Supporting Information (SI)

Insights into the mechanisms and kinetics of the hydroperoxyl radical scavenging activity of Artepillin C

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Table S1. 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):[1-5]

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

Where: σ is the reaction symmetry number ,[6, 7]

κ contains the tunneling corrections calculated using the Eckart barrier,[8]

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.[9-12] 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.[13, 14]

For rate constants that were close to the diffusion limit a correction was applied to yield realistic results[15]. The apparent rate constants (k_{app}) were calculated following the Collins–Kimball theory in the solvents at 298.15K;[16] 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).[15, 17]

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

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

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),[16, 18] where D_A or D_B is estimated using the Stokes–Einstein formulation (6).[19, 20]

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

η is the viscosity of the solvents (i.e. $\eta(H_2O) = 8.91\times10^{-4}$ Pa s, η(pentyl ethanoate) $= 8.62\times10^{-4}$ 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 ($\varepsilon = 4.73$) are the *de facto* standard solvents in the literature to mimic the polar and nonpolar environments in the human body.[15, 21-23] Thus, these solvents were used to model the physiological environments. The solvent cage effects were included following the corrections proposed by Okuno,[24] adjusted with the free volume theory according to the Benson correction[15, 25-27] 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.[22, 23] The hindered internal rotation treatment was also applied to the single bonds to ensure that the obtained conformer has the lowest electronic energy.[23, 28] 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 S2. The Calculated Free Energy (ΔG^{o}, in kcal/mol at 298.15 k) of the Reaction Between AC with $HOO^{\bullet}$ Radical via the Formal Hydrogen Transfer (FHT), Sequential Proton (SA), single electron transfer (SET) and radical adduct formation (RAF) Processes in the Gas Phase.

The Formal Hydrogen Transfer (FHT) mechanism: $R\text{-}H + HOO^{\bullet} \rightarrow R^{\bullet} + HOOH$

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

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

The radical adduct formation mechanism: $R\text{-}H + HOO^{\bullet} \rightarrow RH(HOO)^{\bullet}$

Positions	Mechanism			
	FHT	SA	SET	RAF
1OH	21.9	174.9	207.3	
10CH	-6.8	174.9	205.3	
7OH	-0.5	174.9	173.4	
C2				-2.9
C3				1.7
C11				1.8
C12				3.7

Table S3. Selected parameters at the bond critical points (BCPs) at intermolecular contacts for TS-C10-H-OOH and TS-O7-H-OOH (M06-2X/6-311++G(d,p)).

Contacts	ρ(r) (au)	$\nabla^2\rho(r)$ (au)	G(r)[a) (au)]	V(r)[b) (au)]	G(r)/|V(r)|	H(r)[c) (au)]	E_{HB}[d) (kcal/mol)]
TS-C10-H-OOH							
H10···O1'	0.1575	−0.0481	0.0909	−0.1939	0.4690	−0.1030	−60.8
H6···O1'	0.0102	0.0377	0.0082	−0.0070	1.1780	0.0012	−2.2
TS-O7-H-OOH							
H7···O1'	0.1403	−0.0134	0.0872	−0.1778	0.4906	-0.0906	−55.8
C11···O1'	0.0066	0.0222	0.0049	−0.0042	1.1547	0.0007	−1.3
H10···O1'	0.0082	0.0260	0.0060	−0.0054	1.0972	0.0005	−1.7
C7···O2'	0.0157	0.0530	0.0121	−0.0110	1.1006	0.0011	−3.5
C12···O2'	0.0083	0.0297	0.0065	−0.0055	1.1733	0.0010	−1.7
H13···O2'	0.0067	0.0252	0.0054	-0.0045	1.2081	0.0009	−1.4
RCP1 (C7-O7-H7-O1'-O2')	0.0146	0.0695	0.0155	−0.0136	1.1387	0.0019	−4.3
RCP2 (O2'-C12-C13-H13-O2')	0.0066	0.0268	0.0056	−0.0045	1.2420	0.0011	−1.4
RCP3 (O2'-C7-C8-C10-C11-C12-O2')	0.0056	0.0198	0.0043	−0.0037	1.1718	0.0006	−1.2

a) electron kinetic energy density; b) electron potential energy density; c) total electron energy density; d) individual energies of each hydrogen bond.

Table S4. Calculated ΔH (kcal/mol), ΔG≠ (kcal/mol), κ, k_{Eck} (M^{-1} s^{-1}) and branching ratios (Γ, %) at 298.15 K for the HOO• scavenging of the AC-ANION in the gas phase.

Mechanisms	Positions	DG≠	k	keck	Γ
HAT	O7-H	4.9	3.7	5.96×10^{9}	100.0
	C10-H	19.0	133.4	1.02×10^{1}	0.0
RAF	C2	17.8	2.6	1.44	0.0
	C3	18.1	1.4	0.518	0.0
	C11	18.0	1.6	0.663	0.0
	C12	18.5	1.5	0.253	0.0
$k_{overall}$				**5.96×10^{9}**	

Table S5: The cartesian coordinates and energies of TS of the reaction between AC with HOO• at the M06-2x/6-311++G(d,p) calculating method following the mechanisms in the studied environments

Name				**TS-AC-O7-H-OOH-FHT (gas phase)**
Cartesian Coordinates				Frequency and Energy
C	-0.20921700	-0.89840200	1.18448500	Zero-point correction= 0.401912 (Hartree/Particle)
C	1.17127300	-0.91251900	1.11476300	Thermal correction to Energy= 0.428623
C	1.88576700	0.00425500	0.32719400	Thermal correction to Enthalpy= 0.429568
C	1.17663400	0.96134300	-0.41814200	Thermal correction to Gibbs Free Energy= 0.342616
C	-0.20103600	1.02592800	-0.36864700	Sum of electronic and zero-point Energies= -1114.452812
C	-0.90914200	0.09822200	0.45286700	Sum of electronic and thermal Energies= -1114.426100
C	-0.98350300	2.06667600	-1.13326100	Sum of electronic and thermal Enthalpies= -1114.425156
C	-1.44037200	3.17516300	-0.21635700	Sum of electronic and thermal Free Energies= -1114.512107
C	-2.68980600	3.44347700	0.16754900	
C	-2.97010900	4.57403700	1.12187600	
C	-3.91246500	2.67988800	-0.25931100	
C	-0.99316100	-1.89826300	1.99931900	
C	-2.00228600	-2.65501200	1.15983000	
C	-1.69423900	-3.49499300	0.17145000	
C	3.34505400	-0.08736000	0.30486300	
O	-2.21687800	0.17274600	0.54079000	
C	-0.27991400	-3.83908900	-0.21000100	
C	-2.75889700	-4.10575700	-0.69476600	
C	4.18970000	0.75653700	-0.30181300	
C	5.67262500	0.65027700	-0.23727700	
O	6.38554800	1.59979800	-0.37970700	
O	6.19945100	-0.57076800	0.00795600	
H	1.72052900	-1.66130700	1.67843500	
H	1.70984800	1.66270800	-1.05036500	
H	-0.34093100	2.48155300	-1.91557800	
H	-1.84318600	1.60024900	-1.62037500	
H	-0.63555900	3.78845800	0.18396500	
H	-2.05642500	5.08615900	1.42480000	
H	-3.64375100	5.30518100	0.66462100	
H	-3.47115900	4.19710200	2.01894200	
H	-4.67185400	3.37104000	-0.63712800	
H	-3.71850000	1.92819800	-1.02184700	
H	-4.34204400	2.16764100	0.60709800	
H	-0.29174000	-2.58073500	2.48782700	
H	-1.52265300	-1.36209400	2.79072400	
H	-3.04782900	-2.43174300	1.34563700	
H	3.74983700	-0.92041300	0.87796800	
H	-2.67473200	-0.31000000	-0.35187300	
H	0.43025400	-3.65338200	0.59647500	
H	-0.20575200	-4.89110900	-0.49743800	
H	0.02509400	-3.23883400	-1.07425900	
H	-3.75629000	-3.79450800	-0.38390100	
H	-2.61215500	-3.79047700	-1.73299100	
H	-2.70405700	-5.19851900	-0.67281500	
H	3.84817900	1.64679700	-0.81553400	
H	5.52713800	-1.25282800	-0.08227300	
H	-1.25678800	-0.54571000	-2.43215900	
O	-2.84810100	-0.82761700	-1.50561100	
O	-1.59463500	-1.23289400	-1.83538900	
Name				**TS-AC-O7-H-OOH-FHT (pentyl ethanoate)**

Cartesian Coordinates				Frequency and Energy
C	-0.22524100	-0.91327200	1.16565100	Zero-point correction= 0.401277 (Hartree/Particle)
C	1.15602600	-0.92589500	1.10147800	Thermal correction to Energy= 0.428104
C	1.87007400	0.00366200	0.32693600	Thermal correction to Enthalpy= 0.429048
C	1.16364000	0.97196900	-0.40684200	Thermal correction to Gibbs Free Energy= 0.341122
C	-0.21490100	1.03235900	-0.36287000	Sum of electronic and zero-point Energies= -1114.485248
C	-0.92409600	0.08906700	0.43978900	Sum of electronic and thermal Energies= -1114.458422
C	-0.98882000	2.08965500	-1.11329600	Sum of electronic and thermal Enthalpies= -1114.457477
C	-1.41497300	3.20230400	-0.18629900	Sum of electronic and thermal Free Energies= -1114.545404
C	-2.65762100	3.52344800	0.18403600	
C	-2.90364900	4.66183400	1.13837800	
C	-3.90635200	2.81991900	-0.26804800	
C	-1.00402100	-1.92183300	1.97499200	
C	-1.99594300	-2.70059700	1.13532900	
C	-1.67014400	-3.57725600	0.18357500	
C	3.32945300	-0.08902500	0.30836500	
O	-2.23487600	0.16013800	0.52479400	
C	-0.25084800	-3.93106100	-0.16641500	
C	-2.71893000	-4.23457600	-0.66805800	
C	4.16783800	0.76215400	-0.29877500	
C	5.64635400	0.66082200	-0.24569500	
O	6.36064100	1.60920700	-0.43381400	
O	6.19363500	-0.53752000	0.03346500	
H	1.70593300	-1.67987900	1.65763600	
H	1.69733600	1.68624200	-1.02436900	
H	-0.34241300	2.49847100	-1.89520700	
H	-1.85667300	1.64192800	-1.60242500	
H	-0.59107300	3.78134800	0.22803400	
H	-1.97393000	5.14183200	1.44782300	
H	-3.54913400	5.41717600	0.67832400	
H	-3.42409500	4.30295300	2.03250800	
H	-4.59737900	3.53899400	-0.72034400	
H	-3.72494600	2.01909800	-0.98231100	
H	-4.41936100	2.38794700	0.59725400	
H	-0.29391600	-2.59108400	2.46828200	
H	-1.54639900	-1.39295100	2.76294300	
H	-3.04619800	-2.47626500	1.29564800	
H	3.72640100	-0.92923900	0.87623700	
H	-2.68505300	-0.30351800	-0.37521700	
H	0.45374100	-3.69304400	0.63140700	
H	-0.16657000	-4.99817100	-0.39195000	
H	0.05757600	-3.38434600	-1.06493200	
H	-3.72358500	-3.90621800	-0.39765500	
H	-2.54932000	-3.99133600	-1.72237300	
H	-2.66878700	-5.32488300	-0.57829600	
H	3.81682200	1.64816500	-0.81426900	
H	5.52670700	-1.23545400	0.02312500	
H	-1.26669300	-0.54331600	-2.44251800	
O	-2.86701900	-0.83406900	-1.53036700	
O	-1.61563700	-1.24232000	-1.86167300	
Name				**TS-AC-C10-H-OOH-FHT (gas phase)**
Cartesian Coordinates				Frequency and Energy
C	-1.20499500	-1.19969900	-0.76062500	Zero-point correction= 0.401153 (Hartree/Particle)
C	-1.79774000	0.05294200	-0.68116200	Thermal correction to Energy= 0.428915

C	-1.10815700	1.17400900	-0.21018700
C	0.21243300	1.01113900	0.21800400
C	0.83448600	-0.22914200	0.17062500
C	0.11938400	-1.32791800	-0.33409000
C	2.24591200	-0.42924400	0.64309000
C	3.22747100	-0.76997600	-0.39124200
C	4.45535200	-1.30145700	-0.18980900
C	5.36773800	-1.59447800	-1.34571700
C	5.00672300	-1.64175600	1.16468500
C	-1.96214500	-2.41148500	-1.25521400
C	-2.39835000	-3.28860800	-0.10843900
C	-3.63612200	-3.45043400	0.36370500
C	-1.79035800	2.47025700	-0.18227000
O	0.67269700	-2.56975000	-0.41272600
C	-4.86762200	-2.77638000	-0.17907100
C	-3.90139000	-4.35755200	1.53664500
C	-1.23284800	3.66613100	0.04161800
C	-1.97724200	4.95113400	0.00007700
O	-1.45003400	5.99712400	-0.24434200
O	-3.31096900	4.90255200	0.23882300
H	-2.82796400	0.16153100	-1.00914500
H	0.77354900	1.85274800	0.60744600
H	2.64384500	0.70930600	1.07045000
H	2.31609900	-1.01934800	1.56028700
H	2.94254800	-0.51937500	-1.41118300
H	4.90970200	-1.33856000	-2.30095000
H	6.30587700	-1.03882600	-1.24670100
H	5.63522500	-2.65592300	-1.35970600
H	5.16095500	-2.72249000	1.25036600
H	5.98952000	-1.17786000	1.29237500
H	4.37167300	-1.31298100	1.98499900
H	-2.81180700	-2.07953700	-1.85133100
H	-1.30824900	-2.99111300	-1.91263600
H	-1.58678700	-3.81695200	0.38646600
H	-2.85530500	2.41783500	-0.40738000
H	1.62176000	-2.52179300	-0.25227600
H	-4.66885100	-2.11927900	-1.02374000
H	-5.60113600	-3.52499600	-0.49446700
H	-5.34334400	-2.18219900	0.60767400
H	-2.98560900	-4.82470700	1.89979800
H	-4.35582700	-3.79817300	2.36062400
H	-4.60764200	-5.14722700	1.26114100
H	-0.16480000	3.78805900	0.17762600
H	-3.55056500	4.04401700	0.60033100
H	4.54698800	1.82843600	0.01387300
O	3.17871900	1.82629000	1.27735000
O	3.64645700	2.18184800	0.03993500

Thermal correction to Enthalpy= 0.429859
Thermal correction to Gibbs Free Energy= 0.336921
Sum of electronic and zero-point Energies= -1114.443210
Sum of electronic and thermal Energies= -1114.415448
Sum of electronic and thermal Enthalpies= -1114.414504
Sum of electronic and thermal Free Energies= -1114.507442

Name			**TS-AC-C2-H-OOH-RAF (gas phase)**
Cartesian Coordinates			Frequency and Energy
C	-0.85439600	1.11964900	-0.75174800
C	0.52501600	1.18491700	-0.66050500
C	1.27856200	0.18019300	-0.02925600
C	0.59299500	-0.92124100	0.51071800
C	-0.78644600	-1.02103800	0.44361500

Zero-point correction= 0.407165 (Hartree/Particle)
Thermal correction to Energy= 0.433996
Thermal correction to Enthalpy= 0.434941
Thermal correction to Gibbs Free Energy= 0.344687
Sum of electronic and zero-point Energies= -1114.452528

C	-1.50288000	0.00576000	-0.19864800	Sum of electronic and thermal Energies= -1114.425696
C	-1.52170800	-2.18931600	1.06702000	Sum of electronic and thermal Enthalpies= -1114.424752
C	-2.33609100	-2.96942700	0.06374400	Sum of electronic and thermal Free Energies= -1114.515005
C	-3.63779600	-3.27709200	0.12054900	
C	-4.28678000	-4.07856400	-0.97681200	
C	-4.57113700	-2.89949000	1.24122400	
C	-1.66789000	2.21952800	-1.39494100	
C	-2.37310200	3.06046900	-0.35820600	
C	-1.99212800	4.25433900	0.10076500	
C	2.71505300	0.30030600	0.02605900	
O	-2.85517800	-0.02280200	-0.29553700	
C	-0.76410800	5.00047700	-0.34636100	
C	-2.79193700	4.96541000	1.16025600	
C	3.56483700	-0.53330100	0.70891800	
C	5.02158200	-0.20094300	0.80575000	
O	5.59833500	-0.14132400	1.85152100	
O	5.63512900	0.07473400	-0.35825700	
H	1.04064300	2.04157300	-1.08506000	
H	1.15109900	-1.72260600	0.98247900	
H	-0.78151300	-2.85502900	1.51964200	
H	-2.14862000	-1.82188800	1.88333100	
H	-1.77347200	-3.31032800	-0.80350200	
H	-3.57921400	-4.33235400	-1.76608200	
H	-4.70365600	-5.00600100	-0.57271600	
H	-5.11911300	-3.52292100	-1.41912200	
H	-5.44499000	-2.37416800	0.84352400	
H	-4.94578200	-3.80501400	1.72772100	
H	-4.11399100	-2.27317200	2.00505600	
H	-1.01215700	2.82552700	-2.02024200	
H	-2.41740900	1.76648300	-2.04906700	
H	-3.26434500	2.60557300	0.06632900	
H	3.15362800	1.09684700	-0.57082900	
H	-3.17325800	-0.93064200	-0.19305900	
H	-0.21290000	4.49670300	-1.13845600	
H	-1.03499300	6.00000600	-0.70006900	
H	-0.08513600	5.13894900	0.50108700	
H	-3.66393900	4.38556500	1.46377700	
H	-2.17548000	5.15433700	2.04483000	
H	-3.13277800	5.93987800	0.79642900	
H	3.20341800	-1.18090200	1.49722900	
H	5.13309800	-0.29667000	-1.09999100	
H	3.05711300	-1.65613900	-2.18905400	
O	3.72731700	-2.13950600	-0.51319400	
O	3.94113100	-1.71703100	-1.79916300	

Name				**TS-AC-C2-H-OOH-FHT (pentyl ethanoate)**
Cartesian Coordinates				Frequency and Energy
C	-0.82504300	1.11831300	-0.76631600	Zero-point correction= 0.406870 (Hartree/Particle)
C	0.55182700	1.15249100	-0.63318600	Thermal correction to Energy= 0.433454
C	1.26125300	0.13790700	0.03756300	Thermal correction to Enthalpy= 0.434399
C	0.52955500	-0.92712700	0.59534200	Thermal correction to Gibbs Free Energy= 0.346323
C	-0.84823400	-0.99469900	0.48832400	Sum of electronic and zero-point Energies= -1114.486916
C	-1.51739700	0.03065700	-0.21007100	Sum of electronic and thermal Energies= -1114.460331
C	-1.63358800	-2.12456800	1.12133800	Sum of electronic and thermal Enthalpies= -1114.459387
C	-2.41983700	-2.92104200	0.10748000	Sum of electronic and thermal Free Energies= -1114.547463

C	-3.73155400	-3.19421600	0.11211400
C	-4.34707100	-4.01694000	-0.98771000
C	-4.71053000	-2.74672200	1.16461700
C	-1.58808800	2.21949100	-1.46768000
C	-2.36912700	3.07425800	-0.49534300
C	-1.93404400	4.18461500	0.10750400
C	2.69620800	0.22712300	0.10626800
O	-2.86125300	0.02579700	-0.35794100
C	-0.56643500	4.78052100	-0.08492400
C	-2.80564500	4.93342600	1.07965900
C	3.54286700	-0.69677800	0.67176700
C	4.98051400	-0.35640300	0.88237100
O	5.53181800	-0.49678500	1.94038800
O	5.63283600	0.15524900	-0.17164800
H	1.10319900	1.98221600	-1.06609300
H	1.04217000	-1.71836500	1.13127400
H	-0.92444000	-2.78760700	1.62465800
H	-2.28570400	-1.71679400	1.89815600
H	-1.82586400	-3.30932900	-0.71851200
H	-3.60829900	-4.31996400	-1.73065500
H	-4.81327100	-4.91614000	-0.57244500
H	-5.13926200	-3.45335900	-1.49079600
H	-5.52654600	-2.18206200	0.70138500
H	-5.16688400	-3.62242500	1.63686100
H	-4.26997900	-2.13340900	1.94933700
H	-0.88128500	2.82102000	-2.04056500
H	-2.28518600	1.76970600	-2.17934800
H	-3.36507800	2.71382200	-0.25085300
H	3.13713300	1.09318200	-0.38298100
H	-3.20772800	-0.86483900	-0.19883900
H	0.01293100	4.29264400	-0.86780500
H	-0.64654600	5.84494100	-0.32759900
H	0.00293500	4.71221900	0.84852300
H	-3.77407500	4.44845800	1.21199800
H	-2.31620000	5.00546700	2.05666700
H	-2.97429700	5.95880600	0.73429000
H	3.17211000	-1.47267900	1.32933200
H	5.15855700	-0.05350700	-0.99374300
H	3.28986600	-1.27812000	-2.40863500
O	3.86104400	-2.05476500	-0.79974600
O	4.14780000	-1.39146300	-1.96959200

Name	**TS-AC-C3-H-OOH-RAF (gas phase)**
Cartesian Coordinates	Frequency and Energy

C	-0.64915700	1.06046600	-0.93637600
C	0.72652800	0.88205300	-0.94848500
C	1.32446900	-0.26462600	-0.41796000
C	0.50730000	-1.23098600	0.17544700
C	-0.87436300	-1.08154100	0.22271900
C	-1.44245900	0.06361600	-0.35453300
C	-1.75574100	-2.10967400	0.90077600
C	-2.74442200	-2.73763100	-0.05166900
C	-4.07510100	-2.81331700	0.07358800
C	-4.90920100	-3.48734900	-0.98368800
C	-4.86990800	-2.27995000	1.23704500

Zero-point correction= 0.407154 (Hartree/Particle)
Thermal correction to Energy= 0.433870
Thermal correction to Enthalpy= 0.434815
Thermal correction to Gibbs Free Energy= 0.345735
Sum of electronic and zero-point Energies= -1114.450260
Sum of electronic and thermal Energies= -1114.423544
Sum of electronic and thermal Enthalpies= -1114.422600
Sum of electronic and thermal Free Energies= -1114.511680

C	-1.29600400	2.30877600	-1.49132000
C	-1.73878100	3.23318400	-0.38308800
C	-1.11821200	4.33662400	0.03987700
C	2.78642700	-0.39039200	-0.42654500
O	-2.78560700	0.27794000	-0.33972700
C	0.16464600	4.87984100	-0.52951300
C	-1.67753100	5.14860700	1.17843500
C	3.44253900	-1.61131800	-0.36911900
C	4.92059300	-1.71715000	-0.44902000
O	5.46614200	-2.63386700	-0.99784300
O	5.61054900	-0.71279500	0.11363900
H	1.35301200	1.65120300	-1.39059700
H	0.95088000	-2.10886000	0.63393300
H	-1.11388300	-2.89218200	1.31546400
H	-2.26661800	-1.64424100	1.74729100
H	-2.29515300	-3.16869700	-0.94445200
H	-4.29777200	-3.86078600	-1.80506800
H	-5.46182400	-4.32733400	-0.55207300
H	-5.65196000	-2.79356100	-1.38883300
H	-5.65716300	-1.60873300	0.87995600
H	-5.37245800	-3.10653400	1.74816800
H	-4.27213200	-1.74449600	1.97235700
H	-0.59665500	2.80136500	-2.16667900
H	-2.17124900	2.01983800	-2.07883600
H	-2.64724200	2.92451100	0.12820300
H	3.32652600	0.44461600	-0.86535100
H	-3.24902900	-0.56701300	-0.25993000
H	0.54824100	4.30132400	-1.36799900
H	0.02451000	5.91293700	-0.86226700
H	0.93644300	4.90082000	0.24657400
H	-2.59928100	4.71543800	1.56773700
H	-0.95258900	5.21571100	1.99593400
H	-1.88594400	6.17318800	0.85449700
H	2.90965700	-2.54681100	-0.26081200
H	5.02488800	-0.20915900	0.70518300
H	1.71762100	0.17048400	2.25592500
O	3.29176100	0.35036800	1.29962200
O	2.58833700	-0.25520000	2.29584000

Name			**TS-AC-C11-H-OOH-RAF (gas phase)**
Cartesian Coordinates			Frequency and Energy
C	-0.72861700	1.37168000	0.68383800
C	-1.73128500	0.41213300	0.65397600
C	-1.51282400	-0.87385200	0.15098800
C	-0.24842200	-1.17631200	-0.36261500
C	0.77690000	-0.24069000	-0.36837400
C	0.52809200	1.02820700	0.17690800
C	2.12921800	-0.58972500	-0.95368800
C	3.17836200	-0.75669200	0.12139400
C	4.19659000	0.13541300	0.41243200
C	5.00738800	-0.03994400	1.65755200
C	4.73782500	1.12321100	-0.57633100
C	-0.97627100	2.76555200	1.21428900
C	-1.13132100	3.75877200	0.08972200
C	-2.25532000	4.35070200	-0.31952200

Zero-point correction= 0.406049 (Hartree/Particle)
Thermal correction to Energy= 0.433511
Thermal correction to Enthalpy= 0.434455
Thermal correction to Gibbs Free Energy= 0.342908
Sum of electronic and zero-point Energies= -1114.443735
Sum of electronic and thermal Energies= -1114.416273
Sum of electronic and thermal Enthalpies= -1114.415329
Sum of electronic and thermal Free Energies= -1114.506876

C	-2.60924800	-1.84456800	0.17893200
O	1.48547000	1.99750900	0.20610900
C	-3.61741000	4.14020400	0.28550500
C	-2.24216200	5.31246100	-1.47869000
C	-2.52874600	-3.15468200	-0.08241500
C	-3.66750900	-4.10210000	0.02309500
O	-3.51521100	-5.27371600	0.21494000
O	-4.91612700	-3.58917200	-0.09107100
H	-2.71093500	0.67038300	1.04655600
H	-0.05244600	-2.15344800	-0.79104100
H	2.03653600	-1.53951200	-1.48280800
H	2.43262900	0.15686300	-1.69108200
H	2.85441400	-1.38849400	0.94568700
H	4.57346800	-0.78434400	2.32473000
H	6.02290500	-0.36099600	1.39718600
H	5.10300400	0.90657700	2.19874600
H	5.04909200	2.04516000	-0.07716300
H	5.63452600	0.69674900	-1.04363400
H	4.04705200	1.37578500	-1.38040900
H	-1.85513700	2.74939800	1.85836100
H	-0.12383600	3.06331600	1.83098700
H	-0.21082400	3.97754500	-0.44641500
H	-3.56732500	-1.42492200	0.48466500
H	2.36056100	1.59933900	0.14213600
H	-3.62054400	3.44286500	1.12130900
H	-4.02808900	5.09283600	0.63445500
H	-4.30709600	3.76042500	-0.47505000
H	-1.23944300	5.43541600	-1.88873800
H	-2.90290300	4.96123600	-2.27768900
H	-2.61276600	6.29472900	-1.16870100
H	-1.58592100	-3.64036700	-0.30261400
H	-4.87568400	-2.68781600	-0.42447000
H	3.64017900	-3.80441100	-0.06741000
O	4.26475500	-2.15551300	-0.68407000
O	3.44450600	-3.24947500	-0.83460500

Name	**TS-AC-C12-H-OOH-RAF (gas phase)**
Cartesian Coordinates	Frequency and Energy

C	1.04261600	1.24895700	-0.75175600
C	1.95769200	0.20816100	-0.66539800
C	1.61331900	-1.04247400	-0.14526600
C	0.30865200	-1.22782200	0.32309300
C	-0.63120800	-0.20955100	0.26941100
C	-0.25460700	1.02465100	-0.28385200
C	-2.02887300	-0.39326200	0.81677100
C	-3.09353600	-0.22667600	-0.22863600
C	-4.37674900	0.22992300	0.01242900
C	-5.28440800	0.49738300	-1.15861100
C	-4.72452400	0.94182100	1.29589500
C	1.42809600	2.60561900	-1.29608800
C	1.63525300	3.60136500	-0.18224000
C	2.79261300	4.10839000	0.24750000
C	2.62559200	-2.10035900	-0.10900600
O	-1.12442500	2.07088700	-0.35980800

Zero-point correction=	0.406055 (Hartree/Particle)
Thermal correction to Energy=	0.433167
Thermal correction to Enthalpy=	0.434111
Thermal correction to Gibbs Free Energy=	0.343784
Sum of electronic and zero-point Energies=	-1114.444239
Sum of electronic and thermal Energies=	-1114.417127
Sum of electronic and thermal Enthalpies=	-1114.416183
Sum of electronic and thermal Free Energies=	-1114.506510

C	4.14800200	3.78116800	-0.31946600
C	2.82771100	5.08695700	1.39208600
C	2.42777600	-3.39369900	0.17238000
C	3.49051000	-4.43084700	0.13900600
O	3.25310000	-5.59157600	-0.03010800
O	4.77059100	-4.01511300	0.29509000
H	2.96918900	0.37377900	-1.02591200
H	0.01653100	-2.17702700	0.75868500
H	-2.11674200	-1.40061900	1.24169600
H	-2.18961100	0.30527200	1.64469400
H	-2.87644700	-0.64924500	-1.20647300
H	-5.02301000	-0.12511400	-2.01570500
H	-6.32588600	0.31646600	-0.88087900
H	-5.20597300	1.54546800	-1.46221300
H	-4.27653400	1.94041300	1.32116800
H	-5.80564200	1.05244600	1.38044400
H	-4.37466600	0.38174500	2.16349000
H	2.32162500	2.50074600	-1.91094200
H	0.62463000	2.96545200	-1.94467000
H	0.72225200	3.90178300	0.32656400
H	3.62675500	-1.76609300	-0.37981100
H	-2.03144600	1.75404900	-0.26861000
H	4.11640700	3.06967900	-1.14262900
H	4.63980300	4.69215100	-0.67462200
H	4.78784900	3.36393100	0.46463800
H	1.82825200	5.29542200	1.77465700
H	3.43893300	4.69765300	2.21257600
H	3.28260800	6.03167900	1.07769800
H	1.44009900	-3.79815400	0.35747200
H	4.78879000	-3.10462700	0.60461000
H	-6.11012100	-2.13506700	-0.78307000
O	-5.10546300	-1.46553200	0.63435000
O	-5.25520300	-2.35996700	-0.38982100

Name	**TS-AC-ANION-O7-H-OOH-FHT (water)**
Cartesian Coordinates	Frequency and Energy

C	0.16799200	0.92168600	1.17809100
C	-1.21317700	0.87297200	1.13100800
C	-1.89729500	-0.10014600	0.38079100
C	-1.15391200	-1.05336800	-0.33767900
C	0.22698200	-1.05254300	-0.30879700
C	0.89793800	-0.06137200	0.46275100
C	1.03761000	-2.09003900	-1.04712600
C	1.55452800	-3.14880800	-0.10398600
C	2.82791700	-3.41725800	0.20214900
C	3.17096200	-4.51446800	1.17438900
C	4.02374000	-2.69208900	-0.35041100
C	0.90696100	1.98419900	1.95687400
C	1.81942300	2.81365600	1.07678900
C	1.40625500	3.67306600	0.14132000
C	-3.36024000	-0.06629500	0.37752000
O	2.22624800	-0.07297600	0.54148600
C	-0.04360400	3.95441700	-0.14419600
C	2.38292700	4.38396100	-0.75362200
C	-4.17308200	-0.87445400	-0.31381500

Zero-point correction= 0.388719 (Hartree/Particle)
Thermal correction to Energy= 0.414890
Thermal correction to Enthalpy= 0.415834
Thermal correction to Gibbs Free Energy= 0.330669
Sum of electronic and zero-point Energies= -1114.050427
Sum of electronic and thermal Energies= -1114.024256
Sum of electronic and thermal Enthalpies= -1114.023312
Sum of electronic and thermal Free Energies= -1114.108477

C	-5.67412100	-0.75610800	-0.25282000
O	-6.32023400	-1.56470700	-0.97278100
O	-6.18327100	0.11923000	0.49298500
H	-1.78884200	1.61344300	1.67826900
H	-1.66153600	-1.80783800	-0.92864000
H	0.39060400	-2.55728700	-1.79428400
H	1.85840900	-1.60287000	-1.57785100
H	0.77795300	-3.74227300	0.37635700
H	2.27849300	-5.01240500	1.55624000
H	3.81167300	-5.26235000	0.69632900
H	3.73561800	-4.10996300	2.02064400
H	4.69610600	-3.40322600	-0.84088700
H	3.77104800	-1.90823800	-1.06286300
H	4.59093000	-2.23876100	0.46941200
H	0.16933500	2.61296100	2.46164800
H	1.50544000	1.50104500	2.73312200
H	2.88744600	2.65029500	1.19256500
H	-3.81157500	0.70111100	1.00158500
H	2.64347300	0.32617700	-0.36943400
H	-0.70087200	3.66027900	0.67457700
H	-0.19079800	5.01983600	-0.34241500
H	-0.36169700	3.41489900	-1.04417000
H	3.41430700	4.11025300	-0.52511400
H	2.18055300	4.13646400	-1.80161000
H	2.27701800	5.46942300	-0.65995300
H	-3.78961900	-1.65682900	-0.96046600
H	1.26420300	0.46168200	-2.48779800
O	2.81469900	0.93516500	-1.55272200
O	1.53824400	1.20355300	-1.91904700

Name			**TS-AC-ANION-C10-H-OOH-FHT (gas phase)**
Cartesian Coordinates			Frequency and Energy
C	-1.05568000	-1.33199500	-0.82150900
C	-1.81578400	-0.16752900	-0.80193800
C	-1.31096700	1.06054100	-0.35968800
C	0.02257400	1.08599900	0.06592600
C	0.81395300	-0.05976900	0.06594100
C	0.26365800	-1.27058300	-0.37873700
C	2.23705700	-0.03799700	0.54221100
C	3.26922300	-0.41929400	-0.42539800
C	4.54812500	-0.73401900	-0.12328700
C	5.53309700	-1.12015000	-1.18916200
C	5.06647900	-0.73328600	1.29188600
C	-1.64009100	-2.65420800	-1.27069200
C	-1.94849100	-3.54920200	-0.09640200
C	-3.13802600	-3.74963900	0.47471900
C	-2.18726000	2.24195000	-0.36399800
O	0.98026300	-2.44724500	-0.38464400
C	-4.42532200	-3.10680500	0.03369500
C	-3.27738300	-4.64120300	1.68134000
C	-1.93469900	3.44412000	0.15624000
C	-2.95617800	4.59821200	0.09859400
O	-2.55554100	5.65300600	0.63187200
O	-4.04088900	4.34577000	-0.46104500
H	-2.84623000	-0.21010100	-1.14380600

Zero-point correction= 0.386911 (Hartree/Particle)
Thermal correction to Energy= 0.414703
Thermal correction to Enthalpy= 0.415648
Thermal correction to Gibbs Free Energy= 0.320644
Sum of electronic and zero-point Energies= -1113.908101
Sum of electronic and thermal Energies= -1113.880309
Sum of electronic and thermal Enthalpies= -1113.879365
Sum of electronic and thermal Free Energies= -1113.974368

H	0.46182700	2.02070600	0.39727000
H	2.54743300	1.17665000	0.81662100
H	2.37514900	-0.47169200	1.53742200
H	2.97763900	-0.38841700	-1.47355000
H	5.07330000	-1.13322100	-2.17749600
H	6.37997800	-0.42549900	-1.20780000
H	5.94843200	-2.11284000	-0.98404600
H	4.93121000	-1.71658900	1.75662000
H	6.13804400	-0.51898800	1.30783600
H	4.55771500	0.00447500	1.91517500
H	-2.53218300	-2.45993000	-1.86674600
H	-0.91822400	-3.16200700	-1.91659300
H	-1.07949800	-4.03215100	0.34482800
H	-3.16554000	2.12167100	-0.82627900
H	1.90486700	-2.26232500	-0.19427300
H	-4.32149000	-2.50850200	-0.86928500
H	-5.19305200	-3.86782300	-0.14127500
H	-4.80198200	-2.44949700	0.82409900
H	-2.31886100	-5.07070000	1.97575800
H	-3.67942800	-4.07789100	2.53004800
H	-3.97832800	-5.45899100	1.48177500
H	-0.99628300	3.67543800	0.65610800
H	4.71367900	2.00560700	0.03200700
O	3.16921100	2.25186200	1.04165700
O	3.87647000	2.47057700	-0.10944900

Name			**TS-AC-ANION-C2-H-OOH-RAF (gas phase)**
Cartesian Coordinates			Frequency and Energy
C	-1.11670200	1.07813200	-0.75970800
C	0.24510800	1.34379600	-0.82683500
C	1.20836200	0.44933700	-0.33373000
C	0.74751100	-0.75518800	0.22453800
C	-0.60730300	-1.04342700	0.32134100
C	-1.53506100	-0.12152100	-0.18034800
C	-1.08630200	-2.33967000	0.94335900
C	-1.78025000	-3.22665000	-0.05934600
C	-3.02183800	-3.72361200	-0.01140600
C	-3.55051500	-4.59233400	-1.12348600
C	-4.00040500	-3.50319900	1.11418700
C	-2.14363300	2.06537900	-1.27074300
C	-2.82919600	2.78394700	-0.13657700
C	-2.61153300	4.03206200	0.28301400
C	2.62079300	0.76078900	-0.41644500
O	-2.89157400	-0.35349300	-0.10669900
C	-1.61710200	4.98614000	-0.32224900
C	-3.35439400	4.59040200	1.46921400
C	3.60302600	0.10082700	0.29026800
C	5.06759100	0.57354200	0.22996600
O	5.29272100	1.68354000	-0.25186900
O	5.90191500	-0.26023900	0.70117100
H	0.57892800	2.27654800	-1.27318400
H	1.47608800	-1.49019900	0.55160700
H	-0.21339800	-2.86913200	1.33475500
H	-1.73457500	-2.12153100	1.79575200
H	-1.17603900	-3.46027400	-0.93428100

Zero-point correction= 0.392882 (Hartree/Particle)
Thermal correction to Energy= 0.418886
Thermal correction to Enthalpy= 0.419831
Thermal correction to Gibbs Free Energy= 0.332789
Sum of electronic and zero-point Energies= -1113.937684
Sum of electronic and thermal Energies= -1113.911680
Sum of electronic and thermal Enthalpies= -1113.910735
Sum of electronic and thermal Free Energies= -1113.997777

H	-2.80997900	-4.72988600	-1.91171100
H	-3.83444800	-5.57735800	-0.73848200
H	-4.45044700	-4.15202100	-1.56520200
H	-4.94329300	-3.10506700	0.72434400
H	-4.23734100	-4.45810900	1.59439100
H	-3.63540900	-2.82129600	1.88017300
H	-1.65515400	2.76505500	-1.94938400
H	-2.89996400	1.52247900	-1.84504800
H	-3.54375200	2.17493600	0.41295900
H	2.93991900	1.53915800	-1.10318100
H	-3.04366700	-1.30488500	-0.15450100
H	-2.11151500	5.91748700	-0.61840800
H	-0.85735000	5.25136800	0.42013300
H	-1.10245700	4.57896300	-1.19025800
H	-4.05587800	3.86371900	1.88103100
H	-2.65386100	4.88069800	2.25939400
H	-3.91100100	5.49189800	1.19062700
H	3.32119200	-0.44503500	1.18559500
H	5.31282400	-1.64923000	0.55531000
O	3.86315200	-1.60040500	-0.57848300
O	4.56024100	-2.32325100	0.34681500

Name			**TS-AC-ANION-C3-H-OOH-RAF (gas phase)**
Cartesian Coordinates			Frequency and Energy
C	-0.49033700	1.12274700	-0.97661300
C	0.76451100	0.53256700	-1.06494800
C	1.04748000	-0.71068400	-0.49492600
C	0.00082300	-1.39467700	0.12253000
C	-1.28013400	-0.85116300	0.20373300
C	-1.51491400	0.41482400	-0.34425700
C	-2.39674300	-1.58737800	0.91590900
C	-3.53533500	-1.93259500	-0.01081500
C	-4.82782100	-1.60533600	0.10398000
C	-5.82903300	-2.03345400	-0.93754800
C	-5.42417500	-0.81597300	1.24139500
C	-0.68605400	2.56175000	-1.40118800
C	-0.39620500	3.45659700	-0.21643500
C	0.80062900	3.92940700	0.14420900
C	2.44671800	-1.19345400	-0.49029500
O	-2.73938000	1.03142400	-0.22935800
C	2.07752000	3.70778600	-0.62476900
C	0.97695200	4.69676200	1.42825400
C	2.89701500	-2.23980900	0.29055000
C	4.17977500	-3.00837000	-0.03887000
O	4.38812300	-3.98193200	0.71338600
O	4.82337100	-2.59120000	-1.02049900
H	1.57977500	1.07845300	-1.52919300
H	0.18873400	-2.36770200	0.56353100
H	-1.98490500	-2.51259200	1.32846100
H	-2.74399400	-0.99226500	1.76427900
H	-3.23611700	-2.50352200	-0.88818400
H	-5.35743900	-2.60374800	-1.73815800
H	-6.61150600	-2.65160300	-0.48537900
H	-6.32610600	-1.16284500	-1.37745000
H	-6.15103700	-1.43183100	1.78055700

Zero-point correction= 0.393454 (Hartree/Particle)
Thermal correction to Energy= 0.419787
Thermal correction to Enthalpy= 0.420731
Thermal correction to Gibbs Free Energy= 0.333793
Sum of electronic and zero-point Energies= -1113.916186
Sum of electronic and thermal Energies= -1113.889853
Sum of electronic and thermal Enthalpies= -1113.888908
Sum of electronic and thermal Free Energies= -1113.975847

H	-4.68666400	-0.45922600	1.95801100
H	-5.97163300	0.05021100	0.85503700
H	-0.01681600	2.78249500	-2.23459300
H	-1.71157400	2.71718700	-1.73909700
H	-1.24113600	3.63587300	0.44511300
H	3.04219300	-1.00353500	-1.37960700
H	-3.42514800	0.35401200	-0.19820500
H	2.68759800	4.61569400	-0.61180700
H	2.67402500	2.91157900	-0.16243400
H	1.90477100	3.42912900	-1.66396100
H	0.03691100	4.79322700	1.97346800
H	1.70286500	4.18830500	2.07152500
H	1.37210500	5.69875600	1.23089800
H	2.36378000	-2.53329100	1.19024500
H	1.65783400	1.11062100	1.08813900
O	3.23185100	0.36482000	0.39019100
O	2.46971700	0.74680600	1.47870900

Name	**TS-AC-ANION-C11-H-OOH-RAF (gas phase)**
Cartesian Coordinates	Frequency and Energy

C	-0.93904800	1.28516600	0.67336900
C	-1.81224400	0.20225100	0.62577200
C	-1.43890500	-1.04338700	0.10896300
C	-0.14776800	-1.15309600	-0.41979400
C	0.74873800	-0.08959400	-0.40502800
C	0.34966700	1.12234900	0.16782700
C	2.14184500	-0.25291800	-0.97704700
C	3.15604300	-0.40573300	0.12846900
C	4.07585400	0.55326200	0.52472400
C	4.86718000	0.34666100	1.77780800
C	4.55926700	1.65058300	-0.37472100
C	-1.36735000	2.62331100	1.23562300
C	-1.61231000	3.62824400	0.13844500
C	-2.79009500	4.02226300	-0.35025300
C	-2.38820800	-2.16690300	0.14257900
O	1.19817800	2.21177200	0.21664000
C	-4.13029100	3.52785600	0.12374900
C	-2.86556900	5.00822800	-1.48714700
C	-2.09027500	-3.46052100	0.00987500
C	-3.15040200	-4.57640400	0.08190800
O	-2.68514000	-5.72239600	-0.08943400
O	-4.32099100	-4.21045100	0.29955800
H	-2.81575400	0.31913000	1.02548700
H	0.16063400	-2.08894300	-0.87459000
H	2.16216500	-1.16076100	-1.58327700
H	2.39354600	0.58183000	-1.63446000
H	2.84920200	-1.11117100	0.89796900
H	4.46095300	-0.46259600	2.38423800
H	5.90427100	0.09466100	1.52223100
H	4.89947800	1.26021700	2.38016900
H	4.82638600	2.53945200	0.20369200
H	5.46949000	1.31269600	-0.88697700
H	3.84181100	1.93740100	-1.14307300
H	-2.25577800	2.48056600	1.85111700
H	-0.57438300	3.00458900	1.88536200

Zero-point correction= 0.392266 (Hartree/Particle)
Thermal correction to Energy= 0.419534
Thermal correction to Enthalpy= 0.420478
Thermal correction to Gibbs Free Energy= 0.328887
Sum of electronic and zero-point Energies= -1113.912594
Sum of electronic and thermal Energies= -1113.885326
Sum of electronic and thermal Enthalpies= -1113.884382
Sum of electronic and thermal Free Energies= -1113.975974

H	-0.70834100	4.02352900	-0.31989300
H	-3.43367600	-1.93014600	0.33167900
H	2.09936400	1.89628400	0.33955900
H	-4.06331800	2.83444200	0.95969000
H	-4.76531800	4.36900800	0.42142200
H	-4.64631800	3.01319200	-0.69323900
H	-1.87326200	5.33157900	-1.80420400
H	-3.37561800	4.56335800	-2.34810500
H	-3.44337000	5.89256900	-1.19720400
H	-1.06800700	-3.79985500	-0.14667200
H	3.64684500	-3.33307500	-0.50263600
O	4.45574500	-1.65080400	-0.63832300
O	3.76623600	-2.69032900	-1.21581600

Name	**TS-AC-ANION-C12-H-OOH-RAF (gas phase)**
Cartesian Coordinates	Frequency and Energy

C	-0.97537700	1.24871800	0.73529900
C	-1.97158000	0.27975100	0.65364500
C	-1.74063100	-0.99733000	0.13153500
C	-0.45403200	-1.26568000	-0.35243900
C	0.56258700	-0.31899800	-0.30345100
C	0.29524100	0.93452300	0.25950400
C	1.94006600	-0.61234600	-0.86769800
C	2.99464100	-0.61692100	0.19564100
C	4.23312400	-0.00600600	0.12418100
C	5.06094900	0.09805500	1.37911300
C	4.56242800	0.98592400	-0.96505200
C	-1.25490000	2.62699400	1.29426100
C	-1.36714300	3.65276800	0.19515100
C	-2.48135500	4.20690900	-0.28725200
C	-2.83223600	-1.98294200	0.10760400
O	1.26253800	1.91889800	0.32596400
C	-3.87486000	3.90929200	0.19735000
C	-2.42498000	5.19122700	-1.42678400
C	-2.72521000	-3.29425600	-0.11316600
C	-3.94253400	-4.24005000	-0.11236800
O	-3.65897100	-5.42392600	-0.38833900
O	-5.04257300	-3.72058600	0.15632000
H	-2.96496200	0.51657400	1.02450800
H	-0.24740400	-2.23298200	-0.79787000
H	1.91781200	-1.60073800	-1.34004000
H	2.18217900	0.11206400	-1.65021600
H	2.78411000	-1.23675500	1.06361300
H	4.83164800	-0.71269200	2.07277600
H	6.12689500	0.07962300	1.13542100
H	4.85745300	1.04560100	1.88758600
H	4.01568200	1.92508300	-0.82937600
H	5.63003000	1.20817300	-0.95291200
H	4.31307300	0.58351700	-1.94687400
H	-2.16225200	2.58683800	1.89705400
H	-0.43244600	2.91437400	1.95577800
H	-0.41987700	3.91748400	-0.26994500
H	-3.83453000	-1.61359300	0.31719600
H	2.12542700	1.49752100	0.39450400
H	-3.90232800	3.20744900	1.02841600

Zero-point correction= 0.392212 (Hartree/Particle)
Thermal correction to Energy= 0.419266
Thermal correction to Enthalpy= 0.420210
Thermal correction to Gibbs Free Energy= 0.329659
Sum of electronic and zero-point Energies= -1113.912578
Sum of electronic and thermal Energies= -1113.885524
Sum of electronic and thermal Enthalpies= -1113.884579
Sum of electronic and thermal Free Energies= -1113.975130

H	-4.37724600	4.83194100	0.50682600
H	-4.46818300	3.48224800	-0.61759100
H	-1.39919600	5.37175900	-1.75070500
H	-2.99773500	4.82016000	-2.28323300
H	-2.87148800	6.14837100	-1.13614500
H	-1.76582600	-3.77079500	-0.30523000
H	6.16620400	-2.28462700	0.58086600
O	5.20470300	-1.44903100	-0.77827200
O	5.39277500	-2.52465800	0.05247000

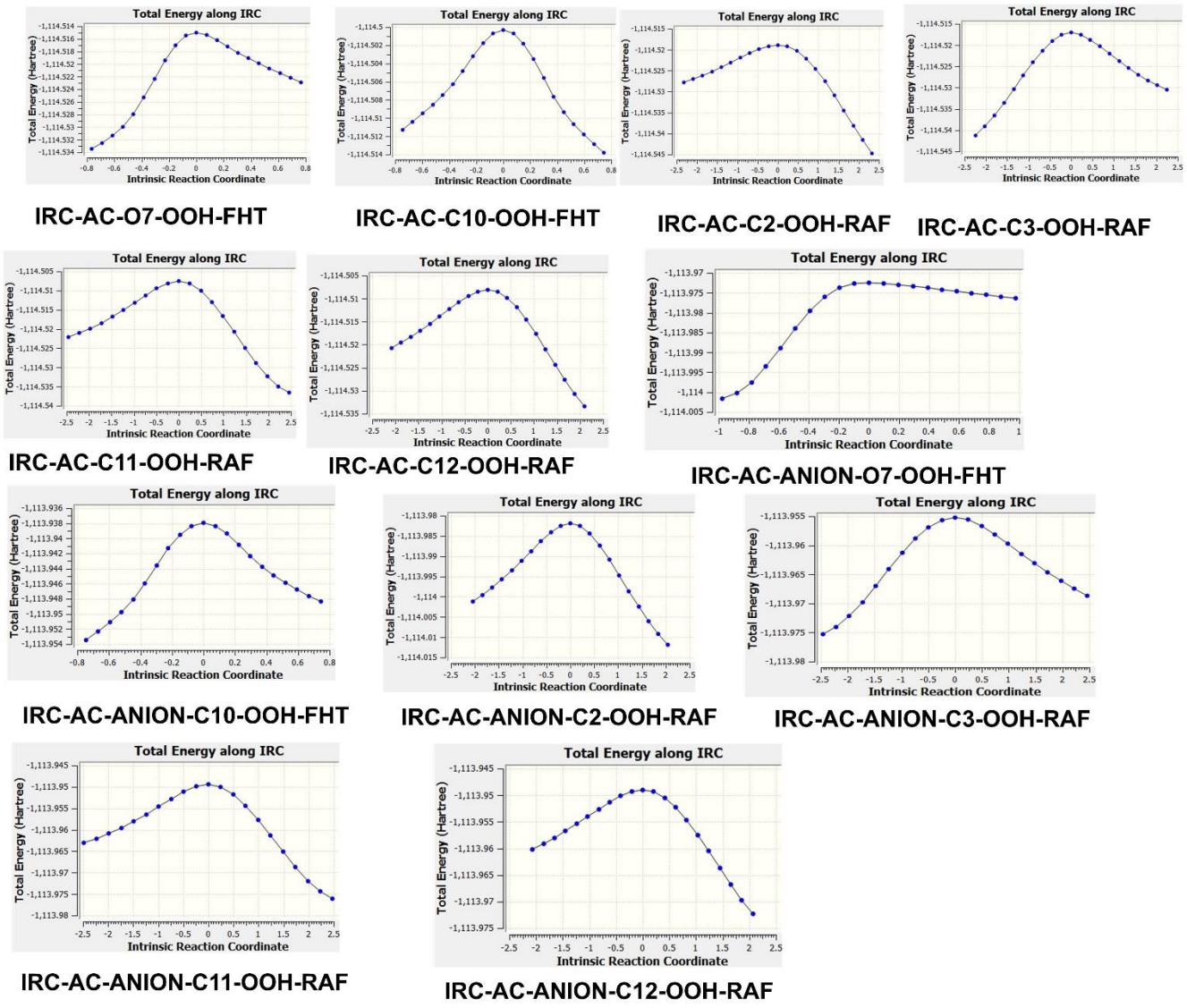

Figure S1. IRC plots for the transition states related to the reaction of HOO• radical with AC compound

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