Supporting Information (SI)

A thermodynamic and kinetic study of the antioxidant activity of natural hydroanthraquinones

Quan V. Vo[1*], Nguyen Minh Thong[2*], Trinh Le Huyen[3], Pham Cam Nam[4], Nguyen Minh Tam[5,6*] Nguyen Thi Hoa[7] and Adam Mechler[8]

[1]Institute of Research and Development, Duy Tan University, Danang 550000, Vietnam

[2]The University of Danang, Campus in Kon Tum, 704 Phan Dinh Phung, Kon Tum, Vietnam

[3]Department of Applied Chemistry, National Chiao Tung University, Hsinchu 30010, Taiwan

[4]Department of Chemical Engineering, The University of Danang - University of Science and Technology, Danang 550000, Vietnam.

[5]Computational Chemistry Research Group, Ton Duc Thang University, Ho Chi Minh City, Vietnam.

[6]Faculty of Applied Sciences, Ton Duc Thang University, Ho Chi Minh City, Vietnam

[7]Academic Affairs, The University of Danang - University of Technology and Education, Da Nang 550000, Vietnam.

[8]Department of Chemistry and Physics, La Trobe University, Victoria 3086, Australia

*Corresponding author: vovanquan2@duytan.edu.vn, nmthong@kontum.udn.vn; nguyenminhtam@tdtu.edu.vn

Table of Contents

Table S1. The method to compute the thermochemical properties

In order to determine the mechanistic pathway of the radical scavenging process, thermochemical properties were used, by assessing the energetics of the determining step of each pathway. The literature recognizes three common mechanisms of antioxidant activity.[1-5] In the formal hydrogen transfer (FHT) mechanism, the first step is the homolytic bond breakage in an appropriate moiety to yield a hydrogen radical, which then reacts with the free radical species; here the bond dissociation energy of the R–H moiety determines the enthalpy of the first step.

$$R{-}H \rightarrow R^{\bullet} + H^{\bullet} \quad (BDE(R{-}H)) \qquad (1)$$

In the "Single electron transfer followed by proton transfer" (SETPT) mechanism the first step is electron loss to form a radical cation, characterized by the ionization energy, followed by a deprotonation step that is described with the proton dissociation energy.

$$R{-}H \rightarrow RH^{+\bullet} + e^{-} \quad (IE) \qquad (2)$$

$$RH^{+\bullet} \rightarrow R^{\bullet} + H^{+} \quad (PDE) \qquad (3)$$

The third mechanism, "Sequential proton loss electron transfer" (SPLET), starts with the dissociation of the acidic moiety, which can be characterized by the proton affinity; this is followed by an electron transfer to the free radical, at a cost of the electron transfer energy

$$R{-}H \rightarrow R^{-} + H^{+} \quad (PA) \qquad (4)$$

$$R^{-} \rightarrow R^{\bullet} + e^{-} \quad (ETE) \qquad (5)$$

Thus the reaction enthalpies of the individual steps in the above described mechanisms of antioxidant activity in gas phase (at 298.15 K and 1 atm) are calculated as follows:[1,6,7]

$$BDE = H(R^{\bullet}) + H(H^{\bullet}) - H(R{-}H) \qquad (6)$$

$$IE = H(RH^{\bullet+}) + H(e^{-}) - H(R{-}H) \qquad (7)$$

$$PDE = H(R^{\bullet}) + H(H^{+}) - H(R^{\bullet+}) \qquad (8)$$

$$PA = H(R^{-}) + H(H^{+}) - H(R{-}H) \qquad (9)$$

$$ETE = H(R^{\bullet}) + H(e^{-}) - H(R^{-}) \qquad (10)$$

In the gas phase, the enthalpy of hydrogen atom was calculated at the same method (the M06-2x/6-311++G(d,p) level of theory. The calculated enthalpies of the electron (e^{-}) and proton (H^{+}) were taken from the

literature[1,8-10].

Table S2. BDE and PA values of the X-H (X = O, C) bonds of the studied compounds in the gas phase at the M06-2X/6-31g level of theory

Compounds	Position	BDEs (kcal/mol)	PAs (kcal/mol)
1			
	C1-H	96.4	391.5
	C2-H	92.5	402.6
	C3-H	93.9	390.2
	C4-H	94.1	391.3
	C4a-H	79.9	342.1
	C6-H	115.8	391.7
	C9-H	**72.3**	354.8
	C9a-H	94.0	384.6
	O2-H	93.9	371.3
	O5-H	99.4	350.1
	O8-H	**70.2**	**322.1**
	O9-H	88.1	367.3
2			
	C1-H	96.3	391.2
	C2-H	91.8	401.7
	C3-H	93.5	390.8
	C4-H	94.1	391.2
	C4a-H	79.2	340.1
	C6-H	114.9	385.1
	C9-H	**69.9**	356.2
	C9a-H	91.8	385.1
	C11-H	79.7	348.2
	O2-H	93.9	371.8
	O5-H	99.1	347.2
	O8-H	**75.2**	**318.1**
	O9-H	99.8	363.2
	O11-H	93.9	371.0
3			
	C1-H	96.1	386.7
	C2-H	93.3	396.1
	C3-H	97.1	380.2
	C4-H	96.4	403.6
	C4a-H	83.1	327.7
	C6-H	116.6	387.1
	C9-H	**73.7**	353.2
	C9a-H	91.4	379.1
	O2-H	94.3	363.5
	O4-H	93.4	348.3

	O5-H	93.1	347.6
	O8-H	**71.2**	**321.1**
	O9-H	84.6	363.1
4			
	C1-H	96.5	390.3
	C2-H	93.1	389.1
	C3-H	96.1	371.8
	C4-H	87.3	388.4
	C4a-H	81.2	334.8
	C6-H	116.1	386.1
	C9-H	**71.1**	345.8
	C9a-H	94.4	365.4
	O2-H	94.4	371.0
	O4-H	96.9	347.2
	O5-H	91.7	343.5
	O8-H	**71.3**	**321.2**
	O9-H	88.5	366.2
5			
	C1-H	97.8	384.3
	C2-H	89.1	389.8
	C3-H	97.9	388.1
	C4-H	89.8	385.0
	C4a-H	95.2	367.9
	C6-H	115.1	385.7
	C9a-H	83.7	334.9
	C10-H	**81.1**	348.2
	O2-H	94.3	361.1
	O4-H	97.1	354.0
	O5-H	**84.5**	**334.1**
	O8-H	89.3	341.6

Table S3. 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.

The Formal Hydrogen Transfer (FHT) mechanism: R-H + HOO• → R• + HOOH

The Sequential Proton (SA) mechanism: R-H + HOO• → R^- + $HOOH^{+\bullet}$

The Single Electron Transfer (SET) mechanism: R-H + HOO• → $RH^{\bullet+}$ + HOO^-

compounds	Position	SA		SET		FHT	
		ΔH	ΔG	ΔH	ΔG	ΔH	ΔG
1	O8-H	197.1	198.1	154.2	153.9	-8.5	-8.6
	C9-H					-7.7	-7.6
2	O8-H	191.5	192.0	151.7	150.8	-6.2	-6.8
	C9-H					-9.0	-9.6
3	O8-H	196.6	196.7	157.5	157.1	-7.7	-7.9
	C9-H					-5.7	-6.5
4	O8-H	196.4	196.8	156.9	156.4	-8.2	-8.7
	C9-H					-8.9	-9.0
5	O5-H	199.8	201.3	154.2	153.9	3.3	2.0
	C10-H					-0.5	-1.4

Table S4. Calculated $\Delta G^{\neq}$ (kcal/mol), κ and k_{Eck} ($M^{-1}s^{-1}$) for the HOO• scavenging of the hydroanthraquinones in the presence of one H_2O molecule in the gas phase.

REACTIONS	$\Delta G^{\neq}$	κ	k_{Eck}
1-O8-H + •OOH	8.5	20.9	7.23×10^{7}
1-O8-H-H_2O + •OOH	11.3	14.6	5.06×10^{5}
1-O8-H + •OOH-H_2O	10.2	14.3	2.89×10^{6}

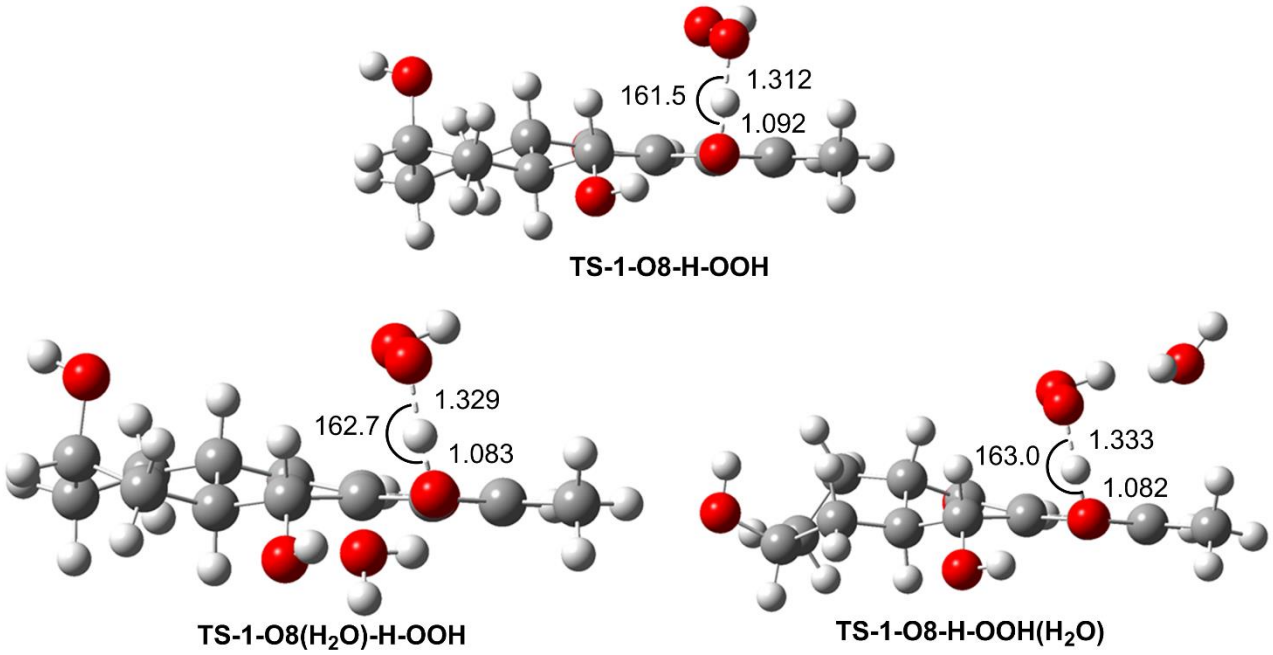

Figure S1. Optimized geometries of TSs between the **1**-O8-H and a HOO• radical in the presence of one H_2O molecule in the gas phase

Table S5: 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-O8-H-OOH**
Cartesian Coordinates				Frequency and Energy
C	3.23384100	0.36574800	-0.45144700	Zero-point correction= 0.328802
C	2.16065900	-0.56546300	-0.52707400	(Hartree/Particle)
C	0.82457800	-0.14021200	-0.37284200	Thermal correction to Energy= 0.349322
C	0.56108400	1.20483700	-0.09843900	Thermal correction to Enthalpy= 0.350266
C	1.63605900	2.13020100	-0.03271800	Thermal correction to Gibbs Free Energy= 0.278822
C	2.95782500	1.69340600	-0.21500100	Sum of electronic and zero-point Energies= -1109.030572
C	-0.29402400	-1.16363500	-0.44634400	
C	-0.80988600	1.66898200	0.19413600	Sum of electronic and thermal Energies= -1109.010051
C	-1.92076900	0.65070600	0.26650600	
C	-1.66617200	-0.53826600	-0.66213500	Sum of electronic and thermal Enthalpies= -1109.009107
C	-2.75298600	-1.62069800	-0.50239800	
H	-2.42886000	-2.36623600	0.22920100	Sum of electronic and thermal Free Energies= -1109.080551
C	-4.09851400	-1.06888800	-0.03553100	
C	-4.31329000	0.33599900	-0.58623000	
C	-3.28418600	1.31859400	-0.00594000	
H	3.74826800	2.43214400	-0.15228600	
H	-4.89809400	-1.73762200	-0.37336400	
H	-4.22634000	0.28657300	-1.67668100	
H	-3.65380000	1.75198600	0.92376900	
H	-3.14464600	2.15359700	-0.69556500	
H	-5.32699300	0.68669100	-0.37017300	
H	-2.87488700	-2.14173900	-1.45311800	
H	-0.29472300	-1.69182100	0.52240900	
C	4.63321300	-0.14762600	-0.61408100	
H	5.35962400	0.65906900	-0.52471700	
H	4.85062100	-0.91172500	0.13833100	
O	2.44530900	-1.85280600	-0.71884600	
H	2.67293100	-2.30329700	0.24992100	
O	-0.12725600	-2.08047700	-1.50686100	
H	0.75701700	-2.45973500	-1.43696000	
O	-4.07218000	-1.05278900	1.39369200	
H	-4.91984100	-0.73344400	1.71497900	
O	1.44624800	3.41934700	0.21082000	
H	0.47688300	3.55994200	0.32970000	
O	-1.03415800	2.85593800	0.40682600	
H	-1.90949900	0.27264300	1.29956800	
H	-1.67426600	-0.16864200	-1.69619600	
O	2.11937200	-1.40766700	2.02741300	
H	2.78632000	-0.73457500	2.23808200	
O	2.81631800	-2.46457200	1.54405400	
H	4.74647500	-0.63169900	-1.58645500	
Name				**1-O8-H-OOH (water)**
Cartesian Coordinates				Frequency and Energy
C	3.22232900	0.36841900	-0.44986300	Zero-point correction= 0.327265
C	2.14415200	-0.55542300	-0.53486100	(Hartree/Particle)

C	0.80737800	-0.12808600	-0.39228100	Thermal correction to Energy= 0.347846
C	0.54608400	1.21712800	-0.11723600	Thermal correction to Enthalpy= 0.348790
C	1.62823200	2.13415400	-0.05124500	Thermal correction to Gibbs Free Energy= 0.277711
C	2.94697900	1.69858300	-0.22452400	Sum of electronic and zero-point Energies= -
C	-0.31268000	-1.14891600	-0.46308700	1109.066563
C	-0.82308500	1.67440600	0.18022400	Sum of electronic and thermal Energies= -
C	-1.92529100	0.65195500	0.27774600	1109.045982
C	-1.68876500	-0.53042200	-0.66607200	Sum of electronic and thermal Enthalpies= -
C	-2.77121500	-1.61697800	-0.49701100	1109.045038
H	-2.43043500	-2.36977600	0.22065900	Sum of electronic and thermal Free Energies= -
C	-4.12023200	-1.08189600	-0.02124600	1109.116117
C	-4.33766800	0.33503000	-0.52762800	
C	-3.30475800	1.30684300	0.06050700	
H	3.74551300	2.42791900	-0.15231100	
H	-4.91651700	-1.73767100	-0.38468700	
H	-4.26020700	0.31066900	-1.61897800	
H	-3.66114100	1.70412700	1.01191000	
H	-3.19608800	2.15869300	-0.61350400	
H	-5.34792800	0.67403000	-0.28429600	
H	-2.91404600	-2.12715800	-1.45097300	
H	-0.30688600	-1.68821500	0.49701100	
C	4.62211000	-0.14544600	-0.56758000	
H	5.34129100	0.66682300	-0.47339400	
H	4.81387200	-0.88620400	0.21544400	
O	2.41998500	-1.84942500	-0.74907100	
H	2.62038500	-2.32076800	0.20179200	
O	-0.13184300	-2.07209000	-1.53034200	
H	0.75192500	-2.45411300	-1.43367000	
O	-4.12396000	-1.11420100	1.41565800	
H	-4.95090600	-0.72189700	1.72006800	
O	1.44068600	3.43577300	0.19028000	
H	0.47422900	3.58379800	0.31043200	
O	-1.05114000	2.86564100	0.39237800	
H	-1.85557600	0.27265100	1.30824800	
H	-1.71854400	-0.14529600	-1.69312200	
O	2.43877500	-1.33403200	2.02060700	
H	3.28288200	-0.85310800	2.09998700	
O	2.75228200	-2.54693900	1.51181600	
H	4.76849300	-0.64843200	-1.52629400	

Name				**1-O8-H-OOH (pentyl ethanoate)**
Cartesian Coordinates				Frequency and Energy
C	3.20501600	0.38929300	-0.47825200	Zero-point correction= 0.327800
C	2.13889800	-0.55292200	-0.52580300	(Hartree/Particle)
C	0.79915700	-0.13858000	-0.36886000	Thermal correction to Energy= 0.348589
C	0.52796100	1.20556500	-0.09998300	Thermal correction to Enthalpy= 0.349533
C	1.59776800	2.13917600	-0.04826000	Thermal correction to Gibbs Free Energy= 0.276847
C	2.91951300	1.71672300	-0.24817800	Sum of electronic and zero-point Energies= -
C	-0.31670800	-1.16635500	-0.43985100	1109.059528
C	-0.84377100	1.65936000	0.20014000	Sum of electronic and thermal Energies= -

C	-1.94716200	0.63602100	0.27891400	1109.038739
C	-1.69184000	-0.54795500	-0.65856000	Sum of electronic and thermal Enthalpies= -
C	-2.77563200	-1.63547700	-0.50510500	1109.037795
H	-2.44057900	-2.39607400	0.20629100	Sum of electronic and thermal Free Energies= -
C	-4.12042700	-1.10065000	-0.01829800	1109.110481
C	-4.35090400	0.30924700	-0.54498900	
C	-3.31986600	1.29349200	0.02840500	
H	3.70845600	2.45883800	-0.20491100	
H	-4.91769400	-1.76780600	-0.36279500	
H	-4.28085600	0.27298900	-1.63697300	
H	-3.68203800	1.71829500	0.96538700	
H	-3.19768100	2.13091400	-0.66176800	
H	-5.36298600	0.64828600	-0.30513900	
H	-2.91381000	-2.13694100	-1.46425600	
H	-0.32172100	-1.69411400	0.52803900	
C	4.60808400	-0.10121100	-0.66396300	
H	4.71774500	-0.57774100	-1.64129000	
H	5.31993700	0.71956800	-0.58447700	
O	2.42911600	-1.84101500	-0.72299600	
H	2.73299600	-2.27669600	0.22138800	
O	-0.13438300	-2.09039200	-1.49723000	
H	0.75330900	-2.45896600	-1.40978100	
O	-4.09075300	-1.11006300	1.41360000	
H	-4.92181200	-0.74461100	1.73509700	
O	1.39262700	3.42788600	0.19533200	
H	0.42039100	3.54792000	0.32674300	
O	-1.07091000	2.84706300	0.41875700	
H	-1.91303500	0.25536900	1.31038600	
H	-1.70413900	-0.16754700	-1.68809000	
O	2.42704400	-1.34502400	2.05146400	
H	3.16554200	-0.71907000	2.15721800	
O	2.97204200	-2.46163800	1.51389600	
H	4.85919100	-0.86150100	0.08220300	
Name				**1-C9-H-OOH**
Cartesian Coordinates				Frequency and Energy
C	3.42618400	-0.31483700	0.11717700	Zero-point correction= 0.330145
C	2.21229900	-0.93577800	-0.21374600	(Hartree/Particle)
C	1.05581400	-0.19469800	-0.39213800	Thermal correction to Energy= 0.350519
C	1.06077600	1.19030400	-0.12169800	Thermal correction to Enthalpy= 0.351463
C	2.27451300	1.82198700	0.19464200	Thermal correction to Gibbs Free Energy= 0.281324
C	3.44272700	1.05921300	0.29690700	Sum of electronic and zero-point Energies= -
C	-0.17335100	-0.87961800	-0.89501400	1109.025951
C	-0.21013800	1.92502400	-0.03655100	Sum of electronic and thermal Energies= -
C	-1.45321900	1.06748500	0.03816700	1109.005577
C	-1.40513200	-0.01680900	-1.04811400	Sum of electronic and thermal Enthalpies= -
C	-2.70538600	-0.86093300	-1.09314900	1109.004632
H	-2.46398500	-1.92501000	-1.03851400	Sum of electronic and thermal Free Energies= -
C	-3.69984100	-0.52057200	0.00812800	1109.074771
C	-3.99374800	0.98078800	0.07766400	

C	-2.74134700	1.87490900	-0.06776200
H	4.36313300	1.57204000	0.55034100
H	-4.63118200	-1.06151700	-0.19036900
H	-4.71224800	1.21606500	-0.71206900
H	-2.73821100	2.67087800	0.67674400
H	-2.74570300	2.37376700	-1.04173600
H	-4.50756100	1.18800700	1.02199800
H	-3.21323400	-0.70261600	-2.04723200
H	-0.42324500	-1.72542000	-0.00137300
C	4.66340000	-1.15118300	0.26849400
H	5.51967800	-0.53310500	0.53607700
H	4.51648900	-1.91072400	1.03917200
H	4.88350300	-1.68234700	-0.65991100
O	2.19522800	-2.30433200	-0.39851200
H	1.50449200	-2.68268400	0.17267800
O	0.00250000	-1.64104900	-2.04354000
H	0.83369300	-2.12958400	-1.96847700
O	-3.17171100	-1.00396000	1.25884400
H	-3.81080300	-0.80532400	1.94968300
O	2.36306200	3.13853700	0.43070100
H	1.47681600	3.52956000	0.31445200
O	-0.25681700	3.14382200	0.05688000
H	-1.39880900	0.57375100	1.01729000
H	-1.28955600	0.49267500	-2.01502700
O	-0.66999200	-2.02178700	2.04447800
H	-1.61685400	-1.79550200	1.99621900
O	-0.47073600	-2.67805800	0.85139900

Name			**2-O8-H-OOH**
Cartesian Coordinates			Frequency and Energy
C	3.04184600	0.49871300	-0.17733600
C	2.00576700	-0.46489200	-0.28931000
C	0.65137600	-0.07667900	-0.25085300
C	0.33573300	1.26652400	-0.02698500
C	1.37656600	2.22549600	0.08367200
C	2.72109600	1.82352700	-0.00704000
C	-0.43057500	-1.13235800	-0.38910600
C	-1.06503200	1.69549600	0.16424200
C	-2.14480500	0.64236300	0.20281900
C	-1.80388900	-0.54890200	-0.69735600
C	-2.86723900	-1.66213400	-0.59622800
H	-2.55834200	-2.40591700	0.14337000
C	-4.24804000	-1.15286700	-0.18974900
C	-4.48478100	0.24144900	-0.75809700
C	-3.51612400	1.26071900	-0.13816200
H	3.48648400	2.58711200	0.06831600
H	-5.00957800	-1.84957900	-0.55685000
H	-4.34759800	0.19058000	-1.84317500
H	-3.94260300	1.68618900	0.77056900
H	-3.37337800	2.09683500	-0.82547300

Zero-point correction= 0.335087
(Hartree/Particle)
Thermal correction to Energy= 0.356486
Thermal correction to Enthalpy= 0.357430
Thermal correction to Gibbs Free Energy= 0.283891
Sum of electronic and zero-point Energies= -1184.238798
Sum of electronic and thermal Energies= -1184.217399
Sum of electronic and thermal Enthalpies= -1184.216455
Sum of electronic and thermal Free Energies= -1184.289993

H	-5.51801600	0.55908400	-0.58943500
H	-2.93140300	-2.17785400	-1.55542100
H	-0.47977100	-1.65890900	0.57859800
C	4.47239400	0.01438800	-0.23467200
H	5.14983700	0.86665400	-0.17809000
H	4.66428100	-0.62926000	0.63550200
O	2.34562600	-1.75484200	-0.41470500
H	2.31663200	-2.22301300	0.57062900
O	-0.16550300	-2.04446000	-1.43460800
H	0.71618000	-2.41036500	-1.30201500
O	-4.28141600	-1.12943800	1.23900100
H	-5.14993500	-0.83245100	1.52397100
O	1.13607600	3.51317200	0.27852100
H	0.15768300	3.63086100	0.32607400
O	-1.33604800	2.88032400	0.32381800
H	-2.16588200	0.27704000	1.24018700
H	-1.75738900	-0.18776500	-1.73311800
O	4.76780000	-0.66474300	-1.43277800
H	4.20457600	-1.44576600	-1.46404600
O	1.57920500	-1.27805900	2.25009200
H	2.27724100	-0.71478400	2.62158900
O	2.20366300	-2.41492200	1.86488200

Name	**2-O8-H-OOH (water)**
Cartesian Coordinates	Frequency and Energy

C	3.01647300	0.50518100	-0.21743900
C	1.98195400	-0.46199400	-0.31571200
C	0.62596700	-0.07675200	-0.26232300
C	0.30968100	1.26770100	-0.04382900
C	1.35357600	2.22419200	0.04910400
C	2.69645100	1.82996500	-0.05224000
C	-0.45554300	-1.13539600	-0.35914300
C	-1.09027600	1.68789400	0.16316800
C	-2.16548900	0.63459700	0.21782100
C	-1.83255500	-0.56643300	-0.67153900
C	-2.89194700	-1.68032200	-0.54134200
H	-2.57956800	-2.40025100	0.22153500
C	-4.28508700	-1.17182400	-0.17603400
C	-4.50547900	0.22215400	-0.74136000
C	-3.54520600	1.24112100	-0.11159900
H	3.46749200	2.58798800	0.02592300
H	-5.03567000	-1.86186600	-0.57176000
H	-4.34881600	0.16835600	-1.82309600
H	-3.97804900	1.65174800	0.80160000
H	-3.41499600	2.07803400	-0.80034600
H	-5.53958600	0.53778400	-0.58104700
H	-2.95431300	-2.22300400	-1.48591400
H	-0.49343300	-1.63769000	0.62015900
C	4.44616800	0.02927300	-0.24969900
H	5.11904300	0.88374300	-0.19253600

Zero-point correction= 0.332984 (Hartree/Particle)
Thermal correction to Energy= 0.354549
Thermal correction to Enthalpy= 0.355494
Thermal correction to Gibbs Free Energy= 0.281543
Sum of electronic and zero-point Energies= -1184.282306
Sum of electronic and thermal Energies= -1184.260741
Sum of electronic and thermal Enthalpies= -1184.259797
Sum of electronic and thermal Free Energies= -1184.333747

H	4.62573200	-0.61239800	0.62112000
O	2.32292900	-1.75162800	-0.45174300
H	2.36546700	-2.20511000	0.53754600
O	-0.18130500	-2.09014000	-1.37724900
H	0.70466600	-2.44421200	-1.21778000
O	-4.38758200	-1.16006400	1.25759200
H	-5.24052600	-0.77452800	1.49089300
O	1.11330000	3.52275200	0.24284600
H	0.13763800	3.64229900	0.31279000
O	-1.36435300	2.87511500	0.33373200
H	-2.15497400	0.28722400	1.26184000
H	-1.80450900	-0.21229000	-1.70968800
O	4.75763900	-0.66780600	-1.44961800
H	4.21213000	-1.46472000	-1.46498300
O	1.94729000	-1.16298500	2.27254300
H	2.77810500	-0.68386800	2.44869000
O	2.31483800	-2.39191600	1.84415200

Name			**2-O8-H-OOH (pentyl ethanoate)**
Cartesian Coordinates			Frequency and Energy
C	3.03816100	0.50616500	-0.17332400
C	2.00282600	-0.45794900	-0.28855000
C	0.64757000	-0.06975400	-0.25846600
C	0.33144700	1.27201500	-0.03084200
C	1.37263700	2.22958800	0.08626400
C	2.71709400	1.83108500	-0.00260400
C	-0.43379100	-1.12330000	-0.41266700
C	-1.06963600	1.69755700	0.16243900
C	-2.14592500	0.64372800	0.20316300
C	-1.81033400	-0.54096700	-0.70959400
C	-2.87203400	-1.65682200	-0.60860400
H	-2.55003500	-2.41199900	0.11438500
C	-4.25047400	-1.15943800	-0.18126100
C	-4.49954900	0.23973700	-0.72735900
C	-3.52402900	1.25747300	-0.11655000
H	3.48738800	2.58974400	0.07808700
H	-5.01248700	-1.85230100	-0.55360200
H	-4.38065100	0.19935800	-1.81493700
H	-3.94082000	1.67881900	0.79911200
H	-3.39459200	2.09281500	-0.80772800
H	-5.53054900	0.55002100	-0.53408300
H	-2.95491300	-2.15686100	-1.57488500
H	-0.48257000	-1.66882800	0.54347900
C	4.47064600	0.03167400	-0.22541900
H	5.14019000	0.89030300	-0.17585200
H	4.67206500	-0.60320000	0.64777400
O	2.34180300	-1.74790900	-0.42735500
H	2.30746000	-2.22859400	0.54778300
O	-0.15674000	-2.02036200	-1.47408500
H	0.72363800	-2.38695600	-1.33126600

Zero-point correction= 0.333979
(Hartree/Particle)
Thermal correction to Energy= 0.355455
Thermal correction to Enthalpy= 0.356399
Thermal correction to Gibbs Free Energy= 0.282794
Sum of electronic and zero-point Energies= -1184.270189
Sum of electronic and thermal Energies= -1184.248712
Sum of electronic and thermal Enthalpies= -1184.247768
Sum of electronic and thermal Free Energies= -1184.321374

O	-4.27914000	-1.15970100	1.25060900	
H	-5.13364700	-0.81874800	1.53552400	
O	1.12421900	3.51679700	0.28450600	
H	0.14242000	3.62084900	0.33215500	
O	-1.33844900	2.88413900	0.32925200	
H	-2.14665000	0.27399600	1.23915200	
H	-1.77573300	-0.16725400	-1.74087700	
O	4.77085900	-0.65808500	-1.42343600	
H	4.21482800	-1.44539500	-1.44260700	
O	1.64777400	-1.29968200	2.27226600	
H	2.39493200	-0.78035000	2.61998900	
O	2.18618200	-2.46271800	1.84057300	
Name				**2-C9-H-OOH**
Cartesian Coordinates				Frequency and Energy
C	3.18517700	0.14760500	0.25586500	Zero-point correction= 0.336127
C	2.06201200	-0.61164300	-0.09755000	(Hartree/Particle)
C	0.83887400	-0.00937100	-0.33939700	Thermal correction to Energy= 0.357352
C	0.68512500	1.37339500	-0.10279500	Thermal correction to Enthalpy= 0.358296
C	1.80976200	2.14396500	0.23574000	Thermal correction to Gibbs Free Energy= 0.286731
C	3.05191400	1.51734200	0.39528500	Sum of electronic and zero-point Energies= -1184.235147
C	-0.29077100	-0.83734800	-0.85962700	
C	-0.66428100	1.96446500	-0.07323800	Sum of electronic and thermal Energies= -1184.213922
C	-1.80414500	0.97357600	-0.00240400	
C	-1.60680600	-0.12190800	-1.05994300	Sum of electronic and thermal Enthalpies= -1184.212978
C	-2.80498100	-1.10607600	-1.11344600	
H	-2.44713500	-2.13624200	-1.04909700	Sum of electronic and thermal Free Energies= -1184.284543
C	-3.84270300	-0.87090800	-0.02474200	
C	-4.31200700	0.58707600	0.02311700	
C	-3.17555200	1.61885000	-0.15617500	
H	3.90448700	2.13331400	0.65742800	
H	-4.70167900	-1.52051500	-0.22287900	
H	-5.06439700	0.72384500	-0.75803400	
H	-3.27757000	2.44194300	0.55087300	
H	-3.22751400	2.06801900	-1.15287400	
H	-4.83136600	0.74968900	0.97303300	
H	-3.31697400	-1.00914500	-2.07354300	
H	-0.46501200	-1.69247000	0.04343400	
C	4.50136300	-0.55566500	0.49426800	
H	5.28171000	0.18426500	0.67369100	
H	4.41065900	-1.17711400	1.39443700	
O	2.20455400	-1.98343700	-0.23091100	
H	1.52627200	-2.42133800	0.31502800	
O	-0.00240700	-1.59116900	-1.98935100	
H	0.88088300	-1.97225000	-1.90000500	
O	-3.27276900	-1.27262100	1.23707000	
H	-3.94439200	-1.15933400	1.91656800	
O	1.74586900	3.46648800	0.43733000	
H	0.82912500	3.75797400	0.27680200	
O	-0.84733900	3.17148700	-0.01857900	

H	-1.71746000	0.51126500	0.98971800
H	-1.52476100	0.37572900	-2.03634600
O	-0.69290100	-1.98551100	2.09227500
H	-1.65892500	-1.87261000	2.02533000
O	-0.39829500	-2.62892000	0.91190100
O	4.92148100	-1.32957700	-0.60863700
H	4.28062800	-2.03907800	-0.72211000

Name				**3-O8-H-OOH**
Cartesian Coordinates				Frequency and Energy
C	3.38650900	0.37992800	-0.50451000	Zero-point correction= 0.334644
C	2.33487300	-0.58134200	-0.47468700	(Hartree/Particle)
C	0.99351700	-0.17736400	-0.33444700	Thermal correction to Energy= 0.355882
C	0.69787300	1.18362800	-0.19245900	Thermal correction to Enthalpy= 0.356827
C	1.74577300	2.13702100	-0.26000200	Thermal correction to Gibbs Free Energy= 0.284618
C	3.07510400	1.71635700	-0.41073700	Sum of electronic and zero-point Energies= -1184.247852
C	-0.10342000	-1.23679600	-0.37681500	
C	-0.67627400	1.63246300	0.12286100	Sum of electronic and thermal Energies= -1184.226614
C	-1.64544500	0.53468000	0.48334200	
C	-1.47063400	-0.59390100	-0.54511600	Sum of electronic and thermal Enthalpies= -1184.225670
C	-2.62130900	-1.58545300	-0.42428500	
H	-2.67438700	-1.94796500	0.60888600	Sum of electronic and thermal Free Energies= -1184.297878
C	-3.96336900	-0.91717400	-0.76105700	
C	-3.92153300	0.60817600	-0.57154500	
C	-3.10860800	0.99382700	0.65995300	
H	3.84690600	2.47627500	-0.43847000	
H	-4.23967100	-1.14349800	-1.79614400	
H	-3.47740900	1.07974200	-1.45366400	
H	-3.11421500	2.07645200	0.79130000	
H	-4.94102400	0.99496800	-0.48275500	
H	-2.44703700	-2.44927800	-1.06555700	
H	-0.08384700	-1.78888200	0.57908900	
C	4.79562900	-0.11049300	-0.62316500	
H	5.49400500	0.72104500	-0.70493300	
H	5.05540500	-0.70702300	0.25621000	
H	4.89944300	-0.76102900	-1.49407400	
O	2.62263400	-1.87436500	-0.60796200	
H	3.09509000	-2.24008600	0.30203200	
O	0.06187800	-2.12893000	-1.45552500	
H	0.94715600	-2.50785000	-1.38995100	
O	-4.92572100	-1.50777100	0.12208300	
H	-5.80861000	-1.24186000	-0.15048900	
O	1.52194600	3.44267200	-0.16706500	
H	0.55573400	3.58447600	-0.07330000	
O	-0.97923800	2.81731000	0.12460300	
H	-1.32123600	0.15484000	1.46293700	
H	-1.47480300	-0.16904400	-1.55856100	
O	-3.66232900	0.44075500	1.84506000	
H	-4.15158500	-0.36096400	1.62340800	
O	3.22357300	-1.12254900	2.03636400	

H	2.40672600	-1.17941500	2.55583400	
O	3.42741200	-2.37865300	1.56546900	
Name				**3-O8-H-OOH (water)**
Cartesian Coordinates				Frequency and Energy
C	3.48957800	0.29653000	-0.42410800	Zero-point correction= 0.332795
C	2.40675500	-0.62543200	-0.46092000	(Hartree/Particle)
C	1.07185800	-0.18070200	-0.37426700	Thermal correction to Energy= 0.354236
C	0.81258000	1.18343700	-0.20310600	Thermal correction to Enthalpy= 0.355180
C	1.89426200	2.09701400	-0.20710500	Thermal correction to Gibbs Free Energy= 0.282466
C	3.21499400	1.64130200	-0.31873700	Sum of electronic and zero-point Energies= -1184.291098
C	-0.04856900	-1.20764600	-0.45859000	
C	-0.55426900	1.65508500	0.10000900	Sum of electronic and thermal Energies= -1184.269658
C	-1.55112700	0.57437700	0.42809600	
C	-1.40224200	-0.53886200	-0.62497700	Sum of electronic and thermal Enthalpies= -1184.268714
C	-2.56925000	-1.51211900	-0.49595700	
H	-2.60614300	-1.87029700	0.53954000	Sum of electronic and thermal Free Energies= -1184.341427
C	-3.90088300	-0.81984000	-0.81893300	
C	-3.83076500	0.69980200	-0.62257500	
C	-3.00158800	1.07094100	0.59861700	
H	4.01545600	2.37193600	-0.29652600	
H	-4.19169400	-1.02953000	-1.85130500	
H	-3.37494100	1.15839800	-1.50452500	
H	-2.98906900	2.15252800	0.72897800	
H	-4.84400400	1.10027000	-0.53222700	
H	-2.42832500	-2.37985000	-1.14058500	
H	-0.04556300	-1.79079100	0.47570100	
C	4.88852000	-0.22783200	-0.48853200	
H	5.60903100	0.58671200	-0.42998700	
H	5.06590600	-0.92383300	0.33615100	
H	5.04787600	-0.78235400	-1.41644800	
O	2.66671200	-1.93235200	-0.58514400	
H	2.69226400	-2.37553900	0.40370000	
O	0.13322300	-2.07745600	-1.56825600	
H	0.99539200	-2.50281900	-1.46151100	
O	-4.87829900	-1.39888000	0.06341000	
H	-5.74143900	-1.02900000	-0.15892200	
O	1.70985300	3.41665800	-0.08117800	
H	0.74658300	3.58874500	-0.00816000	
O	-0.82501700	2.85165300	0.12764800	
H	-1.22511900	0.16266000	1.39414600	
H	-1.41318500	-0.09026800	-1.62674200	
O	-3.58330600	0.54193000	1.79646000	
H	-4.04393600	-0.28039100	1.57763700	
O	2.38967800	-1.28663700	2.14511000	
H	1.42338000	-1.20213400	2.24478900	
O	2.61070700	-2.55251300	1.72104900	
Name				**3-O8-H-OOH (pentyl ethanoate)**
Cartesian Coordinates				Frequency and Energy
C	3.40410500	0.37666800	-0.49966500	Zero-point correction= 0.333717

C	2.34918800	-0.58073500	-0.47728200
C	1.00673900	-0.17437100	-0.34198100
C	0.71562800	1.18607800	-0.18893700
C	1.76839700	2.13525600	-0.24314500
C	3.09672300	1.71439300	-0.39571000
C	-0.09370600	-1.22907000	-0.39039100
C	-0.65735500	1.63586500	0.12707700
C	-1.63561400	0.54169600	0.46923300
C	-1.46035600	-0.58628900	-0.56138900
C	-2.60975800	-1.57935600	-0.42936700
H	-2.65192600	-1.93365400	0.60728400
C	-3.95352300	-0.91611200	-0.76738600
C	-3.90734000	0.61001200	-0.59975100
C	-3.09868400	1.00912100	0.62908500
H	3.87536500	2.46817100	-0.41596700
H	-4.23894800	-1.15479700	-1.79594600
H	-3.45133400	1.06174300	-1.48581900
H	-3.10468100	2.09290900	0.74790600
H	-4.92588100	1.00230200	-0.52669600
H	-2.44122500	-2.44855000	-1.06516700
H	-0.07626500	-1.78343500	0.56267300
C	4.81276500	-0.10985200	-0.62683700
H	5.51185000	0.72532900	-0.64684700
H	5.06495600	-0.76146700	0.21484300
H	4.93267900	-0.70180300	-1.53747600
O	2.63631300	-1.87549100	-0.61715600
H	3.02789700	-2.26233100	0.31724300
O	0.08200400	-2.12126500	-1.47376000
H	0.96674300	-2.49905800	-1.39304100
O	-4.91558000	-1.49256200	0.13120500
H	-5.79750500	-1.21905200	-0.14520600
O	1.54249400	3.44124600	-0.13687000
H	0.57335700	3.57271700	-0.04014700
O	-0.94852000	2.82570400	0.14914600
H	-1.31494800	0.15575500	1.44759300
H	-1.47323800	-0.15758200	-1.57218800
O	-3.66789600	0.47239200	1.82083300
H	-4.15552500	-0.32990000	1.59374300
O	3.11368000	-1.17345800	2.07427000
H	2.24426800	-1.17915100	2.51127600
O	3.28389100	-2.43256200	1.60240900

(Hartree/Particle)
Thermal correction to Energy= 0.355121
Thermal correction to Enthalpy= 0.356065
Thermal correction to Gibbs Free Energy= 0.283404
Sum of electronic and zero-point Energies= -1184.279376
Sum of electronic and thermal Energies= -1184.257972
Sum of electronic and thermal Enthalpies= -1184.257028
Sum of electronic and thermal Free Energies= -1184.329689

Name			**3-C9-H-OOH**
Cartesian Coordinates			Frequency and Energy
C	3.75262500	-0.03849300	0.02658000
C	2.64177700	-0.86617000	-0.19519500
C	1.35678200	-0.35069300	-0.30961200
C	1.17073800	1.04566300	-0.13653600
C	2.28238200	1.88086000	0.09264200
C	3.56052600	1.32398200	0.16540700

Zero-point correction= 0.334921
(Hartree/Particle)
Thermal correction to Energy= 0.356248
Thermal correction to Enthalpy= 0.357192
Thermal correction to Gibbs Free Energy= 0.286100
Sum of electronic and zero-point Energies= -

C	0.18791700	-1.25083800	-0.55035600	1184.247409
C	-0.17823300	1.61740900	-0.10468200	Sum of electronic and thermal Energies= -
C	-1.35517300	0.67963900	-0.14168600	1184.226082
C	-1.09954600	-0.57563700	-0.97802700	Sum of electronic and thermal Enthalpies= -
C	-2.28750900	-1.56843000	-0.90464400	1184.225138
H	-2.04850500	-2.39286200	-0.22917100	Sum of electronic and thermal Free Energies= -
C	-3.58726200	-0.91133600	-0.44277400	1184.296230
C	-3.71669500	0.47038400	-1.06794100	
C	-2.63801400	1.42422100	-0.54778800	
H	4.39760200	1.98848000	0.34221400	
H	-4.43207800	-1.53974200	-0.73775200	
H	-3.63236900	0.36070000	-2.15257300	
H	-2.39603900	2.16069500	-1.32087500	
H	-4.69111500	0.91878500	-0.85880100	
H	-2.44566000	-2.01127100	-1.88973800	
H	-0.07294800	-1.73494100	0.61174800	
C	5.12624200	-0.64530500	0.11769400	
H	5.21354800	-1.30853100	0.98576500	
H	5.36052600	-1.22685900	-0.77828600	
H	5.88266200	0.13002800	0.22679000	
O	2.80613800	-2.22863900	-0.32233300	
H	3.61446600	-2.51685800	0.10960500	
O	0.39130900	-2.33903000	-1.38078400	
H	1.22655300	-2.76460800	-1.15050400	
O	-3.58621300	-0.83162500	0.99221800	
H	-3.86979300	0.04937500	1.26765000	
O	2.18015400	3.20473200	0.25499000	
H	1.23401600	3.44532700	0.20011200	
O	-0.37169900	2.82588500	0.03054100	
H	-1.47327200	0.36939100	0.90398400	
H	-0.95557100	-0.26902500	-2.02458400	
O	-1.19458100	-1.42950600	2.38353200	
H	-2.10069800	-1.46509300	2.01667000	
O	-0.48339700	-2.34467500	1.64639800	
O	-3.18763300	2.09729300	0.58081000	
H	-2.54327600	2.75999300	0.85628300	
Name				**3- C9-H-OOH (water)**
Cartesian Coordinates				Frequency and Energy
C	3.73477600	-0.07739200	0.06686900	Zero-point correction= 0.332236
C	2.60921200	-0.88245800	-0.17916300	(Hartree/Particle)
C	1.33785500	-0.33697700	-0.31247000	Thermal correction to Energy= 0.353893
C	1.16702500	1.05942100	-0.12978200	Thermal correction to Enthalpy= 0.354837
C	2.29299900	1.86628200	0.10628000	Thermal correction to Gibbs Free Energy= 0.282821
C	3.55931300	1.28958700	0.19615500	Sum of electronic and zero-point Energies= -
C	0.16111200	-1.20872400	-0.61286000	1184.289732
C	-0.17619800	1.64734100	-0.11829300	Sum of electronic and thermal Energies= -
C	-1.35998400	0.71566800	-0.12171000	1184.268075
C	-1.11421500	-0.49931400	-1.02297100	Sum of electronic and thermal Enthalpies= -
C	-2.31049900	-1.48380800	-1.03542900	1184.267131

H	-2.04978200	-2.40601800	-0.51220000	Sum of electronic and thermal Free Energies= -1184.339147
C	-3.57699900	-0.91947700	-0.40802100	
C	-3.80258300	0.52079900	-0.83953000	
C	-2.65084900	1.46541500	-0.47550800	
H	4.41130300	1.93240400	0.38583100	
H	-4.42856600	-1.52793900	-0.72355200	
H	-3.94319100	0.51385300	-1.92344800	
H	-2.44473000	2.12071900	-1.32751900	
H	-4.72337100	0.91001900	-0.39737200	
H	-2.54147300	-1.75539600	-2.06647700	
H	-0.11180800	-1.75042600	0.48416900	
C	5.09261900	-0.70380600	0.18910500	
H	5.10687900	-1.44364500	0.99504300	
H	5.37152400	-1.21786400	-0.73686000	
H	5.84573100	0.05370900	0.39913200	
O	2.72817500	-2.24950900	-0.26964300	
H	3.65130900	-2.51723100	-0.36674700	
O	0.38848900	-2.25887900	-1.50520100	
H	1.24592200	-2.66205400	-1.29848400	
O	-3.45347500	-1.03211100	1.02253100	
H	-4.19027800	-0.56993200	1.44094500	
O	2.21248400	3.20891000	0.26772800	
H	1.27328700	3.46726700	0.17329500	
O	-0.34350800	2.86694900	-0.03950900	
H	-1.44133800	0.37165200	0.91615500	
H	-0.94878900	-0.12819900	-2.04349900	
O	-1.13456700	-1.56051800	2.37342700	
H	-2.02613700	-1.42756400	1.97548200	
O	-0.51487300	-2.44824200	1.52607800	
O	-3.06661200	2.27321100	0.62878500	
H	-2.36690600	2.92281500	0.77650000	

Name				**3- C9-H-OOH (pentyl ethanoate)**
Cartesian Coordinates				Frequency and Energy
C	3.76020200	-0.04936300	0.03126400	Zero-point correction= 0.333976 (Hartree/Particle)
C	2.64334300	-0.87355000	-0.18769400	Thermal correction to Energy= 0.355372
C	1.35967500	-0.35197900	-0.29785200	Thermal correction to Enthalpy= 0.356316
C	1.17759100	1.04524300	-0.12273500	Thermal correction to Gibbs Free Energy= 0.285130
C	2.29388300	1.87454600	0.09720800	Sum of electronic and zero-point Energies= -1184.278297
C	3.57075100	1.31463200	0.16264000	
C	0.18517400	-1.24452200	-0.54742600	Sum of electronic and thermal Energies= -1184.256901
C	-0.16849300	1.62248800	-0.09138400	
C	-1.35006700	0.69105700	-0.13414200	Sum of electronic and thermal Enthalpies= -1184.255956
C	-1.09418400	-0.55656100	-0.98411500	
C	-2.28934900	-1.54244000	-0.94472200	Sum of electronic and thermal Free Energies= -1184.327142
H	-2.06145100	-2.39141400	-0.29624100	
C	-3.58663300	-0.89461800	-0.46958400	
C	-3.71577200	0.50057400	-1.05907100	
C	-2.63096500	1.44318400	-0.53385400	
H	4.41572300	1.97100000	0.33557400	

H	-4.43192000	-1.51416600	-0.77925900
H	-3.64078500	0.41262300	-2.14605300
H	-2.38747200	2.18022100	-1.30510200
H	-4.69013200	0.94217500	-0.83439400
H	-2.45336200	-1.94881900	-1.94424800
H	-0.09277200	-1.73447600	0.59847000
C	5.13070500	-0.65786800	0.12948500
H	5.19554000	-1.35334400	0.97308000
H	5.39204600	-1.20317200	-0.78354500
H	5.88225000	0.11580000	0.27970200
O	2.78941700	-2.23464500	-0.28447900
H	3.71499900	-2.49335900	-0.20809500
O	0.39568000	-2.33078900	-1.37894500
H	1.24950900	-2.73013600	-1.16511500
O	-3.58354600	-0.85084600	0.97231500
H	-3.90085900	0.01234700	1.26727300
O	2.19122300	3.20167300	0.25782000
H	1.24103800	3.43323000	0.20800700
O	-0.35288300	2.83359100	0.04502900
H	-1.46833600	0.37527000	0.90971400
H	-0.93445300	-0.23195500	-2.02183300
O	-1.25085100	-1.48878200	2.38282000
H	-2.13458200	-1.45876000	1.95912300
O	-0.52933700	-2.38211300	1.62580800
O	-3.17146000	2.11746100	0.60232900
H	-2.51609500	2.76759900	0.88325600

Name			**4-O8-H-OOH**
Cartesian Coordinates			Frequency and Energy
C	3.33235200	0.52690800	-0.47483100
C	2.32999000	-0.47990600	-0.56607900
C	0.97122300	-0.16615200	-0.35890600
C	0.61673400	1.13992800	-0.00080800
C	1.62365800	2.13786000	0.09460700
C	2.96641200	1.81473500	-0.15654800
C	-0.06894300	-1.26791000	-0.45084300
C	-0.77189700	1.48006800	0.34532700
C	-1.81629100	0.39497000	0.34252300
C	-1.48800900	-0.74246600	-0.62160500
C	-2.48892500	-1.90605100	-0.46509900
H	-2.08153300	-2.66110100	0.21293500
C	-3.84367300	-1.46877800	0.08700300
C	-4.20131000	-0.08031300	-0.42095000
C	-3.22053100	0.99226100	0.06651700
H	3.70098600	2.60726500	-0.07522800
H	-4.60639500	-2.18926800	-0.22766500
H	-4.16360500	-0.08536400	-1.51492900
H	-3.58240100	1.44048400	0.99681900
H	-5.22026100	0.19986000	-0.14016300
H	-2.62605000	-2.38953800	-1.43329400

Zero-point correction= 0.334773
(Hartree/Particle)
Thermal correction to Energy= 0.355925
Thermal correction to Enthalpy= 0.356869
Thermal correction to Gibbs Free Energy= 0.284751
Sum of electronic and zero-point Energies= -1184.248316
Sum of electronic and thermal Energies= -1184.227164
Sum of electronic and thermal Enthalpies= -1184.226220
Sum of electronic and thermal Free Energies= -1184.298339

H	-0.00849700	-1.82496200	0.50014000
C	4.75943800	0.12969900	-0.70304300
H	5.42562600	0.98604000	-0.60745700
H	5.06028300	-0.64170400	0.01232700
O	2.70773300	-1.73187700	-0.81790600
H	2.98154300	-2.20642600	0.13054600
O	0.14221300	-2.13489000	-1.54365500
H	1.05338400	-2.44875700	-1.50638800
O	-3.74841300	-1.48203700	1.51533300
H	-4.60803300	-1.26096600	1.88365600
O	1.35343900	3.39242000	0.42773700
H	0.38596300	3.45672900	0.59890400
O	-1.07252100	2.62939200	0.67178900
H	-1.82242000	-0.00780500	1.36609900
H	-1.55032000	-0.34162200	-1.64088300
O	2.42888100	-1.40991800	1.95135100
H	3.06831900	-0.71698200	2.18165700
O	3.16480800	-2.41003600	1.40872200
H	4.87437100	-0.31073500	-1.69566300
O	-3.19302200	1.97379800	-0.95598700
H	-2.74728000	2.75090700	-0.60407500

Name			**4-O8-H-OOH (water)**
Cartesian Coordinates			Frequency and Energy
C	3.31068100	0.54906900	-0.49643900
C	2.31202100	-0.46189800	-0.57457100
C	0.95170200	-0.15960100	-0.35828200
C	0.59220500	1.14597600	-0.00302700
C	1.59722500	2.14814100	0.06926200
C	2.93668700	1.83821600	-0.19263000
C	-0.08343500	-1.26769600	-0.42169600
C	-0.79216100	1.47154000	0.36823400
C	-1.83534800	0.38653200	0.35300800
C	-1.50605700	-0.75789100	-0.60174800
C	-2.50247600	-1.92197500	-0.42394800
H	-2.09702000	-2.65249400	0.28271300
C	-3.87622100	-1.48264800	0.08081800
C	-4.21341000	-0.09197400	-0.43025700
C	-3.23982900	0.97719600	0.07333700
H	3.67338900	2.62968700	-0.11868300
H	-4.63061400	-2.19164700	-0.27017600
H	-4.15452100	-0.11608300	-1.52330600
H	-3.61293600	1.42435900	0.99725200
H	-5.23549100	0.18470200	-0.16174900
H	-2.62962000	-2.43458500	-1.37857200
H	-0.01931400	-1.80982400	0.53476600
C	4.74013100	0.16275700	-0.70563200
H	5.39552000	1.02319800	-0.58008900
H	5.02556900	-0.61489900	0.00971700
O	2.69218100	-1.71635700	-0.85080300

Zero-point correction= 0.332119 (Hartree/Particle)
Thermal correction to Energy= 0.353658
Thermal correction to Enthalpy= 0.354602
Thermal correction to Gibbs Free Energy= 0.281383
Sum of electronic and zero-point Energies= -1184.290489
Sum of electronic and thermal Energies= -1184.268950
Sum of electronic and thermal Enthalpies= -1184.268006
Sum of electronic and thermal Free Energies= -1184.341225

H	2.96843500	-2.20766700	0.07476300	
O	0.14593000	-2.16751000	-1.49800000	
H	1.06706800	-2.45875300	-1.44155900	
O	-3.85717900	-1.51063100	1.51702700	
H	-4.72166800	-1.21932800	1.83025000	
O	1.31849000	3.41331500	0.39637400	
H	0.35633000	3.47304500	0.59320200	
O	-1.09579900	2.61127100	0.73027400	
H	-1.83506300	-0.00709600	1.37948300	
H	-1.57637500	-0.36771100	-1.62467000	
O	2.82257900	-1.31979900	1.94823200	
H	3.64431100	-0.79829900	2.00679000	
O	3.16953200	-2.48647100	1.35793900	
H	4.88182000	-0.25595800	-1.70492400	
O	-3.20583000	1.97958900	-0.94438800	
H	-2.76934500	2.75765300	-0.57702300	
Name				**4-O8-H-OOH (pentyl ethanoate)**
Cartesian Coordinates				Frequency and Energy
C	3.31801300	0.54710700	-0.48934300	Zero-point correction= 0.333146
C	2.32252300	-0.46901300	-0.56150600	(Hartree/Particle)
C	0.96099400	-0.16506500	-0.35305100	Thermal correction to Energy= 0.354701
C	0.60013600	1.13981400	0.00220700	Thermal correction to Enthalpy= 0.355646
C	1.60217500	2.14420000	0.08924100	Thermal correction to Gibbs Free Energy= 0.282169
C	2.94361500	1.83395400	-0.17515000	Sum of electronic and zero-point Energies= -1184.279030
C	-0.07597200	-1.27101500	-0.44194900	
C	-0.78788000	1.47189200	0.35407000	Sum of electronic and thermal Energies= -1184.257474
C	-1.82993200	0.38633600	0.34518500	
C	-1.49860100	-0.75469500	-0.61522800	Sum of electronic and thermal Enthalpies= -1184.256530
C	-2.49605400	-1.91971200	-0.44755500	
H	-2.08836800	-2.66320100	0.24353500	Sum of electronic and thermal Free Energies= -1184.330006
C	-3.86004000	-1.48372500	0.08436300	
C	-4.21034300	-0.09564000	-0.42820800	
C	-3.23795500	0.97682800	0.07250200	
H	3.67711500	2.62909500	-0.10766100	
H	-4.61789300	-2.20128700	-0.24538200	
H	-4.15826700	-0.10998000	-1.52168300	
H	-3.60651300	1.41278700	1.00522100	
H	-5.23284800	0.18081700	-0.15763600	
H	-2.62971900	-2.41699500	-1.40931700	
H	-0.01775100	-1.82824800	0.50761000	
C	4.74696700	0.17377600	-0.73692400	
H	5.39577800	1.04472000	-0.65231500	
H	5.07994100	-0.58643900	-0.02341100	
O	2.70411900	-1.72043400	-0.82523500	
H	3.01337000	-2.19184600	0.10336500	
O	0.14861000	-2.14378600	-1.53313000	
H	1.06644800	-2.43856400	-1.48722700	
O	-3.79522400	-1.49974100	1.51625000	
H	-4.65836100	-1.24549200	1.85988100	

O	1.31828200	3.39636100	0.42500000	
H	0.34976600	3.44144700	0.60545000	
O	-1.08998100	2.61872700	0.69393800	
H	-1.83086900	-0.01311100	1.36995800	
H	-1.56563100	-0.35953200	-1.63623600	
O	2.62353900	-1.37958600	1.96943200	
H	3.32878300	-0.72712800	2.12840100	
O	3.23429700	-2.43643200	1.38349200	
H	4.85927400	-0.26260600	-1.73229700	
O	-3.21578100	1.97690100	-0.93860500	
H	-2.77300800	2.74923000	-0.57133000	
Name				**4-C9-H-OOH**
Cartesian Coordinates				Frequency and Energy
C	-3.58399300	-0.07051900	-0.06703400	Zero-point correction= 0.335132
C	-2.43234700	-0.79930200	0.27215000	(Hartree/Particle)
C	-1.20058500	-0.17756200	0.38164700	Thermal correction to Energy= 0.356508
C	-1.06927000	1.18346600	0.02791300	Thermal correction to Enthalpy= 0.357452
C	-2.21865400	1.92453600	-0.29337900	Thermal correction to Gibbs Free Energy= 0.285759
C	-3.46279700	1.28560100	-0.32435300	Sum of electronic and zero-point Energies= -1184.246314
C	-0.03477700	-0.95652800	0.90040000	
C	0.26622600	1.76316500	-0.12762500	Sum of electronic and thermal Energies= -1184.224938
C	1.40615100	0.77122600	-0.19274300	
C	1.28785900	-0.22600500	0.96945100	Sum of electronic and thermal Enthalpies= -1184.223994
C	2.48797400	-1.20488000	1.02825700	
H	2.13274100	-2.23787800	1.02413200	Sum of electronic and thermal Free Energies= -1184.295687
C	3.48782600	-1.02057300	-0.10406800	
C	3.92187500	0.43665700	-0.25275300	
C	2.77087200	1.45991900	-0.21320500	
H	-4.33193600	1.87802700	-0.58487200	
H	4.36788200	-1.63518200	0.11053200	
H	4.59212600	0.68295100	0.57462100	
H	2.81551300	2.11004400	-1.09190800	
H	4.50387000	0.54756600	-1.17244400	
H	3.03041000	-1.05678600	1.96405400	
H	0.09669600	-1.87259800	0.05347100	
C	-4.90506800	-0.77881100	-0.14248900	
H	-5.70247600	-0.08656000	-0.40966600	
H	-4.86331300	-1.57934500	-0.88406000	
H	-5.14408000	-1.24759800	0.81423400	
O	-2.55544600	-2.14846500	0.53472200	
H	-1.92298900	-2.62899100	-0.02725900	
O	-0.25612100	-1.62325200	2.09765100	
H	-1.13388800	-2.02773400	2.07397100	
O	2.89477300	-1.51464300	-1.32277300	
H	3.55191800	-1.45501200	-2.02262300	
O	-2.17577500	3.22806100	-0.60288600	
H	-1.25445700	3.53421800	-0.52150900	
O	0.45039700	2.96902100	-0.26970000	
H	1.26972400	0.22679100	-1.13594500	

H	1.26905600	0.35408600	1.89960700
O	0.27372800	-2.27829300	-1.98199700
H	1.24243500	-2.16832700	-1.96173400
O	0.02254000	-2.85925800	-0.75989000
O	2.94849500	2.24395200	0.95801500
H	2.33228700	2.98301900	0.89924900

Name	**4- C9-H-OOH (water)**
Cartesian Coordinates	Frequency and Energy

C	-3.68368900	-0.12753600	0.00156400
C	-2.53284900	-0.87256800	0.31003100
C	-1.27064700	-0.29136800	0.32516900
C	-1.13554100	1.07026400	-0.04627500
C	-2.28636700	1.81980000	-0.34277900
C	-3.54175400	1.21375100	-0.31170700
C	-0.07224100	-1.09720200	0.71362900
C	0.19417800	1.67464700	-0.18430000
C	1.38879300	0.75738800	-0.13432900
C	1.21008500	-0.32193100	0.93863700
C	2.43605200	-1.26581000	1.03321300
H	2.14316900	-2.29319100	0.80667300
C	3.59227700	-0.88259900	0.12121400
C	3.91080100	0.60456000	0.19938500
C	2.69858400	1.53602400	0.02938100
H	-4.41353600	1.81199500	-0.55114100
H	4.47746400	-1.44499500	0.42933800
H	4.33644800	0.79100200	1.18907000
H	2.83158800	2.16528000	-0.85301700
H	4.68454300	0.84763000	-0.53234300
H	2.81630600	-1.26183600	2.05612300
H	0.13919000	-1.82650700	-0.27825900
C	-5.03148500	-0.78722800	0.01670900
H	-5.81009700	-0.07335800	-0.24686700
H	-5.06614000	-1.61695500	-0.69565600
H	-5.25829200	-1.19194600	1.00861800
O	-2.61295500	-2.21493900	0.59298700
H	-3.53014200	-2.49833000	0.69872300
O	-0.25335700	-1.97504800	1.78679700
H	-1.10151500	-2.43085400	1.67383700
O	3.26603600	-1.28538000	-1.22385300
H	3.97591200	-1.00229000	-1.81317600
O	-2.23973800	3.13177700	-0.67881800
H	-1.30426100	3.41643400	-0.64482900
O	0.33335600	2.88114500	-0.39741400
H	1.40402000	0.27817500	-1.12108700
H	1.08568600	0.19085600	1.90095200
O	0.86176800	-1.91316600	-2.28794500
H	1.78848100	-1.68603200	-2.04352900
O	0.43999400	-2.68123500	-1.22908300
O	2.64771700	2.37820900	1.18628800

Zero-point correction= 0.332313
(Hartree/Particle)
Thermal correction to Energy= 0.353940
Thermal correction to Enthalpy= 0.354884
Thermal correction to Gibbs Free Energy= 0.282740
Sum of electronic and zero-point Energies= -1184.288395
Sum of electronic and thermal Energies= -1184.266769
Sum of electronic and thermal Enthalpies= -1184.265824
Sum of electronic and thermal Free Energies= -1184.337969

H	2.00143000	3.07286800	1.00764600	
Name				**4- C9-H-OOH (pentyl ethanoate)**
Cartesian Coordinates				Frequency and Energy
C	-3.59037600	-0.07998100	-0.07022400	Zero-point correction= 0.333848
C	-2.43447300	-0.80295700	0.26826400	(Hartree/Particle)
C	-1.20320500	-0.17685100	0.37337100	Thermal correction to Energy= 0.355449
C	-1.07737600	1.18415700	0.01741400	Thermal correction to Enthalpy= 0.356393
C	-2.23094300	1.91811900	-0.30321300	Thermal correction to Gibbs Free Energy= 0.283834
C	-3.47300600	1.27688300	-0.33122100	Sum of electronic and zero-point Energies= -1184.274698
C	-0.03126200	-0.94822900	0.89339500	
C	0.25667500	1.77309100	-0.13560500	Sum of electronic and thermal Energies= -1184.253097
C	1.40182300	0.79092500	-0.19620600	
C	1.28345600	-0.20292400	0.97017900	Sum of electronic and thermal Enthalpies= -1184.252153
C	2.50006000	-1.15873100	1.05250900	
H	2.16429200	-2.19732200	1.09659800	Sum of electronic and thermal Free Energies= -1184.324712
C	3.48462200	-1.00212200	-0.09592200	
C	3.91174600	0.45181900	-0.29089400	
C	2.76668400	1.47783000	-0.22204400	
H	-4.34858400	1.86153100	-0.59024100	
H	4.37013400	-1.60504200	0.12397600	
H	4.62325000	0.70675100	0.49844600	
H	2.80639900	2.13742300	-1.09314900	
H	4.44772600	0.54117800	-1.23975900	
H	3.05219600	-0.96282700	1.97391200	
H	0.11186400	-1.86865800	0.05181000	
C	-4.91146700	-0.78623700	-0.14196500	
H	-5.70649900	-0.09218500	-0.41310500	
H	-4.87441200	-1.58991000	-0.88137200	
H	-5.15570500	-1.24694400	0.81812500	
O	-2.55164900	-2.15068400	0.53670200	
H	-1.90945900	-2.63178200	-0.01285300	
O	-0.25466700	-1.61435500	2.09073700	
H	-1.13263000	-2.01953100	2.06954500	
O	2.88019600	-1.53222500	-1.29540800	
H	3.52847500	-1.47458800	-2.00714000	
O	-2.18917200	3.22374100	-0.61391600	
H	-1.26553600	3.52557200	-0.52995500	
O	0.42730500	2.98198700	-0.27558700	
H	1.27030200	0.24663700	-1.14010700	
H	1.24064400	0.38258600	1.89629700	
O	0.33194900	-2.36950100	-1.96952900	
H	1.29266100	-2.19508900	-1.90957500	
O	0.05606800	-2.89241200	-0.72576600	
O	2.95442000	2.25402700	0.95866400	
H	2.33153500	2.98882700	0.91434700	
Name				**5-O5-H-OOH**
Cartesian Coordinates				Frequency and Energy
C	-3.50091100	1.14804200	-0.31048700	Zero-point correction= 0.362439
C	-2.24461300	1.79453300	-0.23213900	(Hartree/Particle)

C	-1.04695700	1.04838300	-0.10861500
C	-1.07438800	-0.35361500	-0.10902300
C	-2.33605600	-1.00173200	-0.14957800
C	-3.51680300	-0.22133000	-0.24613200
C	0.22214100	1.77483600	0.09544500
C	0.21473200	-1.16044700	-0.03387800
C	1.46296700	-0.33320200	-0.37136000
C	1.44332800	0.96312200	0.45517900
C	2.71830800	1.79119900	0.31427800
H	2.67444100	2.66794100	0.96152700
C	3.95195800	0.95745900	0.63620500
C	3.99433800	-0.28182300	-0.24646800
C	2.74554800	-1.13583600	-0.08680400
H	-4.45423200	-0.76578900	-0.28593300
H	3.91405800	0.65182000	1.68750200
H	4.07282500	0.01877400	-1.29980800
H	2.68987600	-1.48611300	0.95776300
H	4.87180400	-0.88711200	-0.01084900
H	2.79262600	2.15872400	-0.71741100
C	-4.74109200	1.98284500	-0.43872800
H	-5.62754200	1.35070900	-0.47586100
H	-4.82913500	2.67278500	0.40325600
H	-4.70097300	2.59284800	-1.34371300
O	-2.25559500	3.12213200	-0.26656700
H	-1.32393900	3.43549300	-0.20385100
O	5.13822000	1.72377600	0.52916800
H	5.25011400	1.98411300	-0.39011100
O	-2.46830500	-2.30835800	-0.13242900
H	-1.93859800	-2.72578600	0.72932800
O	0.15551500	-2.36059200	-0.78780400
H	1.45956700	-0.06948400	-1.43767500
H	1.31017900	0.67891900	1.51244200
C	-0.12364000	-2.21977100	-2.17154000
H	-1.01062000	-1.60361700	-2.34193400
H	0.73119600	-1.79615000	-2.70817600
H	-0.31974300	-3.22348800	-2.54454600
H	0.31682300	-1.50810300	1.00172500
O	0.28048000	2.99448400	0.00794600
O	2.89310100	-2.23776000	-0.95733100
H	2.09930200	-2.78037800	-0.87372800
O	-1.53731300	-2.87723800	1.96258300
O	-1.53673300	-1.59937300	2.44766500
H	-2.34615000	-1.53865300	2.97609400

Thermal correction to Energy= 0.385393
Thermal correction to Enthalpy= 0.386337
Thermal correction to Gibbs Free Energy= 0.310636
Sum of electronic and zero-point Energies= -1223.509021
Sum of electronic and thermal Energies= -1223.486068
Sum of electronic and thermal Enthalpies= -1223.485124
Sum of electronic and thermal Free Energies= -1223.560824

Name			**5-O5-H-OOH (water)**
Cartesian Coordinates			Frequency and Energy
C	-3.49411800	1.07065700	-0.29036600
C	-2.24279500	1.73135500	-0.28788500
C	-1.03167200	1.00860700	-0.18654900
C	-1.04868500	-0.39073900	-0.14500000

Zero-point correction= 0.360492 (Hartree/Particle)
Thermal correction to Energy= 0.383639
Thermal correction to Enthalpy= 0.384584

C	-2.29999700	-1.04785800	-0.08921400	Thermal correction to Gibbs Free Energy= 0.308297
C	-3.49467600	-0.29688900	-0.16742200	Sum of electronic and zero-point Energies= -
C	0.23802200	1.73742800	-0.00144100	1223.552130
C	0.23690100	-1.19711100	-0.14152300	Sum of electronic and thermal Energies= -
C	1.49239600	-0.35643700	-0.40735400	1223.528983
C	1.43603900	0.93289900	0.42942800	Sum of electronic and thermal Enthalpies= -
C	2.71821200	1.75620700	0.35442500	1223.528039
H	2.64659700	2.61995900	1.01783100	Sum of electronic and thermal Free Energies= -
C	3.92873100	0.91353200	0.72748100	1223.604325
C	4.01440000	-0.30995600	-0.17187100	
C	2.75809800	-1.15905200	-0.07327700	
H	-4.43250500	-0.84135100	-0.13645500	
H	3.84798800	0.59849000	1.77207000	
H	4.13961400	0.02140900	-1.21036300	
H	2.65699500	-1.53106400	0.95660400	
H	4.88069900	-0.91801800	0.10042800	
H	2.85331300	2.12706400	-0.66885700	
C	-4.75229300	1.87818500	-0.39431300	
H	-5.62344700	1.22451400	-0.37649200	
H	-4.82511900	2.58796300	0.43338400	
H	-4.76330700	2.45786800	-1.32047500	
O	-2.27044600	3.06462800	-0.36448900	
H	-1.34429900	3.39406900	-0.34474600	
O	5.12753900	1.68517000	0.65947400	
H	5.24651300	1.96539500	-0.25698100	
O	-2.38758800	-2.37160900	0.02254800	
H	-2.00642300	-2.66504100	0.98494100	
O	0.18351600	-2.31386500	-1.03160400	
H	1.53688200	-0.07796400	-1.46744200	
H	1.24321000	0.64548200	1.47521600	
C	-0.24272000	-2.03620300	-2.36285000	
H	-1.32430900	-1.88276700	-2.40361000	
H	0.26341500	-1.16188900	-2.77981600	
H	0.01522800	-2.91266400	-2.95589100	
H	0.33743100	-1.64935700	0.85268200	
O	0.29988900	2.95506400	-0.14690600	
O	2.92990200	-2.26319100	-0.96054100	
H	2.06589900	-2.69009300	-1.06085000	
O	-1.65877700	-2.65034700	2.28586300	
O	-1.51483400	-1.31975400	2.51202100	
H	-2.38304100	-1.00851900	2.82428400	

Name			**5-O5-H-OOH (pentyl ethanoate)**
Cartesian Coordinates			Frequency and Energy
C	-3.49666700	1.14803400	-0.30296300	Zero-point correction= 0.361540
C	-2.23846000	1.79246600	-0.23766500	(Hartree/Particle)
C	-1.03971000	1.04664200	-0.12190200	Thermal correction to Energy= 0.384636
C	-1.06915000	-0.35464800	-0.11974700	Thermal correction to Enthalpy= 0.385580
C	-2.33191000	-0.99952300	-0.14264900	Thermal correction to Gibbs Free Energy= 0.309012
C	-3.51330000	-0.22184000	-0.23230400	Sum of electronic and zero-point Energies= -

C	0.23166700	1.76961300	0.07984400	1223.540727
C	0.21771800	-1.16404900	-0.06390000	Sum of electronic and thermal Energies= -
C	1.47062900	-0.33610300	-0.38275200	1223.517631
C	1.44651200	0.95723300	0.44926500	Sum of electronic and thermal Enthalpies= -
C	2.72607800	1.78030000	0.32188400	1223.516687
H	2.67874900	2.65308900	0.97483100	Sum of electronic and thermal Free Energies= -
C	3.95067100	0.94058400	0.65933000	1223.593255
C	4.00075800	-0.29536500	-0.22706900	
C	2.74614200	-1.14233300	-0.08094200	
H	-4.45542300	-0.75948700	-0.25855300	
H	3.89928400	0.63321900	1.70901200	
H	4.09478000	0.01327800	-1.27650700	
H	2.67589400	-1.49166400	0.96178600	
H	4.87288800	-0.90423600	0.02243700	
H	2.81835600	2.14621600	-0.70868900	
C	-4.74075300	1.97635200	-0.42238000	
H	-5.62277800	1.33679300	-0.44824800	
H	-4.82903200	2.66728200	0.41961800	
H	-4.71703500	2.58142700	-1.33198500	
O	-2.24106100	3.12040700	-0.27590400	
H	-1.30319400	3.42109800	-0.21753000	
O	5.14458500	1.70517600	0.56084400	
H	5.24850700	1.97776200	-0.35790500	
O	-2.46094500	-2.31086100	-0.11667500	
H	-1.95572800	-2.71288700	0.74972300	
O	0.15760400	-2.34630700	-0.85217700	
H	1.47891400	-0.06508800	-1.44642700	
H	1.30149000	0.67215700	1.50434400	
C	-0.15139000	-2.16989300	-2.22727800	
H	-1.10678100	-1.65639700	-2.36471500	
H	0.63611000	-1.62114000	-2.75291200	
H	-0.22874000	-3.17018400	-2.65223700	
H	0.32015500	-1.53744700	0.96244500	
O	0.28825700	2.99118000	-0.01166100	
O	2.89671300	-2.25378400	-0.94836400	
H	2.06396400	-2.74320600	-0.92866400	
O	-1.57913800	-2.86671800	2.01808300	
O	-1.54826300	-1.58147000	2.47494300	
H	-2.38540100	-1.46639300	2.95482100	
Name				**5-C10-H-OOH**
Cartesian Coordinates				Frequency and Energy
C	3.70551500	-0.68214300	-0.21557900	Zero-point correction= 0.362551
C	2.53062400	-1.46161200	-0.31902000	(Hartree/Particle)
C	1.27303400	-0.85654300	-0.23831100	Thermal correction to Energy= 0.385549
C	1.15796400	0.55498000	-0.10708200	Thermal correction to Enthalpy= 0.386493
C	2.32773300	1.30940000	0.03077300	Thermal correction to Gibbs Free Energy= 0.310864
C	3.57761200	0.67849300	-0.03419600	Sum of electronic and zero-point Energies= -
C	0.06642300	-1.69823200	-0.18760800	1223.508348
C	-0.16939500	1.19658100	-0.05665100	Sum of electronic and thermal Energies= -

C	-1.36552200	0.34522900	-0.44841500	1223.485350
C	-1.22988000	-1.03284300	0.22353100	Sum of electronic and thermal Enthalpies= -
C	-2.43079600	-1.93592700	-0.04238900	1223.484406
H	-2.31381800	-2.88227000	0.48671300	Sum of electronic and thermal Free Energies= -
C	-3.72875900	-1.25505900	0.37283000	1223.560035
C	-3.87623900	0.08480400	-0.33616600	
C	-2.70032700	1.00689600	-0.05537900	
H	4.45878300	1.30409300	0.05888500	
H	-3.71418700	-1.08922800	1.45541500	
H	-3.93596000	-0.07745000	-1.42086200	
H	-2.66269700	1.22196800	1.02339500	
H	-4.79872600	0.57893100	-0.02558400	
H	-2.47194100	-2.17160600	-1.11421000	
C	5.03736300	-1.36676200	-0.29542200	
H	5.84970500	-0.64936400	-0.18388300	
H	5.12325700	-2.12958300	0.48167600	
H	5.14424700	-1.88200200	-1.25281800	
O	2.70038400	-2.78141300	-0.47453300	
H	1.81498800	-3.19475700	-0.53184700	
O	-4.85082600	-2.09056100	0.15260900	
H	-4.91631300	-2.27100500	-0.78990500	
O	2.33890300	2.64690000	0.25120800	
H	1.43600700	2.99029500	0.16659000	
O	-0.18809100	2.51877100	-0.55991700	
H	-1.37371800	0.20546700	-1.54093700	
H	-1.13675400	-0.85940700	1.30843700	
C	-0.02997600	2.62240000	-1.98234300	
H	0.84392000	2.05212700	-2.30966800	
H	-0.93068300	2.26897200	-2.48800200	
H	0.11940800	3.67935400	-2.19633300	
H	-0.32794900	1.39433400	1.20650100	
O	0.11033300	-2.89965500	-0.41450100	
O	-2.93731200	2.20018400	-0.78126400	
H	-2.27023400	2.84318900	-0.52028100	
O	0.61023400	0.51420700	2.80347000	
H	1.44727100	0.99821100	2.85913100	
O	-0.31573100	1.46803600	2.45744700	

Name				**5- C10-H-OOH (water)**
Cartesian Coordinates				Frequency and Energy
C	-3.67076300	0.79736100	-0.18031500	Zero-point correction= 0.360377
C	-2.48502100	1.55940000	-0.24472600	(Hartree/Particle)
C	-1.23324400	0.93765900	-0.20472500	Thermal correction to Energy= 0.383618
C	-1.13926700	-0.48045500	-0.15551600	Thermal correction to Enthalpy= 0.384562
C	-2.32200000	-1.22151400	-0.06347500	Thermal correction to Gibbs Free Energy= 0.308631
C	-3.56257400	-0.57502700	-0.08454000	Sum of electronic and zero-point Energies= -
C	-0.00942700	1.75088000	-0.12621400	1223.550426
C	0.17763300	-1.14534100	-0.13104400	Sum of electronic and thermal Energies= -
C	1.39396700	-0.29746800	-0.46172600	1223.527184
C	1.26851300	1.05123000	0.26854700	Sum of electronic and thermal Enthalpies= -

C	2.48793800	1.94564400	0.07146900	1223.526240
H	2.37423100	2.86421500	0.64921000	Sum of electronic and thermal Free Energies= -
C	3.75700300	1.22224900	0.49600500	1223.602171
C	3.90487400	-0.08306100	-0.27079700	
C	2.70586900	-0.99230000	-0.05636500	
H	-4.45721100	-1.18544800	-0.02303200	
H	3.71346900	1.01270500	1.56897300	
H	3.99476200	0.13995000	-1.34137600	
H	2.63387500	-1.25215200	1.00917800	
H	4.80973500	-0.60597400	0.04784500	
H	2.57403000	2.21973100	-0.98715100	
C	-4.99763000	1.49384400	-0.20746000	
H	-5.80984300	0.77087100	-0.14157900	
H	-5.08167000	2.19672700	0.62526000	
H	-5.11152100	2.07083700	-1.12867300	
O	-2.63483500	2.90131800	-0.32371200	
H	-1.74336200	3.30167800	-0.37585900	
O	4.90373000	2.05340300	0.32328900	
H	4.97656800	2.26617500	-0.61555600	
O	-2.34728800	-2.57864500	0.07388900	
H	-1.44887700	-2.93157700	-0.05061300	
O	0.18426700	-2.43302900	-0.71226800	
H	1.42318900	-0.11226800	-1.54557400	
H	1.15153900	0.83019200	1.34219600	
C	-0.01690400	-2.46495800	-2.13785700	
H	-0.93296600	-1.93279700	-2.40620600	
H	0.83720800	-2.02532100	-2.65510200	
H	-0.10800900	-3.51614600	-2.40400900	
H	0.29568600	-1.44004000	1.10013500	
O	-0.03456700	2.96576600	-0.31074400	
O	2.94675200	-2.17295900	-0.81714900	
H	2.18647100	-2.75833100	-0.70351000	
O	-0.99240600	-1.28435100	2.74298800	
H	-1.65510900	-1.96472900	2.53752700	
O	0.20234700	-1.81864800	2.32750100	

Name				**5-C10-H-OOH (pentyl ethanoate)**
Cartesian Coordinates				Frequency and Energy
C	-3.66133700	0.83562300	-0.16221800	Zero-point correction= 0.361188
C	-2.47390700	1.59949300	-0.20962000	(Hartree/Particle)
C	-1.22376200	0.97088100	-0.17801500	Thermal correction to Energy= 0.384396
C	-1.13538300	-0.44592800	-0.15355100	Thermal correction to Enthalpy= 0.385340
C	-2.31674600	-1.18772300	-0.07002700	Thermal correction to Gibbs Free Energy= 0.309535
C	-3.55630200	-0.53908700	-0.08401800	Sum of electronic and zero-point Energies= -
C	0.00006300	1.78112100	-0.06780600	1223.539348
C	0.17302200	-1.12347800	-0.16023300	Sum of electronic and thermal Energies= -
C	1.39883400	-0.27272100	-0.43664000	1223.516139
C	1.27552000	1.06339500	0.31750100	Sum of electronic and thermal Enthalpies= -
C	2.50233000	1.95203400	0.13305500	1223.515195
H	2.39461000	2.86592900	0.71870400	Sum of electronic and thermal Free Energies= -

C	3.77304100	1.21752000	0.54123700	1223.591000
C	3.90994300	-0.08382600	-0.23747300	
C	2.70410100	-0.98879700	-0.04088300	
H	-4.45178800	-1.14940700	-0.03187400	
H	3.73086500	0.99536800	1.61243600	
H	4.00605600	0.14141600	-1.30775200	
H	2.62982900	-1.25846100	1.02354700	
H	4.81036900	-0.61721000	0.07518800	
H	2.58104500	2.24492200	-0.92185400	
C	-4.98490600	1.53899700	-0.18575800	
H	-5.80359000	0.82141600	-0.13431500	
H	-5.06829600	2.23214900	0.65509900	
H	-5.09051800	2.13164400	-1.09805000	
O	-2.61295200	2.93242100	-0.26785300	
H	-1.71514600	3.32202700	-0.30041400	
O	4.91999500	2.04102300	0.38302100	
H	5.00454300	2.25807700	-0.55236200	
O	-2.32710200	-2.54054000	0.08026000	
H	-1.44689000	-2.88710900	-0.14783700	
O	0.16105300	-2.37199600	-0.82857800	
H	1.44558000	-0.05936400	-1.51566100	
H	1.15817400	0.82930000	1.38838200	
C	0.02384400	-2.30397600	-2.25809100	
H	-0.82161400	-1.66787100	-2.53448700	
H	0.94211400	-1.92958100	-2.71429800	
H	-0.15866500	-3.32383300	-2.59376200	
H	0.26053600	-1.54870500	1.06474400	
O	-0.02171100	2.99757800	-0.21468100	
O	2.93540100	-2.15282800	-0.81830600	
H	2.18418100	-2.74511700	-0.69832700	
O	-1.05548100	-1.58606800	2.66491900	
H	-1.76785200	-2.14401000	2.31073100	
O	0.09158800	-2.14368400	2.15339300	

Name				**Trolox-H-OOH** (gas)
Cartesian Coordinates				Frequency and Energy
C	-1.91851700	0.94223300	-0.63651500	Zero-point correction= 0.313503
C	-0.61618900	1.42081500	-0.60769000	(Hartree/Particle)
C	0.43886500	0.49222400	-0.59978000	Thermal correction to Energy= 0.334403
C	0.23235200	-0.89550000	-0.62778300	Thermal correction to Enthalpy= 0.335347
C	-1.07279800	-1.37726300	-0.61217100	Thermal correction to Gibbs Free Energy= 0.263330
C	-2.15246300	-0.46104100	-0.62350900	Sum of electronic and zero-point Energies= -995.726218
C	1.40343800	-1.84946300	-0.67742500	
C	2.69321600	-1.12306200	-1.03773600	Sum of electronic and thermal Energies= -995.705318
C	2.80167800	0.17249500	-0.24996700	Sum of electronic and thermal Enthalpies= -995.704374
H	1.52143100	-2.34694300	0.29161300	
H	3.56326000	-1.74382000	-0.82383500	Sum of electronic and thermal Free Energies= -995.776391
C	-1.34820200	-2.85420900	-0.61270500	
H	-1.13447200	-3.28770800	-1.59515700	
H	-0.71813100	-3.37149400	0.11436800	

H	-2.39423000	-3.04630800	-0.38542000
C	-0.34075400	2.90303600	-0.57205500
H	-0.60580500	3.36893500	-1.52540700
H	-0.93871000	3.38597400	0.20370300
H	0.71053700	3.11203800	-0.38742100
C	-3.09448000	1.87436300	-0.63416000
H	-2.88534600	2.77860800	-1.20623200
H	-3.97279400	1.38635900	-1.05348400
H	-3.33736100	2.16908500	0.39231900
C	4.05772000	0.96244400	-0.59329400
H	4.07929600	1.90861400	-0.04920600
H	4.94055400	0.38005600	-0.32775000
H	4.06788400	1.17266700	-1.66371500
H	2.70576900	-0.85937200	-2.09920200
H	1.20068100	-2.63658900	-1.40718100
C	2.82226700	-0.11648700	1.26579600
O	2.17324600	0.76711600	2.03408800
H	1.73152300	1.41609700	1.46859500
O	-3.39017300	-0.92577500	-0.64978000
H	-3.90297900	-0.64973900	0.27091300
O	1.70094300	1.03571300	-0.55182800
O	3.42560100	-1.03764100	1.73050700
O	-2.95467800	0.13925300	1.94416800
O	-4.14606600	-0.36579400	1.52501400
H	-2.53889500	-0.58295300	2.43911100

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

C	-1.90822200	0.98387200	-0.61749300
C	-0.59817800	1.44105000	-0.56881400
C	0.44234100	0.49430500	-0.57703800
C	0.21353900	-0.88988700	-0.61842700
C	-1.10022500	-1.35034700	-0.61632000
C	-2.16286400	-0.41505400	-0.63296800
C	1.37087300	-1.85958000	-0.66882700
C	2.66689400	-1.15325400	-1.04401700
C	2.81088100	0.14240800	-0.26344100
H	1.48129300	-2.35392700	0.30296000
H	3.53067300	-1.78821700	-0.84698700
C	-1.39488200	-2.82273100	-0.62659300
H	-1.21955000	-3.24745800	-1.62092300
H	-0.74770200	-3.35587600	0.07331200
H	-2.43412900	-3.01086900	-0.36445600
C	-0.29937500	2.91640300	-0.50300900
H	-0.47133900	3.39206600	-1.47371300
H	-0.95078600	3.40821800	0.22212200
H	0.73524000	3.10754900	-0.22454100
C	-3.06251600	1.94265800	-0.61568900
H	-2.84394300	2.82238700	-1.22320600
H	-3.96477700	1.46980300	-1.00038800

Zero-point correction= 0.312677 (Hartree/Particle)
Thermal correction to Energy= 0.333797
Thermal correction to Enthalpy= 0.334741
Thermal correction to Gibbs Free Energy= 0.261634
Sum of electronic and zero-point Energies= -995.753273
Sum of electronic and thermal Energies= -995.732154
Sum of electronic and thermal Enthalpies= -995.731210
Sum of electronic and thermal Free Energies= -995.804317

H	-3.27212100	2.28562400	0.40320300
C	4.06466600	0.91912900	-0.64183100
H	4.11765900	1.86378000	-0.09606300
H	4.95084900	0.32630900	-0.41126300
H	4.04289300	1.13090300	-1.71216800
H	2.66956500	-0.89118200	-2.10585300
H	1.15498100	-2.64787100	-1.39315200
C	2.86486500	-0.12835600	1.25277200
O	2.24356900	0.76641400	2.02797700
H	1.80657100	1.42880700	1.47109500
O	-3.41201600	-0.86143700	-0.70359300
H	-3.92588400	-0.63818500	0.21012100
O	1.70963700	1.01846500	-0.53671600
O	3.47184500	-1.04651500	1.72633000
O	-3.00889300	0.05553700	1.96048900
O	-4.19598400	-0.42245900	1.50816300
H	-2.57154400	-0.70559600	2.37888500

Name	**Trolox-H-OOH (**water) (anion)
Cartesian Coordinates	Frequency and Energy

C	-1.85551000	1.34558000	-0.31642900
C	-0.51294600	1.68768100	-0.22354400
C	0.46225200	0.69143700	-0.43703000
C	0.13742900	-0.63633900	-0.76026900
C	-1.20811400	-0.98241800	-0.84246700
C	-2.19466800	0.01151000	-0.64894900
C	1.23679000	-1.63990600	-1.02580600
C	2.56529900	-0.93528900	-1.27261200
C	2.79134300	0.13443200	-0.21141300
H	1.32849300	-2.32183900	-0.17201200
H	3.39208400	-1.64528900	-1.25647300
C	-1.65561600	-2.38882500	-1.12667600
H	-0.85948400	-3.10892900	-0.94732400
H	-2.50662100	-2.65027600	-0.49273600
H	-1.98540300	-2.49234700	-2.16529700
C	-0.04518200	3.07499500	0.12172900
H	-0.87551500	3.77371200	0.19576400
H	0.49230800	3.07318000	1.07450200
H	0.65002500	3.44707500	-0.63459700
C	-2.94415700	2.34873700	-0.04828600
H	-2.79669600	2.82488500	0.92356900
H	-2.94454800	3.14068700	-0.80240200
H	-3.92204400	1.87267400	-0.05343800
C	4.08625700	0.89958800	-0.42679700
H	4.19863900	1.68126700	0.32816700
H	4.93402400	0.21798700	-0.35778900
H	4.08101800	1.35992700	-1.41713800
H	2.55990400	-0.43948600	-2.24820000
H	0.97421200	-2.25294700	-1.88995400
C	2.78488500	-0.49687800	1.20896200

Zero-point correction= 0.299250 (Hartree/Particle)
Thermal correction to Energy= 0.320113
Thermal correction to Enthalpy= 0.321057
Thermal correction to Gibbs Free Energy= 0.248581
Sum of electronic and zero-point Energies= -995.318391
Sum of electronic and thermal Energies= -995.297528
Sum of electronic and thermal Enthalpies= -995.296584
Sum of electronic and thermal Free Energies= -995.369060

O	1.94185800	-0.09150400	2.04074700
O	-3.49122500	-0.32248100	-0.83351300
H	-3.84960900	-0.78552800	0.02192600
O	1.74590800	1.11753800	-0.31565000
O	3.65638700	-1.37956900	1.40744100
O	-2.73783900	-0.89630500	1.85347800
O	-3.94239400	-1.26869900	1.37830400
H	-2.14072800	-1.65241600	1.70451300

References

(1) Rimarčík, J.; Lukeš, V.; Klein, E.; Ilčin, M. Study of the Solvent Effect on the Enthalpies of Homolytic and Heterolytic N–H Bond Cleavage in P-Phenylenediamine and Tetracyano-P-Phenylenediamine. *J. Mol. Struct: THEOCHEM* **2010,** *952*, 25-30.

(2) Wright, J. S.; Johnson, E. R.; DiLabio, G. A. Predicting the Activity of Phenolic Antioxidants: Theoretical Method, Analysis of Substituent Effects, and Application to Major Families of Antioxidants. *J. Am. Chem. Soc.* **2001,** *123*, 1173-1183.

(3) Alvarez-Idaboy, J. R. l.; Galano, A. On the Chemical Repair of DNA Radicals by Glutathione: Hydrogen Vs Electron Transfer. *J. Phys. Chem. B* **2012,** *116*, 9316-9325.

(4) Galano, A.; Alvarez-Idaboy, J. R. Kinetics of Radical-Molecule Reactions in Aqueous Solution: A Benchmark Study of the Performance of Density Functional Methods. *J. Comput. Chem.* **2014,** *35*, 2019-2026.

(5) Galano, A.; Raúl Alvarez-Idaboy, J. Computational Strategies for Predicting Free Radical Scavengers' Protection against Oxidative Stress: Where Are We and What Might Follow? *Int. J. Quantum Chem.* **2019,** *119*, e25665.

(6) Thong, N. M.; Duong, T.; Pham, L. T.; Nam, P. C. Theoretical Investigation on the Bond Dissociation Enthalpies of Phenolic Compounds Extracted from Artocarpus Altilis Using Oniom (Rob3lyp/6-311++ G (2df, 2p): Pm6) Method. *Chem. Phys. Lett.* **2014,** *613*, 139-145.

(7) Thong, N. M.; Quang, D. T.; Bui, N. H. T.; Dao, D. Q.; Nam, P. C. Antioxidant Properties of Xanthones Extracted from the Pericarp of Garcinia Mangostana (Mangosteen): A Theoretical Study. *Chem. Phys. Lett.* **2015,** *625*, 30-35.

(8) Bartmess, J. E. Thermodynamics of the Electron and the Proton. *J. Phys. Chem.* **1994,** *98*, 6420-6424.

(9) Urbaniak, A.; Szeląg, M.; Molski, M. Theoretical Investigation of Stereochemistry and Solvent Influence on Antioxidant Activity of Ferulic Acid. *Comput. Theor. Chem.* **2013,** *1012*, 33-40.

(10) Donald, W. A.; Demireva, M.; Leib, R. D.; Aiken, M. J.; Williams, E. R. Electron Hydration and Ion–Electron Pairs in Water Clusters Containing Trivalent Metal Ions. *J. Am. Chem. Soc.* **2010,** *132*, 4633-4640.