Supporting Information (SI)

Modeling the Antioxidant Behavior of F420 Coenzyme: A Computational Study

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Table S1. The method to calculate rate constant following the conventional transition state theory

The rate constant (k) was calculated by using the conventional transition state theory (TST) (at 298.15 K, 1M standard state) according to the equation (1):[1-5]

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

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

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

k_B is the Boltzmann constant,

h is the Planck constant,

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

The Marcus Theory was used to estimate the reaction barriers of SET reactions.[9-12] The free energy of reaction $\Delta G^{\neq}$ for the SET pathway was computed following the equations (2,3).

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

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

where ΔG_{SET} is the Gibbs energy of reaction, ΔE_{SET} is the non-adiabatic energy difference between reactants and vertical products for SET.[13, 14]

For rate constants that were close to the diffusion limit a correction was applied to yield realistic results[15]. The apparent rate constants (k_{app}) were calculated following the Collins–Kimball theory in the solvents at 298.15K;[16] the steady-state Smoluchowski rate constant (k_D) for an irreversible bimolecular diffusion–controlled reaction was calculated following the literature as corroding to equations (4,5).[15, 17]

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

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

where R_{AB} is the reaction distance, N_A is the Avogadro constant, and $D_{AB} = D_A + D_B$ (D_{AB} is the mutual diffusion coefficient of the reactants A and B),[16, 18] where D_A or D_B is estimated using the Stokes–Einstein formulation (6).[19, 20]

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

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

The kinetic study requires different considerations. Water (dielectric constants, $\varepsilon = 78.35$) and pentyl ethanoate ($\varepsilon = 4.73$) are the *de facto* standard solvents in the literature to mimic the polar and nonpolar environments in the human body.[15, 21-23] Thus, these solvents were used to model the physiological environments. The solvent cage effects were included following the corrections proposed by Okuno,[24] adjusted with the free volume theory according to the Benson correction[15, 25-27] to reduce over-penalizing entropy losses in solution. For the species that have multiple conformers, all of these were investigated and the conformer with the lowest electronic energy was included in the analysis.[22, 23] The hindered internal rotation treatment was also applied to the single bonds to ensure that the obtained conformer has the lowest electronic energy.[23, 28] All transition states were characterized by the existence of only one single imaginary frequency. Intrinsic coordinate calculations (IRCs) were performed to ensure that each transition state is connected correctly with the pre-complex and post-complex.

Table S2. The calculated ΔG^o values (in kcal/mol) for the RAF, FHT, and SET reactions of F0/F0H2 with HO• and HOO•.

Mechanisms	positions	F0		F0H2	
		HO•	HOO•	HO•	HOO•
FHT	C5–H			–40.7	–9.5
	C11–H	–21.3	10.0	–24.3	6.9
	N1–H			–29.7	3.6
	N3–H	3.2	34.5	2.7	27.6
	O8–H	–26.6	4.6	–30.1	1.2
RAF	C2	7.5		15	
	C4	10.1		5.4	
	C5	–15.5			
	C6	–9.7		–6.8	
	C7	–9.9		–11.6	
	C8	–11.9		–11.7	
	C9	–11.9		–11.5	
	C4’	–10.9		–12.4	
	C5’	3.7		–11.7	
	C9’	0.2		–8.4	
	C10’	4.4		–17.3	
	N1	12.6			
SET		163.4	168.1	147.6	152.3

Table S3. The calculated ΔG^{o} values (in kcal/mol) for the RAF, FHT, and SET reactions of F0 with HO· and HOO· in the studied solvents

Mechanisms	Positions	Pentyl ethanoate		water			
		H_2A		H_2A		HA^-	
		$HO^{\bullet}$	$HOO^{\bullet}$	$HO^{\bullet}$	$HOO^{\bullet}$	$HO^{\bullet}$	$HOO^{\bullet}$
FHT	C11–H	–21.6	10.6	–20.5	11.3	–22.8	9.0
	N3–H	2.4	34.6	–3.6	28.1	–20.8	11.0
	O8–H	–27.6	4.6	–24.9	6.9		
RAF	C2	12.6		11.4		2.7	
	C4	14.7		14.1		0.1	
	C5	–10.9		–7.6		–15.5	
	C6	–8.8		–9.0		–9.1	
	C7	–7.9		–7.2		–15.0	
	C8	–8.4		–7.5		0.8	
	C9	–9.6		–8.2		–11.1	
	C4’	–6.6		–2.9		–2.6	
	C5’	5.9		7.7		–1.3	
	C9’	2.9		4.1		0.7	
	C10’	10.3		11.2		–3.5	
	N1	18.9		25.1		31.1	
SET		62.9	82.3	21.4	43.4	–2.8	19.3

Table S4. The calculated ΔG^{o} values (in kcal/mol) for the RAF, FHT, and SET reactions of F0H2 with HO$^{\cdot}$ and HOO$^{\cdot}$ in the studied solvents

Mechanisms	Positions	Pentyl ethanoate		Water			
		H_2A		H_2A		HA^-	
		HO$^{\bullet}$	HOO$^{\bullet}$	HO$^{\bullet}$	HOO$^{\bullet}$	HO$^{\bullet}$	HOO$^{\bullet}$
FHT	C5–H	–42	–9.8	–43.7	–12.0	–47.0	–15.3
	C11–H	–23.8	8.4	–24.0	7.8	–25.6	6.2
	N1–H	–30.2	2	–32.9	–1.1		
	O8–H	–32.2	0.0	–33.7	–2.0	–36.0	–4.2
RAF	C6	–5.0		–6.0		–5.9	
	C7	–9.7		–9.7		–9.9	
	C8	–9.4		–9.5		–10.2	
	C9	–9.0		–9.0		–9.2	
	C4’	–8.2		–7.5		–5.0	
	C5’	–10.1		–10.5		–11.9	
	C9’	–5.5		–6.6		–5.7	
	C10'	–12.1		–13.2		–5.9	
SET		45.7	65.1	1.6	23.6	–10.2	11.8

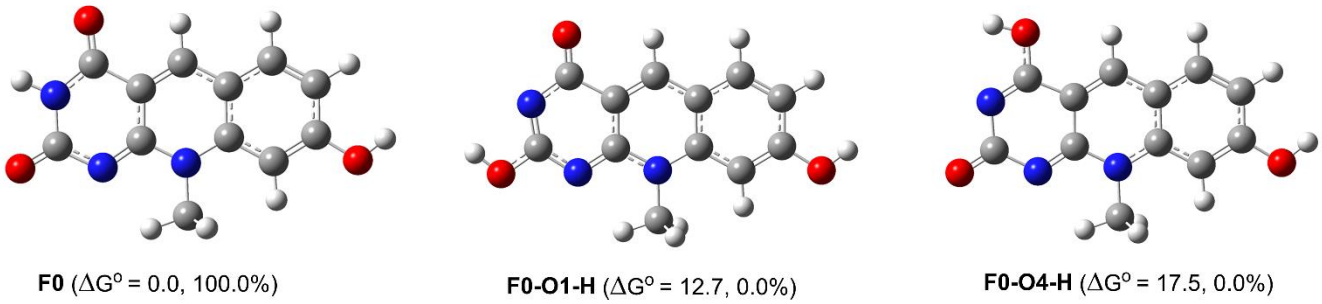

Figure S1. The typical conformers of F0 and the relative free energies ΔG° (in kcal/mol) compared with F0 conformer

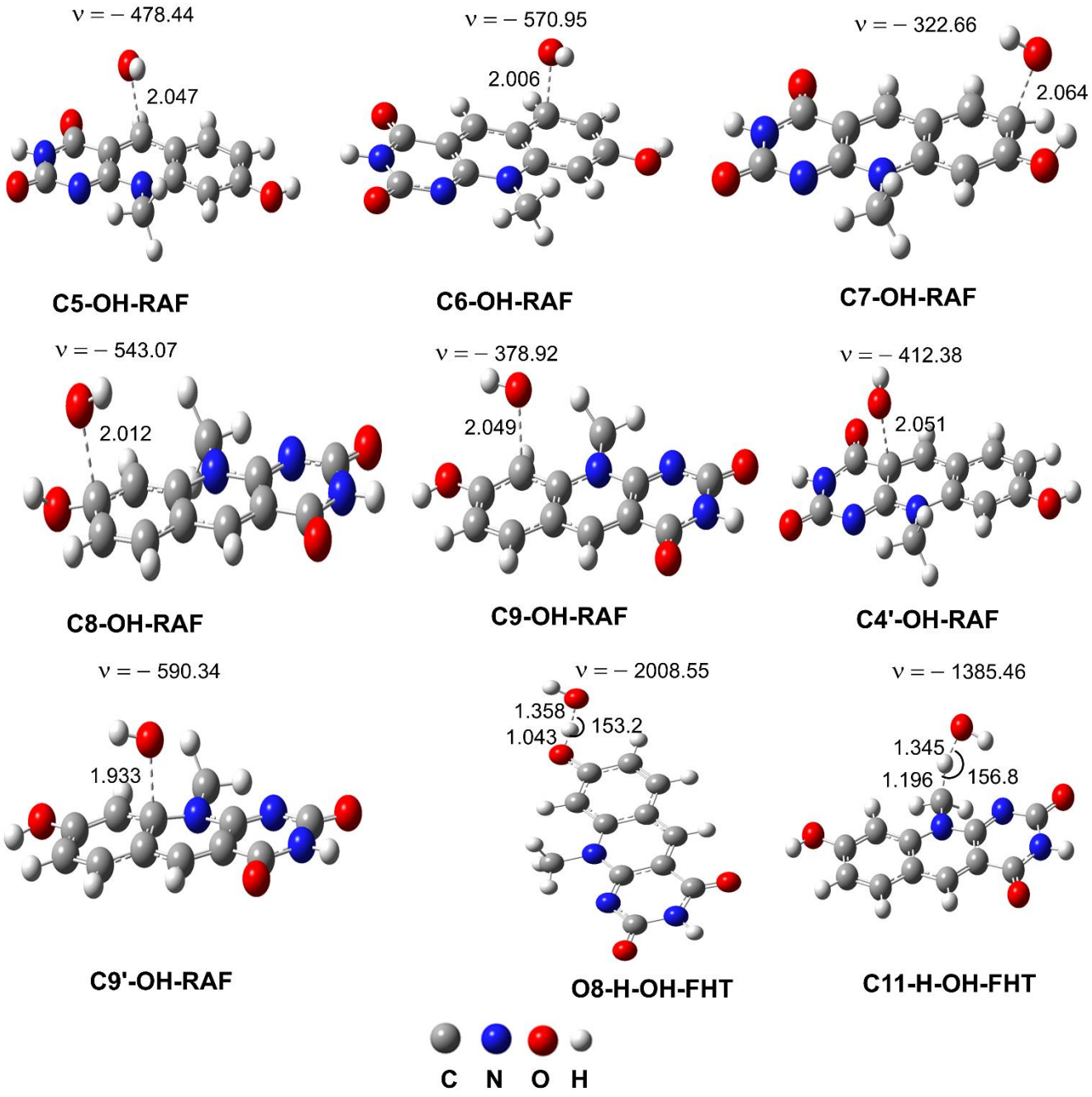

Figure S2. The TS structures of the FHT and RAF reactions between the F0 and HO• radicals in the gas phase

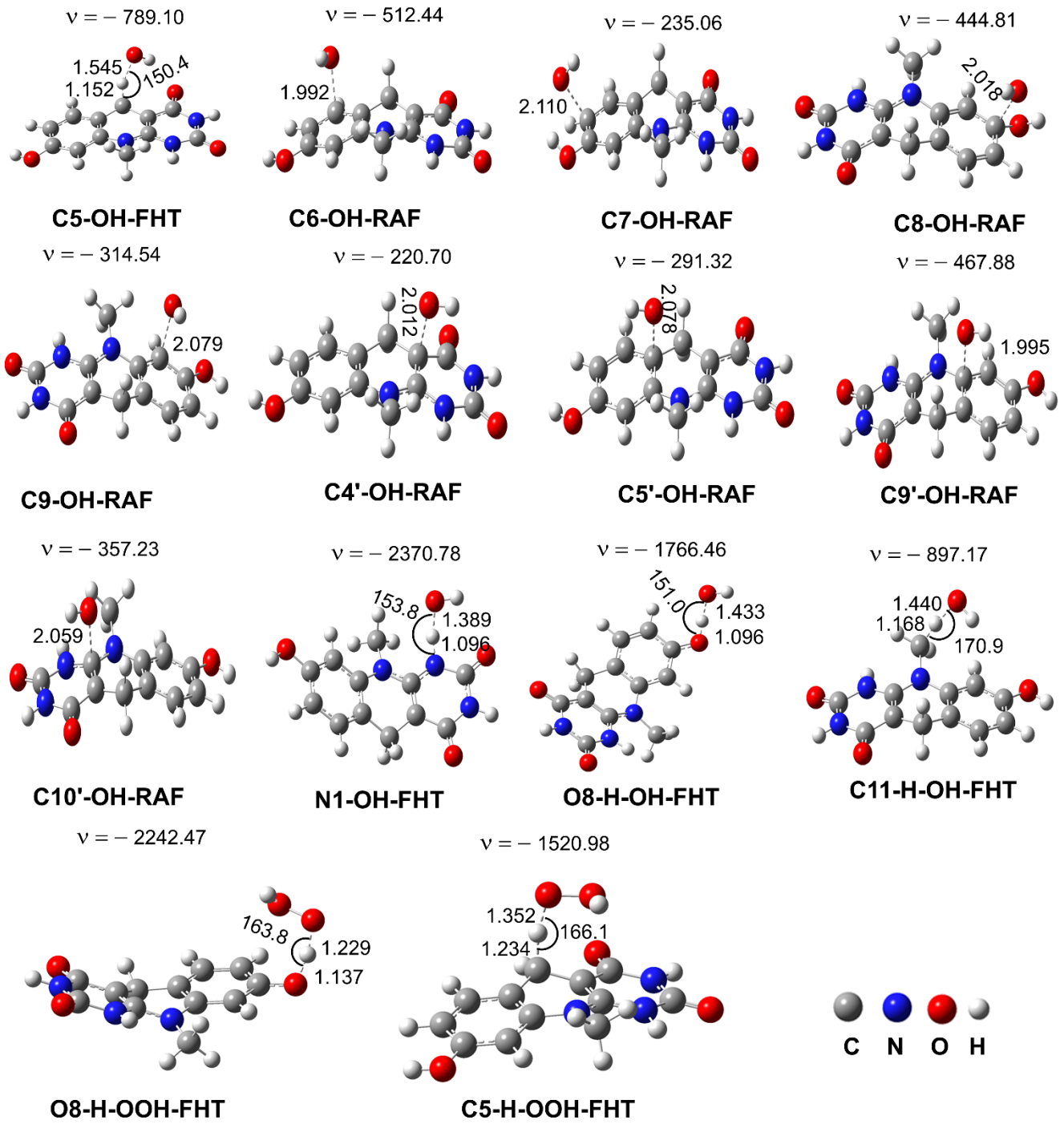

Figure S3. The TS structures of the FHT and RAF reactions between the F0H2 and HO•/HOO• radicals in the gas phase

Table S5: The Cartesian coordinates and energies of TS of the reaction between F0/F0H2 with HO•/HOO• following the RAF and FHT mechanisms in the gas phase

Name				**F0-C5-OH-RAF**
Cartesian Coordinates				Frequency and Energy
N	-5.37997300	2.78574700	-2.51796500	Zero-point correction= 0.213939 (Hartree/Particle)
C	-4.05028800	2.76343800	-2.98675000	Thermal correction to Energy= 0.229964
N	-3.14585300	1.94169400	-2.33666400	Thermal correction to Enthalpy= 0.230908
C	-3.54806100	1.18232100	-1.36245100	Thermal correction to Gibbs Free Energy= 0.170040
C	-4.90995900	1.12934600	-0.88090300	Sum of electronic and zero-point Energies= -928.096281
C	-5.90228700	2.04079500	-1.49110200	Sum of electronic and thermal Energies= -928.080256
N	-2.62668700	0.36079600	-0.73713000	Sum of electronic and thermal Enthalpies= -928.079312
C	-2.95924100	-0.44493700	0.34692900	Sum of electronic and thermal Free Energies= -928.140180
C	-4.30012700	-0.51965700	0.79002800	
C	-5.29829900	0.23670600	0.09599900	
C	-1.97920700	-1.19159300	1.00880200	
C	-2.33374500	-1.99577200	2.08272200	
C	-3.66109500	-2.08289600	2.52442700	
C	-4.62452700	-1.34742400	1.87107800	
O	-7.04796800	2.12598800	-1.11583600	
O	-3.74858900	3.46369300	-3.91896800	
O	-1.33288200	-2.68539700	2.67515600	
C	-1.23638200	0.38915100	-1.19533100	
H	-6.00592600	3.41917000	-2.99992100	
H	-6.30944000	0.29943600	0.47924100	
H	-0.93858800	-1.16647400	0.72278100	
H	-3.91858200	-2.71958800	3.36316000	
H	-5.66017600	-1.40159800	2.18641600	
H	-1.67325300	-3.20796200	3.40690900	
H	-1.18535800	1.02137500	-2.07464700	
H	-0.91413600	-0.62266200	-1.44399400	
H	-0.59491300	0.79784800	-0.41229900	
O	-5.95782400	-0.91846500	-1.45965900	
H	-5.12420700	-1.32436000	-1.74909600	

Name				**F0-C6-OH-RAF**
Cartesian Coordinates				Frequency and Energy
N	-5.42510100	2.76560800	-2.55646400	Zero-point correction= 0.213590 (Hartree/Particle)
C	-4.08367400	2.76934700	-3.00385300	Thermal correction to Energy= 0.229756
N	-3.18522200	1.94647700	-2.35521500	Thermal correction to Enthalpy= 0.230700
C	-3.59171000	1.20624400	-1.36712400	Thermal correction to Gibbs Free Energy= 0.169164
C	-4.94670900	1.16368000	-0.86688700	Sum of electronic and zero-point Energies= -928.095588
C	-5.95097900	2.02964500	-1.52634400	Sum of electronic and thermal Energies= -928.079422
N	-2.66878600	0.38939900	-0.73402900	Sum of electronic and thermal Enthalpies= -928.078478
C	-3.00923300	-0.43498100	0.32292400	Sum of electronic and thermal Free Energies= -928.140014
C	-4.33656100	-0.46160600	0.79562700	
C	-5.30185100	0.35830600	0.16332100	
C	-2.04042100	-1.24610600	0.94153000	
C	-2.38909900	-2.05108700	2.01939100	
C	-3.69495700	-2.08420200	2.50950800	
C	-4.68945800	-1.34671000	1.85527600	
O	-7.11302400	2.08447900	-1.19222700	
O	-3.78409200	3.48501000	-3.92532800	
O	-1.39289700	-2.78541400	2.56687600	
C	-1.28033300	0.40614600	-1.20302600	
H	-6.05388400	3.38338200	-3.05499000	

H	-6.33705700	0.34737500	0.49007900
H	-1.01169900	-1.26731000	0.61431400
H	-3.95618400	-2.71412000	3.35164200
H	-5.65081000	-1.20942700	2.33145500
H	-1.73041600	-3.32584400	3.28708800
H	-1.21457200	1.11195700	-2.02337700
H	-0.99618900	-0.58915100	-1.54770800
H	-0.62274000	0.71900800	-0.39083900
O	-5.56476500	-2.87238300	0.89024900
H	-4.82295600	-3.18746800	0.35019900

Name			**F0-C7-OH-RAF**
Cartesian Coordinates			Frequency and Energy
N	-5.41666200	2.74185700	-2.59572700
C	-4.07701800	2.73121700	-3.04230600
N	-3.17716500	1.92300100	-2.36951600
C	-3.58412000	1.20757800	-1.36728700
C	-4.94255600	1.17260600	-0.87286200
C	-5.94534700	2.02394100	-1.55352400
N	-2.65536800	0.41177700	-0.70752100
C	-2.99056100	-0.39791400	0.35440100
C	-4.33606900	-0.42716000	0.82560600
C	-5.29750100	0.39593600	0.17421700
C	-2.02685200	-1.21725200	0.96630000
C	-2.38750400	-2.02385100	2.02584300
C	-3.71807700	-2.03775100	2.54155100
C	-4.66401600	-1.21863500	1.92729800
O	-7.10899000	2.08162500	-1.22718900
O	-3.77115100	3.41898100	-3.98133900
O	-1.46651600	-2.83965900	2.55352300
C	-1.26249100	0.43730800	-1.16684300
H	-6.04535100	3.34630600	-3.11069100
H	-6.33062200	0.40749800	0.50841500
H	-1.00851800	-1.27647300	0.61383800
H	-3.90097000	-2.43488400	3.53003200
H	-5.67678800	-1.18775700	2.31179200
H	-1.93266500	-3.61423400	2.90140100
H	-1.18686000	1.16544400	-1.96620500
H	-0.97939300	-0.54875300	-1.53804500
H	-0.61336500	0.72180800	-0.33834400
O	-3.97846100	-4.02125100	2.03226200
H	-4.15688600	-3.93780400	1.08371100

Zero-point correction= 0.214350 (Hartree/Particle)
Thermal correction to Energy= 0.230227
Thermal correction to Enthalpy= 0.231171
Thermal correction to Gibbs Free Energy= 0.170353
Sum of electronic and zero-point Energies= -928.103404
Sum of electronic and thermal Energies= -928.087528
Sum of electronic and thermal Enthalpies= -928.086584
Sum of electronic and thermal Free Energies= -928.147402

Name			**F0-C8-OH-RAF**
Cartesian Coordinates			Frequency and Energy
N	-5.41084400	2.79486900	-2.57363300
C	-4.06301400	2.81941500	-3.00395200
N	-3.16049700	2.00260900	-2.35237400
C	-3.56385200	1.24345500	-1.37842900
C	-4.92943500	1.17903400	-0.89676600
C	-5.93871700	2.03695300	-1.56307100
N	-2.64286600	0.43282800	-0.74570500
C	-2.98013500	-0.40194000	0.31114500
C	-4.32623300	-0.44967500	0.77117600
C	-5.28932600	0.37145200	0.12728900
C	-2.02108400	-1.18611600	0.94007200

Zero-point correction= 0.213078 (Hartree/Particle)
Thermal correction to Energy= 0.229278
Thermal correction to Enthalpy= 0.230222
Thermal correction to Gibbs Free Energy= 0.168659
Sum of electronic and zero-point Energies= -928.096021
Sum of electronic and thermal Energies= -928.079821
Sum of electronic and thermal Enthalpies= -928.078877
Sum of electronic and thermal Free Energies= -928.140440

C	-2.38916300	-2.07093500	1.97394600
C	-3.73135700	-2.06768800	2.47016500
C	-4.67009700	-1.28850900	1.85263300
O	-7.10643400	2.06274700	-1.24535600
O	-3.76241700	3.54729600	-3.91440400
O	-1.37357700	-2.58390700	2.70059100
C	-1.25114400	0.45568400	-1.20299700
H	-6.04174500	3.40721400	-3.07635100
H	-6.32647000	0.36551300	0.44849700
H	-0.98110300	-1.18707100	0.65150200
H	-3.97845300	-2.70740100	3.30796900
H	-5.69753800	-1.28869400	2.19742400
H	-1.61373400	-3.47700300	2.97544200
H	-1.18547300	1.13851800	-2.04243400
H	-0.95285700	-0.54681400	-1.51259700
H	-0.60446900	0.80036400	-0.39447400
O	-2.71403400	-3.79894100	0.99440400
H	-3.53273200	-3.71443500	0.48322700

Name			**F0-C9-OH-RAF**
Cartesian Coordinates			Frequency and Energy
N	-5.41365200	2.83035700	-2.52882400
C	-4.06527400	2.85550300	-2.95553400
N	-3.17108400	2.01685700	-2.31942600
C	-3.59109800	1.24280800	-1.36507800
C	-4.95069300	1.18248600	-0.88137600
C	-5.95136100	2.05836900	-1.53211000
N	-2.67409300	0.39699700	-0.75495500
C	-3.01349800	-0.41056500	0.29822800
C	-4.34257200	-0.46403400	0.76476800
C	-5.30971300	0.36204700	0.13273100
C	-2.03261500	-1.25046200	0.89614500
C	-2.39703000	-2.02482100	2.00918700
C	-3.71706100	-2.08969700	2.46267800
C	-4.66800700	-1.31336800	1.83995700
O	-7.12016500	2.09307200	-1.21772000
O	-3.75611100	3.60270300	-3.84801300
O	-1.39771700	-2.73429700	2.57391400
C	-1.29677400	0.36847000	-1.26836700
H	-6.03900200	3.45673900	-3.02090700
H	-6.34650000	0.35251900	0.45533000
H	-0.97897700	-1.08842000	0.72814300
H	-3.97889500	-2.73126800	3.29613700
H	-5.69785600	-1.34262900	2.17696600
H	-1.72742200	-3.25146700	3.31535200
H	-1.27982300	0.92227700	-2.20009500
H	-1.01276900	-0.67023400	-1.42845800
H	-0.62666500	0.85043600	-0.55350400
O	-2.07115500	-2.67277600	-0.57817300
H	-1.57812900	-3.36060600	-0.10573000

Thermal correction to Energy= 0.230233
Thermal correction to Enthalpy= 0.231177
Thermal correction to Gibbs Free Energy= 0.170620
Sum of electronic and zero-point Energies= -928.101826
Sum of electronic and thermal Energies= -928.085929
Sum of electronic and thermal Enthalpies= -928.084985
Sum of electronic and thermal Free Energies= -928.145542

Name			**F0-C4'-OH-RAF**
Cartesian Coordinates			Frequency and Energy
N	-5.39233800	2.82205700	-2.49029100
C	-4.05099200	2.82517500	-2.93749500
N	-3.14942200	1.99440400	-2.29673000

Zero-point correction= 0.214060 (Hartree/Particle)
Thermal correction to Energy= 0.230064
Thermal correction to Enthalpy= 0.231008

C	-3.56201200	1.18553600	-1.37684800
C	-4.95631100	1.03870900	-0.97271500
C	-5.94265900	1.98110700	-1.56722100
N	-2.64550400	0.37010600	-0.74372200
C	-2.98357300	-0.44364300	0.32157500
C	-4.31727000	-0.45099200	0.81509400
C	-5.28583000	0.33653300	0.16240900
C	-2.02194100	-1.24571400	0.94412900
C	-2.37620000	-2.02847700	2.03219900
C	-3.68843200	-2.03617800	2.53899000
C	-4.63474600	-1.25270500	1.92906000
O	-7.11472500	1.98520100	-1.26181900
O	-3.74347500	3.56726400	-3.83307900
O	-1.39708600	-2.77746000	2.58172100
C	-1.25532100	0.39041000	-1.20477200
H	-6.01592100	3.45454800	-2.97646900
H	-6.31318600	0.36804000	0.51192300
H	-0.99551300	-1.28354300	0.61245700
H	-3.93966600	-2.65403400	3.39361500
H	-5.65525200	-1.24391900	2.29454400
H	-1.73731800	-3.28522100	3.32407000
H	-1.19092500	1.07369800	-2.04385900
H	-0.96471100	-0.61273000	-1.51902300
H	-0.60323700	0.73178500	-0.39931000
O	-5.28153400	-0.39670000	-2.40135200
H	-6.22579700	-0.55518000	-2.24194100

Thermal correction to Gibbs Free Energy= 0.170275
Sum of electronic and zero-point Energies= -928.101662
Sum of electronic and thermal Energies= -928.085658
Sum of electronic and thermal Enthalpies= -928.084713
Sum of electronic and thermal Free Energies= -928.145447

Name			**F0-C9'-OH-RAF**
Cartesian Coordinates			Frequency and Energy
N	-5.39552800	2.79955900	-2.54872700
C	-4.03928400	2.84846200	-2.94420000
N	-3.14156300	2.02581900	-2.29139900
C	-3.55230500	1.23743800	-1.34606300
C	-4.93078300	1.15779500	-0.89082600
C	-5.93339900	2.02206800	-1.55869100
N	-2.62756100	0.44895000	-0.69558800
C	-3.01763300	-0.53649500	0.20541200
C	-4.34836500	-0.48088100	0.76443200
C	-5.30268500	0.35422300	0.12967500
C	-2.02071000	-1.26162700	0.93625800
C	-2.37588400	-2.01753600	2.02769000
C	-3.70501200	-2.03880000	2.49996800
C	-4.66460800	-1.27394500	1.86959000
O	-7.10584300	2.03969800	-1.25734200
O	-3.72388700	3.60121800	-3.82927000
O	-1.39537100	-2.73608600	2.62822200
C	-1.25434900	0.40895300	-1.20176100
H	-6.02174900	3.41675000	-3.05103600
H	-6.33685000	0.36630700	0.45936600
H	-0.99459700	-1.28938800	0.60267500
H	-3.96289500	-2.64520000	3.36151700
H	-5.68295200	-1.26454100	2.24014000
H	-1.73058600	-3.17012700	3.41751600
H	-1.16259000	1.15511200	-1.98278100
H	-1.05805000	-0.58472200	-1.60941900

Zero-point correction= 0.213424 (Hartree/Particle)
Thermal correction to Energy= 0.229531
Thermal correction to Enthalpy= 0.230476
Thermal correction to Gibbs Free Energy= 0.169592
Sum of electronic and zero-point Energies= -928.091241
Sum of electronic and thermal Energies= -928.075133
Sum of electronic and thermal Enthalpies= -928.074189
Sum of electronic and thermal Free Energies= -928.135072

H	-0.55670000	0.63564800	-0.39488100
O	-3.38456900	-1.89601100	-1.11817500
H	-3.53799100	-2.72076400	-0.63326100

Name				**F0-C11-OH-FHT**
Cartesian Coordinates				Frequency and Energy
N	-5.28387200	2.45382600	-2.70241000	Zero-point correction= 0.209824 (Hartree/Particle)
C	-3.97398100	2.27212400	-3.19304500	Thermal correction to Energy= 0.225509
N	-3.09301100	1.52826500	-2.42606700	Thermal correction to Enthalpy= 0.226453
C	-3.51597800	0.98708500	-1.31831500	Thermal correction to Gibbs Free Energy= 0.165864
C	-4.86114800	1.07591900	-0.81177700	Sum of electronic and zero-point Energies= -928.100900
C	-5.82745200	1.90190000	-1.56792700	Sum of electronic and thermal Energies= -928.085215
N	-2.59374400	0.28650000	-0.56024700	Sum of electronic and thermal Enthalpies= -928.084271
C	-2.97440900	-0.49980600	0.52351200	Sum of electronic and thermal Free Energies= -928.144860
C	-4.30825200	-0.41745200	0.99639300	
C	-5.23311000	0.41200800	0.30720300	
C	-2.07702700	-1.36639400	1.15573200	
C	-2.49035100	-2.10454800	2.25284000	
C	-3.80035800	-2.00822400	2.75177500	
C	-4.68931200	-1.17773100	2.11577200	
O	-6.97589500	2.07557300	-1.22957300	
O	-3.66984000	2.76421600	-4.24929800	
O	-1.57209400	-2.92335300	2.80942500	
C	-1.22597700	0.34827900	-1.00940300	
H	-5.89557000	3.01214000	-3.28547000	
H	-6.25767500	0.50504100	0.65470600	
H	-1.06776000	-1.52270400	0.80757800	
H	-4.10060300	-2.59230300	3.61431000	
H	-5.71106100	-1.09796400	2.46884800	
H	-1.95870200	-3.42002400	3.53629500	
H	-0.99837900	1.34821600	-1.36623400	
H	-1.10023000	-0.35286700	-1.97052000	
H	-0.53257500	0.01446400	-0.24744400	
O	-1.29548500	-0.76127500	-3.23760200	
H	-1.80493100	0.01726200	-3.53267400	

Name				**F0-O8-OH-FHT**
Cartesian Coordinates				Frequency and Energy
N	-5.42785600	2.73600100	-2.61841700	Zero-point correction= 0.208740 (Hartree/Particle)
C	-4.08273100	2.75160300	-3.05659400	Thermal correction to Energy= 0.225145
N	-3.17642600	1.95258600	-2.38955100	Thermal correction to Enthalpy= 0.226090
C	-3.57614200	1.21993900	-1.39306300	Thermal correction to Gibbs Free Energy= 0.163360
C	-4.93648300	1.16625400	-0.90217100	Sum of electronic and zero-point Energies= -928.101695
C	-5.94990900	2.00476200	-1.58449700	Sum of electronic and thermal Energies= -928.085289
N	-2.64865200	0.42758000	-0.74245200	Sum of electronic and thermal Enthalpies= -928.084345
C	-2.97992000	-0.38008600	0.33333700	Sum of electronic and thermal Free Energies= -928.147075
C	-4.31853800	-0.42130900	0.80005100	
C	-5.28748900	0.38254100	0.14370100	
C	-2.01195000	-1.15317400	0.97999800	
C	-2.37721600	-1.97889200	2.04328100	
C	-3.71017800	-2.02324800	2.51465700	
C	-4.65098500	-1.24513300	1.89520700	
O	-7.11626000	2.04022900	-1.26207300	
O	-3.78799300	3.45706100	-3.98709400	
O	-1.42996900	-2.74688200	2.56912600	
C	-1.25930400	0.44570800	-1.20683700	

H	-6.06229200	3.33479800	-3.13275700
H	-6.32293600	0.38086600	0.47066000
H	-0.97415100	-1.15535600	0.68259100
H	-3.95528900	-2.65148100	3.36164100
H	-5.67973200	-1.25261900	2.23684900
H	-1.66302100	-3.06328600	3.53524100
H	-1.19998400	1.11288700	-2.05929400
H	-0.95947600	-0.56124000	-1.50022300
H	-0.60977400	0.80695600	-0.40803300
O	-1.77224200	-2.88274600	4.87628500
H	-0.90006000	-2.82098400	5.29428100

Name			**F0H2-C6-OH-RAF**
Cartesian Coordinates			Frequency and Energy
N	-5.46593600	2.18878300	-3.06547200
C	-4.18461400	2.14286200	-3.54975500
N	-3.28330500	1.54226200	-2.67661200
C	-3.64387800	0.98415300	-1.46562600
C	-4.92862400	1.02678900	-1.02978500
C	-5.94044100	1.64636100	-1.85470100
N	-2.64205000	0.37962000	-0.73396300
C	-3.01673300	-0.59404400	0.22007900
C	-4.32309700	-0.58919200	0.72567800
C	-5.29561100	0.47806100	0.31658700
C	-2.10449500	-1.55981800	0.63613900
C	-2.48519400	-2.53221600	1.57454400
C	-3.76029500	-2.55309000	2.09131100
C	-4.67168800	-1.53865100	1.71222100
O	-7.11610900	1.73986100	-1.57454400
O	-3.84036600	2.57008500	-4.62522900
O	-1.52642200	-3.43995800	1.90347000
C	-1.23979900	0.55924000	-1.07042400
H	-6.15512500	2.62241300	-3.66664000
H	-6.31356200	0.08327000	0.28381400
H	-1.10000900	-1.61672400	0.23973000
H	-4.06144500	-3.30445100	2.81207900
H	-5.71965100	-1.66449200	1.94969400
H	-1.87807400	-4.07070400	2.53787300
H	-1.08368300	1.56293900	-1.46372700
H	-0.87767200	-0.18249800	-1.79189500
H	-0.64821200	0.47854000	-0.15949500
H	-2.37444600	1.37706900	-3.08179400
H	-5.29768000	1.26234800	1.08547700
O	-4.60698500	-0.24679100	3.22709800
H	-3.64780100	-0.22574500	3.36374500

Zero-point correction= 0.237162 (Hartree/Particle)
Thermal correction to Energy= 0.253935
Thermal correction to Enthalpy= 0.254879
Thermal correction to Gibbs Free Energy= 0.192480
Sum of electronic and zero-point Energies= -929.277510
Sum of electronic and thermal Energies= -929.260737
Sum of electronic and thermal Enthalpies= -929.259793
Sum of electronic and thermal Free Energies= -929.322192

Name			**F0H2-C7-OH-RAF**
Cartesian Coordinates			Frequency and Energy
N	-5.48125200	2.19513300	-3.10969900
C	-4.20672300	2.11739700	-3.61065000
N	-3.30153800	1.52409000	-2.73529800
C	-3.65575700	1.00027900	-1.50815000
C	-4.93263200	1.06811400	-1.05877200
C	-5.94715700	1.68982100	-1.88131600
N	-2.65081400	0.39733400	-0.77083600
C	-3.01768500	-0.56677900	0.18275000

Zero-point correction= 0.237975 (Hartree/Particle)
Thermal correction to Energy= 0.254426
Thermal correction to Enthalpy= 0.255370
Thermal correction to Gibbs Free Energy= 0.193588
Sum of electronic and zero-point Energies= -929.286093
Sum of electronic and thermal Energies= -929.269641
Sum of electronic and thermal Enthalpies= -929.268697
Sum of electronic and thermal Free Energies= -929.330480

C	-4.33359800	-0.54853500	0.70737000
C	-5.27996700	0.55519300	0.30530000
C	-2.09581100	-1.52647100	0.60324100
C	-2.47771000	-2.48365100	1.53213800
C	-3.79586200	-2.51795600	2.03727000
C	-4.70279400	-1.53787100	1.59231500
O	-7.11478000	1.81210800	-1.58145700
O	-3.87192600	2.51384000	-4.69983900
O	-1.55906900	-3.36687100	1.96430500
C	-1.25022000	0.57068200	-1.12765000
H	-6.17083800	2.62753000	-3.71159400
H	-6.31182300	0.19897400	0.30534000
H	-1.08054500	-1.56079800	0.23435400
H	-4.15671000	-3.40710000	2.53378800
H	-5.72096200	-1.55923100	1.96445400
H	-1.78124700	-3.56055400	2.88768400
H	-1.10040700	1.56835900	-1.53761300
H	-0.90141500	-0.18294500	-1.84239000
H	-0.64813200	0.50174400	-0.22334900
H	-2.40164200	1.33319800	-3.14960700
H	-5.23295400	1.36979800	1.04003900
O	-3.07502200	-2.16782500	3.98931600
H	-2.92857700	-1.21263100	3.93212100

Name	**F0H2-C8-OH-RAF**
Cartesian Coordinates	Frequency and Energy

N	-5.47799900	2.18015600	-3.08795600
C	-4.20052800	2.12220500	-3.58341800
N	-3.29266700	1.52912300	-2.71057300
C	-3.64356600	0.99159600	-1.48923900
C	-4.92511600	1.04684600	-1.04392400
C	-5.94203100	1.66349300	-1.86300500
N	-2.64083300	0.39810400	-0.75128500
C	-3.00882400	-0.58529100	0.19477700
C	-4.32483300	-0.56928000	0.72032000
C	-5.27060400	0.53096100	0.31982100
C	-2.11186900	-1.55677000	0.58682100
C	-2.47417900	-2.50467500	1.57187100
C	-3.81838600	-2.54781100	2.02364300
C	-4.70494700	-1.56759700	1.61171900
O	-7.11226600	1.77542700	-1.56555100
O	-3.86515700	2.53389100	-4.66695600
O	-1.63807700	-3.56513800	1.72175400
C	-1.23997800	0.56089600	-1.10657900
H	-6.16979300	2.61124900	-3.68808000
H	-6.30255500	0.17401800	0.32369500
H	-1.10933300	-1.62846000	0.18975900
H	-4.11358300	-3.33253400	2.70856300
H	-5.72348400	-1.57267500	1.98346800
H	-1.53572000	-3.71593600	2.66982000
H	-1.07797300	1.56278200	-1.50218300
H	-0.89820300	-0.18625200	-1.83214400
H	-0.64008600	0.47013900	-0.20227600
H	-2.38624800	1.35834300	-3.11946100
H	-5.22193300	1.34262100	1.05933000

Zero-point correction= 0.236891 (Hartree/Particle)
Thermal correction to Energy= 0.253593
Thermal correction to Enthalpy= 0.254537
Thermal correction to Gibbs Free Energy= 0.192368
Sum of electronic and zero-point Energies= -929.280074
Sum of electronic and thermal Energies= -929.263373
Sum of electronic and thermal Enthalpies= -929.262429
Sum of electronic and thermal Free Energies= -929.324597

O	-1.89310900	-1.69385800	3.32568400
H	-2.52293500	-0.99886500	3.56281700

Name			**F0H2-C9-OH-RAF**
Cartesian Coordinates			Frequency and Energy
N	-5.45892900	2.16567700	-3.08491400
C	-4.16733800	2.12515800	-3.54563000
N	-3.28225400	1.52199900	-2.65909300
C	-3.66152500	0.96981300	-1.45272200
C	-4.95335400	1.01317300	-1.03753300
C	-5.95132800	1.63367600	-1.87817000
N	-2.66986300	0.36091400	-0.70956000
C	-3.05831600	-0.59204200	0.24098900
C	-4.36816900	-0.59817700	0.73267900
C	-5.33639400	0.48077600	0.31111500
C	-2.11106300	-1.53063200	0.70748300
C	-2.53427700	-2.55057200	1.58662500
C	-3.82964700	-2.56755800	2.07442800
C	-4.72641100	-1.59334100	1.63515400
O	-7.13000000	1.73485600	-1.61090700
O	-3.80626500	2.55917500	-4.61248200
O	-1.59999600	-3.47045200	1.90716100
C	-1.25719300	0.56643100	-1.01458300
H	-6.13647300	2.60372000	-3.69603500
H	-6.35584700	0.09211300	0.26707900
H	-1.16170700	-1.66954800	0.21204000
H	-4.14709500	-3.33602400	2.77014200
H	-5.74314700	-1.60458200	2.01333100
H	-1.95589100	-4.09565700	2.54513600
H	-1.10711300	1.59470400	-1.34266300
H	-0.89309600	-0.12477600	-1.78300800
H	-0.69110200	0.43132700	-0.09496400
H	-2.35544700	1.38235000	-3.03253800
H	-5.34418100	1.29096600	1.05193500
O	-1.09678400	-0.28834800	2.03111900
H	-1.83158600	-0.11719200	2.63926300

Zero-point correction= 0.237707 (Hartree/Particle)
Thermal correction to Energy= 0.254315
Thermal correction to Enthalpy= 0.255259
Thermal correction to Gibbs Free Energy= 0.193446
Sum of electronic and zero-point Energies= -929.285642
Sum of electronic and thermal Energies= -929.269034
Sum of electronic and thermal Enthalpies= -929.268090
Sum of electronic and thermal Free Energies= -929.329903

Name			**F0H2-C4'-OH-RAF**
Cartesian Coordinates			Frequency and Energy
N	-5.45354400	2.30079900	-3.03977400
C	-4.17560500	2.22422700	-3.53654500
N	-3.29372600	1.53426700	-2.71092400
C	-3.63645900	0.94672500	-1.51661500
C	-4.90723800	1.14669500	-0.98708600
C	-5.94044100	1.69320800	-1.87061600
N	-2.67080300	0.26251600	-0.85092700
C	-3.04279000	-0.64190700	0.17589300
C	-4.34347000	-0.61453100	0.69189800
C	-5.36765800	0.38422500	0.21899400
C	-2.11243200	-1.57461800	0.63198900
C	-2.46738800	-2.47400900	1.62973700
C	-3.75087500	-2.45985200	2.16342500
C	-4.66822900	-1.53664700	1.67928900
O	-7.12443500	1.68518500	-1.63549400
O	-3.82425500	2.69010000	-4.59205100
O	-1.50775000	-3.35278000	2.02965600

Zero-point correction= 0.237809 (Hartree/Particle)
Thermal correction to Energy= 0.254449
Thermal correction to Enthalpy= 0.255393
Thermal correction to Gibbs Free Energy= 0.193184
Sum of electronic and zero-point Energies= -929.288038
Sum of electronic and thermal Energies= -929.271398
Sum of electronic and thermal Enthalpies= -929.270454
Sum of electronic and thermal Free Energies= -929.332663

C	-1.25984500	0.48985300	-1.13757300
H	-6.13924100	2.73301100	-3.64663200
H	-6.30684100	-0.12166500	-0.02189700
H	-1.11505300	-1.64646100	0.22117300
H	-4.03186900	-3.16147000	2.94125900
H	-5.67259100	-1.52168400	2.08929700
H	-1.86248400	-3.93847700	2.70368500
H	-1.12331500	1.50403000	-1.51033900
H	-0.85789700	-0.23333500	-1.85411800
H	-0.70069300	0.41568800	-0.20683200
H	-2.39044500	1.37381700	-3.13171700
H	-5.58746100	1.11118500	1.00619900
O	-4.39887200	2.84000200	-0.02640500
H	-4.46952700	3.53876700	-0.69174400

Name			**F0H2-C5'-OH-RAF**
Cartesian Coordinates			Frequency and Energy
N	-5.42208100	2.36797900	-2.95785900
C	-4.13627800	2.32802000	-3.43163000
N	-3.27612600	1.58695200	-2.63157600
C	-3.67146300	0.89165600	-1.50310400
C	-4.95907600	0.92741500	-1.08267900
C	-5.93160900	1.68834800	-1.83711800
N	-2.68625200	0.15021000	-0.87833500
C	-3.04821600	-0.73539000	0.13534600
C	-4.31987000	-0.59908000	0.76773500
C	-5.42900400	0.20766000	0.14052500
C	-2.14300900	-1.69790500	0.57076800
C	-2.48204500	-2.54949400	1.61544500
C	-3.73563300	-2.46221400	2.23500800
C	-4.63926800	-1.52536700	1.78309300
O	-7.10853600	1.77724200	-1.55961900
O	-3.75987200	2.87102300	-4.44253100
O	-1.55207500	-3.46195400	1.98578300
C	-1.27386700	0.46746900	-1.07187400
H	-6.08551600	2.89946600	-3.50706200
H	-6.26160700	-0.45100400	-0.12906100
H	-1.17583100	-1.82433200	0.10391800
H	-3.99496600	-3.14045300	3.04071200
H	-5.62420200	-1.46217400	2.23228700
H	-1.89549800	-4.01724000	2.69146000
H	-1.16747400	1.51324700	-1.35669800
H	-0.80277900	-0.17200600	-1.82440800
H	-0.75761400	0.34294600	-0.12153500
H	-2.36646000	1.44014900	-3.04191000
H	-5.81031600	0.92042300	0.87627000
O	-3.57249200	1.01042500	1.84848100
H	-3.13691100	0.54460600	2.57693400

Zero-point correction= 0.237335 (Hartree/Particle)
Thermal correction to Energy= 0.254129
Thermal correction to Enthalpy= 0.255074
Thermal correction to Gibbs Free Energy= 0.192658
Sum of electronic and zero-point Energies= -929.283784
Sum of electronic and thermal Energies= -929.266990
Sum of electronic and thermal Enthalpies= -929.266046
Sum of electronic and thermal Free Energies= -929.328461

Name			**F0H2-C9'-OH-RAF**
Cartesian Coordinates			Frequency and Energy
N	-5.47168900	2.15484600	-3.07534300
C	-4.20184400	2.05668600	-3.58551900
N	-3.30699500	1.43549500	-2.72365800
C	-3.65689200	0.91242200	-1.49397100
C	-4.92872200	1.01449000	-1.03032000

Zero-point correction= 0.236932 (Hartree/Particle)
Thermal correction to Energy= 0.253620
Thermal correction to Enthalpy= 0.254565
Thermal correction to Gibbs Free Energy= 0.192801
Sum of electronic and zero-point Energies= -929.280654

C	-5.93536400	1.65658000	-1.84345500
N	-2.65330600	0.26617400	-0.80948200
C	-2.98831500	-0.53607300	0.29362000
C	-4.34898400	-0.59062300	0.73825000
C	-5.29074500	0.50124300	0.33034900
C	-2.09980600	-1.59002400	0.64603500
C	-2.50368900	-2.56618100	1.52496200
C	-3.82133100	-2.58345900	2.01417300
C	-4.72039700	-1.60879300	1.60321500
O	-7.09975200	1.80096100	-1.53473600
O	-3.86861800	2.45833500	-4.67441600
O	-1.59295300	-3.51519100	1.87262500
C	-1.25023300	0.62577800	-1.00127700
H	-6.15657900	2.60750500	-3.66710800
H	-6.32140000	0.14075100	0.32231000
H	-1.09427000	-1.62547400	0.24980400
H	-4.13508800	-3.36509500	2.69809500
H	-5.74061500	-1.63389300	1.96859300
H	-2.00977100	-4.19114500	2.41343400
H	-1.18267000	1.63492100	-1.40594200
H	-0.73196900	-0.07337800	-1.66410600
H	-0.77160000	0.64058400	-0.02305500
H	-2.40642800	1.23736900	-3.13389800
H	-5.23306400	1.30853100	1.07191800
O	-2.58340400	0.84758000	1.67258900
H	-2.53932000	0.35404700	2.50439000

Sum of electronic and thermal Energies= -929.263965
Sum of electronic and thermal Enthalpies= -929.263021
Sum of electronic and thermal Free Energies= -929.324785

Name			**F0H2-C10'-OH-RAF**
Cartesian Coordinates			Frequency and Energy
N	-5.44575800	2.23096100	-3.07724200
C	-4.17288900	2.12198900	-3.59105500
N	-3.30629400	1.39701300	-2.78595300
C	-3.60178000	0.97788000	-1.50748100
C	-4.93077800	1.01805900	-1.06277700
C	-5.92994000	1.67293200	-1.88351800
N	-2.65478800	0.24200600	-0.86881900
C	-3.03609700	-0.65276500	0.15921400
C	-4.32406300	-0.59620200	0.70676300
C	-5.30371400	0.46279100	0.26783400
C	-2.12350200	-1.61409000	0.58714800
C	-2.48413600	-2.51633000	1.58103000
C	-3.75775000	-2.47828000	2.13730700
C	-4.65986900	-1.52386600	1.68388300
O	-7.10077800	1.77952000	-1.58817800
O	-3.83067200	2.58773900	-4.64864900
O	-1.54128800	-3.42453600	1.95352000
C	-1.24826700	0.57886700	-1.06540500
H	-6.11924900	2.71190100	-3.66021300
H	-6.31775700	0.05969000	0.21270300
H	-1.13747500	-1.70145300	0.15102100
H	-4.04306300	-3.18483800	2.90900600
H	-5.65561000	-1.48849800	2.11301300
H	-1.90073000	-4.01082700	2.62452500
H	-1.17783300	1.62960500	-1.34808000
H	-0.76857500	-0.05853900	-1.81415200

Zero-point correction= 0.237250 (Hartree/Particle)
Thermal correction to Energy= 0.253808
Thermal correction to Enthalpy= 0.254752
Thermal correction to Gibbs Free Energy= 0.193235
Sum of electronic and zero-point Energies= -929.287789
Sum of electronic and thermal Energies= -929.271232
Sum of electronic and thermal Enthalpies= -929.270288
Sum of electronic and thermal Free Energies= -929.331805

H	-0.72642600	0.46747800	-0.11664000
H	-2.36039700	1.34583500	-3.13439500
H	-5.32401100	1.28396000	0.99452400
O	-3.46898300	2.69015700	-0.38651800
H	-3.96432100	3.41255200	-0.79895100

Name			**F0H2-C5-OH-FHT**
Cartesian Coordinates			Frequency and Energy
N	-5.44870100	2.41817100	-2.81317800
C	-4.20446900	2.31047000	-3.38062500
N	-3.31074200	1.56182600	-2.62072000
C	-3.64101900	0.91594700	-1.44706600
C	-4.91400700	0.97954700	-0.96163800
C	-5.87972800	1.82024200	-1.62120000
N	-2.64198500	0.22254000	-0.81383300
C	-2.98895500	-0.69760500	0.20320600
C	-4.27332100	-0.66115100	0.77030300
C	-5.28461100	0.34744600	0.32839200
C	-2.05976300	-1.65024400	0.61753900
C	-2.39349200	-2.55243000	1.62128400
C	-3.65541300	-2.52436600	2.20581600
C	-4.57648100	-1.58562400	1.76415000
O	-6.99899300	2.05102400	-1.19733000
O	-3.88443000	2.80774000	-4.43193900
O	-1.43477900	-3.44897400	1.97628600
C	-1.24363700	0.40151300	-1.17886700
H	-6.11739600	2.99942200	-3.30259800
H	-6.28657000	-0.08477500	0.27325100
H	-1.07973700	-1.73766800	0.16997300
H	-3.91574600	-3.22852600	2.98838100
H	-5.56443900	-1.55586300	2.21068300
H	-1.77179800	-4.03494300	2.65931300
H	-1.08661800	1.41084400	-1.55625300
H	-0.90794300	-0.33051000	-1.92072500
H	-0.63366700	0.30113300	-0.28296100
H	-2.43356500	1.38606700	-3.08707900
H	-5.39907300	1.17534300	1.12064400
O	-6.10891800	2.44318000	1.64567200
H	-6.72575300	2.52545600	0.89399900

Zero-point correction= 0.234205 (Hartree/Particle)
Thermal correction to Energy= 0.250765
Thermal correction to Enthalpy= 0.251709
Thermal correction to Gibbs Free Energy= 0.189626
Sum of electronic and zero-point Energies= -929.288418
Sum of electronic and thermal Energies= -929.271857
Sum of electronic and thermal Enthalpies= -929.270913
Sum of electronic and thermal Free Energies= -929.332996

Name			**F0H2-C11-OH-FHT**
Cartesian Coordinates			Frequency and Energy
N	-5.47984900	2.27847200	-3.06896900
C	-4.23011500	2.15804600	-3.62450400
N	-3.31722900	1.50976000	-2.80031600
C	-3.64199700	0.96030400	-1.57449400
C	-4.89858900	1.05955300	-1.07656400
C	-5.91829600	1.74428300	-1.84601000
N	-2.63185000	0.27916500	-0.91776500
C	-2.98938400	-0.61825400	0.11544700
C	-4.26872700	-0.55688700	0.68697400
C	-5.25090800	0.50952900	0.27070400
C	-2.05536800	-1.55581500	0.55839000
C	-2.39708400	-2.44721000	1.57051500
C	-3.66574400	-2.41359800	2.13815100
C	-4.58103600	-1.47187600	1.68358800

Zero-point correction= 0.232970 (Hartree/Particle)
Thermal correction to Energy= 0.249682
Thermal correction to Enthalpy= 0.250627
Thermal correction to Gibbs Free Energy= 0.187772
Sum of electronic and zero-point Energies= -929.280299
Sum of electronic and thermal Energies= -929.263587
Sum of electronic and thermal Enthalpies= -929.262643
Sum of electronic and thermal Free Energies= -929.325497

O	-7.06927600	1.89168400	-1.49663800
O	-3.92691900	2.56393400	-4.71921700
O	-1.43783000	-3.33211200	1.95122100
C	-1.24242900	0.56115900	-1.14092200
H	-6.17505100	2.75011700	-3.63369600
H	-6.26581300	0.10642400	0.23516700
H	-1.06600000	-1.63442900	0.12852100
H	-3.93546700	-3.11037400	2.92421400
H	-5.56887500	-1.43396700	2.13025800
H	-1.77697200	-3.90773000	2.64198600
H	-1.10858100	1.43640900	-1.77068700
H	-0.67920500	-0.29136500	-1.52495200
H	-0.75237200	0.84503600	-0.11919900
H	-2.45301900	1.26836100	-3.26221800
H	-5.26923100	1.31463900	1.01621200
O	-0.32089900	1.08307700	1.23397600
H	-0.83076900	0.40097300	1.70307300

Name				**F0H2-N1-OH-FHT**
Cartesian Coordinates				Frequency and Energy
N	-5.46346600	2.23546200	-3.04815500	Zero-point correction= 0.232663 (Hartree/Particle)
C	-4.17542400	2.16473900	-3.51720800	Thermal correction to Energy= 0.249383
N	-3.24593100	1.63849800	-2.61522700	Thermal correction to Enthalpy= 0.250327
C	-3.62467600	1.00176700	-1.46489500	Thermal correction to Gibbs Free Energy= 0.187792
C	-4.93275700	1.01801200	-1.04496800	Sum of electronic and zero-point Energies= -929.284275
C	-5.94281500	1.65839000	-1.86431900	Sum of electronic and thermal Energies= -929.267555
N	-2.64278000	0.39948300	-0.72312100	Sum of electronic and thermal Enthalpies= -929.266611
C	-3.02179700	-0.58137500	0.22364600	Sum of electronic and thermal Free Energies= -929.329146
C	-4.33268200	-0.58713400	0.72361000	
C	-5.29923600	0.49134800	0.30368300	
C	-2.10225500	-1.54275100	0.63455000	
C	-2.48428300	-2.51131900	1.55761600	
C	-3.78039300	-2.53869300	2.05827600	
C	-4.68840000	-1.57829000	1.62610200	
O	-7.11932700	1.73031900	-1.58107600	
O	-3.84517800	2.52826100	-4.62112800	
O	-1.53423200	-3.41646500	1.91759900	
C	-1.22817000	0.60599000	-1.02032000	
H	-6.15219200	2.62350900	-3.68060700	
H	-6.32431000	0.11529600	0.27361200	
H	-1.09646500	-1.58469300	0.24066000	
H	-4.07894700	-3.29855400	2.77212200	
H	-5.70184600	-1.59251900	2.01257900	
H	-1.90978400	-4.05981400	2.52443700	
H	-1.09259800	1.59285800	-1.45738400	
H	-0.83950800	-0.14334400	-1.71478600	
H	-0.67381400	0.57018900	-0.08345700	
H	-2.33521700	1.31388100	-3.13228200	
H	-5.29624500	1.31096300	1.03670100	
O	-1.62525400	0.52592800	-4.03061100	
H	-1.94253400	0.86378400	-4.88503600	

Name				**F0H2-O8-OH-FHT**
Cartesian Coordinates				Frequency and Energy
N	-5.47203700	2.01338300	-3.13397900	Zero-point correction= 0.232881 (Hartree/Particle)
C	-4.18370600	1.97367900	-3.60075900	Thermal correction to Energy= 0.249916

N	-3.27725900	1.45059200	-2.68391400
C	-3.63739900	0.95672400	-1.44589500
C	-4.92925500	0.99040800	-1.02842800
C	-5.94628200	1.53635200	-1.89595000
N	-2.63240000	0.42653200	-0.66466500
C	-2.99539200	-0.52324700	0.31954000
C	-4.31067900	-0.52412700	0.81717100
C	-5.28770300	0.52441500	0.35063000
C	-2.07353300	-1.46112500	0.76758100
C	-2.44312700	-2.38580700	1.75024400
C	-3.75020300	-2.40588000	2.24760600
C	-4.66332800	-1.48439200	1.76087700
O	-7.12622800	1.62402800	-1.63000300
O	-3.83802700	2.34610700	-4.69587500
O	-1.49630100	-3.22419400	2.19165700
C	-1.23153000	0.61302000	-1.00363900
H	-6.16416500	2.39426800	-3.76664900
H	-6.30585100	0.13012400	0.34566600
H	-1.06658400	-1.52095100	0.37822300
H	-4.03450300	-3.14798300	2.98352300
H	-5.68164000	-1.49313000	2.13398500
H	-1.89976400	-4.05945300	2.60938300
H	-1.08853700	1.60248900	-1.43644400
H	-0.85606100	-0.15210200	-1.69335200
H	-0.64405500	0.57536000	-0.08757300
H	-2.35809800	1.28964700	-3.06716800
H	-5.28629500	1.36989500	1.05220200
O	-2.47323500	-5.36706800	2.49245000
H	-1.82464400	-6.02979300	2.21031700

Name			**F0H2-C5-OOH-FHT**
Cartesian Coordinates			Frequency and Energy
N	-5.46336900	2.25165000	-3.01154900
C	-4.17887100	2.22889000	-3.48624300
N	-3.28221200	1.56719600	-2.64775000
C	-3.64653300	0.94319800	-1.47387400
C	-4.94569700	0.95439100	-1.05056900
C	-5.95277200	1.63842100	-1.84326600
N	-2.65402800	0.33296800	-0.74424500
C	-3.02199200	-0.63535400	0.22009700
C	-4.33752400	-0.63456300	0.71713000
C	-5.28645500	0.40602300	0.26251300
C	-2.09745300	-1.58186200	0.65371900
C	-2.47339100	-2.52265800	1.60704200
C	-3.76796700	-2.53598100	2.11750400
C	-4.68201900	-1.59728300	1.66135700
O	-7.12637600	1.71261600	-1.56548100
O	-3.82095100	2.71932100	-4.52881100
O	-1.52056500	-3.41456000	1.98858600
C	-1.24930200	0.51519600	-1.07818300
H	-6.14154400	2.73830000	-3.58432800
H	-6.33919700	0.13939300	0.35229100
H	-1.09145100	-1.63720800	0.26200900
H	-4.05743600	-3.27224200	2.85934300
H	-5.69303700	-1.59972300	2.05299400

Thermal correction to Enthalpy= 0.250860
Thermal correction to Gibbs Free Energy= 0.186997
Sum of electronic and zero-point Energies= -929.282654
Sum of electronic and thermal Energies= -929.265619
Sum of electronic and thermal Enthalpies= -929.264675
Sum of electronic and thermal Free Energies= -929.328538

Zero-point correction= 0.237706 (Hartree/Particle)
Thermal correction to Energy= 0.255685
Thermal correction to Enthalpy= 0.256629
Thermal correction to Gibbs Free Energy= 0.190078
Sum of electronic and zero-point Energies= -1004.428894
Sum of electronic and thermal Energies= -1004.410916
Sum of electronic and thermal Enthalpies= -1004.409971
Sum of electronic and thermal Free Energies= -1004.476522

H	-1.88734600	-4.03242200	2.62673100
H	-1.09050200	1.52034700	-1.46643400
H	-0.89177000	-0.22374000	-1.80361500
H	-0.66098300	0.42635400	-0.16671400
H	-2.37669300	1.41694300	-3.06656100
H	-5.18364800	1.36764200	1.02949500
H	-3.64765400	3.37814500	0.53681600
O	-4.92564800	2.56045700	1.61246100
O	-4.61454600	3.36824000	0.55084400

Name	**F0H2-O8-OOH-FHT**
Cartesian Coordinates	Frequency and Energy

N	-5.46229200	2.16788000	-3.08755800
C	-4.17390000	2.14188800	-3.55690500
N	-3.27227100	1.55610100	-2.67239800
C	-3.63724100	0.99746400	-1.46465900
C	-4.92798600	1.02150500	-1.04526900
C	-5.94074800	1.62687000	-1.87898200
N	-2.63772700	0.41229500	-0.71431900
C	-3.00417400	-0.58427100	0.21701400
C	-4.32911500	-0.59857800	0.71837400
C	-5.29211100	0.48109400	0.30363700
C	-2.09487200	-1.54279600	0.62451500
C	-2.46692100	-2.52202000	1.57274300
C	-3.79164600	-2.53994600	2.06671600
C	-4.69579100	-1.58961100	1.62245700
O	-7.11879000	1.70922300	-1.60497400
O	-3.82449000	2.57308900	-4.62813300
O	-1.57366700	-3.38987100	1.97697700
C	-1.23373800	0.60769600	-1.03911700
H	-6.15020400	2.59266200	-3.69669200
H	-6.31475800	0.09911900	0.27930500
H	-1.08410600	-1.59083500	0.24301600
H	-4.06880500	-3.29667200	2.78860300
H	-5.71288300	-1.59659200	1.99836800
H	-1.91538200	-4.45794000	1.78851900
H	-1.08439700	1.61646600	-1.42183100
H	-0.86129900	-0.12506200	-1.76422100
H	-0.65001200	0.52103000	-0.12398800
H	-2.35363300	1.41178100	-3.06371800
H	-5.28160000	1.28446300	1.05378300
H	-3.61050500	-5.09024900	-0.05092800
O	-2.37234400	-5.47884300	1.27898800
O	-3.63362200	-5.10374500	0.91729500

Zero-point correction= 0.237600 (Hartree/Particle)
Thermal correction to Energy= 0.255263
Thermal correction to Enthalpy= 0.256207
Thermal correction to Gibbs Free Energy= 0.190143
Sum of electronic and zero-point Energies= -1004.427237
Sum of electronic and thermal Energies= -1004.409574
Sum of electronic and thermal Enthalpies= -1004.408630
Sum of electronic and thermal Free Energies= -1004.474694

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