

Supporting Information (SI)

The antioxidant activity of tetrahydrofuran lignans from *Anogeissus rivularis*: Theoretical insights into the radical scavenging activity and enzyme inhibition

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Table S1: The Cartesian coordinates and energies of TS of the reaction between HFL with HOO* in the studied media (G: the gas phase; P: pentyl ethanoate; W: water)

Name	1-C2-H-OOH-G			
Cartesian Coordinates	Frequency and Energy			
C	-1.39696500	0.91675400	-1.05228200	Zero-point correction= 0.391033 (Hartree/Particle)
C	0.31615900	0.22893400	0.32787300	Thermal correction to Energy= 0.415247
C	-0.20403100	1.57594000	0.89074700	Thermal correction to Enthalpy= 0.416191
C	-0.89903400	2.18440600	-0.35265300	Thermal correction to Gibbs Free Energy= 0.335722
H	-1.53324400	1.05983600	-2.12789300	Sum of electronic and zero-point Energies= -1188.502404
H	-0.18513600	-0.69602800	1.02944300	Sum of electronic and thermal Energies= -1188.478191
H	-0.98451100	1.35361300	1.62520800	Sum of electronic and thermal Enthalpies= -1188.477246
H	-1.71627900	2.84167300	-0.05612200	Sum of electronic and thermal Free Energies= -1188.557715
O	-0.24310200	0.05187100	-0.93805400	
C	-2.62506900	0.25128000	-0.45779000	
C	-3.55219800	0.92905900	0.33496900	
C	-2.89828700	-1.09172200	-0.77001700	
C	-4.71380800	0.33023800	0.79794300	
H	-3.37981100	1.96556000	0.59744100	
C	-4.06184300	-1.70568300	-0.31594800	
C	-4.96593200	-0.99674800	0.46211200	
H	-5.42530300	0.86787200	1.41041900	
H	-4.22391200	-2.74701300	-0.57202900	
C	1.76382300	-0.11182100	0.33385100	
C	2.49299000	-0.23463600	-0.84523700	
C	2.41316700	-0.37190800	1.55090200	
C	3.84549900	-0.57229800	-0.82613600	
H	1.99497200	-0.06641500	-1.79227200	
C	3.75200500	-0.70858400	1.58413900	
H	1.84808800	-0.32937200	2.47652700	
C	4.48064900	-0.80507100	0.39208100	
H	4.38225000	-0.65433600	-1.76147300	
H	4.26206700	-0.91280400	2.51740300	
O	-2.08240700	-1.84347400	-1.54677800	
H	-1.16675600	-1.55034400	-1.42683000	
O	-6.11305500	-1.55816800	0.93284500	
H	-6.15957400	-2.47699300	0.65560600	
O	5.78716500	-1.13977400	0.52547700	
C	6.55977700	-1.26333100	-0.65142900	
H	6.59599300	-0.31739500	-1.20028200	
H	7.56197300	-1.53233300	-0.32659800	
H	6.16421600	-2.04909500	-1.30215000	
C	0.84573500	2.46520600	1.54734500	
H	1.21819100	2.01990800	2.47108400	
H	1.70201000	2.63055100	0.89107400	
H	0.40697900	3.43415900	1.79889400	
C	0.05887300	2.95449900	-1.26081800	
H	0.44579900	3.84506100	-0.76328800	
H	0.90951000	2.33142800	-1.55042200	
H	-0.45486900	3.27423100	-2.17007900	
H	0.98830800	-2.80020000	0.76536300	
O	-0.49169800	-1.87254000	1.42728100	
O	0.07823500	-2.66769700	0.46002600	
Name	1-C2-H-OOH-P			
Cartesian Coordinates	Frequency and Energy			

C	-1.39178400	0.91743800	-1.05477700	Zero-point correction=	0.390562 (Hartree/Particle)
C	0.31644900	0.20088600	0.33773500	Thermal correction to Energy=	0.414702
C	-0.21691000	1.53804800	0.91289300	Thermal correction to Enthalpy=	0.415646
C	-0.89192000	2.16759100	-0.32972400	Thermal correction to Gibbs Free Energy=	0.335332
H	-1.50094600	1.08057200	-2.13066300	Sum of electronic and zero-point Energies=	-1188.533530
H	-0.15262800	-0.71005500	1.05972200	Sum of electronic and thermal Energies=	-1188.509390
H	-1.00939600	1.30074600	1.62960400	Sum of electronic and thermal Enthalpies=	-1188.508446
H	-1.70730500	2.82595600	-0.03139000	Sum of electronic and thermal Free Energies=	-1188.588760
O	-0.25843900	0.02398400	-0.92527000		
C	-2.64596100	0.25915700	-0.50363000		
C	-3.59782200	0.94409600	0.25266600		
C	-2.91576700	-1.08447300	-0.81868400		
C	-4.77764700	0.34964200	0.67826100		
H	-3.42981000	1.98138700	0.51490700		
C	-4.09461500	-1.69673100	-0.40119100		
C	-5.02285300	-0.97920500	0.34246000		
H	-5.50571400	0.89807300	1.26259000		
H	-4.26164900	-2.73787700	-0.65710900		
C	1.76933000	-0.11956600	0.32499200		
C	2.48295400	-0.26117400	-0.86277900		
C	2.44245600	-0.34146100	1.53792400		
C	3.83849800	-0.58660100	-0.85821500		
H	1.97612700	-0.11263200	-1.80864500		
C	3.78491600	-0.66718200	1.55689400		
H	1.89849600	-0.26928300	2.47455400		
C	4.49545400	-0.78886100	0.35501600		
H	4.36265200	-0.68241500	-1.79979300		
H	4.30715800	-0.83993200	2.49065800		
O	-2.06953300	-1.84060600	-1.56029200		
H	-1.17489800	-1.47471100	-1.47593100		
O	-6.18563200	-1.53592200	0.77404000		
H	-6.22823100	-2.45769900	0.49512600		
O	5.80428300	-1.11133600	0.47071600		
C	6.55581300	-1.26160000	-0.72398300		
H	6.57812600	-0.32922600	-1.29553200		
H	7.56619600	-1.51901200	-0.41295300		
H	6.15110400	-2.06578200	-1.34523400		
C	0.81138400	2.42283200	1.60592900		
H	1.16319800	1.96742200	2.53320600		
H	1.68044300	2.61072900	0.97252300		
H	0.35572600	3.38319500	1.86184200		
C	0.08079700	2.94216800	-1.21672900		
H	0.46468300	3.82548300	-0.70342900		
H	0.93383600	2.32140400	-1.50645000		
H	-0.42251900	3.27624100	-2.12723900		
H	1.17632200	-2.73829900	1.28607700		
O	-0.41955800	-1.83595100	1.65240400		
O	0.28274500	-2.75315800	0.90637800		
Name				1-C2-H-OOH-W	
Cartesian Coordinates				Frequency and Energy	
C	-1.38931300	0.91533100	-1.08326000	Zero-point correction=	0.390033 (Hartree/Particle)
C	0.31303600	0.17456800	0.29935300	Thermal correction to Energy=	0.414009
C	-0.19953200	1.51810000	0.88000100	Thermal correction to Enthalpy=	0.414953
C	-0.87503800	2.15846300	-0.35590300	Thermal correction to Gibbs Free Energy=	0.335453

H	-1.51887100	1.08335900	-2.15507100	Sum of electronic and zero-point Energies=	-1188.536597
H	-0.18766400	-0.70552000	0.99691900	Sum of electronic and thermal Energies=	-1188.512621
H	-0.98753100	1.28909100	1.60379900	Sum of electronic and thermal Enthalpies=	-1188.511677
H	-1.68208300	2.82214900	-0.04945100	Sum of electronic and thermal Free Energies=	-1188.591177
O	-0.25509000	0.01933900	-0.97323000		
C	-2.63539700	0.26006700	-0.50438000		
C	-3.59999100	0.98134100	0.20244700		
C	-2.89218500	-1.10335300	-0.72672600		
C	-4.77214000	0.40048200	0.66758200		
H	-3.44777500	2.03629500	0.39243200		
C	-4.05897600	-1.70704300	-0.26630000		
C	-4.99657900	-0.95116600	0.42467200		
H	-5.50843900	0.97993000	1.21048400		
H	-4.22149300	-2.76376200	-0.44939000		
C	1.76260900	-0.16058700	0.29570100		
C	2.50545800	-0.21220400	-0.88193900		
C	2.40709300	-0.44605100	1.50954500		
C	3.86560600	-0.51711400	-0.86407900		
H	2.02545100	0.00012300	-1.82956100		
C	3.75437400	-0.75086900	1.54189300		
H	1.83688800	-0.43643000	2.43305900		
C	4.49162900	-0.78468100	0.35194700		
H	4.41665800	-0.54045900	-1.79458000		
H	4.25636200	-0.97394200	2.47606900		
O	-2.02818500	-1.91136800	-1.41593300		
H	-1.15355100	-1.48560300	-1.43253000		
O	-6.16050000	-1.49964000	0.89490900		
H	-6.20285400	-2.43394600	0.65532200		
O	5.81279600	-1.09390600	0.47824700		
C	6.59292500	-1.14913700	-0.71283500		
H	6.60315700	-0.17896000	-1.21511100		
H	7.60082900	-1.40890100	-0.39762100		
H	6.21072600	-1.91517800	-1.39170200		
C	0.85149200	2.38058600	1.56520900		
H	1.21414600	1.90388500	2.47760100		
H	1.70895800	2.56654100	0.91538600		
H	0.41141800	3.34232200	1.84069300		
C	0.09896000	2.92767400	-1.24543400		
H	0.48555400	3.80850000	-0.73031700		
H	0.94958400	2.30397600	-1.53610300		
H	-0.40707400	3.26182900	-2.15403200		
H	0.92467200	-2.90524100	1.36275600		
O	-0.61237600	-1.84840600	1.55438500		
O	0.08986200	-2.81418000	0.87455300		
Name				1-C5-H-OOH-G	
Cartesian Coordinates				Frequency and Energy	
C	-1.18637600	0.40501100	-0.10194400	Zero-point correction=	0.391567 (Hartree/Particle)
C	0.51550600	-0.20620100	1.39119100	Thermal correction to Energy=	0.415637
C	-0.00419400	1.17972400	1.83434300	Thermal correction to Enthalpy=	0.416581
C	-0.74391600	1.71004500	0.58475700	Thermal correction to Gibbs Free Energy=	0.336773
H	-0.77391200	0.48275700	-1.28788800	Sum of electronic and zero-point Energies=	-1188.504835
H	0.51920100	-0.89310700	2.24206200	Sum of electronic and thermal Energies=	-1188.480766
H	-0.77168800	0.97116500	2.58695800	Sum of electronic and thermal Enthalpies=	-1188.479822
H	-1.63061000	2.26182700	0.90630400	Sum of electronic and thermal Free Energies=	-1188.559629

O	-0.51600700	-0.66928000	0.51125400	
C	-2.62995400	0.14668200	-0.33037200	
C	-3.41209400	1.19820500	-0.83790000	
C	-3.23968900	-1.11930300	-0.21095300	
C	-4.74005200	1.04202900	-1.18160300	
H	-2.94567100	2.16855400	-0.97521400	
C	-4.58746000	-1.28186600	-0.54117600	
C	-5.32995100	-0.21580300	-1.02172100	
H	-5.33283700	1.86210100	-1.56420100	
H	-5.02265400	-2.26816900	-0.42175600	
C	1.87822400	-0.25498800	0.73452000	
C	2.04281400	-0.37008200	-0.63901200	
C	3.02280700	-0.20324100	1.53900000	
C	3.31453000	-0.39893100	-1.21361200	
H	1.18064400	-0.44515400	-1.29092000	
C	4.28890200	-0.22826800	0.98577200	
H	2.92025900	-0.14932800	2.61843800	
C	4.44207800	-0.31999200	-0.40130000	
H	3.40008200	-0.48899200	-2.28792900	
H	5.17821500	-0.18978900	1.60259100	
O	-2.60228600	-2.22361300	0.21644300	
H	-1.67661500	-1.99984900	0.40261300	
O	-6.63937400	-0.33495400	-1.36074500	
H	-6.93539900	-1.23716100	-1.21130500	
O	5.72125600	-0.33728100	-0.85599100	
C	5.91919900	-0.44046600	-2.25090300	
H	5.47078900	0.40776500	-2.77721300	
H	6.99590000	-0.43390600	-2.40382600	
H	5.50122600	-1.37339900	-2.64128500	
C	1.02284700	2.12631200	2.43688500	
H	1.45583800	1.70460300	3.34692800	
H	1.83773100	2.33385100	1.74182600	
H	0.54817400	3.07309300	2.70501300	
C	0.08925100	2.61269900	-0.32919400	
H	0.35264100	3.54132100	0.18062900	
H	1.01137600	2.12165900	-0.64745600	
H	-0.47717000	2.86476200	-1.22860300	
H	-2.34140800	-0.11740400	-3.06424500	
O	-0.64486000	0.49485600	-2.58419200	
O	-1.46829100	-0.53027600	-2.97960500	
Name				1-C5-H-OOH-P
Cartesian Coordinates				Frequency and Energy
C	-1.19077400	0.42392600	-0.15328400	Zero-point correction= 0.390733 (Hartree/Particle)
C	0.51057700	-0.20644500	1.34361400	Thermal correction to Energy= 0.414848
C	-0.01588700	1.17244300	1.79675700	Thermal correction to Enthalpy= 0.415792
C	-0.74659800	1.72009400	0.54906700	Thermal correction to Gibbs Free Energy= 0.335793
H	-0.80000200	0.50877200	-1.33778900	Sum of electronic and zero-point Energies= -1188.535022
H	0.49482800	-0.90506900	2.18407600	Sum of electronic and thermal Energies= -1188.510907
H	-0.78847200	0.95398900	2.54072000	Sum of electronic and thermal Enthalpies= -1188.509963
H	-1.63275900	2.27106400	0.87100900	Sum of electronic and thermal Free Energies= -1188.589962
O	-0.50287100	-0.65673600	0.42960000	
C	-2.64000100	0.15771300	-0.35073900	
C	-3.44084800	1.20654900	-0.83399900	
C	-3.24254500	-1.10996800	-0.21058400	

C	-4.77879800	1.04400800	-1.13508700	
H	-2.98492100	2.18048400	-0.98249800	
C	-4.59831900	-1.28129900	-0.49881200	
C	-5.35879800	-0.21648900	-0.95751400	
H	-5.38238700	1.86521400	-1.50027700	
H	-5.03462400	-2.26586000	-0.36561100	
C	1.88529500	-0.25454500	0.71245200	
C	2.07748700	-0.33849000	-0.66032100	
C	3.01468300	-0.23371400	1.54014300	
C	3.35929800	-0.37414700	-1.21317100	
H	1.22516100	-0.38443500	-1.32842500	
C	4.29164600	-0.26430700	1.00956200	
H	2.89095000	-0.19946300	2.61812200	
C	4.47236500	-0.33021100	-0.37668600	
H	3.46727900	-0.44152500	-2.28761900	
H	5.16606000	-0.24999300	1.64975500	
O	-2.58097100	-2.20791500	0.20352800	
H	-1.65632100	-1.96123600	0.37634500	
O	-6.67572300	-0.34357400	-1.25388800	
H	-6.96253500	-1.25078800	-1.09604700	
O	5.75769400	-0.35865900	-0.80901000	
C	5.97811700	-0.44495100	-2.20733900	
H	5.55741800	0.42037200	-2.72794200	
H	7.05797000	-0.45718600	-2.34213200	
H	5.55086400	-1.36430100	-2.61842400	
C	1.00553000	2.10973600	2.42072600	
H	1.43673600	1.66800500	3.32247500	
H	1.82176500	2.34020300	1.73378200	
H	0.52476700	3.04782600	2.70938600	
C	0.09069800	2.63344900	-0.34791600	
H	0.36040700	3.54933700	0.18198000	
H	1.01124300	2.14804400	-0.68001900	
H	-0.47969900	2.91541700	-1.23634800	
H	-2.37384200	-0.16639200	-3.08744100	
O	-0.67211400	0.47572200	-2.65392000	
O	-1.49200500	-0.56645300	-3.01479100	
Name				1-C5-H-OOH-W
Cartesian Coordinates				Frequency and Energy
C	-1.19255400	0.40522900	-0.19192300	Zero-point correction= 0.390143 (Hartree/Particle)
C	0.50936400	-0.23306300	1.30493000	Thermal correction to Energy= 0.414167
C	-0.01290600	1.14688900	1.75595100	Thermal correction to Enthalpy= 0.415111
C	-0.74154700	1.69915100	0.51027800	Thermal correction to Gibbs Free Energy= 0.335457
H	-0.82616300	0.49230400	-1.36423000	Sum of electronic and zero-point Energies= -1188.536003
H	0.47930800	-0.93394200	2.14187300	Sum of electronic and thermal Energies= -1188.511979
H	-0.78488500	0.93241700	2.50063600	Sum of electronic and thermal Enthalpies= -1188.511035
H	-1.62556900	2.25255800	0.83205600	Sum of electronic and thermal Free Energies= -1188.590689
O	-0.48990000	-0.67887800	0.36980700	
C	-2.64654700	0.14558600	-0.36051600	
C	-3.43378800	1.18732200	-0.88217700	
C	-3.27333800	-1.09633600	-0.14574300	
C	-4.77789800	1.03435900	-1.15782600	
H	-2.95907400	2.14279800	-1.08307400	
C	-4.63245400	-1.26215700	-0.41032200	
C	-5.37632500	-0.20572800	-0.91300000	

H	-5.37079900	1.84853200	-1.55512100	
H	-5.09528900	-2.22473400	-0.22071500	
C	1.89351800	-0.28046500	0.69662700	
C	2.11313700	-0.31353900	-0.67467800	
C	3.00459200	-0.29933600	1.54843000	
C	3.40544700	-0.34021300	-1.20373500	
H	1.27299900	-0.32219900	-1.35964300	
C	4.29271300	-0.31999700	1.04232300	
H	2.85559500	-0.30091100	2.62355300	
C	4.49771400	-0.33544300	-0.34079400	
H	3.53904100	-0.36692500	-2.27690500	
H	5.15326200	-0.33364300	1.70120000	
O	-2.62022800	-2.19067800	0.33499200	
H	-1.69332400	-1.94309500	0.50628300	
O	-6.70815300	-0.32591300	-1.18686600	
H	-7.01157600	-1.21814100	-0.97489800	
O	5.80057900	-0.35608200	-0.75391000	
C	6.04089100	-0.36905600	-2.15705500	
H	5.62452300	0.52315100	-2.63114800	
H	7.12208100	-0.37539000	-2.27575500	
H	5.61595400	-1.26474200	-2.61668300	
C	1.01601300	2.07747400	2.37664100	
H	1.45647400	1.62460200	3.26803700	
H	1.82401400	2.31205700	1.68108100	
H	0.53884900	3.01380900	2.67540800	
C	0.09223300	2.61100800	-0.38999500	
H	0.37537100	3.51985000	0.14438900	
H	1.00354400	2.11937200	-0.73781400	
H	-0.49292900	2.90307600	-1.26549700	
H	-2.46332000	-0.04849200	-3.15814800	
O	-0.70554500	0.44412500	-2.72060200	
O	-1.61608000	-0.51835600	-3.08025600	
Name				1-O9-H-OOH-G
Cartesian Coordinates				Frequency and Energy
C	-1.32934900	1.02960800	-0.99645300	Zero-point correction= 0.391242 (Hartree/Particle)
C	0.27133700	0.03050000	0.38143300	Thermal correction to Energy= 0.415079
C	-0.10362300	1.41715900	1.00030900	Thermal correction to Enthalpy= 0.416023
C	-0.71680000	2.18488500	-0.19092600	Thermal correction to Gibbs Free Energy= 0.334382
H	-1.43432800	1.28464500	-2.05609000	Sum of electronic and zero-point Energies= -1188.500289
H	-0.21578500	-0.75955200	0.96697500	Sum of electronic and thermal Energies= -1188.476452
H	-0.91417700	1.23635300	1.71230900	Sum of electronic and thermal Enthalpies= -1188.475507
H	-1.47777400	2.87690400	0.17040200	Sum of electronic and thermal Free Energies= -1188.557148
O	-0.30662100	0.03022200	-0.93466700	
C	-2.66174700	0.51263400	-0.46697300	
C	-3.65794500	1.42796100	-0.07720100	
C	-2.97083700	-0.86287100	-0.42027000	
C	-4.89295300	1.02690500	0.37588400	
H	-3.45267400	2.48910200	-0.15163500	
C	-4.20134800	-1.28626200	0.06921800	
C	-5.17477600	-0.35667600	0.48320900	
H	-5.65464600	1.73479400	0.67590100	
H	-4.41424400	-2.34667200	0.11757500	
C	1.74106700	-0.29284800	0.28108700	
C	2.46315500	-0.12308100	-0.89115400	

C	2.41343200	-0.76641000	1.41304500	
C	3.83205000	-0.39092200	-0.94369000	
H	1.95051700	0.20249600	-1.78789900	
C	3.76967700	-1.02896500	1.38158200	
H	1.86174000	-0.93594900	2.33285500	
C	4.49089300	-0.83660000	0.19899100	
H	4.36087200	-0.25517600	-1.87734300	
H	4.29681800	-1.39603100	2.25345300	
O	-2.12971200	-1.83437400	-0.84094300	
H	-1.28330800	-1.42694700	-1.09079000	
O	-6.32279700	-0.74842700	0.97821300	
H	-6.89484000	-1.40530600	0.23281000	
O	5.81673100	-1.12196700	0.26115900	
C	6.58000500	-0.95504200	-0.91508500	
H	6.55797800	0.08471800	-1.25619400	
H	7.59970800	-1.22874200	-0.65454100	
H	6.22070800	-1.60927300	-1.71551100	
C	1.01937900	2.14785200	1.72555500	
H	1.34949000	1.58777700	2.60240100	
H	1.88962500	2.29182500	1.08272900	
H	0.67054400	3.12627200	2.06544100	
C	0.30108900	2.95441000	-1.03066000	
H	0.76148800	3.75625400	-0.45142600	
H	1.09755800	2.29714400	-1.38557400	
H	-0.18450000	3.40511400	-1.89934600	
H	-6.63714200	-1.11266800	-2.29206700	
O	-7.41751200	-1.84289000	-0.77304100	
O	-6.40547600	-1.83390200	-1.68879600	
Name				1-O9-H-OOH-P
Cartesian Coordinates				Frequency and Energy
C	-1.34121800	0.81355800	-1.02566300	Zero-point correction= 0.390752 (Hartree/Particle)
C	0.30664700	-0.03786900	0.39936300	Thermal correction to Energy= 0.414368
C	-0.12347300	1.36584800	0.93876600	Thermal correction to Enthalpy= 0.415312
C	-0.78541000	2.03591600	-0.28580700	Thermal correction to Gibbs Free Energy= 0.335588
H	-1.46635900	1.00597400	-2.09626100	Sum of electronic and zero-point Energies= -1188.532210
H	-0.15049200	-0.81075800	1.02871700	Sum of electronic and thermal Energies= -1188.508594
H	-0.91381800	1.19052700	1.67405600	Sum of electronic and thermal Enthalpies= -1188.507649
H	-1.57389000	2.71219400	0.04251100	Sum of electronic and thermal Free Energies= -1188.587374
O	-0.26749100	-0.13214400	-0.91756100	
C	-2.64002900	0.23202600	-0.47747000	
C	-3.64670900	1.06156400	0.02950100	
C	-2.89697800	-1.16489000	-0.54688200	
C	-4.85119900	0.55815200	0.48346800	
H	-3.48870000	2.13180600	0.06590600	
C	-4.10159900	-1.68238100	-0.10304100	
C	-5.09066100	-0.83746500	0.42880700	
H	-5.61505100	1.20715400	0.89782200	
H	-4.28528100	-2.74820100	-0.16437300	
C	1.78737700	-0.31311300	0.31770200	
C	2.51622100	-0.14954000	-0.85269700	
C	2.46564700	-0.72648600	1.46993300	
C	3.89452500	-0.37005400	-0.88626200	
H	2.00672400	0.13979300	-1.76390200	
C	3.83198400	-0.94200200	1.45722900	

H	1.91185100	-0.88373700	2.39075200	
C	4.55836800	-0.76026400	0.27510000	
H	4.42806600	-0.23949000	-1.81837300	
H	4.35851500	-1.26207100	2.34878500	
O	-2.01039900	-2.03761600	-1.06854000	
H	-1.15967100	-1.57274100	-1.18739900	
O	-6.21860800	-1.33884100	0.88351800	
H	-7.05807000	-1.03371000	0.19313000	
O	5.89184900	-0.99655100	0.35294200	
C	6.65928700	-0.82799800	-0.82742500	
H	6.60270400	0.20219100	-1.19159000	
H	7.68729400	-1.05782800	-0.55417900	
H	6.33144400	-1.51434900	-1.61373900	
C	0.97363800	2.18543800	1.60472600	
H	1.34080500	1.68752300	2.50487300	
H	1.82640500	2.34209900	0.94105700	
H	0.58219600	3.16246700	1.90074800	
C	0.18223400	2.80837000	-1.17959300	
H	0.60933100	3.66108300	-0.64875000	
H	1.00591000	2.17610300	-1.51863900	
H	-0.33982200	3.19040900	-2.06040900	
H	-6.69797900	0.75617900	-1.45383700	
O	-7.75010200	-0.62190900	-0.75733000	
O	-6.82506700	-0.18638300	-1.65542500	
Name				1-O9-H-OOH-W
Cartesian Coordinates				Frequency and Energy
C	-0.71811500	0.85378000	-0.88206800	Zero-point correction= 0.389618 (Hartree/Particle)
C	0.98907800	-0.03217900	0.45067600	Thermal correction to Energy= 0.413287
C	0.58800100	1.35944300	1.03694200	Thermal correction to Enthalpy= 0.414231
C	-0.12648400	2.05756700	-0.14038000	Thermal correction to Gibbs Free Energy= 0.334230
H	-0.89366500	1.07030800	-1.94004100	Sum of electronic and zero-point Energies= -1188.531853
H	0.55805000	-0.81805300	1.08095600	Sum of electronic and thermal Energies= -1188.508184
H	-0.16794500	1.16972600	1.80365400	Sum of electronic and thermal Enthalpies= -1188.507240
H	-0.89958700	2.72390100	0.23918300	Sum of electronic and thermal Free Energies= -1188.587242
O	0.35341300	-0.10115600	-0.84164600	
C	-1.99818800	0.27737400	-0.28829800	
C	-2.98824900	1.12182900	0.22099500	
C	-2.26599100	-1.12061200	-0.31544300	
C	-4.18338400	0.63275900	0.71726000	
H	-2.82962800	2.19229800	0.22157500	
C	-3.45615300	-1.62625800	0.17175400	
C	-4.42414900	-0.76159200	0.70486300	
H	-4.94136700	1.29425500	1.12083300	
H	-3.64236000	-2.69317000	0.14420700	
C	2.46480400	-0.30456000	0.30237100	
C	3.15860100	-0.08555600	-0.88132900	
C	3.17802300	-0.76451500	1.41512700	
C	4.53560200	-0.30196000	-0.96705000	
H	2.62943600	0.25229200	-1.76395600	
C	4.54473700	-0.97577500	1.35165700	
H	2.65190300	-0.95744100	2.34501000	
C	5.23094300	-0.74081800	0.15653200	
H	5.04173000	-0.12587200	-1.90678800	
H	5.09756700	-1.32994800	2.21408200	

O	-1.38881000	-2.01557400	-0.84300900	
H	-0.54665300	-1.54875600	-1.02104200	
O	-5.55290700	-1.25121200	1.20226700	
H	-6.39733400	-0.93345600	0.55600600	
O	6.57756400	-0.97683000	0.18147900	
C	7.30548000	-0.74072600	-1.01895300	
H	7.22430000	0.30564200	-1.32361300	
H	8.34283600	-0.97569200	-0.79143200	
H	6.95047400	-1.38915500	-1.82385400	
C	1.71695700	2.16152000	1.66908400	
H	2.12414100	1.63971700	2.53803400	
H	2.53562500	2.33469100	0.96729400	
H	1.34089300	3.13139900	2.00448300	
C	0.79785600	2.85165500	-1.05981000	
H	1.24948000	3.69015200	-0.52689500	
H	1.60366300	2.22908600	-1.45524600	
H	0.23120900	3.25384700	-1.90283200	
H	-6.21818600	0.99010700	-0.97354200	
O	-7.13645200	-0.54555600	-0.41214300	
O	-6.24540700	0.05606100	-1.24565500	
Name				2-C2-H-OOH-G
Cartesian Coordinates				Frequency and Energy
C	-0.81978100	1.88631900	0.47856300	Zero-point correction= 0.365509 (Hartree/Particle)
C	0.56139400	2.35781400	-0.03973300	Thermal correction to Energy= 0.390177
C	0.98554800	1.17699100	-0.93878600	Thermal correction to Enthalpy= 0.391121
C	-1.30475900	1.09508800	-0.75317500	Thermal correction to Gibbs Free Energy= 0.309716
H	0.33997200	3.21657900	-0.68313900	Sum of electronic and zero-point Energies= -1224.460149
H	1.20614500	1.67700200	-2.07871100	Sum of electronic and thermal Energies= -1224.435481
H	-1.56286500	1.83421600	-1.52447500	Sum of electronic and thermal Enthalpies= -1224.434537
O	-0.14393600	0.37467700	-1.15102500	Sum of electronic and thermal Free Energies= -1224.515941
C	-2.46052600	0.16334600	-0.52750800	
C	-3.73148400	0.69965800	-0.32738500	
C	-2.29771100	-1.21965500	-0.46956000	
C	-4.81632000	-0.12614400	-0.06109500	
H	-3.86847600	1.77455200	-0.36878500	
C	-3.37713700	-2.05429900	-0.21162300	
H	-1.31703000	-1.64472600	-0.64330000	
C	-4.63887400	-1.50672400	-0.00249200	
H	-5.80182900	0.30166500	0.09468500	
H	-3.26309000	-3.13055800	-0.17358100	
C	2.18990700	0.36295300	-0.63281500	
C	3.46275900	0.91615100	-0.78188700	
C	2.07172000	-0.96379900	-0.20663500	
C	4.59806600	0.17626600	-0.48170100	
H	3.56582800	1.92563000	-1.16331300	
C	3.20551000	-1.70016100	0.08635400	
H	1.08847300	-1.41197000	-0.10953700	
C	4.47792000	-1.13472100	-0.04226800	
H	5.59124600	0.59105300	-0.60005200	
C	1.55585500	2.78527500	1.02967600	
H	1.87483500	1.94294900	1.64603400	
H	2.44863200	3.22568800	0.58386600	
H	1.10490100	3.54467600	1.67548000	
C	-0.72683000	1.01553800	1.72217700	

H	-0.32572300	1.58947600	2.56199500	
H	-1.71535500	0.63876200	1.98956800	
H	-0.06016800	0.16606700	1.55077700	
O	-1.71905300	2.96197200	0.67058500	
H	-1.58511900	3.33062200	1.54783400	
O	-5.66330400	-2.36853800	0.24917200	
H	-6.48272200	-1.87864700	0.35702300	
O	5.58528400	-1.85941700	0.24568500	
H	5.31198700	-2.74897500	0.49908300	
O	3.19238900	-3.00155800	0.51686500	
H	2.30013100	-3.35585300	0.49073200	
H	0.23237100	0.24508100	-3.68626000	
O	1.08493600	1.86170800	-3.32749900	
O	1.13196300	0.57815800	-3.81800900	
Name				2-C5-H-OOH-G
Cartesian Coordinates				Frequency and Energy
C	-0.77922000	1.88344700	0.42919200	Zero-point correction= 0.365703 (Hartree/Particle)
C	0.49844700	2.41519000	-0.25368500	Thermal correction to Energy= 0.390271
C	0.92844900	1.24870100	-1.18358500	Thermal correction to Enthalpy= 0.391215
C	-1.34193300	1.02177300	-0.71021900	Thermal correction to Gibbs Free Energy= 0.310810
H	0.14570600	3.21845600	-0.90798400	Sum of electronic and zero-point Energies= -1224.460834
H	1.20766800	1.65658100	-2.15713000	Sum of electronic and thermal Energies= -1224.436266
H	-1.81443200	1.88536300	-1.50187500	Sum of electronic and thermal Enthalpies= -1224.435322
O	-0.26171200	0.46284300	-1.37114500	Sum of electronic and thermal Free Energies= -1224.515727
C	-2.42596800	0.04190200	-0.45205200	
C	-3.59297000	0.45510200	0.19797300	
C	-2.32165300	-1.28836100	-0.86876100	
C	-4.61785300	-0.44530900	0.44818200	
H	-3.68998000	1.49005200	0.50542600	
C	-3.34506400	-2.19271200	-0.62412900	
H	-1.43014500	-1.60838500	-1.39412600	
C	-4.49474300	-1.77247600	0.03828600	
H	-5.51980700	-0.11640900	0.95503000	
H	-3.27500300	-3.22529700	-0.94320400	
C	2.04990900	0.35406400	-0.70191100	
C	3.36990300	0.78209900	-0.82369700	
C	1.79933900	-0.90085600	-0.14682000	
C	4.42257000	-0.00507300	-0.36949400	
H	3.58407800	1.74000300	-1.28522500	
C	2.84814600	-1.68803900	0.30016300	
H	0.78048200	-1.27080500	-0.08488400	
C	4.16859800	-1.24332900	0.20040000	
H	5.45172200	0.31977200	-0.46000900	
C	1.56070700	2.96180900	0.68717100	
H	1.98443600	2.18269100	1.32313600	
H	2.38103100	3.41815700	0.12986900	
H	1.13339000	3.74096200	1.32578400	
C	-0.51939500	1.07936400	1.69935800	
H	-0.10166200	1.72857600	2.47453200	
H	-1.45446900	0.65366600	2.06587900	
H	0.19548400	0.27460100	1.52250300	
O	-1.71617300	2.91524300	0.69347900	
H	-1.40114000	3.43136700	1.44096500	
O	-5.46813100	-2.69891100	0.25472900	

H	-6.21625900	-2.28895700	0.69693000	
O	5.19357200	-2.01696500	0.63795100	
H	4.82929000	-2.84154700	0.98021500	
O	2.69464100	-2.93254300	0.85370900	
H	1.76613400	-3.17766300	0.87739200	
H	-1.23975900	1.68778900	-3.89648200	
O	-2.00169500	2.67713900	-2.50834900	
O	-0.93456800	2.41462800	-3.33664000	
Name				2-O9-H-OOH-G
Cartesian Coordinates				Frequency and Energy
C	-0.79268700	1.77740600	0.39112300	Zero-point correction= 0.365563 (Hartree/Particle)
C	0.56806600	2.29641500	-0.12530300	Thermal correction to Energy= 0.389829
C	1.03444200	1.18271200	-1.11693800	Thermal correction to Enthalpy= 0.390773
C	-1.25873700	0.98248200	-0.84939600	Thermal correction to Gibbs Free Energy= 0.309176
H	0.31643200	3.17843300	-0.72155400	Sum of electronic and zero-point Energies= -1224.462086
H	1.27564100	1.64795000	-2.07953300	Sum of electronic and thermal Energies= -1224.437820
H	-1.59414200	1.72734800	-1.58733600	Sum of electronic and thermal Enthalpies= -1224.436876
O	-0.09439500	0.32545900	-1.29833900	Sum of electronic and thermal Free Energies= -1224.518473
C	-2.36619400	-0.00200300	-0.60880000	
C	-3.63933700	0.47783400	-0.27625600	
C	-2.14353200	-1.38387200	-0.68583300	
C	-4.66842100	-0.40081400	-0.00095700	
H	-3.80343000	1.54816300	-0.22553900	
C	-3.16918000	-2.27276700	-0.43056500	
H	-1.16165200	-1.73953200	-0.97140700	
C	-4.44905700	-1.79932200	-0.06382800	
H	-5.65906200	-0.04859700	0.25958900	
H	-3.02414800	-3.34482700	-0.49048300	
C	2.22824400	0.36442400	-0.68693200	
C	3.51247400	0.86611900	-0.88065000	
C	2.07587500	-0.87793000	-0.07174200	
C	4.62940100	0.16169400	-0.44396100	
H	3.64735500	1.81840400	-1.38279600	
C	3.18854400	-1.58335700	0.35691000	
H	1.08455700	-1.30287800	0.04647900	
C	4.47472700	-1.06549900	0.18212700	
H	5.63235100	0.54274400	-0.59134000	
C	1.56362600	2.70638300	0.95020400	
H	1.89345000	1.85332700	1.54598000	
H	2.45262500	3.16018400	0.50839800	
H	1.11401800	3.44789700	1.61742600	
C	-0.68915800	0.91398000	1.63931000	
H	-0.29949900	1.50027800	2.47604400	
H	-1.67189200	0.52490500	1.91090000	
H	-0.00769000	0.07636100	1.47857500	
O	-1.72326700	2.83058200	0.58678900	
H	-1.58353800	3.21400600	1.45699100	
O	-5.40434900	-2.65264000	0.22364900	
H	-6.27554300	-2.53239300	-0.49089700	
O	5.56189600	-1.75908000	0.60207800	
H	5.26385000	-2.59009200	0.98992400	
O	3.13655900	-2.81141900	0.96268500	
H	2.22829500	-3.11663800	1.02892700	
H	-5.87433500	-1.69081000	-2.85842600	

O	-6.95743700	-2.36528400	-1.50632100	
O	-6.35462400	-1.30283000	-2.11174300	
Name				2-O9-H-OOH-P
Cartesian Coordinates				Frequency and Energy
C	-0.78363100	1.79100000	0.47985700	Zero-point correction= 0.364760 (Hartree/Particle)
C	0.57608000	2.29452200	-0.03883700	Thermal correction to Energy= 0.388939
C	1.00437100	1.20535400	-1.07542300	Thermal correction to Enthalpy= 0.389883
C	-1.27544500	1.03340900	-0.78577500	Thermal correction to Gibbs Free Energy= 0.308755
H	0.34049100	3.20205200	-0.60223600	Sum of electronic and zero-point Energies= -1224.496542
H	1.20167000	1.69694400	-2.03440900	Sum of electronic and thermal Energies= -1224.472363
H	-1.57703600	1.80181300	-1.51258700	Sum of electronic and thermal Enthalpies= -1224.471419
O	-0.12932500	0.34366400	-1.23397600	Sum of electronic and thermal Free Energies= -1224.552546
C	-2.41918800	0.09471900	-0.55836000	
C	-3.71383700	0.62080000	-0.45097800	
C	-2.21607100	-1.28269700	-0.38765300	
C	-4.78456600	-0.20049600	-0.15622000	
H	-3.87470000	1.68127100	-0.61587300	
C	-3.27939300	-2.11741000	-0.10711100	
H	-1.21539100	-1.68396700	-0.49066200	
C	-4.58267700	-1.58822400	0.03237500	
H	-5.79143300	0.19229800	-0.07274800	
H	-3.14151600	-3.18454900	0.02610600	
C	2.21865700	0.38301600	-0.71850100	
C	3.48911000	0.88979200	-0.98206000	
C	2.10250000	-0.86206100	-0.09958200	
C	4.63062200	0.18359400	-0.61415700	
H	3.59333900	1.84763700	-1.48097300	
C	3.23922400	-1.56973700	0.25968500	
H	1.12317800	-1.29063800	0.08608500	
C	4.51239000	-1.04804000	0.01166000	
H	5.62174000	0.57306400	-0.81589400	
C	1.59100700	2.64817100	1.03701900	
H	1.91597600	1.77066900	1.59996200	
H	2.47894300	3.10672800	0.59619500	
H	1.15349700	3.36847600	1.73331500	
C	-0.68807300	0.88931200	1.70038700	
H	-0.25720900	1.44001000	2.53838000	
H	-1.68065700	0.53446800	1.99427200	
H	-0.06042100	0.01802600	1.50172400	
O	-1.60002800	2.91634900	0.75786700	
H	-2.33218000	2.63358200	1.31752700	
O	-5.58717600	-2.38123400	0.34785000	
H	-6.24852900	-2.52507000	-0.54567600	
O	5.62393200	-1.74422800	0.36411000	
H	5.35115700	-2.57564900	0.77243000	
O	3.22198600	-2.79670700	0.86142500	
H	2.31591700	-3.09966100	0.98763800	
H	-5.24116500	-2.32021600	-2.84146400	
O	-6.69133100	-2.63985600	-1.71310800	
O	-5.91768600	-1.76739100	-2.41437500	
Name				2-O9-H-OOH-W
Cartesian Coordinates				Frequency and Energy
C	-0.77887300	1.85988300	0.54634600	Zero-point correction= 0.365019 (Hartree/Particle)
C	0.58265700	2.35481100	0.02741700	Thermal correction to Energy= 0.388748

C	0.97446500	1.30910500	-1.06081000	Thermal correction to Enthalpy=	0.389692
C	-1.32181600	1.18368800	-0.74409300	Thermal correction to Gibbs Free Energy=	0.310790
H	0.36320700	3.28903300	-0.49709600	Sum of electronic and zero-point Energies=	-1224.505662
H	1.20640900	1.84349400	-1.98702000	Sum of electronic and thermal Energies=	-1224.481933
H	-1.64068900	1.99299500	-1.41485300	Sum of electronic and thermal Enthalpies=	-1224.480989
O	-0.19838300	0.50940200	-1.28035400	Sum of electronic and thermal Free Energies=	-1224.559891
C	-2.46360800	0.23836200	-0.52973900		
C	-3.75860700	0.76681100	-0.40230300		
C	-2.26107500	-1.14118800	-0.39019200		
C	-4.83135000	-0.05664200	-0.12996300		
H	-3.91132200	1.83332300	-0.53029800		
C	-3.32616700	-1.97791300	-0.11806200		
H	-1.26380600	-1.54965300	-0.49617600		
C	-4.62714800	-1.44516300	0.02706200		
H	-5.83700000	0.33521900	-0.03271300		
H	-3.18921800	-3.04788100	-0.00644300		
C	2.14613800	0.41295800	-0.73752500		
C	3.43989700	0.87599800	-0.97282500		
C	1.97164300	-0.85512400	-0.18362900		
C	4.54536700	0.09844300	-0.64056800		
H	3.58841100	1.85368100	-1.41866500		
C	3.07264400	-1.63578000	0.13790000		
H	0.97943100	-1.25703300	-0.01066200		
C	4.36665900	-1.15851900	-0.08243900		
H	5.55424300	0.45198800	-0.81963300		
C	1.62339100	2.63616500	1.09969800		
H	1.92637400	1.72709300	1.62338200		
H	2.51638700	3.08464000	0.65902500		
H	1.21934000	3.34008300	1.83178400		
C	-0.69164700	0.90158900	1.72250000		
H	-0.21241300	1.39496200	2.56951100		
H	-1.69377200	0.58738500	2.02761300		
H	-0.11394500	0.01135800	1.46519400		
O	-1.55915500	2.99591200	0.89743600		
H	-2.35002000	2.69451800	1.36264400		
O	-5.65029300	-2.24161400	0.32127300		
H	-5.96697500	-2.76781600	-0.60645500		
O	5.45991200	-1.92535800	0.23093100		
H	5.16046900	-2.76824600	0.59831200		
O	2.97691500	-2.89505000	0.67374200		
H	2.04818400	-3.13998000	0.77481100		
H	-4.43892300	-2.78967400	-2.54096100		
O	-6.13160600	-3.13329800	-1.81381100		
O	-5.28720700	-2.31405600	-2.49206400		
Name				2-O14-H-OOH-G	
Cartesian Coordinates				Frequency and Energy	
C	-0.78631800	1.83181000	0.44870800	Zero-point correction=	0.366588 (Hartree/Particle)
C	0.58329300	2.31431600	-0.08145800	Thermal correction to Energy=	0.390442
C	0.99424300	1.19231600	-1.08705200	Thermal correction to Enthalpy=	0.391386
C	-1.29722700	1.05956100	-0.78648900	Thermal correction to Gibbs Free Energy=	0.311454
H	0.35191100	3.20829800	-0.66746900	Sum of electronic and zero-point Energies=	-1224.468607
H	1.23456900	1.65495900	-2.05245600	Sum of electronic and thermal Energies=	-1224.444752
H	-1.60785800	1.81700300	-1.52140400	Sum of electronic and thermal Enthalpies=	-1224.443808
O	-0.15395500	0.36569500	-1.25010400	Sum of electronic and thermal Free Energies=	-1224.523740

C	-2.43432300	0.11056600	-0.53458200	
C	-3.70721100	0.62642200	-0.29818900	
C	-2.24783000	-1.26976100	-0.48024900	
C	-4.77086900	-0.21598500	0.00129500	
H	-3.86274200	1.69901800	-0.33742200	
C	-3.30534000	-2.12084200	-0.18827100	
H	-1.26689700	-1.68080500	-0.68335300	
C	-4.56905100	-1.59313400	0.05745800	
H	-5.75844500	0.19603500	0.18470300	
H	-3.17113300	-3.19476200	-0.15068500	
C	2.17105500	0.33735500	-0.68232800	
C	3.47838100	0.81837200	-0.90048200	
C	2.00559600	-0.90229300	-0.09788000	
C	4.59631700	0.09389700	-0.52857400	
H	3.61067000	1.78098100	-1.38443800	
C	3.12471200	-1.66864200	0.28185700	
H	1.01799700	-1.31847000	0.06214500	
C	4.43101000	-1.15730600	0.06175500	
H	5.59863600	0.46241800	-0.70592200	
C	1.60743900	2.68437000	0.98195200	
H	1.91519000	1.81829100	1.57102800	
H	2.50495300	3.11602200	0.53395800	
H	1.18861000	3.43436800	1.65904000	
C	-0.69391700	0.95728600	1.68906400	
H	-0.26960800	1.52134000	2.52461100	
H	-1.68647500	0.60038600	1.96877100	
H	-0.05088400	0.09262000	1.51247300	
O	-1.67467600	2.91765800	0.66433600	
H	-1.59011500	3.21667600	1.57329700	
O	-5.57251600	-2.47051300	0.34131700	
H	-6.39456900	-1.99187200	0.47558800	
O	5.48973100	-1.88989300	0.41523800	
H	5.15589700	-2.71882700	0.79141700	
O	3.02329900	-2.86594700	0.83017000	
H	2.76669500	-3.59055100	0.02040800	
H	2.40177400	-2.59499900	-2.20936300	
O	2.61521800	-4.10220100	-1.13295400	
O	3.14771800	-3.16081500	-1.95040400	
Name				2-O14-H-OOH-P
Cartesian Coordinates				Frequency and Energy
C	-0.78285700	1.82607200	0.46908700	Zero-point correction= 0.365878 (Hartree/Particle)
C	0.57935800	2.31564000	-0.07369900	Thermal correction to Energy= 0.389721
C	0.98282700	1.20249500	-1.09039900	Thermal correction to Enthalpy= 0.390666
C	-1.31117100	1.07476200	-0.77175400	Thermal correction to Gibbs Free Energy= 0.310999
H	0.34228800	3.20986600	-0.65671500	Sum of electronic and zero-point Energies= -1224.502123
H	1.22856500	1.67424500	-2.04898100	Sum of electronic and thermal Energies= -1224.478280
H	-1.63217500	1.84264200	-1.49045800	Sum of electronic and thermal Enthalpies= -1224.477335
O	-0.17491800	0.38586800	-1.26428400	Sum of electronic and thermal Free Energies= -1224.557002
C	-2.44643000	0.12165000	-0.52476200	
C	-3.73816900	0.62572200	-0.38051500	
C	-2.24319600	-1.25020600	-0.37457500	
C	-4.80456400	-0.21410900	-0.08005600	
H	-3.91321000	1.68984800	-0.49818600	
C	-3.30175900	-2.10121200	-0.08206400	

H	-1.24725300	-1.65853100	-0.49697800	
C	-4.58460100	-1.58166700	0.07092300	
H	-5.80622900	0.19003900	0.03051400	
H	-3.14784800	-3.16829500	0.02892400	
C	2.15396300	0.33569000	-0.69376400	
C	3.46281300	0.82644100	-0.88760300	
C	1.98670600	-0.91620200	-0.13697400	
C	4.57903100	0.10137200	-0.51242300	
H	3.59699000	1.79904000	-1.35038900	
C	3.10521000	-1.68097500	0.24551400	
H	0.99904400	-1.33832800	0.00807800	
C	4.41119100	-1.15916500	0.05741700	
H	5.58054300	0.48418200	-0.66709800	
C	1.61310100	2.68634600	0.97915600	
H	1.92982000	1.82246500	1.56733800	
H	2.50259300	3.12290700	0.51889700	
H	1.19976900	3.43493900	1.66176300	
C	-0.67392000	0.93720000	1.69721600	
H	-0.23412900	1.49136500	2.53119700	
H	-1.66415000	0.58729000	1.99583900	
H	-0.04076100	0.06812600	1.50430400	
O	-1.66959400	2.90789200	0.71715900	
H	-1.51800900	3.22995500	1.61186600	
O	-5.58869500	-2.45486700	0.35979600	
H	-6.42200700	-1.97726200	0.43958000	
O	5.47226100	-1.88671500	0.42220800	
H	5.14681700	-2.71964600	0.79840700	
O	2.99991300	-2.88668000	0.78799700	
H	2.79710900	-3.60315700	-0.01469400	
H	2.47642400	-2.63879400	-2.27172800	
O	2.70993700	-4.14916300	-1.19784700	
O	3.23232900	-3.18866600	-1.99817400	
Name				2-O14-H-OOH-W
Cartesian Coordinates				Frequency and Energy
C	-0.80962600	1.79814400	0.51732300	Zero-point correction= 0.365132 (Hartree/Particle)
C	0.53725500	2.29652200	-0.04818400	Thermal correction to Energy= 0.388878
C	0.92549100	1.19238500	-1.07874000	Thermal correction to Enthalpy= 0.389822
C	-1.36966600	1.07411200	-0.72381400	Thermal correction to Gibbs Free Energy= 0.310957
H	0.29141900	3.19221700	-0.62464700	Sum of electronic and zero-point Energies= -1224.511727
H	1.15676200	1.67209400	-2.03527600	Sum of electronic and thermal Energies= -1224.487981
H	-1.68812700	1.85475200	-1.42792600	Sum of electronic and thermal Enthalpies= -1224.487037
O	-0.24323500	0.37979400	-1.24589700	Sum of electronic and thermal Free Energies= -1224.565902
C	-2.51425800	0.13165400	-0.48370300	
C	-3.81990400	0.61707800	-0.54048600	
C	-2.31226100	-1.20830500	-0.14608400	
C	-4.90530800	-0.20562400	-0.25681900	
H	-3.99498200	1.65254300	-0.81393800	
C	-3.38699200	-2.04390900	0.12904200	
H	-1.30538700	-1.60608600	-0.09820300	
C	-4.68390100	-1.53813700	0.07786000	
H	-5.91956500	0.17640400	-0.30443400	
H	-3.23349100	-3.08573600	0.38538800	
C	2.10274200	0.32603100	-0.70496700	
C	3.40287200	0.83927300	-0.90947600	

C	1.95910800	-0.93537500	-0.16605900	
C	4.53152500	0.12576000	-0.55588600	
H	3.51545800	1.82051200	-1.35875600	
C	3.09132400	-1.68516900	0.19902700	
H	0.98348600	-1.38003700	-0.01276200	
C	4.38703900	-1.14186700	0.00635500	
H	5.52628600	0.52392700	-0.71439100	
C	1.58432900	2.66253200	0.99221700	
H	1.91485400	1.79292600	1.56411300	
H	2.46101300	3.11234900	0.52113900	
H	1.16839500	3.39522800	1.68995800	
C	-0.66877100	0.89392900	1.73062200	
H	-0.21871600	1.44910500	2.55721600	
H	-1.64971800	0.53539000	2.04803700	
H	-0.03257200	0.03311600	1.51179900	
O	-1.69044800	2.87726700	0.81307300	
H	-1.38015800	3.30480300	1.62095100	
O	-5.71343700	-2.40053200	0.35941700	
H	-6.55643500	-1.93529900	0.28807900	
O	5.47772000	-1.85166500	0.34780300	
H	5.19990900	-2.68715300	0.75566000	
O	2.98953200	-2.90307200	0.73756300	
H	3.13341300	-3.63066000	-0.04790200	
H	2.85102300	-2.78674900	-2.38192600	
O	3.36346200	-4.18552800	-1.24604800	
O	3.68550000	-3.09852300	-1.98725700	
Name				2-O15-H-OOH-G
Cartesian Coordinates				Frequency and Energy
C	-0.78179400	1.83766000	0.46349100	Zero-point correction= 0.366291 (Hartree/Particle)
C	0.58680900	2.32586800	-0.06541900	Thermal correction to Energy= 0.390251
C	0.98854000	1.21563200	-1.09082000	Thermal correction to Enthalpy= 0.391195
C	-1.30032700	1.08665600	-0.78090600	Thermal correction to Gibbs Free Energy= 0.310814
H	0.35468600	3.22789000	-0.63849400	Sum of electronic and zero-point Energies= -1224.468737
H	1.22673800	1.69100800	-2.05058600	Sum of electronic and thermal Energies= -1224.444776
H	-1.61091600	1.85616800	-1.50334300	Sum of electronic and thermal Enthalpies= -1224.443832
O	-0.16116500	0.39611100	-1.25873000	Sum of electronic and thermal Free Energies= -1224.524213
C	-2.43885900	0.13610700	-0.54082400	
C	-3.70495700	0.65038900	-0.26701100	
C	-2.25915400	-1.24613700	-0.53881700	
C	-4.76871300	-0.19649900	0.01910500	
H	-3.85494200	1.72449300	-0.26681400	
C	-3.31733000	-2.10110200	-0.26023200	
H	-1.28412100	-1.65419300	-0.77389900	
C	-4.57378500	-1.57584300	0.02402100	
H	-5.75111800	0.21389800	0.23169600	
H	-3.18907300	-3.17640800	-0.26316000	
C	2.17088400	0.36379100	-0.69928300	
C	3.46932100	0.87591000	-0.90469600	
C	1.99979400	-0.88932700	-0.13177500	
C	4.57819400	0.15460100	-0.51980400	
H	3.58963300	1.84814700	-1.37054800	
C	3.11347900	-1.63185000	0.25357900	
H	1.01171800	-1.31191800	-0.00678000	
C	4.42313600	-1.11337000	0.07241600	

H	5.58462000	0.53280300	-0.65848100	
C	1.61235400	2.68116500	1.00183300	
H	1.92593600	1.80633900	1.57491700	
H	2.50638600	3.12629400	0.56104800	
H	1.18936200	3.41574100	1.69315300	
C	-0.68500000	0.94257700	1.68878800	
H	-0.25601500	1.49176500	2.53179900	
H	-1.67701500	0.58304400	1.96693900	
H	-0.04469600	0.07975300	1.49427900	
O	-1.66451300	2.92331700	0.70157900	
H	-1.57300300	3.20772700	1.61456600	
O	-5.57808500	-2.45736100	0.29270500	
H	-6.39386600	-1.97885700	0.46131500	
O	5.44284200	-1.86225600	0.45813700	
H	5.85203000	-2.37206900	-0.43481100	
O	2.95913600	-2.83988500	0.80064400	
H	3.84196100	-3.18608400	1.00090700	
H	4.72904300	-1.82126600	-2.58927000	
O	5.94339600	-2.85369800	-1.62348500	
O	4.69233700	-2.66400500	-2.10895700	
Name				2-O15-H-OOH-P
Cartesian Coordinates				Frequency and Energy
C	-0.77997400	1.82736800	0.48231400	Zero-point correction= 0.365821 (Hartree/Particle)
C	0.58648200	2.31646000	-0.05225200	Thermal correction to Energy= 0.389675
C	0.98158700	1.21332900	-1.08638500	Thermal correction to Enthalpy= 0.390619
C	-1.30988700	1.09054400	-0.76611700	Thermal correction to Gibbs Free Energy= 0.310906
H	0.35620800	3.21977900	-0.62353100	Sum of electronic and zero-point Energies= -1224.502302
H	1.22244700	1.69627700	-2.04068100	Sum of electronic and thermal Energies= -1224.478448
H	-1.62497700	1.86639100	-1.47894000	Sum of electronic and thermal Enthalpies= -1224.477504
O	-0.17599500	0.40027400	-1.26188000	Sum of electronic and thermal Free Energies= -1224.557217
C	-2.44989700	0.14022100	-0.53077000	
C	-3.73809300	0.64941400	-0.37339200	
C	-2.25386400	-1.23523800	-0.40647900	
C	-4.80848200	-0.18960900	-0.08527900	
H	-3.90714900	1.71652800	-0.47106600	
C	-3.31682900	-2.08511600	-0.12648700	
H	-1.26079800	-1.64695300	-0.54067000	
C	-4.59614800	-1.56103700	0.03959300	
H	-5.80738800	0.21831500	0.03573100	
H	-3.16889600	-3.15499400	-0.03636300	
C	2.15940900	0.35162000	-0.70424200	
C	3.45939800	0.86198300	-0.90804500	
C	1.98570300	-0.90682500	-0.14676900	
C	4.56644300	0.13470200	-0.53059500	
H	3.58188000	1.83789400	-1.36527800	
C	3.09782300	-1.65487700	0.22911700	
H	0.99592000	-1.32454000	-0.01436900	
C	4.40699700	-1.13810400	0.04956700	
H	5.57265100	0.51523700	-0.66977000	
C	1.61922100	2.66658400	1.00884900	
H	1.93276900	1.79233000	1.58347700	
H	2.51062000	3.10932100	0.55910400	
H	1.20449600	3.40375500	1.70290300	
C	-0.67805100	0.92577400	1.70166300	

H	-0.23742600	1.46910400	2.54226600	
H	-1.67082200	0.57806700	1.99427800	
H	-0.04928900	0.05529900	1.50096300	
O	-1.66042100	2.91203200	0.73927200	
H	-1.51179100	3.22177300	1.63881800	
O	-5.60493100	-2.43342400	0.31483800	
H	-6.43542300	-1.95248900	0.40332000	
O	5.42763700	-1.88998200	0.44094500	
H	5.86750300	-2.35252700	-0.44259500	
O	2.93932700	-2.86849500	0.76972200	
H	3.81894400	-3.21971800	0.97874500	
H	4.85791200	-1.70967100	-2.62195500	
O	6.01910200	-2.81490600	-1.66324700	
O	4.79993900	-2.58914200	-2.20835300	
Name				2-O15-H-OOH-W
Cartesian Coordinates				Frequency and Energy
C	-0.76704100	1.81113400	0.54794100	Zero-point correction= 0.365126 (Hartree/Particle)
C	0.57940200	2.33670200	0.00351000	Thermal correction to Energy= 0.388921
C	0.98087000	1.26433500	-1.05768100	Thermal correction to Enthalpy= 0.389865
C	-1.31205900	1.10822000	-0.71182400	Thermal correction to Gibbs Free Energy= 0.310771
H	0.32934800	3.24556100	-0.54972400	Sum of electronic and zero-point Energies= -1224.512395
H	1.20428700	1.77264000	-2.00122300	Sum of electronic and thermal Energies= -1224.488601
H	-1.63672300	1.90038100	-1.40003200	Sum of electronic and thermal Enthalpies= -1224.487657
O	-0.17446500	0.43970100	-1.24371900	Sum of electronic and thermal Free Energies= -1224.566751
C	-2.44436200	0.14412700	-0.50100900	
C	-3.75733500	0.60915200	-0.55873900	
C	-2.22298500	-1.20013300	-0.19388800	
C	-4.83170500	-0.23843600	-0.30702300	
H	-3.94713900	1.64803800	-0.80835600	
C	-3.28594800	-2.06022800	0.04827200	
H	-1.21018800	-1.58227900	-0.14498400	
C	-4.59081200	-1.57552700	-0.00498000	
H	-5.85169300	0.12806000	-0.35500800	
H	-3.11737900	-3.10555200	0.27965600	
C	2.17439500	0.41273800	-0.70760800	
C	3.46081700	0.95447300	-0.92092000	
C	2.03691500	-0.86052700	-0.17610300	
C	4.58803300	0.23770200	-0.59037500	
H	3.55316000	1.94418000	-1.35422800	
C	3.17148100	-1.59201900	0.16424400	
H	1.06224000	-1.30637800	-0.02502600	
C	4.46556600	-1.04733700	-0.03243900	
H	5.58342900	0.63599700	-0.74884500	
C	1.61725500	2.68253500	1.05991400	
H	1.95467600	1.79985200	1.60751100	
H	2.49096700	3.15626000	0.60763900	
H	1.18842400	3.38869400	1.77683300	
C	-0.62604900	0.88366200	1.74318800	
H	-0.18799300	1.42598500	2.58463400	
H	-1.60580600	0.50910600	2.04531600	
H	0.02011800	0.03378700	1.51214200	
O	-1.66029300	2.87526200	0.85980300	
H	-1.37401800	3.27367400	1.69104800	
O	-5.60693900	-2.46403900	0.24171600	

H	-6.45814800	-2.01469700	0.16825100	
O	5.52750200	-1.77537600	0.32458800	
H	5.72236500	-2.49406200	-0.45434100	
O	3.03091600	-2.82921500	0.67817700	
H	3.90553400	-3.18475400	0.90048100	
H	4.79713400	-1.94121800	-2.69831200	
O	5.63803700	-3.19973800	-1.59675800	
O	4.51009400	-2.68771900	-2.14174400	
Name				3-C2-H-OOH-G
Cartesian Coordinates				Frequency and Energy
C	-0.92064500	2.04107200	0.01370400	Zero-point correction= 0.362249 (Hartree/Particle)
C	0.50521400	1.68210200	0.50461200	Thermal correction to Energy= 0.385005
C	0.99277500	0.80751000	-0.65244300	Thermal correction to Enthalpy= 0.385949
C	-1.29594800	0.80325200	-0.89004800	Thermal correction to Gibbs Free Energy= 0.308972
H	1.08829900	2.60408300	0.57787200	Sum of electronic and zero-point Energies= -1149.242951
H	1.23228100	1.60806300	-1.55376300	Sum of electronic and thermal Energies= -1149.220195
H	-1.58618000	1.21240100	-1.86366100	Sum of electronic and thermal Enthalpies= -1149.219250
O	-0.09148500	0.04662900	-1.05898100	Sum of electronic and thermal Free Energies= -1149.296227
C	-2.38939900	-0.10635400	-0.39367400	
C	-3.71912800	0.25221600	-0.60141600	
C	-2.11775000	-1.28911200	0.29335900	
C	-4.75745300	-0.52975700	-0.11063200	
H	-3.95018000	1.15680000	-1.15528500	
C	-3.14568900	-2.08262100	0.78358200	
H	-1.08836000	-1.59957600	0.42802300	
C	-4.46920600	-1.69901600	0.58857700	
H	-5.78903400	-0.23736800	-0.28017900	
H	-2.94289500	-3.00510300	1.31345600	
C	2.24664800	0.02582800	-0.54121900	
C	2.33590300	-1.27354400	-1.04194700	
C	3.38832100	0.61159100	0.02383900	
C	3.53113900	-1.97705500	-0.97165000	
H	1.45942400	-1.73048700	-1.48413100	
C	4.58468800	-0.08239600	0.09246900	
H	3.33125800	1.62000400	0.41964300	
C	4.65746300	-1.38216900	-0.40754300	
H	3.58978200	-2.99024900	-1.35702800	
C	0.54376000	0.92131400	1.83198100	
H	-0.05730100	0.01033900	1.77916200	
H	1.56636300	0.63620800	2.08301800	
H	0.15329800	1.54002800	2.64097900	
C	-1.91300900	2.33349900	1.12465800	
H	-1.53438500	3.15876700	1.73083300	
H	-2.86317700	2.64290800	0.68632300	
H	-2.09153700	1.46415000	1.75723700	
O	-0.89913600	3.21696800	-0.77955400	
H	-0.13943600	3.20951300	-1.37948800	
O	-5.43968600	-2.51220200	1.09197900	
H	-6.30583500	-2.14603000	0.89526700	
O	5.85423600	-2.01963100	-0.31236800	
H	5.78377600	-2.90627500	-0.67644200	
H	5.46981400	0.35727800	0.53494900	
H	3.37142500	2.81259600	-2.11884300	
O	1.52787700	2.68158100	-2.32828900	

O	2.61267200	3.23542000	-1.69201300	
Name				3-C2-H-OOH-P
Cartesian Coordinates				Frequency and Energy
C	-0.91262400	2.04192800	0.03501900	Zero-point correction= 0.361406 (Hartree/Particle)
C	0.51193700	1.67577300	0.52321500	Thermal correction to Energy= 0.384277
C	0.99845400	0.81088300	-0.64293000	Thermal correction to Enthalpy= 0.385221
C	-1.29388300	0.81580500	-0.87917500	Thermal correction to Gibbs Free Energy= 0.307365
H	1.09816900	2.59436400	0.60659900	Sum of electronic and zero-point Energies= -1149.275152
H	1.23899300	1.61145000	-1.53768600	Sum of electronic and thermal Energies= -1149.252281
H	-1.59026100	1.23063400	-1.84859000	Sum of electronic and thermal Enthalpies= -1149.251337
O	-0.08908800	0.06027300	-1.06143500	Sum of electronic and thermal Free Energies= -1149.329193
C	-2.38744300	-0.09914400	-0.39042100	
C	-3.71771600	0.25463400	-0.61130700	
C	-2.11759800	-1.28060300	0.30013100	
C	-4.75870200	-0.53186000	-0.13249800	
H	-3.94796600	1.15832800	-1.16737500	
C	-3.14834300	-2.07953900	0.77882700	
H	-1.08974200	-1.58859900	0.45289900	
C	-4.47182800	-1.70093300	0.56932100	
H	-5.79071200	-0.24602100	-0.31163100	
H	-2.94100900	-3.00039100	1.31135000	
C	2.24951600	0.02215000	-0.53548400	
C	2.33494700	-1.28200700	-1.02662600	
C	3.39446900	0.61100400	0.01981300	
C	3.52862800	-1.98884200	-0.95492100	
H	1.45939000	-1.74709700	-1.46278200	
C	4.58976200	-0.08511600	0.09032700	
H	3.34382100	1.62162800	0.41136500	
C	4.65789600	-1.39025600	-0.39860100	
H	3.58472100	-3.00583200	-1.33126500	
C	0.55308700	0.90895000	1.84583900	
H	-0.03524100	-0.01048600	1.79284800	
H	1.57936900	0.63857200	2.09998300	
H	0.15612700	1.52224400	2.65643600	
C	-1.90437200	2.33364800	1.14456700	
H	-1.52712900	3.15541700	1.75738700	
H	-2.85812900	2.64081600	0.71048500	
H	-2.07924200	1.46371100	1.77769100	
O	-0.87703700	3.22620800	-0.75526300	
H	-0.13867100	3.18452900	-1.38027500	
O	-5.44601500	-2.51469900	1.06005200	
H	-6.31258600	-2.14811600	0.85090500	
O	5.85048000	-2.03142400	-0.30262300	
H	5.77419500	-2.92230200	-0.66381100	
H	5.47481500	0.36290500	0.52604500	
H	3.33179800	2.86747800	-2.19305300	
O	1.48825000	2.66130400	-2.38415800	
O	2.55607800	3.30180400	-1.80427000	
Name				3-C2-H-OOH-W
Cartesian Coordinates				Frequency and Energy
C	-0.89989300	2.05989700	0.04199300	Zero-point correction= 0.360650 (Hartree/Particle)
C	0.51978000	1.66586800	0.51536000	Thermal correction to Energy= 0.383583
C	1.00364500	0.84208500	-0.68027300	Thermal correction to Enthalpy= 0.384527
C	-1.30470600	0.87098800	-0.90093800	Thermal correction to Gibbs Free Energy= 0.306624

H	1.11641200	2.57398000	0.62903000	Sum of electronic and zero-point Energies=	-1149.283036
H	1.28070000	1.67015000	-1.52965300	Sum of electronic and thermal Energies=	-1149.260102
H	-1.63873800	1.31409400	-1.84421400	Sum of electronic and thermal Enthalpies=	-1149.259158
O	-0.09915200	0.13313400	-1.15356900	Sum of electronic and thermal Free Energies=	-1149.337062
C	-2.37353000	-0.06972000	-0.40459300		
C	-3.71347700	0.27880300	-0.57732500		
C	-2.07205100	-1.26999900	0.23835300		
C	-4.73411900	-0.53454400	-0.09987700		
H	-3.96493300	1.19969700	-1.09412300		
C	-3.08287400	-2.09736600	0.71424400		
H	-1.03835500	-1.57201100	0.36084200		
C	-4.41339500	-1.72438000	0.54975400		
H	-5.77486100	-0.26017900	-0.23651200		
H	-2.85103200	-3.03326700	1.20923600		
C	2.23079900	0.01550000	-0.57471100		
C	2.26766000	-1.31591400	-0.99218400		
C	3.40195700	0.60345600	-0.07679700		
C	3.44374200	-2.05236100	-0.90553700		
H	1.37312200	-1.78528800	-1.38268500		
C	4.57878100	-0.12171100	0.00926600		
H	3.38507500	1.63716900	0.25306800		
C	4.59730500	-1.45343400	-0.40656200		
H	3.47191000	-3.08942300	-1.22266900		
C	0.55786200	0.85620100	1.81185600		
H	-0.03002900	-0.06083500	1.72630600		
H	1.58598400	0.58230000	2.05431700		
H	0.16110800	1.44481400	2.64029300		
C	-1.88236700	2.34313600	1.16076400		
H	-1.49326200	3.14863000	1.78764000		
H	-2.83922700	2.65894000	0.73943100		
H	-2.05225400	1.46262800	1.77997000		
O	-0.84520300	3.26841600	-0.72572400		
H	-0.17516500	3.19129200	-1.42253200		
O	-5.37659600	-2.57284100	1.03497000		
H	-6.25256100	-2.20989700	0.85297000		
O	5.78113800	-2.13111600	-0.29877700		
H	5.66592900	-3.04012300	-0.60355100		
H	5.48554900	0.32578700	0.39856100		
H	3.31381700	3.12566700	-1.81960300		
O	1.56549800	2.73292900	-2.36243900		
O	2.43957000	3.51202100	-1.64845300		
Name				3-C5-H-OOH-G	
Cartesian Coordinates				Frequency and Energy	
C	-0.76228700	2.03974700	0.22337800	Zero-point correction=	0.360953 (Hartree/Particle)
C	0.67620300	1.70582400	0.68846700	Thermal correction to Energy=	0.384176
C	1.20579200	0.99493700	-0.57211100	Thermal correction to Enthalpy=	0.385120
C	-1.05939500	0.84768700	-0.73365700	Thermal correction to Gibbs Free Energy=	0.306845
H	1.22331600	2.63560600	0.87110700	Sum of electronic and zero-point Energies=	-1149.235091
H	1.33512900	1.73508600	-1.37128200	Sum of electronic and thermal Energies=	-1149.211868
H	-1.34575100	1.40331200	-1.84729600	Sum of electronic and thermal Enthalpies=	-1149.210923
O	0.11663000	0.14021100	-0.92078200	Sum of electronic and thermal Free Energies=	-1149.289198
C	-2.22027800	-0.04877800	-0.49442300		
C	-3.51858400	0.43378100	-0.68418900		
C	-2.05191800	-1.38286100	-0.11308400		

C	-4.62119200	-0.38315700	-0.47028100	
H	-3.66132000	1.45531600	-1.02357500	
C	-3.14655800	-2.20579000	0.10322700	
H	-1.04807500	-1.77044100	0.01045400	
C	-4.43480700	-1.70584700	-0.07060500	
H	-5.62451300	0.00270500	-0.62187900	
H	-3.02567600	-3.23946800	0.40271600	
C	2.46703100	0.19841100	-0.39832900	
C	2.46354600	-1.18977600	-0.33462000	
C	3.68066200	0.87374300	-0.25293400	
C	3.64608000	-1.89317300	-0.12198200	
H	1.53154300	-1.72508200	-0.46538500	
C	4.86311600	0.18536200	-0.03410100	
H	3.70133900	1.95760700	-0.31538900	
C	4.84516700	-1.20648700	0.03291900	
H	3.63376400	-2.97804500	-0.08162700	
C	0.73409200	0.80481400	1.91881400	
H	0.18189800	-0.12442200	1.74824600	
H	1.76756800	0.54130000	2.14951300	
H	0.30555400	1.30068900	2.79100400	
C	-1.76786900	2.23302700	1.34840600	
H	-1.41347600	3.01358900	2.02964600	
H	-2.72875500	2.54507600	0.93775200	
H	-1.91854000	1.31723900	1.92061600	
O	-0.73758200	3.19951800	-0.60881400	
H	-0.57825800	3.96874400	-0.05363500	
O	-5.47211800	-2.55674400	0.15409100	
H	-6.30655200	-2.10511600	0.00201200	
O	6.03405500	-1.83764400	0.24615900	
H	5.89975200	-2.78892600	0.25480500	
H	5.80790000	0.70248400	0.07764000	
H	-2.84535800	0.11597800	-3.26891400	
O	-1.79112800	1.63397900	-3.00825000	
O	-1.95710600	0.38229700	-3.54968700	
Name				3-O9-H-OOH-G
Cartesian Coordinates				Frequency and Energy
C	-0.79693800	2.10360900	0.22399700	Zero-point correction= 0.361330 (Hartree/Particle)
C	0.61325100	1.68923500	0.70068600	Thermal correction to Energy= 0.384105
C	1.16944900	1.07282100	-0.59858100	Thermal correction to Enthalpy= 0.385049
C	-1.10955700	1.03291400	-0.88440500	Thermal correction to Gibbs Free Energy= 0.306874
H	1.17634100	2.58778800	0.97197600	Sum of electronic and zero-point Energies= -1149.239455
H	1.37008900	1.88460400	-1.31047900	Sum of electronic and thermal Energies= -1149.216680
H	-1.33726100	1.60595200	-1.79143200	Sum of electronic and thermal Enthalpies= -1149.215736
O	0.08202000	0.29196200	-1.07491600	Sum of electronic and thermal Free Energies= -1149.293911
C	-2.25625300	0.10244400	-0.59681100	
C	-3.56862300	0.55158000	-0.82387700	
C	-2.05075100	-1.18345500	-0.09435000	
C	-4.65064300	-0.25077900	-0.53675700	
H	-3.72307000	1.54273700	-1.23928400	
C	-3.12660200	-1.99952700	0.20961000	
H	-1.03727100	-1.53786600	0.04419200	
C	-4.45052000	-1.54299200	0.00540700	
H	-5.66901100	0.07737900	-0.70591700	
H	-2.98427100	-2.99878000	0.60238700	

C	2.39905900	0.22275700	-0.44241200	
C	2.34703000	-1.16523200	-0.49267400	
C	3.62747300	0.83855800	-0.19378100	
C	3.49492000	-1.92675400	-0.29011500	
H	1.40382200	-1.65291900	-0.70458100	
C	4.77577000	0.09178900	0.01625800	
H	3.68719400	1.92249500	-0.16509900	
C	4.70843000	-1.29943500	-0.03079700	
H	3.44442500	-3.01022700	-0.33825900	
C	0.61890700	0.70278600	1.86506500	
H	0.06061700	-0.20379000	1.61795000	
H	1.64131900	0.40858700	2.10778300	
H	0.17102800	1.14453400	2.75658900	
C	-1.83432500	2.23277900	1.32838900	
H	-1.48838800	2.95071100	2.07898100	
H	-2.77669700	2.59455000	0.91394000	
H	-2.02117900	1.28046300	1.82587000	
O	-0.71127700	3.33342700	-0.50090900	
H	-0.53655000	4.04322500	0.12437800	
O	-5.48537600	-2.28650200	0.31654100	
H	-5.47444000	-3.26106000	-0.26437800	
O	5.86512400	-1.98883800	0.17850600	
H	5.69674000	-2.93266900	0.11588100	
H	5.73144700	0.56293000	0.20933300	
H	-4.34161000	-3.41400600	-2.54716300	
O	-5.36678600	-4.10317300	-1.15749900	
O	-4.14349000	-3.83059000	-1.69519700	
Name				3-O9-H-OOH-P
Cartesian Coordinates				Frequency and Energy
C	-0.80458800	2.10413700	0.21529600	Zero-point correction= 0.360601 (Hartree/Particle)
C	0.60356800	1.69060900	0.69887100	Thermal correction to Energy= 0.383435
C	1.16934700	1.08119500	-0.59874500	Thermal correction to Enthalpy= 0.384379
C	-1.11884300	1.02715400	-0.88398300	Thermal correction to Gibbs Free Energy= 0.305345
H	1.16282400	2.58970200	0.97427200	Sum of electronic and zero-point Energies= -1149.272962
H	1.38535600	1.89671600	-1.30062500	Sum of electronic and thermal Energies= -1149.250129
H	-1.37988600	1.58884400	-1.78889600	Sum of electronic and thermal Enthalpies= -1149.249185
O	0.08412600	0.30698200	-1.09956400	Sum of electronic and thermal Free Energies= -1149.328218
C	-2.24243400	0.07373500	-0.57512200	
C	-3.56670500	0.49487600	-0.78796000	
C	-2.00379500	-1.20851400	-0.07349200	
C	-4.62867900	-0.33040300	-0.48723700	
H	-3.74839200	1.48214100	-1.20124900	
C	-3.05870100	-2.04766500	0.23818000	
H	-0.98326400	-1.54433400	0.06055200	
C	-4.39247500	-1.61764400	0.04898100	
H	-5.65420800	-0.01713800	-0.64544600	
H	-2.88759200	-3.04405500	0.62937300	
C	2.39488300	0.22434400	-0.44095700	
C	2.32514800	-1.16457300	-0.38837700	
C	3.64031300	0.83726100	-0.28689500	
C	3.47068900	-1.92890600	-0.18234300	
H	1.36892200	-1.65686400	-0.51856500	
C	4.78842800	0.08833900	-0.07298800	
H	3.71464800	1.91961400	-0.33645600	

C	4.70259400	-1.30199500	-0.02042400	
H	3.40646000	-3.01243900	-0.15038100	
C	0.60239500	0.70810400	1.86545700	
H	0.05179500	-0.20490700	1.62332500	
H	1.62456200	0.42453100	2.12461100	
H	0.14451400	1.15437900	2.75004500	
C	-1.84335900	2.25059500	1.31481700	
H	-1.49642400	2.98138500	2.05234000	
H	-2.78505200	2.60919000	0.89425800	
H	-2.03230900	1.30757800	1.82974100	
O	-0.70886300	3.33091900	-0.51753800	
H	-0.51154500	4.03626000	0.10929100	
O	-5.40822100	-2.39178200	0.37437800	
H	-5.44609400	-3.27820800	-0.30626600	
O	5.85594700	-1.99612200	0.18496900	
H	5.66878900	-2.94158800	0.19457600	
H	5.75504100	0.56369000	0.04584100	
H	-4.48856500	-3.09565600	-2.63746300	
O	-5.37411600	-4.04622400	-1.29944900	
O	-4.21267100	-3.65923900	-1.89470800	
Name				3-O9-H-OOH-W
Cartesian Coordinates				Frequency and Energy
C	0.12359400	2.39915400	0.02979500	Zero-point correction= 0.359648 (Hartree/Particle)
C	1.48690400	1.84592800	0.49805500	Thermal correction to Energy= 0.381617
C	1.85333100	0.95751300	-0.70435500	Thermal correction to Enthalpy= 0.382561
C	-0.44377400	1.22947200	-0.84696500	Thermal correction to Gibbs Free Energy= 0.307078
H	2.19177000	2.67749500	0.58187800	Sum of electronic and zero-point Energies= -1149.280394
H	2.14188800	1.60380000	-1.54142700	Sum of electronic and thermal Energies= -1149.258426
H	-0.71039400	1.66922200	-1.81451500	Sum of electronic and thermal Enthalpies= -1149.257481
O	0.62201700	0.30345000	-1.02481900	Sum of electronic and thermal Free Energies= -1149.332965
C	-1.65854000	0.52940900	-0.29973400	
C	-2.91534000	1.12279400	-0.49465300	
C	-1.56743200	-0.67920900	0.40347200	
C	-4.05505300	0.54574100	0.02515400	
H	-2.98436800	2.04519800	-1.06177100	
C	-2.70157800	-1.27627200	0.91964200	
H	-0.60208500	-1.15222600	0.53246600	
C	-3.96160900	-0.66387300	0.75115000	
H	-5.03214900	0.99451900	-0.11420800	
H	-2.64914900	-2.21301100	1.46239500	
C	2.93955400	-0.05482200	-0.47181800	
C	2.66851600	-1.34896000	-0.03099600	
C	4.27042800	0.32904800	-0.64455500	
C	3.70188000	-2.24353400	0.23110000	
H	1.64234500	-1.66787500	0.11003000	
C	5.31209800	-0.54959700	-0.37664100	
H	4.49570900	1.33160500	-0.99470100	
C	5.02301500	-1.83968600	0.06071700	
H	3.48966200	-3.25293900	0.56796400	
C	1.43128900	1.08305600	1.81695300	
H	0.73112600	0.24462500	1.77117600	
H	2.41756400	0.68703200	2.06692700	
H	1.11944100	1.74197500	2.62878900	
C	-0.78544100	2.89164400	1.14193400	

H	-0.26812800	3.67004500	1.70996500	
H	-1.69593100	3.31917600	0.71706700	
H	-1.06466800	2.08906800	1.82595200	
O	0.35005200	3.46830100	-0.90113800	
H	0.74838200	4.19957000	-0.41225900	
O	-5.05139000	-1.21416300	1.27931300	
H	-5.58301800	-1.77694200	0.48196200	
O	6.08080000	-2.68037500	0.30444500	
H	5.75303100	-3.54129100	0.59367000	
H	6.34534700	-0.25180200	-0.51155600	
H	-5.03047800	-1.30033800	-1.88438400	
O	-5.90098500	-2.35771000	-0.60660200	
O	-4.82386400	-2.11747200	-1.39681800	
Name				3-O15-H-OOH-G
Cartesian Coordinates				Frequency and Energy
C	-0.79409900	2.01054500	0.13503400	Zero-point correction= 0.361387 (Hartree/Particle)
C	0.62560000	1.61044900	0.59582200	Thermal correction to Energy= 0.384139
C	1.13237900	0.92106000	-0.68958500	Thermal correction to Enthalpy= 0.385083
C	-1.15749400	0.88779000	-0.89978100	Thermal correction to Gibbs Free Energy= 0.306852
H	1.20575100	2.51547900	0.80045300	Sum of electronic and zero-point Energies= -1149.239560
H	1.33022200	1.69581000	-1.44341700	Sum of electronic and thermal Energies= -1149.216808
H	-1.41181000	1.41294400	-1.82748100	Sum of electronic and thermal Enthalpies= -1149.215864
O	0.03033900	0.13148600	-1.09682300	Sum of electronic and thermal Free Energies= -1149.294095
C	-2.29330700	-0.02875100	-0.52486900	
C	-3.60516300	0.37819400	-0.75465700	
C	-2.07749000	-1.26957800	0.07370500	
C	-4.68062500	-0.41402700	-0.37077500	
H	-3.79302500	1.32902000	-1.24405000	
C	-3.14147500	-2.07428600	0.45594100	
H	-1.06184200	-1.61449800	0.22367800	
C	-4.44739800	-1.64306500	0.24069900	
H	-5.69757900	-0.08338400	-0.55754200	
H	-2.98115900	-3.04178700	0.91537600	
C	2.35631900	0.07134100	-0.51479800	
C	2.28154700	-1.32806100	-0.50736000	
C	3.59109600	0.69744800	-0.30718900	
C	3.41396100	-2.08691900	-0.28831800	
H	1.32450500	-1.80026100	-0.68944100	
C	4.72885900	-0.04681100	-0.06866200	
H	3.65099000	1.78097700	-0.33240800	
C	4.65746100	-1.46199900	-0.04191800	
H	3.38157000	-3.16980300	-0.27828400	
C	0.65876400	0.68695800	1.81051700	
H	0.08527200	-0.22528300	1.62993900	
H	1.68512700	0.39826000	2.04461500	
H	0.23923200	1.18152900	2.68786800	
C	-1.79778300	2.21392400	1.25829600	
H	-1.42887800	2.97386800	1.95495400	
H	-2.74916200	2.55378400	0.84557800	
H	-1.97714800	1.29302900	1.81384700	
O	-0.71027500	3.19923900	-0.65766600	
H	-0.52621200	3.94132000	-0.07404800	
O	-5.45473400	-2.46986200	0.63690700	
H	-6.30418400	-2.07493500	0.42367800	

O	5.71367200	-2.19243800	0.22721300	
H	6.53175200	-2.01007000	-0.53204900	
H	5.69081600	0.42270800	0.09658400	
H	5.94626500	-1.36598900	-2.92734200	
O	7.15054600	-1.82289200	-1.58627400	
O	6.40155000	-0.87824900	-2.22495200	
Name				3-O15-H-OOH-P
Cartesian Coordinates				Frequency and Energy
C	-0.78218600	2.07220300	0.16417000	Zero-point correction= 0.360557 (Hartree/Particle)
C	0.63434100	1.69924900	0.65724300	Thermal correction to Energy= 0.383304
C	1.19741900	1.05878000	-0.62953900	Thermal correction to Enthalpy= 0.384248
C	-1.09158800	0.96249300	-0.89899200	Thermal correction to Gibbs Free Energy= 0.305603
H	1.18226000	2.61429200	0.89949500	Sum of electronic and zero-point Energies= -1149.273413
H	1.40941300	1.85832400	-1.35206300	Sum of electronic and thermal Energies= -1149.250667
H	-1.36005800	1.49536500	-1.81814100	Sum of electronic and thermal Enthalpies= -1149.249723
O	0.12898700	0.25672900	-1.10379300	Sum of electronic and thermal Free Energies= -1149.328368
C	-2.19524000	-0.00863900	-0.56228800	
C	-3.51984100	0.35414100	-0.80190000	
C	-1.94116900	-1.25633800	0.00665300	
C	-4.57041600	-0.48868000	-0.45840500	
H	-3.73817200	1.31086800	-1.26679100	
C	-2.98040600	-2.11292500	0.34789400	
H	-0.91707900	-1.56839600	0.17191800	
C	-4.29871800	-1.72589200	0.12195100	
H	-5.59725500	-0.19278700	-0.65001300	
H	-2.78401700	-3.08501600	0.78495400	
C	2.43424600	0.23236600	-0.43898100	
C	2.39156900	-1.16639700	-0.43316700	
C	3.65462100	0.88877800	-0.21414000	
C	3.54103000	-1.89833400	-0.19562500	
H	1.44934900	-1.66755000	-0.61687000	
C	4.80941700	0.17219600	0.01704400	
H	3.68510300	1.97382700	-0.23174800	
C	4.77104900	-1.24161600	0.04018400	
H	3.52342300	-2.98328200	-0.17702900	
C	0.65871200	0.75183700	1.85269400	
H	0.12490100	-0.17831800	1.64213900	
H	1.68702400	0.49782500	2.11966000	
H	0.19496200	1.21686300	2.72438100	
C	-1.81940500	2.23631700	1.26171700	
H	-1.48852900	3.00030800	1.97265800	
H	-2.76920200	2.55697500	0.82866100	
H	-1.98783000	1.30697600	1.80717200	
O	-0.70224800	3.28005900	-0.60329000	
H	-0.52433300	4.00693600	0.00429900	
O	-5.28214100	-2.59834000	0.47471100	
H	-6.14351300	-2.22060900	0.26410200	
O	5.86458400	-1.93451700	0.29025900	
H	6.25142400	-2.35255100	-0.67591900	
H	5.76021900	0.66501500	0.18365700	
H	4.79098900	-2.22321100	-2.66148800	
O	6.44472600	-2.61845800	-1.88782700	
O	5.62633000	-1.74265400	-2.52859300	
Name				3-O15-H-OOH-W

Cartesian Coordinates				Frequency and Energy	
C	-1.68669700	2.10475600	-0.06067700	Zero-point correction=	0.360427 (Hartree/Particle)
C	-0.28490600	2.01091900	0.58048500	Thermal correction to Energy=	0.382077
C	0.48321600	1.31028000	-0.55970000	Thermal correction to Enthalpy=	0.383021
C	-1.74726100	0.84333300	-0.98423000	Thermal correction to Gibbs Free Energy=	0.308991
H	0.10412700	3.02063500	0.73361500	Sum of electronic and zero-point Energies=	-1149.279946
H	0.66536100	2.03759600	-1.36041400	Sum of electronic and thermal Energies=	-1149.258296
H	-2.01533700	1.20554500	-1.98248000	Sum of electronic and thermal Enthalpies=	-1149.257352
O	-0.42078500	0.31285900	-1.02089900	Sum of electronic and thermal Free Energies=	-1149.331382
C	-2.72195000	-0.23749400	-0.58863200		
C	-4.05878100	-0.11572000	-0.96925300		
C	-2.34240700	-1.34584200	0.16798300		
C	-5.00554600	-1.05737600	-0.58366900		
H	-4.36698400	0.72990300	-1.57628800		
C	-3.27652800	-2.30057700	0.55413900		
H	-1.30533100	-1.47438800	0.45386400		
C	-4.60949100	-2.14960300	0.18464000		
H	-6.04430400	-0.95665600	-0.88014400		
H	-2.98256200	-3.16431400	1.13920900		
C	1.78868000	0.69584400	-0.15443200		
C	1.90452700	-0.66676300	0.14282500		
C	2.90664800	1.53548000	-0.01442800		
C	3.10961500	-1.18378900	0.58115100		
H	1.04448200	-1.31553800	0.03312200		
C	4.11668900	1.03267700	0.41246400		
H	2.81046300	2.58961200	-0.25310400		
C	4.23293000	-0.33923500	0.72870700		
H	3.21798500	-2.23617400	0.82004100		
C	-0.24454200	1.23830000	1.89481100		
H	-0.62176800	0.21913700	1.77818800		
H	0.77895300	1.18124600	2.27171300		
H	-0.85001800	1.74004800	2.65111200		
C	-2.83305300	2.24824900	0.92391400		
H	-2.68027200	3.14582000	1.53009500		
H	-3.77551300	2.34983100	0.38161200		
H	-2.90785900	1.38631900	1.58785900		
O	-1.70278800	3.21837100	-0.96843500		
H	-1.63278800	4.02472300	-0.44205200		
O	-5.49703200	-3.11304100	0.59441300		
H	-6.38294400	-2.89212700	0.28104700		
O	5.38601300	-0.82171200	1.18070700		
H	5.84331400	-1.45410600	0.39302600		
H	4.98834700	1.66725100	0.52105700		
H	4.49426600	-2.15983100	-1.55534100		
O	6.16232300	-2.00138300	-0.71776200		
O	5.22621100	-1.51824000	-1.57581500		
Name				4-C2-H-OOH-G	
Cartesian Coordinates				Frequency and Energy	
C	0.57017500	1.65724600	-0.14641400	Zero-point correction=	0.366893 (Hartree/Particle)
C	-0.84782900	1.89097400	0.43243000	Thermal correction to Energy=	0.391255
C	-1.15572700	0.54330200	1.10721400	Thermal correction to Enthalpy=	0.392199
C	1.13219200	0.71720200	0.93938100	Thermal correction to Gibbs Free Energy=	0.311155
H	-0.72495700	2.65856500	1.20708200	Sum of electronic and zero-point Energies=	-1224.451633
H	-1.43173100	0.81638600	2.30972200	Sum of electronic and thermal Energies=	-1224.427270

H	1.32077200	1.33337500	1.82966500	Sum of electronic and thermal Enthalpies=	-1224.426326
O	0.04411400	-0.16850300	1.19535200	Sum of electronic and thermal Free Energies=	-1224.507371
C	2.36923000	-0.05272700	0.57664000		
C	2.34599500	-1.42206800	0.34041500		
C	3.57622500	0.63804600	0.43549600		
C	3.50571300	-2.09656200	-0.03333600		
H	1.41868700	-1.96859100	0.45866800		
C	4.73315500	-0.02311800	0.05705500		
H	3.59806000	1.70809800	0.61099200		
C	4.69834400	-1.39675700	-0.17791800		
H	3.48017200	-3.16766700	-0.20869100		
H	5.67286700	0.50262500	-0.05746000		
C	-2.27853500	-0.31032600	0.63546800		
C	-2.05101600	-1.50405600	-0.04812100		
C	-3.60017100	0.07572900	0.88919800		
C	-3.11443300	-2.27635700	-0.50008500		
H	-1.03259000	-1.82670500	-0.22632100		
C	-4.66562500	-0.68371200	0.44037500		
H	-3.79103900	0.97042900	1.47319600		
C	-4.42229800	-1.86401600	-0.26196600		
H	-2.92695400	-3.20170300	-1.03586600		
C	-1.85837400	2.39031000	-0.58814900		
H	-2.82827000	2.59190800	-0.12479800		
H	-2.02177500	1.64661700	-1.36927600		
C	0.55512100	1.00228300	-1.52207100		
H	0.11062100	1.67803900	-2.25609500		
H	1.57749600	0.77597800	-1.82751900		
H	-0.02158900	0.07309300	-1.50979600		
O	1.34754400	2.83515800	-0.15454100		
H	0.95010100	3.42545300	-0.80495800		
O	5.86542700	-1.99830400	-0.54202800		
H	5.72056900	-2.93955300	-0.66887900		
O	-5.50416200	-2.57400300	-0.67926100		
H	-5.21827700	-3.37434400	-1.12774700		
H	-5.69031000	-0.39575800	0.63857200		
O	-1.35303000	3.55911600	-1.23294800		
H	-1.53919800	4.32237600	-0.68031900		
H	-0.35940400	-0.75640200	3.71354200		
O	-1.37332900	0.80049900	3.57501000		
O	-1.29517600	-0.54541600	3.84502700		
Name				4-C5-H-OOH-G	
Cartesian Coordinates				Frequency and Energy	
C	0.53825700	1.65636700	-0.19282000	Zero-point correction=	0.367337 (Hartree/Particle)
C	-0.80880400	1.90573500	0.52393200	Thermal correction to Energy=	0.391565
C	-1.09579000	0.57278400	1.26441400	Thermal correction to Enthalpy=	0.392509
C	1.17358900	0.67325500	0.79443700	Thermal correction to Gibbs Free Energy=	0.312419
H	-0.59094100	2.66471500	1.28306600	Sum of electronic and zero-point Energies=	-1224.450322
H	-1.33583600	0.79612200	2.30976800	Sum of electronic and thermal Energies=	-1224.426094
H	1.44886900	1.38863000	1.81155900	Sum of electronic and thermal Enthalpies=	-1224.425150
O	0.14294000	-0.15095900	1.24182000	Sum of electronic and thermal Free Energies=	-1224.505240
C	2.40305400	-0.07385500	0.46831400		
C	2.51436700	-1.43855800	0.73808300		
C	3.50245900	0.60040200	-0.08416100		
C	3.68731700	-2.12344200	0.44558800		

H	1.67543300	-1.96355800	1.17708600	
C	4.67043300	-0.07775300	-0.37983600	
H	3.42692900	1.66454700	-0.27543300	
C	4.76522600	-1.44447100	-0.11453300	
H	3.76561700	-3.18544700	0.65662400	
H	5.52552400	0.43045500	-0.80763400	
C	-2.19691900	-0.29250600	0.69514800	
C	-1.93274100	-1.38622200	-0.12258200	
C	-3.52809500	0.01222400	0.99030500	
C	-2.97150900	-2.14044300	-0.66026400	
H	-0.90512300	-1.66330800	-0.32506000	
C	-4.57190100	-0.72606700	0.45648600	
H	-3.75378500	0.83813100	1.65854400	
C	-4.29200900	-1.80557300	-0.37945400	
H	-2.75166200	-2.99466600	-1.29311300	
C	-1.89884900	2.43572000	-0.39284700	
H	-2.82336900	2.63404000	0.15816200	
H	-2.13983000	1.71669400	-1.17700400	
C	0.39636200	1.04384000	-1.58534800	
H	-0.08319600	1.75712000	-2.26015900	
H	1.38584000	0.80273600	-1.97550800	
H	-0.20475900	0.13270300	-1.55934400	
O	1.32547300	2.82956500	-0.25229700	
H	0.85216900	3.44620400	-0.82295000	
O	5.93875300	-2.05948100	-0.42359400	
H	5.89615500	-2.98663500	-0.17480600	
O	-5.35085700	-2.50101100	-0.87672400	
H	-5.03813200	-3.22379100	-1.42725700	
H	-5.60492800	-0.49357400	0.68287100	
O	-1.44145600	3.61726200	-1.05116800	
H	-1.54471700	4.36257200	-0.45372600	
H	0.79864600	-0.02969000	3.60029800	
O	1.32878100	1.67568700	3.05649800	
O	1.62274400	0.47522900	3.66198000	
Name				4-O9-H-OOH-G
Cartesian Coordinates				Frequency and Energy
C	0.57066400	1.58159900	-0.03013700	Zero-point correction= 0.367361 (Hartree/Particle)
C	-0.82833900	1.83426500	0.57482700	Thermal correction to Energy= 0.391078
C	-1.16501700	0.50863900	1.31884000	Thermal correction to Enthalpy= 0.392022
C	1.13084000	0.61631900	1.03858600	Thermal correction to Gibbs Free Energy= 0.311504
H	-0.68421200	2.62339100	1.31927800	Sum of electronic and zero-point Energies= -1224.454750
H	-1.43745700	0.74543800	2.35402900	Sum of electronic and thermal Energies= -1224.431033
H	1.38196700	1.23168300	1.91574300	Sum of electronic and thermal Enthalpies= -1224.430088
O	0.04652300	-0.24330300	1.32841300	Sum of electronic and thermal Free Energies= -1224.510607
C	2.34037100	-0.17155600	0.62831000	
C	2.28166100	-1.55918400	0.44102500	
C	3.54222600	0.51102200	0.40159800	
C	3.40185700	-2.25617500	0.03285700	
H	1.35041500	-2.07534700	0.63691200	
C	4.66407300	-0.17212500	-0.02367900	
H	3.57468400	1.58522100	0.54570100	
C	4.61196100	-1.57386400	-0.22521900	
H	3.38376300	-3.32925800	-0.11543900	
H	5.60152800	0.33807600	-0.20826700	

C	-2.27896300	-0.31856400	0.71979100	
C	-2.02976900	-1.40164900	-0.11639100	
C	-3.60679400	0.01867500	0.99290200	
C	-3.07771600	-2.11434100	-0.69139600	
H	-1.00667100	-1.70166100	-0.30552400	
C	-4.66028200	-0.67782000	0.42200200	
H	-3.82218400	0.83760900	1.67315600	
C	-4.39388900	-1.74772300	-0.43015100	
H	-2.86915100	-2.96120700	-1.33789500	
C	-1.85127900	2.33335300	-0.42559200	
H	-2.79966500	2.56298500	0.07160500	
H	-2.04666400	1.57895800	-1.19511100	
C	0.54084400	0.95254900	-1.41846100	
H	0.08184200	1.64101800	-2.13032400	
H	1.56068500	0.74664500	-1.74634400	
H	-0.02538900	0.01844500	-1.41977700	
O	1.36315100	2.75219200	-0.02980900	
H	0.87980000	3.41651900	-0.53599000	
O	5.65641100	-2.23904800	-0.66256000	
H	6.51765100	-2.15294600	0.06357300	
O	-5.46159700	-2.40206500	-0.96445100	
H	-5.15750400	-3.13011100	-1.51286900	
H	-5.69086400	-0.42124300	0.63332700	
O	-1.28724100	3.51211600	-1.00026500	
H	-1.90200300	3.88754000	-1.63439400	
H	6.05714400	-1.81806700	2.54183200	
O	7.19575300	-2.10111100	1.09924200	
O	6.48672100	-1.24512200	1.88929900	
Name				4-O9-H-OOH-P
Cartesian Coordinates				Frequency and Energy
C	0.57407500	1.69963400	-0.10408800	Zero-point correction= 0.366632 (Hartree/Particle)
C	-0.82328700	1.91804800	0.51546100	Thermal correction to Energy= 0.390255
C	-1.09113300	0.61308900	1.31866700	Thermal correction to Enthalpy= 0.391200
C	1.19739700	0.81625200	1.00219900	Thermal correction to Gibbs Free Energy= 0.311874
H	-0.70171100	2.73733200	1.23063600	Sum of electronic and zero-point Energies= -1224.489482
H	-1.36619400	0.88494300	2.34339300	Sum of electronic and thermal Energies= -1224.465859
H	1.43691700	1.48190800	1.84432700	Sum of electronic and thermal Enthalpies= -1224.464915
O	0.16050300	-0.07905900	1.35191100	Sum of electronic and thermal Free Energies= -1224.544240
C	2.43336000	0.06791900	0.60083500	
C	2.39988200	-1.30058500	0.30934000	
C	3.63819800	0.77713900	0.46987600	
C	3.54323300	-1.95038100	-0.11795800	
H	1.46998600	-1.84381700	0.42202900	
C	4.78841200	0.13856600	0.05678200	
H	3.65544700	1.83692700	0.69952500	
C	4.75913300	-1.24015300	-0.25666100	
H	3.53199300	-3.00794500	-0.36196100	
H	5.72815600	0.66924400	-0.04146600	
C	-2.16716500	-0.29846900	0.77391200	
C	-1.87627700	-1.41107200	-0.01025200	
C	-3.50683300	-0.01255900	1.05114500	
C	-2.89441600	-2.20809500	-0.52685000	
H	-0.84369300	-1.67028200	-0.20967100	
C	-4.53189700	-0.79262100	0.53672300	

H	-3.75380700	0.83271500	1.68677100	
C	-4.22375200	-1.89412200	-0.26035600	
H	-2.65457800	-3.07726600	-1.13184900	
C	-1.88234400	2.33709600	-0.48326600	
H	-2.83107100	2.54417000	0.02260500	
H	-2.05722300	1.55344900	-1.22778300	
C	0.54912700	1.00221300	-1.45827100	
H	0.03999100	1.62884600	-2.19339100	
H	1.57082000	0.83279400	-1.80397800	
H	0.03132000	0.04160900	-1.40514800	
O	1.31002700	2.90668500	-0.18411700	
H	0.77359400	3.51557500	-0.70817500	
O	5.84650900	-1.84944800	-0.68333500	
H	6.21530100	-2.53156800	0.12880800	
O	-5.26082800	-2.63318100	-0.73962400	
H	-4.92245100	-3.36894300	-1.26245300	
H	-5.57019800	-0.57026200	0.75332300	
O	-1.38140100	3.52177300	-1.10682500	
H	-2.00808600	3.81561700	-1.77495200	
H	4.78255900	-2.88262300	2.10119800	
O	6.41527500	-3.11239000	1.22170600	
O	5.63701500	-2.41793100	2.09405600	
Name				4-O9-H-OOH-W
Cartesian Coordinates				Frequency and Energy
C	0.57581400	1.70552100	-0.14419400	Zero-point correction= 0.365799 (Hartree/Particle)
C	-0.82813700	1.93114900	0.45535000	Thermal correction to Energy= 0.389625
C	-1.08927700	0.65691300	1.30692300	Thermal correction to Enthalpy= 0.390570
C	1.20429400	0.86754900	0.99542600	Thermal correction to Gibbs Free Energy= 0.311069
H	-0.72529800	2.77646100	1.14190600	Sum of electronic and zero-point Energies= -1224.499451
H	-1.36723600	0.96744500	2.31825100	Sum of electronic and thermal Energies= -1224.475624
H	1.43019100	1.56090800	1.81663700	Sum of electronic and thermal Enthalpies= -1224.474680
O	0.17171400	-0.02656600	1.37218400	Sum of electronic and thermal Free Energies= -1224.554181
C	2.44848500	0.11982000	0.62224900	
C	2.40285200	-1.21200700	0.19118900	
C	3.67681000	0.79958100	0.65384300	
C	3.55784900	-1.85219600	-0.21513200	
H	1.45661500	-1.73834400	0.17363000	
C	4.83850800	0.17204900	0.25548100	
H	3.70735100	1.82512000	1.00504500	
C	4.79287500	-1.16418000	-0.19918000	
H	3.54279500	-2.88176000	-0.55572700	
H	5.79461500	0.68147500	0.27799800	
C	-2.15820900	-0.28097700	0.79570900	
C	-1.87243400	-1.39065500	0.00280900	
C	-3.49296100	-0.01243600	1.11063100	
C	-2.89314700	-2.20498600	-0.48079200	
H	-0.84518200	-1.63775100	-0.23584900	
C	-4.52154200	-0.80973800	0.62795300	
H	-3.73128200	0.83534700	1.74554100	
C	-4.21681800	-1.90705300	-0.17416200	
H	-2.66645500	-3.07116400	-1.09384200	
C	-1.89788000	2.28603100	-0.55627000	
H	-2.85427700	2.45921200	-0.05332400	
H	-2.03647100	1.48247200	-1.28631000	

C	0.57244800	0.97733300	-1.48034100	
H	0.05580400	1.57829000	-2.23129700	
H	1.59857200	0.81497100	-1.81633800	
H	0.06943000	0.01064700	-1.40602800	
O	1.30738800	2.92018500	-0.25316100	
H	0.81537000	3.48903800	-0.86086600	
O	5.90096900	-1.76107100	-0.62384700	
H	6.22153700	-2.50348500	0.14127500	
O	-5.26072500	-2.67310700	-0.62911900	
H	-4.91983200	-3.39232100	-1.17577200	
H	-5.55619200	-0.59855400	0.87163800	
O	-1.45956200	3.48014400	-1.20890500	
H	-2.10364400	3.71006700	-1.88724700	
H	4.65193100	-3.17765600	1.90845900	
O	6.39339800	-3.15628400	1.21755500	
O	5.44882800	-2.63466900	2.04282600	
Name				4-O15-H-OOH-G
Cartesian Coordinates				Frequency and Energy
C	0.57994700	1.66474400	-0.12287200	Zero-point correction= 0.367243 (Hartree/Particle)
C	-0.80216500	1.96924400	0.50041500	Thermal correction to Energy= 0.391003
C	-1.11809600	0.69331300	1.33913600	Thermal correction to Enthalpy= 0.391948
C	1.16796900	0.76610400	0.98532900	Thermal correction to Gibbs Free Energy= 0.311836
H	-0.63496100	2.80234600	1.18956400	Sum of electronic and zero-point Energies= -1224.453919
H	-1.36264600	0.99785800	2.36456400	Sum of electronic and thermal Energies= -1224.430159
H	1.43853500	1.43110400	1.81863400	Sum of electronic and thermal Enthalpies= -1224.429215
O	0.08118700	-0.06649800	1.35756000	Sum of electronic and thermal Free Energies= -1224.509327
C	2.35949500	-0.06276000	0.59603100	
C	2.29103700	-1.44629600	0.48672000	
C	3.56507500	0.58030800	0.30102200	
C	3.40346100	-2.18150800	0.08409700	
H	1.36651400	-1.95461900	0.73004800	
C	4.67500000	-0.14205300	-0.10584100	
H	3.62159900	1.66085300	0.37745700	
C	4.59402200	-1.52940400	-0.21500500	
H	3.34296200	-3.26288900	0.00797100	
H	5.61265800	0.34642400	-0.34007200	
C	-2.25754800	-0.15322800	0.82700700	
C	-2.03728900	-1.29878300	0.06035700	
C	-3.57705900	0.23573200	1.11811200	
C	-3.10400300	-2.02234400	-0.44485600	
H	-1.02011700	-1.61869400	-0.12594000	
C	-4.65019400	-0.47851000	0.63327400	
H	-3.74783400	1.10570700	1.74527200	
C	-4.43380100	-1.61654500	-0.18069900	
H	-2.94876400	-2.90957400	-1.04631200	
C	-1.85082800	2.40852200	-0.50235000	
H	-2.78448900	2.67856100	0.00279700	
H	-2.07056300	1.60622100	-1.21544500	
C	0.50738200	0.95140500	-1.46780600	
H	0.03335500	1.59604500	-2.21040800	
H	1.51726800	0.71574600	-1.80526900	
H	-0.06179200	0.02169200	-1.39522800	
O	1.37587800	2.82934800	-0.21708000	
H	0.89075700	3.45644000	-0.76668900	

O	5.71628300	-2.19219700	-0.61502800	
H	5.53968900	-3.13584400	-0.65118900	
O	-5.45899900	-2.26283200	-0.68014900	
H	-5.45737300	-3.35224600	-0.34941500	
H	-5.67317500	-0.19464400	0.84853500	
O	-1.29776600	3.54189300	-1.16861300	
H	-1.92382200	3.87141100	-1.81717800	
H	-4.39588800	-4.07256200	1.86508700	
O	-5.37637100	-4.37931800	0.31595100	
O	-4.17018300	-4.25344100	0.94053300	
Name				4-O15-H-OOH-P
Cartesian Coordinates				Frequency and Energy
C	0.57332200	1.65243800	-0.13432000	Zero-point correction= 0.366254 (Hartree/Particle)
C	-0.80584300	1.95748300	0.49240200	Thermal correction to Energy= 0.390108
C	-1.12216000	0.67960400	1.32557200	Thermal correction to Enthalpy= 0.391052
C	1.16973100	0.76799100	0.98137500	Thermal correction to Gibbs Free Energy= 0.310479
H	-0.63712100	2.78123100	1.19216600	Sum of electronic and zero-point Energies= -1224.489077
H	-1.38331300	0.98323700	2.34597800	Sum of electronic and thermal Energies= -1224.465223
H	1.43833300	1.43991200	1.80894500	Sum of electronic and thermal Enthalpies= -1224.464279
O	0.08844900	-0.07006800	1.36137600	Sum of electronic and thermal Free Energies= -1224.544852
C	2.36705400	-0.05595300	0.59945200	
C	2.26866400	-1.41402800	0.31158400	
C	3.61087400	0.56817900	0.47674300	
C	3.38591300	-2.13892500	-0.09487500	
H	1.31356500	-1.91482500	0.41430700	
C	4.72949600	-0.14142900	0.06525800	
H	3.70073200	1.62610100	0.70004200	
C	4.61612000	-1.50076300	-0.22215900	
H	3.30131100	-3.19991100	-0.31044000	
H	5.69508900	0.34071700	-0.03233700	
C	-2.24707000	-0.17939200	0.80250100	
C	-2.01112800	-1.33526400	0.05392500	
C	-3.57222800	0.20803000	1.07144400	
C	-3.06801100	-2.07220700	-0.45158500	
H	-0.99207900	-1.65546800	-0.12184800	
C	-4.63557200	-0.51860400	0.58220200	
H	-3.75571700	1.08728600	1.68121300	
C	-4.40109000	-1.66715200	-0.20968200	
H	-2.89758600	-2.96676200	-1.03952800	
C	-1.85408700	2.41016400	-0.50415600	
H	-2.78509100	2.68062000	0.00494400	
H	-2.07841600	1.62070400	-1.22970500	
C	0.49768100	0.92897400	-1.47253500	
H	0.01279500	1.56345700	-2.21749200	
H	1.50680000	0.70068000	-1.82024700	
H	-0.06416700	-0.00508300	-1.39428400	
O	1.36270500	2.82293600	-0.24993300	
H	0.85349200	3.44035200	-0.79039600	
O	5.74269900	-2.15614300	-0.61646000	
H	5.53780200	-3.08318500	-0.78254800	
O	-5.41758800	-2.33130400	-0.71907200	
H	-5.45814300	-3.36584600	-0.29105300	
H	-5.66098600	-0.22952900	0.78140300	
O	-1.29811300	3.55139900	-1.15923000	

H	-1.91489100	3.86226200	-1.82897100	
H	-4.56651800	-3.81881300	2.04221200	
O	-5.41344300	-4.35948400	0.47170300	
O	-4.26792100	-4.14938700	1.17813800	
Name				4-O15-H-OOH-W
Cartesian Coordinates				Frequency and Energy
C	0.57954400	1.60519500	-0.15553300	Zero-point correction= 0.366194 (Hartree/Particle)
C	-0.81465700	1.86171700	0.45718100	Thermal correction to Energy= 0.389807
C	-1.10420000	0.56411500	1.26981200	Thermal correction to Enthalpy= 0.390751
C	1.19094900	0.71843200	0.94999900	Thermal correction to Gibbs Free Energy= 0.311926
H	-0.68368800	2.67806400	1.17278100	Sum of electronic and zero-point Energies= -1224.499204
H	-1.37298500	0.84689100	2.29233200	Sum of electronic and thermal Energies= -1224.475592
H	1.42243400	1.37983600	1.79544200	Sum of electronic and thermal Enthalpies= -1224.474648
O	0.12771200	-0.16088300	1.29964300	Sum of electronic and thermal Free Energies= -1224.553473
C	2.42121400	-0.05821500	0.57821500	
C	2.34852300	-1.33489900	0.02126300	
C	3.67560900	0.53077300	0.74400300	
C	3.50135300	-2.01142100	-0.36172500	
H	1.38449000	-1.81140200	-0.11341600	
C	4.83480800	-0.12916600	0.35499000	
H	3.74844900	1.51835300	1.18769300	
C	4.74348200	-1.40346800	-0.19781600	
H	3.44493000	-3.00811000	-0.78685300	
H	5.80924700	0.32706700	0.48433000	
C	-2.20852900	-0.30879300	0.72933200	
C	-1.95229500	-1.42755400	-0.07509800	
C	-3.53550500	0.02978600	1.03918600	
C	-2.99511800	-2.18089900	-0.57917200	
H	-0.93023700	-1.70949300	-0.29332800	
C	-4.58738500	-0.70435200	0.53259700	
H	-3.72965000	0.87911000	1.68585600	
C	-4.32967300	-1.81938800	-0.29793200	
H	-2.81370000	-3.05083700	-1.19963600	
C	-1.87733400	2.28326100	-0.53725500	
H	-2.82480700	2.47842700	-0.02590300	
H	-2.04741100	1.50595800	-1.28937500	
C	0.54132200	0.92280800	-1.51452000	
H	0.04811100	1.56884200	-2.24373300	
H	1.55887800	0.72789900	-1.85785400	
H	-0.00067700	-0.02471700	-1.47070100	
O	1.34924600	2.79958700	-0.23162700	
H	0.87955900	3.39842800	-0.82755700	
O	5.91157300	-2.02562800	-0.56005400	
H	5.71567400	-2.89733200	-0.92626300	
O	-5.33513500	-2.51501900	-0.82010900	
H	-5.72993200	-3.20512600	-0.04136300	
H	-5.61694500	-0.45129400	0.75975800	
O	-1.39831800	3.47795300	-1.15784700	
H	-2.03249200	3.74537400	-1.83181400	
H	-5.12670400	-2.80539100	2.31517900	
O	-5.89631900	-3.90370700	1.00721900	
O	-4.82906400	-3.55655100	1.77170900	