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Supporting Information (SI)

Another look at reactions of 4-hydroxycoumarin with hydroxyl radical in the environment: Deprotonation and diffusion effects

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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) = 8.62×10^{-4} Pa s) and a is the radius of the solute.

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. The kinetic calculations were performed by the *Eyringpy* code[29, 30]

Table S2. Calculated $\Delta G^{\neq}$ (kcal/mol), tunneling corrections (κ), diffusion rate (k_D), rate constants (k_{app}, k_r, and $k_{overall}$ (r) M^{-1} s^{-1}), and branching ratios (Γ, %) at 298.15 K, in all of the reactions of the 4HC products with HO• in water

Reactions	Mechanism		$\Delta G^{\neq}$	κ	k_D	k_{app}	k_r
1 + HO•	FHT	C3-H	8.2	9	2.90E+09	5.00E+07	4.96E+07
		O3-H	30	13.1	2.60E+09	6.00E-10	5.95E-10
		O4-H	21.3	23.7	2.60E+09	3.55E-02	3.53E-02
	RAF	C2	16.8	1.6	2.10E+09	5.10E+00	5.06E+00
		C4	24.1	1.7	2.20E+09	2.30E-05	2.28E-05
		C4'	11.2	1.2	2.20E+09	4.50E+04	4.46E+04
		C5	13.1	1.3	2.20E+09	2.10E+03	2.08E+03
		C6	5.9	1.1	2.40E+09	2.70E+08	2.68E+08
		C7	17.9	1.4	2.10E+09	6.90E-01	6.84E-01
		C8	6.5	1.1	2.40E+09	1.20E+08	1.19E+08
		C8'	14.7	1.4	2.20E+09	1.40E+02	1.39E+02
	$k_{overall}$(r) (4HC + HO•, step 2)						**4.37E+08**
10 + HO•	RAF	C2	18.9	1.5	2.10E+09	1.30E-01	7.80E-02
		C3	28.2	1.2	2.10E+09	1.32E-08	7.93E-09
		C4	18.1	1.4	2.10E+09	5.20E-01	3.12E-01
		C4'	10	1.2	2.30E+09	3.20E+05	1.92E+05
		C5	10.1	1.3	2.40E+09	3.20E+05	1.92E+05
		C6	9.2	1.2	2.40E+09	1.20E+06	7.20E+05
		C7	11.5	1.3	2.30E+09	3.20E+04	1.92E+04
		C8	8.2	1.2	2.40E+09	7.60E+06	4.56E+06
		C8'	10.6	1.3	2.40E+09	1.30E+05	7.80E+04
	Σk_r(**10** + HO•)						**5.76E+06**
11 + HO•	SET		42.4	5.9	8.10E+09	5.00E-19	8.45E-20
	FHT	O2-H	15.6	1.4	2.20E+09	2.42E+01	4.09E+00
		C3	-15.8	1	2.20E+09	2.20E+09	3.72E+08
		C4	20	1.4	2.10E+09	2.00E-02	3.38E-03
		C4'	7.5	1.1	2.30E+09	2.00E+07	3.38E+06
		C5	8.7	1.2	2.40E+09	3.00E+06	5.07E+05
		C6	5.5	1.1	2.50E+09	4.80E+08	8.11E+07

		C7	9.3	1.2	2.40E+09	1.10E+06	1.86E+05
		C8	5.4	1.1	2.50E+09	5.70E+08	9.63E+07
		C8'	9.3	1.2	2.40E+09	1.10E+06	1.86E+05
	Σk_r(**11** + HO•)						**5.54E+08**
12 + HO•	SET		161.8	4.3	8.20E+09	1.70E-106	3.01E-107
	FHT	C3-H	7.7	3.4	2.90E+09	4.80E+07	8.50E+06
		O3-H	25.2	1.5	2.90E+09	3.14E-06	5.55E-07
	RAF	C2	18.4	1.5	2.10E+09	3.30E-01	5.84E-02
		C4	29.4	1.5	1.90E+09	2.80E-09	4.96E-10
		C4'	9.9	1.2	2.10E+09	4.40E+05	7.79E+04
		C5	12.1	1.3	2.20E+09	1.10E+04	1.95E+03
		C6	4.3	1.1	2.30E+09	1.60E+09	2.83E+08
		C7	16.8	1.3	2.10E+09	3.90E+00	6.90E-01
		C8	4.5	1.1	2.50E+09	1.40E+09	2.48E+08
		C8'	10.9	1.2	2.30E+09	7.30E+04	1.29E+04
	Σk_r(**12** + HO•)						**5.40E+08**
	$k_{overall}$(r) (4HC-ANION + HO•, step 2)					**6.33E+09**	**1.10E+09**

$k_r = r.k_{app}$; $k_{overall}(r) = \Sigma k_r$; $\Gamma = k_r.100/k_{overall}(r)$

Table S3: The Cartesian coordinates and energies of TSs in the studied media (B: benzene; P: pentyl ethanoate; H: water)

Name				**4HC-O4-H-OH-FHT-B**
Cartesian Coordinates				Frequency and Energy
O	-0.12442500	1.74430000	0.10002000	Zero-point correction= 0.142504 (Hartree/Particle)
O	-1.04451900	-2.20331900	-0.35418500	Thermal correction to Energy= 0.152764
O	-2.23937800	2.31151800	-0.18896500	Thermal correction to Enthalpy= 0.153708
C	0.64259700	-0.53431800	-0.16913100	Thermal correction to Gibbs Free Energy= 0.105608
C	0.87869400	0.82861900	0.04808300	Sum of electronic and zero-point Energies= -647.789558
C	-0.72330900	-0.94984600	-0.35034200	Sum of electronic and thermal Energies= -647.779299
C	1.72015400	-1.43461000	-0.16770800	Sum of electronic and thermal Enthalpies= -647.778354
C	2.17235500	1.29858300	0.25293700	Sum of electronic and thermal Free Energies= -647.826454
C	-1.72890700	0.02199900	-0.44210000	
C	3.00426400	-0.97001500	0.02366600	
C	3.22379200	0.39830800	0.23339100	
C	-1.43417800	1.42353800	-0.17680100	
H	1.51598800	-2.48726100	-0.32117900	
H	2.32644000	2.35617800	0.42562500	
H	-2.64767800	-0.17163000	-0.97480700	
H	3.83974800	-1.65832700	0.01878300	
H	4.23267600	0.76213800	0.38849700	
H	-2.00237100	-2.14129300	0.10304200	
O	-2.84521900	-1.35241500	0.95499900	
H	-3.76923100	-1.15402000	0.75310400	
Name				**4HC-C2-OH-RAF-B**
Cartesian Coordinates				Frequency and Energy
O	0.77287700	-1.20961000	-0.47261900	Zero-point correction= 0.144882 (Hartree/Particle)
O	-0.02648700	2.80373600	-0.03851400	Thermal correction to Energy= 0.155074
O	2.96187500	-0.85123000	-0.60918600	Thermal correction to Enthalpy= 0.156018
C	-0.78947500	0.57104800	-0.03484100	Thermal correction to Gibbs Free Energy= 0.108579
C	-0.49765900	-0.78068900	-0.22520000	Sum of electronic and zero-point Energies= -647.767682
C	0.31970900	1.50781600	-0.11064600	Sum of electronic and thermal Energies= -647.757490
C	-2.11505900	0.95752400	0.18888500	Sum of electronic and thermal Enthalpies= -647.756546
C	-1.50192300	-1.74136100	-0.20484500	Sum of electronic and thermal Free Energies= -647.803984
C	1.57897100	1.05691700	-0.25194900	
C	-3.11979800	0.00594900	0.22135900	
C	-2.80971800	-1.34157400	0.02164800	
C	1.84446100	-0.37864100	-0.26523400	
H	-2.33653900	2.00737000	0.33456600	
H	-1.24042400	-2.78013800	-0.36385300	
H	2.44399800	1.70601300	-0.29135800	
H	-4.14486100	0.30639900	0.39861500	
H	-3.59623600	-2.08649900	0.04503300	
H	0.76041600	3.36129800	-0.06336900	
O	2.31435100	-0.73777800	1.43077200	
H	2.47567900	-1.69732100	1.42166900	
Name				**4HC-C3-OH-RAF-B**
Cartesian Coordinates				Frequency and Energy
O	0.45551600	-1.60840600	-0.11005000	Zero-point correction= 0.144331 (Hartree/Particle)
O	0.60503200	2.47650200	-0.50209400	Thermal correction to Energy= 0.155339
O	2.63005600	-1.78742400	-0.43645000	Thermal correction to Enthalpy= 0.156284

C	-0.67070400	0.52561100	-0.17812700	Thermal correction to Gibbs Free Energy= 0.106118
C	-0.68170700	-0.86645300	-0.04056300	Sum of electronic and zero-point Energies= -647.792192
C	0.60277600	1.15447300	-0.39389000	Sum of electronic and thermal Energies= -647.781184
C	-1.87909900	1.23494600	-0.09267200	Sum of electronic and thermal Enthalpies= -647.780239
C	-1.87183400	-1.55230200	0.17655100	Sum of electronic and thermal Free Energies= -647.830405
C	1.75548700	0.40320400	-0.40974000	
C	-3.06255800	0.55782700	0.12060200	
C	-3.05424300	-0.83607200	0.25437200	
C	1.68669800	-1.05230400	-0.33759800	
H	-1.86094800	2.31292400	-0.19186900	
H	-1.84581800	-2.62951600	0.28148100	
H	2.69483100	0.81680500	-0.75097300	
H	-3.99539900	1.10300500	0.18822800	
H	-3.98407400	-1.36573500	0.42427000	
H	1.51048700	2.81433000	-0.47163000	
O	2.25574300	0.83929700	1.58520800	
H	2.96125500	0.17485200	1.63396800	

Name				**4HC-C4-OH-RAF-B**
Cartesian Coordinates				Frequency and Energy
O	0.55812600	-1.65630300	0.02450300	Zero-point correction= 0.144364 (Hartree/Particle)
O	0.69879400	2.39880100	-0.65256800	Thermal correction to Energy= 0.154982
O	2.74249800	-1.85426500	-0.23982700	Thermal correction to Enthalpy= 0.155927
C	-0.57040800	0.47134100	-0.17929400	Thermal correction to Gibbs Free Energy= 0.107587
C	-0.58595500	-0.91285400	-0.00840600	Sum of electronic and zero-point Energies= -647.786866
C	0.72727900	1.11665800	-0.30854300	Sum of electronic and thermal Energies= -647.776248
C	-1.77716000	1.17732800	-0.19523900	Sum of electronic and thermal Enthalpies= -647.775304
C	-1.78640900	-1.59880100	0.14179000	Sum of electronic and thermal Free Energies= -647.823644
C	1.86346900	0.32128000	-0.41374000	
C	-2.97483400	0.50159200	-0.04819900	
C	-2.97417700	-0.88607600	0.12114400	
C	1.79786600	-1.11236200	-0.21368500	
H	-1.75250600	2.25244100	-0.32056200	
H	-1.76447900	-2.67370100	0.26994400	
H	2.83748800	0.74148900	-0.62447400	
H	-3.91007500	1.04674600	-0.06130200	
H	-3.91216500	-1.41585800	0.23731600	
H	1.58646200	2.77747700	-0.60206500	
O	1.40912200	1.39162200	1.57439900	
H	1.32892300	0.56392500	2.07410700	

Name				**4HC-C5-OH-RAF-B**
Cartesian Coordinates				Frequency and Energy
O	1.32823700	-1.38322800	0.14671600	Zero-point correction= 0.144196 (Hartree/Particle)
O	0.28409200	2.54354300	-0.46362500	Thermal correction to Energy= 0.154993
O	3.47487700	-0.88040800	0.27136400	Thermal correction to Enthalpy= 0.155937
C	-0.34155300	0.28559700	-0.28988800	Thermal correction to Gibbs Free Energy= 0.106857
C	0.03182100	-1.02810300	-0.04051600	Sum of electronic and zero-point Energies= -647.782873
C	0.70428700	1.27961800	-0.29113000	Sum of electronic and thermal Energies= -647.772076
C	-1.71633000	0.60733200	-0.44182700	Sum of electronic and thermal Enthalpies= -647.771131
C	-0.92130100	-2.04600400	0.01447600	Sum of electronic and thermal Free Energies= -647.820212
C	1.99399700	0.91741700	-0.10897500	
C	-2.66084600	-0.43657600	-0.45311800	
C	-2.26212900	-1.73897400	-0.19672100	
C	2.35909600	-0.46814400	0.11102900	
H	-1.97860800	1.57253900	-0.85502400	

H	-0.59278800	-3.05811000	0.21526100	
H	2.80564000	1.63365000	-0.10384500	
H	-3.70392900	-0.20107200	-0.61940600	
H	-2.99701300	-2.53419900	-0.16881600	
H	1.03157400	3.15457400	-0.45422800	
O	-2.10296800	1.35143100	1.40488800	
H	-1.56103500	2.14894200	1.29132400	
Name				**4HC-C6-OH-RAF-B**
Cartesian Coordinates				Frequency and Energy
O	1.27230400	-1.41465600	0.04408300	Zero-point correction= 0.144019 (Hartree/Particle)
O	0.76082300	2.65676800	-0.18184000	Thermal correction to Energy= 0.154952
O	3.44854700	-1.20220300	0.35012700	Thermal correction to Enthalpy= 0.155896
C	-0.16452700	0.49456000	-0.23197900	Thermal correction to Gibbs Free Energy= 0.106439
C	0.04509200	-0.88941700	-0.15717900	Sum of electronic and zero-point Energies= -647.785517
C	1.00367900	1.34433700	-0.09851900	Sum of electronic and thermal Energies= -647.774584
C	-1.45097800	0.98079700	-0.44692600	Sum of electronic and thermal Enthalpies= -647.773640
C	-1.01739400	-1.79049700	-0.30127300	Sum of electronic and thermal Free Energies= -647.823097
C	2.22631900	0.80151600	0.09328400	
C	-2.54177900	0.09514800	-0.52058800	
C	-2.28592300	-1.30357500	-0.50871700	
C	2.40853200	-0.63186700	0.17659800	
H	-1.61309700	2.04852600	-0.51715800	
H	-0.80915600	-2.85210000	-0.25743100	
H	3.12073100	1.40321300	0.19298300	
H	-3.49323200	0.45674700	-0.88302600	
H	-3.11560000	-1.98946300	-0.62658000	
H	1.57892900	3.16050600	-0.08786200	
O	-3.29127100	0.35107600	1.32654700	
H	-2.52992700	0.03868500	1.83954500	
Name				**4HC-C7-OH-RAF-B**
Cartesian Coordinates				Frequency and Energy
O	0.95314000	-1.48785600	-0.17363200	Zero-point correction= 0.143986 (Hartree/Particle)
O	1.33743500	2.59137200	0.22041800	Thermal correction to Energy= 0.154906
O	3.12199400	-1.79045000	0.10072300	Thermal correction to Enthalpy= 0.155850
C	-0.03506400	0.71352500	-0.13946400	Thermal correction to Gibbs Free Energy= 0.106404
C	-0.13628800	-0.67910500	-0.26524600	Sum of electronic and zero-point Energies= -647.783752
C	1.28313700	1.25834600	0.10006500	Sum of electronic and thermal Energies= -647.772832
C	-1.19034500	1.50838300	-0.26238500	Sum of electronic and thermal Enthalpies= -647.771888
C	-1.35645900	-1.28475500	-0.50587400	Sum of electronic and thermal Free Energies= -647.821334
C	2.35510300	0.43807500	0.18461000	
C	-2.40968200	0.92099100	-0.49552500	
C	-2.52208800	-0.49535900	-0.56271200	
C	2.22171400	-0.99890500	0.04277100	
H	-1.09491100	2.58351700	-0.18003000	
H	-1.40619900	-2.36115700	-0.60855000	
H	3.35693100	0.80881100	0.35886200	
H	-3.30312000	1.52441100	-0.58978100	
H	-3.42974900	-0.93640900	-0.95054000	
H	2.24588300	2.88134800	0.36952700	
O	-3.29594800	-0.84626600	1.25524100	
H	-2.56196400	-0.52210600	1.80105800	
Name				**4HC-C8-OH-RAF-B**
Cartesian Coordinates				Frequency and Energy
O	0.73748200	-1.36656900	-0.37437900	Zero-point correction= 0.144117 (Hartree/Particle)

O	1.26205100	2.63911100	0.36778800	Thermal correction to Energy= 0.154993
O	2.90693700	-1.75951800	-0.23150600	Thermal correction to Enthalpy= 0.155937
C	-0.17926500	0.83309000	-0.07677900	Thermal correction to Gibbs Free Energy= 0.106692
C	-0.31926200	-0.52963100	-0.32185300	Sum of electronic and zero-point Energies= -647.784458
C	1.16700900	1.32514000	0.13504300	Sum of electronic and thermal Energies= -647.773581
C	-1.32044700	1.64285500	-0.04760300	Sum of electronic and thermal Enthalpies= -647.772637
C	-1.59525400	-1.11755200	-0.47205200	Sum of electronic and thermal Free Energies= -647.821882
C	2.22006200	0.47742800	0.09248600	
C	-2.57969700	1.09420300	-0.27950700	
C	-2.71439200	-0.26110400	-0.52235700	
C	2.04057000	-0.93302000	-0.17007700	
H	-1.20574700	2.70154800	0.14850300	
H	-1.65477900	-2.12742800	-0.85659500	
H	3.23873800	0.80720800	0.25099300	
H	-3.45198600	1.73540500	-0.27761700	
H	-3.68973400	-0.69337800	-0.70749600	
H	2.18290200	2.89315500	0.50689100	
O	-1.74661500	-1.77487200	1.42890200	
H	-1.01416900	-2.41017900	1.38507100	
Name				**4HC-C4'-OH-RAF-B**
Cartesian Coordinates				Frequency and Energy
O	0.91898100	-1.49631300	-0.01632400	Zero-point correction= 0.144414 (Hartree/Particle)
O	0.55901100	2.58378100	-0.43554400	Thermal correction to Energy= 0.155138
O	3.12073300	-1.37183900	-0.03742700	Thermal correction to Enthalpy= 0.156082
C	-0.44608600	0.49173300	-0.01674200	Thermal correction to Gibbs Free Energy= 0.107610
C	-0.29714000	-0.92426400	-0.08540500	Sum of electronic and zero-point Energies= -647.781715
C	0.76639100	1.27461000	-0.28001000	Sum of electronic and thermal Energies= -647.770991
C	-1.74841900	1.03311500	-0.24785300	Sum of electronic and thermal Enthalpies= -647.770047
C	-1.40346000	-1.75800300	-0.16475500	Sum of electronic and thermal Free Energies= -647.818519
C	1.96432300	0.66444600	-0.32974300	
C	-2.83539200	0.20176900	-0.33508300	
C	-2.66441100	-1.19611500	-0.28056900	
C	2.09167600	-0.76357000	-0.11387600	
H	-1.84998200	2.10920100	-0.30389400	
H	-1.25250200	-2.82988100	-0.15387700	
H	2.88828100	1.20572200	-0.48700500	
H	-3.82694500	0.61711900	-0.46412600	
H	-3.52950500	-1.84442500	-0.35117600	
H	1.39862800	3.04724000	-0.54575800	
O	-0.25211800	0.66458600	1.89537700	
H	-1.16573300	0.51099200	2.18139400	
Name				**4HC-C8'-OH-RAF-B**
Cartesian Coordinates				Frequency and Energy
O	0.85184600	-1.34421600	-0.44166100	Zero-point correction= 0.143972 (Hartree/Particle)
O	0.67892000	2.74352300	0.09215400	Thermal correction to Energy= 0.154835
O	3.05512300	-1.33024700	-0.31501100	Thermal correction to Enthalpy= 0.155780
C	-0.43704100	0.68561800	-0.14991500	Thermal correction to Gibbs Free Energy= 0.106760
C	-0.32813900	-0.73451900	-0.16916000	Sum of electronic and zero-point Energies= -647.783397
C	0.80374800	1.41494100	-0.03410000	Sum of electronic and thermal Energies= -647.772533
C	-1.69338900	1.27418100	-0.13809800	Sum of electronic and thermal Enthalpies= -647.771589
C	-1.49385600	-1.51886200	-0.35291100	Sum of electronic and thermal Free Energies= -647.820608
C	1.98180500	0.75199200	-0.04619400	
C	-2.83407000	0.48516400	-0.23101600	
C	-2.72872500	-0.90699900	-0.34606000	

C	2.04643000	-0.68423400	-0.25045600
H	-1.76970300	2.35175500	-0.06607300
H	-1.37643300	-2.58904500	-0.47520300
H	2.93256400	1.25646200	0.07130100
H	-3.81114100	0.95191400	-0.22848300
H	-3.62341200	-1.50857100	-0.45024000
H	1.54738700	3.15797800	0.16402200
O	-0.24110100	-0.87431900	1.83121300
H	-0.55814400	-1.78211000	1.95857900

Name	**4HC-O4-H-OH-FHT-P**
Cartesian Coordinates	Frequency and Energy

O	-0.12545000	1.74255100	0.10021200	Zero-point correction= 0.142439 (Hartree/Particle)
O	-1.04341400	-2.20531900	-0.34582500	Thermal correction to Energy= 0.152710
O	-2.23898500	2.30939500	-0.18802100	Thermal correction to Enthalpy= 0.153654
C	0.64418100	-0.53608600	-0.16590900	Thermal correction to Gibbs Free Energy= 0.105525
C	0.88054500	0.82737400	0.04827000	Sum of electronic and zero-point Energies= -647.792404
C	-0.72104400	-0.95079200	-0.34571700	Sum of electronic and thermal Energies= -647.782133
C	1.72286400	-1.43569500	-0.16512500	Sum of electronic and thermal Enthalpies= -647.781188
C	2.17317400	1.29967500	0.25074200	Sum of electronic and thermal Free Energies= -647.829317
C	-1.72795300	0.01933300	-0.44261900	
C	3.00684700	-0.96909000	0.02334200	
C	3.22565800	0.39986900	0.23087900	
C	-1.43270100	1.41977500	-0.17751500	
H	1.52234900	-2.48922200	-0.31810000	
H	2.32888300	2.35753700	0.42161500	
H	-2.64174700	-0.17501000	-0.98439900	
H	3.84325400	-1.65648100	0.01736600	
H	4.23457200	0.76486300	0.38355200	
H	-2.00144100	-2.14241600	0.09941100	
O	-2.85961800	-1.34209400	0.94988100	
H	-3.77555800	-1.14170200	0.71249400	

Name	**4HC-C2-OH-RAF-P**
Cartesian Coordinates	Frequency and Energy

O	0.77442100	-1.20634800	-0.47695900	Zero-point correction= 0.144756 (Hartree/Particle)
O	-0.02591400	2.80450800	-0.03824400	Thermal correction to Energy= 0.154914
O	2.96342300	-0.84922600	-0.60712200	Thermal correction to Enthalpy= 0.155858
C	-0.78933100	0.57216500	-0.03455000	Thermal correction to Gibbs Free Energy= 0.108485
C	-0.49772100	-0.77925400	-0.22756500	Sum of electronic and zero-point Energies= -647.770614
C	0.31972700	1.50962300	-0.10906900	Sum of electronic and thermal Energies= -647.760456
C	-2.11532700	0.95746900	0.19091400	Sum of electronic and thermal Enthalpies= -647.759511
C	-1.50070400	-1.74126800	-0.20833500	Sum of electronic and thermal Free Energies= -647.806885
C	1.58034600	1.05921800	-0.24770900	
C	-3.11952300	0.00484200	0.22242100	
C	-2.80890600	-1.34246700	0.02004100	
C	1.84418000	-0.37547000	-0.26251500	
H	-2.33949000	2.00652100	0.33917000	
H	-1.24038300	-2.78038700	-0.36865900	
H	2.44323900	1.71166700	-0.28595000	
H	-4.14474900	0.30443700	0.40109100	
H	-3.59495800	-2.08806900	0.04305600	
H	0.76231900	3.36275600	-0.06657900	
O	2.31284000	-0.74800200	1.42924700	
H	2.43941900	-1.71353800	1.42070700	

Name	**4HC-C3-OH-RAF-P**

Cartesian Coordinates				Frequency and Energy
O	0.52576800	-1.56833400	-0.16791100	Zero-point correction= 0.144256 (Hartree/Particle)
O	0.53506700	2.52861400	-0.48324200	Thermal correction to Energy= 0.155202
O	2.70283300	-1.66565000	-0.50467200	Thermal correction to Enthalpy= 0.156146
C	-0.66968300	0.53066300	-0.18156000	Thermal correction to Gibbs Free Energy= 0.106430
C	-0.63419300	-0.86361600	-0.07059900	Sum of electronic and zero-point Energies= -647.796031
C	0.58354900	1.20749700	-0.37553700	Sum of electronic and thermal Energies= -647.785085
C	-1.90178500	1.19677800	-0.08500300	Sum of electronic and thermal Enthalpies= -647.784141
C	-1.80006500	-1.59326200	0.13518200	Sum of electronic and thermal Free Energies= -647.833857
C	1.75889900	0.49303300	-0.36786200	
C	-3.06153800	0.47632100	0.11860700	
C	-3.00596800	-0.91866400	0.22866600	
C	1.73740900	-0.96395100	-0.36603800	
H	-1.92309000	2.27632500	-0.16670500	
H	-1.73952200	-2.67119900	0.21873100	
H	2.70039100	0.95623700	-0.63404200	
H	-4.01213200	0.98865200	0.19677400	
H	-3.91694300	-1.48253600	0.39118500	
H	1.42727100	2.90208500	-0.52210100	
O	2.04640300	0.62807900	1.73212700	
H	2.94372300	0.25995700	1.69060600	
Name				**4HC-C4-OH-RAF-P**
Cartesian Coordinates				Frequency and Energy
O	0.56607900	-1.65123100	0.01825800	Zero-point correction= 0.144236 (Hartree/Particle)
O	0.69500300	2.40416800	-0.64594100	Thermal correction to Energy= 0.154832
O	2.74964900	-1.84302100	-0.24561700	Thermal correction to Enthalpy= 0.155776
C	-0.57068300	0.47313700	-0.17987600	Thermal correction to Gibbs Free Energy= 0.107517
C	-0.58225600	-0.91132300	-0.01158800	Sum of electronic and zero-point Energies= -647.790528
C	0.72534500	1.12293900	-0.30524400	Sum of electronic and thermal Energies= -647.779932
C	-1.78018300	1.17482600	-0.19655500	Sum of electronic and thermal Enthalpies= -647.778988
C	-1.77971200	-1.60235000	0.13759600	Sum of electronic and thermal Free Energies= -647.827247
C	1.86614400	0.33212800	-0.40679200	
C	-2.97570400	0.49437100	-0.05068700	
C	-2.97035700	-0.89358500	0.11772700	
C	1.80243800	-1.10122600	-0.21580100	
H	-1.76206800	2.25026700	-0.32172200	
H	-1.75611900	-2.67756100	0.26468900	
H	2.83807200	0.75880900	-0.61589600	
H	-3.91291600	1.03639300	-0.06425100	
H	-3.90649400	-1.42693400	0.23338800	
H	1.58943400	2.77380800	-0.64574100	
O	1.39253600	1.36744200	1.59131700	
H	1.27377100	0.53286500	2.07272400	
Name				**4HC-C5-OH-RAF-P**
Cartesian Coordinates				Frequency and Energy
O	1.32627900	-1.38384200	0.14692800	Zero-point correction= 0.144030 (Hartree/Particle)
O	0.28932700	2.54216500	-0.46707700	Thermal correction to Energy= 0.154828
O	3.47242900	-0.88681600	0.27322700	Thermal correction to Enthalpy= 0.155772
C	-0.34134500	0.28684900	-0.28994100	Thermal correction to Gibbs Free Energy= 0.106683
C	0.02895800	-1.02737900	-0.04090000	Sum of electronic and zero-point Energies= -647.787320
C	0.70600100	1.27960600	-0.29263500	Sum of electronic and thermal Energies= -647.776522
C	-1.71581800	0.61010700	-0.44292000	Sum of electronic and thermal Enthalpies= -647.775578
C	-0.92504500	-2.04474000	0.01387400	Sum of electronic and thermal Free Energies= -647.824667
C	1.99615200	0.91507600	-0.11011600	

C	-2.66190700	-0.43243200	-0.45486400
C	-2.26550800	-1.73603500	-0.19851500
C	2.35621800	-0.46915400	0.11098500
H	-1.97825300	1.57614000	-0.85442200
H	-0.59991500	-3.05833100	0.21391600
H	2.80699000	1.63249400	-0.10711000
H	-3.70431000	-0.19641900	-0.62598700
H	-3.00111300	-2.53082500	-0.17287200
H	1.03893500	3.15319800	-0.45464100
O	-2.09665800	1.35116500	1.41430900
H	-1.55957900	2.15098300	1.29221700

Name			**4HC-C6-OH-RAF-P**
Cartesian Coordinates			Frequency and Energy
O	1.26986400	-1.41457300	0.04417600
O	0.76375500	2.65552100	-0.18242100
O	3.44475000	-1.20666400	0.35113000
C	-0.16539800	0.49526000	-0.23333200
C	0.04179400	-0.88885900	-0.15794900
C	1.00347800	1.34391900	-0.09971100
C	-1.45143500	0.98232200	-0.44922900
C	-1.02032500	-1.79015200	-0.30274300
C	2.22658300	0.79990800	0.09233800
C	-2.54252700	0.09691700	-0.52275600
C	-2.28843800	-1.30219800	-0.51051500
C	2.40472500	-0.63156500	0.17633800
H	-1.61389000	2.04989800	-0.52329200
H	-0.81460600	-2.85247300	-0.25972300
H	3.11979000	1.40374000	0.19139500
H	-3.49424000	0.45946500	-0.88394700
H	-3.11785700	-1.98811700	-0.63127300
H	1.58489100	3.15765800	-0.08921500
O	-3.27957600	0.35200700	1.33781900
H	-2.50517200	0.04617700	1.83578400

Zero-point correction= 0.143846 (Hartree/Particle)
Thermal correction to Energy= 0.154782
Thermal correction to Enthalpy= 0.155726
Thermal correction to Gibbs Free Energy= 0.106249
Sum of electronic and zero-point Energies= -647.789784
Sum of electronic and thermal Energies= -647.778848
Sum of electronic and thermal Enthalpies= -647.777904
Sum of electronic and thermal Free Energies= -647.827381

Name			**4HC-C7-OH-RAF-P**
Cartesian Coordinates			Frequency and Energy
O	0.95391000	-1.48707000	-0.17446400
O	1.33553000	2.59045600	0.22148400
O	3.12080600	-1.79026100	0.10053800
C	-0.03687900	0.71337500	-0.13996900
C	-0.13779600	-0.67898000	-0.26644100
C	1.28097500	1.25912100	0.10011400
C	-1.19254400	1.50764700	-0.26416500
C	-1.35662100	-1.28632300	-0.50776000
C	2.35447900	0.43918600	0.18401700
C	-2.41140000	0.91914100	-0.49810400
C	-2.52263200	-0.49727700	-0.56496700
C	2.22005100	-0.99540400	0.04234300
H	-1.09979900	2.58320100	-0.18296400
H	-1.40692700	-2.36266900	-0.61315200
H	3.35517000	0.81374200	0.35761200
H	-3.30444300	1.52289100	-0.59606600
H	-3.43036600	-0.93944700	-0.95165600
H	2.24568100	2.88008700	0.37161200
O	-3.28497500	-0.84729500	1.26575900

Zero-point correction= 0.143817 (Hartree/Particle)
Thermal correction to Energy= 0.154728
Thermal correction to Enthalpy= 0.155672
Thermal correction to Gibbs Free Energy= 0.106225
Sum of electronic and zero-point Energies= -647.787991
Sum of electronic and thermal Energies= -647.777080
Sum of electronic and thermal Enthalpies= -647.776136
Sum of electronic and thermal Free Energies= -647.825582

H	-2.54728400	-0.50735600	1.79767300	
Name				**4HC-C8-OH-RAF-P**
Cartesian Coordinates				Frequency and Energy
O	0.73808100	-1.36666500	-0.37414200	Zero-point correction= 0.143962 (Hartree/Particle)
O	1.26486100	2.63653000	0.36965800	Thermal correction to Energy= 0.154834
O	2.90578700	-1.76188800	-0.23508900	Thermal correction to Enthalpy= 0.155778
C	-0.17822200	0.83259800	-0.07567300	Thermal correction to Gibbs Free Energy= 0.106528
C	-0.31941800	-0.52983000	-0.32085800	Sum of electronic and zero-point Energies= -647.788745
C	1.16819800	1.32431000	0.13662700	Sum of electronic and thermal Energies= -647.777873
C	-1.31944600	1.64311400	-0.04863400	Sum of electronic and thermal Enthalpies= -647.776929
C	-1.59551200	-1.11690800	-0.47367900	Sum of electronic and thermal Free Energies= -647.826179
C	2.22173200	0.47562800	0.09393300	
C	-2.57900700	1.09561300	-0.28335400	
C	-2.71423400	-0.25990000	-0.52629800	
C	2.03971300	-0.93188900	-0.17045700	
H	-1.20660200	2.70228900	0.14673400	
H	-1.65679500	-2.12746700	-0.85690900	
H	3.23977400	0.80796000	0.25247200	
H	-3.45036100	1.73830700	-0.28486500	
H	-3.68927100	-0.69100600	-0.71682000	
H	2.18799000	2.88976400	0.50676000	
O	-1.74925100	-1.76849400	1.43789400	
H	-1.04337500	-2.43211600	1.37641400	
Name				**4HC-C4'-OH-RAF-P**
Cartesian Coordinates				Frequency and Energy
O	0.92050400	-1.49516400	-0.01568000	Zero-point correction= 0.144226 (Hartree/Particle)
O	0.56129200	2.58300500	-0.43583600	Thermal correction to Energy= 0.154951
O	3.12075300	-1.37237300	-0.03579500	Thermal correction to Enthalpy= 0.155895
C	-0.44604300	0.49247000	-0.01430500	Thermal correction to Gibbs Free Energy= 0.107416
C	-0.29805200	-0.92358500	-0.08641800	Sum of electronic and zero-point Energies= -647.786042
C	0.76627300	1.27500000	-0.27931700	Sum of electronic and thermal Energies= -647.775318
C	-1.74886800	1.03435300	-0.24492800	Sum of electronic and thermal Enthalpies= -647.774373
C	-1.40269600	-1.75796100	-0.16903900	Sum of electronic and thermal Free Energies= -647.822853
C	1.96539400	0.66470800	-0.33047900	
C	-2.83525900	0.20280400	-0.33495200	
C	-2.66407200	-1.19546400	-0.28408000	
C	2.09055800	-0.76135100	-0.11452800	
H	-1.85312200	2.11041300	-0.29918600	
H	-1.25389700	-2.83039100	-0.16120800	
H	2.88727400	1.20903000	-0.49070800	
H	-3.82707000	0.61796500	-0.46339000	
H	-3.52908200	-1.84376300	-0.35679100	
H	1.40226400	3.04359100	-0.56173100	
O	-0.25455100	0.65813800	1.90036300	
H	-1.17376900	0.51846000	2.17687200	
Name				**4HC-C8'-OH-RAF-P**
Cartesian Coordinates				Frequency and Energy
O	0.85104800	-1.34443300	-0.44093600	Zero-point correction= 0.143723 (Hartree/Particle)
O	0.68434900	2.74117400	0.09438300	Thermal correction to Energy= 0.154647
O	3.05293800	-1.33512000	-0.31973300	Thermal correction to Enthalpy= 0.155592
C	-0.43599300	0.68593300	-0.14773300	Thermal correction to Gibbs Free Energy= 0.106237
C	-0.32982100	-0.73417200	-0.16832000	Sum of electronic and zero-point Energies= -647.787952
C	0.80596300	1.41389200	-0.03243000	Sum of electronic and thermal Energies= -647.777028
C	-1.69190600	1.27693900	-0.14064800	Sum of electronic and thermal Enthalpies= -647.776084

C	-1.49588900	-1.51807100	-0.35238400	Sum of electronic and thermal Free Energies= -647.825438
C	1.98432800	0.74938000	-0.04538700	
C	-2.83319400	0.48912900	-0.23596500	
C	-2.72968300	-0.90418100	-0.34810900	
C	2.04437200	-0.68463500	-0.25221300	
H	-1.76921200	2.35473600	-0.07135400	
H	-1.38177700	-2.58922400	-0.47045800	
H	2.93447300	1.25587800	0.07020200	
H	-3.80974700	0.95724700	-0.23752300	
H	-3.62517100	-1.50462200	-0.45277800	
H	1.55557100	3.15475900	0.16028100	
O	-0.23545700	-0.87705500	1.83745900	
H	-0.63622900	-1.75057900	1.97138200	
Name				**4HC-O4-H-OH-FHT-H**
Cartesian Coordinates				Frequency and Energy
O	-0.13231200	1.73767400	0.10044100	Zero-point correction= 0.142025 (Hartree/Particle)
O	-1.04070000	-2.21314500	-0.30700500	Thermal correction to Energy= 0.152244
O	-2.24637700	2.29565900	-0.18360900	Thermal correction to Enthalpy= 0.153188
C	0.65228600	-0.54213500	-0.15830400	Thermal correction to Gibbs Free Energy= 0.105269
C	0.88724100	0.82221700	0.04819500	Sum of electronic and zero-point Energies= -647.794196
C	-0.71012100	-0.95875900	-0.32977800	Sum of electronic and thermal Energies= -647.783977
C	1.73589300	-1.43693800	-0.15900200	Sum of electronic and thermal Enthalpies= -647.783033
C	2.17427700	1.30562200	0.24304100	Sum of electronic and thermal Free Energies= -647.830952
C	-1.72474900	0.00667700	-0.44432000	
C	3.01779200	-0.96110000	0.02050700	
C	3.23123600	0.40988800	0.22131600	
C	-1.43140800	1.40149200	-0.17870600	
H	1.54355400	-2.49210800	-0.31010400	
H	2.32473900	2.36507600	0.40752500	
H	-2.62220500	-0.19436800	-1.01115300	
H	3.85822000	-1.64314000	0.01126500	
H	4.23910200	0.78007500	0.36596500	
H	-2.00830600	-2.13971500	0.10840500	
O	-2.89991000	-1.29802400	0.92783900	
H	-3.77538600	-1.13492700	0.54908000	
Name				**4HC-C2-OH-RAF-H**
Cartesian Coordinates				Frequency and Energy
O	0.77819800	-1.20530100	-0.46160100	Zero-point correction= 0.144193 (Hartree/Particle)
O	-0.03300600	2.80865300	-0.03334800	Thermal correction to Energy= 0.154334
O	2.96415900	-0.83731200	-0.62852900	Thermal correction to Enthalpy= 0.155278
C	-0.79575400	0.57266800	-0.02946400	Thermal correction to Gibbs Free Energy= 0.107931
C	-0.50463000	-0.77834000	-0.21821000	Sum of electronic and zero-point Energies= -647.774035
C	0.31186300	1.51230300	-0.10079200	Sum of electronic and thermal Energies= -647.763894
C	-2.12466100	0.95419300	0.18883400	Sum of electronic and thermal Enthalpies= -647.762950
C	-1.50096600	-1.74541600	-0.20315200	Sum of electronic and thermal Free Energies= -647.810297
C	1.57631200	1.06540100	-0.23526100	
C	-3.12599200	-0.00197700	0.21579400	
C	-2.81172700	-1.34938000	0.01732200	
C	1.84015900	-0.36256800	-0.25535000	
H	-2.35575400	2.00183100	0.33548200	
H	-1.23525600	-2.78352400	-0.35977300	
H	2.43093400	1.72774900	-0.27496300	
H	-4.15279500	0.29523000	0.38807100	
H	-3.59598400	-2.09655600	0.03725500	

H	0.75366500	3.37135800	-0.06677800
O	2.36637100	-0.76344600	1.40378600
H	2.36177700	-1.73815100	1.41992200

Name			**4HC-C3-OH-RAF-H**
Cartesian Coordinates			Frequency and Energy
O	0.53319300	-1.57069400	-0.16756800
O	0.55004500	2.52109800	-0.50911800
O	2.70491600	-1.68332200	-0.51481500
C	-0.66246700	0.53015600	-0.18745100
C	-0.63607400	-0.86187200	-0.07473400
C	0.59802700	1.20201000	-0.39160000
C	-1.89112300	1.20117300	-0.09253400
C	-1.80029800	-1.59114600	0.13425800
C	1.76662000	0.48294900	-0.41721400
C	-3.05322400	0.48373100	0.11384300
C	-3.00374000	-0.91127400	0.22703200
C	1.74095800	-0.96010800	-0.38417900
H	-1.91048500	2.28016700	-0.18045600
H	-1.74299200	-2.66914500	0.21796700
H	2.71339900	0.95521500	-0.64161000
H	-4.00218800	0.99916600	0.18908700
H	-3.91685800	-1.47105000	0.38984900
H	1.43608900	2.89296600	-0.63706900
O	2.18431300	0.63270100	1.81742700
H	1.29123200	0.36069000	2.09030800

Zero-point correction= 0.143663 (Hartree/Particle)
Thermal correction to Energy= 0.154521
Thermal correction to Enthalpy= 0.155466
Thermal correction to Gibbs Free Energy= 0.106057
Sum of electronic and zero-point Energies= -647.804660
Sum of electronic and thermal Energies= -647.793802
Sum of electronic and thermal Enthalpies= -647.792857
Sum of electronic and thermal Free Energies= -647.842266

Name			**4HC-C4-OH-RAF-H**
Cartesian Coordinates			Frequency and Energy
O	0.58017400	-1.64642000	0.00086000
O	0.69518000	2.41308600	-0.63984700
O	2.76288200	-1.82640000	-0.25037600
C	-0.57166100	0.47815800	-0.17641000
C	-0.58005200	-0.90673100	-0.01871200
C	0.72066100	1.13478400	-0.30133400
C	-1.78541600	1.17308600	-0.19185000
C	-1.76996600	-1.60819300	0.12457600
C	1.87202000	0.34874800	-0.38697100
C	-2.97696500	0.48395600	-0.05036200
C	-2.96471500	-0.90508000	0.10921600
C	1.80667300	-1.08014600	-0.21633800
H	-1.77620300	2.24902000	-0.31391000
H	-1.74003700	-2.68408100	0.24311600
H	2.83792800	0.78877300	-0.59564900
H	-3.91720100	1.02030500	-0.06240700
H	-3.89777900	-1.44419300	0.22018900
H	1.59271300	2.75929200	-0.76252400
O	1.36890800	1.32302200	1.62073900
H	1.13995200	0.49309600	2.06929300

Zero-point correction= 0.144679 (Hartree/Particle)
Thermal correction to Energy= 0.154924
Thermal correction to Enthalpy= 0.155868
Thermal correction to Gibbs Free Energy= 0.108519
Sum of electronic and zero-point Energies= -647.797426
Sum of electronic and thermal Energies= -647.787182
Sum of electronic and thermal Enthalpies= -647.786238
Sum of electronic and thermal Free Energies= -647.833586

Name			**4HC-C5-OH-RAF-H**
Cartesian Coordinates			Frequency and Energy
O	1.30896600	-1.39295600	0.13779100
O	0.34431800	2.54490700	-0.50299400
O	3.45589900	-0.93061500	0.30746800
C	-0.33594900	0.30412700	-0.29225700
C	0.01062100	-1.01676800	-0.05680600

Zero-point correction= 0.143394 (Hartree/Particle)
Thermal correction to Energy= 0.154183
Thermal correction to Enthalpy= 0.155127
Thermal correction to Gibbs Free Energy= 0.106087
Sum of electronic and zero-point Energies= -647.796786

C	0.72691900	1.28158700	-0.30286600	Sum of electronic and thermal Energies= -647.785997
C	-1.70787600	0.64300600	-0.43885100	Sum of electronic and thermal Enthalpies= -647.785052
C	-0.95303000	-2.02684400	-0.01870800	Sum of electronic and thermal Free Energies= -647.834093
C	2.01348800	0.89474100	-0.10761300	
C	-2.66692700	-0.38701500	-0.46828500	
C	-2.28797000	-1.70145800	-0.23266400	
C	2.34100800	-0.48301200	0.12200300	
H	-1.96367200	1.62920300	-0.80348600	
H	-0.63865100	-3.04622100	0.16824500	
H	2.82962000	1.60545500	-0.11112800	
H	-3.70582100	-0.13566500	-0.63881200	
H	-3.03249900	-2.48770100	-0.22376300	
H	1.10803100	3.14065200	-0.49038800	
O	-2.09382100	1.29632100	1.49326200	
H	-1.56161300	2.10283900	1.39139900	
Name				**4HC-C6-OH-RAF-H**
Cartesian Coordinates				Frequency and Energy
O	1.25174200	-1.41884700	0.03602000	Zero-point correction= 0.143689 (Hartree/Particle)
O	0.78256600	2.65385600	-0.19375600	Thermal correction to Energy= 0.154483
O	3.42281900	-1.23412100	0.35746700	Thermal correction to Enthalpy= 0.155427
C	-0.16941400	0.50175000	-0.24053500	Thermal correction to Gibbs Free Energy= 0.106403
C	0.02160500	-0.88370700	-0.16981800	Sum of electronic and zero-point Energies= -647.798287
C	1.00443800	1.34179100	-0.10339300	Sum of electronic and thermal Energies= -647.787493
C	-1.45251000	0.99710500	-0.45380200	Sum of electronic and thermal Enthalpies= -647.786549
C	-1.04061600	-1.78185800	-0.32434900	Sum of electronic and thermal Free Energies= -647.835573
C	2.22489800	0.78686900	0.10063100	
C	-2.54475300	0.11572800	-0.53680300	
C	-2.30457600	-1.28501100	-0.53117900	
C	2.38246700	-0.63536500	0.17820300	
H	-1.61150600	2.06550200	-0.52394600	
H	-0.83848900	-2.84480200	-0.28784900	
H	3.11650600	1.39045000	0.20746000	
H	-3.50347500	0.48955200	-0.86745100	
H	-3.13806100	-1.96403300	-0.66104100	
H	1.61059100	3.15044400	-0.11632400	
O	-3.20312300	0.34509000	1.41342600	
H	-2.39684200	0.00124600	1.83017100	
Name				**4HC-C7-OH-RAF-H**
Cartesian Coordinates				Frequency and Energy
O	0.96004800	-1.48440300	-0.18519900	Zero-point correction= 0.143621 (Hartree/Particle)
O	1.31360900	2.59350700	0.22444800	Thermal correction to Energy= 0.154358
O	3.12170100	-1.77949600	0.10129800	Thermal correction to Enthalpy= 0.155302
C	-0.04890100	0.71084000	-0.15262500	Thermal correction to Gibbs Free Energy= 0.106347
C	-0.14485000	-0.68016000	-0.27926500	Sum of electronic and zero-point Energies= -647.796141
C	1.26434000	1.26478200	0.09713000	Sum of electronic and thermal Energies= -647.785403
C	-1.20885000	1.49854600	-0.28116600	Sum of electronic and thermal Enthalpies= -647.784459
C	-1.35567100	-1.29986500	-0.51891100	Sum of electronic and thermal Free Energies= -647.833414
C	2.34457800	0.44879100	0.18839600	
C	-2.42347000	0.90109000	-0.51273900	
C	-2.52437400	-0.51587200	-0.57480300	
C	2.21325800	-0.97419800	0.04113200	
H	-1.12507700	2.57480300	-0.20363300	
H	-1.39754900	-2.37647100	-0.62469100	
H	3.33767200	0.83731800	0.37267400	

H	-3.31985000	1.49900600	-0.61531300
H	-3.43821500	-0.96799300	-0.93528800
H	2.21906500	2.89293000	0.39420500
O	-3.21123600	-0.84403400	1.33116000
H	-2.44538000	-0.46791400	1.79549400

Name			**4HC-C8-OH-RAF-H**
Cartesian Coordinates			Frequency and Energy
O	0.74205300	-1.36476400	-0.38443500
O	1.26527900	2.63471500	0.37263000
O	2.90344300	-1.76583200	-0.23623400
C	-0.17812300	0.83195000	-0.07811500
C	-0.32104200	-0.52786800	-0.32966200
C	1.16691400	1.32552700	0.13726500
C	-1.32226000	1.64000300	-0.04738600
C	-1.59466500	-1.11547900	-0.49208200
C	2.22310400	0.47384500	0.09767900
C	-2.58178600	1.09267200	-0.28258700
C	-2.71591500	-0.26223700	-0.53343600
C	2.03465700	-0.92045800	-0.17107700
H	-1.21345500	2.69862200	0.15292100
H	-1.65347300	-2.13271100	-0.85669300
H	3.23731300	0.81438700	0.25925300
H	-3.45312700	1.73478200	-0.27938100
H	-3.69016900	-0.69324800	-0.72768500
H	2.18796500	2.89617000	0.50890400
O	-1.74015700	-1.76753700	1.46911600
H	-1.04530400	-2.43839700	1.37046700

Zero-point correction= 0.143552 (Hartree/Particle)
Thermal correction to Energy= 0.154427
Thermal correction to Enthalpy= 0.155371
Thermal correction to Gibbs Free Energy= 0.106140
Sum of electronic and zero-point Energies= -647.797761
Sum of electronic and thermal Energies= -647.786885
Sum of electronic and thermal Enthalpies= -647.785941
Sum of electronic and thermal Free Energies= -647.835172

Name			**4HC-C4'-OH-RAF-H**
Cartesian Coordinates			Frequency and Energy
O	0.93098100	-1.49456700	0.01323000
O	0.57102400	2.58072000	-0.41973800
O	3.12769800	-1.37861600	-0.04631200
C	-0.44516900	0.49157100	-0.02011600
C	-0.29863500	-0.92553000	-0.07365000
C	0.76988300	1.27251700	-0.27948000
C	-1.74732200	1.02962500	-0.27470400
C	-1.39592900	-1.76450900	-0.15150700
C	1.97277200	0.66179900	-0.32961700
C	-2.82913300	0.19506100	-0.36467700
C	-2.65680700	-1.20271200	-0.28705400
C	2.09152100	-0.75496500	-0.11658100
H	-1.85400800	2.10432900	-0.34574300
H	-1.24636300	-2.83638300	-0.12838900
H	2.88872100	1.21429900	-0.49258500
H	-3.82015500	0.60499900	-0.51160700
H	-3.52063800	-1.85234000	-0.35711600
H	1.41085600	3.04547600	-0.55157400
O	-0.30745700	0.70202300	1.90480400
H	-1.20346700	0.42599800	2.15545900

Zero-point correction= 0.144061 (Hartree/Particle)
Thermal correction to Energy= 0.154629
Thermal correction to Enthalpy= 0.155573
Thermal correction to Gibbs Free Energy= 0.107516
Sum of electronic and zero-point Energies= -647.793485
Sum of electronic and thermal Energies= -647.782917
Sum of electronic and thermal Enthalpies= -647.781973
Sum of electronic and thermal Free Energies= -647.830030

Name			**4HC-C8'-OH-RAF-H**
Cartesian Coordinates			Frequency and Energy
O	0.85178400	-1.34886900	-0.41223100
O	0.71631800	2.73656600	0.11620500
O	3.05153300	-1.35314400	-0.34100600

Zero-point correction= 0.143276 (Hartree/Particle)
Thermal correction to Energy= 0.154074
Thermal correction to Enthalpy= 0.155018

C	-0.42224400	0.69420700	-0.13802100	Thermal correction to Gibbs Free Energy= 0.106310
C	-0.33759600	-0.72487800	-0.17523100	Sum of electronic and zero-point Energies= -647.795950
C	0.82569000	1.41235200	-0.01673000	Sum of electronic and thermal Energies= -647.785152
C	-1.67196500	1.29685700	-0.13396600	Sum of electronic and thermal Enthalpies= -647.784208
C	-1.50460900	-1.49976600	-0.38029600	Sum of electronic and thermal Free Energies= -647.832917
C	2.00360100	0.73988500	-0.03642400	
C	-2.82030100	0.51964300	-0.25352600	
C	-2.73199000	-0.87248400	-0.38477600	
C	2.04518800	-0.68140000	-0.25318200	
H	-1.74273500	2.37407900	-0.05320600	
H	-1.39834200	-2.57110100	-0.50128900	
H	2.95269500	1.24834300	0.07206300	
H	-3.79115400	0.99895800	-0.26003400	
H	-3.63228500	-1.46123300	-0.50778800	
H	1.58943800	3.15169600	0.16545700	
O	-0.33075600	-0.93260100	1.86233100	
H	-0.60330500	-1.86285200	1.91531200	
Name				**1-C3H-OH-FHT-B**
Cartesian Coordinates				Frequency and Energy
O	-0.16915100	-1.69294100	-0.16348400	Zero-point correction= 0.153909 (Hartree/Particle)
O	-0.66634400	2.41774400	-0.48076800	Thermal correction to Energy= 0.166854
O	-2.31491100	-1.94404100	-0.63041900	Thermal correction to Enthalpy= 0.167798
C	0.80703500	0.55070100	-0.23887500	Thermal correction to Gibbs Free Energy= 0.112910
C	0.93511500	-0.85329400	-0.09019900	Sum of electronic and zero-point Energies= -723.552362
C	-0.47591800	1.09861000	-0.33335300	Sum of electronic and thermal Energies= -723.539417
C	2.00123700	1.31571800	-0.25477700	Sum of electronic and thermal Enthalpies= -723.538473
C	2.15869100	-1.46275200	0.06826500	Sum of electronic and thermal Free Energies= -723.593361
C	-1.65702100	0.24182300	-0.01208800	
C	3.22829300	0.70168600	-0.09859500	
C	3.31653100	-0.68343500	0.07183400	
C	-1.41311200	-1.22408100	-0.31570900	
H	1.92536700	2.38842600	-0.38170100	
H	2.19799600	-2.54014400	0.17234100	
H	-1.78804200	0.25254400	1.16489700	
H	4.13030400	1.30161900	-0.10650200	
H	4.28067700	-1.15943400	0.19669700	
H	-1.60754400	2.59164800	-0.62272200	
O	-2.79457900	0.72755600	-0.61997700	
H	-3.43904800	0.00845600	-0.69615100	
O	-1.37859700	0.28157000	2.52437200	
H	-0.51616100	0.72792700	2.45632200	
Name				**1-O3H-OH-FHT-B**
Cartesian Coordinates				Frequency and Energy
O	-0.03105900	-1.66711000	-0.20825300	Zero-point correction= 0.153001 (Hartree/Particle)
O	0.51132900	2.42923700	-0.19063800	Thermal correction to Energy= 0.165224
O	2.15307800	-1.92418600	-0.11317500	Thermal correction to Enthalpy= 0.166168
C	-0.97706700	0.57265300	-0.03696100	Thermal correction to Gibbs Free Energy= 0.113288
C	-1.13152000	-0.83015000	-0.09502000	Sum of electronic and zero-point Energies= -723.550952
C	0.30433200	1.10552400	-0.23619000	Sum of electronic and thermal Energies= -723.538730
C	-2.13832400	1.34880700	0.19311800	Sum of electronic and thermal Enthalpies= -723.537786
C	-2.36101400	-1.43924900	0.02974300	Sum of electronic and thermal Free Energies= -723.590665
C	1.38317100	0.24187400	-0.80708400	
C	-3.37128700	0.73969400	0.32312600	
C	-3.49251900	-0.65067300	0.23428700	

C	1.22303500	-1.20577100	-0.33099400
H	-2.03761100	2.42527500	0.25199100
H	-2.42018700	-2.51975000	-0.01569800
H	1.29410500	0.19260300	-1.91200900
H	-4.25231900	1.34686300	0.49242200
H	-4.46157200	-1.12261200	0.33522000
H	1.45294300	2.60503000	-0.32898500
O	2.65708600	0.74622300	-0.58893700
H	3.00486300	0.63776000	0.46848800
O	3.14368600	0.15644600	1.56052800
H	3.31396400	-0.78630800	1.38822400

Name			**1-O4H-OH-FHT-B**
Cartesian Coordinates			Frequency and Energy
O	-0.55925300	1.85668500	0.10544900
O	1.10923500	-1.94247000	-0.10895000
O	1.42368000	2.75277400	-0.22796400
C	-0.79274600	-0.56239000	-0.05677200
C	-1.35675400	0.72330700	0.07242500
C	0.61510000	-0.70786400	-0.05885500
C	-1.68790400	-1.65462300	-0.15153800
C	-2.71844400	0.93024500	0.12158400
C	1.46344700	0.45867200	0.34941500
C	-3.05367700	-1.45102900	-0.10571200
C	-3.57735100	-0.16328000	0.03642900
C	0.77055700	1.78287900	0.03234700
H	-1.27936700	-2.65168100	-0.25689800
H	-3.09075900	1.94301400	0.21595000
H	1.61255800	0.43916400	1.44501000
H	-3.72227200	-2.30022100	-0.17876500
H	-4.64799500	-0.00749700	0.07300900
H	2.20961100	-2.09634000	0.27610200
O	2.72325000	0.45597300	-0.28469300
H	2.97061200	1.37754800	-0.45140700
O	3.35253100	-2.08359900	0.19699500
H	3.57870200	-1.15440000	-0.00563100

Zero-point correction= 0.153229 (Hartree/Particle)
Thermal correction to Energy= 0.165459
Thermal correction to Enthalpy= 0.166403
Thermal correction to Gibbs Free Energy= 0.113216
Sum of electronic and zero-point Energies= -723.547656
Sum of electronic and thermal Energies= -723.535425
Sum of electronic and thermal Enthalpies= -723.534481
Sum of electronic and thermal Free Energies= -723.587669

Name			**1-C2-OH-RAF-B**
Cartesian Coordinates			Frequency and Energy
O	0.23551400	-1.51373800	-0.48926400
O	0.46400800	2.59438500	-0.03024700
O	2.43252400	-1.72231800	-0.30090800
C	-0.87506700	0.61877500	-0.07832100
C	-0.92029100	-0.78384400	-0.25460300
C	0.36377200	1.26333100	-0.17767400
C	-2.09961900	1.28174000	0.18182900
C	-2.10060200	-1.49170100	-0.19998400
C	1.59033300	0.52328400	-0.60665100
C	-3.28364200	0.57184700	0.23757400
C	-3.29489300	-0.81280700	0.04365100
C	1.44897400	-0.96460300	-0.27986300
H	-2.08523600	2.35467600	0.32690100
H	-2.07540800	-2.56508200	-0.34342400
H	1.71181100	0.57886000	-1.69951600
H	-4.21189600	1.09555200	0.43247700
H	-4.22545500	-1.36440400	0.08668300

Zero-point correction= 0.159502 (Hartree/Particle)
Thermal correction to Energy= 0.171241
Thermal correction to Enthalpy= 0.172185
Thermal correction to Gibbs Free Energy= 0.121183
Sum of electronic and zero-point Energies= -723.544169
Sum of electronic and thermal Energies= -723.532431
Sum of electronic and thermal Enthalpies= -723.531487
Sum of electronic and thermal Free Energies= -723.582488

H	1.40430800	2.82470900	-0.00367500
O	2.75462300	1.08685800	-0.06084500
H	2.85864500	0.74087400	0.83643800
O	1.60849800	-0.83748000	1.54721800
H	1.68810400	-1.76298400	1.84074700

Name	**1-C4-OH-RAF-B**
Cartesian Coordinates	Frequency and Energy

O	-0.17595800	1.75329000	-0.09434000
O	-0.74017800	-2.34468100	-0.38472500
O	-2.34542300	2.00975300	0.19083900
C	0.74175200	-0.52948000	-0.16230300
C	0.91701300	0.94161700	-0.10398700
C	-0.54982800	-1.02749300	-0.20676500
C	1.94386300	-1.35152800	-0.05094700
C	2.15167900	1.50734300	-0.06520400
C	-1.66639600	-0.12162000	-0.67575500
C	3.15430800	-0.75841500	-0.00741300
C	3.29732400	0.68351700	-0.03172700
C	-1.45820600	1.28918900	-0.13459900
H	1.82909400	-2.42741800	-0.03796600
H	2.23517200	2.58669900	-0.04060900
H	-1.64922800	-0.07000600	-1.77097800
H	4.05024300	-1.36562100	0.04996000
H	4.28255800	1.12602600	0.00340300
H	-1.69373000	-2.51174100	-0.35175100
O	-2.90804300	-0.64130500	-0.31330900
H	-2.97272900	-0.57259900	0.65046500
O	-0.94616900	-0.68924400	1.60581600
H	-0.34427500	-1.26662700	2.09542700

Zero-point correction= 0.158503 (Hartree/Particle)
Thermal correction to Energy= 0.170762
Thermal correction to Enthalpy= 0.171706
Thermal correction to Gibbs Free Energy= 0.119621
Sum of electronic and zero-point Energies= -723.529269
Sum of electronic and thermal Energies= -723.517010
Sum of electronic and thermal Enthalpies= -723.516066
Sum of electronic and thermal Free Energies= -723.568151

Name	**1-C5-OH-RAF-B**
Cartesian Coordinates	Frequency and Energy

O	0.67328700	-1.73861200	0.16220000
O	0.69481200	2.34389400	-0.27118400
O	2.81601600	-1.56930800	0.68591100
C	-0.55704500	0.29664500	-0.27069100
C	-0.51480600	-1.07541900	-0.09612300
C	0.66739100	1.00240100	-0.27687100
C	-1.84650900	0.92980900	-0.35895100
C	-1.67735000	-1.86892000	-0.08375900
C	1.91529100	0.24322500	-0.56600600
C	-2.98946400	0.11934600	-0.43464800
C	-2.90665900	-1.27087800	-0.25835200
C	1.85197100	-1.09020800	0.16478600
H	-1.88848500	1.93388200	-0.76294600
H	-1.57491600	-2.93615800	0.07055500
H	1.98334200	0.00836300	-1.64557600
H	-3.95203600	0.59194500	-0.58497300
H	-3.80481700	-1.87455200	-0.26867300
H	1.61671800	2.62927200	-0.17946800
O	3.03657300	0.98760600	-0.17763300
H	3.64733400	0.39775300	0.28560500
O	-2.02132600	1.63592100	1.44840800
H	-1.27895500	2.25748100	1.38754300

Zero-point correction= 0.158528 (Hartree/Particle)
Thermal correction to Energy= 0.171168
Thermal correction to Enthalpy= 0.172113
Thermal correction to Gibbs Free Energy= 0.118499
Sum of electronic and zero-point Energies= -723.540842
Sum of electronic and thermal Energies= -723.528202
Sum of electronic and thermal Enthalpies= -723.527257
Sum of electronic and thermal Free Energies= -723.580871

Name	**1-C6-OH-RAF-B**

Cartesian Coordinates				Frequency and Energy
O	0.72996100	-1.68146400	0.00940000	Zero-point correction= 0.158503 (Hartree/Particle)
O	0.95963700	2.43398800	-0.08642800	Thermal correction to Energy= 0.171143
O	2.82776900	-1.65464100	0.70720900	Thermal correction to Enthalpy= 0.172087
C	-0.39006400	0.46884700	-0.25261800	Thermal correction to Gibbs Free Energy= 0.118450
C	-0.41578600	-0.95382100	-0.25102400	Sum of electronic and zero-point Energies= -723.554785
C	0.85207900	1.10228700	-0.16456600	Sum of electronic and thermal Energies= -723.542145
C	-1.62555100	1.13933100	-0.37401900	Sum of electronic and thermal Enthalpies= -723.541201
C	-1.58384200	-1.67487700	-0.42005600	Sum of electronic and thermal Free Energies= -723.594838
C	2.08907900	0.30466100	-0.42111300	
C	-2.82584800	0.41706600	-0.46985400	
C	-2.78635700	-0.99944800	-0.56580800	
C	1.92545500	-1.08564100	0.16741900	
H	-1.64031900	2.22145800	-0.36540500	
H	-1.53477300	-2.75689200	-0.41833500	
H	2.22830400	0.17036200	-1.50965600	
H	-3.73147300	0.94078900	-0.74130700	
H	-3.70832100	-1.55050800	-0.69454000	
H	1.88760200	2.65701700	0.08016700	
O	3.20468500	0.95998500	0.11618800	
H	3.76673400	0.30231400	0.54839400	
O	-3.47002800	0.63078700	1.46737300	
H	-2.71894100	0.19578600	1.90057800	
Name				**1-C7-OH-RAF-B**
Cartesian Coordinates				Frequency and Energy
O	0.48502100	-1.61728500	-0.08675300	Zero-point correction= 0.158687 (Hartree/Particle)
O	1.35249900	2.37057300	0.39093800	Thermal correction to Energy= 0.171195
O	2.61560200	-2.00975600	0.35413900	Thermal correction to Enthalpy= 0.172139
C	-0.30924900	0.68207600	-0.05725600	Thermal correction to Gibbs Free Energy= 0.118995
C	-0.54085000	-0.69199600	-0.23915000	Sum of electronic and zero-point Energies= -723.536515
C	1.06539800	1.07790800	0.18487000	Sum of electronic and thermal Energies= -723.524007
C	-1.38594200	1.56954900	-0.17396000	Sum of electronic and thermal Enthalpies= -723.523062
C	-1.79168000	-1.19063500	-0.52322800	Sum of electronic and thermal Free Energies= -723.576207
C	2.10228500	0.18740700	-0.40856700	
C	-2.65721600	1.09244900	-0.44379300	
C	-2.90807400	-0.30747100	-0.53568300	
C	1.77238100	-1.24044700	-0.00264200	
H	-1.20137400	2.63102200	-0.06490400	
H	-1.92860200	-2.25584500	-0.65921300	
H	2.05398100	0.22404900	-1.51504200	
H	-3.49073800	1.77791700	-0.52928000	
H	-3.81580400	-0.64198100	-1.02046700	
H	2.31352700	2.45538000	0.48412700	
O	3.38022600	0.56312000	0.01681100	
H	3.83861200	-0.22717000	0.33492200	
O	-3.69148700	-0.64125500	1.12911700	
H	-2.98681000	-0.35957800	1.73229400	
Name				**1-C8-OH-RAF-B**
Cartesian Coordinates				Frequency and Energy
O	0.24798400	-1.48770500	-0.43040800	Zero-point correction= 0.158307 (Hartree/Particle)
O	1.38118900	2.38769300	0.43213900	Thermal correction to Energy= 0.171025
O	2.30937800	-2.09453300	0.09124100	Thermal correction to Enthalpy= 0.171969
C	-0.36866200	0.84042800	-0.06425400	Thermal correction to Gibbs Free Energy= 0.118013
C	-0.70777200	-0.48962600	-0.39416100	Sum of electronic and zero-point Energies= -723.553380

C	0.98237100	1.16084100	0.07121100	Sum of electronic and thermal Energies= -723.540661
C	-1.43692700	1.76455400	0.08606900	Sum of electronic and thermal Enthalpies= -723.539717
C	-2.03223800	-0.91220400	-0.53513900	Sum of electronic and thermal Free Energies= -723.593674
C	2.01324300	0.20631000	-0.43452500	
C	-2.75167100	1.37278300	-0.12971700	
C	-3.05856500	0.06609200	-0.47548700	
C	1.55061700	-1.22212900	-0.21075900	
H	-1.19931000	2.78551400	0.35720000	
H	-2.22362100	-1.88978800	-0.95796500	
H	2.12919300	0.32669500	-1.52787300	
H	-3.54474000	2.10402600	-0.03214100	
H	-4.08246000	-0.24112200	-0.64126600	
H	2.33459500	2.36363600	0.60075000	
O	3.24104000	0.45201500	0.19579500	
H	3.66824700	-0.39598100	0.37749000	
O	-2.26605200	-1.68913000	1.34366300	
H	-1.53258800	-2.32199800	1.28493500	
Name				**1-C4'-OH-RAF-B**
Cartesian Coordinates				Frequency and Energy
O	0.31364600	-1.71723000	-0.08824100	Zero-point correction= 0.158749 (Hartree/Particle)
O	0.87928400	2.37338300	-0.16739500	Thermal correction to Energy= 0.171164
O	2.45716300	-1.78810800	0.46559500	Thermal correction to Enthalpy= 0.172108
C	-0.63372200	0.52047200	0.00650500	Thermal correction to Gibbs Free Energy= 0.119381
C	-0.79137400	-0.90676900	-0.20280400	Sum of electronic and zero-point Energies= -723.548001
C	0.62662900	1.07047500	-0.35569300	Sum of electronic and thermal Energies= -723.535586
C	-1.84937600	1.30785700	-0.03215200	Sum of electronic and thermal Enthalpies= -723.534642
C	-2.01655500	-1.49576200	-0.34077500	Sum of electronic and thermal Free Energies= -723.587369
C	1.75063900	0.15479600	-0.71663700	
C	-3.06728900	0.70018300	-0.16276000	
C	-3.16680700	-0.69639200	-0.32450700	
C	1.55121400	-1.18879200	-0.03029500	
H	-1.75649500	2.38345900	0.05704700	
H	-2.07752300	-2.57303900	-0.43322400	
H	1.74462600	-0.05134000	-1.80126000	
H	-3.96886100	1.30072700	-0.16154000	
H	-4.13857400	-1.16096100	-0.43012700	
H	1.84146900	2.49392800	-0.15526300	
O	2.97915300	0.73071300	-0.36283600	
H	3.48124200	0.08024000	0.14827000	
O	-0.29329300	0.33371300	1.85713500	
H	-0.23364600	1.27080800	2.09674900	
Name				**1-C8'-OH-RAF-B**
Cartesian Coordinates				Frequency and Energy
O	0.30911600	-1.50334100	-0.61572600	Zero-point correction= 0.158324 (Hartree/Particle)
O	0.89801500	2.55638600	0.02340100	Thermal correction to Energy= 0.170911
O	2.43038100	-1.89917200	-0.10887500	Thermal correction to Enthalpy= 0.171855
C	-0.61922600	0.72328600	-0.14819900	Thermal correction to Gibbs Free Energy= 0.118702
C	-0.75575900	-0.71690400	-0.20476300	Sum of electronic and zero-point Energies= -723.540607
C	0.69473800	1.23733900	-0.10632800	Sum of electronic and thermal Energies= -723.528019
C	-1.76959500	1.47871800	-0.02994000	Sum of electronic and thermal Enthalpies= -723.527075
C	-2.02144300	-1.29408200	-0.35291300	Sum of electronic and thermal Free Energies= -723.580229
C	1.86429000	0.38247500	-0.43280000	
C	-3.04564200	0.86119700	-0.04999500	
C	-3.17383200	-0.49910400	-0.21122600	

C	1.56475300	-1.10450900	-0.31139500
H	-1.68593200	2.55233000	0.08180800
H	-2.07996200	-2.36163700	-0.53035100
H	2.13126100	0.51979700	-1.49955300
H	-3.92875100	1.48108900	0.04783100
H	-4.15065600	-0.96217500	-0.26045700
H	1.83355800	2.71184600	0.21589300
O	2.95027800	0.76863900	0.37238900
H	3.62784000	0.08262800	0.32091100
O	-0.50644700	-0.98952600	1.69306400
H	-0.82780400	-1.89826000	1.79524100

Name			**1-C3H-OH-FHT-P**
Cartesian Coordinates			Frequency and Energy
O	-0.16978500	-1.69051200	-0.16920500
O	-0.66045100	2.42294200	-0.46761900
O	-2.31446500	-1.94432400	-0.63147500
C	0.80847800	0.55252800	-0.23453700
C	0.93643300	-0.85191700	-0.09366500
C	-0.47391200	1.10243300	-0.32778100
C	2.00340400	1.31680000	-0.24519700
C	2.15918400	-1.46405300	0.06147300
C	-1.65810400	0.24549000	-0.01788500
C	3.23038000	0.70094300	-0.09234500
C	3.31790800	-0.68550400	0.06957700
C	-1.41329600	-1.22074500	-0.32091700
H	1.93044600	2.39070800	-0.36461200
H	2.19949900	-2.54215900	0.16016900
H	-1.79810300	0.25058300	1.15704900
H	4.13273500	1.30068600	-0.09597000
H	4.28170500	-1.16321100	0.19195400
H	-1.60147900	2.60463500	-0.60524100
O	-2.78944300	0.73628100	-0.63291600
H	-3.45396400	0.03274500	-0.68189600
O	-1.39214500	0.25329800	2.52354200
H	-0.54337300	0.72868500	2.46758500

Zero-point correction= 0.153579 (Hartree/Particle)
Thermal correction to Energy= 0.166561
Thermal correction to Enthalpy= 0.167505
Thermal correction to Gibbs Free Energy= 0.112666
Sum of electronic and zero-point Energies= -723.555235
Sum of electronic and thermal Energies= -723.542253
Sum of electronic and thermal Enthalpies= -723.541309
Sum of electronic and thermal Free Energies= -723.596148

Name			**1-O3H-OH-FHT-P**
Cartesian Coordinates			Frequency and Energy
O	-0.02645400	-1.66842500	-0.21148600
O	0.50943300	2.43092800	-0.20997500
O	2.15638400	-1.93171400	-0.13508300
C	-0.97195900	0.57196700	-0.04426300
C	-1.12682600	-0.83109000	-0.09515100
C	0.30846700	1.10565300	-0.24823700
C	-2.13345300	1.34876900	0.18484900
C	-2.35543300	-1.44048300	0.03754700
C	1.39174200	0.24159600	-0.80913000
C	-3.36613000	0.73977100	0.32266900
C	-3.48705800	-0.65136100	0.24248100
C	1.22722700	-1.20793300	-0.34215400
H	-2.03539800	2.42596800	0.23720400
H	-2.41628700	-2.52132800	-0.00319500
H	1.31754100	0.19931100	-1.91502100
H	-4.24689900	1.34781100	0.49132800
H	-4.45548700	-1.12361400	0.34947000

Zero-point correction= 0.152775 (Hartree/Particle)
Thermal correction to Energy= 0.165071
Thermal correction to Enthalpy= 0.166015
Thermal correction to Gibbs Free Energy= 0.112835
Sum of electronic and zero-point Energies= -723.553702
Sum of electronic and thermal Energies= -723.541405
Sum of electronic and thermal Enthalpies= -723.540461
Sum of electronic and thermal Free Energies= -723.593641

H	1.44795600	2.61597400	-0.36018900
O	2.66583500	0.73996300	-0.56899200
H	2.97333400	0.65151100	0.49648800
O	3.09414500	0.16820600	1.59812100
H	3.30104300	-0.76861800	1.43156300

Name			**1-O4H-OH-FHT-P**
Cartesian Coordinates			Frequency and Energy
O	-0.55576700	1.85587300	0.10895300
O	1.10625800	-1.94847000	-0.08762500
O	1.42568900	2.76270100	-0.19050600
C	-0.79284000	-0.56322200	-0.05281200
C	-1.35519400	0.72404100	0.07010800
C	0.61382300	-0.71050100	-0.05006800
C	-1.68982700	-1.65453100	-0.14715300
C	-2.71677900	0.93365000	0.11298900
C	1.47152200	0.45555600	0.33248600
C	-3.05576400	-1.44837900	-0.10767900
C	-3.57768000	-0.15886900	0.02755800
C	0.77530600	1.78356900	0.04281700
H	-1.28476700	-2.65369700	-0.24755200
H	-3.08951500	1.94676900	0.20452500
H	1.65689300	0.43522600	1.42214000
H	-3.72560100	-2.29682500	-0.18043400
H	-4.64827500	-0.00066600	0.05959800
H	2.20383600	-2.09272500	0.29767600
O	2.70868900	0.44482900	-0.35027200
H	3.00873500	1.36217100	-0.43224400
O	3.34957500	-2.07941800	0.20956300
H	3.56773900	-1.15226100	-0.01408100

Zero-point correction= 0.153047 (Hartree/Particle)
Thermal correction to Energy= 0.165312
Thermal correction to Enthalpy= 0.166256
Thermal correction to Gibbs Free Energy= 0.112860
Sum of electronic and zero-point Energies= -723.550147
Sum of electronic and thermal Energies= -723.537882
Sum of electronic and thermal Enthalpies= -723.536937
Sum of electronic and thermal Free Energies= -723.590334

Name			**1-C2-OH-RAF-P**
Cartesian Coordinates			Frequency and Energy
O	0.23648700	-1.51254500	-0.49889800
O	0.46312000	2.59662300	-0.03636400
O	2.43203700	-1.72477200	-0.29944600
C	-0.87177200	0.61961300	-0.08013600
C	-0.91830300	-0.78312300	-0.25817200
C	0.36731900	1.26448300	-0.17926500
C	-2.09633400	1.28279500	0.18162200
C	-2.09887700	-1.49081600	-0.20152700
C	1.59568800	0.52390500	-0.60239500
C	-3.28102700	0.57313800	0.23898900
C	-3.29301900	-0.81175500	0.04499400
C	1.45028200	-0.96474000	-0.27941900
H	-2.08368300	2.35580400	0.32751200
H	-2.07585200	-2.56437600	-0.34573200
H	1.72242800	0.58236000	-1.69429300
H	-4.20881200	1.09735700	0.43575700
H	-4.22352900	-1.36359900	0.08993200
H	1.40210500	2.83492400	-0.01803100
O	2.75874700	1.08275000	-0.04831500
H	2.83762800	0.76370500	0.86176800
O	1.59096300	-0.84407100	1.54694300
H	1.65514000	-1.77105900	1.84358300

Zero-point correction= 0.159214 (Hartree/Particle)
Thermal correction to Energy= 0.170986
Thermal correction to Enthalpy= 0.171930
Thermal correction to Gibbs Free Energy= 0.120853
Sum of electronic and zero-point Energies= -723.547001
Sum of electronic and thermal Energies= -723.535229
Sum of electronic and thermal Enthalpies= -723.534285
Sum of electronic and thermal Free Energies= -723.585362

Name	**1-C4-OH-RAF-P**

Cartesian Coordinates				Frequency and Energy	
O	-0.17763500	1.75373900	-0.08073700	Zero-point correction=	0.158306 (Hartree/Particle)
O	-0.73659600	-2.34374600	-0.39122900	Thermal correction to Energy=	0.170554
O	-2.34683300	2.01312200	0.18577800	Thermal correction to Enthalpy=	0.171498
C	0.74173900	-0.52846500	-0.15770200	Thermal correction to Gibbs Free Energy=	0.119472
C	0.91764800	0.94210100	-0.09968200	Sum of electronic and zero-point Energies=	-723.532887
C	-0.55006600	-1.02658500	-0.20839000	Sum of electronic and thermal Energies=	-723.520640
C	1.94393900	-1.35073300	-0.04555800	Sum of electronic and thermal Enthalpies=	-723.519695
C	2.15120900	1.50879200	-0.06692500	Sum of electronic and thermal Free Energies=	-723.571721
C	-1.66516500	-0.11993200	-0.67773200		
C	3.15489900	-0.75795300	-0.00818400		
C	3.29793500	0.68427300	-0.03808000		
C	-1.45750700	1.28978500	-0.13419200		
H	1.83060400	-2.42679700	-0.02613800		
H	2.23735300	2.58823200	-0.04386200		
H	-1.64590300	-0.06424800	-1.77268100		
H	4.05123200	-1.36470100	0.04923600		
H	4.28339500	1.12699700	-0.00906600		
H	-1.68987200	-2.51657200	-0.37145900		
O	-2.90812600	-0.63904200	-0.31555800		
H	-2.95427900	-0.60740200	0.65181300		
O	-0.95079900	-0.69529100	1.60835800		
H	-0.36039900	-1.29346600	2.08791800		
Name				**1-C5-OH-RAF-P**	
Cartesian Coordinates				Frequency and Energy	
O	0.67515000	-1.73811100	0.16267800	Zero-point correction=	0.158172 (Hartree/Particle)
O	0.68831000	2.34526600	-0.28053700	Thermal correction to Energy=	0.170924
O	2.81891700	-1.57626700	0.67679800	Thermal correction to Enthalpy=	0.171868
C	-0.55620900	0.29639200	-0.26973700	Thermal correction to Gibbs Free Energy=	0.117872
C	-0.51388800	-1.07557100	-0.09479500	Sum of electronic and zero-point Energies=	-723.544694
C	0.66683600	1.00373000	-0.27723000	Sum of electronic and thermal Energies=	-723.531942
C	-1.84679500	0.92795900	-0.35963900	Sum of electronic and thermal Enthalpies=	-723.530998
C	-1.67596200	-1.87052000	-0.08236100	Sum of electronic and thermal Free Energies=	-723.584994
C	1.91729200	0.24692000	-0.56150800		
C	-2.98957800	0.11639200	-0.43510200		
C	-2.90625700	-1.27402100	-0.25778300		
C	1.85410100	-1.08946600	0.16252300		
H	-1.89083500	1.93118800	-0.76558800		
H	-1.57405100	-2.93825000	0.07055800		
H	1.98981200	0.01477500	-1.64112900		
H	-3.95228800	0.58752000	-0.59067900		
H	-3.80366800	-1.87897700	-0.27008500		
H	1.60787700	2.63931000	-0.18848800		
O	3.03390300	0.99469100	-0.16350900		
H	3.66253300	0.40027900	0.26905600		
O	-2.02306200	1.63621100	1.45281200		
H	-1.28235400	2.25893700	1.38419500		
Name				**1-C6-OH-RAF-P**	
Cartesian Coordinates				Frequency and Energy	
O	0.74152300	-1.68341300	-0.00045700	Zero-point correction=	0.158209 (Hartree/Particle)
O	0.91616400	2.44690700	-0.18055600	Thermal correction to Energy=	0.170944
O	2.86268700	-1.70132800	0.60281100	Thermal correction to Enthalpy=	0.171888
C	-0.39302100	0.45748600	-0.27140700	Thermal correction to Gibbs Free Energy=	0.118122
C	-0.41166000	-0.96408500	-0.23727000	Sum of electronic and zero-point Energies=	-723.558431

C	0.83987400	1.10874600	-0.19295400	Sum of electronic and thermal Energies= -723.545696
C	-1.63292100	1.11832100	-0.40592200	Sum of electronic and thermal Enthalpies= -723.544752
C	-1.57862900	-1.69403700	-0.37640200	Sum of electronic and thermal Free Energies= -723.598518
C	2.10003200	0.33401500	-0.36927000	
C	-2.83089900	0.38888000	-0.47143400	
C	-2.78656900	-1.02917400	-0.52619700	
C	1.94405400	-1.08995900	0.14479400	
H	-1.65393700	2.20017400	-0.42883200	
H	-1.52438400	-2.77573900	-0.35420300	
H	2.33821400	0.24482000	-1.44556300	
H	-3.74177000	0.90173300	-0.74670500	
H	-3.70622700	-1.58899100	-0.63364900	
H	1.83400800	2.70608000	-0.01130700	
O	3.13214300	1.00941700	0.30120700	
H	3.91941800	0.45052300	0.31091000	
O	-3.43918500	0.65912800	1.48254200	
H	-2.67355100	0.23455400	1.90134700	
Name				**1-C7-OH-RAF-P**
Cartesian Coordinates				Frequency and Energy
O	0.48622100	-1.61716900	-0.08212000	Zero-point correction= 0.158300 (Hartree/Particle)
O	1.34737400	2.37191000	0.39323200	Thermal correction to Energy= 0.170927
O	2.61661700	-2.01115500	0.34963000	Thermal correction to Enthalpy= 0.171871
C	-0.31044000	0.68149600	-0.05757100	Thermal correction to Gibbs Free Energy= 0.118391
C	-0.54144800	-0.69319000	-0.23787800	Sum of electronic and zero-point Energies= -723.540135
C	1.06386800	1.07839800	0.18610000	Sum of electronic and thermal Energies= -723.527509
C	-1.38721500	1.56818700	-0.17836200	Sum of electronic and thermal Enthalpies= -723.526565
C	-1.79068700	-1.19383700	-0.52240100	Sum of electronic and thermal Free Energies= -723.580045
C	2.10193400	0.18904000	-0.40810100	
C	-2.65814400	1.08934700	-0.44864700	
C	-2.90802800	-0.31113100	-0.53694700	
C	1.77318000	-1.23883200	-0.00345900	
H	-1.20547300	2.63064800	-0.07326300	
H	-1.92715600	-2.25906800	-0.66061600	
H	2.05123000	0.22585200	-1.51407100	
H	-3.49098500	1.77517200	-0.53999700	
H	-3.81479700	-0.64736500	-1.02252800	
H	2.30865900	2.46272100	0.48357300	
O	3.38043500	0.56597000	0.01693500	
H	3.84215700	-0.22313600	0.33353100	
O	-3.68645100	-0.63837300	1.13578400	
H	-2.97531900	-0.35116000	1.72927700	
Name				**1-C8-OH-RAF-P**
Cartesian Coordinates				Frequency and Energy
O	0.25479900	-1.48909900	-0.44666600	Zero-point correction= 0.158114 (Hartree/Particle)
O	1.34736700	2.42548400	0.35278900	Thermal correction to Energy= 0.170870
O	2.32604600	-2.12414300	-0.03394000	Thermal correction to Enthalpy= 0.171814
C	-0.37235000	0.83628300	-0.08519400	Thermal correction to Gibbs Free Energy= 0.117944
C	-0.70557400	-0.50159800	-0.38727100	Sum of electronic and zero-point Energies= -723.557119
C	0.97450300	1.17359900	0.04763800	Sum of electronic and thermal Energies= -723.544363
C	-1.44561100	1.75811100	0.04667300	Sum of electronic and thermal Enthalpies= -723.543419
C	-2.02895500	-0.93377700	-0.50646800	Sum of electronic and thermal Free Energies= -723.597289
C	2.03204400	0.21469400	-0.37733400	
C	-2.76064000	1.35469900	-0.14975500	
C	-3.06259200	0.03751800	-0.45757100	

C	1.56538500	-1.22776900	-0.24164500
H	-1.21432300	2.78738900	0.29086900
H	-2.21828600	-1.92138500	-0.90690000
H	2.25868900	0.35886600	-1.45012000
H	-3.55650400	2.08486600	-0.06580400
H	-4.08574400	-0.27990500	-0.60976400
H	2.30010400	2.43344700	0.52665500
O	3.18079700	0.45518700	0.39499400
H	3.85806000	-0.19260000	0.16362800
O	-2.23451700	-1.67031900	1.40585800
H	-1.51519400	-2.31811600	1.33271600

Name			**1-C4'-OH-RAF-P**
Cartesian Coordinates			Frequency and Energy
O	0.31843100	-1.71656100	-0.07454800
O	0.87650500	2.37383800	-0.16633400
O	2.46336500	-1.78562900	0.46699200
C	-0.63332500	0.51957000	0.01424400
C	-0.78848400	-0.90800200	-0.19775900
C	0.62815900	1.06909100	-0.34296600
C	-1.85050300	1.30589600	-0.03278300
C	-2.01121000	-1.49906600	-0.34614300
C	1.74894300	0.15500000	-0.71817900
C	-3.06640300	0.69647900	-0.17434000
C	-3.16307500	-0.70064700	-0.33860000
C	1.55554200	-1.18678800	-0.02877600
H	-1.76166300	2.38160500	0.06068000
H	-2.07202900	-2.57622100	-0.44309700
H	1.72841100	-0.05125100	-1.80241900
H	-3.96890100	1.29588100	-0.17991100
H	-4.13332000	-1.16640500	-0.45379400
H	1.83813200	2.50255900	-0.16813000
O	2.98130700	0.73250000	-0.37866900
H	3.49018000	0.08684100	0.13202100
O	-0.31380400	0.33841900	1.87056400
H	-0.24510900	1.27726100	2.10241300

Zero-point correction= 0.158366 (Hartree/Particle)
Thermal correction to Energy= 0.170891
Thermal correction to Enthalpy= 0.171835
Thermal correction to Gibbs Free Energy= 0.118792
Sum of electronic and zero-point Energies= -723.551748
Sum of electronic and thermal Energies= -723.539223
Sum of electronic and thermal Enthalpies= -723.538279
Sum of electronic and thermal Free Energies= -723.591321

Name			**1-C8'-OH-RAF-P**
Cartesian Coordinates			Frequency and Energy
O	0.30827700	-1.50292800	-0.61304300
O	0.89416400	2.55978000	0.00047200
O	2.43284500	-1.91075800	-0.14909400
C	-0.61787300	0.72284300	-0.14932200
C	-0.75507500	-0.71692300	-0.20089800
C	0.69584300	1.23809700	-0.11124400
C	-1.76876000	1.47931300	-0.03767600
C	-2.02120900	-1.29547800	-0.34377200
C	1.87114400	0.38341700	-0.41527600
C	-3.04548900	0.86197100	-0.05544100
C	-3.17370600	-0.49979800	-0.20689400
C	1.56903100	-1.10657100	-0.32153700
H	-1.68798800	2.55415200	0.06571900
H	-2.08177800	-2.36417000	-0.51469700
H	2.16861600	0.53543400	-1.47099200
H	-3.92833500	1.48343200	0.03602600
H	-4.15039700	-0.96371300	-0.25398900

Zero-point correction= 0.158204 (Hartree/Particle)
Thermal correction to Energy= 0.170780
Thermal correction to Enthalpy= 0.171724
Thermal correction to Gibbs Free Energy= 0.118434
Sum of electronic and zero-point Energies= -723.544696
Sum of electronic and thermal Energies= -723.532120
Sum of electronic and thermal Enthalpies= -723.531176
Sum of electronic and thermal Free Energies= -723.584466

H	1.83328400	2.72408800	0.17002000
O	2.93015600	0.76207600	0.43182800
H	3.69524300	0.20609300	0.23747800
O	-0.50745400	-0.99272400	1.70294900
H	-0.83598700	-1.90011100	1.79790700

Name			**1-C3H-OH-FHT-H**
Cartesian Coordinates			Frequency and Energy
O	-0.17807600	-1.70055300	-0.16593600
O	-0.68548400	2.40532100	-0.52219400
O	-2.33416300	-1.93866800	-0.61397000
C	0.79600700	0.54516800	-0.25649100
C	0.92413400	-0.85786000	-0.09454400
C	-0.48803100	1.08942300	-0.35250700
C	1.98861500	1.31167700	-0.28122500
C	2.14909600	-1.46303500	0.06949600
C	-1.65705100	0.23556500	0.01704000
C	3.21632200	0.70072800	-0.11935900
C	3.30598200	-0.68236000	0.06533700
C	-1.42522600	-1.22908300	-0.30005500
H	1.90714800	2.38245200	-0.41880500
H	2.18642400	-2.53919100	0.18215700
H	-1.73241900	0.25557800	1.20295200
H	4.11747400	1.30128100	-0.13341800
H	4.27062800	-1.15544700	0.19462000
H	-1.63145400	2.56750500	-0.63871800
O	-2.82234200	0.71773300	-0.54242300
H	-3.43440500	-0.02450200	-0.65327400
O	-1.25337900	0.34406400	2.51956600
H	-0.35492300	0.68780800	2.37797400

Zero-point correction= 0.151441 (Hartree/Particle)
Thermal correction to Energy= 0.163596
Thermal correction to Enthalpy= 0.164540
Thermal correction to Gibbs Free Energy= 0.111224
Sum of electronic and zero-point Energies= -723.561646
Sum of electronic and thermal Energies= -723.549491
Sum of electronic and thermal Enthalpies= -723.548547
Sum of electronic and thermal Free Energies= -723.601864

Name			**1-O3H-OH-FHT-H**
Cartesian Coordinates			Frequency and Energy
O	-0.04073400	-1.66960300	-0.20125700
O	0.51997800	2.42315700	-0.16051400
O	2.14619500	-1.91603000	-0.06951100
C	-0.98285800	0.57271400	-0.02635200
C	-1.13997400	-0.82929900	-0.09431900
C	0.30066300	1.10148400	-0.21909200
C	-2.14171900	1.35141500	0.20376800
C	-2.37250200	-1.43458500	0.01824500
C	1.37001200	0.23612100	-0.80587300
C	-3.37715900	0.74563000	0.32168900
C	-3.50239500	-0.64361700	0.22086300
C	1.21621000	-1.20728100	-0.31116800
H	-2.03348700	2.42647100	0.26999200
H	-2.43143300	-2.51435900	-0.03409000
H	1.25518000	0.17579900	-1.90815900
H	-4.25717800	1.35402600	0.48988100
H	-4.47369000	-1.11237800	0.31152900
H	1.46493300	2.58205500	-0.29285300
O	2.64532000	0.75024600	-0.62398500
H	3.05348000	0.61889900	0.41908700
O	3.21270600	0.15139200	1.50100700
H	3.33280600	-0.79931000	1.33212000

Zero-point correction= 0.153330 (Hartree/Particle)
Thermal correction to Energy= 0.163843
Thermal correction to Enthalpy= 0.164788
Thermal correction to Gibbs Free Energy= 0.116503
Sum of electronic and zero-point Energies= -723.530307
Sum of electronic and thermal Energies= -723.519793
Sum of electronic and thermal Enthalpies= -723.518849
Sum of electronic and thermal Free Energies= -723.567134

Name	**1-O4H-OH-FHT-H**

Cartesian Coordinates				Frequency and Energy	
O	-0.56867000	1.86282700	0.06146300	Zero-point correction=	0.153309 (Hartree/Particle)
O	1.11491800	-1.92870800	-0.14598600	Thermal correction to Energy=	0.164372
O	1.42655500	2.72815700	-0.30789500	Thermal correction to Enthalpy=	0.165316
C	-0.79234400	-0.55944700	-0.06453900	Thermal correction to Gibbs Free Energy=	0.114124
C	-1.36100900	0.72388800	0.06236900	Sum of electronic and zero-point Energies=	-723.541881
C	0.61842400	-0.69962000	-0.07457600	Sum of electronic and thermal Energies=	-723.530818
C	-1.68193800	-1.65606500	-0.14631700	Sum of electronic and thermal Enthalpies=	-723.529874
C	-2.72328800	0.92401100	0.12637300	Sum of electronic and thermal Free Energies=	-723.581066
C	1.43630100	0.46848300	0.40251800		
C	-3.04808400	-1.45962400	-0.08551800		
C	-3.57701200	-0.17429900	0.05820300		
C	0.76204400	1.78274900	0.00421200		
H	-1.26495900	-2.64934900	-0.25118400		
H	-3.09689600	1.93631000	0.21540500		
H	1.47962800	0.45223900	1.50736800		
H	-3.71284600	-2.31235300	-0.14696600		
H	-4.64776900	-0.02477400	0.10725300		
H	2.22989700	-2.10780300	0.21937300		
O	2.75045000	0.48042500	-0.09674100		
H	2.94015000	1.38358500	-0.39273200		
O	3.36186500	-2.09593900	0.11758600		
H	3.59329200	-1.15241800	0.01772100		
Name				**1-C2-OH-RAF-H**	
Cartesian Coordinates				Frequency and Energy	
O	0.24258600	-1.50994300	-0.53079100	Zero-point correction=	0.158881 (Hartree/Particle)
O	0.45931900	2.60895900	-0.04358200	Thermal correction to Energy=	0.170836
O	2.43549800	-1.73119300	-0.28697400	Thermal correction to Enthalpy=	0.171781
C	-0.85865400	0.62214100	-0.07979100	Thermal correction to Gibbs Free Energy=	0.120245
C	-0.91385400	-0.77843100	-0.26979500	Sum of electronic and zero-point Energies=	-723.551652
C	0.38191100	1.26809700	-0.17614100	Sum of electronic and thermal Energies=	-723.539697
C	-2.08168100	1.28765700	0.18542500	Sum of electronic and thermal Enthalpies=	-723.538752
C	-2.09565400	-1.48369100	-0.21605600	Sum of electronic and thermal Free Energies=	-723.590288
C	1.61262800	0.52540400	-0.58470300		
C	-3.26968200	0.58175900	0.23863400		
C	-3.28754900	-0.80203700	0.03699100		
C	1.45857500	-0.96177400	-0.26777700		
H	-2.06880300	2.35973300	0.33779000		
H	-2.07659900	-2.55585100	-0.37070000		
H	1.74938400	0.57814400	-1.67394000		
H	-4.19503600	1.10880500	0.43845000		
H	-4.21981100	-1.35074800	0.07932000		
H	1.38993000	2.87926200	-0.06302500		
O	2.78591200	1.06692600	-0.02690200		
H	2.75233800	0.96021500	0.93474000		
O	1.53539100	-0.89939000	1.55146100		
H	1.32270600	-1.81718900	1.81094600		
Name				**1-C4-OH-RAF-H**	
Cartesian Coordinates				Frequency and Energy	
O	0.18924100	-1.75948000	-0.02847900	Zero-point correction=	0.157522 (Hartree/Particle)
O	0.72026600	2.34642800	-0.40867800	Thermal correction to Energy=	0.169990
O	2.36021900	-2.01565500	0.17558200	Thermal correction to Enthalpy=	0.170934
C	-0.74010600	0.52092200	-0.14883900	Thermal correction to Gibbs Free Energy=	0.118317
C	-0.91857100	-0.94604500	-0.08551200	Sum of electronic and zero-point Energies=	-723.539393

C	0.55111000	1.02506100	-0.21356200	Sum of electronic and thermal Energies= -723.526925
C	-1.94360100	1.34271900	-0.03547200	Sum of electronic and thermal Enthalpies= -723.525981
C	-2.14526500	-1.51810000	-0.07354800	Sum of electronic and thermal Free Energies= -723.578598
C	1.66133400	0.11544500	-0.67997600	
C	-3.15462900	0.74985100	-0.01874400	
C	-3.29628300	-0.69224200	-0.06531800	
C	1.45705400	-1.28950700	-0.12852800	
H	-1.83068500	2.41805800	0.00214400	
H	-2.23074400	-2.59747200	-0.05125400	
H	1.63122600	0.04489400	-1.77318500	
H	-4.05203100	1.35443600	0.03722200	
H	-4.28102700	-1.13671600	-0.05964400	
H	1.66852800	2.54494300	-0.44544600	
O	2.92233500	0.61938700	-0.33192000	
H	2.93270800	0.73243800	0.63153300	
O	0.92931300	0.73303400	1.63196500	
H	0.36476100	1.40108300	2.04787000	
Name				**1-C5-OH-RAF-H**
Cartesian Coordinates				Frequency and Energy
O	0.70053700	-1.73050500	0.10266100	Zero-point correction= 0.158338 (Hartree/Particle)
O	0.66730800	2.37692600	-0.41956900	Thermal correction to Energy= 0.171046
O	2.85161500	-1.67417400	0.55041100	Thermal correction to Enthalpy= 0.171990
C	-0.52595900	0.31679600	-0.27661500	Thermal correction to Gibbs Free Energy= 0.118364
C	-0.49000900	-1.05625000	-0.11157200	Sum of electronic and zero-point Energies= -723.556172
C	0.68142700	1.03665000	-0.28785900	Sum of electronic and thermal Energies= -723.543464
C	-1.82500300	0.93770100	-0.36628200	Sum of electronic and thermal Enthalpies= -723.542520
C	-1.65153100	-1.85974800	-0.10166800	Sum of electronic and thermal Free Energies= -723.596146
C	1.97525600	0.31924600	-0.44754700	
C	-2.96484100	0.12258400	-0.45991600	
C	-2.88120000	-1.27489300	-0.27951200	
C	1.89336700	-1.09004100	0.12793900	
H	-1.87453300	1.95880400	-0.71940400	
H	-1.53851900	-2.92748500	0.04316200	
H	2.20926100	0.19403200	-1.51885900	
H	-3.92712200	0.59074400	-0.62906300	
H	-3.77723300	-1.88077300	-0.29874000	
H	1.57437600	2.71232800	-0.34515900	
O	2.99596100	1.06013600	0.18039700	
H	3.83783200	0.85466200	-0.24373200	
O	-2.06499800	1.46664700	1.51796300	
H	-2.97649400	1.79317400	1.47506900	
Name				**1-C6-OH-RAF-H**
Cartesian Coordinates				Frequency and Energy
O	0.72479800	-1.68747900	-0.01107500	Zero-point correction= 0.158055 (Hartree/Particle)
O	0.90843200	2.44851100	-0.21403000	Thermal correction to Energy= 0.170811
O	2.84043400	-1.75336300	0.57850600	Thermal correction to Enthalpy= 0.171755
C	-0.39639600	0.45963700	-0.28035600	Thermal correction to Gibbs Free Energy= 0.117861
C	-0.42959400	-0.95920300	-0.24334900	Sum of electronic and zero-point Energies= -723.567324
C	0.83959100	1.10508500	-0.19946400	Sum of electronic and thermal Energies= -723.554568
C	-1.63148300	1.12743900	-0.42273500	Sum of electronic and thermal Enthalpies= -723.553624
C	-1.59797600	-1.68513500	-0.38313600	Sum of electronic and thermal Free Energies= -723.607519
C	2.10836200	0.33431400	-0.33817200	
C	-2.83012100	0.40334800	-0.49839300	
C	-2.80155100	-1.01296800	-0.53827100	

C	1.93604300	-1.10288500	0.13564700
H	-1.64811700	2.20934100	-0.45154600
H	-1.54872800	-2.76687400	-0.36067300
H	2.38617000	0.26865300	-1.40308400
H	-3.74498600	0.92516400	-0.74415000
H	-3.72450700	-1.56656800	-0.64917400
H	1.83055700	2.72112600	-0.08615800
O	3.12554100	0.98554900	0.38585900
H	3.97783000	0.78494100	-0.01923800
O	-3.36488500	0.65963700	1.56476500
H	-2.58402400	0.18356900	1.89120400

Name			**1-C7-OH-RAF-H**
Cartesian Coordinates			Frequency and Energy
O	0.48989200	-1.62570300	-0.12337500
O	1.29905200	2.40870800	0.27736000
O	2.60487000	-2.08404400	0.25742600
C	-0.31546500	0.67285800	-0.08918300
C	-0.54750200	-0.70285800	-0.25267300
C	1.05207900	1.09152600	0.15466300
C	-1.39447400	1.55721300	-0.21248800
C	-1.79738300	-1.21112800	-0.50666400
C	2.13814900	0.19682500	-0.32610000
C	-2.66832500	1.07377300	-0.45810500
C	-2.91805800	-0.32952900	-0.51318800
C	1.78456100	-1.25453200	-0.02174000
H	-1.21514400	2.62142000	-0.12726200
H	-1.93186000	-2.27798300	-0.63409400
H	2.23014600	0.26361100	-1.42560800
H	-3.50170200	1.75814500	-0.55443900
H	-3.83311900	-0.67608200	-0.97554200
H	2.25700400	2.54477600	0.35352300
O	3.34747700	0.56822700	0.28785300
H	4.08218300	0.28548000	-0.26988500
O	-3.64046500	-0.61344800	1.20535300
H	-2.89559900	-0.31417500	1.74923200

Zero-point correction= 0.158291 (Hartree/Particle)
Thermal correction to Energy= 0.170917
Thermal correction to Enthalpy= 0.171861
Thermal correction to Gibbs Free Energy= 0.118419
Sum of electronic and zero-point Energies= -723.548667
Sum of electronic and thermal Energies= -723.536041
Sum of electronic and thermal Enthalpies= -723.535097
Sum of electronic and thermal Free Energies= -723.588539

Name			**1-C8-OH-RAF-H**
Cartesian Coordinates			Frequency and Energy
O	0.25796000	-1.49033100	-0.46222600
O	1.32556100	2.43301700	0.34974500
O	2.31819200	-2.14176300	-0.06024900
C	-0.37742600	0.83097500	-0.09120700
C	-0.70825200	-0.50564800	-0.39740400
C	0.96831000	1.17168500	0.04786500
C	-1.45474600	1.74884500	0.03729600
C	-2.02820600	-0.93771000	-0.52922000
C	2.04075700	0.21786200	-0.35574300
C	-2.76942400	1.34288300	-0.16005500
C	-3.06777500	0.02461900	-0.47039600
C	1.56980400	-1.22636300	-0.25398000
H	-1.23014900	2.77979200	0.28041700
H	-2.21339700	-1.93912200	-0.89599300
H	2.29289800	0.37497700	-1.41760100
H	-3.56617900	2.07182900	-0.07685700
H	-4.08923100	-0.29525800	-0.62846900

Zero-point correction= 0.158066 (Hartree/Particle)
Thermal correction to Energy= 0.170832
Thermal correction to Enthalpy= 0.171777
Thermal correction to Gibbs Free Energy= 0.117998
Sum of electronic and zero-point Energies= -723.566607
Sum of electronic and thermal Energies= -723.553841
Sum of electronic and thermal Enthalpies= -723.552897
Sum of electronic and thermal Free Energies= -723.606675

H	2.28612600	2.46815500	0.47939400
O	3.17784000	0.43557500	0.44605100
H	3.96331100	0.15629100	-0.03978100
O	-2.20260600	-1.65048800	1.47402600
H	-1.49719800	-2.30763600	1.35718600

Name	**1-C4'-OH-RAF-H**
Cartesian Coordinates	Frequency and Energy

O	0.34975800	-1.72132600	-0.08694400	Zero-point correction= 0.158656 (Hartree/Particle)
O	0.78216000	2.40215300	-0.31225100	Thermal correction to Energy= 0.171102
O	2.50328600	-1.88539700	0.32607300	Thermal correction to Enthalpy= 0.172046
C	-0.62929900	0.50693900	0.02734000	Thermal correction to Gibbs Free Energy= 0.118830
C	-0.77275800	-0.92184300	-0.17687500	Sum of electronic and zero-point Energies= -723.559322
C	0.63231200	1.06757900	-0.31087300	Sum of electronic and thermal Energies= -723.546875
C	-1.85243600	1.28528000	-0.06463500	Sum of electronic and thermal Enthalpies= -723.545931
C	-1.98720500	-1.52797800	-0.31641200	Sum of electronic and thermal Free Energies= -723.599148
C	1.79995700	0.19778300	-0.63839600	
C	-3.06214200	0.66294800	-0.20037000	
C	-3.14786000	-0.73946000	-0.32573100	
C	1.60187500	-1.20399100	-0.07103100	
H	-1.77263900	2.36253800	0.00920700	
H	-2.03496100	-2.60557000	-0.41374200	
H	1.87973600	0.07006400	-1.72864500	
H	-3.96844500	1.25536200	-0.23099100	
H	-4.11310700	-1.21596600	-0.43627200	
H	1.71878800	2.62378100	-0.43467800	
O	3.02647400	0.75378100	-0.23004700	
H	3.04721900	0.80697800	0.73631100	
O	-0.40392800	0.37779200	1.90998500	
H	-0.31326700	1.32324700	2.10618100	

Name	**1-C8'-OH-RAF-H**
Cartesian Coordinates	Frequency and Energy

O	0.30684200	-1.51059300	-0.57897100	Zero-point correction= 0.158309 (Hartree/Particle)
O	0.89643300	2.56326900	0.00328900	Thermal correction to Energy= 0.170863
O	2.43341600	-1.93476000	-0.19817300	Thermal correction to Enthalpy= 0.171807
C	-0.60488800	0.72495900	-0.14049200	Thermal correction to Gibbs Free Energy= 0.118605
C	-0.76052500	-0.70981600	-0.19663300	Sum of electronic and zero-point Energies= -723.553818
C	0.71144500	1.23502600	-0.09714000	Sum of electronic and thermal Energies= -723.541263
C	-1.75276800	1.48907500	-0.04152600	Sum of electronic and thermal Enthalpies= -723.540319
C	-2.02859900	-1.28266100	-0.36131800	Sum of electronic and thermal Free Energies= -723.593521
C	1.89203500	0.38231200	-0.39450300	
C	-3.03486200	0.88112400	-0.07956200	
C	-3.17525400	-0.47958600	-0.23867200	
C	1.57810200	-1.10797200	-0.33600800	
H	-1.67023500	2.56383900	0.05932200	
H	-2.09097400	-2.35102400	-0.53137200	
H	2.21354600	0.55747400	-1.43554800	
H	-3.91217100	1.51149800	0.00067700	
H	-4.15483600	-0.93431000	-0.30248800	
H	1.84159500	2.75648000	0.09875200	
O	2.94499200	0.71652000	0.48388700	
H	3.78444800	0.50483800	0.05706500	
O	-0.59315200	-1.01667300	1.73877100	
H	-0.86774300	-1.94566900	1.77829500	

Name	**4HC-ANION-C2-OH-RAF-H**

Cartesian Coordinates				Frequency and Energy	
O	0.72889600	-1.33113200	-0.42344800	Zero-point correction=	0.131331 (Hartree/Particle)
O	0.32064600	2.75003500	-0.23461200	Thermal correction to Energy=	0.141425
O	2.93662300	-1.15673500	-0.53960700	Thermal correction to Enthalpy=	0.142370
C	-0.70484500	0.60312900	-0.11025000	Thermal correction to Gibbs Free Energy=	0.095127
C	-0.50445600	-0.77586400	-0.20855300	Sum of electronic and zero-point Energies=	-647.367790
C	0.45150600	1.51440300	-0.21772200	Sum of electronic and thermal Energies=	-647.357695
C	-2.00303600	1.08797400	0.08246600	Sum of electronic and thermal Enthalpies=	-647.356751
C	-1.57773000	-1.66005900	-0.12838300	Sum of electronic and thermal Free Energies=	-647.403994
C	1.72706500	0.87978300	-0.29708400		
C	-3.07529400	0.21738900	0.17077400		
C	-2.85629800	-1.15946900	0.06149500		
C	1.88837100	-0.56589300	-0.27203800		
H	-2.14865700	2.15892800	0.16206000		
H	-1.39124600	-2.72359700	-0.21477800		
H	2.62911600	1.47729100	-0.32907800		
H	-4.07736900	0.59846300	0.32282200		
H	-3.69111300	-1.84729000	0.12751800		
O	1.75701000	-0.31943400	1.64683900		
H	2.66216200	-0.05402800	1.85384500		
Name				**4HC-ANION-C3-OH-RAF-H**	
Cartesian Coordinates				Frequency and Energy	
O	0.53981100	-1.53574900	-0.16398100	Zero-point correction=	0.131326 (Hartree/Particle)
O	0.59021000	2.53849400	-0.57386900	Thermal correction to Energy=	0.141850
O	2.70400400	-1.62233600	-0.56198900	Thermal correction to Enthalpy=	0.142794
C	-0.67226900	0.56118800	-0.17334000	Thermal correction to Gibbs Free Energy=	0.094013
C	-0.63500900	-0.82810600	-0.05607900	Sum of electronic and zero-point Energies=	-647.376868
C	0.58001800	1.30500500	-0.37313600	Sum of electronic and thermal Energies=	-647.366345
C	-1.91472000	1.20407500	-0.08534700	Sum of electronic and thermal Enthalpies=	-647.365400
C	-1.78996700	-1.57501100	0.15059600	Sum of electronic and thermal Free Energies=	-647.414181
C	1.78305800	0.53696300	-0.24153100		
C	-3.07249200	0.47562200	0.12207600		
C	-3.00686400	-0.91724000	0.24069300		
C	1.74010900	-0.90169000	-0.35596400		
H	-1.94504300	2.28350400	-0.17568900		
H	-1.71625200	-2.65257700	0.23274800		
H	2.70462100	0.99004600	-0.58225700		
H	-4.02754300	0.98106200	0.19485300		
H	-3.91139800	-1.49110400	0.40301800		
O	2.13877400	0.66935300	1.66330200		
H	3.04204700	0.32613300	1.65181100		
Name				**4HC-ANION-C4-OH-RAF-H**	
Cartesian Coordinates				Frequency and Energy	
O	0.65273300	-1.58458400	0.06235200	Zero-point correction=	0.131137 (Hartree/Particle)
O	0.71659000	2.47422500	-0.62949800	Thermal correction to Energy=	0.141284
O	2.82695400	-1.73204900	-0.26372200	Thermal correction to Enthalpy=	0.142229
C	-0.56742700	0.50740300	-0.15835700	Thermal correction to Gibbs Free Energy=	0.094828
C	-0.53459200	-0.87238600	0.01029100	Sum of electronic and zero-point Energies=	-647.363854
C	0.71598700	1.27093800	-0.26569600	Sum of electronic and thermal Energies=	-647.353707
C	-1.80579000	1.14316100	-0.21577500	Sum of electronic and thermal Enthalpies=	-647.352763
C	-1.69937500	-1.61994000	0.13209100	Sum of electronic and thermal Free Energies=	-647.400163
C	1.88755200	0.41977700	-0.44150300		
C	-2.98166900	0.41461400	-0.09558700		
C	-2.92448200	-0.96819400	0.08167400		

C	1.85594600	-0.99298400	-0.22157300	
H	-1.83058900	2.21782400	-0.35407800	
H	-1.63023800	-2.69330400	0.26116800	
H	2.84710800	0.86795800	-0.66425400	
H	-3.93971500	0.91783200	-0.14006600	
H	-3.83775900	-1.54349200	0.17567200	
O	1.15489200	1.17211900	1.59764900	
H	1.90492600	1.78116700	1.63391800	
Name				**4HC-ANION-C5-OH-RAF-H**
Cartesian Coordinates				Frequency and Energy
O	1.34333000	-1.34262800	0.15160700	Zero-point correction= 0.130418 (Hartree/Particle)
O	0.32230900	2.57786200	-0.48306700	Thermal correction to Energy= 0.140928
O	3.48598000	-0.84348500	0.27640100	Thermal correction to Enthalpy= 0.141872
C	-0.33982200	0.31013100	-0.31095400	Thermal correction to Gibbs Free Energy= 0.093143
C	0.03759900	-0.99413800	-0.04125500	Sum of electronic and zero-point Energies= -647.358867
C	0.67875400	1.37981000	-0.32460900	Sum of electronic and thermal Energies= -647.348357
C	-1.71784600	0.60071900	-0.47656300	Sum of electronic and thermal Enthalpies= -647.347413
C	-0.90508800	-2.02391700	0.03854600	Sum of electronic and thermal Free Energies= -647.396142
C	2.00087600	0.95346100	-0.13594100	
C	-2.66162200	-0.44395400	-0.44856500	
C	-2.25192600	-1.73893400	-0.16619700	
C	2.35460700	-0.38811200	0.09847200	
H	-1.99047500	1.56562600	-0.88425400	
H	-0.56709900	-3.03009600	0.25575700	
H	2.80709600	1.67528100	-0.14228200	
H	-3.70681200	-0.22217800	-0.62384700	
H	-2.97737700	-2.54164100	-0.11677500	
O	-2.06492000	1.41919900	1.41476100	
H	-1.43211900	2.13503100	1.23618500	
Name				**4HC-ANION-C6-OH-RAF-H**
Cartesian Coordinates				Frequency and Energy
O	1.29876300	-1.36172500	0.05607400	Zero-point correction= 0.130513 (Hartree/Particle)
O	0.78987800	2.69660100	-0.21811100	Thermal correction to Energy= 0.141112
O	3.46881100	-1.14027000	0.37540500	Thermal correction to Enthalpy= 0.142056
C	-0.16323500	0.52277900	-0.25082500	Thermal correction to Gibbs Free Energy= 0.093219
C	0.06283600	-0.85412200	-0.15858500	Sum of electronic and zero-point Energies= -647.359535
C	0.98155200	1.45826800	-0.12550900	Sum of electronic and thermal Energies= -647.348937
C	-1.46019200	0.96678900	-0.47530500	Sum of electronic and thermal Enthalpies= -647.347992
C	-0.97913400	-1.78687400	-0.30139200	Sum of electronic and thermal Free Energies= -647.396830
C	2.23125000	0.85896500	0.09357600	
C	-2.53262200	0.05814000	-0.54508600	
C	-2.25543100	-1.33593700	-0.51716200	
C	2.41748100	-0.52811300	0.18733000	
H	-1.64337100	2.03126600	-0.56440300	
H	-0.74497800	-2.84305300	-0.24921900	
H	3.11374200	1.47654700	0.19687800	
H	-3.50054600	0.40156500	-0.88326100	
H	-3.06876000	-2.04139700	-0.63546400	
O	-3.15819900	0.25434100	1.44328700	
H	-3.16514200	1.22412700	1.43997900	
Name				**4HC-ANION-C7-OH-RAF-H**
Cartesian Coordinates				Frequency and Energy
O	1.00904200	-1.43189300	-0.18793800	Zero-point correction= 0.130235 (Hartree/Particle)
O	1.33193400	2.63900700	0.25939200	Thermal correction to Energy= 0.140849

O	3.17543700	-1.69933900	0.09600100	Thermal correction to Enthalpy= 0.141793
C	-0.04311700	0.74490700	-0.14324400	Thermal correction to Gibbs Free Energy= 0.092826
C	-0.10734400	-0.64609100	-0.27922700	Sum of electronic and zero-point Energies= -647.357869
C	1.26478800	1.38982000	0.12163400	Sum of electronic and thermal Energies= -647.347255
C	-1.22423700	1.49660500	-0.27402800	Sum of electronic and thermal Enthalpies= -647.346311
C	-1.30540600	-1.29249300	-0.52644800	Sum of electronic and thermal Free Energies= -647.395278
C	2.36112900	0.51998800	0.19777800	
C	-2.42786800	0.87777500	-0.51362800	
C	-2.49505300	-0.54047800	-0.58333500	
C	2.26051800	-0.87565900	0.04533000	
H	-1.15950700	2.57434800	-0.18893700	
H	-1.32187300	-2.36972500	-0.63682200	
H	3.35031100	0.91767500	0.38348500	
H	-3.33763500	1.45578600	-0.61575300	
H	-3.39595600	-1.01453100	-0.94859200	
O	-3.19187100	-0.89593600	1.32643300	
H	-2.43213700	-0.50450900	1.78652500	

Name				**4HC-ANION-C8-OH-RAF-H**
Cartesian Coordinates				Frequency and Energy
O	0.81837800	-1.31497000	-0.38449200	Zero-point correction= 0.130535 (Hartree/Particle)
O	1.25098600	2.68469100	0.39955600	Thermal correction to Energy= 0.141128
O	2.99033500	-1.65738900	-0.21825800	Thermal correction to Enthalpy= 0.142072
C	-0.17960000	0.85001800	-0.07830000	Thermal correction to Gibbs Free Energy= 0.093230
C	-0.26931900	-0.51281400	-0.33718200	Sum of electronic and zero-point Energies= -647.361211
C	1.15203500	1.45325700	0.16744700	Sum of electronic and thermal Energies= -647.350618
C	-1.35730200	1.60453500	-0.06030500	Sum of electronic and thermal Enthalpies= -647.349674
C	-1.51854800	-1.14471900	-0.52819500	Sum of electronic and thermal Free Energies= -647.398516
C	2.23649700	0.56255000	0.12169200	
C	-2.59622000	1.01641600	-0.30628400	
C	-2.67424300	-0.34393500	-0.56505400	
C	2.10199400	-0.80670200	-0.15134000	
H	-1.28353000	2.66614700	0.14469700	
H	-1.53648500	-2.17092800	-0.86945400	
H	3.23994600	0.92821900	0.29579700	
H	-3.49294400	1.62303600	-0.30410900	
H	-3.62901300	-0.81405900	-0.76672700	
O	-1.66435500	-1.87461900	1.46124900	
H	-1.83248200	-1.00575100	1.86048600	

Name				**4HC-ANION-C4'-OH-RAF-H**
Cartesian Coordinates				Frequency and Energy
O	0.97312000	-1.43921700	0.05757300	Zero-point correction= 0.130760 (Hartree/Particle)
O	0.57414800	2.60658700	-0.48497000	Thermal correction to Energy= 0.141224
O	3.17008500	-1.30123900	-0.04067800	Thermal correction to Enthalpy= 0.142169
C	-0.45009100	0.50628900	-0.05289500	Thermal correction to Gibbs Free Energy= 0.094044
C	-0.26459600	-0.90576000	-0.05802800	Sum of electronic and zero-point Energies= -647.356740
C	0.74191000	1.37582000	-0.32347900	Sum of electronic and thermal Energies= -647.346275
C	-1.76809700	0.99262100	-0.30437600	Sum of electronic and thermal Enthalpies= -647.345331
C	-1.34128700	-1.77688100	-0.11170300	Sum of electronic and thermal Free Energies= -647.393456
C	1.97631600	0.71660700	-0.35796800	
C	-2.83241200	0.13033000	-0.36692600	
C	-2.61965900	-1.25783800	-0.25600600	
C	2.12539700	-0.65761400	-0.11679200	
H	-1.90034800	2.06273100	-0.40891100	
H	-1.16266500	-2.84377400	-0.06185600	

H	2.88338700	1.28260300	-0.52327100
H	-3.83506600	0.50916700	-0.52033700
H	-3.46373100	-1.93516400	-0.30707600
O	-0.36847300	0.70558000	1.91378500
H	-0.71750400	1.60930800	1.94480500

Name			**4HC-ANION-C8'-OH-RAF-H**
Cartesian Coordinates			Frequency and Energy
O	0.89049500	-1.29794700	-0.40103300
O	0.72940700	2.77860600	0.13886000
O	3.09224800	-1.27277500	-0.34797400
C	-0.42266600	0.72214100	-0.13559900
C	-0.30550200	-0.69550100	-0.17002200
C	0.81095600	1.53075600	-0.00112700
C	-1.68882400	1.28278800	-0.14424800
C	-1.45642100	-1.50165200	-0.37835100
C	2.01068000	0.80783500	-0.04196200
C	-2.82156200	0.48095200	-0.27103800
C	-2.69982200	-0.90989900	-0.39543500
C	2.07919700	-0.58241200	-0.25281800
H	-1.78354400	2.35920300	-0.06862400
H	-1.32172300	-2.57087900	-0.49251800
H	2.95470000	1.32645600	0.06264700
H	-3.80365500	0.93741800	-0.28812300
H	-3.58398700	-1.52220600	-0.52186500
O	-0.32405600	-0.89723600	1.87693700
H	-0.60276100	-1.82522500	1.91775000

Zero-point correction= 0.130237 (Hartree/Particle)
Thermal correction to Energy= 0.140785
Thermal correction to Enthalpy= 0.141730
Thermal correction to Gibbs Free Energy= 0.093295
Sum of electronic and zero-point Energies= -647.357311
Sum of electronic and thermal Energies= -647.346763
Sum of electronic and thermal Enthalpies= -647.345819
Sum of electronic and thermal Free Energies= -647.394254

Name			**10-C2-OH-RAF-H**
Cartesian Coordinates			Frequency and Energy
O	0.76157100	-1.21872900	-0.47167900
O	0.13769400	2.81035300	-0.08414900
O	2.96226600	-0.91543600	-0.57847100
C	-0.78639700	0.61458500	-0.05553300
C	-0.51043100	-0.74309200	-0.22148500
C	0.30796100	1.59380700	-0.13832800
C	-2.10957500	1.01459600	0.16744700
C	-1.51983700	-1.69598800	-0.17453500
C	1.63207700	1.03188900	-0.29052400
C	-3.12342900	0.07650600	0.21994500
C	-2.82312100	-1.27876700	0.04634700
C	1.84356900	-0.41165400	-0.27798200
H	-2.31660000	2.07046100	0.29551600
H	-1.26930200	-2.74053500	-0.31091800
H	2.50537000	1.66967900	-0.33125700
H	-4.14571700	0.38773100	0.39307800
H	-3.61537200	-2.01677700	0.08609600
O	2.19381500	-0.73128300	1.45003400
H	2.93394500	-0.14109400	1.68948300

Zero-point correction= 0.130913 (Hartree/Particle)
Thermal correction to Energy= 0.141006
Thermal correction to Enthalpy= 0.141950
Thermal correction to Gibbs Free Energy= 0.094133
Sum of electronic and zero-point Energies= -647.137626
Sum of electronic and thermal Energies= -647.127533
Sum of electronic and thermal Enthalpies= -647.126589
Sum of electronic and thermal Free Energies= -647.174405

Name			**10-C3-OH-RAF-H**
Cartesian Coordinates			Frequency and Energy
O	0.61223900	-1.49497700	-0.22352600
O	0.50750400	2.57771500	-0.51669100
O	2.81081000	-1.49319800	-0.50550200
C	-0.67240600	0.55637800	-0.18911100
C	-0.56840000	-0.83779000	-0.09852900

Zero-point correction= 0.129268 (Hartree/Particle)
Thermal correction to Energy= 0.139038
Thermal correction to Enthalpy= 0.139982
Thermal correction to Gibbs Free Energy= 0.093052
Sum of electronic and zero-point Energies= -647.121464

C	0.56784500	1.28431000	-0.37628300	Sum of electronic and thermal Energies= -647.111694
C	-1.93013900	1.17277100	-0.08374600	Sum of electronic and thermal Enthalpies= -647.110750
C	-1.70833400	-1.61583300	0.09948100	Sum of electronic and thermal Free Energies= -647.157679
C	1.77833000	0.62149700	-0.32672900	
C	-3.06039100	0.39991300	0.11307500	
C	-2.94359900	-0.99462500	0.20560100	
C	1.81019600	-0.84028100	-0.37205800	
H	-2.00130200	2.25429800	-0.14971900	
H	-1.59608900	-2.69255600	0.16704300	
H	2.70709000	1.13721500	-0.53124800	
H	-4.03282800	0.87263600	0.19889300	
H	-3.83055800	-1.60034600	0.36313200	
O	1.85938300	0.56802000	1.78225800	
H	2.79558200	0.29023100	1.82938200	
Name				**10-C4-OH-RAF-H**
Cartesian Coordinates				Frequency and Energy
O	0.62088700	-1.68257000	0.11306800	Zero-point correction= 0.130925 (Hartree/Particle)
O	0.83062500	2.34140100	-0.75220700	Thermal correction to Energy= 0.141118
O	2.80926000	-1.86692200	-0.07563700	Thermal correction to Enthalpy= 0.142062
C	-0.53309700	0.44414000	-0.17113900	Thermal correction to Gibbs Free Energy= 0.094039
C	-0.54073300	-0.93160000	0.03341800	Sum of electronic and zero-point Energies= -647.138827
C	0.76201000	1.14570800	-0.29422100	Sum of electronic and thermal Energies= -647.128634
C	-1.74783600	1.12853100	-0.24262800	Sum of electronic and thermal Enthalpies= -647.127689
C	-1.73036500	-1.63498500	0.16634300	Sum of electronic and thermal Free Energies= -647.175713
C	1.92587700	0.28550100	-0.37870300	
C	-2.94272500	0.44106700	-0.11165300	
C	-2.92895600	-0.94073700	0.09407500	
C	1.84409300	-1.13748000	-0.11107400	
H	-1.73375000	2.20028100	-0.40167800	
H	-1.69843700	-2.70611000	0.32208900	
H	2.89808500	0.70630100	-0.59893200	
H	-3.88402900	0.97275700	-0.16868000	
H	-3.86165400	-1.48218100	0.19637700	
O	0.96285700	1.86058900	1.38670600	
H	1.84114000	2.28810400	1.36887300	
Name				**10-C5-OH-RAF-H**
Cartesian Coordinates				Frequency and Energy
O	1.34459000	-1.34567500	0.14889700	Zero-point correction= 0.129891 (Hartree/Particle)
O	0.40422300	2.58268600	-0.50011800	Thermal correction to Energy= 0.140719
O	3.48592000	-0.84357000	0.30555400	Thermal correction to Enthalpy= 0.141663
C	-0.34499300	0.33818300	-0.30175400	Thermal correction to Gibbs Free Energy= 0.091843
C	0.03323900	-0.96851500	-0.05311900	Sum of electronic and zero-point Energies= -647.150346
C	0.67072000	1.39460800	-0.33132400	Sum of electronic and thermal Energies= -647.139518
C	-1.72424700	0.64030200	-0.45122400	Sum of electronic and thermal Enthalpies= -647.138574
C	-0.90719500	-2.00195600	-0.00216900	Sum of electronic and thermal Free Energies= -647.188394
C	2.03646300	0.95337300	-0.12775500	
C	-2.66073400	-0.40912000	-0.46962000	
C	-2.24801000	-1.71237500	-0.21824100	
C	2.36223400	-0.44065300	0.12137000	
H	-1.99470000	1.61794200	-0.83014300	
H	-0.56781600	-3.01118900	0.19529000	
H	2.85147300	1.66485000	-0.14385400	
H	-3.70540000	-0.18524400	-0.64259800	
H	-2.97262000	-2.51686400	-0.20004000	

O	-2.14467800	1.29994800	1.45602900
H	-1.63623400	2.12031700	1.34146400

Name			**10-C6-OH-RAF-H**
Cartesian Coordinates			Frequency and Energy
O	1.30862000	-1.36514800	0.06150500
O	0.81467300	2.69016600	-0.20268700
O	3.47834400	-1.11146400	0.36370000
C	-0.18127400	0.52817100	-0.24954400
C	0.05977500	-0.84597500	-0.15259500
C	0.93951500	1.47235500	-0.13054100
C	-1.48243600	0.96789500	-0.47316700
C	-0.96870000	-1.78529900	-0.29139400
C	2.24018800	0.86560900	0.08303100
C	-2.54471300	0.04879600	-0.53112600
C	-2.24957600	-1.34243600	-0.50629200
C	2.41399800	-0.57188200	0.18143100
H	-1.67119400	2.03068700	-0.56826700
H	-0.72556900	-2.83899500	-0.23972000
H	3.12279800	1.48398700	0.17931400
H	-3.51491300	0.37898300	-0.87597500
H	-3.05552800	-2.05584700	-0.62549000
O	-3.12287300	0.25854500	1.42609800
H	-3.34638100	1.20098900	1.36239000

Zero-point correction= 0.130115 (Hartree/Particle)
Thermal correction to Energy= 0.140933
Thermal correction to Enthalpy= 0.141877
Thermal correction to Gibbs Free Energy= 0.092083
Sum of electronic and zero-point Energies= -647.151741
Sum of electronic and thermal Energies= -647.140923
Sum of electronic and thermal Enthalpies= -647.139979
Sum of electronic and thermal Free Energies= -647.189772

Name			**10-C7-OH-RAF-H**
Cartesian Coordinates			Frequency and Energy
O	1.04758800	-1.42965600	-0.17058000
O	1.33130100	2.63071100	0.23548600
O	3.22174000	-1.64121900	0.12027800
C	-0.06435700	0.74357800	-0.14195700
C	-0.09481700	-0.65484400	-0.26426000
C	1.22083500	1.41264100	0.10874000
C	-1.25011000	1.47405500	-0.28198400
C	-1.26830700	-1.32866800	-0.50478400
C	2.37909000	0.54944400	0.19973700
C	-2.43978500	0.82249700	-0.52022900
C	-2.47536000	-0.59750300	-0.56593400
C	2.27532800	-0.89294900	0.05298900
H	-1.20674300	2.55401200	-0.21305400
H	-1.26215200	-2.40638100	-0.60644900
H	3.35995700	0.96820700	0.38111900
H	-3.36060300	1.37954400	-0.63977300
H	-3.36146900	-1.09294600	-0.93937100
O	-3.10459000	-0.85478600	1.34095100
H	-3.83240200	-0.21233500	1.31454100

Zero-point correction= 0.129941 (Hartree/Particle)
Thermal correction to Energy= 0.140737
Thermal correction to Enthalpy= 0.141682
Thermal correction to Gibbs Free Energy= 0.091947
Sum of electronic and zero-point Energies= -647.148210
Sum of electronic and thermal Energies= -647.137413
Sum of electronic and thermal Enthalpies= -647.136469
Sum of electronic and thermal Free Energies= -647.186204

Name			**10-C8-OH-RAF-H**
Cartesian Coordinates			Frequency and Energy
O	0.82708900	-1.32108200	-0.37616800
O	1.26554100	2.67738200	0.38961900
O	3.00664300	-1.62092000	-0.21846700
C	-0.19935200	0.85865400	-0.07409200
C	-0.26952800	-0.50626300	-0.32405300
C	1.10975900	1.48214000	0.16317900
C	-1.38476900	1.60738400	-0.05806400
C	-1.50895000	-1.15517900	-0.50544800

Zero-point correction= 0.130191 (Hartree/Particle)
Thermal correction to Energy= 0.141005
Thermal correction to Enthalpy= 0.141949
Thermal correction to Gibbs Free Energy= 0.092180
Sum of electronic and zero-point Energies= -647.153485
Sum of electronic and thermal Energies= -647.142670
Sum of electronic and thermal Enthalpies= -647.141726
Sum of electronic and thermal Free Energies= -647.191496

C	2.24229100	0.57525600	0.11827200
C	-2.61156500	1.00271200	-0.30174400
C	-2.67076100	-0.36097000	-0.55416000
C	2.08748800	-0.84091800	-0.16021000
H	-1.31903600	2.67048700	0.14124400
H	-1.51321900	-2.17599200	-0.86195200
H	3.24518100	0.94376800	0.28928400
H	-3.51592100	1.59704700	-0.30657000
H	-3.61888100	-0.84235400	-0.75959800
O	-1.62579700	-1.87775600	1.43195800
H	-1.83361900	-1.03084500	1.85998500

Name	**10-C4'-OH-RAF-H**
Cartesian Coordinates	Frequency and Energy

O	0.92851500	-1.45868200	-0.06421400	Zero-point correction= 0.130182 (Hartree/Particle)
O	0.58941100	2.58489300	-0.59123500	Thermal correction to Energy= 0.140922
O	3.12664300	-1.30480700	-0.00853000	Thermal correction to Enthalpy= 0.141866
C	-0.48049500	0.52164600	-0.04041100	Thermal correction to Gibbs Free Energy= 0.092601
C	-0.31296600	-0.88999100	-0.13012100	Sum of electronic and zero-point Energies= -647.150938
C	0.68658600	1.39297900	-0.34807400	Sum of electronic and thermal Energies= -647.140198
C	-1.80306700	1.03944600	-0.14468400	Sum of electronic and thermal Enthalpies= -647.139254
C	-1.39414100	-1.74478900	-0.19125800	Sum of electronic and thermal Free Energies= -647.188519
C	1.96880000	0.71320900	-0.32743100	
C	-2.87753100	0.18956600	-0.19718900	
C	-2.67343000	-1.20320700	-0.21887100	
C	2.07712200	-0.71991100	-0.11950800	
H	-1.92742500	2.11553900	-0.16100400	
H	-1.22547100	-2.81370300	-0.21702400	
H	2.88572500	1.26794900	-0.47614200	
H	-3.88395400	0.58495400	-0.24514900	
H	-3.52670100	-1.86852200	-0.26835500	
O	-0.01349400	0.61620900	1.86353700	
H	-0.51603800	1.41919800	2.07650500	

Name	**10-C8'-OH-RAF-H**
Cartesian Coordinates	Frequency and Energy

O	0.89857800	-1.27873800	-0.46175000	Zero-point correction= 0.129946 (Hartree/Particle)
O	0.72994200	2.77298900	0.09349200	Thermal correction to Energy= 0.140710
O	3.10079600	-1.22737300	-0.34488000	Thermal correction to Enthalpy= 0.141654
C	-0.46162300	0.72877700	-0.15500600	Thermal correction to Gibbs Free Energy= 0.092234
C	-0.31249700	-0.68453000	-0.18884000	Sum of electronic and zero-point Energies= -647.149816
C	0.74826800	1.54871900	-0.01193300	Sum of electronic and thermal Energies= -647.139052
C	-1.73369500	1.27007600	-0.13418100	Sum of electronic and thermal Enthalpies= -647.138107
C	-1.44343000	-1.51325800	-0.35581100	Sum of electronic and thermal Free Energies= -647.187528
C	2.00054200	0.81861900	0.00856700	
C	-2.85278100	0.44184300	-0.22678200	
C	-2.70184900	-0.94253600	-0.34105800	
C	2.06755100	-0.60913000	-0.25687700	
H	-1.84597000	2.34461200	-0.05289000	
H	-1.29130100	-2.57978400	-0.46959400	
H	2.93265000	1.34042700	0.18063900	
H	-3.84391200	0.87738800	-0.22017100	
H	-3.57444300	-1.57620800	-0.43716800	
O	-0.21725300	-0.88108200	1.84826000	
H	-0.33644700	-1.84428900	1.88973600	

Name	**11-O2-OH-FHT-H**

Cartesian Coordinates				Frequency and Energy
O	0.67009200	-1.10610400	-0.09219900	Zero-point correction= 0.142830 (Hartree/Particle)
O	-0.32208400	2.82865300	0.47629700	Thermal correction to Energy= 0.154344
O	1.56679400	0.00799600	-1.98005900	Thermal correction to Enthalpy= 0.155288
C	-1.03468000	0.58680600	0.07080300	Thermal correction to Gibbs Free Energy= 0.103455
C	-0.62087900	-0.75329400	-0.06151600	Sum of electronic and zero-point Energies= -723.093955
C	-0.01279600	1.66347700	0.17013400	Sum of electronic and thermal Energies= -723.082441
C	-2.39620500	0.88843700	0.14924700	Sum of electronic and thermal Enthalpies= -723.081497
C	-1.59321900	-1.76600000	-0.10696300	Sum of electronic and thermal Free Energies= -723.133330
C	1.33476800	1.26171700	-0.08975100	
C	-3.35615100	-0.11476800	0.10009100	
C	-2.94187100	-1.44684500	-0.02543500	
C	1.65911000	-0.07037500	-0.71001300	
H	-2.67202600	1.93408900	0.25856500	
H	-1.25566400	-2.79242700	-0.21479800	
H	2.11596800	2.01460300	-0.08026400	
H	-4.41314400	0.12929500	0.15874000	
H	-3.68168500	-2.24324300	-0.06721200	
O	2.89736500	-0.59391700	-0.32554700	
H	2.97295400	-0.58291100	0.71789300	
O	2.56565300	-0.96924100	1.98874600	
H	1.68256400	-1.29343500	1.70959300	
Name				**11-C3-OH-RAF-H**
Cartesian Coordinates				Frequency and Energy
O	0.12357500	-1.33737900	1.06721500	Zero-point correction= 0.144323 (Hartree/Particle)
O	0.33666800	2.63357400	0.33131200	Thermal correction to Energy= 0.156315
O	1.14930100	-0.75675000	-1.93275700	Thermal correction to Enthalpy= 0.157259
C	-0.83128600	0.58785400	0.06155800	Thermal correction to Gibbs Free Energy= 0.104725
C	-0.88555300	-0.77893900	0.57418500	Sum of electronic and zero-point Energies= -723.148723
C	0.43035900	1.39348900	0.06657200	Sum of electronic and thermal Energies= -723.136731
C	-1.98898500	1.16584500	-0.40433800	Sum of electronic and thermal Enthalpies= -723.135786
C	-2.15323500	-1.47623200	0.52408600	Sum of electronic and thermal Free Energies= -723.188321
C	1.69360100	0.79716400	-0.18876300	
C	-3.20247400	0.45489200	-0.43374800	
C	-3.27674800	-0.87128900	0.02812500	
C	1.80924500	-0.50285600	-0.94159600	
H	-1.96205700	2.18528500	-0.77066400	
H	-2.16996000	-2.48921600	0.90951600	
H	2.48312600	1.50198100	-0.43164900	
H	-4.09053500	0.93935800	-0.82084000	
H	-4.22061900	-1.40120800	-0.00356500	
O	2.73367200	-1.31354100	-0.47171300	
H	2.94485500	-0.86017700	0.43927900	
O	2.60598500	0.23099000	1.39314200	
H	1.85203000	-0.15073500	1.86383600	
Name				**11-C4-OH-RAF-H**
Cartesian Coordinates				Frequency and Energy
O	0.71243800	-1.27765300	0.63928500	Zero-point correction= 0.144799 (Hartree/Particle)
O	0.19743400	2.57306800	-0.70002100	Thermal correction to Energy= 0.156472
O	1.78890300	-1.28301400	-1.41743800	Thermal correction to Enthalpy= 0.157416
C	-0.78345400	0.43328800	-0.13777800	Thermal correction to Gibbs Free Energy= 0.106532
C	-0.54075800	-0.87484100	0.29988800	Sum of electronic and zero-point Energies= -723.093106
C	0.36798500	1.36941700	-0.21652200	Sum of electronic and thermal Energies= -723.081432
C	-2.08219200	0.83488000	-0.44309400	Sum of electronic and thermal Enthalpies= -723.080488

C	-1.60145700	-1.76883200	0.43657800	Sum of electronic and thermal Free Energies= -723.131373
C	1.66388300	0.75733400	-0.29363500	
C	-3.13966700	-0.05532400	-0.31077900	
C	-2.89296600	-1.35434500	0.13588400	
C	1.81660700	-0.73873800	-0.23335400	
H	-2.25249300	1.85086200	-0.78019900	
H	-1.39789900	-2.77669600	0.77851200	
H	2.52926700	1.36546600	-0.52758700	
H	-4.14835100	0.25714900	-0.55081100	
H	-3.71372300	-2.05426800	0.24295500	
O	2.96863900	-1.03367700	0.53008600	
H	3.24965200	-1.91680400	0.25401500	
O	0.30050900	2.14876300	1.41082900	
H	1.14227200	2.63734800	1.45807100	
Name				**11-C5-OH-RAF-H**
Cartesian Coordinates				Frequency and Energy
O	-1.17240600	-1.12170000	-0.56554000	Zero-point correction= 0.144330 (Hartree/Particle)
O	0.14142400	2.63451200	0.28028900	Thermal correction to Energy= 0.156440
O	-2.42698700	-0.52147900	1.29534200	Thermal correction to Enthalpy= 0.157384
C	0.58061600	0.30286600	0.24620500	Thermal correction to Gibbs Free Energy= 0.105237
C	0.10409500	-0.93343500	-0.17840200	Sum of electronic and zero-point Energies= -723.110163
C	-0.30738200	1.47657000	0.18546800	Sum of electronic and thermal Energies= -723.098052
C	1.94842200	0.45118100	0.58955000	Sum of electronic and thermal Enthalpies= -723.097108
C	0.98272000	-2.03229900	-0.25218300	Sum of electronic and thermal Free Energies= -723.149255
C	-1.69093500	1.20637300	-0.04539300	
C	2.79659200	-0.67277000	0.57704000	
C	2.31178600	-1.89447300	0.12335500	
C	-2.20374000	-0.20110500	0.05425500	
H	2.25307300	1.35072300	1.10945000	
H	0.59403300	-2.98213000	-0.59981900	
H	-2.40089500	2.02207400	-0.10930400	
H	3.82722900	-0.56798000	0.89108500	
H	2.96817600	-2.75511700	0.07915400	
O	-3.29889600	-0.35647600	-0.81751400	
H	-3.81882700	-1.09226700	-0.46566500	
O	2.67655200	1.32984000	-1.15366000	
H	2.08666000	2.08967200	-1.01560000	
Name				**11-C6-OH-RAF-H**
Cartesian Coordinates				Frequency and Energy
O	1.09027200	-1.18993400	0.45556500	Zero-point correction= 0.144095 (Hartree/Particle)
O	0.30350900	2.78369800	-0.05652100	Thermal correction to Energy= 0.156426
O	2.53387300	-0.55147800	-1.24759900	Thermal correction to Enthalpy= 0.157371
C	-0.44674200	0.52809700	-0.22780800	Thermal correction to Gibbs Free Energy= 0.104442
C	-0.12688500	-0.81899500	0.04858100	Sum of electronic and zero-point Energies= -723.114704
C	0.58069600	1.57274600	-0.02740500	Sum of electronic and thermal Energies= -723.102372
C	-1.73749500	0.85661000	-0.62135100	Sum of electronic and thermal Enthalpies= -723.101428
C	-1.11593400	-1.81352600	-0.06487100	Sum of electronic and thermal Free Energies= -723.154356
C	1.90702600	1.10646000	0.23069200	
C	-2.73633800	-0.12424300	-0.70446000	
C	-2.39069700	-1.47298900	-0.45335500	
C	2.26924900	-0.33041600	0.00236400	
H	-1.97379400	1.89246800	-0.83512100	
H	-0.84308500	-2.84007700	0.14722700	
H	2.70450700	1.82033600	0.39882600	

H	-3.70074600	0.11796700	-1.12836500
H	-3.14725800	-2.24225000	-0.55348400
O	3.27016100	-0.70630200	0.91626900
H	3.72645400	-1.46135200	0.51979800
O	-3.59826300	0.36107100	1.26178500
H	-2.77976400	0.11400400	1.72081800

Name	**11-C7-OH-RAF-H**
Cartesian Coordinates	Frequency and Energy

O	-0.88281100	-1.25735600	-0.33840300	Zero-point correction= 0.144119 (Hartree/Particle)
O	-0.78847600	2.80005800	-0.42943000	Thermal correction to Energy= 0.156378
O	-2.32249600	-0.64578900	1.37609300	Thermal correction to Enthalpy= 0.157322
C	0.34165400	0.77281000	0.09859300	Thermal correction to Gibbs Free Energy= 0.104640
C	0.26368100	-0.63411700	0.03070600	Sum of electronic and zero-point Energies= -723.108850
C	-0.85909300	1.57212800	-0.24372000	Sum of electronic and thermal Energies= -723.096591
C	1.54372600	1.39447900	0.46067100	Sum of electronic and thermal Enthalpies= -723.095647
C	1.38461100	-1.39970700	0.30332900	Sum of electronic and thermal Free Energies= -723.148329
C	-2.08550700	0.85272700	-0.36520500	
C	2.66495700	0.64164000	0.73284700	
C	2.61321400	-0.77122100	0.59584400	
C	-2.15703900	-0.57779300	0.08496400	
H	1.57118700	2.47553300	0.52740800	
H	1.31689800	-2.47966100	0.25458000	
H	-3.00058400	1.38074400	-0.60471100	
H	3.59625800	1.11515000	1.01608800	
H	3.42499500	-1.37150500	0.98472600	
O	-3.12692300	-1.25184100	-0.68407600	
H	-3.41902200	-2.00219500	-0.14851700	
O	3.54230200	-0.87692600	-1.23563000	
H	2.87628200	-0.36891000	-1.72618500	

Name	**11-C8-OH-RAF-H**
Cartesian Coordinates	Frequency and Energy

O	0.71718600	-1.21306100	-0.02201500	Zero-point correction= 0.143631 (Hartree/Particle)
O	0.63498100	2.81087000	0.71010200	Thermal correction to Energy= 0.156220
O	2.24773000	-0.33643500	-1.53454400	Thermal correction to Enthalpy= 0.157164
C	-0.50589500	0.85832200	-0.04137500	Thermal correction to Gibbs Free Energy= 0.103594
C	-0.41977500	-0.53809700	-0.18943100	Sum of electronic and zero-point Energies= -723.114536
C	0.69256200	1.61605500	0.37384800	Sum of electronic and thermal Energies= -723.101947
C	-1.73426300	1.48905200	-0.22481100	Sum of electronic and thermal Enthalpies= -723.101003
C	-1.59243000	-1.28496800	-0.45268800	Sum of electronic and thermal Free Energies= -723.154573
C	1.92009000	0.88286400	0.39734800	
C	-2.88044200	0.76468300	-0.56005200	
C	-2.80356000	-0.61065600	-0.68645800	
C	2.02864700	-0.45860700	-0.26360800	
H	-1.78428000	2.56511800	-0.10200400	
H	-1.49083700	-2.33957700	-0.67363100	
H	2.83260200	1.37479800	0.71249300	
H	-3.81887500	1.27990300	-0.72027100	
H	-3.68211200	-1.18973000	-0.94500500	
O	2.95007000	-1.25142800	0.44342800	
H	3.27266600	-1.91288600	-0.18436300	
O	-1.86931200	-1.74792900	1.66400700	
H	-1.00401700	-2.18565600	1.70832400	

Name	**11-C4'-OH-RAF-H**
Cartesian Coordinates	Frequency and Energy

O	0.86565900	-1.18878500	0.50567600	Zero-point correction=	0.144056 (Hartree/Particle)
O	0.08886100	2.70514000	-0.48583700	Thermal correction to Energy=	0.156360
O	2.13169900	-0.85939300	-1.41586700	Thermal correction to Enthalpy=	0.157304
C	-0.73781600	0.51497200	-0.03499400	Thermal correction to Gibbs Free Energy=	0.104927
C	-0.37800300	-0.86333900	0.16665800	Sum of electronic and zero-point Energies=	-723.112010
C	0.34974300	1.51789100	-0.25605500	Sum of electronic and thermal Energies=	-723.099706
C	-2.06072600	0.80802600	-0.48051800	Sum of electronic and thermal Enthalpies=	-723.098761
C	-1.36316700	-1.84948700	0.12244500	Sum of electronic and thermal Free Energies=	-723.151139
C	1.69071300	1.03303500	-0.16515100		
C	-3.01024000	-0.17796800	-0.53045600		
C	-2.66164100	-1.50895400	-0.21208200		
C	2.00950100	-0.43215700	-0.20158200		
H	-2.29485100	1.83333900	-0.74130900		
H	-1.08334100	-2.87425200	0.33362300		
H	2.51236300	1.72850800	-0.28940600		
H	-4.02371000	0.05302400	-0.83380600		
H	-3.41844900	-2.28324500	-0.25876100		
O	3.09145800	-0.69051300	0.65636400		
H	3.49571500	-1.51090000	0.34083100		
O	-0.78453900	0.92162200	1.88612100		
H	-1.36301300	1.69684900	1.82758700		
Name				**11-C8'-OH-RAF-H**	
Cartesian Coordinates				Frequency and Energy	
O	0.77600200	-1.24633700	0.09607300	Zero-point correction=	0.143504 (Hartree/Particle)
O	0.30312300	2.82566100	0.33592100	Thermal correction to Energy=	0.155914
O	2.06103900	-0.34232200	-1.61395500	Thermal correction to Enthalpy=	0.156858
C	-0.65419400	0.69912400	-0.13548500	Thermal correction to Gibbs Free Energy=	0.104095
C	-0.44420800	-0.71182800	0.05244000	Sum of electronic and zero-point Energies=	-723.108913
C	0.47580500	1.60895300	0.15180200	Sum of electronic and thermal Energies=	-723.096503
C	-1.91756200	1.16751900	-0.42925700	Sum of electronic and thermal Enthalpies=	-723.095559
C	-1.54171100	-1.59975600	-0.17473100	Sum of electronic and thermal Free Energies=	-723.148322
C	1.76314600	0.99680200	0.23879800		
C	-2.98421700	0.28192300	-0.61074800		
C	-2.78748700	-1.09798400	-0.48149000		
C	1.96442300	-0.37911700	-0.32079100		
H	-2.07186400	2.23607200	-0.52365200		
H	-1.35515600	-2.66404300	-0.09037500		
H	2.63194700	1.59214100	0.49196000		
H	-3.96594600	0.66717900	-0.85643300		
H	-3.61472100	-1.77910300	-0.63927200		
O	3.02891700	-1.00499500	0.35253400		
H	3.36934000	-1.68082900	-0.25004700		
O	-0.84202600	-0.56323600	2.06479500		
H	-0.85400900	-1.51540000	2.24165000		
Name				**12-C3-OH-FHT-H**	
Cartesian Coordinates				Frequency and Energy	
O	0.13801800	1.73436000	-0.19912300	Zero-point correction=	0.141671 (Hartree/Particle)
O	-0.96487900	-2.21936400	-0.22826900	Thermal correction to Energy=	0.153761
O	-1.96647100	2.19164900	-0.66949000	Thermal correction to Enthalpy=	0.154706
C	0.80866600	-0.60479400	-0.06188500	Thermal correction to Gibbs Free Energy=	0.101552
C	1.13450300	0.76952600	-0.06171100	Sum of electronic and zero-point Energies=	-723.118906
C	-0.55844600	-1.01754800	-0.04304900	Sum of electronic and thermal Energies=	-723.106816
C	1.89802900	-1.51179400	-0.08172600	Sum of electronic and thermal Enthalpies=	-723.105872
C	2.43396500	1.23170400	-0.02379700	Sum of electronic and thermal Free Energies=	-723.159025

C	-1.53253000	0.05132800	0.35632300
C	3.20410800	-1.05805800	-0.04879400
C	3.48474800	0.31369100	-0.00627400
C	-1.16817000	1.39317800	-0.23387000
H	1.68229600	-2.57357900	-0.10174000
H	2.61402500	2.30043000	-0.03322600
H	-2.57547000	-0.23263900	-0.08456800
H	4.01894800	-1.77304000	-0.05115500
H	4.50786700	0.66646000	0.02313600
O	-1.63091900	0.13027100	1.76564400
H	-2.24157400	0.84307800	2.00485800
O	-3.50249000	-1.18006800	-0.65570200
H	-2.82140200	-1.88889600	-0.63308600

Name			**12-O3-OH-FHT-H**
Cartesian Coordinates			Frequency and Energy
O	-0.07930600	-1.68076300	-0.08352700
O	0.68020100	2.34815800	-0.07417900
O	2.09487500	-1.90520800	0.20147600
C	-0.94465400	0.60018400	-0.00238500
C	-1.16191600	-0.80229100	-0.07431700
C	0.34897500	1.15589400	-0.20744800
C	-2.10773200	1.40037300	0.20487800
C	-2.41195500	-1.37102500	-0.01073800
C	1.34029400	0.15269200	-0.82675400
C	-3.36312800	0.83442100	0.26693300
C	-3.54292700	-0.55545100	0.14620800
C	1.17865700	-1.21920000	-0.18249000
H	-1.96185700	2.47075000	0.28934700
H	-2.49021400	-2.45178400	-0.04810600
H	1.08091500	0.02596200	-1.89712700
H	-4.22862300	1.47410900	0.40873000
H	-4.53057100	-0.99626200	0.19479800
O	2.66348300	0.56575600	-0.84552300
H	2.99781500	0.83202900	0.16827300
O	3.37085600	0.42363400	1.27827900
H	3.27797600	-0.54099600	1.18855500

Zero-point correction= 0.139145 (Hartree/Particle)
Thermal correction to Energy= 0.149184
Thermal correction to Enthalpy= 0.150129
Thermal correction to Gibbs Free Energy= 0.102337
Sum of electronic and zero-point Energies= -723.090040
Sum of electronic and thermal Energies= -723.080001
Sum of electronic and thermal Enthalpies= -723.079056
Sum of electronic and thermal Free Energies= -723.126847

Name			**12-C2-OH-RAF-H**
Cartesian Coordinates			Frequency and Energy
O	0.27724200	-1.47254000	-0.53558500
O	0.47958700	2.63886800	0.00371000
O	2.46821900	-1.65111000	-0.25489800
C	-0.84431000	0.65312200	-0.07320700
C	-0.89461100	-0.75170600	-0.27828700
C	0.37396700	1.37195100	-0.15420800
C	-2.09666700	1.28256500	0.19214900
C	-2.06117700	-1.47727700	-0.24340900
C	1.60353900	0.58697100	-0.56788400
C	-3.27406900	0.55762300	0.22721700
C	-3.27792200	-0.82583000	0.00848300
C	1.46877900	-0.89725800	-0.24718900
H	-2.10688800	2.35307500	0.35876900
H	-2.01692000	-2.54765500	-0.41023400
H	1.71644700	0.62287000	-1.66405400

Zero-point correction= 0.146100 (Hartree/Particle)
Thermal correction to Energy= 0.157792
Thermal correction to Enthalpy= 0.158737
Thermal correction to Gibbs Free Energy= 0.107529
Sum of electronic and zero-point Energies= -723.103454
Sum of electronic and thermal Energies= -723.091761
Sum of electronic and thermal Enthalpies= -723.090817
Sum of electronic and thermal Free Energies= -723.142025

H	-4.20817000	1.07137400	0.42715900
H	-4.20029800	-1.39151400	0.03635000
O	2.75531900	1.12634500	0.04171900
H	3.52993900	0.72198600	-0.36725700
O	1.52498700	-0.89419400	1.57657600
H	1.25788400	-1.81004500	1.78510300

Name	**12-C4-OH-RAF-H**
Cartesian Coordinates	Frequency and Energy

O	-0.11927400	1.78026200	0.09849100	Zero-point correction= 0.146014 (Hartree/Particle)
O	-0.78694300	-2.31144900	-0.48704000	Thermal correction to Energy= 0.157558
O	-2.29765100	2.04439900	0.30110100	Thermal correction to Enthalpy= 0.158502
C	0.74106900	-0.50785200	-0.06050400	Thermal correction to Gibbs Free Energy= 0.107794
C	0.96842100	0.90222400	-0.01564300	Sum of electronic and zero-point Energies= -723.086287
C	-0.58826800	-1.02039600	-0.10131000	Sum of electronic and thermal Energies= -723.074743
C	1.92136000	-1.32822300	-0.04146600	Sum of electronic and thermal Enthalpies= -723.073799
C	2.21490100	1.46622300	-0.00555600	Sum of electronic and thermal Free Energies= -723.124507
C	-1.59030300	-0.01993600	-0.66808400	
C	3.17708600	-0.76420900	-0.03586800	
C	3.35881800	0.63777000	-0.02878800	
C	-1.36902200	1.33829400	-0.03675900	
H	1.80458900	-2.40576400	-0.04815400	
H	2.29967200	2.54659200	0.03876600	
H	-1.39505100	0.07779600	-1.74567100	
H	4.04651800	-1.41360100	-0.03565400	
H	4.34885800	1.07372600	-0.02296200	
O	-2.92007300	-0.44133500	-0.46503200	
H	-3.43102600	0.32718800	-0.17157100	
O	-1.19177300	-1.43778800	1.38984900	
H	**-2.15222000**	**-1.50201600**	**1.25017300**	

Name	**12-C5-OH-RAF-H**
Cartesian Coordinates	Frequency and Energy

O	0.72835600	-1.69332200	0.13687200	Zero-point correction= 0.145761 (Hartree/Particle)
O	0.68928600	2.39913600	-0.36814100	Thermal correction to Energy= 0.158069
O	2.86404600	-1.56141200	0.63119300	Thermal correction to Enthalpy= 0.159014
C	-0.51528800	0.34273700	-0.26759200	Thermal correction to Gibbs Free Energy= 0.105818
C	-0.47671900	-1.03890400	-0.11393200	Sum of electronic and zero-point Energies= -723.112078
C	0.66916100	1.12522600	-0.30962700	Sum of electronic and thermal Energies= -723.099769
C	-1.83855300	0.93676300	-0.35408600	Sum of electronic and thermal Enthalpies= -723.098825
C	-1.62181900	-1.84854400	-0.11421200	Sum of electronic and thermal Free Energies= -723.152020
C	1.95622300	0.34744800	-0.50212400	
C	-2.96978800	0.10825100	-0.46491500	
C	-2.87413500	-1.28681300	-0.29413300	
C	1.89386300	-1.02237600	0.15218300	
H	-1.89898400	1.95459600	-0.71663200	
H	-1.49610600	-2.91615600	0.02920900	
H	2.11502700	0.16318300	-1.58012800	
H	-3.93516900	0.57081100	-0.63621700	
H	-3.75677400	-1.91110700	-0.32186500	
O	3.04482900	1.07988100	0.01716800	
H	3.85807300	0.60920400	-0.20326000	
O	-1.98852800	1.50197900	1.52346800	
H	-2.92765400	1.73665800	1.51504100	

Name	**12-C6-OH-RAF-H**
Cartesian Coordinates	Frequency and Energy

O	0.74493100	-1.64487200	-0.01030500	Zero-point correction= 0.144729 (Hartree/Particle)
O	0.97030000	2.47651700	-0.10251200	Thermal correction to Energy= 0.157454
O	2.83451900	-1.67009800	0.66215700	Thermal correction to Enthalpy= 0.158398
C	-0.36719800	0.50952200	-0.26777700	Thermal correction to Gibbs Free Energy= 0.103492
C	-0.40822600	-0.91524500	-0.26698900	Sum of electronic and zero-point Energies= -723.123261
C	0.86033000	1.20873700	-0.17891700	Sum of electronic and thermal Energies= -723.110535
C	-1.61961800	1.15902300	-0.40874800	Sum of electronic and thermal Enthalpies= -723.109591
C	-1.56538400	-1.64824900	-0.43525800	Sum of electronic and thermal Free Energies= -723.164497
C	2.11347400	0.37124300	-0.37257800	
C	-2.80880500	0.43163800	-0.52307900	
C	-2.78054300	-0.98654300	-0.59206700	
C	1.93933000	-1.04005700	0.15616800	
H	-1.64720100	2.24179300	-0.40665400	
H	-1.50491000	-2.73019300	-0.42371400	
H	2.31238600	0.26725000	-1.45332200	
H	-3.72741800	0.95654700	-0.75161800	
H	-3.69877900	-1.54429200	-0.71813700	
O	3.21209800	0.99017500	0.25836600	
H	4.00939500	0.49697500	0.02980500	
O	-3.42481000	0.55798100	1.59077700	
H	-2.61992800	0.09386700	1.87124900	
Name				**12-C7-OH-RAF-H**
Cartesian Coordinates				Frequency and Energy
O	0.54559700	-1.58560400	-0.15618900	Zero-point correction= 0.145148 (Hartree/Particle)
O	1.32053200	2.43259400	0.32385500	Thermal correction to Energy= 0.157598
O	2.64848700	-1.99652900	0.31457800	Thermal correction to Enthalpy= 0.158542
C	-0.27766300	0.70332500	-0.08968000	Thermal correction to Gibbs Free Energy= 0.104843
C	-0.51093800	-0.68455800	-0.27296800	Sum of electronic and zero-point Energies= -723.104187
C	1.07292700	1.19076600	0.11602700	Sum of electronic and thermal Energies= -723.091737
C	-1.39316400	1.56157000	-0.18113400	Sum of electronic and thermal Enthalpies= -723.090793
C	-1.74647600	-1.21043700	-0.51521400	Sum of electronic and thermal Free Energies= -723.144492
C	2.17033200	0.26353700	-0.33817300	
C	-2.65776400	1.05777900	-0.42326700	
C	-2.89776700	-0.35325100	-0.48701900	
C	1.82359900	-1.17855200	-0.01343200	
H	-1.23208100	2.62825900	-0.08978100	
H	-1.86135900	-2.27957100	-0.64798700	
H	2.29898300	0.31313700	-1.43760800	
H	-3.50256900	1.73113800	-0.51312100	
H	-3.78630500	-0.69444700	-1.00371200	
O	3.38685000	0.61755900	0.28592900	
H	4.09355400	0.09407600	-0.11143700	
O	-3.56094300	-0.70355600	1.20313100	
H	-4.23292100	-0.00937600	1.26239000	
Name				**12-C8-OH-RAF-H**
Cartesian Coordinates				Frequency and Energy
O	0.32466000	-1.46663600	-0.44754900	Zero-point correction= 0.145145 (Hartree/Particle)
O	1.34126800	2.44318800	0.43078700	Thermal correction to Energy= 0.157689
O	2.38609400	-2.05795400	0.01856700	Thermal correction to Enthalpy= 0.158633
C	-0.35014200	0.84298200	-0.07490600	Thermal correction to Gibbs Free Energy= 0.104419
C	-0.66248000	-0.49370300	-0.40929300	Sum of electronic and zero-point Energies= -723.123315
C	0.98947700	1.26711700	0.08600900	Sum of electronic and thermal Energies= -723.110772
C	-1.46726700	1.72897300	0.04248900	Sum of electronic and thermal Enthalpies= -723.109828
C	-1.96312400	-0.95340600	-0.58267900	Sum of electronic and thermal Free Energies= -723.164042

C	2.05873200	0.28633900	-0.36168700
C	-2.76705700	1.30012100	-0.18474400
C	-3.03688400	-0.02361600	-0.52333600
C	1.61857500	-1.15961500	-0.22161800
H	-1.27168400	2.76153100	0.30582000
H	-2.11545500	-1.96320800	-0.94115500
H	2.25304500	0.43705600	-1.43776100
H	-3.58163000	2.01041600	-0.10192000
H	-4.04742700	-0.36660700	-0.70050900
O	3.24586500	0.49912500	0.37028700
H	3.94412600	-0.04134000	-0.01882900
O	-2.22649000	-1.75952500	1.43326200
H	-2.27112600	-0.87457800	1.83010900

Name			**12-C4'-OH-RAF-H**
Cartesian Coordinates			Frequency and Energy
O	0.41677200	-1.68922600	-0.04162300
O	0.74228400	2.44253400	-0.35946100
O	2.57495000	-1.75964300	0.36036400
C	-0.60905900	0.51980400	0.12289500
C	-0.72519200	-0.91809400	-0.14338200
C	0.60913800	1.16672900	-0.29446700
C	-1.87626200	1.25667500	-0.01153500
C	-1.90889700	-1.55010100	-0.36462700
C	1.78210500	0.27622000	-0.63819700
C	-3.05459200	0.61116600	-0.23744800
C	-3.09835800	-0.79440000	-0.41075700
C	1.64281100	-1.11355700	-0.04247600
H	-1.83322700	2.33215800	0.10721300
H	-1.91982400	-2.62450800	-0.50429400
H	1.83708800	0.12629100	-1.73105300
H	-3.97533100	1.17962300	-0.29905400
H	-4.04211000	-1.29350000	-0.58648300
O	2.98515300	0.86711700	-0.18805600
H	3.72350600	0.35638200	-0.54221100
O	-0.49476700	0.38082200	1.92283900
H	-0.15540800	1.26407200	2.12334400

Zero-point correction= 0.145502 (Hartree/Particle)
Thermal correction to Energy= 0.157684
Thermal correction to Enthalpy= 0.158628
Thermal correction to Gibbs Free Energy= 0.106022
Sum of electronic and zero-point Energies= -723.116102
Sum of electronic and thermal Energies= -723.103920
Sum of electronic and thermal Enthalpies= -723.102976
Sum of electronic and thermal Free Energies= -723.155581

Name			**12-C8'-OH-RAF-H**
Cartesian Coordinates			Frequency and Energy
O	0.45380500	-1.47555900	-0.50142600
O	0.76959000	2.63390400	-0.42178300
O	2.61641400	-1.66070500	-0.78689700
C	-0.61330900	0.70619500	-0.22192900
C	-0.65772200	-0.73756600	-0.13251100
C	0.65325400	1.36692900	-0.29404800
C	-1.84133100	1.37284500	-0.17839400
C	-1.87542100	-1.43512500	-0.19783000
C	1.89383700	0.53623200	-0.17779800
C	-3.04560100	0.65999200	-0.12425800
C	-3.07624800	-0.73686500	-0.13050100
C	1.69109000	-0.93365900	-0.50731300
H	-1.84955700	2.45544500	-0.19107300
H	-1.83905300	-2.51693600	-0.24959600
H	2.64113000	0.90294900	-0.88915800
H	-3.97832000	1.21207500	-0.09054600

Zero-point correction= 0.145275 (Hartree/Particle)
Thermal correction to Energy= 0.157579
Thermal correction to Enthalpy= 0.158523
Thermal correction to Gibbs Free Energy= 0.105677
Sum of electronic and zero-point Energies= -723.114289
Sum of electronic and thermal Energies= -723.101985
Sum of electronic and thermal Enthalpies= -723.101040
Sum of electronic and thermal Free Energies= -723.153886

H	-4.01762800	-1.26959200	-0.11772100
O	2.44194700	0.64606200	1.14841200
H	3.37774100	0.41128500	1.10572300
O	-0.29077000	-0.84973300	1.81739400
H	-1.03349000	-0.34083900	2.17425100

References

1. Evans, M. G.; Polanyi, M., Some Applications of the Transition State Method to the Calculation of Reaction Velocities, Especially in Solution. *Trans. Faraday Soc.* **1935**, 31, 875-894.

2. Eyring, H., The Activated Complex in Chemical Reactions. *J. Chem. Phys.* **1935**, 3, 107-115.

3. Truhlar, D. G.; Hase, W. L.; Hynes, J. T., Current Status of Transition-State Theory. *J. Phys. Chem.* **1983**, 87, 2664-2682.

4. Furuncuoglu, T.; Ugur, I.; Degirmenci, I.; Aviyente, V., Role of Chain Transfer Agents in Free Radical Polymerization Kinetics. *Macromolecules* **2010**, 43, 1823-1835.

5. Vélez, E.; Quijano, J.; Notario, R.; Pabón, E.; Murillo, J.; Leal, J.; Zapata, E.; Alarcón, G., A Computational Study of Stereospecifity in the Thermal Elimination Reaction of Menthyl Benzoate in the Gas Phase. *J. Phys. Org. Chem.* **2009**, 22, 971-977.

6. Pollak, E.; Pechukas, P., Symmetry Numbers, Not Statistical Factors, Should Be Used in Absolute Rate Theory and in Broensted Relations. *J. Am. Chem. Soc.* **1978**, 100, 2984-2991.

7. Fernández-Ramos, A.; Ellingson, B. A.; Meana-Pañeda, R.; Marques, J. M.; Truhlar, D. G., Symmetry Numbers and Chemical Reaction Rates. *Theor. Chem. Acc.* **2007**, 118, 813-826.

8. Eckart, C., The Penetration of A Potential Barrier by Electrons. *Phy. Rev.* **1930**, 35, 1303.

9. Marcus, R. A., Chemical and Electrochemical Electron-Transfer Theory. *Annu. Rev. Phys. Chem.* **1964**, 15, 155-196.

10. Marcus, R. A., Electron Transfer Reactions in Chemistry. Theory and Experiment. *Rev. Mod. Phys.* **1993**, 65, 599.

11. Lu, Y.; Wang, A.; Shi, P.; Zhang, H., A Theoretical Study on the Antioxidant Activity of Piceatannol and Isorhapontigenin Scavenging Nitric Oxide and Nitrogen Dioxide Radicals. *PloS one* **2017**, 12, e0169773.

12. Lu, Y.; Wang, A.; Shi, P.; Zhang, H.; Li, Z., Quantum Chemical Study on the Antioxidation Mechanism of Piceatannol and Isorhapontigenin toward Hydroxyl and Hydroperoxyl Radicals. *PloS one* **2015**, 10, e0133259.

13. Nelsen, S. F.; Blackstock, S. C.; Kim, Y., Estimation of inner shell Marcus terms for amino nitrogen compounds by molecular orbital calculations. *J. Am. Chem. Soc.* **1987**, 109, 677-682.

14. Nelsen, S. F.; Weaver, M. N.; Luo, Y.; Pladziewicz, J. R.; Ausman, L. K.; Jentzsch, T. L.; O'Konek, J. J., Estimation of electronic coupling for intermolecular electron transfer from cross-reaction data. *J. Phys. Chem. A* **2006**, 110, 11665-11676.

15. Galano, A.; Alvarez-Idaboy, J. R., A computational methodology for accurate predictions of rate constants in solution: Application to the assessment of primary antioxidant activity. *J. Comput. Chem.* **2013**, 34, 2430-2445.

16. Collins, F. C.; Kimball, G. E., Diffusion-Controlled Reaction Rates. *J. Colloid Sci.* **1949**, 4, 425-437.

17. Von Smoluchowski, M., Mathematical Theory of the Kinetics of the Coagulation of Colloidal Solutions. *Z. Phys. Chem* **1917**, 92, 129-68.

18. Truhlar, D. G., Nearly encounter-controlled reactions: The equivalence of the steady-state and diffusional viewpoints. *J. Chem. Educ.* **1985**, 62, 104.

19. Einstein, A., On the motion of small particles suspended in liquids at rest required by the molecular-kinetic theory of heat. *Ann. Phys.* **1905**, 17, 549-560.

20. Stokes, G. G., *Mathematical and Physical Papers*. University Press: Cambridge, 1905.

21. 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.

22. Vo, Q. V.; Gon, T. V.; Bay, M. V.; Mechler, A., The Antioxidant Activity of Monosubstituted Indolinonic Hydroxylamines: A Thermodynamic and Kinetic Study. *J. Phys. Chem. B* **2019**, 123, 10672-10679.

23. Vo, Q. V.; Mechler, A., In silico study of the radical scavenging activities of natural indole-3-carbinols. *J. Chem. Inf. Model.* **2020**, 60, 316-321.

24. Okuno, Y., Theoretical Investigation of the Mechanism of the Baeyer-Villiger Reaction in Nonpolar Solvents. *Chem.: Eur. J.* **1997**, 3, 212-218.

25. Benson, S., *The foundations of chemical kinetics:* . Malabar, Florida, 1982.

26. Iuga, C.; Alvarez-Idaboy, J. R.; Vivier-Bunge, A., ROS Initiated Oxidation of Dopamine under Oxidative Stress Conditions in Aqueous and Lipidic Environments. *J. Phys. Chem. B* **2011**, 115, 12234-12246.

27. Alvarez-Idaboy, J. R.; Reyes, L.; Mora-Diez, N., The mechanism of the Baeyer–Villiger rearrangement: quantum chemistry and TST study supported by experimental kinetic data. *Org. Biomol. Chem.* **2007**, 5, 3682-3689.

28. Le, T. H.; Tran, T. T.; Huynh, L. K., Identification of Hindered Internal Rotational Mode for Complex Chemical Species: A Data Mining Approach with Multivariate Logistic Regression Model. *Chemom. Intell. Lab. Syst.* **2018**, 172, 10-16.

29. Dzib, E.; Cabellos, J. L.; Ortíz-Chi, F.; Pan, S.; Galano, A.; Merino, G., Eyringpy: A Program for Computing Rate Constants in the Gas Phase and in Solution. *Int. J. Quantum Chem.* **2019**, 119, e25686.

30. E. Dzib; J. L. Cabellos; F. Ortiz-Chi; S. Pan; A. Galano; G. Merino, *Eyringpy 1.0.2* **2018**, Cinvestav, Mérida, Yucatán.