Supporting Information (SI)

The radical scavenging activity of 4-mercaptoimidazole: 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.

Table S2: The Cartesian coordinates and energies of TS of the reaction between 4MC with HO•/HOO• following the RAF and FHT mechanisms (G: the gas phase; P: pentyl ethanoate; W: water)

Name				**4MC-C2-OH-RAF-G**
Cartesian Coordinates				Frequency and Energy
C	-1.38976200	-0.02056500	-0.75043600	Zero-point correction= 0.082189 (Hartree/Particle)
C	0.63831200	0.15786000	-0.09666500	Thermal correction to Energy= 0.089695
C	-0.01611800	1.28898800	0.36757000	Thermal correction to Enthalpy= 0.090639
N	-1.28891900	1.17527200	-0.09636600	Thermal correction to Gibbs Free Energy= 0.049212
H	-2.06985900	1.75620500	0.16568800	Sum of electronic and zero-point Energies= -700.022053
H	-2.23911000	-0.27558400	-1.36110600	Sum of electronic and thermal Energies= -700.014547
H	0.31991600	2.11561100	0.96951600	Sum of electronic and thermal Enthalpies= -700.013603
N	-0.20107900	-0.62431800	-0.80629100	Sum of electronic and thermal Free Energies= -700.055030
S	2.32571800	-0.25589400	0.18762800	
H	2.31516100	-1.26235100	-0.69919400	
O	-2.34697900	-1.10112100	0.79447200	
H	-1.72637800	-1.84498300	0.76305900	
Name				**4MC-C2-OH-RAF-P**
Cartesian Coordinates				Frequency and Energy
C	-1.40667900	-0.00218900	-0.75206200	Zero-point correction= 0.081810 (Hartree/Particle)
C	0.62348800	0.15483200	-0.09336000	Thermal correction to Energy= 0.089367
C	-0.02472200	1.29261300	0.37063600	Thermal correction to Enthalpy= 0.090311
N	-1.29470000	1.18142000	-0.08704000	Thermal correction to Gibbs Free Energy= 0.048737
H	-2.05613100	1.81577600	0.11531100	Sum of electronic and zero-point Energies= -700.040498
H	-2.26313500	-0.24976800	-1.35560600	Sum of electronic and thermal Energies= -700.032941
H	0.31645100	2.12260500	0.96696000	Sum of electronic and thermal Enthalpies= -700.031997
N	-0.22011800	-0.61965500	-0.80352800	Sum of electronic and thermal Free Energies= -700.073570
S	2.30806000	-0.27315400	0.20215000	
H	2.30476000	-1.28570400	-0.68133700	
O	-2.30727400	-1.15540500	0.81952200	
H	-1.65909800	-1.87225200	0.73622900	
Name				**4MC-C2-OH-RAF-W**
Cartesian Coordinates				Frequency and Energy
C	-1.43234100	-0.02832000	-0.73689000	Zero-point correction= 0.081520 (Hartree/Particle)
C	0.58837400	0.02172800	-0.04062600	Thermal correction to Energy= 0.089196
C	0.01203100	1.22171400	0.34408100	Thermal correction to Enthalpy= 0.090140
N	-1.25547300	1.17613000	-0.12585200	Thermal correction to Gibbs Free Energy= 0.048125
H	-1.96683000	1.88698600	-0.00445000	Sum of electronic and zero-point Energies= -700.047031
H	-2.30148100	-0.24948600	-1.33356900	Sum of electronic and thermal Energies= -700.039355
H	0.40807100	2.06085200	0.89195800	Sum of electronic and thermal Enthalpies= -700.038411
N	-0.29984800	-0.73695100	-0.72556400	Sum of electronic and thermal Free Energies= -700.080427
S	2.22498300	-0.50157500	0.36448000	
H	2.63450300	-0.69936300	-0.90207600	
O	-2.41107100	-1.12211600	0.92919100	
H	-1.88001400	-1.92047900	0.77719200	
Name				**4MC-C4-OH-RAF-G**
Cartesian Coordinates				Frequency and Energy
C	-1.80474400	-0.25865000	0.75934300	Zero-point correction= 0.082552 (Hartree/Particle)
C	0.20689300	-0.11390600	0.01963100	Thermal correction to Energy= 0.089739
C	-0.62950400	-0.25662300	-1.10077100	Thermal correction to Enthalpy= 0.090683
N	-1.89214800	-0.29975100	-0.61520900	Thermal correction to Gibbs Free Energy= 0.050454
H	-2.74067200	-0.32947500	-1.15845700	Sum of electronic and zero-point Energies= -700.016314
H	-2.68399300	-0.29247900	1.38513800	Sum of electronic and thermal Energies= -700.009126
H	-0.38796600	-0.25468200	-2.14954000	Sum of electronic and thermal Enthalpies= -700.008182

N	-0.57906800	-0.19511200	1.17326400	Sum of electronic and thermal Free Energies= -700.048411
S	1.92019900	-0.58505400	0.01496300	
H	2.38852300	0.66486800	0.15449800	
O	0.41822700	1.84520100	-0.14487700	
H	0.01775900	2.05013500	0.71236800	
Name				**4MC-C4-OH-RAF-P**
Cartesian Coordinates				Frequency and Energy
C	-1.78910700	-0.27309500	0.76851100	Zero-point correction= 0.082184 (Hartree/Particle)
C	0.21529100	-0.11787200	0.00659900	Thermal correction to Energy= 0.089547
C	-0.63944300	-0.23355700	-1.10567500	Thermal correction to Enthalpy= 0.090492
N	-1.88869200	-0.28549900	-0.60066100	Thermal correction to Gibbs Free Energy= 0.049658
H	-2.74819300	-0.32132000	-1.13396100	Sum of electronic and zero-point Energies= -700.038941
H	-2.66247700	-0.31590400	1.40138400	Sum of electronic and thermal Energies= -700.031578
H	-0.42001500	-0.22431000	-2.16036000	Sum of electronic and thermal Enthalpies= -700.030634
N	-0.55318300	-0.21529500	1.16718800	Sum of electronic and thermal Free Energies= -700.071467
S	1.92508000	-0.59918900	-0.02733900	
H	2.40793900	0.61350700	0.28863200	
O	0.47944000	1.85698600	-0.14958200	
H	-0.09313200	2.09001900	0.59561500	
Name				**4MC-C4-OH-RAF-W**
Cartesian Coordinates				Frequency and Energy
C	-1.73007800	-0.31829300	0.80775900	Zero-point correction= 0.082678 (Hartree/Particle)
C	0.24800800	-0.17323200	0.00582600	Thermal correction to Energy= 0.089783
C	-0.63471700	-0.17098700	-1.08811300	Thermal correction to Enthalpy= 0.090727
N	-1.86969800	-0.23109600	-0.55324400	Thermal correction to Gibbs Free Energy= 0.050673
H	-2.74704900	-0.19988600	-1.05971100	Sum of electronic and zero-point Energies= -700.047304
H	-2.58709200	-0.37844800	1.46075600	Sum of electronic and thermal Energies= -700.040200
H	-0.44367000	-0.09756600	-2.14610700	Sum of electronic and thermal Enthalpies= -700.039256
N	-0.47998000	-0.32980700	1.17791900	Sum of electronic and thermal Free Energies= -700.079309
S	1.95539800	-0.61257300	-0.12167800	
H	2.41713300	0.44470500	0.56953000	
O	0.50221600	1.88001500	-0.11441500	
H	-0.39696600	2.16164000	0.11182900	
Name				**4MC-C5-OH-RAF-G**
Cartesian Coordinates				Frequency and Energy
C	-1.53203200	-1.16511000	0.33853100	Zero-point correction= 0.082210 (Hartree/Particle)
C	0.35348300	-0.30846300	-0.13776600	Thermal correction to Energy= 0.089796
C	-0.58862800	0.45061100	-0.82061100	Thermal correction to Enthalpy= 0.090740
N	-1.78502400	-0.16541300	-0.53768000	Thermal correction to Gibbs Free Energy= 0.049065
H	-2.69371000	0.19292200	-0.78450100	Sum of electronic and zero-point Energies= -700.026866
H	-2.31136100	-1.77803200	0.76385100	Sum of electronic and thermal Energies= -700.019280
H	-0.48640400	1.21686800	-1.56715900	Sum of electronic and thermal Enthalpies= -700.018336
N	-0.24834300	-1.28947800	0.59078000	Sum of electronic and thermal Free Energies= -700.060012
S	2.08998000	-0.05911600	-0.13664000	
H	2.31194200	-1.03555400	0.75658400	
O	-0.69153800	2.09776200	0.65097400	
H	0.10879100	1.88956100	1.15704400	
Name				**4MC-C5-OH-RAF-P**
Cartesian Coordinates				Frequency and Energy
C	-1.55368100	-1.16728400	0.33317600	Zero-point correction= 0.081761 (Hartree/Particle)
C	0.33188300	-0.29936400	-0.14518200	Thermal correction to Energy= 0.089427
C	-0.61549900	0.44014700	-0.84057700	Thermal correction to Enthalpy= 0.090372
N	-1.80533200	-0.17116200	-0.54014400	Thermal correction to Gibbs Free Energy= 0.048411
H	-2.71804300	0.12981000	-0.85394900	Sum of electronic and zero-point Energies= -700.046853

H	-2.33240500	-1.78318100	0.75480000	Sum of electronic and thermal Energies=	-700.039187
H	-0.52304400	1.21142400	-1.58461200	Sum of electronic and thermal Enthalpies=	-700.038243
N	-0.26500000	-1.27814900	0.59025400	Sum of electronic and thermal Free Energies=	-700.080203
S	2.07158600	-0.04781300	-0.16073900		
H	2.30294900	-0.93178700	0.82504300		
O	-0.60332000	2.09579400	0.73899000		
H	0.23706300	1.84812300	1.15634700		
Name				**4MC-C5-OH-RAF-W**	
Cartesian Coordinates				Frequency and Energy	
C	-1.64846300	-1.00132300	0.43279300	Zero-point correction=	0.081410 (Hartree/Particle)
C	0.30794700	-0.33873900	-0.09656500	Thermal correction to Energy=	0.089358
C	-0.56548300	0.34240600	-0.92379700	Thermal correction to Enthalpy=	0.090302
N	-1.80520100	-0.12671200	-0.58398200	Thermal correction to Gibbs Free Energy=	0.047171
H	-2.68570500	0.16385900	-0.99009000	Sum of electronic and zero-point Energies=	-700.052124
H	-2.48375900	-1.49329100	0.90557300	Sum of electronic and thermal Energies=	-700.044176
H	-0.39733500	1.02353200	-1.74035600	Sum of electronic and thermal Enthalpies=	-700.043232
N	-0.37911600	-1.16959300	0.74870600	Sum of electronic and thermal Free Energies=	-700.086362
S	2.06509800	-0.26573900	-0.17844700		
H	2.26382200	-0.09594400	1.14172800		
O	-0.35419300	2.25281900	0.57071200		
H	-0.17882200	1.69118700	1.34494700		
Name				**4MC-NH-OH-FHT-G**	
Cartesian Coordinates				Frequency and Energy	
C	1.68515200	0.31970700	-0.52065700	Zero-point correction=	0.078013 (Hartree/Particle)
C	-0.21238300	-0.39765900	0.08277100	Thermal correction to Energy=	0.085903
C	0.71366600	-0.99310300	0.93514700	Thermal correction to Enthalpy=	0.086848
N	1.91105500	-0.49437000	0.56468900	Thermal correction to Gibbs Free Energy=	0.044170
H	2.90308500	-0.88229500	0.71990400	Sum of electronic and zero-point Energies=	-700.017767
H	2.50091000	0.80466200	-1.03425400	Sum of electronic and thermal Energies=	-700.009876
H	0.58215000	-1.66236800	1.76813000	Sum of electronic and thermal Enthalpies=	-700.008932
N	0.41597100	0.41975200	-0.82020900	Sum of electronic and thermal Free Energies=	-700.051610
S	-1.94194700	-0.56939100	0.13517300		
H	-2.15150200	0.35688400	-0.81343500		
O	4.14008500	-1.33306200	0.09029700		
H	4.13306200	-2.22497400	-0.28314400		
Name				**4MC-NH-OH-FHT-P**	
Cartesian Coordinates				Frequency and Energy	
C	-0.94266800	1.08435500	-0.18509800	Zero-point correction=	0.077345 (Hartree/Particle)
C	0.86424500	-0.00531900	-0.02061700	Thermal correction to Energy=	0.085087
C	-0.12699300	-0.94251600	-0.29949500	Thermal correction to Enthalpy=	0.086032
N	-1.26253300	-0.22842000	-0.44207500	Thermal correction to Gibbs Free Energy=	0.043945
H	-2.29090200	-0.53442200	-0.35535100	Sum of electronic and zero-point Energies=	-700.044465
H	-1.69863400	1.85436900	-0.18941100	Sum of electronic and thermal Energies=	-700.036723
H	-0.07384900	-2.00760000	-0.44729700	Sum of electronic and thermal Enthalpies=	-700.035778
N	0.33299900	1.25627600	0.04659200	Sum of electronic and thermal Free Energies=	-700.077865
S	2.56612400	-0.30886000	0.16673800		
H	2.87997000	0.99379000	0.24647500		
O	-3.56152700	-0.33147000	0.33318900		
H	-3.64312000	-0.72673500	1.21189400		
Name				**4MC-NH-OH-FHT-W**	
Cartesian Coordinates				Frequency and Energy	
C	-0.94266800	1.08435500	-0.18509800	Zero-point correction=	0.078653 (Hartree/Particle)
C	0.86424500	-0.00531900	-0.02061700	Thermal correction to Energy=	0.086502
C	-0.12699300	-0.94251600	-0.29949500	Thermal correction to Enthalpy=	0.087447

N	-1.26253300	-0.22842000	-0.44207500	Thermal correction to Gibbs Free Energy= 0.044589
H	-2.29090200	-0.53442200	-0.35535100	Sum of electronic and zero-point Energies= -700.050752
H	-1.69863400	1.85436900	-0.18941100	Sum of electronic and thermal Energies= -700.042902
H	-0.07384900	-2.00760000	-0.44729700	Sum of electronic and thermal Enthalpies= -700.041958
N	0.33299900	1.25627600	0.04659200	Sum of electronic and thermal Free Energies= -700.084815
S	2.56612400	-0.30886000	0.16673800	
H	2.87997000	0.99379000	0.24647500	
O	-3.56152700	-0.33147000	0.33318900	
H	-3.64312000	-0.72673500	1.21189400	
Name				**4MC-SH-OH-FHT-G**
Cartesian Coordinates				Frequency and Energy
C	1.88102400	0.27662400	-0.77239500	Zero-point correction= 0.080066 (Hartree/Particle)
C	-0.03572900	-0.41460400	-0.15334000	Thermal correction to Energy= 0.088154
C	0.84330800	-0.85894300	0.80231700	Thermal correction to Enthalpy= 0.089099
N	2.07181500	-0.41397200	0.38822800	Thermal correction to Gibbs Free Energy= 0.043861
H	2.95146300	-0.56749000	0.85474700	Sum of electronic and zero-point Energies= -700.021403
H	2.69399100	0.74306100	-1.30704100	Sum of electronic and thermal Energies= -700.013314
H	0.69558800	-1.43085500	1.70208700	Sum of electronic and thermal Enthalpies= -700.012370
N	0.62557400	0.28870900	-1.12942000	Sum of electronic and thermal Free Energies= -700.057608
S	-1.75797400	-0.75266200	-0.20454200	
H	-2.15998800	0.56743500	-0.30103200	
O	-2.52985100	1.67619300	0.80213000	
H	-2.01707500	1.44330400	1.59263500	
Name				**4MC-SH-OH-FHT-P**
Cartesian Coordinates				Frequency and Energy
C	1.89379100	0.26638300	-0.77932300	Zero-point correction= 0.080142 (Hartree/Particle)
C	-0.03443800	-0.42091100	-0.17779600	Thermal correction to Energy= 0.088136
C	0.83491300	-0.84656300	0.79619200	Thermal correction to Enthalpy= 0.089080
N	2.06134400	-0.40288300	0.39046100	Thermal correction to Gibbs Free Energy= 0.045014
H	2.93727300	-0.54622200	0.87485700	Sum of electronic and zero-point Energies= -700.042618
H	2.71592500	0.72515900	-1.30571200	Sum of electronic and thermal Energies= -700.034625
H	0.68175500	-1.40470500	1.70468100	Sum of electronic and thermal Enthalpies= -700.033681
N	0.63894800	0.26878500	-1.15641900	Sum of electronic and thermal Free Energies= -700.077746
S	-1.75659700	-0.76043100	-0.24965600	
H	-2.17244400	0.55399100	-0.28482500	
O	-2.53724000	1.68295900	0.84319500	
H	-2.00108400	1.44123900	1.61871800	
Name				**4MC-SH-OH-FHT-W**
Cartesian Coordinates				Frequency and Energy
C	1.86875600	0.25458700	-0.75534700	Zero-point correction= 0.080237 (Hartree/Particle)
C	-0.06862500	-0.43626100	-0.19244900	Thermal correction to Energy= 0.088128
C	0.77529400	-0.82010400	0.81806300	Thermal correction to Enthalpy= 0.089072
N	2.00839500	-0.37454700	0.43731000	Thermal correction to Gibbs Free Energy= 0.045575
H	2.87284400	-0.49012600	0.95104900	Sum of electronic and zero-point Energies= -700.046648
H	2.70269300	0.70579100	-1.26901900	Sum of electronic and thermal Energies= -700.038757
H	0.60053300	-1.35090400	1.73886700	Sum of electronic and thermal Enthalpies= -700.037813
N	0.62467600	0.23316200	-1.17615900	Sum of electronic and thermal Free Energies= -700.081311
S	-1.78301700	-0.79447200	-0.28794100	
H	-2.21287700	0.51463900	-0.32704300	
O	-2.41888000	1.66308500	0.85285100	
H	-1.70764600	1.45195100	1.48419100	
Name				**4MC-ANION-C2-OH-RAF-W**
Cartesian Coordinates				Frequency and Energy
C	-1.36062000	-0.15600300	-0.63748400	Zero-point correction= 0.073251 (Hartree/Particle)

C	0.71348900	0.04926800	-0.06274000	Thermal correction to Energy=	0.079914
C	0.04141900	1.23195900	0.34184200	Thermal correction to Enthalpy=	0.080858
N	-1.22280500	1.11666100	-0.09347800	Thermal correction to Gibbs Free Energy=	0.041365
H	-1.99045400	1.73948500	0.12147900	Sum of electronic and zero-point Energies=	-699.620896
H	-2.20116400	-0.38235200	-1.27169900	Sum of electronic and thermal Energies=	-699.614234
H	0.40974700	2.09201400	0.87729700	Sum of electronic and thermal Enthalpies=	-699.613290
N	-0.17982200	-0.75711300	-0.73451200	Sum of electronic and thermal Free Energies=	-699.652783
S	2.34922500	-0.28022900	0.22248000		
O	-2.41251200	-0.96594600	0.93945700		
H	-2.46009900	-1.87926300	0.63731000		
Name				**4MC-ANION-C4-OH-RAF-W**	
Cartesian Coordinates				Frequency and Energy	
C	-1.71548700	-0.27728400	0.79272700	Zero-point correction=	0.073241 (Hartree/Particle)
C	0.29202600	-0.08730700	-0.02530800	Thermal correction to Energy=	0.079690
C	-0.63418400	-0.17949000	-1.11630500	Thermal correction to Enthalpy=	0.080634
N	-1.87224400	-0.24109900	-0.57064300	Thermal correction to Gibbs Free Energy=	0.041974
H	-2.75371100	-0.28277800	-1.06549100	Sum of electronic and zero-point Energies=	-699.603602
H	-2.57132900	-0.35788900	1.44696400	Sum of electronic and thermal Energies=	-699.597153
H	-0.45449100	-0.14910800	-2.17756000	Sum of electronic and thermal Enthalpies=	-699.596209
N	-0.47424600	-0.23007500	1.16693400	Sum of electronic and thermal Free Energies=	-699.634869
S	1.91580100	-0.68663700	-0.14278700		
O	0.47902200	1.85736900	-0.05143300		
H	-0.39478500	2.16406400	0.22372500		
Name				**4MC-ANION-C5-OH-RAF-W**	
Cartesian Coordinates				Frequency and Energy	
C	-1.67775100	-1.13245300	0.36052500	Zero-point correction=	0.073474 (Hartree/Particle)
C	0.31296200	-0.39629300	-0.00958600	Thermal correction to Energy=	0.080153
C	-0.59719000	0.46320000	-0.70249900	Thermal correction to Enthalpy=	0.081097
N	-1.82604100	-0.10411700	-0.52484000	Thermal correction to Gibbs Free Energy=	0.041508
H	-2.70422600	0.25489200	-0.87346000	Sum of electronic and zero-point Energies=	-699.626643
H	-2.52542100	-1.69906200	0.71541900	Sum of electronic and thermal Energies=	-699.619964
H	-0.38711100	1.10698400	-1.53832900	Sum of electronic and thermal Enthalpies=	-699.619020
N	-0.42810700	-1.34544800	0.68631900	Sum of electronic and thermal Free Energies=	-699.658609
S	1.99769600	-0.23731700	0.02525000		
O	-0.60926700	2.12545000	0.55309200		
H	0.31942400	2.04257000	0.79760200		
Name				**4MC-NH-OOH-FHT-G**	
Cartesian Coordinates				Frequency and Energy	
C	0.47946300	0.99977700	0.06239100	Zero-point correction=	0.082668 (Hartree/Particle)
C	-1.37870100	0.00778200	0.01189800	Thermal correction to Energy=	0.091414
C	-0.38233700	-0.97973400	-0.12211500	Thermal correction to Enthalpy=	0.092358
N	0.78395400	-0.32846500	-0.12084800	Thermal correction to Gibbs Free Energy=	0.046809
H	1.89751100	-0.68552300	0.06967200	Sum of electronic and zero-point Energies=	-775.155985
H	1.25644500	1.74420200	0.14933800	Sum of electronic and thermal Energies=	-775.147239
H	-0.46986600	-2.04497900	-0.26014100	Sum of electronic and thermal Enthalpies=	-775.146295
N	-0.81148600	1.24097100	0.12107600	Sum of electronic and thermal Free Energies=	-775.191843
S	-3.09089500	-0.24449400	-0.00864000		
H	-3.37835200	1.06747300	0.00354500		
O	3.60166000	0.29014100	-0.38450100		
O	3.11636700	-0.71795500	0.42208100		
H	4.28653200	0.69875200	0.16055700		
Name				**4MC-SH-OOH-FHT-G**	
Cartesian Coordinates				Frequency and Energy	
C	1.98719300	0.23503900	-0.77296700	Zero-point correction=	0.084412 (Hartree/Particle)

C	0.23432400	-0.72534800	-0.02678900	Thermal correction to Energy= 0.092798
C	1.09433000	-0.61982800	1.04674000	Thermal correction to Enthalpy= 0.093742
N	2.21185900	-0.00638900	0.55584100	Thermal correction to Gibbs Free Energy= 0.049115
H	3.05019400	0.21415400	1.06955700	Sum of electronic and zero-point Energies= -775.168418
H	2.71978700	0.72107500	-1.39903900	Sum of electronic and thermal Energies= -775.160032
H	0.99468100	-0.93989200	2.07005500	Sum of electronic and thermal Enthalpies= -775.159088
N	0.81580900	-0.18651900	-1.15302500	Sum of electronic and thermal Free Energies= -775.203715
S	-1.36181000	-1.41809800	-0.00114400	
H	-2.00786800	-0.09144000	-0.00383400	
O	-1.10809200	1.75778000	0.66851600	
O	-2.27468700	1.19818300	0.31479200	
H	-1.09957900	1.72157800	1.63803200	
Name				**4MC-SH-OOH-FHT-P**
Cartesian Coordinates				Frequency and Energy
C	2.02410300	0.21858400	-0.77626200	Zero-point correction= 0.084444 (Hartree/Particle)
C	0.23564900	-0.71298500	-0.06457600	Thermal correction to Energy= 0.092749
C	1.06879300	-0.59121000	1.03121800	Thermal correction to Enthalpy= 0.093693
N	2.19745000	0.00351800	0.55883900	Thermal correction to Gibbs Free Energy= 0.049355
H	3.02214500	0.23358600	1.09757500	Sum of electronic and zero-point Energies= -775.195193
H	2.78358000	0.68257600	-1.38617800	Sum of electronic and thermal Energies= -775.186889
H	0.94386500	-0.88709600	2.05995500	Sum of electronic and thermal Enthalpies= -775.185944
N	0.85592100	-0.20114300	-1.18382300	Sum of electronic and thermal Free Energies= -775.230282
S	-1.35862200	-1.41208000	-0.08212600	
H	-2.03784900	-0.11390700	0.07226300	
O	-1.16073800	1.77976600	0.64207600	
O	-2.33411900	1.16633400	0.44172500	
H	-0.98403700	1.69435100	1.59605000	
Name				**4MC-SH-OOH-FHT-W**
Cartesian Coordinates				Frequency and Energy
C	2.05039400	0.16439400	-0.75391900	Zero-point correction= 0.084888 (Hartree/Particle)
C	0.22852900	-0.73522800	-0.08955700	Thermal correction to Energy= 0.093042
C	0.99604600	-0.53134400	1.04056800	Thermal correction to Enthalpy= 0.093986
N	2.14566700	0.04163500	0.59776600	Thermal correction to Gibbs Free Energy= 0.050058
H	2.93445000	0.32461800	1.16611500	Sum of electronic and zero-point Energies= -775.200493
H	2.84403700	0.59175100	-1.34632300	Sum of electronic and thermal Energies= -775.192338
H	0.80841600	-0.74796300	2.07924800	Sum of electronic and thermal Enthalpies= -775.191394
N	0.90991500	-0.29420000	-1.20774400	Sum of electronic and thermal Free Energies= -775.235322
S	-1.36910000	-1.41853000	-0.13938800	
H	-2.02921100	-0.12130600	0.06386400	
O	-1.07344800	1.74733100	0.63091200	
O	-2.26793400	1.20247800	0.37727000	
H	-0.92162000	1.63665800	1.58792300	
Name				**4MC-N3H-C2-OH-RAF-P**
Cartesian Coordinates				Frequency and Energy
C	1.42493800	0.01438300	0.83281900	Zero-point correction= 0.086019 (Hartree/Particle)
C	-0.67692400	0.17188400	0.07743600	Thermal correction to Energy= 0.092286
C	0.09264700	1.21944500	-0.43622500	Thermal correction to Enthalpy= 0.093231
N	1.34599500	1.09654400	0.06017800	Thermal correction to Gibbs Free Energy= 0.054657
H	2.14068900	1.67887400	-0.17453000	Sum of electronic and zero-point Energies= -700.037291
H	2.31845000	-0.38454900	1.27532900	Sum of electronic and thermal Energies= -700.031024
H	-0.19251400	2.01532800	-1.10245600	Sum of electronic and thermal Enthalpies= -700.030080
N	0.22474600	-0.53719200	0.86599800	Sum of electronic and thermal Free Energies= -700.068654
S	-2.30574800	-0.22329000	-0.12726600	
H	-0.01601700	-1.37667700	1.37744500	

O	1.77644900	-1.10726500	-0.96842200	
H	2.39061100	-1.85194700	-0.91956400	
Name				**4MC-N3H-C2-OH-RAF-W**
Cartesian Coordinates				Frequency and Energy
C	1.42493800	0.01438300	0.83281900	Zero-point correction= 0.085936 (Hartree/Particle)
C	-0.67692400	0.17188400	0.07743600	Thermal correction to Energy= 0.092264
C	0.09264700	1.21944500	-0.43622500	Thermal correction to Enthalpy= 0.093208
N	1.34599500	1.09654400	0.06017800	Thermal correction to Gibbs Free Energy= 0.054455
H	2.14068900	1.67887400	-0.17453000	Sum of electronic and zero-point Energies= -700.052255
H	2.31845000	-0.38454900	1.27532900	Sum of electronic and thermal Energies= -700.045927
H	-0.19251400	2.01532800	-1.10245600	Sum of electronic and thermal Enthalpies= -700.044983
N	0.22474600	-0.53719200	0.86599800	Sum of electronic and thermal Free Energies= -700.083735
S	-2.30574800	-0.22329000	-0.12726600	
H	-0.01601700	-1.37667700	1.37744500	
O	1.77644900	-1.10726500	-0.96842200	
H	2.39061100	-1.85194700	-0.91956400	
Name				**4MC-N3H-C4-OH-RAF-P**
Cartesian Coordinates				Frequency and Energy
C	-1.91984000	-0.38589100	0.75483900	Zero-point correction= 0.086407 (Hartree/Particle)
C	0.23251300	-0.07689400	0.14916100	Thermal correction to Energy= 0.093035
C	-0.60114700	-0.12970400	-1.00190900	Thermal correction to Enthalpy= 0.093979
N	-1.88923400	-0.27057900	-0.57576800	Thermal correction to Gibbs Free Energy= 0.055047
H	-2.71139000	-0.27502900	-1.16758000	Sum of electronic and zero-point Energies= -700.037008
H	-2.81073000	-0.51671600	1.34646400	Sum of electronic and thermal Energies= -700.030380
H	-0.33238700	-0.02503300	-2.03832900	Sum of electronic and thermal Enthalpies= -700.029436
N	-0.67852400	-0.34487500	1.19990500	Sum of electronic and thermal Free Energies= -700.068368
S	1.91229000	-0.40744900	0.28273800	
O	-0.04013100	1.86139700	0.14019200	
H	0.82387000	2.05453800	-0.24588100	
H	-0.40117000	-0.37674600	2.17327600	
Name				**4MC-N3H-C4-OH-RAF-W**
Cartesian Coordinates				Frequency and Energy
C	-1.92079800	-0.39400900	0.75177400	Zero-point correction= 0.086223 (Hartree/Particle)
C	0.22701500	-0.06971800	0.16212300	Thermal correction to Energy= 0.092926
C	-0.60238200	-0.12279600	-0.99612100	Thermal correction to Enthalpy= 0.093871
N	-1.88876700	-0.27549000	-0.57941200	Thermal correction to Gibbs Free Energy= 0.054707
H	-2.71154100	-0.30053900	-1.17331700	Sum of electronic and zero-point Energies= -700.050175
H	-2.81302100	-0.54035600	1.33965400	Sum of electronic and thermal Energies= -700.043472
H	-0.32851100	-0.01574700	-2.03150200	Sum of electronic and thermal Enthalpies= -700.042528
N	-0.68560900	-0.33833100	1.20984500	Sum of electronic and thermal Free Energies= -700.081691
S	1.89375200	-0.43522000	0.27462900	
O	0.03205500	1.91038800	0.20962300	
H	0.80767900	2.08006500	-0.33848600	
H	-0.42575300	-0.39123000	2.18829800	
Name				**4MC-N3H-C5-OH-RAF-P**
Cartesian Coordinates				Frequency and Energy
C	1.60499700	-1.00821800	-0.29498900	Zero-point correction= 0.086705 (Hartree/Particle)
C	-0.45687700	-0.23760100	0.17529000	Thermal correction to Energy= 0.093422
C	0.49506200	0.46530200	0.91946000	Thermal correction to Enthalpy= 0.094366
N	1.73452500	-0.04661600	0.60282000	Thermal correction to Gibbs Free Energy= 0.054934
H	2.60817500	0.18850500	1.05696700	Sum of electronic and zero-point Energies= -700.048693
H	2.40623800	-1.58755500	-0.72204900	Sum of electronic and thermal Energies= -700.041976
H	0.37376500	1.33207800	1.54198500	Sum of electronic and thermal Enthalpies= -700.041032
N	0.30968200	-1.14412300	-0.56198500	Sum of electronic and thermal Free Energies= -700.080464

S	-2.13971300	-0.13356000	0.09889300	
H	-0.08284100	-1.78563100	-1.24062300	
O	0.63425800	1.86781800	-0.80615700	
H	-0.31252600	2.06529100	-0.85373300	
Name				**4MC-N3H-C5-OH-RAF-W**
Cartesian Coordinates				Frequency and Energy
C	-1.87661100	-0.68121900	-0.11147100	Zero-point correction= 0.086068 (Hartree/Particle)
C	0.29280000	-0.15347300	-0.07646900	Thermal correction to Energy= 0.093232
C	-0.47589400	1.02080100	-0.02066000	Thermal correction to Enthalpy= 0.094177
N	-1.78329300	0.65156000	-0.10125400	Thermal correction to Gibbs Free Energy= 0.053025
H	-2.58027300	1.28018800	-0.08226200	Sum of electronic and zero-point Energies= -700.065988
H	-2.79576700	-1.24436500	-0.13739700	Sum of electronic and thermal Energies= -700.058824
H	-0.15400200	2.04504900	-0.07434800	Sum of electronic and thermal Enthalpies= -700.057880
N	-0.65710100	-1.18355600	-0.09769300	Sum of electronic and thermal Free Energies= -700.099031
S	1.94824100	-0.35511100	-0.09599500	
H	-0.43986900	-2.17559000	-0.11799700	
O	-0.29756800	1.30485800	2.43919300	
H	0.64695600	1.23780600	2.26998300	
Name				**4MC-N3H-N1-H-OH-FHT-P**
Cartesian Coordinates				Frequency and Energy
C	0.83117900	1.28096700	-0.03395700	Zero-point correction= 0.081836 (Hartree/Particle)
C	-0.96271000	-0.03892500	-0.01433400	Thermal correction to Energy= 0.088356
C	0.19994700	-0.80374600	-0.12975400	Thermal correction to Enthalpy= 0.089300
N	1.26422700	0.02524300	-0.13398000	Thermal correction to Gibbs Free Energy= 0.049576
H	2.33901700	-0.26299000	-0.17579100	Sum of electronic and zero-point Energies= -700.082439
H	1.45333300	2.16105700	-0.00668500	Sum of electronic and thermal Energies= -700.075920
H	0.30227100	-1.87476300	-0.19756500	Sum of electronic and thermal Enthalpies= -700.074976
N	-0.49326200	1.27388400	0.03937300	Sum of electronic and thermal Free Energies= -700.114700
S	-2.57905600	-0.49193500	0.04981600	
H	-1.08544500	2.09218400	0.13238100	
O	3.61296700	-0.55992100	0.10441600	
H	3.54473500	-1.48883700	0.34580100	
Name				**4MC-N3H-N1-H-OH-FHT-W**
Cartesian Coordinates				Frequency and Energy
C	-0.73856900	1.42692200	0.01090500	Zero-point correction= 0.082565 (Hartree/Particle)
C	0.93700400	-0.03197400	0.00023100	Thermal correction to Energy= 0.089894
C	-0.28639200	-0.70663200	-0.00074000	Thermal correction to Enthalpy= 0.090838
N	-1.28295300	0.20690800	0.01130400	Thermal correction to Gibbs Free Energy= 0.048700
H	-2.35776500	-0.08997500	-0.04790700	Sum of electronic and zero-point Energies= -700.095892
H	-1.28629300	2.35589500	0.01565700	Sum of electronic and thermal Energies= -700.088563
H	-0.47524000	-1.76825500	-0.00476200	Sum of electronic and thermal Enthalpies= -700.087619
N	0.58057500	1.31819700	0.00776700	Sum of electronic and thermal Free Energies= -700.129757
S	2.50815000	-0.62360900	-0.00632400	
H	1.23082600	2.09829900	0.00870600	
O	-3.53752700	-0.76818500	-0.09808500	
H	-3.49733700	-1.27837700	0.71829900	
Name				**4MC-N3H-N3-H-OH-FHT-P**
Cartesian Coordinates				Frequency and Energy
S	-2.29103700	0.53427200	-0.37814100	Zero-point correction= 0.084912 (Hartree/Particle)
N	0.33973400	1.11168000	-0.26423400	Thermal correction to Energy= 0.091355
C	-0.60811400	0.11676200	-0.16642800	Thermal correction to Enthalpy= 0.092300
C	1.54491600	0.59604600	-0.07536600	Thermal correction to Gibbs Free Energy= 0.053360
H	-0.10547100	2.08424800	-0.46255400	Sum of electronic and zero-point Energies= -700.069106
H	-0.28145000	-2.05434500	0.24095400	Sum of electronic and thermal Energies= -700.062663

H	2.48064000	1.12862500	-0.09343800	Sum of electronic and thermal Enthalpies= -700.061718
H	2.16795700	-1.34961900	0.31735600	Sum of electronic and thermal Free Energies= -700.100658
O	-1.41616600	2.79421300	-0.74808900	
H	-1.79674200	3.14282900	0.06662100	
N	1.40270700	-0.70867700	0.14219800	
C	0.06211700	-1.04604600	0.09176200	
Name				**4MC-N3H-N3-H-OH-FHT-W**
Cartesian Coordinates				Frequency and Energy
S	-2.29103700	0.53427200	-0.37814100	Zero-point correction= 0.084747 (Hartree/Particle)
N	0.33973400	1.11168000	-0.26423400	Thermal correction to Energy= 0.091272
C	-0.60811400	0.11676200	-0.16642800	Thermal correction to Enthalpy= 0.092216
C	1.54491600	0.59604600	-0.07536600	Thermal correction to Gibbs Free Energy= 0.053022
H	-0.10547100	2.08424800	-0.46255400	Sum of electronic and zero-point Energies= -700.075527
H	-0.28145000	-2.05434500	0.24095400	Sum of electronic and thermal Energies= -700.069003
H	2.48064000	1.12862500	-0.09343800	Sum of electronic and thermal Enthalpies= -700.068059
H	2.16795700	-1.34961900	0.31735600	Sum of electronic and thermal Free Energies= -700.107252
O	-1.41616600	2.79421300	-0.74808900	
H	-1.79674200	3.14282900	0.06662100	
N	1.40270700	-0.70867700	0.14219800	
C	0.06211700	-1.04604600	0.09176200	
Name				**4MC-N3H-N1-H-OOH-FHT-P**
Cartesian Coordinates				Frequency and Energy
C	0.53830000	0.90782900	0.20216300	Zero-point correction= 0.088997 (Hartree/Particle)
C	-1.48335600	-0.07002300	0.00440900	Thermal correction to Energy= 0.095633
C	-0.47486600	-1.03050600	-0.03145800	Thermal correction to Enthalpy= 0.096577
N	0.72997500	-0.40055100	0.08327100	Thermal correction to Gibbs Free Energy= 0.056217
H	1.71742000	-0.78575700	0.16346400	Sum of electronic and zero-point Energies= -775.189557
H	1.32385300	1.63549400	0.31304600	Sum of electronic and thermal Energies= -775.182921
H	-0.56546100	-2.09614100	-0.14021600	Sum of electronic and thermal Enthalpies= -775.181977
N	-0.77530200	1.13360800	0.15065000	Sum of electronic and thermal Free Energies= -775.222337
S	-3.16196300	-0.16057200	-0.10618800	
O	3.46759500	0.32069700	-0.52924600	
O	3.26181800	-0.67577300	0.37881400	
H	4.35378800	0.65040700	-0.32412900	
H	-1.23666900	2.03056500	0.20216600	
Name				**4MC-N3H-N1-H-OOH-FHT-W**
Cartesian Coordinates				Frequency and Energy
C	0.53830000	0.90782900	0.20216300	Zero-point correction= 0.089529 (Hartree/Particle)
C	-1.48335600	-0.07002300	0.00440900	Thermal correction to Energy= 0.097034
C	-0.47486600	-1.03050600	-0.03145800	Thermal correction to Enthalpy= 0.097978
N	0.72997500	-0.40055100	0.08327100	Thermal correction to Gibbs Free Energy= 0.055186
H	1.71742000	-0.78575700	0.16346400	Sum of electronic and zero-point Energies= -775.205503
H	1.32385300	1.63549400	0.31304600	Sum of electronic and thermal Energies= -775.197998
H	-0.56546100	-2.09614100	-0.14021600	Sum of electronic and thermal Enthalpies= -775.197054
N	-0.77530200	1.13360800	0.15065000	Sum of electronic and thermal Free Energies= -775.239846
S	-3.16196300	-0.16057200	-0.10618800	
O	3.46759500	0.32069700	-0.52924600	
O	3.26181800	-0.67577300	0.37881400	
H	4.35378800	0.65040700	-0.32412900	
H	-1.23666900	2.03056500	0.20216600	
Name				**4MC-N3H-N3-H-OOH-FHT-P**
Cartesian Coordinates				Frequency and Energy
S	-0.70119600	1.70813600	-0.00174200	Zero-point correction= 0.089188 (Hartree/Particle)
N	0.36730100	-0.81597700	-0.00750300	Thermal correction to Energy= 0.094869

C	0.58582300	0.55841800	-0.00094800	Thermal correction to Enthalpy= 0.095813
C	1.54144400	-1.40394400	-0.00460900	Thermal correction to Gibbs Free Energy= 0.057749
H	-1.00573900	-1.30835900	-0.00191700	Sum of electronic and zero-point Energies= -775.203759
H	2.52036700	1.67654300	0.00970100	Sum of electronic and thermal Energies= -775.198077
H	1.72050700	-2.46685900	-0.00641200	Sum of electronic and thermal Enthalpies= -775.197133
H	3.51425900	-0.67716400	0.00652700	Sum of electronic and thermal Free Energies= -775.235197
H	-2.02244900	0.40026400	-0.00339000	
O	-2.05555400	-1.54197800	0.00604000	
O	-2.72055400	-0.38376700	0.00080600	
C	1.94788900	0.76633600	0.00580800	
N	2.52557500	-0.48023800	0.00280200	
Name				**4MC-N3H-N3-H-OOH-FHT-W**
Cartesian Coordinates				Frequency and Energy
S	-0.70119600	1.70813600	-0.00174200	Zero-point correction= 0.089040 (Hartree/Particle)
N	0.36730100	-0.81597700	-0.00750300	Thermal correction to Energy= 0.094724
C	0.58582300	0.55841800	-0.00094800	Thermal correction to Enthalpy= 0.095668
C	1.54144400	-1.40394400	-0.00460900	Thermal correction to Gibbs Free Energy= 0.057584
H	-1.00573900	-1.30835900	-0.00191700	Sum of electronic and zero-point Energies= -775.214438
H	2.52036700	1.67654300	0.00970100	Sum of electronic and thermal Energies= -775.208753
H	1.72050700	-2.46685900	-0.00641200	Sum of electronic and thermal Enthalpies= -775.207809
H	3.51425900	-0.67716400	0.00652700	Sum of electronic and thermal Free Energies= -775.245893
H	-2.02244900	0.40026400	-0.00339000	
O	-2.05555400	-1.54197800	0.00604000	
O	-2.72055400	-0.38376700	0.00080600	
C	1.94788900	0.76633600	0.00580800	
N	2.52557500	-0.48023800	0.00280200	

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