04762300	-2.60706600
H	-2.41367600	-0.83071900	-2.30971700
H	-2.01987000	2.05194800	-1.20547900
H	-1.57555800	0.40388400	1.30995700
O	4.30662700	1.35440100	-0.27579900
H	4.86193900	0.64279800	-0.63728500
H	-0.36453400	2.59809700	1.28968400
H	-0.18792600	3.35846200	-0.28192600

Zero-point correction= 0.394961 (Hartree/Particle)
Thermal correction to Energy= 0.415330
Thermal correction to Enthalpy= 0.416274
Thermal correction to Gibbs Free Energy= 0.346558
Sum of electronic and zero-point Energies= -962.873505
Sum of electronic and thermal Energies= -962.853136
Sum of electronic and thermal Enthalpies= -962.852192
Sum of electronic and thermal Free Energies= -962.921907

O	3.77908200	-0.69096900	1.84521700		
H	4.12381400	0.22086400	1.86686700		
O	4.74458000	-1.39826600	1.19703600		
Name				**6-O12-H-OOH (water)**	
Cartesian Coordinates				Frequency and Energy	
C	-1.98673000	0.46840900	0.32021500	Zero-point correction=	0.393242 (Hartree/Particle)
C	-1.07981700	-0.39965500	-0.60310500	Thermal correction to Energy=	0.413795
C	0.36773100	0.09018800	-0.44845900	Thermal correction to Enthalpy=	0.414739
C	0.66393600	1.43114400	-0.07683400	Thermal correction to Gibbs Free Energy=	0.344765
C	-0.41643200	2.41179700	0.31442000	Sum of electronic and zero-point Energies=	-962.893320
C	-1.82833100	1.94935700	-0.03124700	Sum of electronic and thermal Energies=	-962.872767
H	1.26465300	-1.79095800	-1.03791800	Sum of electronic and thermal Enthalpies=	-962.871823
C	1.42798700	-0.75979300	-0.74118600	Sum of electronic and thermal Free Energies=	-962.941797
C	1.98741800	1.87425200	-0.02161000		
H	-2.54294500	2.56239900	0.52454100		
C	3.03567600	1.01812300	-0.32393000		
C	2.75948900	-0.32537600	-0.68247000		
H	2.20871200	2.89976400	0.26211800		
O	3.79071900	-1.13119500	-0.98767500		
H	4.25446000	-1.44825100	-0.08119400		
C	-1.20595900	-1.87522000	-0.16901700		
H	-0.75923900	-1.98891200	0.82905100		
H	-0.64027400	-2.51819700	-0.85129800		
C	-2.65853600	-2.34851200	-0.11933100		
H	-3.09708700	-2.32691400	-1.12452200		
H	-2.68539400	-3.39447600	0.20541900		
C	-3.48053000	-1.49119400	0.83774900		
H	-3.07341800	-1.61453200	1.85242300		
H	-4.52223100	-1.83649900	0.86945000		
C	-3.46335100	0.00847600	0.49041400		
C	-4.07892300	0.75973000	1.68329900		
H	-4.27332500	1.81250000	1.45602400		
H	-5.03783200	0.30092900	1.95054200		
H	-3.42466700	0.71248400	2.56161200		
C	-4.35792800	0.28418700	-0.72885100		
H	-5.40835000	0.16844600	-0.43704100		
H	-4.22906300	1.30776600	-1.09752100		
H	-4.17777200	-0.40073900	-1.55963700		
C	-1.39891500	-0.29174200	-2.11095700		
H	-1.31825300	0.73645000	-2.47451400		
H	-0.67262000	-0.89363200	-2.66820300		
H	-2.39389000	-0.66354200	-2.35803200		
H	-2.03342400	2.11592200	-1.09387200		
H	-1.55041800	0.33803100	1.32643100		
O	4.31656600	1.45276600	-0.25574000		
H	4.90828100	0.74380400	-0.56189600		
H	-0.34777500	2.55241400	1.40228100		
H	-0.19426300	3.38632800	-0.13319500		
O	3.58134500	-0.89993900	1.83511200		
H	3.96686700	-0.01795500	2.00607900		
O	4.56869100	-1.61759000	1.24558600		
Name				**6-O12-H-OOH (pentyl ethanoate)**	
Cartesian Coordinates				Frequency and Energy	
C	-2.00716700	0.47895100	0.30579900	Zero-point correction=	0.394159 (Hartree/Particle)

C	-1.10266800	-0.43613600	-0.57419000	Thermal correction to Energy= 0.414603
C	0.34895400	0.05218900	-0.44108800	Thermal correction to Enthalpy= 0.415547
C	0.65533600	1.40263700	-0.11731700	Thermal correction to Gibbs Free Energy= 0.345831
C	-0.41844600	2.40587200	0.23481800	Sum of electronic and zero-point Energies= -962.896524
C	-1.83177000	1.94277100	-0.10480800	Sum of electronic and thermal Energies= -962.876081
H	1.23036800	-1.85588100	-0.96590500	Sum of electronic and thermal Enthalpies= -962.875137
C	1.40154000	-0.81581600	-0.70792900	Sum of electronic and thermal Free Energies= -962.944852
C	1.98250300	1.83865700	-0.07847500	
H	-2.54571400	2.58534600	0.41772200	
C	3.02072000	0.96501600	-0.35936900	
C	2.73678300	-0.38908500	-0.67507200	
H	2.21233700	2.87188500	0.16842000	
O	3.75969000	-1.19491500	-0.95783100	
H	4.26491800	-1.45620500	-0.03615400	
C	-1.23846200	-1.88840300	-0.06775800	
H	-0.79018900	-1.95688900	0.93361100	
H	-0.67783700	-2.56878700	-0.71746800	
C	-2.69374700	-2.35171400	0.00456400	
H	-3.13012200	-2.38640100	-1.00123200	
H	-2.72549500	-3.37835400	0.38622100	
C	-3.51763000	-1.44145400	0.91002700	
H	-3.12071300	-1.51627800	1.93353300	
H	-4.56111600	-1.78075800	0.95100300	
C	-3.48915100	0.03951300	0.48849800	
C	-4.10783500	0.85270700	1.63921000	
H	-4.30401100	1.89205200	1.35740200	
H	-5.06736100	0.40940800	1.92973600	
H	-3.45739800	0.85326800	2.52186600	
C	-4.37408800	0.26254000	-0.74894500	
H	-5.42789900	0.16764600	-0.46143300	
H	-4.23742600	1.26677600	-1.16532000	
H	-4.19394800	-0.46028000	-1.54694700	
C	-1.42103100	-0.40209300	-2.08590800	
H	-1.35689800	0.60838100	-2.49916700	
H	-0.68509700	-1.01582200	-2.61686700	
H	-2.40897800	-0.80208900	-2.31642300	
H	-2.02508400	2.06820000	-1.17544600	
H	-1.57699300	0.38684400	1.31890900	
O	4.30642200	1.37562500	-0.29358300	
H	4.86966400	0.68201900	-0.67780700	
H	-0.35668600	2.58554400	1.31767700	
H	-0.18773700	3.36252700	-0.24669200	
O	3.76579200	-0.72119200	1.85385200	
H	4.12246900	0.18752900	1.89533500	
O	4.72733500	-1.44034300	1.21794600	

Name	**6-O12-H-OOH (6-311++G(d,); pentyl ethanoate)**
Cartesian Coordinates	Frequency and Energy

C	-2.00175700	0.47826100	0.30844500	Zero-point correction= 0.393784 (Hartree/Particle)
C	-1.10085900	-0.43342300	-0.57705000	Thermal correction to Energy= 0.414221
C	0.35068700	0.05155000	-0.44245300	Thermal correction to Enthalpy= 0.415166
C	0.65776000	1.39969800	-0.11973500	Thermal correction to Gibbs Free Energy= 0.345425
C	-0.41341400	2.40353600	0.23376100	Sum of electronic and zero-point Energies= -963.119410
C	-1.82821400	1.94223100	-0.09912500	Sum of electronic and thermal Energies= -963.098973
H	1.22943000	-1.85372800	-0.96433900	Sum of electronic and thermal Enthalpies= -963.098029

C	1.40051300	-0.81555800	-0.70702300	Sum of electronic and thermal Free Energies= -963.167770
C	1.98298400	1.83340500	-0.08223600	
H	-2.53681200	2.58221000	0.42920300	
C	3.01946300	0.96101400	-0.36038900	
C	2.73455100	-0.39146500	-0.67567700	
H	2.21361300	2.86479600	0.16362600	
O	3.75284100	-1.19878000	-0.95561200	
H	4.26512700	-1.44453300	-0.03523100	
C	-1.23771200	-1.88725800	-0.07840800	
H	-0.78934700	-1.96052300	0.92007000	
H	-0.68090000	-2.56341800	-0.73187100	
C	-2.69314200	-2.34795400	-0.00685200	
H	-3.13016500	-2.37575100	-1.00996700	
H	-2.72563300	-3.37478000	0.36841700	
C	-3.51250200	-1.44227600	0.90606000	
H	-3.11275500	-1.52185900	1.92558600	
H	-4.55435900	-1.77914800	0.94783700	
C	-3.48302100	0.03936000	0.49062600	
C	-4.09856600	0.84823800	1.64515200	
H	-4.29824900	1.88552900	1.36594200	
H	-5.05414700	0.40211500	1.93723800	
H	-3.44555900	0.84794500	2.52342000	
C	-4.36989200	0.26705400	-0.74357100	
H	-5.42126500	0.18133000	-0.45117400	
H	-4.22753600	1.26772700	-1.16140000	
H	-4.19985500	-0.45846700	-1.53850300	
C	-1.41740100	-0.38954000	-2.08783000	
H	-1.33946200	0.62001100	-2.49578700	
H	-0.68826700	-1.00861000	-2.61841600	
H	-2.40763200	-0.77658400	-2.32073500	
H	-2.02751400	2.07020300	-1.16580500	
H	-1.57014900	0.38224500	1.31766700	
O	4.30304000	1.37279800	-0.29627400	
H	4.86566800	0.67667900	-0.66837200	
H	-0.34593800	2.58372700	1.31420800	
H	-0.18274200	3.35719600	-0.24917200	
O	3.74353900	-0.73862400	1.86477600	
H	4.07263200	0.17550300	1.92947500	
O	4.71994900	-1.42052500	1.21784800	

Name	**6-O13-H-OOH (gas phase)**
Cartesian Coordinates	Frequency and Energy

C	-2.00003300	0.54955400	0.22814000	Zero-point correction= 0.395023 (Hartree/Particle)
C	-1.15388300	-0.54687000	-0.48729900	Thermal correction to Energy= 0.415400
C	0.32164000	-0.12107100	-0.45000300	Thermal correction to Enthalpy= 0.416344
C	0.70011700	1.24504100	-0.34248200	Thermal correction to Gibbs Free Energy= 0.346630
C	-0.31666700	2.35127400	-0.15150800	Sum of electronic and zero-point Energies= -962.873070
C	-1.75236200	1.91266400	-0.42252100	Sum of electronic and thermal Energies= -962.852694
H	1.07330100	-2.14375600	-0.69914300	Sum of electronic and thermal Enthalpies= -962.851749
C	1.31708000	-1.09198400	-0.59929200	Sum of electronic and thermal Free Energies= -962.921463
C	2.04348500	1.58978600	-0.37100000	
H	-2.43510600	2.66813600	-0.02418900	
C	3.04679300	0.62331700	-0.52509900	
C	2.65731500	-0.73779700	-0.63968000	
H	2.35298400	2.62769200	-0.28150600	

O	3.61441800	-1.68731200	-0.73994100
H	4.46368100	-1.23897400	-0.89157900
C	-1.35796600	-1.88243000	0.26154200
H	-0.89862100	-1.80180000	1.25683100
H	-0.84331700	-2.69416800	-0.26295500
C	-2.83384600	-2.25006900	0.41975700
H	-3.28539200	-2.43465800	-0.56259300
H	-2.91291400	-3.19366900	0.97034500
C	-3.59789700	-1.15658600	1.15966500
H	-3.19160200	-1.07554400	2.17886000
H	-4.65594500	-1.42942200	1.26491500
C	-3.49984800	0.22603000	0.48879000
C	-4.06315500	1.25603800	1.48459300
H	-4.21180900	2.23870500	1.02747600
H	-5.03894800	0.91844600	1.85083200
H	-3.40229700	1.37570000	2.35056300
C	-4.38726700	0.27791900	-0.76637200
H	-5.44040800	0.29372500	-0.46438400
H	-4.20002100	1.18356800	-1.35307000
H	-4.25559800	-0.58275300	-1.42401200
C	-1.49053400	-0.75339400	-1.98261200
H	-1.37337300	0.16634200	-2.56098900
H	-0.79942600	-1.48987500	-2.40493200
H	-2.50384800	-1.12484300	-2.13500900
H	-1.93845300	1.86403400	-1.50070900
H	-1.56122900	0.60692000	1.24040900
O	4.33897800	0.91140500	-0.58662500
H	4.81720500	0.61650700	0.37180100
H	-0.24688600	2.69778800	0.88883600
H	-0.04250600	3.20544200	-0.77974800
O	3.83994000	-0.33434300	1.91706300
H	3.72648900	-1.26538400	1.65051200
O	5.08244100	-0.00683700	1.46771900

Name	**6-O13-H-OOH (water)**
Cartesian Coordinates	Frequency and Energy

C	-1.98964600	0.56829800	0.19780800
C	-1.15670900	-0.57818300	-0.44946300
C	0.32208500	-0.16594900	-0.44734400
C	0.71666000	1.20120700	-0.40004900
C	-0.28641100	2.32601500	-0.26379700
C	-1.72312900	1.88879600	-0.52820500
H	1.04373300	-2.20400300	-0.63451800
C	1.30478400	-1.15294000	-0.56971300
C	2.06545200	1.52562100	-0.45044500
H	-2.40034600	2.67300500	-0.17949100
C	3.05202800	0.53912900	-0.56683700
C	2.65137600	-0.81994400	-0.63383200
H	2.38361300	2.56442200	-0.40816000
O	3.58415300	-1.79580600	-0.74626800
H	4.46040200	-1.38860500	-0.85917200
C	-1.36615100	-1.86141500	0.38443900
H	-0.91053200	-1.71580700	1.37413100
H	-0.85469300	-2.70671700	-0.08685000
C	-2.84510100	-2.20654900	0.56313000

Zero-point correction= 0.393560 (Hartree/Particle)
Thermal correction to Energy= 0.413959
Thermal correction to Enthalpy= 0.414903
Thermal correction to Gibbs Free Energy= 0.345611
Sum of electronic and zero-point Energies= -962.892605
Sum of electronic and thermal Energies= -962.872206
Sum of electronic and thermal Enthalpies= -962.871261
Sum of electronic and thermal Free Energies= -962.940553

H	-3.29564800	-2.44912400	-0.40704800
H	-2.93024900	-3.11060800	1.17604600
C	-3.60364600	-1.06153100	1.22708900
H	-3.19903800	-0.91532700	2.23970200
H	-4.66490200	-1.31785100	1.34297000
C	-3.49251000	0.27315100	0.46790100
C	-4.05312400	1.37027100	1.38878800
H	-4.18662800	2.32223700	0.86571900
H	-5.03549400	1.06474900	1.76692300
H	-3.39619600	1.53987300	2.24991800
C	-4.37060600	0.24835400	-0.79370800
H	-5.42499800	0.30901600	-0.49975300
H	-4.15953800	1.10348000	-1.44558700
H	-4.25267200	-0.66353900	-1.38205800
C	-1.50149600	-0.87684500	-1.92656700
H	-1.39457900	0.00787500	-2.56015500
H	-0.81241900	-1.63900600	-2.30564600
H	-2.51440800	-1.26170200	-2.04597000
H	-1.89571500	1.77970600	-1.60430800
H	-1.55681300	0.67851400	1.20794000
O	4.35976800	0.82893900	-0.65359300
H	4.82390800	0.60043300	0.28210900
H	-0.22122300	2.71451400	0.76163500
H	0.00658500	3.14798700	-0.92516100
O	3.79483400	-0.12144300	1.96970900
H	3.69572600	-1.08597500	1.84477600
O	5.05486800	0.16925300	1.55975800

Name			**6-O13-H-OOH (pentyl ethanoate)**
Cartesian Coordinates			Frequency and Energy
C	-1.99614600	0.55466200	0.22357400
C	-1.15429000	-0.55344200	-0.47859800
C	0.32204500	-0.13017500	-0.45296700
C	0.70438400	1.23742800	-0.35740700
C	-0.30912700	2.34757700	-0.17772700
C	-1.74534000	1.90879500	-0.44400400
H	1.06424600	-2.15574600	-0.69538100
C	1.31471400	-1.10466600	-0.60022500
C	2.04962100	1.57760400	-0.39122400
H	-2.42493600	2.67100400	-0.05311600
C	3.04721400	0.60547500	-0.53660100
C	2.65659600	-0.75453800	-0.64710400
H	2.35865800	2.61686800	-0.31008900
O	3.60756600	-1.70857600	-0.75725700
H	4.45931000	-1.27394000	-0.93471700
C	-1.35735400	-1.87898600	0.28863400
H	-0.89748400	-1.78535800	1.28273500
H	-0.84561400	-2.69808200	-0.22740000
C	-2.83391500	-2.24062100	0.45450700
H	-3.28666000	-2.43669700	-0.52519500
H	-2.91270200	-3.17585800	1.02002700
C	-3.59639300	-1.13542200	1.17853100
H	-3.18987400	-1.03857300	2.19639900
H	-4.65528000	-1.40532000	1.28597000

Zero-point correction= 0.394318 (Hartree/Particle)
Thermal correction to Energy= 0.414692
Thermal correction to Enthalpy= 0.415636
Thermal correction to Gibbs Free Energy= 0.346164
Sum of electronic and zero-point Energies= -962.896011
Sum of electronic and thermal Energies= -962.875636
Sum of electronic and thermal Enthalpies= -962.874692
Sum of electronic and thermal Free Energies= -962.944165

C	-3.49674400	0.23623600	0.48588900
C	-4.06072200	1.28343500	1.46209600
H	-4.20981400	2.25800000	0.98675800
H	-5.03677300	0.95179300	1.83485500
H	-3.39972200	1.42058800	2.32605200
C	-4.38089500	0.26625100	-0.77184300
H	-5.43495200	0.30359400	-0.47254900
H	-4.18185400	1.15325800	-1.38364000
H	-4.25922100	-0.61472800	-1.40497100
C	-1.49681900	-0.77928100	-1.96923700
H	-1.39180300	0.13503400	-2.55956000
H	-0.80487500	-1.51796000	-2.38786300
H	-2.50853900	-1.16065300	-2.10964200
H	-1.93061700	1.84758000	-1.52174200
H	-1.55958100	0.62315900	1.23584000
O	4.34558900	0.89383200	-0.59973800
H	4.80924800	0.61726600	0.34171200
H	-0.23720500	2.70401400	0.85911600
H	-0.03125400	3.19404300	-0.81480600
O	3.82343200	-0.29979300	1.93601600
H	3.72602400	-1.24249700	1.69842100
O	5.07095200	0.03544000	1.51285700

Name			**6-O13-H-OOH (6-311++G(d,); pentyl ethanoate)**
Cartesian Coordinates			Frequency and Energy
C	-1.99121400	0.55364100	0.22562100
C	-1.15099000	-0.55136400	-0.48126400
C	0.32425300	-0.12864600	-0.45426300
C	0.70533500	1.23702600	-0.35868400
C	-0.30735800	2.34672200	-0.17917000
C	-1.74396500	1.90834100	-0.44010700
H	1.06696200	-2.14977700	-0.69619600
C	1.31592800	-1.10040500	-0.60090200
C	2.04761700	1.57640200	-0.39080700
H	-2.42002400	2.66799500	-0.04433000
C	3.04517600	0.60741800	-0.53647700
C	2.65555700	-0.75139500	-0.64718000
H	2.35591800	2.61389800	-0.30880600
O	3.60382400	-1.70550400	-0.75916200
H	4.45570700	-1.27283200	-0.92238300
C	-1.35308700	-1.87934400	0.28021100
H	-0.89378600	-1.78902600	1.27235200
H	-0.84351300	-2.69447100	-0.23932800
C	-2.82911300	-2.24087600	0.44512200
H	-3.28156600	-2.43235000	-0.53293300
H	-2.90715700	-3.17658700	1.00604300
C	-3.58947300	-1.13925100	1.17530200
H	-3.18113400	-1.04604000	2.19025700
H	-4.64619200	-1.40838800	1.28282900
C	-3.49066000	0.23363300	0.48715000
C	-4.05344700	1.27716400	1.46693000
H	-4.20715500	2.24983500	0.99375900
H	-5.02537900	0.94188200	1.84161600
H	-3.39047700	1.41404600	2.32688600
C	-4.37603000	0.26700700	-0.76868700

Zero-point correction= 0.393851 (Hartree/Particle)
Thermal correction to Energy= 0.414248
Thermal correction to Enthalpy= 0.415192
Thermal correction to Gibbs Free Energy= 0.345672
Sum of electronic and zero-point Energies= -963.118960
Sum of electronic and thermal Energies= -963.098564
Sum of electronic and thermal Enthalpies= -963.097620
Sum of electronic and thermal Free Energies= -963.167140

H	-5.42718500	0.31220300	-0.46685800
H	-4.17294700	1.15024100	-1.38108400
H	-4.26281400	-0.61495400	-1.39841700
C	-1.49090600	-0.77035300	-1.97248200
H	-1.37505800	0.14294100	-2.55870900
H	-0.80395500	-1.51233100	-2.38897700
H	-2.50318000	-1.14277600	-2.11655000
H	-1.93417800	1.84920200	-1.51457700
H	-1.55386900	0.61907700	1.23484000
O	4.33990500	0.89786400	-0.59493500
H	4.80251200	0.60049400	0.33912000
H	-0.23122700	2.70381300	0.85496800
H	-0.03056500	3.18971300	-0.81781300
O	3.80702500	-0.28693600	1.95031500
H	3.67664700	-1.22599000	1.72835900
O	5.05273100	0.01156000	1.50554100

Name			**7-O12-H-OOH (gas phase)**
Cartesian Coordinates			Frequency and Energy
C	-4.91656400	-1.69360600	0.06634700
C	-5.03035700	-0.14856600	0.23490200
C	-3.67830200	0.47769200	-0.14162800
C	-2.46489300	-0.25117300	-0.04462400
C	-2.43392300	-1.71390300	0.33456500
C	-3.75251200	-2.22924300	0.90372600
H	-4.49556100	2.44256200	-0.54878600
C	-3.61111300	1.81662500	-0.50090600
C	-1.24038500	0.36128600	-0.33889800
H	-3.73458200	-3.32248400	0.89993200
C	-1.19430400	1.68522400	-0.74398600
C	-2.39580300	2.45242900	-0.81289300
H	-0.32416700	-0.21632800	-0.26078100
O	-2.34612600	3.71818100	-1.15686500
H	-1.70144200	4.23474300	-0.44832600
C	-6.14345300	0.36024100	-0.70654500
H	-5.81265800	0.22768200	-1.74627200
H	-6.30361100	1.43321800	-0.55830200
C	-7.46773900	-0.37697700	-0.50423000
H	-7.86574000	-0.17345100	0.49733100
H	-8.20958500	0.01385800	-1.20890800
C	-7.29993400	-1.87889000	-0.71485800
H	-7.01085400	-2.05399700	-1.76189100
H	-8.25474400	-2.39870400	-0.56257800
C	-6.23157700	-2.51551300	0.19381200
C	-5.97901100	-3.94098900	-0.32945000
H	-5.37610500	-4.53741500	0.36167100
H	-6.93468500	-4.46128000	-0.45690500
H	-5.47323300	-3.92478500	-1.30155900
C	-6.75944800	-2.64802000	1.63212800
H	-7.52557400	-3.43067300	1.66540700
H	-5.96369700	-2.93763400	2.32671500
H	-7.21883900	-1.73298600	2.00882000
C	-5.33076600	0.32894700	1.67388200
H	-4.58267600	-0.02327600	2.38870900
H	-5.30514800	1.42305300	1.69710200

Zero-point correction= 0.735095 (Hartree/Particle)
Thermal correction to Energy= 0.772081
Thermal correction to Enthalpy= 0.773026
Thermal correction to Gibbs Free Energy= 0.667439
Sum of electronic and zero-point Energies= -1772.523489
Sum of electronic and thermal Energies= -1772.486503
Sum of electronic and thermal Enthalpies= -1772.485559
Sum of electronic and thermal Free Energies= -1772.591146

H	-6.31275400	0.01301800	2.02587100
H	-3.85873900	-1.92430000	1.95016800
H	-4.62235900	-1.82614300	-0.99044800
O	-0.07060100	2.37439900	-1.08054600
H	-2.19313600	-2.28682300	-0.57246000
H	-1.60639600	-1.88832100	1.03109700
C	5.04630800	-1.30693900	-0.10060600
C	5.07247600	0.22487600	0.18960700
C	3.67134600	0.77080500	-0.12479900
C	2.98372200	0.31241300	-1.26583500
C	3.58035800	-0.74946100	-2.12256900
C	4.64451200	-1.57573600	-1.54230700
H	3.57679600	2.17926800	1.52684100
C	3.08391600	1.77084700	0.65190600
C	1.73774900	0.84222100	-1.59716000
C	1.16158100	1.81003700	-0.79160400
C	1.83563500	2.30007900	0.32686400
H	1.19974800	0.49301500	-2.47494500
O	1.28812300	3.25690500	1.11775300
H	0.64929000	3.81954400	0.62396300
C	5.43268300	0.43805600	1.67259600
H	4.58792400	0.10435500	2.29151100
H	5.57161200	1.50743400	1.87045900
C	6.68628300	-0.32470100	2.10552300
H	7.57096300	0.07453500	1.59518000
H	6.85479700	-0.15672000	3.17454600
C	6.54656800	-1.82187600	1.83418800
H	5.71193700	-2.21232800	2.43470900
H	7.44707900	-2.35841000	2.15966300
C	6.27443200	-2.14128200	0.35388900
C	5.89760600	-3.62586400	0.23021800
H	5.73990000	-3.91882000	-0.81352600
H	6.69776500	-4.25443600	0.63613000
H	4.97692800	-3.84579700	0.78097100
C	7.55489800	-1.91426900	-0.46883800
H	8.29254700	-2.67741000	-0.19746600
H	7.37919400	-2.00376500	-1.54527800
H	8.01502700	-0.94215400	-0.28833700
C	6.05581800	1.01002400	-0.70587200
H	5.93203100	0.74914800	-1.76191100
H	5.86185600	2.08238600	-0.60401400
H	7.09682000	0.83380400	-0.43127600
H	5.39030000	-1.99583700	-2.21483500
H	4.20826200	-1.68822700	0.50180400
H	3.54533500	-0.58761400	-3.19910800
O	3.33690000	-2.10692600	-1.74014000
O	-1.04393100	4.52516400	0.68366300
O	-1.52628500	3.54621100	1.51216000
H	-0.73932700	3.00826600	1.73183300

Name			**7-O12-H-OOH (water)**	
Cartesian Coordinates			Frequency and Energy	
C	-4.86551501	-1.66197044	0.13849986	Zero-point correction= 0.735095 (Hartree/Particle)
C	-4.97930801	-0.11693044	0.30705486	Thermal correction to Energy= 0.771281

C	-3.62725301	0.50932756	-0.06947514
C	-2.41384401	-0.21953744	0.02752886
C	-2.38287401	-1.68226744	0.40671786
C	-3.70146301	-2.19760744	0.97587886
H	-4.44451201	2.47419756	-0.47663314
C	-3.56006401	1.84826056	-0.42875314
C	-1.18933601	0.39292156	-0.26674514
H	-3.68353301	-3.29084844	0.97208486
C	-1.14325501	1.71685956	-0.67183314
C	-2.34475401	2.48406456	-0.74074014
H	-0.27311801	-0.18469244	-0.18862814
O	-2.29507701	3.74981656	-1.08471214
H	-1.70144200	4.23474300	-0.44832600
C	-6.09240401	0.39187656	-0.63439214
H	-5.76160901	0.25931756	-1.67411914
H	-6.25256201	1.46485356	-0.48614914
C	-7.41669001	-0.34534144	-0.43207714
H	-7.81469101	-0.14181544	0.56948386
H	-8.15853601	0.04549356	-1.13675514
C	-7.24888501	-1.84725444	-0.64270514
H	-6.95980501	-2.02236144	-1.68973814
H	-8.20369501	-2.36706844	-0.49042514
C	-6.18052801	-2.48387744	0.26596486
C	-5.92796201	-3.90935344	-0.25729714
H	-5.32505601	-4.50577944	0.43382386
H	-6.88363601	-4.42964444	-0.38475214
H	-5.42218401	-3.89314944	-1.22940614
C	-6.70839901	-2.61638444	1.70428086
H	-7.47452501	-3.39903744	1.73755986
H	-5.91264801	-2.90599844	2.39886786
H	-7.16779001	-1.70135044	2.08097286
C	-5.27971701	0.36058256	1.74603486
H	-4.53162701	0.00835956	2.46086186
H	-5.25409901	1.45468856	1.76925486
H	-6.26170501	0.04465356	2.09802386
H	-3.80769001	-1.89266444	2.02232086
H	-4.57131001	-1.79450744	-0.91829514
O	-0.01955201	2.40603456	-1.00839314
H	-2.14208701	-2.25518744	-0.50030714
H	-1.55534701	-1.85668544	1.10324986
C	5.09735699	-1.27530344	-0.02845314
C	5.12352499	0.25651156	0.26175986
C	3.72239499	0.80244056	-0.05264614
C	3.03477099	0.34404856	-1.19368214
C	3.63140699	-0.71782544	-2.05041614
C	4.69556099	-1.54410044	-1.47015414
H	3.62784499	2.21090356	1.59899386
C	3.13496499	1.80248256	0.72405886
C	1.78879799	0.87385656	-1.52500714
C	1.21262999	1.84167256	-0.71945114
C	1.88668399	2.33171456	0.39901686
H	1.25079699	0.52465056	-2.40279214
O	1.33917199	3.28854056	1.18990586
H	0.70033899	3.85117956	0.69611586
C	5.48373199	0.46969156	1.74474886

Thermal correction to Enthalpy= 0.771126
Thermal correction to Gibbs Free Energy= 0.665939
Sum of electronic and zero-point Energies= -1772.521729
Sum of electronic and thermal Energies= -1772.485967
Sum of electronic and thermal Enthalpies= -1772.483986
Sum of electronic and thermal Free Energies= -1772.599076

H	4.63897299	0.13599056	2.36366386
H	5.62266099	1.53906956	1.94261186
C	6.73733199	-0.29306544	2.17767586
H	7.62201199	0.10617056	1.66733286
H	6.90584599	-0.12508444	3.24669886
C	6.59761699	-1.79024044	1.90634086
H	5.76298599	-2.18069244	2.50686186
H	7.49812799	-2.32677444	2.23181586
C	6.32548099	-2.10964644	0.42604186
C	5.94865499	-3.59422844	0.30237086
H	5.79094899	-3.88718444	-0.74137314
H	6.74881399	-4.22280044	0.70828286
H	5.02797699	-3.81416144	0.85312386
C	7.60594699	-1.88263344	-0.39668514
H	8.34359599	-2.64577444	-0.12531314
H	7.43024299	-1.97212944	-1.47312514
H	8.06607599	-0.91051844	-0.21618414
C	6.10686699	1.04165956	-0.63371914
H	5.98307999	0.78078356	-1.68975814
H	5.91290499	2.11402156	-0.53186114
H	7.14786899	0.86543956	-0.35912314
H	5.44134899	-1.96420144	-2.14268214
H	4.25931099	-1.65659144	0.57395686
H	3.59638399	-0.55597844	-3.12695514
O	3.38794899	-2.07529044	-1.66798714
O	-1.04393100	4.52516400	0.68366300
O	-1.52628500	3.54621100	1.51216000
H	-0.73932700	3.00826600	1.73183300

Name			**7-O12-H-OOH (pentyl ethanoate)**
Cartesian Coordinates			Frequency and Energy
C	-4.93774900	-1.68825400	0.09359400
C	-5.06165800	-0.13943900	0.21297200
C	-3.69858000	0.48099800	-0.13217000
C	-2.48655700	-0.24537700	0.01361400
C	-2.46513300	-1.69508800	0.43618400
C	-3.79902600	-2.19502400	0.98176400
H	-4.50991700	2.43366000	-0.59680100
C	-3.62295800	1.81357200	-0.51724700
C	-1.25551400	0.35970900	-0.26862900
H	-3.77809100	-3.28781600	1.01002900
C	-1.20145600	1.67351500	-0.70473000
C	-2.40005500	2.43785800	-0.81011900
H	-0.34283900	-0.21772600	-0.15590000
O	-2.33989100	3.70380500	-1.18456500
H	-1.69236500	4.21233500	-0.51571900
C	-6.14017400	0.33847100	-0.78393200
H	-5.77268700	0.17215400	-1.80655800
H	-6.30658800	1.41540500	-0.67474700
C	-7.46936700	-0.39648300	-0.60655500
H	-7.90326000	-0.16283100	0.37340700
H	-8.18440100	-0.03056100	-1.35185200
C	-7.29250500	-1.90422600	-0.76116900
H	-6.96644900	-2.11427400	-1.79089600
H	-8.25188200	-2.42007300	-0.62286600

Zero-point correction= 0.734184 (Hartree/Particle)
Thermal correction to Energy= 0.771208
Thermal correction to Enthalpy= 0.772152
Thermal correction to Gibbs Free Energy= 0.666485
Sum of electronic and zero-point Energies= -1772.559627
Sum of electronic and thermal Energies= -1772.522604
Sum of electronic and thermal Enthalpies= -1772.521659
Sum of electronic and thermal Free Energies= -1772.627326

C	-6.25591200	-2.50740400	0.20535600
C	-5.98432500	-3.94955300	-0.25747900
H	-5.41120300	-4.52208700	0.47856900
H	-6.93529600	-4.47409200	-0.40626300
H	-5.43797800	-3.96811500	-1.20794200
C	-6.83296500	-2.58939300	1.62797300
H	-7.59330300	-3.37844700	1.66511300
H	-6.06019000	-2.84397500	2.36200000
H	-7.31417400	-1.66474600	1.95171800
C	-5.41686600	0.37670800	1.62547400
H	-4.70132400	0.03850400	2.38027700
H	-5.39051600	1.47177700	1.62258800
H	-6.41477100	0.07369600	1.94337000
H	-3.93588700	-1.85791500	2.01474700
H	-4.61218700	-1.85225600	-0.94912600
O	-0.07286700	2.35556500	-1.04191500
H	-2.19696300	-2.29223300	-0.44720500
H	-1.65715100	-1.84499000	1.16083300
C	5.06459800	-1.31748000	-0.08949400
C	5.09384500	0.22158500	0.15869400
C	3.68381300	0.75750200	-0.13131700
C	2.96518900	0.26874100	-1.24113800
C	3.54139400	-0.81522900	-2.08450100
C	4.62030500	-1.62540500	-1.51063500
H	3.63872400	2.21011300	1.48203500
C	3.11822800	1.78040500	0.63305400
C	1.71196100	0.79201200	-1.55791900
C	1.16058000	1.78456700	-0.76463700
C	1.86348600	2.30248500	0.32261600
H	1.15367600	0.41898600	-2.41344000
O	1.33611500	3.28713000	1.09589300
H	0.67868600	3.82277900	0.59969200
C	5.49610800	0.47634000	1.62417500
H	4.67243000	0.15507100	2.27724900
H	5.63559100	1.55144700	1.78760000
C	6.76591700	-0.26963100	2.03808800
H	7.63169700	0.12056900	1.48958000
H	6.96379800	-0.07384600	3.09765200
C	6.62790100	-1.77397800	1.80930800
H	5.81456900	-2.15474900	2.44451300
H	7.54319600	-2.29563200	2.11800400
C	6.31340200	-2.13177500	0.34625500
C	5.94504700	-3.62092500	0.26997400
H	5.77509500	-3.94471600	-0.76346800
H	6.75703000	-4.23293600	0.67896700
H	5.03584300	-3.83400500	0.84347600
C	7.56589100	-1.91660100	-0.52077500
H	8.30563400	-2.68691100	-0.27410900
H	7.35296100	-2.00391600	-1.59122800
H	8.04192900	-0.94902800	-0.35428900
C	6.04862400	0.98235000	-0.78641600
H	5.88957100	0.70082000	-1.83299500
H	5.86505700	2.05864400	-0.70075800
H	7.09740100	0.80639300	-0.54242000
H	5.34523800	-2.06560400	-2.19235900

H	4.25228800	-1.68658300	0.55406000
H	3.47564000	-0.68197300	-3.16306900
O	3.30339300	-2.16414000	-1.65650100
O	-1.01958600	4.54697600	0.67009100
O	-1.50868400	3.58006100	1.50345500
H	-0.73739700	3.01120000	1.70547800

Name	**8-C3-H-OOH (gas phase)**
Cartesian Coordinates	Frequency and Energy

C	-1.38317900	1.72132500	0.25538900
C	-0.17460700	2.38758500	-0.30193300
C	0.96061100	1.78260400	-0.69535100
C	1.44265600	0.34812600	-0.67229700
C	0.93393800	-0.50226300	0.51725100
C	-0.54316000	-0.67619200	0.48603500
C	-1.51998200	0.24330400	0.36092000
O	-2.34246100	2.40629400	0.59566100
C	-0.35059500	3.87646000	-0.46259700
C	1.49541600	0.01624700	1.83167900
C	3.00427400	0.05476700	1.82692200
C	0.76176300	0.40694200	2.87421000
C	3.51408300	0.88727000	0.64336100
C	2.98894300	0.34407000	-0.70121300
C	3.62735300	-0.98111300	-1.09576500
C	2.95773000	-2.04113100	-1.55750000
C	5.13357400	-1.01844400	-0.99795900
C	-2.88017400	-0.39030900	0.30834800
C	-1.17073700	-2.03279300	0.55183300
C	-2.68164200	-1.86445600	0.64288700
O	-0.56470100	-3.07987200	0.49111300
H	-0.32343200	0.38151100	2.86520200
H	1.23999100	0.76010000	3.78305700
H	1.35400300	-1.50881700	0.39297000
H	1.08349400	-0.12337900	-1.60041400
H	1.69201900	2.45982900	-1.14130500
H	3.30369600	1.05480600	-1.48173200
H	4.60685500	0.92575800	0.64337100
H	3.16384800	1.92001500	0.76477400
H	3.37502700	0.46406600	2.77105400
H	3.38724700	-0.97252700	1.73675000
H	3.48985100	-2.93419400	-1.87107100
H	1.87600400	-2.08086700	-1.63505200
H	5.46309700	-1.06396200	0.04612500
H	5.53557900	-1.89216100	-1.51428600
H	5.58084400	-0.11940900	-1.43797800
H	0.54386900	4.32628700	-0.89702600
H	-1.20998800	4.09261800	-1.10359400
H	-0.55307600	4.34527900	0.50417600
H	-3.13788200	-0.31525800	-0.91116000
O	-3.90727200	0.20037300	1.00613200
H	-3.78373800	1.16497500	0.95899100
H	-2.95047900	-1.97759900	1.70322600
C	-3.45594700	-2.86725700	-0.20399500
H	-3.19792600	-3.88553000	0.09476100
H	-4.53091900	-2.71885300	-0.07740100

Zero-point correction= 0.413527 (Hartree/Particle)
Thermal correction to Energy= 0.438446
Thermal correction to Enthalpy= 0.439390
Thermal correction to Gibbs Free Energy= 0.358540
Sum of electronic and zero-point Energies= -1152.243295
Sum of electronic and thermal Energies= -1152.218376
Sum of electronic and thermal Enthalpies= -1152.217432
Sum of electronic and thermal Free Energies= -1152.298281

H	-3.21281900	-2.74449100	-1.26332000
O	-2.15449200	0.80225500	-2.41396700
H	-1.43968600	0.24086200	-2.75475300
O	-3.19574600	-0.07499000	-2.20852800

Name	**8-C3-H-OOH (water)**
Cartesian Coordinates	Frequency and Energy

C	-1.38770700	1.85386900	-0.05985000
C	-0.09006000	2.56431900	-0.01139900
C	1.10572400	1.98120800	-0.21236500
C	1.45027900	0.54476900	-0.52715600
C	0.88535900	-0.46658000	0.49668300
C	-0.60007000	-0.52465400	0.51310500
C	-1.54514700	0.40273800	0.22952200
O	-2.41662700	2.49626200	-0.28913200
C	-0.21025200	4.05674000	0.16515400
C	1.52752600	-0.28832900	1.86136000
C	3.02843400	-0.41627400	1.80013400
C	0.85085400	-0.01719800	2.98004500
C	3.60254400	0.57588500	0.77978400
C	2.98331300	0.39149900	-0.62101800
C	3.45754100	-0.87959300	-1.31345500
C	2.66131400	-1.72081200	-1.98427200
C	4.94485200	-1.12428400	-1.25957300
C	-2.90502000	-0.22137800	0.16717200
C	-1.28878000	-1.81755000	0.80265900
C	-2.78455500	-1.59358300	0.81113800
O	-0.72243300	-2.88385800	0.97596400
H	-0.23117300	0.08989400	2.99054700
H	1.37280100	0.10027500	3.92627200
H	1.20602900	-1.46136100	0.15629000
H	1.00163000	0.31220700	-1.50243000
H	1.95467700	2.66607200	-0.21511100
H	3.35650400	1.21720000	-1.24561400
H	4.69053800	0.48510200	0.73288100
H	3.38969200	1.59461300	1.12573500
H	3.46315200	-0.24383700	2.78886700
H	3.28677500	-1.44009400	1.49190000
H	3.08317900	-2.57880200	-2.50151600
H	1.58366400	-1.59964500	-2.05126100
H	5.25783400	-1.42914400	-0.25454200
H	5.23477200	-1.91182600	-1.95877700
H	5.50112900	-0.21236500	-1.50543500
H	0.78007900	4.50590200	0.25772300
H	-0.72136800	4.51025700	-0.68933100
H	-0.79384200	4.29905200	1.05862300
H	-3.00420200	-0.41478700	-1.06274300
O	-4.01348500	0.49428300	0.59538800
H	-3.91029900	1.40870800	0.27515200
H	-3.07135100	-1.46743300	1.86611100
C	-3.58642200	-2.72246600	0.17898300
H	-3.44290100	-3.64804000	0.74120500
H	-4.65111300	-2.47618600	0.18596600
H	-3.27179700	-2.88862700	-0.85501600
O	-1.70832400	0.15173000	-2.65602000

Zero-point correction= 0.412210 (Hartree/Particle)
Thermal correction to Energy= 0.437042
Thermal correction to Enthalpy= 0.437986
Thermal correction to Gibbs Free Energy= 0.357664
Sum of electronic and zero-point Energies= -1152.270681
Sum of electronic and thermal Energies= -1152.245849
Sum of electronic and thermal Enthalpies= -1152.244905
Sum of electronic and thermal Free Energies= -1152.325227

H	-0.98205200	-0.49032600	-2.54995300
O	-2.84922100	-0.55801300	-2.37438300

Name	**8-C3-H-OOH (pentyl ethanoate)**
Cartesian Coordinates	Frequency and Energy

C	-1.38635800	1.75397100	0.19705500
C	-0.14079300	2.43974600	-0.22647200
C	1.01054500	1.84425100	-0.59180500
C	1.45469900	0.40118200	-0.65575700
C	0.93650500	-0.49217100	0.49685900
C	-0.54295900	-0.64425000	0.48015900
C	-1.51801900	0.27577600	0.32461500
O	-2.38650400	2.42919200	0.43940000
C	-0.27833800	3.94033600	-0.29007300
C	1.51971600	-0.05311300	1.83096400
C	3.02832200	-0.05603400	1.81586700
C	0.79970400	0.31450100	2.89280200
C	3.55329900	0.81330100	0.66581200
C	3.00021300	0.35621900	-0.69934200
C	3.59606900	-0.96421500	-1.17050600
C	2.89182400	-1.96894700	-1.70286200
C	5.09783700	-1.06404800	-1.06463100
C	-2.87847800	-0.36038900	0.29179200
C	-1.17912700	-1.99143600	0.62137900
C	-2.68665400	-1.81611700	0.70010600
O	-0.57809100	-3.04553900	0.63265900
H	-0.28683000	0.32450300	2.88632900
H	1.29157900	0.61349500	3.81490300
H	1.33965500	-1.49796000	0.32111900
H	1.06681800	-0.00728600	-1.60077600
H	1.77710000	2.53906700	-0.93900000
H	3.32895800	1.09784800	-1.44358300
H	4.64657500	0.81486600	0.65858000
H	3.24021300	1.85080900	0.83892300
H	3.41614800	0.30230200	2.77385500
H	3.38092100	-1.08884000	1.67772300
H	3.39493000	-2.86013100	-2.06890700
H	1.80969800	-1.95907600	-1.79548100
H	5.41539200	-1.17707700	-0.02173800
H	5.47115400	-1.92439400	-1.62474600
H	5.58195000	-0.15958000	-1.45166500
H	0.65801700	4.39601900	-0.61766100
H	-1.07506500	4.23053400	-0.98152200
H	-0.54388400	4.34764700	0.69016400
H	-3.13251900	-0.34414900	-0.92967000
O	-3.91541600	0.26389500	0.94648700
H	-3.78136200	1.22418400	0.84715300
H	-2.95418200	-1.87576400	1.76525500
C	-3.46545000	-2.85812000	-0.09255500
H	-3.26644300	-3.85771100	0.30086900
H	-4.53907100	-2.66390700	-0.02229300
H	-3.17883900	-2.83951000	-1.14819200
O	-2.18063200	0.66323000	-2.53589700
H	-1.48883800	0.05104900	-2.84175800
O	-3.24528300	-0.15572800	-2.23618600

Zero-point correction= 0.412842 (Hartree/Particle)
Thermal correction to Energy= 0.437763
Thermal correction to Enthalpy= 0.438707
Thermal correction to Gibbs Free Energy= 0.357743
Sum of electronic and zero-point Energies= -1152.272386
Sum of electronic and thermal Energies= -1152.247465
Sum of electronic and thermal Enthalpies= -1152.246521
Sum of electronic and thermal Free Energies= -1152.327485

Name				9-C13-H-OOH (gas phase)
Cartesian Coordinates				Frequency and Energy
C	2.23878300	0.74773100	1.26299200	Zero-point correction= 0.461677 (Hartree/Particle)
C	1.12491900	1.19798600	0.36496800	Thermal correction to Energy= 0.489119
C	1.40334100	0.62626300	-1.01571700	Thermal correction to Enthalpy= 0.490063
C	2.83902400	0.12078300	-0.87044000	Thermal correction to Gibbs Free Energy= 0.406422
C	3.30000300	0.16714500	0.38511100	Sum of electronic and zero-point Energies= -1229.804053
C	4.61097200	-0.24976100	0.95858800	Sum of electronic and thermal Energies= -1229.776612
O	2.30113400	0.86979100	2.46602400	Sum of electronic and thermal Enthalpies= -1229.775668
C	0.27156700	2.13814100	0.78897700	Sum of electronic and thermal Free Energies= -1229.859308
C	-0.79530300	2.89738600	0.00232400	
C	-1.53254800	3.85201900	0.93592600	
C	-1.76980700	1.92210900	-0.67238300	
C	-2.60532100	1.09709200	0.31595200	
C	-3.08833100	-0.19496200	-0.30128200	
C	0.55290600	-0.60262000	-1.44514500	
C	0.25035700	-1.75886000	-0.53004800	
C	-0.90698200	-1.54942300	0.44553900	
C	-2.25436300	-1.46220800	-0.26437500	
C	-3.54791700	-1.37460500	0.51565800	
C	-3.50238600	-1.32012400	2.03018700	
C	-4.72407700	-2.16953000	-0.01440200	
C	0.24405400	-3.08411500	-1.26272100	
O	0.21108700	-0.64181400	-2.61341500	
H	0.41596800	2.43179800	1.83129800	
H	-3.63416600	-0.04392900	-1.23288700	
H	1.24757300	-1.93833800	0.32223700	
H	3.37427600	-0.22891300	-1.75014800	
H	-2.42010700	2.50995700	-1.33071100	
H	-1.20239500	1.24841400	-1.32598200	
H	-3.46748600	1.68278300	0.65754000	
H	-2.01177900	0.89248700	1.21422800	
H	-0.90290000	-2.40906300	1.12816200	
H	-0.71889000	-0.66119100	1.05484800	
H	5.09781200	0.60319100	1.44036100	
H	4.44627400	-0.99442900	1.74637900	
H	5.28575900	-0.64910700	0.19640900	
H	-2.30492900	4.38564900	0.37548400	
H	-1.99977300	3.31901600	1.76874800	
H	-0.82731200	4.58477300	1.33692000	
H	-3.48572700	-2.33539900	2.44249000	
H	-2.62788900	-0.79407100	2.41869400	
H	-4.39497400	-0.81797200	2.41956500	
H	-4.68831200	-3.20502500	0.34276100	
H	-5.67082000	-1.72949800	0.31918900	
H	-4.72794800	-2.18831100	-1.10858200	
H	0.04364400	-3.89526100	-0.55830100	
H	-0.51975200	-3.08972300	-2.04720000	
H	1.20926700	-3.27241000	-1.74096400	
O	1.31409600	1.59234900	-2.03659100	
H	0.93432400	1.14253100	-2.81347500	
O	-0.17185300	3.72868700	-0.96484800	
H	0.40170400	3.17263200	-1.51602400	
H	-2.31359100	-2.07639700	-1.16054600	

O	2.94814600	-3.05311100	0.27002100
H	3.63266100	-2.38087500	0.11089600
O	2.04440800	-2.40415300	1.08885300

Name			**9-C13-H-OOH (water)**
Cartesian Coordinates			Frequency and Energy
C	-2.26475600	0.72641000	-1.24486400
C	-1.15024500	1.19475300	-0.36785600
C	-1.41895800	0.62961400	1.01912200
C	-2.84242800	0.09783300	0.88265700
C	-3.31635400	0.15114600	-0.36997000
C	-4.63028200	-0.28302900	-0.91924400
O	-2.32152700	0.82030400	-2.46307500
C	-0.29508000	2.12633800	-0.80858100
C	0.77292300	2.89455900	-0.03466500
C	1.48232900	3.86174700	-0.97211900
C	1.76444900	1.93981900	0.63681300
C	2.59307000	1.11176100	-0.35295700
C	3.09876800	-0.16036000	0.28756700
C	-0.53549900	-0.57088400	1.45285500
C	-0.23619400	-1.74635800	0.56032000
C	0.92668400	-1.55389400	-0.41356100
C	2.27441000	-1.43539500	0.29046000
C	3.55781100	-1.35497100	-0.50800300
C	3.49208100	-1.33751700	-2.02203800
C	4.74554500	-2.12844000	0.02602000
C	-0.23104500	-3.05554000	1.31945000
O	-0.14731900	-0.57283600	2.61025300
H	-0.42749200	2.41266800	-1.85370200
H	3.65780800	0.01540700	1.20700700
H	-1.21530600	-1.93050000	-0.28496400
H	-3.36331500	-0.28332300	1.75702700
H	2.42362200	2.53954300	1.27569300
H	1.20775200	1.27094700	1.30394900
H	3.44185000	1.70593900	-0.71249900
H	1.99016200	0.88373800	-1.23853700
H	0.93173800	-2.43691900	-1.06528500
H	0.73079400	-0.68763700	-1.05142300
H	-5.14847800	0.56479500	-1.37813900
H	-4.47796300	-1.03101200	-1.70602000
H	-5.26499700	-0.70598800	-0.13762400
H	2.26029400	4.40367200	-0.42635700
H	1.94458400	3.32750900	-1.80640400
H	0.76500700	4.58126700	-1.37824200
H	3.45996400	-2.36332100	-2.40775700
H	2.61829400	-0.81003400	-2.41114600
H	4.38647500	-0.85645700	-2.43476200
H	4.71344200	-3.17206400	-0.30873800
H	5.68552600	-1.69023600	-0.33030400
H	4.76056400	-2.12171100	1.12040400
H	-0.11011000	-3.88586900	0.61837100
H	0.59732700	-3.08639900	2.03610700
H	-1.16012400	-3.19220600	1.88003900
O	-1.35402600	1.61885100	2.02542500

Zero-point correction= 0.460137 (Hartree/Particle)
Thermal correction to Energy= 0.487642
Thermal correction to Enthalpy= 0.488587
Thermal correction to Gibbs Free Energy= 0.405035
Sum of electronic and zero-point Energies= -1229.837311
Sum of electronic and thermal Energies= -1229.809805
Sum of electronic and thermal Enthalpies= -1229.808861
Sum of electronic and thermal Free Energies= -1229.892412

H	-0.95852100	1.20583400	2.81579000
O	0.13307400	3.70813300	0.95709600
H	-0.38519000	3.11310800	1.53012500
H	2.34983700	-2.03248500	1.19713700
O	-2.87969200	-3.15478400	-0.34457200
H	-3.56946600	-2.52370300	-0.06632500
O	-2.00144000	-2.40218400	-1.09910800

Name	**9-C3-H-OOH (pentyl ethanoate)**
Cartesian Coordinates	Frequency and Energy

C	-2.22125100	0.75695500	-1.28832100
C	-1.11759500	1.20332200	-0.37682200
C	-1.41590800	0.62740200	0.99815100
C	-2.84658500	0.11853600	0.83189400
C	-3.29428400	0.17706600	-0.42919200
C	-4.60458100	-0.23548200	-1.00552400
O	-2.26145100	0.87939600	-2.49566600
C	-0.25457700	2.14155900	-0.78637700
C	0.80665700	2.89188000	0.01582300
C	1.55055500	3.85438900	-0.90188400
C	1.77255000	1.90862900	0.68928500
C	2.61401800	1.09513000	-0.30281000
C	3.10126700	-0.20066500	0.30335600
C	-0.57367200	-0.59864300	1.45539700
C	-0.24416500	-1.76108500	0.55695100
C	0.90699900	-1.54741300	-0.42643600
C	2.26327700	-1.46608400	0.26872000
C	3.54523200	-1.37515700	-0.53088800
C	3.47650600	-1.30802800	-2.04390600
C	4.72654400	-2.17779700	-0.02530400
C	-0.21440100	-3.07681300	1.30498100
O	-0.27209300	-0.63096500	2.63586300
H	-0.37646700	2.44232300	-1.82920200
H	3.66294400	-0.05817800	1.22695000
H	-1.23916100	-1.96195800	-0.28224400
H	-3.39265500	-0.24640400	1.69921300
H	2.42093500	2.48462000	1.36020800
H	1.19538800	1.22821900	1.32752700
H	3.47502100	1.68940900	-0.63260400
H	2.02614100	0.89643800	-1.20554900
H	0.89963900	-2.40717400	-1.10901700
H	0.71689900	-0.65828400	-1.03335700
H	-5.11413700	0.62974800	-1.44183500
H	-4.44943800	-0.94976400	-1.82246500
H	-5.26036000	-0.67491300	-0.24877000
H	2.32561200	4.37981300	-0.33598800
H	2.01969700	3.32732200	-1.73736100
H	0.85148400	4.59289500	-1.30545300
H	3.45474100	-2.32049300	-2.46435900
H	2.59592800	-0.77907000	-2.41601300
H	4.36378500	-0.80297000	-2.44359600
H	4.68204000	-3.21142500	-0.38889500
H	5.67055400	-1.74008000	-0.37183300
H	4.74829300	-2.20394400	1.06894100
H	-0.01140800	-3.89447600	0.60813500

Zero-point correction= 0.460995 (Hartree/Particle)
Thermal correction to Energy= 0.488268
Thermal correction to Enthalpy= 0.489212
Thermal correction to Gibbs Free Energy= 0.406487
Sum of electronic and zero-point Energies= -1229.834904
Sum of electronic and thermal Energies= -1229.807631
Sum of electronic and thermal Enthalpies= -1229.806687
Sum of electronic and thermal Free Energies= -1229.889412

H	0.56380100	-3.07124300	2.07571800
H	-1.16827500	-3.26993600	1.80449900
O	-1.34867900	1.60215300	2.01631900
H	-1.01099000	1.15200700	2.81270400
O	0.16995300	3.71197000	0.99222000
H	-0.39563700	3.13612600	1.53288800
H	2.33733600	-2.09153600	1.15586700
O	-2.97567100	-3.05322200	-0.25598900
H	-3.64171200	-2.35860600	-0.10327500
O	-2.03824800	-2.43741600	-1.06067400

Table S5. The method to calculate rate constant following the conventional transition state theory

The rate constant (k) was calculated by using the conventional transition state theory (TST) and 1M standard state as:[1-6]

$$k = \sigma\kappa \frac{k_B T}{h} e^{-(\Delta G^{\neq})/RT}$$

Where k_B and h are the Boltzmann and Planck constants, respectively, $\Delta G^{\neq}$ is Gibbs free energy of activation of the studied reaction, σ is the reaction symmetry number that represents reaction path degeneracy (which was calculated following the literature[7,8]), the number of possible different but equivalent reaction pathways, and κ accounts for tunneling corrections which were calculated using Eckart barrier[9]. The Marcus Theory was used to estimate the reaction barriers of SET reactions[10-13]. To avoid over-penalizing entropy losses in solution, in this study the solvent cage effects were included following the corrections proposed by Okuno[14], adjusted with the free volume theory according to the Benson correction[15,16]. These corrections have been successfully used to study the radical scavenging activity of antioxidants in solution[16-19] and are in good agreement with activity data independently obtained by Ardura *et al*[20]. For rate constants that were close to the diffusion limit a correction was applied to yield realistic results[16]. The apparent rate constants (k_{app}) were calculated following the Collins–Kimball theory in the solvents at 298.15K[21]; the steady-state Smoluchowski rate constant (k_D) for an irreversible bimolecular diffusion–controlled reaction was calculated following the literature[16,22].

For the species that have multiple conformers, all of these were investigated and the conformer with the lowest electronic energy was included in the analysis. The hindered internal rotation treatment was also applied to the single bonds to ensure that the obtained conformer has the lowest electronic energy[23,24]. All transition states were characterized by the existence of only one single imaginary frequency. Intrinsic coordinate calculations (IRCs) were performed to ensure that each transition state is corrected.

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