Supporting Information (SI)

The radical scavenging activity of 1-methyl-1,4-dihydronicotinamide: Theoretical insights into the mechanism, kinetics and solvent 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) $= 8.62\times10^{-4}$ 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.

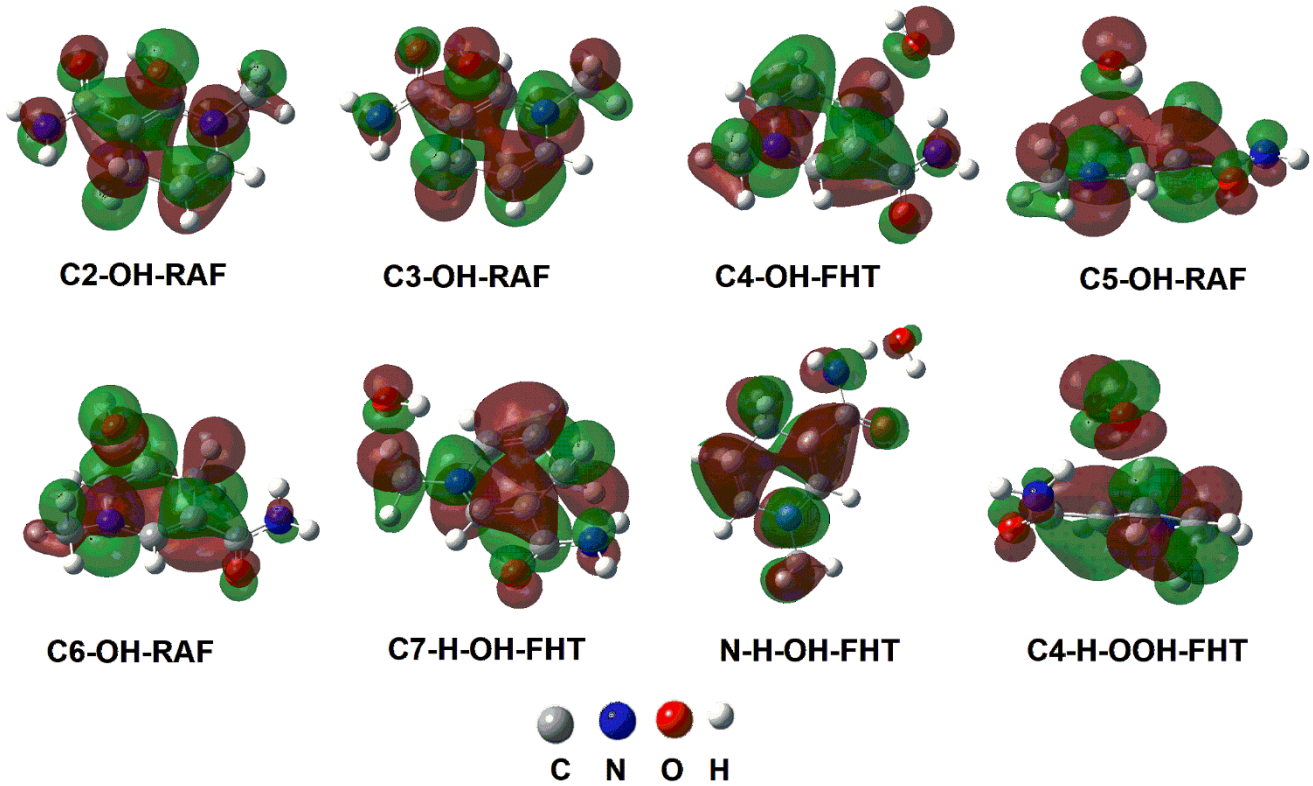

Figure S1. The SOMO orbitals of the transition states following the RAF and FHT mechanisms in the MNAH + HO•/HOO• reactions

Table S2: The Cartesian coordinates and energies of TS of the reaction between MNAH with HO•/HOO• following the FHT and FHT mechanisms (G: the gas phase; P: pentyl ethanoate; W: water)

Name				**C2-OH-RAF-G**
Cartesian Coordinates				Frequency and Energy
O	2.13692100	-1.62515900	-0.02642600	Zero-point correction= 0.179200 (Hartree/Particle)
N	-1.81627600	-0.55708500	-0.30959300	Thermal correction to Energy= 0.190867
N	2.85107400	0.51750200	0.05031800	Thermal correction to Enthalpy= 0.191811
C	0.16219500	1.54214700	0.10133500	Thermal correction to Gibbs Free Energy= 0.141054
C	0.48362200	0.07954500	-0.04239100	Sum of electronic and zero-point Energies= -532.977866
C	-0.50965800	-0.86544500	-0.16505000	Sum of electronic and thermal Energies= -532.966199
C	-1.32058600	1.77504100	-0.00358000	Sum of electronic and thermal Enthalpies= -532.965255
C	-2.19457600	0.78728300	-0.17573600	Sum of electronic and thermal Free Energies= -533.016012
C	-2.81288400	-1.58763500	-0.06070600	
C	1.87134600	-0.43329900	-0.00533300	
H	0.68310700	2.12786500	-0.66913200	
H	0.52363200	1.90580500	1.07385700	
H	-0.23439900	-1.90765100	-0.26789600	
H	-1.69164900	2.78957600	0.06388900	
H	-3.26057100	0.96286300	-0.24421500	
H	-3.74149900	-1.32278500	-0.56651600	
H	-2.99173600	-1.69722700	1.01263500	
H	-2.45502900	-2.53513500	-0.46216600	
H	3.79318700	0.19012300	0.19391000	
H	2.64564300	1.48067100	0.25250900	
O	-0.22547900	-0.78687500	1.99321300	
H	0.52654900	-1.39649400	2.04087800	
Name				**C3-OH-RAF-G**
Cartesian Coordinates				Frequency and Energy
O	2.27227600	-1.51221300	0.19873800	Zero-point correction= 0.178700 (Hartree/Particle)
N	-1.70736600	-0.53670900	-0.21386900	Thermal correction to Energy= 0.190680
N	2.94067600	0.61399900	-0.15165400	Thermal correction to Enthalpy= 0.191624
C	0.24568300	1.61557300	0.00215600	Thermal correction to Gibbs Free Energy= 0.139829
C	0.58148100	0.14438700	-0.04583000	Sum of electronic and zero-point Energies= -532.979068
C	-0.37914800	-0.80808300	-0.15279200	Sum of electronic and thermal Energies= -532.967088
C	-1.24810400	1.80417500	0.05577100	Sum of electronic and thermal Enthalpies= -532.966144
C	-2.10945400	0.79374800	-0.04364700	Sum of electronic and thermal Free Energies= -533.017939
C	-2.68052100	-1.59684100	-0.01025200	
C	1.98041300	-0.33894800	0.00894800	
H	0.65185500	2.14335500	-0.87420300	
H	0.70776500	2.07181700	0.88717500	
H	-0.09066700	-1.85259400	-0.18826300	
H	-1.64034000	2.80590400	0.17600800	
H	-3.18133900	0.94103600	-0.00430600	
H	-3.59980900	-1.35493900	-0.54473400	
H	-2.90324400	-1.73068600	1.05280400	
H	-2.28346100	-2.52862900	-0.41090500	
H	3.90124600	0.33260000	-0.04063200	
H	2.72422800	1.59146600	-0.23674200	
O	0.29735200	-0.42616100	2.32741900	
H	0.95761300	-1.11786900	2.14893400	
Name				**C5-OH-RAF-G**
Cartesian Coordinates				Frequency and Energy
O	2.26964500	-1.52589700	0.12671500	Zero-point correction= 0.178658 (Hartree/Particle)

N	-1.72369800	-0.52366800	-0.18820300	Thermal correction to Energy= 0.190634
N	2.93211900	0.63114700	0.10176400	Thermal correction to Enthalpy= 0.191578
C	0.24414900	1.61743600	-0.11300700	Thermal correction to Gibbs Free Energy= 0.139786
C	0.57465200	0.14396300	-0.03002200	Sum of electronic and zero-point Energies= -532.976702
C	-0.38022700	-0.80223100	-0.08531600	Sum of electronic and thermal Energies= -532.964726
C	-1.24101500	1.81559800	0.01834300	Sum of electronic and thermal Enthalpies= -532.963782
C	-2.11888700	0.79355200	-0.05999700	Sum of electronic and thermal Free Energies= -533.015574
C	-2.70140400	-1.58268100	0.01498100	
C	1.97619800	-0.34548000	0.06576100	
H	0.60612200	2.04671000	-1.05940300	
H	0.73440100	2.17529200	0.69453600	
H	-0.10026500	-1.84886600	-0.04983200	
H	-1.62750300	2.81908500	0.12269500	
H	-3.18568500	0.95497500	0.02112400	
H	-3.62134200	-1.33037200	-0.51208700	
H	-2.92353300	-1.72155100	1.07742600	
H	-2.31152200	-2.51277500	-0.39605300	
H	3.89396400	0.33199200	0.08295400	
H	2.72521800	1.59695800	-0.08412500	
O	-1.34664100	1.57458900	2.30224200	
H	-0.74244500	0.81475700	2.28051100	
Name				**C6-OH-RAF-G**
Cartesian Coordinates				Frequency and Energy
O	2.28505000	-1.49566700	-0.31522000	Zero-point correction= 0.178904 (Hartree/Particle)
N	-1.75017800	-0.58652500	-0.25529900	Thermal correction to Energy= 0.190629
N	2.88925500	0.64325200	0.08469700	Thermal correction to Enthalpy= 0.191573
C	0.18032800	1.57700000	0.03070600	Thermal correction to Gibbs Free Energy= 0.140836
C	0.54238100	0.11730800	-0.10392800	Sum of electronic and zero-point Energies= -532.974830
C	-0.39427400	-0.83706800	-0.20121400	Sum of electronic and thermal Energies= -532.963105
C	-1.30115400	1.76498300	-0.08998700	Sum of electronic and thermal Enthalpies= -532.962161
C	-2.16869300	0.71405200	-0.14076600	Sum of electronic and thermal Free Energies= -533.012899
C	-2.68937100	-1.64440800	0.08795900	
C	1.95516500	-0.34099600	-0.11692000	
H	0.69383500	2.17517400	-0.73374000	
H	0.50327200	1.97199600	1.00588900	
H	-0.09588300	-1.87661400	-0.27112100	
H	-1.70780500	2.76791100	-0.10438900	
H	-3.23565800	0.86750800	-0.23615900	
H	-3.64505200	-1.45134500	-0.40074800	
H	-2.83721700	-1.68518400	1.17020100	
H	-2.30091500	-2.59645000	-0.27133500	
H	3.84099200	0.33383900	0.20571600	
H	2.63522200	1.53526000	0.47406600	
O	-2.07376900	0.89808300	2.00739700	
H	-2.59119000	1.68781100	2.21840100	
Name				**C4-OH-FHT-G**
Cartesian Coordinates				Frequency and Energy
O	2.34281200	-1.44949200	-0.32946400	Zero-point correction= 0.176165 (Hartree/Particle)
N	-1.70843500	-0.54556500	-0.04992300	Thermal correction to Energy= 0.187810
N	2.87423600	0.73564600	0.00046600	Thermal correction to Enthalpy= 0.188754
C	0.24924400	1.57506400	-0.18248600	Thermal correction to Gibbs Free Energy= 0.137548
C	0.57846700	0.13161300	-0.10339600	Sum of electronic and zero-point Energies= -532.982112
C	-0.37011700	-0.82450600	-0.03738100	Sum of electronic and thermal Energies= -532.970467
C	-1.22326900	1.79564900	-0.18283200	Sum of electronic and thermal Enthalpies= -532.969523

C	-2.10027900	0.78246800	-0.10647300	Sum of electronic and thermal Free Energies= -533.020729
C	-2.69258900	-1.58477600	0.20206800	
C	1.99721900	-0.29535200	-0.14455800	
H	0.72390900	2.03955800	-1.06224000	
H	0.74078000	2.12098700	0.70049700	
H	-0.08104200	-1.86858100	0.00098700	
H	-1.60771700	2.80500000	-0.25735300	
H	-3.17085400	0.94564200	-0.11048100	
H	-3.59434000	-1.38078000	-0.37615500	
H	-2.95190500	-1.64231500	1.26292800	
H	-2.28776600	-2.54391500	-0.11727100	
H	3.84511000	0.46679800	0.04313000	
H	2.61061500	1.58012400	0.50009300	
O	1.41335700	2.95904200	1.67623400	
H	0.67324600	3.57859300	1.75251600	
Name				**C7-OH-FHT-G**
Cartesian Coordinates				Frequency and Energy
O	2.11830900	-1.64186400	0.17012600	Zero-point correction= 0.175022 (Hartree/Particle)
N	-1.81715400	-0.51452100	-0.35827900	Thermal correction to Energy= 0.187361
N	2.83083000	0.49278700	0.33735200	Thermal correction to Enthalpy= 0.188305
C	0.18306100	1.56264400	0.05357100	Thermal correction to Gibbs Free Energy= 0.134088
C	0.47594100	0.07969500	0.01725000	Sum of electronic and zero-point Energies= -532.968900
C	-0.49189200	-0.83276300	-0.17821400	Sum of electronic and thermal Energies= -532.956562
C	-1.30445100	1.79979400	0.01473600	Sum of electronic and thermal Enthalpies= -532.955617
C	-2.18910900	0.82202100	-0.18339200	Sum of electronic and thermal Free Energies= -533.009835
C	-2.82480700	-1.52827400	-0.25295600	
C	1.85553800	-0.45309400	0.16983100	
H	0.66219400	2.07728300	-0.79317000	
H	0.60505400	2.01676200	0.95979000	
H	-0.23701300	-1.88613900	-0.20501600	
H	-1.67345200	2.81007100	0.13768700	
H	-3.25637700	1.00213600	-0.21279700	
H	-3.70525200	-1.26032500	-0.83740100	
H	-3.17888200	-1.63683200	0.82754200	
H	-2.43139100	-2.49050200	-0.57621600	
H	3.78371500	0.16585800	0.35606800	
H	2.66405900	1.47170200	0.18232800	
O	-3.45505000	-1.30961400	2.34169900	
H	-2.60809100	-0.86972100	2.52482800	
Name				**N9-OH-FHT-G**
Cartesian Coordinates				Frequency and Energy
O	2.46637700	-1.16633000	-0.36151300	Zero-point correction= 0.174066 (Hartree/Particle)
N	-1.56935600	-0.56301800	0.18513400	Thermal correction to Energy= 0.185742
N	2.88827100	1.06430600	-0.56889300	Thermal correction to Enthalpy= 0.186686
C	0.15342600	1.77118300	-0.13335200	Thermal correction to Gibbs Free Energy= 0.134552
C	0.62483500	0.33074800	-0.14739700	Sum of electronic and zero-point Energies= -532.962331
C	-0.23023900	-0.70653400	0.00102900	Sum of electronic and thermal Energies= -532.950655
C	-1.34957700	1.81865900	-0.00890400	Sum of electronic and thermal Enthalpies= -532.949710
C	-2.10285300	0.72982000	0.13994000	Sum of electronic and thermal Free Energies= -533.001845
C	-2.46653600	-1.70414500	0.21409300	
C	2.03997500	-0.02183300	-0.33528700	
H	0.47118300	2.29290900	-1.04425200	
H	0.60469500	2.32742500	0.70217100	
H	0.15543000	-1.71962000	-0.02116500	

H	-1.84101900	2.78301100	-0.03401200
H	-3.18050200	0.77968700	0.23461800
H	-3.00016400	-1.81632400	-0.73453500
H	-3.19348200	-1.58693800	1.01989100
H	-1.88773000	-2.60708300	0.40097200
H	4.04307500	0.74966200	-0.55096000
H	2.71253600	1.86734500	0.03120500
O	4.91334700	0.20148100	0.05050500
H	4.51813500	-0.68750000	0.09664000

Name			**C2-OH-RAF-P**
Cartesian Coordinates			Frequency and Energy
O	2.14483300	-1.62604200	-0.05222900
N	-1.81620800	-0.56125300	-0.23514200
N	2.84447000	0.52122000	0.05049200
C	0.16529900	1.53839400	0.09539700
C	0.48530700	0.07399800	-0.01026000
C	-0.52023100	-0.87816400	-0.09209100
C	-1.31755100	1.77364700	0.01986800
C	-2.19756100	0.78583100	-0.12704900
C	-2.84038700	-1.58845800	-0.11003800
C	1.87493100	-0.42899600	-0.00520000
H	0.66883200	2.09769200	-0.70541600
H	0.55841500	1.94033500	1.03964700
H	-0.25838900	-1.92342000	-0.19211100
H	-1.68342700	2.79109000	0.08019900
H	-3.26523700	0.95613700	-0.18509700
H	-3.68986000	-1.33240100	-0.74360500
H	-3.17281800	-1.67672100	0.92797100
H	-2.43010300	-2.54261200	-0.43756900
H	3.80213100	0.21539800	0.14121300
H	2.63964600	1.49220600	0.22484700
O	-0.15988700	-0.78684600	2.03665800
H	0.59073000	-1.39740300	2.06331900

Zero-point correction= 0.178935 (Hartree/Particle)
Thermal correction to Energy= 0.190558
Thermal correction to Enthalpy= 0.191502
Thermal correction to Gibbs Free Energy= 0.141080
Sum of electronic and zero-point Energies= -532.998854
Sum of electronic and thermal Energies= -532.987231
Sum of electronic and thermal Enthalpies= -532.986287
Sum of electronic and thermal Free Energies= -533.036709

Name			**C3-OH-RAF-P**
Cartesian Coordinates			Frequency and Energy
O	2.28186200	-1.45766700	0.38954900
N	-1.70351300	-0.52148300	-0.17338900
N	2.93032400	0.63833300	-0.14007100
C	0.24039900	1.63768400	-0.02431800
C	0.58122500	0.16505500	0.00567700
C	-0.37945700	-0.79304500	-0.08682000
C	-1.25247400	1.82210100	0.07228100
C	-2.11332100	0.80739700	-0.01085800
C	-2.69181700	-1.58393500	-0.05954100
C	1.97997100	-0.29921500	0.09219900
H	0.61231400	2.11263300	-0.94505500
H	0.73713000	2.15841800	0.80333500
H	-0.10339600	-1.84112200	-0.10098200
H	-1.64471800	2.82399900	0.19658200
H	-3.18600400	0.94665800	0.04459500
H	-3.55481200	-1.34755900	-0.68296700
H	-3.01835900	-1.70725800	0.97750800
H	-2.25338600	-2.51754300	-0.40908700
H	3.90005800	0.36174800	-0.09810000

Zero-point correction= 0.178834 (Hartree/Particle)
Thermal correction to Energy= 0.190497
Thermal correction to Enthalpy= 0.191442
Thermal correction to Gibbs Free Energy= 0.140684
Sum of electronic and zero-point Energies= -532.998833
Sum of electronic and thermal Energies= -532.987169
Sum of electronic and thermal Enthalpies= -532.986225
Sum of electronic and thermal Free Energies= -533.036982

H	2.70877000	1.56706600	-0.46196200
O	0.33488300	-0.67814800	2.46934400
H	1.03145400	-1.23973100	2.08220400

Name			**C5-OH-RAF-P**
Cartesian Coordinates			Frequency and Energy
O	2.27847200	-1.50877800	0.20627100
N	-1.71358200	-0.49950000	-0.18822000
N	2.94274700	0.64195100	0.05732400
C	0.26409500	1.63517700	-0.14204600
C	0.58708900	0.15965900	-0.02722100
C	-0.37791100	-0.78209900	-0.07408600
C	-1.22310200	1.84342600	-0.04847500
C	-2.10043400	0.82687100	-0.06715300
C	-2.70306800	-1.54293500	0.04704200
C	1.98468000	-0.32556300	0.08377200
H	0.64277200	2.04838200	-1.08861800
H	0.76140700	2.20784000	0.65167000
H	-0.11369200	-1.83185200	-0.01841900
H	-1.60343200	2.84974600	0.07020000
H	-3.16829100	0.98997900	0.00489900
H	-3.60766400	-1.31637200	-0.51745600
H	-2.95157400	-1.61954800	1.11019200
H	-2.30539700	-2.49566300	-0.29972200
H	3.90874300	0.34959900	0.06242400
H	2.74044800	1.60374900	-0.16325400
O	-1.55230800	1.21055300	2.42388700
H	-0.75769800	0.67791100	2.24799700

Zero-point correction= 0.177835 (Hartree/Particle)
Thermal correction to Energy= 0.190036
Thermal correction to Enthalpy= 0.190980
Thermal correction to Gibbs Free Energy= 0.138081
Sum of electronic and zero-point Energies= -532.998001
Sum of electronic and thermal Energies= -532.985800
Sum of electronic and thermal Enthalpies= -532.984856
Sum of electronic and thermal Free Energies= -533.037755

Name			**C6-OH-RAF-P**
Cartesian Coordinates			Frequency and Energy
O	2.29331400	-1.52025400	-0.20286300
N	-1.74505500	-0.59124600	-0.19065300
N	2.89030000	0.63929900	0.06289200
C	0.18946700	1.56800400	0.03639900
C	0.54904600	0.10413300	-0.06115400
C	-0.39403200	-0.84979400	-0.14353300
C	-1.29259500	1.75712300	-0.04313100
C	-2.16640500	0.70597800	-0.07807700
C	-2.69920000	-1.67071700	0.02139100
C	1.96226900	-0.34811900	-0.06900700
H	0.67414100	2.14137000	-0.76571000
H	0.55544900	1.99986800	0.97940500
H	-0.11207000	-1.89453000	-0.19836700
H	-1.69652100	2.76115100	-0.05591200
H	-3.23324900	0.85912600	-0.17112200
H	-3.64300200	-1.41525800	-0.46070400
H	-2.87046100	-1.83275900	1.08881900
H	-2.31135300	-2.58386200	-0.42876600
H	3.85862900	0.36762600	0.14917000
H	2.64300300	1.58410100	0.31000900
O	-2.08317000	0.98678900	2.06964900
H	-2.63416400	1.77189100	2.19546800

Zero-point correction= 0.178077 (Hartree/Particle)
Thermal correction to Energy= 0.190043
Thermal correction to Enthalpy= 0.190988
Thermal correction to Gibbs Free Energy= 0.139394
Sum of electronic and zero-point Energies= -532.997432
Sum of electronic and thermal Energies= -532.985466
Sum of electronic and thermal Enthalpies= -532.984521
Sum of electronic and thermal Free Energies= -533.036115

Name			**C4-OH-FHT-P**
Cartesian Coordinates			Frequency and Energy
O	2.29181300	-1.45858400	-0.22026100

Zero-point correction= 0.175118 (Hartree/Particle)

N	-1.72424900	-0.56442700	-0.04714000	Thermal correction to Energy= 0.186761
N	2.87433600	0.71439300	0.07132900	Thermal correction to Enthalpy= 0.187705
C	0.17492800	1.56989300	-0.16162900	Thermal correction to Gibbs Free Energy= 0.136183
C	0.54741500	0.14995300	-0.06840600	Sum of electronic and zero-point Energies= -533.012263
C	-0.38999200	-0.83099800	-0.02627600	Sum of electronic and thermal Energies= -533.000621
C	-1.27711700	1.77482000	-0.09700000	Sum of electronic and thermal Enthalpies= -532.999677
C	-2.14924800	0.74742400	-0.04283500	Sum of electronic and thermal Free Energies= -533.051199
C	-2.69785000	-1.64183000	0.09509000	
C	1.97823000	-0.28521000	-0.06716900	
H	0.62382200	2.04529700	-1.04715200	
H	0.70923900	2.20765700	0.71800200	
H	-0.09977000	-1.87379600	0.00794300	
H	-1.67152400	2.78367100	-0.09406300	
H	-3.22185900	0.88784000	-0.00711600	
H	-3.58162500	-1.40812500	-0.49761600	
H	-2.98204100	-1.76055600	1.14315700	
H	-2.25764200	-2.56779100	-0.26973200	
H	3.84289300	0.43445000	0.13227500	
H	2.61980800	1.62543500	0.46166400	
O	1.53574300	2.99053600	1.63122700	
H	1.11537200	3.84084900	1.46461100	
Name				**C7-OH-FHT-P**
Cartesian Coordinates				Frequency and Energy
O	2.11883000	-1.64853200	0.13889500	Zero-point correction= 0.174446 (Hartree/Particle)
N	-1.82715300	-0.50745200	-0.34610600	Thermal correction to Energy= 0.186931
N	2.81983300	0.48752000	0.31852800	Thermal correction to Enthalpy= 0.187875
C	0.18503600	1.56123600	0.04731800	Thermal correction to Gibbs Free Energy= 0.133142
C	0.47055800	0.07564900	0.01358700	Sum of electronic and zero-point Energies= -532.991048
C	-0.50614900	-0.83363200	-0.17087500	Sum of electronic and thermal Energies= -532.978562
C	-1.29820200	1.81057200	-0.03009500	Sum of electronic and thermal Enthalpies= -532.977618
C	-2.19133900	0.83695600	-0.21554700	Sum of electronic and thermal Free Energies= -533.032351
C	-2.84163500	-1.51608700	-0.25074000	
C	1.85091600	-0.45245400	0.15642800	
H	0.69145600	2.07442300	-0.78279300	
H	0.58645700	2.01265500	0.96426400	
H	-0.27008600	-1.89128900	-0.19480700	
H	-1.65691500	2.82933200	0.05213500	
H	-3.25608100	1.02588000	-0.27907500	
H	-3.72494200	-1.22733600	-0.82071900	
H	-3.17684500	-1.65198700	0.82372200	
H	-2.45975400	-2.47426900	-0.60011500	
H	3.77796600	0.17981700	0.39294400	
H	2.63583100	1.47704800	0.28924800	
O	-3.36625200	-1.41134600	2.45038400	
H	-2.55575100	-0.87960100	2.53878600	
Name				**N9-OH-FHT-P**
Cartesian Coordinates				Frequency and Energy
O	2.48812300	-1.17752200	-0.30517100	Zero-point correction= 0.174010 (Hartree/Particle)
N	-1.57534100	-0.56930600	0.04133400	Thermal correction to Energy= 0.185602
N	2.89408500	1.04718300	-0.56230000	Thermal correction to Enthalpy= 0.186546
C	0.15801300	1.76131600	-0.20707300	Thermal correction to Gibbs Free Energy= 0.135012
C	0.63208400	0.31997700	-0.18684400	Sum of electronic and zero-point Energies= -532.981284
C	-0.24048600	-0.71960700	-0.08439300	Sum of electronic and thermal Energies= -532.969692
C	-1.33363200	1.81675100	0.00890600	Sum of electronic and thermal Enthalpies= -532.968747

C	-2.09740100	0.72955700	0.11289600	Sum of electronic and thermal Free Energies= -533.020282
C	-2.46832900	-1.70276000	0.22929500	
C	2.04339700	-0.03247300	-0.32062400	
H	0.41290700	2.24751400	-1.15718100	
H	0.65825100	2.35326800	0.57225000	
H	0.13011100	-1.73816700	-0.09573800	
H	-1.80992400	2.78765700	0.07126700	
H	-3.16933900	0.77799600	0.25909500	
H	-3.30375700	-1.63713100	-0.47016100	
H	-2.85628800	-1.72464500	1.25102300	
H	-1.91960700	-2.62286800	0.03627300	
H	4.02216300	0.75681200	-0.47103100	
H	2.67332400	1.89100800	-0.03541600	
O	4.91697400	0.22814200	0.18808900	
H	4.51449700	-0.65579000	0.26143100	
Name				**C2-OH-RAF-W**
Cartesian Coordinates				Frequency and Energy
O	2.14498700	-1.61920100	-0.05038600	Zero-point correction= 0.178389 (Hartree/Particle)
N	-1.80390700	-0.55768400	-0.22098600	Thermal correction to Energy= 0.190134
N	2.84306700	0.52423200	0.09555200	Thermal correction to Enthalpy= 0.191078
C	0.16187000	1.54090100	0.05986800	Thermal correction to Gibbs Free Energy= 0.140340
C	0.48972500	0.08383500	-0.00713900	Sum of electronic and zero-point Energies= -533.012533
C	-0.52483100	-0.88240800	-0.06739300	Sum of electronic and thermal Energies= -533.000788
C	-1.31840400	1.77659200	0.05094600	Sum of electronic and thermal Enthalpies= -532.999844
C	-2.19984400	0.79014200	-0.08772500	Sum of electronic and thermal Free Energies= -533.050582
C	-2.84100600	-1.58465500	-0.15017100	
C	1.88078000	-0.40955800	0.00923400	
H	0.62602500	2.06810500	-0.78609100	
H	0.60804400	1.98884000	0.95830700	
H	-0.27127100	-1.92981700	-0.15664200	
H	-1.67923300	2.79289600	0.14301100	
H	-3.26992600	0.94698500	-0.11436400	
H	-3.64015900	-1.33758800	-0.84750800	
H	-3.24482200	-1.63580000	0.86334800	
H	-2.40726900	-2.54516800	-0.41937600	
H	3.80834400	0.22578300	0.11434900	
H	2.64095400	1.51040300	0.16302700	
O	-0.16569700	-0.84844200	2.11219300	
H	0.58550700	-1.45476100	2.12175100	
Name				**C3-OH-RAF-W**
Cartesian Coordinates				Frequency and Energy
O	2.25930000	-1.55345600	0.00478400	Zero-point correction= 0.177611 (Hartree/Particle)
N	-1.70360700	-0.55414200	-0.07398300	Thermal correction to Energy= 0.189618
N	2.92304900	0.60154200	-0.12275000	Thermal correction to Enthalpy= 0.190563
C	0.21056100	1.56007300	-0.01282900	Thermal correction to Gibbs Free Energy= 0.138739
C	0.56955100	0.11594700	-0.00553700	Sum of electronic and zero-point Energies= -533.016600
C	-0.40440400	-0.85748500	-0.10455200	Sum of electronic and thermal Energies= -533.004592
C	-1.25452800	1.77497400	0.14190200	Sum of electronic and thermal Enthalpies= -533.003648
C	-2.13080000	0.76547300	0.09919900	Sum of electronic and thermal Free Energies= -533.055472
C	-2.72685400	-1.59881000	-0.15251100	
C	1.98562400	-0.35047200	-0.03503200	
H	0.54488800	2.02131600	-0.95773300	
H	0.75469600	2.09752000	0.77242600	
H	-0.14667800	-1.90550400	-0.18062800	

H	-1.62210100	2.78505900	0.26813000
H	-3.20111600	0.89000900	0.18875900
H	-3.40451300	-1.36731000	-0.97375800
H	-3.28362600	-1.61872100	0.78472800
H	-2.24290300	-2.55629400	-0.32311600
H	3.89546300	0.32502500	-0.12326700
H	2.70252800	1.58618000	-0.13554500
O	0.73187900	-0.10321600	2.55603600
H	0.98072600	-1.00331900	2.32540100

Name			**C5-OH-RAF-W**
Cartesian Coordinates			Frequency and Energy
O	2.27460500	-1.54195600	0.26238100
N	-1.72975500	-0.52531700	-0.05673100
N	2.92656000	0.60059900	-0.00727400
C	0.22348400	1.56166500	-0.08716800
C	0.57180600	0.10996400	0.02875800
C	-0.38206200	-0.83662500	0.02940000
C	-1.23900800	1.79210800	0.01304900
C	-2.14031600	0.75709300	-0.04974900
C	-2.68856900	-1.63212600	-0.10169300
C	1.98912400	-0.35084400	0.10597300
H	0.57791200	1.96119500	-1.05187700
H	0.73708500	2.15780000	0.67608000
H	-0.15411700	-1.89276100	0.08805200
H	-1.61385500	2.80467600	-0.00677200
H	-3.20894100	0.92335700	-0.06221800
H	-3.69286300	-1.22597400	-0.18277700
H	-2.59611900	-2.22176600	0.81043600
H	-2.46775300	-2.25848500	-0.96562300
H	3.89953200	0.32830200	0.02996000
H	2.70554400	1.57483400	-0.15106200
O	-1.27908200	1.92808100	2.54806500
H	-0.78091000	1.10871300	2.46179800

Zero-point correction= 0.178389 (Hartree/Particle)
Thermal correction to Energy= 0.190251
Thermal correction to Enthalpy= 0.191196
Thermal correction to Gibbs Free Energy= 0.139485
Sum of electronic and zero-point Energies= -533.014826
Sum of electronic and thermal Energies= -533.002964
Sum of electronic and thermal Enthalpies= -533.002019
Sum of electronic and thermal Free Energies= -533.053730

Name			**C6-OH-RAF-W**
Cartesian Coordinates			Frequency and Energy
O	2.28328000	-1.53719800	0.03063600
N	-1.74645300	-0.57694600	-0.20617900
N	2.88539900	0.63215300	0.10099900
C	0.18697800	1.56636500	-0.01759000
C	0.54715200	0.10326300	-0.02287800
C	-0.39414000	-0.85045800	-0.11569700
C	-1.28911000	1.75968500	-0.01175900
C	-2.16976900	0.70122000	-0.04558200
C	-2.70029300	-1.67571200	-0.06112500
C	1.95931200	-0.34067200	0.03831200
H	0.61322300	2.07623200	-0.89392500
H	0.61919300	2.07882900	0.85275200
H	-0.13471400	-1.90131800	-0.13659200
H	-1.69275600	2.76196900	0.03038600
H	-3.23880900	0.85776100	-0.09163300
H	-3.66033400	-1.36668100	-0.47005600
H	-2.81918100	-1.93817000	0.99247100
H	-2.33530600	-2.53946100	-0.61377500
H	3.86040000	0.37054900	0.14550000

Zero-point correction= 0.178363 (Hartree/Particle)
Thermal correction to Energy= 0.190132
Thermal correction to Enthalpy= 0.191077
Thermal correction to Gibbs Free Energy= 0.140230
Sum of electronic and zero-point Energies= -533.011586
Sum of electronic and thermal Energies= -532.999817
Sum of electronic and thermal Enthalpies= -532.998872
Sum of electronic and thermal Free Energies= -533.049719

H	2.64886000	1.61263800	0.10998700	
O	-2.06535900	0.98057000	2.18257900	
H	-2.62323000	1.76530400	2.24737200	
Name				**C4-OH-FHT-W**
Cartesian Coordinates				Frequency and Energy
O	2.34391400	-1.37666700	-0.33115900	Zero-point correction= 0.175098 (Hartree/Particle)
N	-1.73099600	-0.56199600	-0.05379100	Thermal correction to Energy= 0.186794
N	2.81418000	0.79635500	0.14195900	Thermal correction to Enthalpy= 0.187739
C	0.15727700	1.57903600	-0.19714000	Thermal correction to Gibbs Free Energy= 0.135269
C	0.53333200	0.15533400	-0.11316000	Sum of electronic and zero-point Energies= -533.023636
C	-0.39274500	-0.83001400	-0.04646200	Sum of electronic and thermal Energies= -533.011940
C	-1.29939300	1.77944200	-0.18108000	Sum of electronic and thermal Enthalpies= -533.010996
C	-2.16421800	0.74575700	-0.10030600	Sum of electronic and thermal Free Energies= -533.063466
C	-2.69741300	-1.63509000	0.15851900	
C	1.97259300	-0.22850600	-0.10603700	
H	0.61789200	2.05646400	-1.07741400	
H	0.70994400	2.13183400	0.65686800	
H	-0.10387900	-1.87235700	0.00340100	
H	-1.70126100	2.78240700	-0.24905800	
H	-3.23821100	0.87866600	-0.09330100	
H	-3.59686900	-1.42531400	-0.41852700	
H	-2.95180100	-1.70884600	1.21789000	
H	-2.26364000	-2.57395800	-0.17879400	
H	3.79221700	0.55507800	0.21954200	
H	2.49171400	1.63598500	0.62830000	
O	1.74087600	2.84159600	1.57257900	
H	1.22717100	3.65569400	1.62607600	
Name				**C7-OH-FHT-W**
Cartesian Coordinates				Frequency and Energy
O	2.08189700	-1.60250500	0.29131100	Zero-point correction= 0.173804 (Hartree/Particle)
N	-1.82448900	-0.39016800	-0.22696900	Thermal correction to Energy= 0.185423
N	2.85253000	0.51739600	0.28436600	Thermal correction to Enthalpy= 0.186367
C	0.22320400	1.61403500	-0.08927700	Thermal correction to Gibbs Free Energy= 0.134854
C	0.48763300	0.14789100	0.01845900	Sum of electronic and zero-point Energies= -533.011956
C	-0.51294000	-0.75695600	-0.05068800	Sum of electronic and thermal Energies= -533.000337
C	-1.22354900	1.91325800	-0.25267800	Sum of electronic and thermal Enthalpies= -532.999393
C	-2.15988300	0.95260200	-0.31076000	Sum of electronic and thermal Free Energies= -533.050906
C	-2.85185800	-1.37524700	-0.14249000	
C	1.86914400	-0.38957500	0.20775600	
H	0.78239500	2.04543400	-0.93352700	
H	0.60615500	2.14227000	0.79666900	
H	-0.33189000	-1.82063700	0.02867900	
H	-1.53299900	2.94744700	-0.33153900	
H	-3.21528900	1.15508500	-0.43038100	
H	-3.73808700	-1.04138800	-0.67892000	
H	-3.13905200	-1.50375700	1.01948100	
H	-2.48738600	-2.33353800	-0.50795400	
H	3.80162500	0.19213300	0.40958500	
H	2.69110400	1.51078900	0.20949700	
O	-3.45413700	-1.64016900	2.47830200	
H	-2.91834700	-2.40729600	2.70644300	
Name				**N9-OH-FHT-W**
Cartesian Coordinates				Frequency and Energy
O	2.34304200	-1.28420700	-0.03202700	Zero-point correction= 0.172224 (Hartree/Particle)

N	-1.67604000	-0.52292400	0.04219200	Thermal correction to Energy= 0.183663
N	2.91068400	0.89251400	-0.27994300	Thermal correction to Enthalpy= 0.184608
C	0.09417200	1.69492400	0.02253800	Thermal correction to Gibbs Free Energy= 0.132404
C	0.56142400	0.28677900	-0.03247700	Sum of electronic and zero-point Energies= -533.032619
C	-0.33376700	-0.73851300	-0.02484400	Sum of electronic and thermal Energies= -533.021179
C	-1.37336200	1.82375700	0.15344500	Sum of electronic and thermal Enthalpies= -533.020235
C	-2.18874400	0.74777300	0.15170900	Sum of electronic and thermal Free Energies= -533.072439
C	-2.59538000	-1.66216500	0.13020700	
C	2.02380100	-0.07185600	-0.12108900	
H	0.41780600	2.23709400	-0.88445200	
H	0.59044100	2.24517400	0.83756600	
H	-0.01914400	-1.77123500	-0.07669600	
H	-1.80633100	2.81130700	0.24482000	
H	-3.26538600	0.81191200	0.23203600	
H	-2.14214500	-2.51927700	-0.35952500	
H	-3.53008000	-1.39774800	-0.36000700	
H	-2.78099500	-1.88489600	1.18201700	
H	4.12715400	0.59339000	-0.27864800	
H	2.53650400	1.82829300	-0.35954100	
O	5.31965900	0.32702700	-0.18523600	
H	5.55651500	-0.31021400	-0.86611500	
Name				**C4-OOH-FHT-G**
Cartesian Coordinates				Frequency and Energy
O	2.17832300	-1.36602600	0.03304700	Zero-point correction= 0.181100 (Hartree/Particle)
N	-1.81796800	-0.34222800	0.11237900	Thermal correction to Energy= 0.193663
N	2.82827600	0.80857300	0.12678700	Thermal correction to Enthalpy= 0.194607
C	0.14303800	1.70419700	-0.36088300	Thermal correction to Gibbs Free Energy= 0.140999
C	0.47888800	0.29407100	-0.05223500	Sum of electronic and zero-point Energies= -608.124680
C	-0.48358200	-0.62986200	0.17312200	Sum of electronic and thermal Energies= -608.112117
C	-1.31112800	1.89740000	-0.55502000	Sum of electronic and thermal Enthalpies= -608.111173
C	-2.20233900	0.92757200	-0.29686000	Sum of electronic and thermal Free Energies= -608.164781
C	-2.81674400	-1.39363400	0.22036300	
C	1.89033800	-0.18307900	0.05349800	
H	0.75288000	2.12949300	-1.16473000	
H	0.50239200	2.35495400	0.56819500	
H	-0.20839400	-1.65219300	0.40410700	
H	-1.67918800	2.85985500	-0.88658200	
H	-3.26957300	1.07076900	-0.41015200	
H	-3.13428900	-1.74109600	-0.76703100	
H	-3.68509200	-1.02101800	0.76493800	
H	-2.39396200	-2.23147200	0.77187200	
H	3.76000800	0.48125900	0.33663400	
H	2.56429600	1.69141100	0.55023100	
H	0.27112500	1.58469100	3.02029000	
O	1.15794500	2.71856700	1.83529100	
O	1.09994400	1.53543700	2.52466800	
Name				**C4-OOH-FHT-P**
Cartesian Coordinates				Frequency and Energy
O	2.21034900	-1.36149000	0.07260500	Zero-point correction= 0.180996 (Hartree/Particle)
N	-1.80341000	-0.35202600	0.06774300	Thermal correction to Energy= 0.193619
N	2.82837100	0.82033800	0.13324900	Thermal correction to Enthalpy= 0.194563
C	0.16123200	1.69818100	-0.37077100	Thermal correction to Gibbs Free Energy= 0.140842
C	0.49264300	0.28452200	-0.05941700	Sum of electronic and zero-point Energies= -608.148734
C	-0.47921500	-0.63987900	0.15651800	Sum of electronic and thermal Energies= -608.136111

C	-1.29249900	1.89007400	-0.58333700	Sum of electronic and thermal Enthalpies= -608.135167
C	-2.18643200	0.91901600	-0.33856000	Sum of electronic and thermal Free Energies= -608.188888
C	-2.82375500	-1.37560700	0.25604200	
C	1.90009100	-0.17726300	0.06808000	
H	0.77141500	2.11822900	-1.17819700	
H	0.50031200	2.34802000	0.54559700	
H	-0.22100600	-1.66244300	0.40419200	
H	-1.65522200	2.85287600	-0.92130700	
H	-3.25302800	1.05818900	-0.46495800	
H	-3.31523900	-1.60291600	-0.69285000	
H	-3.56848400	-1.02921200	0.97431300	
H	-2.35342500	-2.27827500	0.64047800	
H	3.76743400	0.52579500	0.36517900	
H	2.54806800	1.72232400	0.50095000	
H	0.20154900	1.49647700	2.97133000	
O	1.11916100	2.72231300	1.90120000	
O	1.07628300	1.52040200	2.55385000	

Name				**C4-OOH-FHT-W**
Cartesian Coordinates				Frequency and Energy
O	2.22301300	-1.31563000	0.35581200	Zero-point correction= 0.180404 (Hartree/Particle)
N	-1.77431100	-0.31410100	0.09524500	Thermal correction to Energy= 0.193445
N	2.86273300	0.82373800	0.02935100	Thermal correction to Enthalpy= 0.194389
C	0.19108500	1.72485200	-0.35327700	Thermal correction to Gibbs Free Energy= 0.139329
C	0.52100500	0.31353400	-0.02691100	Sum of electronic and zero-point Energies= -608.156805
C	-0.46005700	-0.60454600	0.20934300	Sum of electronic and thermal Energies= -608.143764
C	-1.25788200	1.90904300	-0.61030000	Sum of electronic and thermal Enthalpies= -608.142820
C	-2.15515100	0.94517500	-0.35924800	Sum of electronic and thermal Free Energies= -608.197880
C	-2.80604200	-1.32609500	0.30847600	
C	1.91753700	-0.13103700	0.14251900	
H	0.81022000	2.14656000	-1.15216900	
H	0.48428400	2.36132600	0.57143600	
H	-0.21876100	-1.62033600	0.49664000	
H	-1.61060400	2.86200600	-0.98374300	
H	-3.21908300	1.07295400	-0.51269200	
H	-3.30473400	-1.55684900	-0.63441800	
H	-3.54098900	-0.95529000	1.02320100	
H	-2.34151800	-2.22629900	0.70345600	
H	3.82082900	0.56931300	0.22593500	
H	2.62539300	1.80495200	0.02274900	
H	0.04250000	1.05700200	2.75567200	
O	0.86157800	2.62136400	2.12338900	
O	0.95414900	1.33600800	2.57146200	

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