Supporting Information (SI)

Mechanistic and Kinetic Studies of the Radical Scavenging Activity of 5-*O*-methyl-norbergenin: Theoretical and Experimental insights

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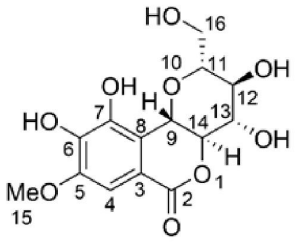
Table S1. Isolation and identification of 5-OMB from *Rourea harmandiana*

Isolation

The leaves of *R.harmandiana* were dried in shade and then ground into powder. The dried powders (2.0 kg) were extracted with MeOH at room temperature for 24 h (10 L×3 times). The extracts were combined and concentrated under reduced pressure to obtain a MeOH residue. Then, the MeOH residue was mixed with 1 liter of distilled water and extracted with ethyl acetate solvent (1L x3 times). The remaining aqueous solution was added to the Dianion column, eluted with water (100%), Water-MeOH (1:1) and MeOH (100%), respectively. After distillation of the solvents obtained the extract residue (32.8 g).

The aqueous residue (32.8 g) was separated on a silica gel column, eluted with the solvent system CH_2Cl_2/MeOH (0-100% MeOH) obtained 5 fractions (F1-F5). The F4 fraction (5.6 g) was separated on the Sephadex column with the eluent system CH_2Cl_2/MeOH (1/9) to obtain 2 sub-fractions F4.1 and F4.2. The sub-fraction F4.2 was purified on a silica gel reversed phase column, eluted with solvent system MeOH/water (1/3), then further purified on a normal phase silica gel column with EtOAc /MeOH (8/2) obtained **5OMB**.



5-O-Methyl-norBergenin (**5OMB**)

C	**5-OMB** (CD_3OD)	
	δ_C[a]	δ_H[b] (m, *J*, Hz)
2	166.3	-
3	119.3	-
4	107.1	7.24 (1H, s)
5	149.7	-
6	142.2	-
7	143.5	-
8	114.2	-
9	74.2	4.99 (1H, d, *J* = 10.5 Hz)
11	83.0	3.68 (1H, m)
12	71.9	3.46 (1H, t, *J* = 9.0 Hz)
13	75.6	3.84 (1H, t, *J* = 9.5 Hz)
14	81.3	4.09 (1H, d, *J* =9.5 Hz)

15-OMe	56.7	3.90 (3H, s)
16	62.7	4.04 (1H, dd, *J* =11.5 Hz, 1.5 Hz)
		3.71 (1H, m)

Identification

Compound **5-OMB** was isolated from the MeOH extract as a light brown solid. The ^{1}H and ^{13}C-NMR spectrum (Figure S1-S2) showed signals of a 1,2,3,4,5-pentasubstituted benzene ring with an aromatic proton signal at δ_H 7.24 (1H, s, H-4) and six signals of aromatic carbon at δ_C 149.7 (C-5), 143.5 (C-7), 142.2 (C-6), 119.3 (C-3), 114.2 (C-8), 107.1 (C-4). Combined with HSQC spectrum, a methoxy group (δ_C 56.7, δ_H 3.90, 3H, s), an oxymethylene group (δ_C 62.7, δ_H 4.04 and 3.71) and five oxymethine groups (δ_C 83.0, δ_H 3.84, 1H, m; δ_C 81.3, δ_H 4.09, 1H, d, *J* =9.5 Hz; δ_C 75.6, δ_H 3.84, 1H, t, *J* = 9.5 Hz; δ_C 74.2, δ_H 4.99, 1H, d, *J* = 10.5 Hz and δ_C 71.9, δ_H 3.46, 1H, t, *J* = 9.0 Hz) were observed. There was an ester carbonyl carbon at δ_C 166.3 (C-2). The NMR data of 5-OMB were very similar to those of bergenin [29]. In the HMBC spectrum (Figure S3-S4), the proton H-4 (δ_H 7.24) correlated with C-2 (δ_C 166.3), C-3 (δ_C 119.3), C-5 (δ_C 149.7), C-6 (δ_C 142.2) and C-8 (δ_C 114.2). Additionally, the correlations of H-9 (δ_H 4.99) to C-8 (δ_C 114.2) and C-7 (δ_C 143.5) and of H-15 (δ_H 3.90) to C-5 (δ_C 149.7) suggested the methoxy group was at C-5 position. The relative stereochemistry of compound 5-OMB was determined by comparison of the

NMR spectral data with those of bergenin[1] and the coupling constants observed in the ^{1}H-NMR spectrum. Thus, **5-OMB** was identified as 5-O-methyl-nor-bergenin. The NMR data are in the agreement with those reported in the literature.[2]

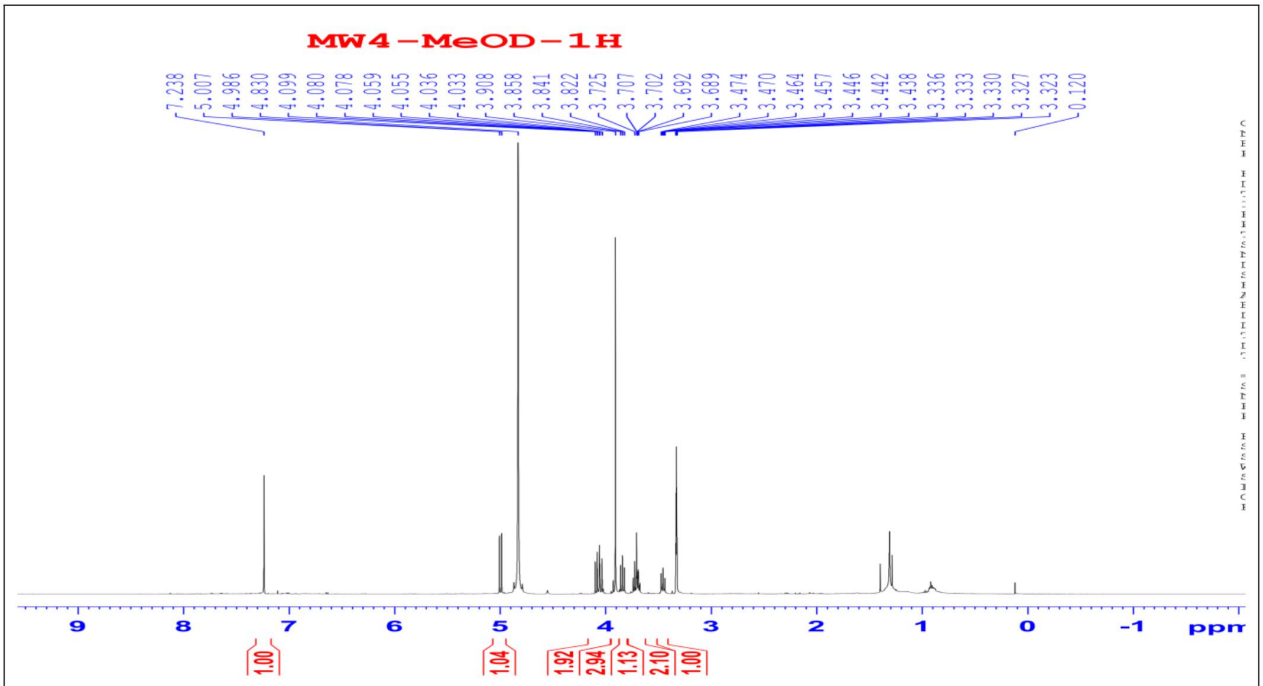


Figure S1. The 1H-NMR spectrum of compound 5OMB

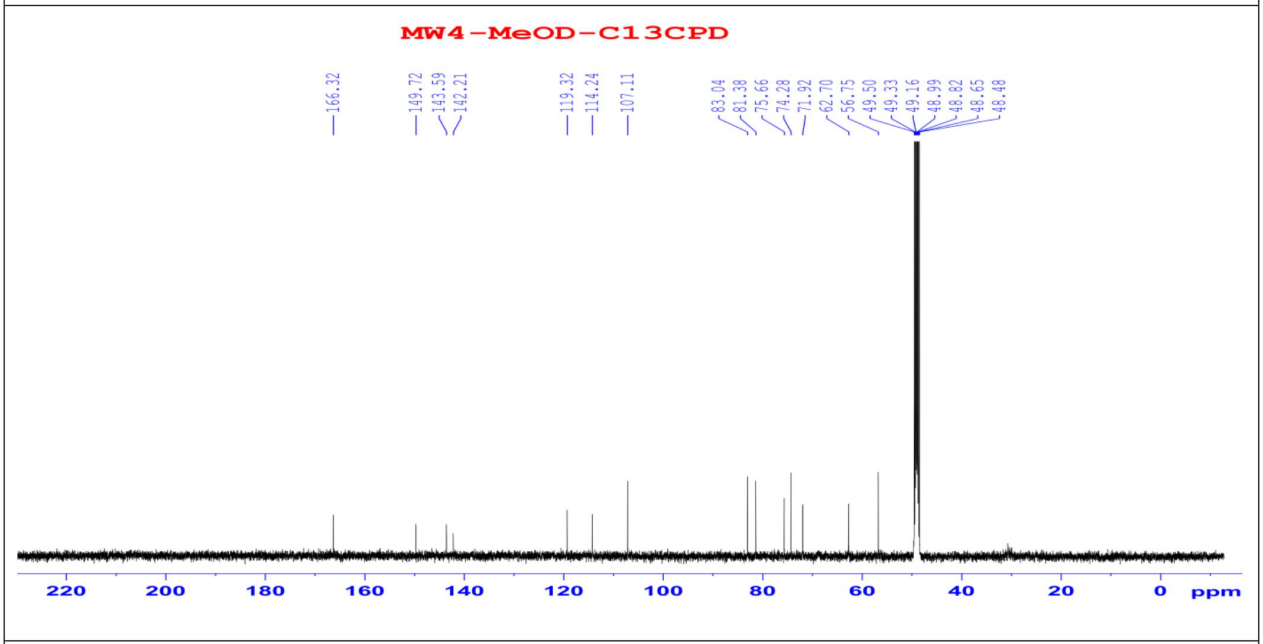


Figure S2. The 13C-NMR spectrum of compound 5OMB

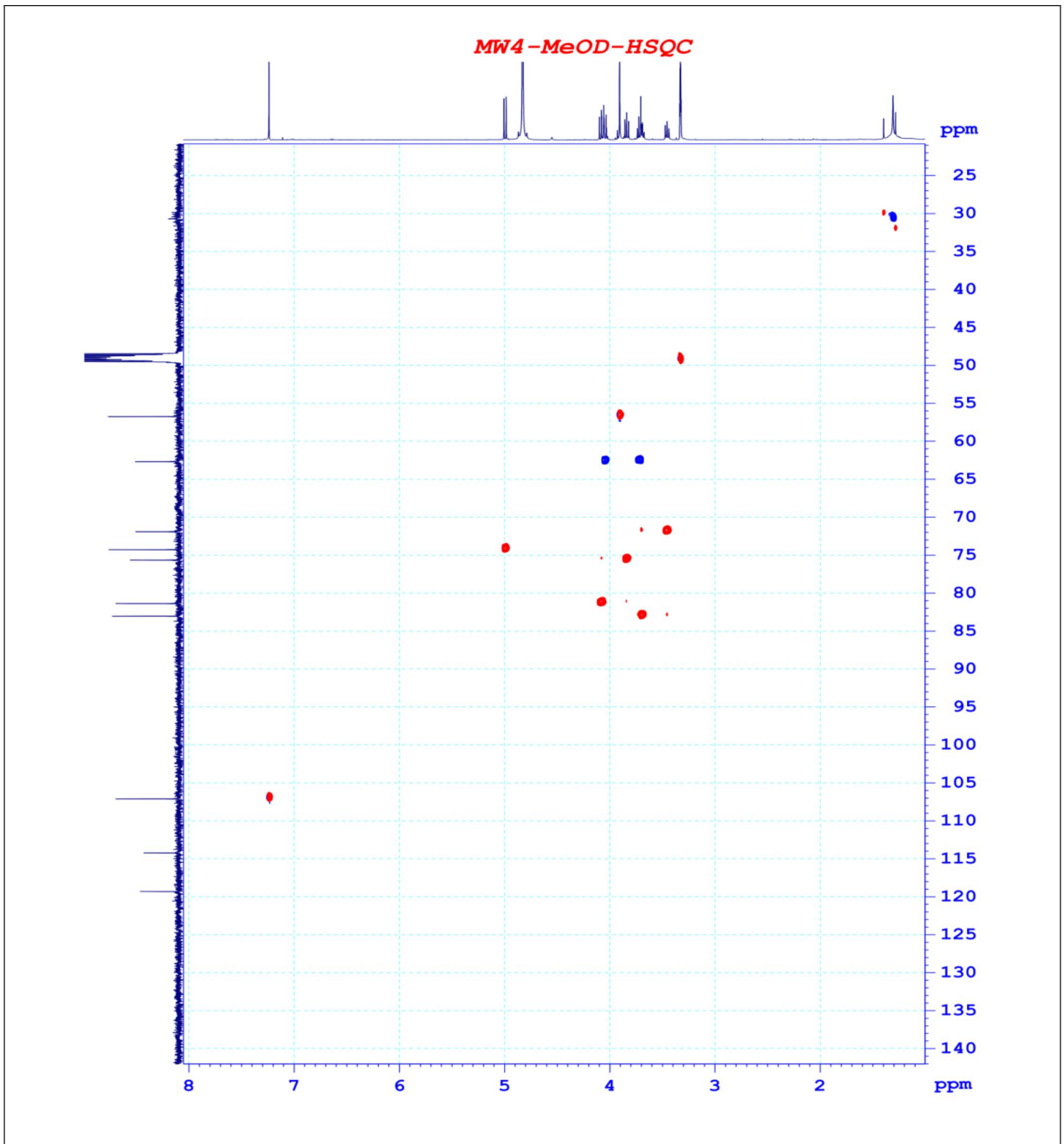


Figure S3. The HSQC spectrum of compound 5OMB

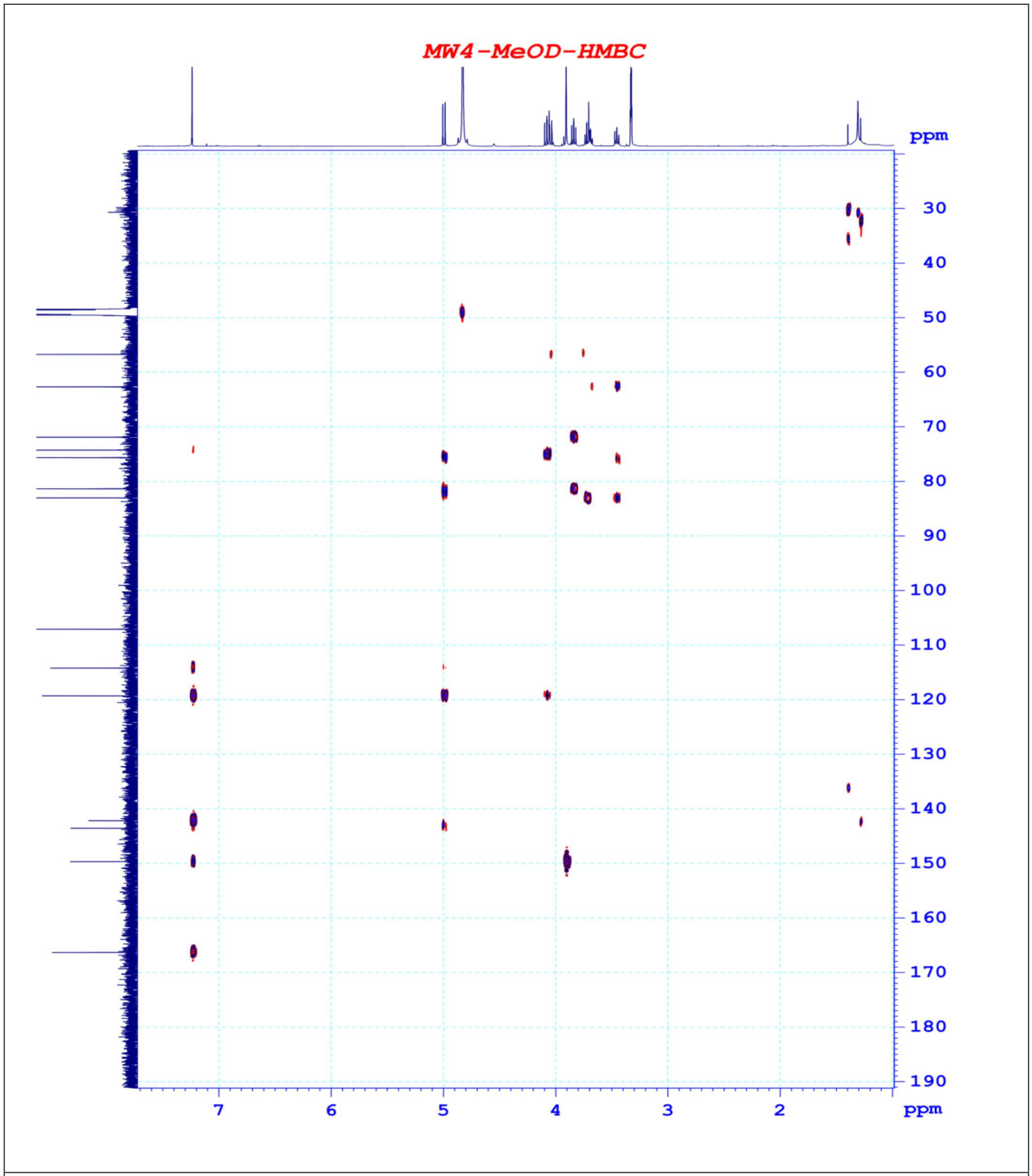


Figure S4. The HMBC spectrum of compound 5OMB

Table S2. 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) (at 298.15 K, 1M standard state) according to the equation (1):[3-7]

$$k = \sigma\kappa\frac{k_B T}{h}e^{-(\Delta G^{\neq})/RT} \quad (1)$$

Where: σ is the reaction symmetry number ,[8-9]

κ contains the tunneling corrections calculated using the Eckart barrier,[10]

k_B is the Boltzmann constant,

h is the Planck constant,

$\Delta G^{\neq}$ is the Gibbs free energy of activation.

The Marcus Theory was used to estimate the reaction barriers of SET reactions.[11-14] The free energy of reaction $\Delta G^{\neq}$ for the SET pathway was computed following the equations (2,3).

$$\Delta G_{SET}^{\neq} = \frac{\lambda}{4}\left(1 + \frac{\Delta G_{SET}^{0}}{\lambda}\right)^2 \quad (2)$$

$$\lambda \approx \Delta E_{SET} - \Delta G_{SET}^{0} \quad (3)$$

where ΔG_{SET} is the Gibbs energy of reaction, ΔE_{SET} is the non-adiabatic energy difference between reactants and vertical products for SET.[15-16]

For rate constants that were close to the diffusion limit a correction was applied to yield realistic results[17]. The apparent rate constants (k_{app}) were calculated following the Collins–Kimball theory in the solvents at 298.15K;[18] the steady-state Smoluchowski rate constant (k_D) for an irreversible bimolecular diffusion–controlled reaction was calculated following the literature as corroding to equations (4,5).[17, 19]

$$k_{app} = \frac{k_{TST}k_D}{k_{TST} + k_D} \quad (4)$$

$$k_D = 4\pi R_{AB} D_{AB} N_A \quad (5)$$

where R_{AB} is the reaction distance, N_A is the Avogadro constant, and $D_{AB} = D_A + D_B$ (D_{AB} is the mutual diffusion coefficient of the reactants A and B),[18, 20] where D_A or D_B is estimated using the Stokes–Einstein formulation (6).[21-22]

$$D_{A\ or\ B} = \frac{k_B T}{6\pi\eta a_{A\ or\ B}} \quad (6)$$

η is the viscosity of the solvents (i.e. $\eta(H_2O) = 8.91\times10^{-4}$ Pa s, η(pentyl ethanoate) = 8.62×10^{-4} Pa s) and *a* is the radius of the solute.

The kinetic study requires different considerations. Water (dielectric constants, ε = 78.35) and pentyl ethanoate (ε = 4.73) are the *de facto* standard solvents in the literature to mimic the polar and nonpolar environments in the human body.[17, 23-25] Thus, these solvents were used to model the physiological environments. The solvent cage effects were included following the corrections proposed by Okuno,[26] adjusted with the free volume theory according to the Benson correction[17, 27-29] to reduce over-penalizing entropy losses in solution. 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.[24-25] The hindered internal rotation treatment was also applied to the single bonds to ensure that the obtained conformer has the lowest electronic energy.[25, 30] 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 connected correctly with the pre-complex and post-complex.

Table S3: The calculated BDEs and IEs and ΔG^o (kcal/mol) of the 5-OMB + HOO• reactions according to the selected mechanisms (FHT and SET) in pentyl ethanoate and water.

Positions	Pentyl ethanoate				Water			
	FHT		SET		FHT		SET	
	BDE	G	IE	ΔG	BDE	G	IE	ΔG
O6–H	86.5	0.0	138.4	76.6	85.7	–4.1	115.4	35.4
O7–H	90.5	3.9			89.3	1.5		
C9–H	85.4	–0.9			87.1	–2.5		
C14–H	98.0	11.7			99.9	10.4		

Table S4: The Cartesian coordinates and energies of molecules, radicals, anions and radical cation of 5-OMB and TS of the reaction between 5-OMB with HOO• in the studied environments at the M06-2X/6-311++G(d,p) level of theory.

Name				**5OMB (gas phase)**
Cartesian Coordinates				Frequency and Energy
O	-1.48450200	1.03033200	0.07030400	Zero-point correction= 0.308302 (Hartree/Particle)
O	-0.48670000	-2.44987000	-0.32054400	Thermal correction to Energy= 0.329004
O	-3.20321900	-2.66347500	0.61151200	Thermal correction to Enthalpy= 0.329949
O	-4.81088000	-0.40497200	0.04121900	Thermal correction to Gibbs Free Energy= 0.259897
O	-2.93299100	3.37315500	-0.17158100	Sum of electronic and zero-point Energies= -1219.726876
O	0.69551500	2.56415900	-0.28675200	Sum of electronic and thermal Energies= -1219.706174
O	1.50531100	-3.39496600	-0.44628900	Sum of electronic and thermal Enthalpies= -1219.705230
O	4.80818900	0.48502200	0.29995400	Sum of electronic and thermal Free Energies= -1219.775282
C	-1.20686600	-1.33210400	0.18443700	
C	-0.75869900	-0.04759500	-0.49099700	
C	-2.68182500	-1.54834100	-0.07691000	
C	-3.45401700	-0.32700100	0.41160000	
C	-2.87961000	0.95366700	-0.19551800	
C	0.71082500	0.12151300	-0.25949400	
C	-3.50040900	2.20660700	0.39199100	
C	1.48870800	-1.03347400	-0.15690800	
C	0.88157300	-2.38452300	-0.30672200	
C	1.32960000	1.36478100	-0.17585700	
C	2.87102000	-0.95665600	0.01972100	
C	2.70915400	1.45044900	0.01932100	
C	3.48638500	0.28433100	0.11595800	
H	-1.02915300	-1.24337400	1.26315500	
H	-0.97264400	-0.10738400	-1.57076500	
H	-2.83995200	-1.65825200	-1.15962300	
H	-3.35079900	-0.27756200	1.50547700	
H	-3.04241400	0.93064200	-1.28439800	
H	-3.27594100	2.24045900	1.46041100	
H	-4.58514900	2.16546400	0.26264900	
H	-2.71486200	-3.44786800	0.33959900	
H	-5.13942200	-1.26567700	0.32371100	
H	3.43175700	-1.87932500	0.07295400	
H	-3.32552400	3.53145200	-1.03353400	
H	-0.26100000	2.45328300	-0.15721800	
O	3.30600500	2.65098100	0.11663100	
H	2.61815100	3.32671300	0.04987300	
C	5.62912700	-0.66176600	0.40457700	
H	5.33704100	-1.27773800	1.26037100	
H	5.58543700	-1.26154300	-0.50938400	
H	6.64085800	-0.29155500	0.54989800	
Name				**5-OMB-RAD-CATION (gas phase)**
Cartesian Coordinates				Frequency and Energy
O	-1.46845700	1.01306400	0.01274800	Zero-point correction= 0.307501 (Hartree/Particle)
O	-0.49419300	-2.47290700	-0.30105400	Thermal correction to Energy= 0.328309
O	-3.24008500	-2.60168900	0.73864500	Thermal correction to Enthalpy= 0.329253
O	-4.80921100	-0.34602300	0.04743500	Thermal correction to Gibbs Free Energy= 0.258427
O	-2.61725600	3.28683700	-0.27969200	Sum of electronic and zero-point Energies= -1219.439126
O	0.65251700	2.55007500	-0.21989400	Sum of electronic and thermal Energies= -1219.418318
O	1.51278700	-3.38693800	-0.51423400	Sum of electronic and thermal Enthalpies= -1219.417374
O	4.74611400	0.47478000	0.30882100	Sum of electronic and thermal Free Energies= -1219.488199

C	-1.22193500	-1.34965300	0.20871600
C	-0.78071400	-0.08662200	-0.51229100
C	-2.70945000	-1.55088500	-0.02654600
C	-3.45823600	-0.28365800	0.41162600
C	-2.87349100	0.96257700	-0.25071100
C	0.68195200	0.11700800	-0.29292100
C	-3.42723700	2.26494600	0.28322200
C	1.49230400	-1.04410900	-0.18718100
C	0.85112300	-2.41396900	-0.33465200
C	1.24647700	1.36052200	-0.16379800
C	2.86132600	-1.00254600	0.00275200
C	2.66117000	1.44279200	0.04853100
C	3.47772300	0.24335300	0.12481500
H	-1.02765600	-1.25348300	1.28303000
H	-0.98654200	-0.19667200	-1.59022300
H	-2.88402100	-1.71307700	-1.09956100
H	-3.34380700	-0.19313400	1.50204200
H	-3.02955200	0.91575700	-1.33669500
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H	-4.47468300	2.35261500	-0.01371500
H	-2.95133500	-3.44885900	0.38444000
H	-5.19402700	-1.14059100	0.43460700
H	3.41636200	-1.92984400	0.04842600
H	-3.03895600	4.14008700	-0.15156000
H	-0.32878200	2.47240000	-0.20459800
O	3.23933700	2.59474900	0.17546100
H	2.57795400	3.31047400	0.11098100
C	5.66225400	-0.63270600	0.39684300
H	5.39635900	-1.26001600	1.24859000
H	5.63703500	-1.20268000	-0.53274700
H	6.63846600	-0.18320100	0.54351400

Name			**5-OMB-O6-RAD (gas phase)**
Cartesian Coordinates			Frequency and Energy
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O	-4.79494000	-0.50766800	0.02742400
O	-3.27630600	3.34325400	-0.08821000
O	0.70320600	2.57186000	-0.46964200
O	1.59911700	-3.29158900	-0.46763100
O	4.84742400	0.51413900	0.36412500
C	-1.16844400	-1.30823700	0.15073100
C	-0.76530500	0.01876200	-0.47823400
C	-2.63346200	-1.56812900	-0.11454200
C	-3.44573000	-0.39626400	0.42017400
C	-2.89932500	0.92982600	-0.11811400
C	0.71343200	0.20185300	-0.27364500
C	-3.58952700	2.11581600	0.53191000
C	1.51535200	-0.94087200	-0.13966600
C	0.93201000	-2.30855800	-0.32384900
C	1.34318500	1.43601300	-0.25824000
C	2.91020600	-0.88956400	0.06787300
C	2.78640400	1.55946900	-0.02082500
C	3.54810300	0.32342900	0.15300500

Zero-point correction= 0.294738 (Hartree/Particle)
Thermal correction to Energy= 0.315478
Thermal correction to Enthalpy= 0.316423
Thermal correction to Gibbs Free Energy= 0.244969
Sum of electronic and zero-point Energies= -1219.091661
Sum of electronic and thermal Energies= -1219.070920
Sum of electronic and thermal Enthalpies= -1219.069976
Sum of electronic and thermal Free Energies= -1219.141429

H	-0.99114000	-1.25106800	1.23125200
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H	-2.79181500	-1.64107600	-1.20025600
H	-3.35860300	-0.39573900	1.51670300
H	-3.06858000	0.95538700	-1.20685700
H	-3.23820800	2.19319400	1.56305100
H	-4.66761700	1.92676400	0.54051400
H	-2.60867100	-3.48766800	0.20906500
H	-5.09899400	-1.38570600	0.28163400
H	3.43917800	-1.82941000	0.14167500
H	-3.68931000	3.36721500	-0.95464600
H	1.36623300	3.28179600	-0.38935500
O	3.28313900	2.68782000	0.00321600
C	5.66212600	-0.63564500	0.53121400
H	5.33079100	-1.22028200	1.39353700
H	5.64016700	-1.25750300	-0.36760000
H	6.66896000	-0.26412600	0.69984200

Name			**5-OMB-O7-RAD (gas phase)**
Cartesian Coordinates			Frequency and Energy
O	-1.50213200	1.03921000	0.19338400
O	-0.47429700	-2.40511200	-0.37401100
O	-3.19785300	-2.69316500	0.44484800
O	-4.82228200	-0.41637500	-0.05451300
O	-3.17676300	3.40455000	0.08678700
O	0.82326700	2.53089100	-0.62317000
O	1.53688100	-3.32001300	-0.37060500
O	4.85551800	0.46592900	0.37073200
C	-1.22212200	-1.30217600	0.13789300
C	-0.78383000	0.02503400	-0.46664200
C	-2.68439400	-1.52928100	-0.16644900
C	-3.48242800	-0.35133000	0.37870300
C	-2.89112800	0.98175300	-0.09514600
C	0.69654000	0.16387900	-0.26944500
C	-3.56625900	2.15137600	0.59901700
C	1.46266000	-0.96035700	-0.10524400
C	0.87380500	-2.32994900	-0.26816900
C	1.35915800	1.44994100	-0.33112900
C	2.87231500	-0.90880100	0.10523900
C	2.79392700	1.47259600	-0.06342000
C	3.53828700	0.29379400	0.15700000
H	-1.07353600	-1.25042700	1.22285600
H	-1.01334700	0.04382900	-1.54540400
H	-2.82110300	-1.57664400	-1.25643200
H	-3.42717500	-0.38981500	1.47665600
H	-3.04458000	1.05830500	-1.18416900
H	-3.26919000	2.14553600	1.65002300
H	-4.64977700	2.00432300	0.53946200
H	-2.70121500	-3.45382200	0.12586100
H	-5.15787300	-1.29053400	0.17159400
H	3.38991800	-1.85226500	0.21224900
H	-3.44269500	3.46285800	-0.83409900
O	3.38117200	2.64758600	-0.08079800
H	2.67773400	3.29415500	-0.28772600
C	5.63423200	-0.70074100	0.57068800

Zero-point correction= 0.294804 (Hartree/Particle)
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Thermal correction to Enthalpy= 0.316541
Thermal correction to Gibbs Free Energy= 0.244790
Sum of electronic and zero-point Energies= -1219.085353
Sum of electronic and thermal Energies= -1219.064560
Sum of electronic and thermal Enthalpies= -1219.063615
Sum of electronic and thermal Free Energies= -1219.135367

H	5.28916200	-1.25378100	1.44910800	
H	5.59906200	-1.34890800	-0.30967800	
H	6.65193800	-0.35524800	0.73108200	
Name				**5-OMB-C9-RAD (gas phase)**
Cartesian Coordinates				Frequency and Energy
O	-1.51450400	1.03093900	0.39339900	Zero-point correction= 0.294166 (Hartree/Particle)
O	-0.51868700	-2.46064600	-0.04926000	Thermal correction to Energy= 0.315205
O	-3.38330600	-2.64483800	0.21789900	Thermal correction to Enthalpy= 0.316149
O	-4.76051900	-0.31393700	-0.50343700	Thermal correction to Gibbs Free Energy= 0.244438
O	-2.75931000	3.39368300	-0.19537000	Sum of electronic and zero-point Energies= -1219.096178
O	0.69223400	2.56552300	0.07323100	Sum of electronic and thermal Energies= -1219.075139
O	1.45775900	-3.42268800	-0.20018700	Sum of electronic and thermal Enthalpies= -1219.074195
O	4.81958200	0.45099100	-0.07326800	Sum of electronic and thermal Free Energies= -1219.145905
C	-1.30781400	-1.38979300	0.45350900	
C	-0.71028300	-0.05002100	0.18851500	
C	-2.67713400	-1.49983400	-0.20236600	
C	-3.52458600	-0.29179700	0.16979200	
C	-2.79890000	0.98359500	-0.24160200	
C	0.67134600	0.10714200	0.09572900	
C	-3.51209400	2.25361100	0.17465200	
C	1.47283000	-1.06448200	0.04567100	
C	0.85056700	-2.40057100	-0.05279600	
C	1.32779400	1.36424500	0.06079100	
C	2.85963000	-0.98384600	-0.01421900	
C	2.70855000	1.43357900	0.00720200	
C	3.48855300	0.25560800	-0.02399300	
H	-1.43180100	-1.53586200	1.53978200	
H	-2.53622500	-1.51017000	-1.29203200	
H	-3.67282100	-0.28831000	1.26012600	
H	-2.64892300	0.97331900	-1.33004200	
H	-3.59261500	2.27475600	1.26368800	
H	-4.51804700	2.25847800	-0.25237600	
H	-2.87131200	-3.42568900	-0.01897500	
H	-5.13679000	-1.19363200	-0.38564700	
H	3.41867900	-1.90773000	-0.06751800	
H	-2.92261500	3.59655000	-1.11973100	
H	-0.26456400	2.45750300	0.19284300	
O	3.33388200	2.62599100	-0.01181000	
H	2.65765500	3.31437400	0.03286800	
C	5.64597500	-0.69716300	-0.10780700	
H	5.50123300	-1.31113300	0.78590200	
H	5.44681500	-1.29699200	-1.00060100	
H	6.66768400	-0.32723400	-0.13632000	
Name				**5-OMB-C14-RAD (gas phase)**
Cartesian Coordinates				Frequency and Energy
O	-1.47606200	1.01146700	0.05668300	Zero-point correction= 0.294133 (Hartree/Particle)
O	-0.50563300	-2.45615600	-0.32992300	Thermal correction to Energy= 0.315146
O	-3.15234200	-2.68936900	0.58870100	Thermal correction to Enthalpy= 0.316091
O	-4.81411700	-0.38157100	0.21185800	Thermal correction to Gibbs Free Energy= 0.244503
O	-2.91025800	3.36126800	-0.08772300	Sum of electronic and zero-point Energies= -1219.076988
O	0.68598800	2.54784600	-0.37682600	Sum of electronic and thermal Energies= -1219.055974
O	1.47997400	-3.41900800	-0.31025700	Sum of electronic and thermal Enthalpies= -1219.055030
O	4.78567800	0.48063300	0.34449900	Sum of electronic and thermal Free Energies= -1219.126618
C	-1.25904300	-1.34000700	-0.11079800	

C	-0.76000600	-0.02341300	-0.60091000
C	-2.73141000	-1.56353300	-0.14864800
C	-3.42685900	-0.34476600	0.45536600
C	-2.87860300	0.94341900	-0.15659800
C	0.70391500	0.10943300	-0.31237500
C	-3.46807200	2.18967100	0.47704000
C	1.47582800	-1.04190700	-0.16742100
C	0.87643500	-2.39074000	-0.26957100
C	1.32188100	1.35363200	-0.22997800
C	2.85509500	-0.96356900	0.04374100
C	2.69508000	1.44308100	-0.00254900
C	3.46957100	0.27718100	0.13100800
H	-0.93621000	0.08178600	-1.69087800
H	-3.06867900	-1.65827900	-1.19828700
H	-3.21213700	-0.34326900	1.53259400
H	-3.08509400	0.94234900	-1.23926600
H	-3.20301600	2.20091300	1.53652900
H	-4.55679200	2.16106700	0.38794400
H	-2.59498400	-3.44006900	0.35776100
H	-5.14361600	-1.23137800	0.52363000
H	3.41203900	-1.88517800	0.13720000
H	-3.34628400	3.54836000	-0.92244600
H	-0.26628400	2.44428500	-0.20945600
O	3.29005100	2.64357100	0.09087000
H	2.60327000	3.31850900	0.00477900
C	5.60189600	-0.66406000	0.50004800
H	5.28436000	-1.25865900	1.36180400
H	5.58347300	-1.28537500	-0.40028800
H	6.60948400	-0.29104800	0.66518500

Name	**5-OMB-O6-ANION (gas phase)**
Cartesian Coordinates	Frequency and Energy

O	-1.51584900	1.04982100	0.13694800
O	-0.51404900	-2.40451600	-0.36093900
O	-3.20839900	-2.66636700	0.48260200
O	-4.84765000	-0.39371000	0.02139200
O	-2.79551600	3.37752200	-0.08642800
O	0.70308700	2.57507400	-0.38730800
O	1.46267200	-3.39866100	-0.33404500
O	4.84307000	0.44212300	0.30988800
C	-1.22459600	-1.29103600	0.14607300
C	-0.76637700	0.01910800	-0.47570300
C	-2.69680600	-1.49829400	-0.13737100
C	-3.48415300	-0.30767700	0.39177200
C	-2.89457700	0.98288400	-0.17257800
C	0.70405700	0.16870300	-0.24324500
C	-3.47856700	2.25286100	0.41800200
C	1.46156100	-1.02544500	-0.11161100
C	0.87505600	-2.34481900	-0.26080700
C	1.34190500	1.38141500	-0.21661400
C	2.85788100	-0.93831400	0.06503500
C	2.76771800	1.51394400	-0.01831600
C	3.49454200	0.28030600	0.12757000
H	-1.06400000	-1.22057700	1.23016500
H	-0.98323900	0.01021000	-1.55726100

Zero-point correction= 0.295369 (Hartree/Particle)
Thermal correction to Energy= 0.315455
Thermal correction to Enthalpy= 0.316399
Thermal correction to Gibbs Free Energy= 0.247406
Sum of electronic and zero-point Energies= -1219.215221
Sum of electronic and thermal Energies= -1219.195135
Sum of electronic and thermal Enthalpies= -1219.194191
Sum of electronic and thermal Free Energies= -1219.263184

H	-2.84291200	-1.56239700	-1.22565800
H	-3.38566900	-0.29239500	1.48662900
H	-3.03241400	0.99431200	-1.26475800
H	-3.39509600	2.19801600	1.51250600
H	-4.53173200	2.34414400	0.14959900
H	-2.59257000	-3.38116100	0.28437600
H	-5.13475000	-1.28828700	0.23268800
H	3.40152200	-1.87093400	0.14253200
H	-1.84916100	3.16983800	-0.04968100
H	1.44128400	3.21253800	-0.31646400
O	3.26552200	2.66561500	0.00063800
C	5.60355900	-0.72736600	0.43705000
H	5.28888400	-1.32193000	1.30373800
H	5.53284800	-1.35512200	-0.45981500
H	6.63667800	-0.40907400	0.57387800

Name			**5-OMB-O7-ANION (gas phase)**
Cartesian Coordinates			Frequency and Energy
O	-1.50637000	1.03592100	0.18599100
O	-0.54679900	-2.41289000	-0.35764400
O	-3.26341800	-2.63301600	0.47550800
O	-4.86277100	-0.33120200	0.00522800
O	-2.68172900	3.39888600	-0.06358200
O	0.76265100	2.55601300	-0.47060900
O	1.42076200	-3.40578500	-0.36493400
O	4.81741900	0.41127000	0.33383100
C	-1.25456700	-1.28617900	0.14335600
C	-0.77678000	0.01885600	-0.46915000
C	-2.72968400	-1.47147800	-0.14153300
C	-3.50268300	-0.26860200	0.39293000
C	-2.87788300	1.01693200	-0.14573500
C	0.69142900	0.15204800	-0.25292700
C	-3.41415700	2.30861400	0.44331800
C	1.44558300	-1.02708600	-0.11029100
C	0.82781800	-2.36307300	-0.26825900
C	1.31475400	1.42334100	-0.27286300
C	2.82785800	-0.99037600	0.08057900
C	2.73335700	1.41494000	-0.03810900
C	3.46823800	0.25149700	0.13474600
H	-1.09577200	-1.22163800	1.22716100
H	-1.02165500	0.04542600	-1.54535300
H	-2.87840900	-1.52903000	-1.22954900
H	-3.41705800	-0.27014600	1.48895900
H	-3.00000400	1.04566600	-1.23957400
H	-3.33497100	2.25017100	1.53847900
H	-4.46262400	2.44474200	0.17331800
H	-2.67429400	-3.36426700	0.25984300
H	-5.16983200	-1.21878000	0.21728100
H	3.36306700	-1.92523000	0.15806500
H	-1.74092200	3.15008500	-0.05423900
O	3.30510100	2.63603800	-0.02888500
H	2.52905100	3.21214300	-0.20311500
C	5.57540400	-0.76003200	0.48726600
H	5.24631900	-1.34251300	1.35560500
H	5.52058800	-1.39597100	-0.40381500

Zero-point correction= 0.295137 (Hartree/Particle)
Thermal correction to Energy= 0.315247
Thermal correction to Enthalpy= 0.316191
Thermal correction to Gibbs Free Energy= 0.246981
Sum of electronic and zero-point Energies= -1219.210342
Sum of electronic and thermal Energies= -1219.190232
Sum of electronic and thermal Enthalpies= -1219.189288
Sum of electronic and thermal Free Energies= -1219.258498

H	6.60561300	-0.43895100	0.63774600	
Name				**5-OMB (pentyl ethanoate)**
Cartesian Coordinates				Frequency and Energy
O	-1.47739100	1.02619600	0.06679000	Zero-point correction= 0.307272 (Hartree/Particle)
O	-0.48254000	-2.45664700	-0.31087700	Thermal correction to Energy= 0.328100
O	-3.21651100	-2.64965200	0.64774900	Thermal correction to Enthalpy= 0.329044
O	-4.81185900	-0.39484500	0.04095600	Thermal correction to Gibbs Free Energy= 0.258836
O	-2.88578400	3.38181800	-0.17225600	Sum of electronic and zero-point Energies= -1219.756243
O	0.68120000	2.55143600	-0.28974900	Sum of electronic and thermal Energies= -1219.735416
O	1.50075400	-3.39703300	-0.48735900	Sum of electronic and thermal Enthalpies= -1219.734471
O	4.80369300	0.48701100	0.30678300	Sum of electronic and thermal Free Energies= -1219.804680
C	-1.20996700	-1.33536600	0.19516700	
C	-0.76161900	-0.05824800	-0.49402000	
C	-2.68761900	-1.54815200	-0.06199000	
C	-3.45353700	-0.31444200	0.41327500	
C	-2.87516200	0.96014500	-0.20378100	
C	0.70893900	0.11250300	-0.26754000	
C	-3.48300300	2.22068000	0.37955600	
C	1.49060700	-1.03934700	-0.16576900	
C	0.87553900	-2.38556100	-0.32068100	
C	1.32393600	1.35790400	-0.18139600	
C	2.87324900	-0.96002600	0.01412500	
C	2.70209000	1.44674000	0.01848400	
C	3.48388900	0.28351600	0.11578900	
H	-1.02471500	-1.24730800	1.27191500	
H	-0.97951400	-0.12400500	-1.57173800	
H	-2.84936000	-1.67302800	-1.14157800	
H	-3.35392400	-0.25229300	1.50640100	
H	-3.03166000	0.93487900	-1.29261000	
H	-3.28167600	2.24849100	1.45299100	
H	-4.56538500	2.20706000	0.22697600	
H	-2.82436600	-3.45966600	0.30221800	
H	-5.14864500	-1.24171100	0.35715300	
H	3.44536000	-1.87559100	0.07102800	
H	-3.23212300	3.51434700	-1.06072500	
H	-0.27676900	2.42115000	-0.17429800	
O	3.29642800	2.65045700	0.12138500	
H	2.60853300	3.32841300	0.06205400	
C	5.62739000	-0.66356500	0.42831000	
H	5.32763800	-1.27226300	1.28620500	
H	5.59633300	-1.26759300	-0.48290100	
H	6.63796000	-0.29149900	0.58239800	
Name				**5-OMB (water)**
Cartesian Coordinates				Frequency and Energy
O	-1.48209800	1.02673900	0.09047900	Zero-point correction= 0.306571 (Hartree/Particle)
O	-0.46615700	-2.44952700	-0.30949100	Thermal correction to Energy= 0.327679
O	-3.18115200	-2.66693400	0.67881000	Thermal correction to Enthalpy= 0.328623
O	-4.81350100	-0.41768000	0.01848300	Thermal correction to Gibbs Free Energy= 0.257788
O	-2.99220600	3.37872300	-0.20155300	Sum of electronic and zero-point Energies= -1219.772089
O	0.68174100	2.56159500	-0.30245700	Sum of electronic and thermal Energies= -1219.750981
O	1.51038500	-3.37955200	-0.53927100	Sum of electronic and thermal Enthalpies= -1219.750037
O	4.81424400	0.49439000	0.31808000	Sum of electronic and thermal Free Energies= -1219.820872
C	-1.20336200	-1.33001900	0.20353200	
C	-0.76062000	-0.04989200	-0.48418800	

C	-2.67979000	-1.55871700	-0.04751700
C	-3.45709200	-0.32768800	0.41584200
C	-2.88064800	0.95266400	-0.19332900
C	0.71326400	0.12283900	-0.26539100
C	-3.51349200	2.19792800	0.39239400
C	1.49859900	-1.02820300	-0.17047200
C	0.88209300	-2.36469400	-0.33968500
C	1.33246600	1.36642200	-0.18470500
C	2.88184300	-0.95609100	0.00995400
C	2.70917300	1.44929400	0.01949100
C	3.48737000	0.28642800	0.11818000
H	-1.00954800	-1.25059200	1.27837900
H	-0.98449200	-0.10872100	-1.55923300
H	-2.84384400	-1.70032300	-1.12274100
H	-3.38214900	-0.26378500	1.50949500
H	-3.02415400	0.93396900	-1.28269100
H	-3.27916300	2.25175400	1.45762800
H	-4.59757800	2.14387500	0.27166600
H	-2.88108300	-3.47861600	0.25316100
H	-5.18795900	-1.21061100	0.42168100
H	3.45738900	-1.86946200	0.06710200
H	-3.30819300	3.42462900	-1.11143600
H	-0.27713300	2.41131700	-0.21934800
O	3.32615400	2.65157200	0.12737700
H	2.66036200	3.35300700	0.06945700
C	5.63942500	-0.66243300	0.44201200
H	5.32598700	-1.26962600	1.29430600
H	5.60897200	-1.25788700	-0.47320900
H	6.64792800	-0.29057500	0.60542400

Name	**5-OMB-O6-RAD (pentyl ethanoate)**
Cartesian Coordinates	Frequency and Energy

O	-1.50499500	1.03461300	0.15922100	Zero-point correction= 0.293742 (Hartree/Particle)
O	-0.41502500	-2.39539400	-0.39376500	Thermal correction to Energy= 0.314518
O	-3.11136700	-2.72721000	0.53616900	Thermal correction to Enthalpy= 0.315462
O	-4.79664000	-0.50592100	0.02787700	Thermal correction to Gibbs Free Energy= 0.244359
O	-3.27311800	3.35434200	-0.03781500	Sum of electronic and zero-point Energies= -1219.122738
O	0.71539100	2.56819800	-0.53295000	Sum of electronic and thermal Energies= -1219.101963
O	1.59488100	-3.28889300	-0.50406500	Sum of electronic and thermal Enthalpies= -1219.101018
O	4.84003100	0.51121200	0.39326400	Sum of electronic and thermal Free Energies= -1219.172122
C	-1.16887700	-1.30647200	0.14891100	
C	-0.76659300	0.02017000	-0.48281600	
C	-2.63498500	-1.56673300	-0.11552300	
C	-3.44521700	-0.39382900	0.42189000	
C	-2.89878400	0.93557300	-0.11001400	
C	0.71453900	0.20256700	-0.28550400	
C	-3.58992800	2.11073700	0.55603900	
C	1.51736500	-0.94175000	-0.13918800	
C	0.92862200	-2.30429000	-0.33719200	
C	1.34926000	1.43169300	-0.29058600	
C	2.90758500	-0.89322000	0.08130400	
C	2.78933100	1.55428900	-0.04258500	
C	3.54682600	0.32137400	0.16253800	
H	-0.98464000	-1.25592100	1.22807600	
H	-1.00358600	0.00571000	-1.55873200	

H	-2.79517900	-1.64177800	-1.20000500
H	-3.36165100	-0.39556500	1.51825800
H	-3.06689300	0.97226800	-1.19785600
H	-3.25652500	2.16843300	1.59467900
H	-4.66921400	1.92938600	0.54703800
H	-2.69072400	-3.50012300	0.14293700
H	-5.10283800	-1.38088800	0.29414800
H	3.44338000	-1.82764500	0.17333300
H	-3.64384600	3.36996200	-0.92575500
H	1.37967000	3.27855000	-0.46649100
O	3.29249700	2.68291800	-0.03347600
C	5.65256000	-0.64291800	0.59688300
H	5.30561900	-1.20736000	1.46587500
H	5.64514700	-1.27923500	-0.29140500
H	6.65780300	-0.26984000	0.77528100

Name	**5-OMB-O6-RAD (water)**
Cartesian Coordinates	Frequency and Energy

O	-1.51308900	1.03858800	0.13589800
O	-0.42398800	-2.40026000	-0.36299800
O	-3.10404500	-2.71330700	0.63157300
O	-4.81036300	-0.49246800	0.02365000
O	-3.13339500	3.35475500	-0.10434100
O	0.68917000	2.57400400	-0.44836900
O	1.57350100	-3.28597600	-0.59324600
O	4.83414300	0.50087800	0.38144500
C	-1.17640600	-1.30239800	0.17696100
C	-0.76860200	0.00806200	-0.48255800
C	-2.64656000	-1.57029300	-0.06925200
C	-3.45743200	-0.37771700	0.42795200
C	-2.90848600	0.93181900	-0.14343000
C	0.71067800	0.19915800	-0.28048400
C	-3.58070400	2.13878700	0.47850100
C	1.51622200	-0.94828200	-0.16349000
C	0.91396100	-2.29910000	-0.37008600
C	1.33950600	1.42883000	-0.25277200
C	2.90562200	-0.90967700	0.04873100
C	2.77813800	1.54146900	-0.01399400
C	3.53756500	0.30599500	0.15205400
H	-0.97617000	-1.24361800	1.25181500
H	-1.00215000	-0.02841300	-1.55660900
H	-2.81258900	-1.69069800	-1.14687700
H	-3.38717500	-0.34423600	1.52325900
H	-3.06040700	0.94002500	-1.23242300
H	-3.32275700	2.18509700	1.53868800
H	-4.66414600	2.03602800	0.38417600
H	-2.75853500	-3.50167700	0.19653800
H	-5.16862600	-1.30050400	0.41091500
H	3.44845600	-1.84127500	0.12589000
H	-3.44936500	3.38653500	-1.01465400
H	1.33568000	3.29987600	-0.38008600
O	3.30005300	2.66641200	0.03024500
C	5.65565100	-0.65602300	0.57253200
H	5.30188100	-1.22901000	1.43159700
H	5.64836100	-1.27523000	-0.32617600

Zero-point correction= 0.293581 (Hartree/Particle)
Thermal correction to Energy= 0.314622
Thermal correction to Enthalpy= 0.315566
Thermal correction to Gibbs Free Energy= 0.243694
Sum of electronic and zero-point Energies= -1219.140977
Sum of electronic and thermal Energies= -1219.119937
Sum of electronic and thermal Enthalpies= -1219.118992
Sum of electronic and thermal Free Energies= -1219.190865

H	6.65671500	-0.27768700	0.75912200	
Name				**5-OMB-C9-RAD (pentyl ethanoate)**
Cartesian Coordinates				Frequency and Energy
O	-1.51107800	1.02194300	0.42796200	Zero-point correction= 0.293119 (Hartree/Particle)
O	-0.51787100	-2.46812300	-0.02113500	Thermal correction to Energy= 0.314267
O	-3.40889500	-2.63183000	0.19273900	Thermal correction to Enthalpy= 0.315212
O	-4.74786700	-0.29008100	-0.55617600	Thermal correction to Gibbs Free Energy= 0.243428
O	-2.68916800	3.40136100	-0.16604500	Sum of electronic and zero-point Energies= -1219.124924
O	0.67438600	2.55112600	0.09139700	Sum of electronic and thermal Energies= -1219.103776
O	1.45064000	-3.43303400	-0.17496900	Sum of electronic and thermal Enthalpies= -1219.102832
O	4.81127300	0.45290900	-0.09905400	Sum of electronic and thermal Free Energies= -1219.174615
C	-1.32363300	-1.39805200	0.47311600	
C	-0.71317300	-0.06022700	0.23335400	
C	-2.68092200	-1.49386800	-0.21478500	
C	-3.52554300	-0.27683500	0.14455100	
C	-2.78172600	0.99377300	-0.24735100	
C	0.66528900	0.09460500	0.12242400	
C	-3.48377100	2.27199100	0.15964500	
C	1.47110500	-1.07453100	0.06440000	
C	0.84298000	-2.40488900	-0.02716700	
C	1.31779900	1.35565700	0.07445200	
C	2.85860000	-0.98914000	-0.01265300	
C	2.69615800	1.42805700	0.00248500	
C	3.48233400	0.25245300	-0.03349900	
H	-1.46798500	-1.55415300	1.55425400	
H	-2.51978000	-1.50428800	-1.30097100	
H	-3.69792700	-0.27355300	1.23076200	
H	-2.59574700	0.98820100	-1.32979100	
H	-3.61345100	2.28142300	1.24422700	
H	-4.46853300	2.31338800	-0.31194600	
H	-2.96314700	-3.42153900	-0.13479400	
H	-5.14314100	-1.16113600	-0.42873700	
H	3.42893400	-1.90613200	-0.06907800	
H	-2.79430200	3.59433600	-1.10354000	
H	-0.28360900	2.43104200	0.20271900	
O	3.31887700	2.62366900	-0.03152900	
H	2.64422000	3.31483400	0.01808100	
C	5.64399200	-0.69796200	-0.14175800	
H	5.51393400	-1.30862700	0.75610800	
H	5.43633500	-1.29836400	-1.03179900	
H	6.66490900	-0.32514100	-0.18431600	
Name				**5-OMB-C9-RAD (water)**
Cartesian Coordinates				Frequency and Energy
O	-1.51495900	1.02609900	0.43176400	Zero-point correction= 0.292009 (Hartree/Particle)
O	-0.49952900	-2.46190700	-0.01095400	Thermal correction to Energy= 0.313654
O	-3.37986300	-2.65469400	0.20603300	Thermal correction to Enthalpy= 0.314599
O	-4.74631800	-0.31538100	-0.56840900	Thermal correction to Gibbs Free Energy= 0.241189
O	-2.80537200	3.41069500	-0.17942300	Sum of electronic and zero-point Energies= -1219.140404
O	0.67372200	2.56260100	0.08078100	Sum of electronic and thermal Energies= -1219.118759
O	1.46159900	-3.42146500	-0.19988900	Sum of electronic and thermal Enthalpies= -1219.117815
O	4.82399700	0.46232800	-0.09481800	Sum of electronic and thermal Free Energies= -1219.191225
C	-1.31756000	-1.39176200	0.47596900	
C	-0.70838600	-0.05108800	0.24234600	
C	-2.67293600	-1.50314900	-0.21286100	

C	-3.52468500	-0.29182800	0.14459100
C	-2.79238800	0.98847400	-0.23969000
C	0.66897700	0.10483300	0.12283300
C	-3.52597800	2.24223800	0.18340400
C	1.47919200	-1.06443000	0.06518700
C	0.85242700	-2.38416700	-0.03235200
C	1.32596100	1.36581400	0.06704300
C	2.86923600	-0.98373800	-0.01033200
C	2.70264200	1.43152700	-0.00274900
C	3.48720900	0.25577900	-0.03245100
H	-1.45870000	-1.54663800	1.55587700
H	-2.51590200	-1.52168000	-1.29769000
H	-3.70958300	-0.29148700	1.22718200
H	-2.60697300	0.99938800	-1.32064500
H	-3.62140300	2.25426100	1.27103600
H	-4.52399700	2.23985600	-0.26009400
H	-3.00625100	-3.42752900	-0.23367300
H	-5.17562300	-1.16059100	-0.38381500
H	3.44558000	-1.89702500	-0.06206800
H	-2.82166100	3.49120400	-1.14030400
H	-0.28396300	2.42000600	0.16833800
O	3.35063100	2.62452400	-0.04137600
H	2.70035900	3.34052700	0.00213000
C	5.65953000	-0.69395500	-0.12418600
H	5.51628000	-1.29378900	0.77731200
H	5.45127300	-1.29537300	-1.01177300
H	6.67985200	-0.32080600	-0.16199700

Name			**TS-5-OMB-O6-H-OOH-FHT (gas phase)**
Cartesian Coordinates			Frequency and Energy
O	1.72616300	-1.07274500	-0.06581900
O	1.23681700	2.52397400	-0.21186900
O	3.84078500	2.27816500	0.96286600
O	5.20637000	-0.12305900	0.30227700
O	2.78026100	-3.52984600	-0.47223400
O	-0.58994500	-2.18580700	-0.96473200
O	-0.59967500	3.74257200	-0.33829400
O	-4.43886200	0.38584300	-0.27958900
C	1.75268200	1.26816800	0.22665900
C	1.20588100	0.11651000	-0.60522000
C	3.26268200	1.30568500	0.11936600
C	3.82264400	-0.04732200	0.54849300
C	3.13960000	-1.16928900	-0.22838100
C	-0.29360600	0.14836200	-0.53260500
C	3.49911200	-2.56072700	0.25444100
C	-0.91734500	1.38627300	-0.31944600
C	-0.11185200	2.65316100	-0.27443900
C	-1.09839500	-0.97240000	-0.69840200
C	-2.30276900	1.53002100	-0.22982000
C	-2.50949800	-0.85802900	-0.60486800
C	-3.10770400	0.40935900	-0.35901600
H	1.46328400	1.11100400	1.27261200
H	1.53442600	0.22727100	-1.65167700
H	3.54337000	1.48891500	-0.92768900
H	3.60914400	-0.17584200	1.61981800

Zero-point correction= 0.320299 (Hartree/Particle)
Thermal correction to Energy= 0.343855
Thermal correction to Enthalpy= 0.344799
Thermal correction to Gibbs Free Energy= 0.266779
Sum of electronic and zero-point Energies= -1370.593663
Sum of electronic and thermal Energies= -1370.570106
Sum of electronic and thermal Enthalpies= -1370.569162
Sum of electronic and thermal Free Energies= -1370.647183

H	3.39004000	-1.07966800	-1.29522200
H	3.28252500	-2.62726400	1.32930200
H	4.56245900	-2.74122300	0.09928200
H	3.51793700	3.14652600	0.70093600
H	5.61820100	0.64321400	0.71584000
H	-2.70894600	2.52009600	-0.07786500
H	1.85528000	-3.25393300	-0.47274200
H	-1.34198300	-2.79045300	-1.06520500
O	-3.22148100	-1.94535600	-0.77089700
H	-3.84283700	-2.11946000	0.14211100
C	-5.09586600	1.57097300	0.14313900
H	-4.71799200	1.88724400	1.11875400
H	-4.96163200	2.37191300	-0.58833500
H	-6.14895000	1.31480900	0.21851800
H	-2.77980500	-1.62859400	2.47248500
O	-4.13986100	-2.24070100	1.36921300
O	-3.46906200	-1.20541900	1.93779000

Name			**TS-5-OMB-O6-H-OOH-FHT (pentyl ethanoate)**
Cartesian Coordinates			Frequency and Energy
O	1.71199200	-1.06530200	-0.08380800
O	1.22314100	2.53304400	-0.19199700
O	3.83287700	2.26056300	1.00676000
O	5.19633500	-0.12870400	0.29098900
O	2.72557200	-3.51567300	-0.51755900
O	-0.60152600	-2.16564600	-0.98852700
O	-0.60068800	3.75444600	-0.36010900
O	-4.44913400	0.39806000	-0.24349800
C	1.74158600	1.27149100	0.24178800
C	1.19309900	0.13343000	-0.60807400
C	3.25335800	1.30825800	0.13760200
C	3.81037000	-0.05532100	0.54114700
C	3.12429900	-1.16149100	-0.25538900
C	-0.30640000	0.16242000	-0.53132900
C	3.47860200	-2.56125200	0.20519500
C	-0.93080900	1.39878800	-0.30855800
C	-0.11839500	2.65981500	-0.27141900
C	-1.11181600	-0.95666400	-0.70334600
C	-2.31505100	1.54202500	-0.20755600
C	-2.52182100	-0.84384600	-0.59773800
C	-3.12069000	0.41998500	-0.33462500
H	1.44563000	1.11105300	1.28490300
H	1.52060800	0.25773500	-1.65220700
H	3.53734000	1.51374100	-0.90341800
H	3.60091900	-0.20623500	1.60984700
H	3.36802100	-1.05127300	-1.32150100
H	3.28463100	-2.64269800	1.28275100
H	4.53491600	-2.75946600	0.02354700
H	3.59313300	3.14425200	0.70558000
H	5.61063300	0.62408900	0.72904000
H	-2.73049200	2.52640700	-0.04412500
H	1.81080500	-3.20489700	-0.51378200
H	-1.34834800	-2.77705800	-1.09275600
O	-3.23843000	-1.92954700	-0.77816900
H	-3.78800900	-2.15645900	0.15641400

Zero-point correction= 0.318900 (Hartree/Particle)
Thermal correction to Energy= 0.342679
Thermal correction to Enthalpy= 0.343623
Thermal correction to Gibbs Free Energy= 0.265091
Sum of electronic and zero-point Energies= -1370.628264
Sum of electronic and thermal Energies= -1370.604485
Sum of electronic and thermal Enthalpies= -1370.603541
Sum of electronic and thermal Free Energies= -1370.682073

C	-5.10803700	1.60690700	0.12661200	
H	-4.74535900	1.95914100	1.09544400	
H	-4.95971400	2.37679000	-0.63447700	
H	-6.16418600	1.35868000	0.19627000	
H	-2.56375400	-1.73228600	2.39566900	
O	-4.02622500	-2.32264400	1.40794600	
O	-3.32598300	-1.30469700	1.96759100	
Name				**TS-5-OMB-O6-H-OOH-FHT (water)**
Cartesian Coordinates				Frequency and Energy
O	1.69242500	-1.05180400	-0.08560800	Zero-point correction= 0.318545 (Hartree/Particle)
O	1.16000300	2.54680900	-0.17702100	Thermal correction to Energy= 0.342479
O	3.77412400	2.31577900	0.99816800	Thermal correction to Enthalpy= 0.343424
O	5.17478900	-0.06398400	0.24671700	Thermal correction to Gibbs Free Energy= 0.264768
O	2.88986300	-3.51542000	-0.56752400	Sum of electronic and zero-point Energies= -1370.645772
O	-0.62618500	-2.15257400	-1.01242200	Sum of electronic and thermal Energies= -1370.621838
O	-0.66480300	3.75430500	-0.36364800	Sum of electronic and thermal Enthalpies= -1370.620894
O	-4.49296100	0.37416500	-0.17864400	Sum of electronic and thermal Free Energies= -1370.699550
C	1.70110000	1.28693000	0.24682200	
C	1.15589400	0.14886600	-0.60581400	
C	3.21079700	1.34966300	0.12882100	
C	3.78702800	-0.00696900	0.52281800	
C	3.10721400	-1.12504600	-0.26534400	
C	-0.34563100	0.16748000	-0.52163100	
C	3.51677700	-2.50337000	0.20772400	
C	-0.97997700	1.39623400	-0.28949700	
C	-0.17578300	2.65497000	-0.26088600	
C	-1.14903000	-0.95192900	-0.70691500	
C	-2.36459500	1.53336600	-0.17448000	
C	-2.55857700	-0.84648500	-0.59611900	
C	-3.16062000	0.40718500	-0.30111000	
H	1.41251000	1.12342000	1.29045300	
H	1.47796100	0.27703000	-1.64964900	
H	3.48255300	1.56681200	-0.91127600	
H	3.60346800	-0.16292600	1.59416900	
H	3.34024100	-1.01213100	-1.33271800	
H	3.25878200	-2.61161100	1.26721700	
H	4.59261400	-2.62889300	0.09128200	
H	3.62253700	3.19289300	0.62707400	
H	5.60237800	0.65221400	0.73247100	
H	-2.78875300	2.51040900	0.00820600	
H	1.93551400	-3.38259500	-0.50584300	
H	-1.35708700	-2.78251500	-1.12601400	
O	-3.28699500	-1.92811400	-0.79917800	
H	-3.68223700	-2.26627800	0.17207500	
C	-5.15616900	1.59787000	0.15265200	
H	-4.79246000	1.97807600	1.10912800	
H	-5.00108000	2.33843800	-0.63398700	
H	-6.21122900	1.34886300	0.22684300	
H	-2.16630400	-1.85135400	2.11100800	
O	-3.81189000	-2.44505500	1.45141200	
O	-3.04086700	-1.45191300	1.95116300	
Name				**TS-5-OMB-O7-H-OOH-FHT (gas phase)**
Cartesian Coordinates				Frequency and Energy
O	1.50488800	-0.80099100	-0.21603000	Zero-point correction= 0.319560 (Hartree/Particle)

O	0.47796600	2.69167800	-0.21575300	Thermal correction to Energy= 0.343379
O	3.16143500	2.82410600	0.78604000	Thermal correction to Enthalpy= 0.344324
O	4.81516600	0.66858700	-0.00462500	Thermal correction to Gibbs Free Energy= 0.265786
O	3.17732100	-3.08242200	-0.76804500	Sum of electronic and zero-point Energies= -1370.586447
O	-0.72643300	-2.26626800	-0.83626200	Sum of electronic and thermal Energies= -1370.562627
O	-1.52651200	3.61861100	-0.26432500	Sum of electronic and thermal Enthalpies= -1370.561683
O	-4.82005800	-0.28650400	0.12029000	Sum of electronic and thermal Free Energies= -1370.640221
C	1.20045700	1.52109600	0.16585900	
C	0.78085400	0.31431000	-0.66169400	
C	2.67524000	1.78383700	-0.03510900	
C	3.45305300	0.52521800	0.32903800	
C	2.90173100	-0.68463000	-0.42998300	
C	-0.69633200	0.12479400	-0.47131900	
C	3.53282900	-1.98244100	0.04204000	
C	-1.47302200	1.24337700	-0.23002500	
C	-0.87846400	2.61347300	-0.22577200	
C	-1.33155000	-1.13721900	-0.54718000	
C	-2.86713900	1.15173900	-0.04049600	
C	-2.72889200	-1.22554600	-0.31749900	
C	-3.50203500	-0.07462600	-0.06781800	
H	1.00105100	1.30413400	1.22214700	
H	0.99450300	0.50670800	-1.72700000	
H	2.85656600	2.01647500	-1.09452400	
H	3.33221000	0.35086800	1.40825600	
H	3.10314600	-0.53959700	-1.50401100	
H	3.14901900	-2.20201800	1.04066700	
H	4.61756300	-1.84728700	0.09642100	
H	2.67990200	3.63125700	0.57696000	
H	5.12432000	1.49102000	0.39038500	
H	-3.41190400	2.07212000	0.12162700	
H	3.61853800	-2.99832700	-1.61668800	
H	-0.07172400	-2.60174700	0.05070300	
O	-3.31151900	-2.42062900	-0.35200200	
H	-2.62032500	-3.05975100	-0.59377300	
C	-5.62968700	0.85161900	0.35205300	
H	-5.32030300	1.37403500	1.26219500	
H	-5.58968100	1.53996100	-0.49717200	
H	-6.64288600	0.47706800	0.47185500	
H	-0.98456600	-2.05683300	2.41236800	
O	0.16997700	-2.88406000	1.22189200	
O	-0.22944000	-1.76311900	1.87969900	

Name				**TS-5-OMB-ANION-O7-H-OOH-FHT (water)**
Cartesian Coordinates				Frequency and Energy
O	-1.53249200	0.88747700	0.06644900	Zero-point correction= 0.305981 (Hartree/Particle)
O	-1.01836800	-2.69063100	-0.24054300	Thermal correction to Energy= 0.327550
O	-3.70697100	-2.53218600	0.63726100	Thermal correction to Enthalpy= 0.328495
O	-5.03408000	-0.08615200	0.04765500	Thermal correction to Gibbs Free Energy= 0.252595
O	-2.58015700	3.37862200	-0.30923200	Sum of electronic and zero-point Energies= -1370.216970
O	0.79875900	1.94326600	-0.97598900	Sum of electronic and thermal Energies= -1370.195401
O	0.81691700	-3.91561200	-0.15454500	Sum of electronic and thermal Enthalpies= -1370.194456
O	4.66214700	-0.54826100	0.18045900	Sum of electronic and thermal Free Energies= -1370.270356
C	-1.56907800	-1.45283900	0.18692000	
C	-0.95219000	-0.25798800	-0.52499100	
C	-3.06027000	-1.48314500	-0.06333800	

C	-3.66833400	-0.16887900	0.40698100
C	-2.91430700	1.00094400	-0.22317200
C	0.53482300	-0.31064900	-0.34401000
C	-3.32244900	2.35891100	0.31337500
C	1.12119300	-1.55296500	-0.10353300
C	0.34961500	-2.80581900	-0.14825300
C	1.32937200	0.83977300	-0.52070500
C	2.52320500	-1.66562600	0.06002100
C	2.76347100	0.76394600	-0.27053500
C	3.31330600	-0.54698200	0.00612400
H	-1.37968600	-1.33288700	1.26106200
H	-1.20565500	-0.27844500	-1.59775000
H	-3.23999300	-1.58976800	-1.14299200
H	-3.55560400	-0.11462300	1.49931000
H	-3.06852500	0.98549400	-1.31273900
H	-3.17025700	2.36227300	1.40182800
H	-4.37842800	2.53635600	0.10525600
H	-3.22006400	-3.34275400	0.45201800
H	-5.44591800	-0.90980700	0.32876000
H	2.92807300	-2.65472200	0.22395100
H	-1.64563100	3.13123300	-0.25725700
H	1.18444100	2.93308600	-0.49665700
O	3.49689500	1.78924000	-0.31525800
C	5.26708000	-1.79003300	0.43279800
H	4.87815500	-2.24513900	1.35107100
H	5.11333600	-2.48707400	-0.39907600
H	6.33158400	-1.59243000	0.54828700
H	2.87470900	2.79523500	0.63851100
O	1.44245600	3.89888800	0.17644600
O	2.24324900	3.40435500	1.15608600

Name			**TS-5-OMB-C9-H-OOH-FHT (gas phase)**
Cartesian Coordinates			Frequency and Energy
O	-1.39532100	-0.85232800	-0.52230300
O	-0.37139200	2.54350700	0.29028000
O	-3.10503600	2.88535500	-0.62418500
O	-4.71544800	0.58935300	-0.36350600
O	-2.75389300	-3.18605000	-0.33971600
O	0.75112800	-2.46556700	-0.26650500
O	1.62997900	3.43197800	0.57369800
O	4.91344300	-0.40969100	-0.35227800
C	-1.10651200	1.52191400	-0.36877300
C	-0.64916800	0.14915100	0.07195800
C	-2.58355200	1.69620200	-0.07444900
C	-3.35397000	0.53916000	-0.71132900
C	-2.79251600	-0.78653300	-0.20617800
C	0.79765600	-0.02575200	-0.06948900
C	-3.41678300	-2.02738200	-0.80802000
C	1.59637400	1.12136400	0.02499200
C	0.99367500	2.45749000	0.30239500
C	1.40818400	-1.27338000	-0.22311400
C	2.98249100	1.03389300	-0.05823600
C	2.79433500	-1.36377000	-0.32883600
C	3.58839400	-0.20530400	-0.24509400
H	-0.94360100	1.60907100	-1.45256000

Zero-point correction= 0.320184 (Hartree/Particle)
Thermal correction to Energy= 0.343940
Thermal correction to Enthalpy= 0.344884
Thermal correction to Gibbs Free Energy= 0.267607
Sum of electronic and zero-point Energies= -1370.592488
Sum of electronic and thermal Energies= -1370.568732
Sum of electronic and thermal Enthalpies= -1370.567788
Sum of electronic and thermal Free Energies= -1370.645065

H	-0.86794000	0.01910200	1.32982300
H	-2.73895600	1.66772300	1.01306300
H	-3.22578300	0.59724500	-1.80235100
H	-2.90565200	-0.81737100	0.88483200
H	-3.29590000	-2.01894400	-1.89334300
H	-4.48474800	-2.03645200	-0.57163800
H	-2.66066000	3.63651500	-0.21752800
H	-5.02782000	1.48327000	-0.54263100
H	3.55949200	1.94337900	0.03465700
H	-2.73290800	-3.15916200	0.62335300
H	-0.20255900	-2.33127400	-0.41059900
O	3.38938600	-2.55599800	-0.50461200
H	2.69660600	-3.22502500	-0.58461200
C	5.75959200	0.72326800	-0.27258500
H	5.53998800	1.43293400	-1.07530500
H	5.65834900	1.22050600	0.69619500
H	6.77226200	0.34519500	-0.38546800
H	-0.19800400	-2.16910000	2.23617200
O	-1.10489600	-0.54166000	2.45475200
O	-1.11937100	-1.88384100	2.14418800

Name			**TS-5-OMB-C9-H-OOH-FHT (pentyl ethanoate)**
Cartesian Coordinates			Frequency and Energy
O	-1.39488800	-0.89162800	-0.47139900
O	-0.37751500	2.53388300	0.22888600
O	-3.12957600	2.83818200	-0.71055800
O	-4.72108600	0.54821100	-0.34778900
O	-2.77685100	-3.23592800	-0.36922300
O	0.75265000	-2.47619300	-0.26749600
O	1.60906100	3.42479400	0.55252800
O	4.90875600	-0.41458700	-0.37382100
C	-1.11688800	1.49812800	-0.41503100
C	-0.65563700	0.14181500	0.07196100
C	-2.59383600	1.67505700	-0.11652100
C	-3.36041600	0.49094900	-0.70667300
C	-2.79752100	-0.82756800	-0.17931100
C	0.79229600	-0.03806900	-0.06845800
C	-3.41225000	-2.05350800	-0.82273200
C	1.59179300	1.11107800	0.00999800
C	0.97922200	2.44389500	0.26908600
C	1.40395400	-1.28659100	-0.21579400
C	2.97748300	1.02713500	-0.08090000
C	2.79132600	-1.37242100	-0.32653100
C	3.58455100	-0.21385500	-0.25907400
H	-0.94945000	1.56436200	-1.49854800
H	-0.87100400	0.10179900	1.32841800
H	-2.74542400	1.69038000	0.97118500
H	-3.24523000	0.51682900	-1.80000300
H	-2.92851500	-0.86801500	0.90959600
H	-3.25861900	-2.01485400	-1.90343300
H	-4.48688500	-2.06359600	-0.62109800
H	-2.77984300	3.61288200	-0.25578000
H	-5.04295100	1.42889000	-0.57546800
H	3.56218600	1.93351900	-0.00700100
H	-2.96545300	-3.34474000	0.56954700

Zero-point correction= 0.318432 (Hartree/Particle)
Thermal correction to Energy= 0.342656
Thermal correction to Enthalpy= 0.343601
Thermal correction to Gibbs Free Energy= 0.264673
Sum of electronic and zero-point Energies= -1370.624818
Sum of electronic and thermal Energies= -1370.600594
Sum of electronic and thermal Enthalpies= -1370.599650
Sum of electronic and thermal Free Energies= -1370.678577

H	-0.20987300	-2.33834700	-0.32022500
O	3.38880800	-2.56604800	-0.49582300
H	2.70049300	-3.24329500	-0.55738900
C	5.75326700	0.72858300	-0.31809200
H	5.52571200	1.42280300	-1.13167100
H	5.65820400	1.23876200	0.64422300
H	6.76763000	0.35338500	-0.43266000
H	-0.03051500	-1.87755000	2.53871700
O	-1.08146000	-0.32732300	2.51950400
O	-0.96846600	-1.69098800	2.37144300

Name	**TS-5-OMB-C9-H-OOH-FHT (water)**
Cartesian Coordinates	Frequency and Energy

O	-1.48517600	-1.05959000	-0.38765900
O	-0.47635600	2.43428000	-0.08288500
O	-3.24837000	2.63215800	-0.92602500
O	-4.81669700	0.38212800	-0.19250100
O	-2.93496100	-3.32331400	0.17708500
O	0.71517600	-2.58305100	-0.07482300
O	1.48963000	3.36910600	0.18989400
O	4.84494200	-0.47700300	-0.46237700
C	-1.22845000	1.32429300	-0.58643100
C	-0.72690100	0.03029600	0.01975800
C	-2.68936400	1.53093000	-0.23510000
C	-3.47901400	0.28991100	-0.64428000
C	-2.87134900	-0.96613900	-0.02060200
C	0.71777400	-0.14206600	-0.14411700
C	-3.53095700	-2.23079100	-0.51114700
C	1.50269200	1.02174000	-0.18315800
C	0.87067100	2.35278600	-0.02683700
C	1.35510100	-1.38671900	-0.16779100
C	2.88893500	0.95826600	-0.28249500
C	2.74122200	-1.45505100	-0.28743000
C	3.51127000	-0.28354300	-0.34885400
H	-1.10449700	1.28527700	-1.67537900
H	-0.86445100	0.17175600	1.27519600
H	-2.78019000	1.67003800	0.84922100
H	-3.44728700	0.19866500	-1.73792700
H	-2.93651000	-0.90307800	1.07263500
H	-3.37702200	-2.32119800	-1.59159400
H	-4.60230200	-2.17493700	-0.30517800
H	-2.95070400	3.44730200	-0.50516200
H	-5.20282900	1.17902000	-0.57676900
H	3.46182200	1.87473200	-0.30541000
H	-3.32902700	-4.13813400	-0.15252900
H	-0.24777000	-2.44811300	-0.11086600
O	3.38052900	-2.64814300	-0.33811500
H	2.72728400	-3.36197300	-0.29110600
C	5.67233800	0.68551700	-0.51858800
H	5.41903000	1.29464300	-1.38885300
H	5.56969400	1.27407500	0.39560500
H	6.69124100	0.31778000	-0.60884400
H	1.03655800	0.72391400	2.75144600
O	-0.78070800	0.30762700	2.55803100
O	0.50345200	-0.08281100	2.84478800

Zero-point correction= 0.317297 (Hartree/Particle)
Thermal correction to Energy= 0.341991
Thermal correction to Enthalpy= 0.342935
Thermal correction to Gibbs Free Energy= 0.263081
Sum of electronic and zero-point Energies= -1370.644348
Sum of electronic and thermal Energies= -1370.619654
Sum of electronic and thermal Enthalpies= -1370.618710
Sum of electronic and thermal Free Energies= -1370.698564

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