Supporting Information (SI)

The radical scavenging activity of monocaffeoylquinic acids: The role of neighboring hydroxyl groups and pH levels

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Table of Contents

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]

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

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. 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. BDEs, PAs, and IEs (kcal/mol) of the CQAs and ΔG° (kcal/mol) of the CQAs + HOO• reactions in the examined media according to the FHT, SET, and PL mechanisms.

Comp.	positions	Pentyl ethanoate						water					
		FHT		PL		SET		FHT		PL		SET	
		BDE	ΔG°	PA	ΔG°	IE	ΔG°	BDE	ΔG°	PA	ΔG°	IE	ΔG°
3CQA	C2-RAD	99.8	13.3			136.9	74.5	100.6	10.8			103.3	22.8
	C3-RAD	95.9	8.9					97.5	7.3				
	C4-RAD	94.4	7.7					96.5	6.5				
	C5-RAD	96.8	10.2					98.3	8.4				
	C6-RAD	101.4	14.8					102.6	12.7				
	COO-RAD	113.8	27.5	66.7	85.2			111.7	22.1	30.9	38.5		
	O1-RAD	108.3	22.2	89.0	107.2			127.8	38.4	50.3	57.6		
	O4-RAD	106.4	20.3	104.1	122.9			108.5	19.2	58.8	66.6		
	O5-RAD	106.6	20.4	104.8	122.2			107.5	18.0	59.1	65.7		
	O61-RAD	81.1	-4.4	77.3	96.4			84.5	-4.2	42.9	51.0		
	O71-RAD	79.1	-6.2	73.7	92.9			82.8	-5.8	40.8	49.1		
4CQA	C2-RAD	97.3	11.1			130.3	68.2	97.7	8.2			93.5	13.2
	C3-RAD	92.1	4.9					93.8	3.4				
	C4-RAD	91.3	3.3					92.8	1.5				
	C5-RAD	88.3	1.7					90.2	0.4				
	C6-RAD	97.3	11.1					97.7	8.2				
	COO-RAD	114.1	27.3	55.7	74.2			112.3	22.3	27.2	34.7		
	O1-RAD	106.1	20.2	89.8	107.6			130.4	41.2	51.3	58.1		
	O3-RAD	107.5	20.4	88.7	108.6			108.8	18.5	49.3	58.3		
	O5-RAD	105.4	19.0	97.7	116.7			108.0	18.3	55.2	63.3		
	O61-RAD	81.3	-4.3	76.5	95.2			84.5	-4.4	43.2	51.0		
	O71-RAD	79.4	-5.9	72.6	91.5			82.7	-5.9	41.2	49.3		
5CQA	C2-RAD	99.3	12.8			139.6	76.9	100.3	10.5			102.1	21.3
	C3-RAD	93.3	7.5					95.7	6.6				
	C4-RAD	95.9	10.4					98.0	9.1				
	C5-RAD	98.5	11.7					99.5	9.4				
	C6-RAD	99.5	12.7					100.7	10.7				
	COO-RAD	113.9	27.9	64.0	82.7			114.4	25.2	29.0	36.8		
	O1-RAD	107.0	20.6	97.8	115.2			131.6	42.0	54.4	60.9		
	O3-RAD	107.3	21.0	92.0	111.9			108.9	19.4	51.7	60.7		
	O4-RAD	104.9	19.1	104.5	122.7			107.9	18.9	58.6	65.8		
	O61-RAD	81.9	-3.9	75.4	94.0			85.4	-3.6	42.7	50.4		

	O71-RAD	79.6	-6.1	74.0	92.7			83.2	-5.8	40.6	48.4		

Table S3. Selected BCP intermolecular contact parameters for the TSs-O6'-H-OOH

Contacts	ρ(r) (au)	$\nabla^2\rho(r)$ (au)	G(r)[a] (au)	V(r)[b] (au)	G(r)/|V(r)|	H(r)[c] (au)	E_{HB}[d] (kcal/.mol)
3CQA-ANION-O6'-H-OOH							
O6'···H41	0.2322	0.9017	0.0894	−0.4135	0.2163	−0.3241	−129.7
O44···H41	0.1262	0.0485	0.0832	−0.1543	0.5393	−0.0711	−48.4
C6'···O45	0.0182	0.0584	0.0135	−0.0123	1.0908	0.0011	−3.9
RCP	0.0156	0.0765	0.0171	−0.0151	1.1341	0.0020	−4.7
3CQA-DIANION-O6'-H-OOH							
O6'···H41	0.2008	−0.6287	0.1027	−0.3626	0.2833	−0.2599	−113.8
O43···H41	0.1551	−0.1450	0.0914	−0.2191	0.4173	−0.1277	−68.7
O7'···H42	0.0751	0.1730	0.0653	−0.0874	0.7473	−0.0221	−27.4
RCP	0.0105	0.0485	0.0108	−0.0096	1.1331	0.0013	−3.0
4CQA-ANION-O6'-H-OOH							
O6'···H41	0.2322	−0.9399	0.0893	−0.4136	0.2160	−0.3243	−129.8
O44···H41	0.1260	0.0488	0.0831	−0.1540	0.5396	−0.0709	−48.3
C6'···O45	0.0181	0.0584	0.0134	−0.0122	1.0966	0.0012	−3.8
RCP	0.0155	0.0760	0.0170	−0.0150	1.1345	0.0020	−4.7

4CQA-DIANION-O6'-H-OOH							
O6'···H41	0.1990	−0.6012	0.1033	−0.3568	0.2894	−0.2536	−112.0
O43···H41	0.1573	−0.1615	0.0918	−0.2239	0.4098	−0.1322	−70.3
O7'···H42	0.0740	0.1729	0.0645	−0.0858	0.7518	−0.0213	−26.9
RCP	0.0105	0.0484	0.0108	−0.0096	1.1332	0.0013	−3.0
5CQA-ANION-O6'-H-OOH							
O6'···H41	0.2285	−0.8867	0.0900	−0.4017	0.2241	−0.3117	−126.0
O44···H41	0.1293	0.0357	0.0842	−0.1594	0.5280	−0.0753	−50.0
C6'···O45	0.0182	0.0590	0.0135	−0.0123	1.0981	0.0012	−3.9
RCP	0.0156	0.0765	0.0171	−0.0151	1.1343	0.0020	−4.7
5CQA-DIANION-O6'-H-OOH							
O6'···H41	0.1926	−0.5154	0.1041	−0.3371	0.3089	−0.2330	−105.8
O43···H41	0.1632	−0.2127	0.0922	−0.2376	0.3881	−0.1454	−74.5
O7'···H42	0.0754	0.1733	0.0656	−0.0879	0.7465	−0.0223	−27.6
RCP	0.0107	0.0490	0.0110	−0.0097	1.1300	0.0013	−3.1

a) electron kinetic energy density; b) electron potential energy density; c) total electron energy density; d) individual energies of each hydrogen bond.

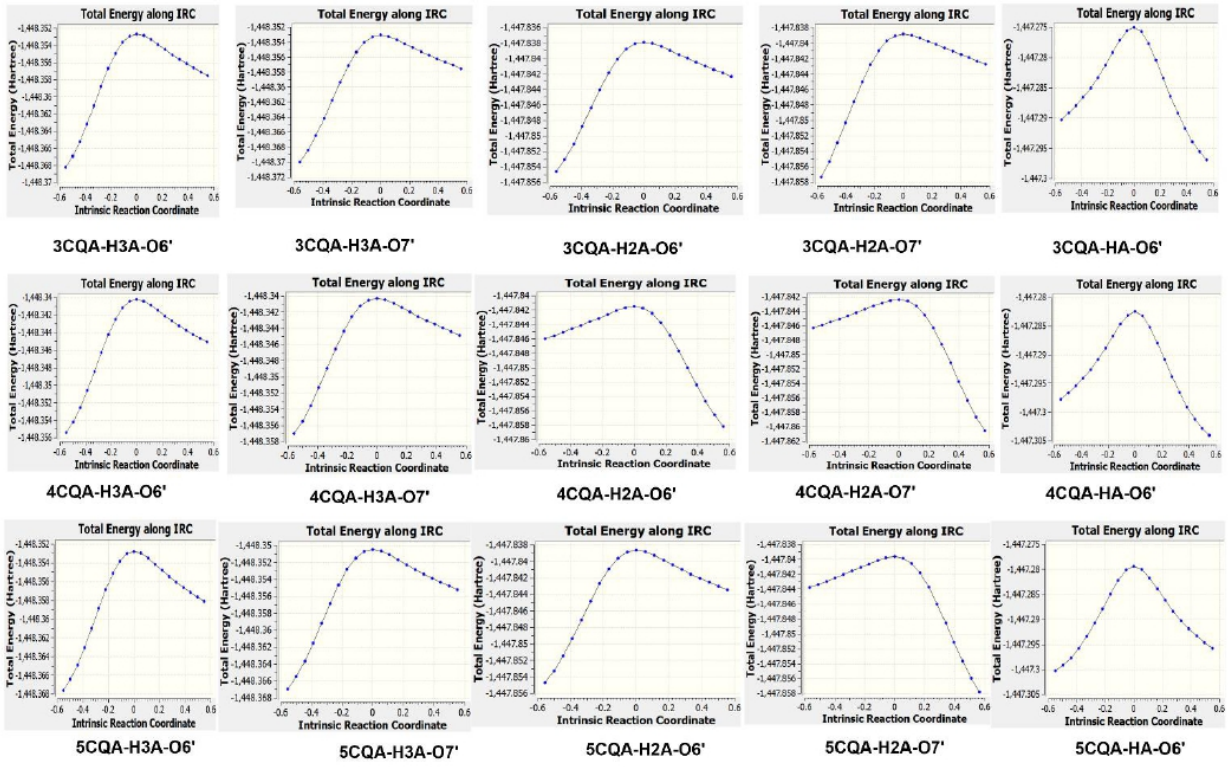

Figure S1. The IRC plots for the transition states of CQAs + HOO• reactions.

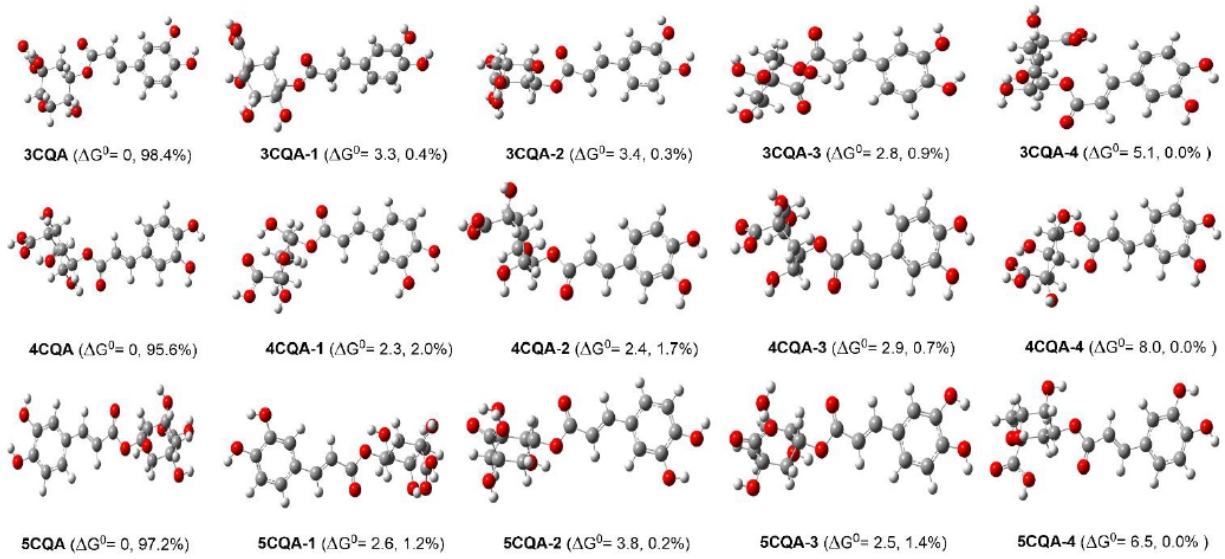

Figure S2. The typical conformers of CQA and the relative free energies ΔG° (in kcal/mol) compared with CQA conformers (3CQA, 4CQA, 5CQA)

Table S4: The Cartesian coordinates and energies of transition states of the reaction between the CQAs with HOO• in the studied media (P: pentyl ethanoate; W: water)

Name				**3CQA-O6'-H-OOH-P**
Cartesian Coordinates				Frequency and Energy
O	1.39807900	-0.84195200	0.73943600	Zero-point correction= 0.351552
O	5.43114500	0.16832800	1.36928400	(Hartree/Particle)
O	2.77676800	-2.85098600	-0.74976100	Thermal correction to Energy= 0.377817
O	5.35064000	-2.26039200	0.01674100	Thermal correction to Enthalpy= 0.378762
O	5.44937700	2.77953900	1.31510400	Thermal correction to Gibbs Free Energy= 0.291733
O	5.23836500	2.85049800	-0.91138900	Sum of electronic and zero-point Energies= -1448.040192
O	0.74357400	0.15291900	-1.17532700	Sum of electronic and thermal Energies= -1448.013926
O	-6.64098400	0.27123700	-1.41572800	Sum of electronic and thermal Enthalpies= -1448.012982
O	-7.37053400	-0.95431800	0.86646600	Sum of electronic and thermal Free Energies= -1448.100010
C	4.79568500	0.76611800	0.24381400	
C	2.80013000	-0.73343200	0.43850600	
C	3.26326800	0.72123300	0.38498800	
C	5.24614600	-0.01421300	-0.99020100	
C	3.20734200	-1.51012200	-0.81624300	
C	4.73295100	-1.45102300	-0.98094300	
C	5.19876800	2.23471600	0.11677500	
C	0.48131700	-0.39909000	-0.13353500	
C	-0.88292000	-0.67212300	0.36969600	
C	-1.94053800	-0.27827000	-0.34770200	
C	-3.35126700	-0.46369700	-0.00679200	
C	-4.31575600	0.00454300	-0.88738800	
C	-3.77194600	-1.10659200	1.18359800	
C	-5.68256600	-0.15008100	-0.60530900	
C	-5.10733400	-1.27645200	1.48181500	
C	-6.07547800	-0.80002000	0.59530300	
H	3.25873300	-1.22213100	1.30164100	
H	2.81349800	1.23268200	-0.46821300	
H	2.95739300	1.23860000	1.29993800	
H	6.33749700	-0.00956900	-1.04701900	
H	4.86031700	0.49334700	-1.87641300	
H	2.73998600	-1.06384300	-1.69484100	
H	4.97620700	-1.92212700	-1.93584100	
H	5.25670800	0.69407800	2.15978000	
H	3.40274500	-3.31233600	-0.17582200	
H	5.53037000	-1.70554900	0.78680400	
H	5.65289800	3.72053500	1.19510600	
H	-0.95961900	-1.19377000	1.31547700	
H	-1.74663300	0.23206700	-1.28842900	
H	-4.03410700	0.49525600	-1.81371700	
H	-3.03247600	-1.47839600	1.88271000	
H	-5.42337200	-1.76950300	2.39293200	
H	-6.78461300	1.35069000	-1.25009100	
H	-7.88003800	-0.58774800	0.12586200	
H	-5.20767800	2.47652100	0.31606700	
O	-6.76323300	2.52830600	-0.71497200	

O	-6.15127500	2.29460000	0.47211600	
Name				**3CQA-O7'-H-OOH-P**
Cartesian Coordinates				Frequency and Energy
O	-1.38916300	0.54916200	0.78192500	Zero-point correction= 0.351542
O	-5.52375200	0.05656000	1.36899100	(Hartree/Particle)
O	-2.48269300	2.84200300	-0.52279200	Thermal correction to Energy= 0.377821
O	-5.11494600	2.54732800	0.20737400	Thermal correction to Enthalpy= 0.378765
O	-5.90354400	-2.51302700	1.11916600	Thermal correction to Gibbs Free Energy= 0.291849
O	-5.69515200	-2.44713800	-1.10800700	Sum of electronic and zero-point Energies= -1448.040407
O	-0.87357700	-0.37008200	-1.21215700	Sum of electronic and thermal Energies= -1448.014128
O	6.33222500	-1.80180800	-1.38626300	Sum of electronic and thermal Enthalpies= -1448.013184
O	7.27826500	-0.70088600	0.88584700	Sum of electronic and thermal Free Energies= -1448.100099
C	-4.97469400	-0.53523900	0.19609900	
C	-2.79372200	0.65753500	0.48978000	
C	-3.45078600	-0.71156200	0.32667700	
C	-5.31152000	0.39191700	-0.97080800	
C	-3.08938400	1.58086500	-0.69475800	
C	-4.60839500	1.74107600	-0.85354100	
C	-5.57538600	-1.92088900	-0.03731100	
C	-0.54303900	0.05290600	-0.13094700	
C	0.84548600	0.08794100	0.38405900	
C	1.83978500	-0.40804600	-0.36031300	
C	3.25586900	-0.45364500	0.00542000	
C	4.13455300	-1.10350000	-0.86115800	
C	3.74827000	0.13200500	1.19624200	
C	5.48809700	-1.17756400	-0.55803600	
C	5.08584500	0.06224700	1.50498700	
C	5.98332700	-0.59130100	0.63587900	
H	-3.17990800	1.13257700	1.39473900	
H	-3.07404700	-1.21108300	-0.56796900	
H	-3.21980100	-1.33592300	1.19560500	
H	-6.39326500	0.53973200	-1.01937100	
H	-4.99515400	-0.09296000	-1.89640900	
H	-2.68297900	1.14842700	-1.60978500	
H	-4.78171700	2.31309200	-1.76768100	
H	-5.42712500	-0.54779800	2.11543700	
H	-3.04746100	3.33725000	0.08540900	
H	-5.37028000	1.96415300	0.93403700	
H	-6.23348100	-3.40596500	0.93167400	
H	0.99088500	0.51882100	1.36672200	
H	1.58377700	-0.82816000	-1.32995300	
H	3.77378800	-1.55287700	-1.77934800	
H	3.07122300	0.64005500	1.87117100	
H	5.48086300	0.50015100	2.41508200	
H	7.21821200	-1.76999000	-0.99293900	
H	7.76207400	0.24566200	0.62767000	
H	6.26456500	2.10258100	-0.11601200	
O	7.98893200	1.41982100	0.09930600	
O	6.89015400	1.60229000	-0.66985600	

Name				**3CQA-HA-O6'-H-OOH-W**
Cartesian Coordinates				Frequency and Energy
O	1.43993400	-0.79221900	0.72140200	Zero-point correction= 0.337209
O	5.41576200	0.16818200	1.42475000	(Hartree/Particle)
O	2.80768500	-2.79129600	-0.77589300	Thermal correction to Energy= 0.363276
O	5.41370300	-2.20385100	-0.00092300	Thermal correction to Enthalpy= 0.364220
O	6.19806200	2.58813400	1.08109600	Thermal correction to Gibbs Free Energy= 0.277766
O	4.91258200	2.98470000	-0.71061700	Sum of electronic and zero-point Energies= -1447.622799
O	0.77567100	0.17799400	-1.20372100	Sum of electronic and thermal Energies= -1447.596733
O	-6.61166000	-0.03204300	-1.48596600	Sum of electronic and thermal Enthalpies= -1447.595789
O	-7.31310100	-0.79375700	1.03827700	Sum of electronic and thermal Free Energies= -1447.682242
C	4.85016800	0.79950800	0.27200000	
C	2.85165700	-0.67987000	0.42768900	
C	3.32311600	0.76923000	0.39428800	
C	5.29169400	0.04227200	-0.98868700	
C	3.25896000	-1.44734000	-0.82988600	
C	4.78365300	-1.39653000	-0.99844300	
C	5.35892700	2.25960100	0.20466000	
C	0.51594700	-0.34032800	-0.13714900	
C	-0.84179600	-0.56146400	0.39620100	
C	-1.90765300	-0.24407600	-0.34825500	
C	-3.31086900	-0.39813900	0.03267500	
C	-4.28868500	-0.11797900	-0.90917600	
C	-3.70787100	-0.81575000	1.32788200	
C	-5.64841900	-0.26187500	-0.59597400	
C	-5.03697500	-0.94999500	1.66482400	
C	-6.02068300	-0.67383300	0.71175300	
H	3.29891000	-1.18334500	1.28804100	
H	2.89026500	1.29359400	-0.45786700	
H	3.01775400	1.27522500	1.31383000	
H	6.38303100	0.04590000	-1.05694500	
H	4.89246300	0.55837400	-1.86508300	
H	2.80295400	-0.99737900	-1.71150600	
H	5.02153200	-1.86510800	-1.95573400	
H	6.05047100	0.81646500	1.77601400	
H	3.35909700	-3.24964900	-0.12652100	
H	5.58136500	-1.63993900	0.76957800	
H	-0.91148800	-0.98907400	1.38848800	
H	-1.73551900	0.16345700	-1.34159200	
H	-4.02351600	0.20811400	-1.90909500	
H	-2.95648200	-1.02869200	2.07856800	
H	-5.33907000	-1.26085400	2.65728800	
H	-7.01006500	0.97011100	-1.30815600	
H	-7.86251500	-0.58209300	0.26631600	
H	-5.55803700	2.52421400	-0.02077400	
O	-7.22045900	2.16768500	-0.80808400	
O	-6.40920200	2.15648400	0.27827100	
Name				**3CQA-HA-O7'-H-OOH-W**
Cartesian Coordinates				Frequency and Energy

O	-1.39932900	0.43570800	0.79042200	Zero-point correction= 0.337795
O	-5.48966300	0.04216900	1.41436800	(Hartree/Particle)
O	-2.41888300	2.76437000	-0.48384500	Thermal correction to Energy= 0.363713
O	-5.09047800	2.52014600	0.24552800	Thermal correction to Enthalpy= 0.364657
O	-6.64482800	-2.16769300	0.81632700	Thermal correction to Gibbs Free Energy= 0.278908
O	-5.40761100	-2.58167700	-1.00501700	Sum of electronic and zero-point Energies= -1447.622267
O	-0.87442900	-0.44944400	-1.21741200	Sum of electronic and thermal Energies= -1447.596349
O	6.42191800	-1.30403600	-1.57493700	Sum of electronic and thermal Enthalpies= -1447.595405
O	7.27451700	-0.70466200	0.95195200	Sum of electronic and thermal Free Energies= -1447.681154
C	-5.01472900	-0.54628800	0.19964000	
C	-2.80902400	0.57423600	0.49671100	
C	-3.50341700	-0.77084200	0.31754300	
C	-5.31666600	0.39814300	-0.97275400	
C	-3.07573500	1.52145100	-0.67272800	
C	-4.58740500	1.73119200	-0.83517900	
C	-5.74766500	-1.89151100	-0.01981500	
C	-0.54924400	-0.06473200	-0.11387600	
C	0.82820100	-0.07666800	0.42142300	
C	1.83966600	-0.49040400	-0.35087300	
C	3.25001700	-0.54119700	0.03408600	
C	4.17797100	-0.91434100	-0.93681500	
C	3.68906700	-0.21984900	1.34150900	
C	5.53136900	-0.95985700	-0.62673400	
C	5.02572400	-0.26035100	1.65492900	
C	5.97325700	-0.63335300	0.68201600	
H	-3.17973900	1.05136600	1.40691500	
H	-3.14971600	-1.26744700	-0.58611200	
H	-3.29224000	-1.41005900	1.17867100	
H	-6.39405400	0.57431000	-1.03484600	
H	-4.99416300	-0.08061800	-1.90042600	
H	-2.68813500	1.09746800	-1.59904800	
H	-4.73872300	2.32884800	-1.73652600	
H	-6.22160300	-0.53304900	1.69794800	
H	-2.89946300	3.23369200	0.21220100	
H	-5.34579500	1.91358800	0.95733800	
H	0.95666300	0.27174300	1.43841000	
H	1.61477200	-0.81050000	-1.36519100	
H	3.85780000	-1.16295600	-1.94228100	
H	2.97169300	0.06067700	2.10201300	
H	5.38298700	-0.01638200	2.64838600	
H	7.31330500	-1.31411300	-1.19184800	
H	7.75972700	0.17684100	0.54485800	
H	6.29709300	2.16969400	0.19576600	
O	7.96704200	1.35705100	-0.03359000	
O	6.73094100	1.64668400	-0.50249500	

Name				**3CQA-A-O6'-H-OOH-W**
Cartesian Coordinates				Frequency and Energy
O	1.52922800	-0.63425700	0.73724800	Zero-point correction= 0.325042
O	5.55344200	0.11545200	1.39062300	(Hartree/Particle)

O	2.83854500	-2.74912600	-0.69665500	Thermal correction to Energy= 0.347784
O	5.41875200	-2.22482400	0.02356800	Thermal correction to Enthalpy= 0.348728
O	6.42527400	2.43539500	1.15516400	Thermal correction to Gibbs Free Energy= 0.270799
O	5.33272900	2.92803300	-0.76248200	Sum of electronic and zero-point Energies= -1447.192147
O	0.87479800	0.26699400	-1.22758200	Sum of electronic and thermal Energies= -1447.169405
O	-6.45996500	0.28766400	-1.54797900	Sum of electronic and thermal Enthalpies= -1447.168461
O	-7.24137600	-0.66559300	0.98246300	Sum of electronic and thermal Free Energies= -1447.246390
C	5.01694300	0.77532000	0.23893400	
C	2.93495900	-0.58579100	0.42355900	
C	3.48946600	0.83479900	0.35052700	
C	5.40241600	-0.00924400	-1.01882600	
C	3.30022700	-1.41443600	-0.81179300	
C	4.82559700	-1.42039200	-0.99873000	
C	5.64739600	2.21004700	0.19198000	
C	0.60939800	-0.20957800	-0.14815600	
C	-0.74884600	-0.41270700	0.39246600	
C	-1.83009900	-0.07100400	-0.32857900	
C	-3.22955400	-0.22014900	0.03982400	
C	-4.21773200	0.15766800	-0.86593100	
C	-3.63903800	-0.75436700	1.28935300	
C	-5.59091500	0.00962600	-0.60659700	
C	-4.96781700	-0.89238800	1.59298100	
C	-6.01066500	-0.52419000	0.68300100	
H	3.37917100	-1.07678700	1.29357600	
H	3.08795000	1.37207400	-0.51033700	
H	3.21385400	1.37558700	1.25999800	
H	6.49286300	-0.06090000	-1.09603800	
H	5.02650900	0.54025100	-1.88574500	
H	2.82594100	-0.98480500	-1.69476400	
H	5.03381600	-1.93724400	-1.94117200	
H	6.13258000	0.83362700	1.74581900	
H	3.46734200	-3.18072000	-0.10461300	
H	5.64552500	-1.61805100	0.74905100	
H	-0.81070500	-0.85834800	1.37680500	
H	-1.63688700	0.36215300	-1.30843300	
H	-3.94205500	0.56206800	-1.83498900	
H	-2.89053900	-1.05416400	2.01439900	
H	-5.28688900	-1.29756800	2.54723500	
H	-7.46459000	0.69164000	-1.21256600	
H	-7.92386500	0.65084400	0.79255300	
O	-8.49887800	1.30410400	-0.86379400	
O	-8.31010400	1.54128900	0.46756600	
Name				**4CQA-O6'-H-OOH-P**
Cartesian Coordinates				Frequency and Energy
O	1.54059300	-0.32550800	0.66207800	Zero-point correction= 0.351106
O	4.36600000	2.10221700	-1.56592900	(Hartree/Particle)
O	4.29925000	-2.36033700	-0.59042800	Thermal correction to Energy= 0.377346
O	3.28877300	0.20688000	2.76153900	Thermal correction to Enthalpy= 0.378290
O	6.76305400	1.62001500	-0.66674900	Thermal correction to Gibbs Free Energy= 0.291246

O	6.39167000	-0.56813900	-0.51891900	Sum of electronic and zero-point Energies= -1448.039066
O	0.40746000	-2.26623400	0.54361200	Sum of electronic and thermal Energies= -1448.012826
O	-6.84822300	-0.72151500	0.57503200	Sum of electronic and thermal Enthalpies= -1448.011882
O	-6.91056800	1.96178300	0.34540700	Sum of electronic and thermal Free Energies= -1448.098925
C	4.48961100	0.93544500	-0.77476000	
C	2.79469900	-1.02990100	0.73611900	
C	3.65308300	-0.13881600	-1.48408900	
C	3.96345500	1.19246500	0.65080100	
C	3.27900800	-1.38868800	-0.67605700	
C	3.75103400	-0.08842900	1.45802300	
C	5.96589300	0.55288400	-0.65955000	
C	0.41230000	-1.06203200	0.57158000	
C	-0.77510900	-0.18556200	0.51770300	
C	-1.99681300	-0.72852200	0.46996700	
C	-3.26918600	-0.00840900	0.42295700	
C	-4.45044300	-0.73099900	0.50855700	
C	-3.34054200	1.40114600	0.30062400	
C	-5.69444100	-0.07981000	0.48177100	
C	-4.54795100	2.06566700	0.27474400	
C	-5.73538800	1.33598800	0.36580500	
H	2.65790600	-1.94558600	1.31194200	
H	4.14093900	-0.43979600	-2.41438500	
H	2.72389600	0.36939700	-1.75523700	
H	3.00449400	1.70617000	0.53327400	
H	4.63860700	1.86006100	1.19384100	
H	2.44650100	-1.87249200	-1.19238700	
H	4.69845900	-0.61768600	1.59310300	
H	4.93158100	2.79254500	-1.19939300	
H	5.15226100	-1.90992900	-0.51834100	
H	2.40612800	0.58715600	2.67815000	
H	7.68060900	1.33023800	-0.53670900	
H	-0.59583100	0.88233800	0.53118300	
H	-2.06546600	-1.81391000	0.47899900	
H	-4.43822200	-1.81166700	0.60800900	
H	-2.42750600	1.97861600	0.21971300	
H	-4.59741000	3.14319000	0.17752600	
H	-7.11519400	-1.10562600	-0.42490000	
H	-7.61050100	1.29650600	0.44571200	
H	-5.43766300	-0.81899600	-2.24916600	
O	-7.16109600	-1.28206300	-1.70128700	
O	-6.28551800	-0.35023400	-2.15261900	

Name				**4CQA-O7'-H-OOH-P**
Cartesian Coordinates				Frequency and Energy
O	1.57574900	-0.74592400	0.43367600	Zero-point correction= 0.351066
O	4.10917400	2.70116300	-0.33105000	(Hartree/Particle)
O	4.44264200	-1.66574100	-1.62971800	Thermal correction to Energy= 0.377411
O	3.34822200	-1.12648000	2.53978700	Thermal correction to Enthalpy= 0.378355
O	6.56828900	2.06038400	0.24735900	Thermal correction to Gibbs Free Energy= 0.290803
O	6.38495100	0.05364200	-0.69496100	Sum of electronic and zero-point Energies= -1448.039110

O	0.60751000	-2.45485200	-0.66409300	Sum of electronic and thermal Energies= -1448.012766
O	-6.68344400	-1.49911900	-0.68008400	Sum of electronic and thermal Enthalpies= -1448.011822
O	-7.06914600	0.67238800	0.86697800	Sum of electronic and thermal Free Energies= -1448.099373
C	4.35713500	1.31411500	-0.19963200	
C	2.88712400	-1.27960000	0.16510900	
C	3.58500800	0.64385000	-1.34425800	
C	3.86498800	0.80613600	1.16943200	
C	3.34464900	-0.86814100	-1.24199600	
C	3.78744200	-0.71829700	1.25900200	
C	5.86318100	1.05757700	-0.27365600	
C	0.51348600	-1.43179200	-0.03632800	
C	-0.74755000	-0.75071500	0.32914000	
C	-1.91583600	-1.26628700	-0.07028000	
C	-3.24469400	-0.71903000	0.20282900	
C	-4.34456100	-1.36679300	-0.35935600	
C	-3.44068200	0.42680000	1.01056900	
C	-5.62780700	-0.88324200	-0.13895000	
C	-4.70746400	0.90788400	1.24020700	
C	-5.82629600	0.26694200	0.66872700	
H	2.84947100	-2.36770500	0.22638400	
H	4.05988800	0.87198600	-2.30155600	
H	2.60828200	1.13490600	-1.34264900	
H	2.86363800	1.22524400	1.30768200	
H	4.50346500	1.18781700	1.97126200	
H	2.53542500	-1.11516000	-1.93296000	
H	4.77925800	-1.16120300	1.13154500	
H	4.62932000	3.17786300	0.32706400	
H	5.25898300	-1.22966600	-1.34846300	
H	2.43539100	-0.83198500	2.64230700	
H	7.51107400	1.82905000	0.22622100	
H	-0.66226500	0.15855700	0.91113000	
H	-1.88915000	-2.17889200	-0.66087800	
H	-4.21126200	-2.24644800	-0.97884600	
H	-2.59212300	0.92507800	1.46174300	
H	-4.87937300	1.77689100	1.86588000	
H	-7.48403300	-1.03170500	-0.39458100	
H	-7.25517400	1.54818000	0.23478400	
H	-5.32275300	2.40973400	-1.08865200	
O	-7.15184200	2.43235800	-0.71616200	
O	-6.11045500	1.95730800	-1.43932700	

Name				**4CQA-HA-O6'-H-OOH-W**
Cartesian Coordinates				Frequency and Energy
O	1.59867800	-0.63393600	0.57558700	Zero-point correction= 0.337497
O	4.21240100	2.62928200	-0.52755900	(Hartree/Particle)
O	4.40172800	-1.81580500	-1.45312300	Thermal correction to Energy= 0.363317
O	3.44573400	-0.91172000	2.65479500	Thermal correction to Enthalpy= 0.364261
O	6.69862700	1.97006800	-0.43528200	Thermal correction to Gibbs Free Energy= 0.278305
O	6.33882400	-0.21814400	-0.66604200	Sum of electronic and zero-point Energies= -1447.625496
O	0.52594500	-2.39025200	-0.32795600	Sum of electronic and thermal Energies= -1447.599677

O	-6.74594100	-1.00861800	-0.24254500	Sum of electronic and thermal Enthalpies= -1447.598733
O	-6.91679000	1.35334400	1.10612700	Sum of electronic and thermal Free Energies= -1447.684689
C	4.43270800	1.23349400	-0.34476200	
C	2.87769600	-1.25045100	0.32164200	
C	3.55742600	0.50446400	-1.37517300	
C	4.01286300	0.86056300	1.09036600	
C	3.29870600	-0.98559000	-1.13080400	
C	3.85271500	-0.63911000	1.31954900	
C	5.95110400	0.96970100	-0.50909800	
C	0.49504500	-1.30024200	0.20575300	
C	-0.72015400	-0.53603000	0.53362100	
C	-1.92110300	-1.01916500	0.19257600	
C	-3.21375400	-0.38367700	0.44122200	
C	-4.35948700	-1.00163800	-0.03551900	
C	-3.33740300	0.83917000	1.14791100	
C	-5.62334400	-0.43471200	0.18416600	
C	-4.56642000	1.41939600	1.37152800	
C	-5.72056000	0.79178500	0.89531600	
H	2.79224600	-2.32432300	0.49135500	
H	3.97100900	0.63800500	-2.37828300	
H	2.58645900	1.00840700	-1.35171000	
H	3.04895800	1.34564500	1.27696800	
H	4.73561300	1.26591100	1.80368900	
H	2.47522800	-1.29426900	-1.77844400	
H	4.80989800	-1.14797600	1.19047500	
H	5.08844100	3.03889800	-0.44178400	
H	5.21152300	-1.33734000	-1.15853300	
H	2.59828400	-0.47230300	2.80242500	
H	-0.57772900	0.40982000	1.04119000	
H	-1.96089300	-1.97443300	-0.32528600	
H	-4.30316200	-1.93632000	-0.58279900	
H	-2.45076000	1.33339600	1.52647900	
H	-4.66056100	2.35375000	1.91086400	
H	-7.07751700	-0.48263400	-1.14175000	
H	-7.61181000	0.77993900	0.74395000	
H	-5.34008500	0.76127400	-2.40402200	
O	-7.15088300	0.35073100	-2.15682500	
O	-6.08850100	1.16134800	-1.92555500	

Name				**4CQA-HA-O7'-H-OOH-W**
Cartesian Coordinates				Frequency and Energy
O	1.61468800	-0.72053700	0.40059400	Zero-point correction= 0.337308
O	4.20034300	2.72167200	-0.10145900	(Hartree/Particle)
O	4.51666100	-1.53035500	-1.67126700	Thermal correction to Energy= 0.363148
O	3.38590000	-1.26706500	2.48651100	Thermal correction to Enthalpy= 0.364092
O	6.69281400	2.08498000	0.01679300	Thermal correction to Gibbs Free Energy= 0.278026
O	6.38618000	-0.04070000	-0.58152000	Sum of electronic and zero-point Energies= -1447.625553
O	0.62094400	-2.35827300	-0.77481600	Sum of electronic and thermal Energies= -1447.599714
O	-6.66415100	-1.40657200	-0.57534500	Sum of electronic and thermal Enthalpies= -1447.598770
O	-6.99865500	0.78192700	1.02462100	Sum of electronic and thermal Free Energies= -

C	4.44009600	1.31731500	-0.11702200	1447.684836
C	2.91902800	-1.26428700	0.10786500	
C	3.62097500	0.73765600	-1.27964900	
C	3.96913500	0.72980200	1.22746900	
C	3.38521000	-0.77605200	-1.27100800	
C	3.83868400	-0.79001100	1.22548200	
C	5.96893800	1.10087500	-0.25210600	
C	0.54439400	-1.35950600	-0.09072700	
C	-0.70553100	-0.68909200	0.31481300	
C	-1.88242600	-1.17496800	-0.09803900	
C	-3.20063300	-0.62665200	0.21833300	
C	-4.31681200	-1.26861200	-0.31582100	
C	-3.36920700	0.51625400	1.03717600	
C	-5.59217800	-0.78712600	-0.04915200	
C	-4.62692000	0.99997700	1.30229100	
C	-5.76307300	0.35887000	0.77031000	
H	2.85528100	-2.35290400	0.11163300	
H	4.06969600	1.02611600	-2.23384100	
H	2.63925600	1.21733200	-1.22095500	
H	2.98617000	1.16389500	1.43833900	
H	4.65038900	1.03907400	2.02476500	
H	2.59186900	-0.99675300	-1.98849800	
H	4.81258200	-1.25583300	1.06365300	
H	5.06145300	3.12529400	0.09345000	
H	5.30503000	-1.08693300	-1.27852400	
H	2.51602700	-0.88227900	2.65547800	
H	-0.60466800	0.18793700	0.94175100	
H	-1.87929300	-2.05995100	-0.72945500	
H	-4.20291000	-2.14420100	-0.94480900	
H	-2.50639400	1.01614600	1.45838200	
H	-4.77908300	1.87410900	1.92433200	
H	-7.47143500	-0.97345800	-0.25595800	
H	-7.33787500	1.37603200	0.18094200	
H	-5.54475200	2.30131600	-1.28907600	
O	-7.37062300	2.01995200	-0.98004900	
O	-6.20152700	1.62477100	-1.53567600	

Name				**4CQA-A-O6'-H-OOH-W**
Cartesian Coordinates				Frequency and Energy
O	1.68574300	-0.46180000	0.43491000	Zero-point correction= 0.324773
O	4.62119400	2.51578600	-0.83755900	(Hartree/Particle)
O	4.61900700	-2.00580800	-1.11980900	Thermal correction to Energy= 0.347744
O	3.27854700	-0.48191900	2.68800900	Thermal correction to Enthalpy= 0.348688
O	7.01905200	1.73977000	-0.54292500	Thermal correction to Gibbs Free Energy= 0.268946
O	6.52876500	-0.43322000	-0.27153400	Sum of electronic and zero-point Energies= -1447.196836
O	0.59501500	-2.32388800	-0.21466000	Sum of electronic and thermal Energies= -1447.173865
O	-6.63328600	-1.23081800	0.08155500	Sum of electronic and thermal Enthalpies= -1447.172921
O	-6.88326700	1.51948000	0.62092300	Sum of electronic and thermal Free Energies= -1447.252663
C	4.71752900	1.15294400	-0.45568300	
C	2.95819100	-1.14651100	0.38212800	

C	3.89006400	0.32683200	-1.45513300
C	4.12448800	1.00816300	0.95861000
C	3.53968800	-1.10873600	-1.03921500
C	3.85568500	-0.43209100	1.38601400
C	6.23795800	0.77697900	-0.43083600
C	0.57266300	-1.16527900	0.12671300
C	-0.63155200	-0.33120700	0.28216100
C	-1.85118600	-0.86537500	0.08812000
C	-3.14474100	-0.21839900	0.21716500
C	-4.30181800	-0.97042800	0.02410500
C	-3.28710400	1.15388900	0.55145100
C	-5.59322200	-0.43844400	0.17089600
C	-4.52773600	1.71973900	0.67870300
C	-5.73905600	0.97568300	0.49652900
H	2.80655400	-2.18563000	0.67590100
H	4.40025600	0.30160600	-2.42229800
H	2.95342500	0.87818900	-1.59076800
H	3.17635900	1.55875100	0.96008200
H	4.78886600	1.48568100	1.68414800
H	2.76263100	-1.48444600	-1.71278800
H	4.79488600	-0.98392500	1.44422200
H	5.55564200	2.79556500	-0.84171800
H	5.42075600	-1.52246600	-0.79289100
H	2.39708700	-0.10319100	2.60365000
H	-0.47320000	0.70100200	0.56762700
H	-1.87167100	-1.91726700	-0.19166000
H	-4.23057900	-2.02508000	-0.22345500
H	-2.40262600	1.76300700	0.70210500
H	-4.64378400	2.76842600	0.92979400
H	-7.58455300	-0.78098200	-0.34819800
H	-7.66773000	1.25445300	-0.63025700
O	-8.56580000	-0.34787500	-0.98337700
O	-8.15264900	0.86901200	-1.44351400

Name			**5CQA-O6'-H-OOH-P**
Cartesian Coordinates			Frequency and Energy
O	-1.23061200	-0.56911100	-0.46198600
O	-5.10258600	-0.01401900	2.38278300
O	-2.94414600	-2.75440900	-0.22848600
O	-5.20762900	-0.70044100	-2.13186300
O	-4.93392800	2.38781100	1.37650900
O	-5.29001900	1.65328400	-0.69318300
O	-0.88137200	1.64883400	-0.38735500
O	5.99317100	-1.60598000	-0.54649000
O	7.49649700	0.62170500	-0.52708100
C	-4.66395700	0.05237700	1.03952200
C	-2.65401300	-0.35727900	-0.45670200
C	-3.13216300	-0.10338800	0.96802600
C	-5.36555600	-1.10207900	0.31116400
C	-3.27095500	-1.62885800	-1.02524900

Zero-point correction= 0.351323 (Hartree/Particle)
Thermal correction to Energy= 0.377508
Thermal correction to Enthalpy= 0.378452
Thermal correction to Gibbs Free Energy= 0.292101
Sum of electronic and zero-point Energies= -1448.039688
Sum of electronic and thermal Energies= -1448.013503
Sum of electronic and thermal Enthalpies= -1448.012558
Sum of electronic and thermal Free Energies= -1448.098909

C	-4.79935600	-1.51789300	-1.05350400
C	-5.01702800	1.42431200	0.46028400
C	-0.44482600	0.52502300	-0.42612500
C	0.98269800	0.14954700	-0.44481600
C	1.91506100	1.10842100	-0.41422700
C	3.36622200	0.92210300	-0.43595400
C	3.96991000	-0.32837400	-0.47399500
C	4.18857700	2.07269000	-0.42617200
C	5.36655600	-0.44213300	-0.50168800
C	5.56756400	1.99047500	-0.45776100
C	6.17011800	0.73555000	-0.49464100
H	-2.88012300	0.48577500	-1.11513400
H	-2.88135700	-0.96989900	1.58455900
H	-2.64074600	0.77845100	1.38690300
H	-6.43348800	-0.89084600	0.21607900
H	-5.25837200	-1.95747400	0.98256900
H	-2.92042300	-1.76651600	-2.05357700
H	-5.17957600	-2.51941200	-1.26773000
H	-4.73576500	0.73308100	2.87081500
H	-1.98496700	-2.84478000	-0.21736000
H	-5.28068000	0.21230400	-1.82090800
H	-5.10715700	3.24388200	0.95248000
H	1.21240500	-0.90810000	-0.49156000
H	1.57205800	2.13956600	-0.37464600
H	3.39099300	-1.24535100	-0.48883300
H	3.71627600	3.04867800	-0.39640600
H	6.18756800	2.87832800	-0.45124700
H	6.03246200	-2.01912100	0.48186300
H	7.71839100	-0.32218700	-0.57580500
H	4.83244700	-0.75373200	2.26066000
O	6.00080500	-2.12077900	1.75856700
O	5.79568600	-0.83759700	2.14712300

Name			**5CQA-O7'-H-OOH-P**
Cartesian Coordinates			Frequency and Energy
O	-1.38172800	-0.06200300	0.39723000
O	-5.69234200	1.64674200	1.57713400
O	-3.10281500	-1.82245200	1.78891000
O	-4.98840800	-1.85099600	-1.27908800
O	-5.40895300	2.78623400	-0.74748200
O	-5.31851600	0.83869600	-1.81862500
O	-0.76881600	-0.85759100	-1.61739700
O	5.55382800	0.54016400	2.27874600
O	7.36435900	-0.43102900	0.54564800
C	-5.02481700	0.86863300	0.60294100
C	-2.77465200	-0.16807800	0.04466300
C	-3.50216500	0.90103200	0.84477000
C	-5.57637800	-0.55613800	0.75427600
C	-3.27529400	-1.56570600	0.40527600
C	-4.77357000	-1.69339300	0.10814000

Zero-point correction= 0.350826 (Hartree/Particle)
Thermal correction to Energy= 0.377265
Thermal correction to Enthalpy= 0.378209
Thermal correction to Gibbs Free Energy= 0.290530
Sum of electronic and zero-point Energies= -1448.039019
Sum of electronic and thermal Energies= -1448.012580
Sum of electronic and thermal Enthalpies= -1448.011636
Sum of electronic and thermal Free Energies= -1448.099315

C	-5.28366800	1.45998100	-0.78430100
C	-0.47475700	-0.44785600	-0.52347800
C	0.89857000	-0.29135500	0.00215300
C	1.93918700	-0.66304000	-0.75236600
C	3.35254200	-0.58130900	-0.38482600
C	3.77992000	-0.03450800	0.82850200
C	4.30178400	-1.08190200	-1.30342800
C	5.13176800	0.01619800	1.12238300
C	5.64880200	-1.04050500	-1.01831100
C	6.09062700	-0.49015800	0.19869400
H	-2.87472800	-0.01304400	-1.03217700
H	-3.35565400	0.71541900	1.91124900
H	-3.09826100	1.88983900	0.60940200
H	-6.61113900	-0.59443700	0.40520400
H	-5.58611900	-0.73545300	1.83199400
H	-2.74236400	-2.30765600	-0.19847400
H	-5.10400900	-2.62439100	0.57453600
H	-5.43322600	2.57048700	1.47575000
H	-2.16628000	-1.74117100	1.99999900
H	-5.09377300	-0.97793300	-1.68076400
H	-5.51998300	3.11864500	-1.65294100
H	0.99922500	0.11999700	0.99914700
H	1.72776500	-1.07358700	-1.73675000
H	3.07810300	0.36343300	1.55140700
H	3.95554300	-1.50641600	-2.23862900
H	6.38887400	-1.43042300	-1.70854400
H	6.52012900	0.46209500	2.30943700
H	7.83511300	0.40564700	0.01013100
H	6.43165100	1.60923500	-1.66125800
O	8.00096600	1.50641000	-0.65552200
O	6.73013900	1.95061600	-0.79946200

Name			**5CQA-HA-O6'-H-OOH-W**
Cartesian Coordinates			Frequency and Energy
O	1.30314100	0.54650600	-0.47455900
O	5.11047200	0.18534200	2.42918500
O	3.06625100	2.71778000	-0.43298100
O	5.26438700	0.38516800	-2.10898200
O	5.42269900	-2.23072000	1.60314000
O	5.14295700	-1.75004100	-0.55678800
O	0.89719400	-1.66301700	-0.42968600
O	-5.84944400	1.80751300	-0.11739600
O	-7.44254300	-0.31259700	-0.72098400
C	4.74076900	-0.00859800	1.06759900
C	2.72716600	0.30542300	-0.47184900
C	3.20805800	0.12467500	0.96107700
C	5.44232600	1.08802800	0.25019300
C	3.36431100	1.51820300	-1.13540000
C	4.88868100	1.36390500	-1.15238800
C	5.14860800	-1.44895500	0.66563600

Zero-point correction= 0.337567 (Hartree/Particle)
Thermal correction to Energy= 0.363318
Thermal correction to Enthalpy= 0.364262
Thermal correction to Gibbs Free Energy= 0.279115
Sum of electronic and zero-point Energies= -1447.624652
Sum of electronic and thermal Energies= -1447.598901
Sum of electronic and thermal Enthalpies= -1447.597957
Sum of electronic and thermal Free Energies= -1447.683104

C	0.48976300	-0.51953900	-0.44900700
C	-0.92489600	-0.10979700	-0.45664300
C	-1.88646700	-1.03832300	-0.52200900
C	-3.32869000	-0.79188600	-0.54738700
C	-3.88822700	0.45102200	-0.28547400
C	-4.18585800	-1.87744900	-0.84836000
C	-5.27575100	0.62942200	-0.34645500
C	-5.55663800	-1.72929700	-0.91438700
C	-6.11526000	-0.47673000	-0.66798700
H	2.92828300	-0.57761100	-1.07951700
H	2.92330400	1.01078200	1.53455200
H	2.72838000	-0.74552600	1.41692700
H	6.51195400	0.87259400	0.18032900
H	5.33079500	2.00901600	0.82936500
H	3.00780900	1.58875600	-2.16793400
H	5.30340300	2.31396900	-1.49701500
H	5.28169900	-0.70532900	2.77572000
H	2.10947200	2.84131300	-0.43805300
H	5.21684700	-0.48828000	-1.65792500
H	-1.12338200	0.95456200	-0.42803300
H	-1.58777500	-2.08221800	-0.57955000
H	-3.28306500	1.31219600	-0.02612300
H	-3.74545100	-2.85040000	-1.03672400
H	-6.20653100	-2.56317200	-1.14852900
H	-6.25101700	1.79942600	0.90505000
H	-7.65754300	0.61825300	-0.54641900
H	-5.28691200	0.12621600	2.46668900
O	-6.58215100	1.43296100	2.11397100
O	-6.19845700	0.13159900	2.12308600

Name	**5CQA-HA-O7'-H-OOH-W**
Cartesian Coordinates	Frequency and Energy

O	-1.35552500	-0.04064500	0.36328900
O	-5.52350400	2.07139100	1.24055200
O	-3.10675500	-1.42540700	2.11496800
O	-5.05190800	-1.91271100	-0.89475200
O	-5.61004700	2.59652800	-1.28306800
O	-5.18146400	0.50618800	-1.93021100
O	-0.79967800	-1.43487000	-1.31189300
O	5.57477700	0.91729000	1.99408800
O	7.39460900	-0.26598800	0.34648600
C	-4.96437400	1.05398800	0.41528400
C	-2.76144400	-0.17540500	0.05416800
C	-3.43421600	1.07191600	0.59957700
C	-5.55487800	-0.28268300	0.88894500
C	-3.30709700	-1.44347500	0.70741400
C	-4.81492100	-1.55388800	0.45747900
C	-5.29192400	1.40766300	-1.05810600
C	-0.47526700	-0.70884600	-0.39570700
C	0.90865400	-0.42529900	0.02968900

Zero-point correction= 0.337124 (Hartree/Particle)
Thermal correction to Energy= 0.362977
Thermal correction to Enthalpy= 0.363921
Thermal correction to Gibbs Free Energy= 0.278350
Sum of electronic and zero-point Energies= -1447.625062
Sum of electronic and thermal Energies= -1447.599209
Sum of electronic and thermal Enthalpies= -1447.598265
Sum of electronic and thermal Free Energies= -1447.683836

C	1.93572600	-0.98359300	-0.62211000
C	3.35446800	-0.77840800	-0.33104300
C	3.79306200	-0.00784900	0.74818000
C	4.29712800	-1.38347300	-1.19303100
C	5.15029400	0.16440400	0.96155800
C	5.64782300	-1.20985200	-0.99324200
C	6.10165500	-0.43877500	0.09017700
H	-2.87316300	-0.24967500	-1.02850500
H	-3.24118800	1.13608300	1.67356200
H	-3.01369000	1.96177200	0.12411200
H	-6.60313500	-0.35490600	0.58688100
H	-5.53034400	-0.24916800	1.98185700
H	-2.81851500	-2.31966900	0.27056000
H	-5.18170100	-2.38020100	1.07098500
H	-5.68146500	2.82286400	0.64690600
H	-2.15847200	-1.37141000	2.28547000
H	-5.08496200	-1.07393900	-1.40994000
H	1.02896500	0.25237400	0.86577900
H	1.71760500	-1.64382000	-1.45766000
H	3.09912100	0.46602600	1.43186900
H	3.94079200	-1.98272400	-2.02272900
H	6.38386300	-1.66138900	-1.64764100
H	6.54455400	0.90606800	2.02396000
H	7.68279800	0.73170400	0.01435600
H	6.28923200	1.71322900	-1.78165300
O	7.65028500	1.94059400	-0.51591100
O	6.34754000	2.04771100	-0.86802900

Name			**5CQA-A-O6'-H-OOH-W**
Cartesian Coordinates			Frequency and Energy
O	-1.39591900	0.18711200	-0.04558900
O	-5.56462300	2.34991000	-0.68947800
O	-2.70846200	0.84016100	2.29855700
O	-5.11879700	-1.67905300	1.34890500
O	-6.33169100	0.57488400	-2.32657000
O	-5.47459100	-1.16825200	-1.20046300
O	-0.87685800	-2.00671900	-0.03294800
O	5.68317000	1.72080900	-0.63674100
O	7.40354200	-0.49143700	-0.54946200
C	-5.06139900	1.06054600	-0.37801100
C	-2.81577600	-0.10028700	0.06008700
C	-3.53075700	1.09604500	-0.54847800
C	-5.41863600	0.75687100	1.08601700
C	-3.15578200	-0.28011700	1.53881000
C	-4.67006100	-0.40840500	1.74772500
C	-5.69074300	0.05086200	-1.39607400
C	-0.52998700	-0.85130500	-0.08083000
C	0.86038200	-0.36874300	-0.17916200
C	1.87354100	-1.25267300	-0.19368000
C	3.30092800	-0.99427200	-0.28154200

Zero-point correction= 0.324212 (Hartree/Particle)
Thermal correction to Energy= 0.346428
Thermal correction to Enthalpy= 0.347372
Thermal correction to Gibbs Free Energy= 0.270962
Sum of electronic and zero-point Energies= -1447.196189
Sum of electronic and thermal Energies= -1447.173974
Sum of electronic and thermal Enthalpies= -1447.173030
Sum of electronic and thermal Free Energies= -1447.249440

C	3.85167400	0.28405800	-0.35885300
C	4.18278100	-2.10471700	-0.29674900
C	5.23275200	0.50490900	-0.46914000
C	5.54172400	-1.93657700	-0.38256900
C	6.14226700	-0.64348400	-0.46753800
H	-3.03775600	-1.02257000	-0.47716400
H	-3.17951000	2.00603400	-0.05240300
H	-3.28212500	1.17651300	-1.61008900
H	-6.49543600	0.58260400	1.17030700
H	-5.18073300	1.66693000	1.64558500
H	-2.68073300	-1.19820500	1.90172600
H	-4.83319300	-0.33932400	2.82922800
H	-6.06014600	2.18120400	-1.51342000
H	-1.83397200	1.07233400	1.96989400
H	-5.25812700	-1.63934300	0.36970900
H	1.00623600	0.70255200	-0.23693100
H	1.58528000	-2.30096300	-0.13278800
H	3.21961800	1.16538000	-0.36075400
H	3.76071200	-3.10369500	-0.23806400
H	6.21700300	-2.78501000	-0.39356000
H	6.71077900	1.96888500	-0.18963500
H	7.85003200	0.43157000	0.53592600
O	7.72170900	2.29461900	0.43680400
O	8.01435000	1.19781900	1.19478100

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