Supplementary Materials

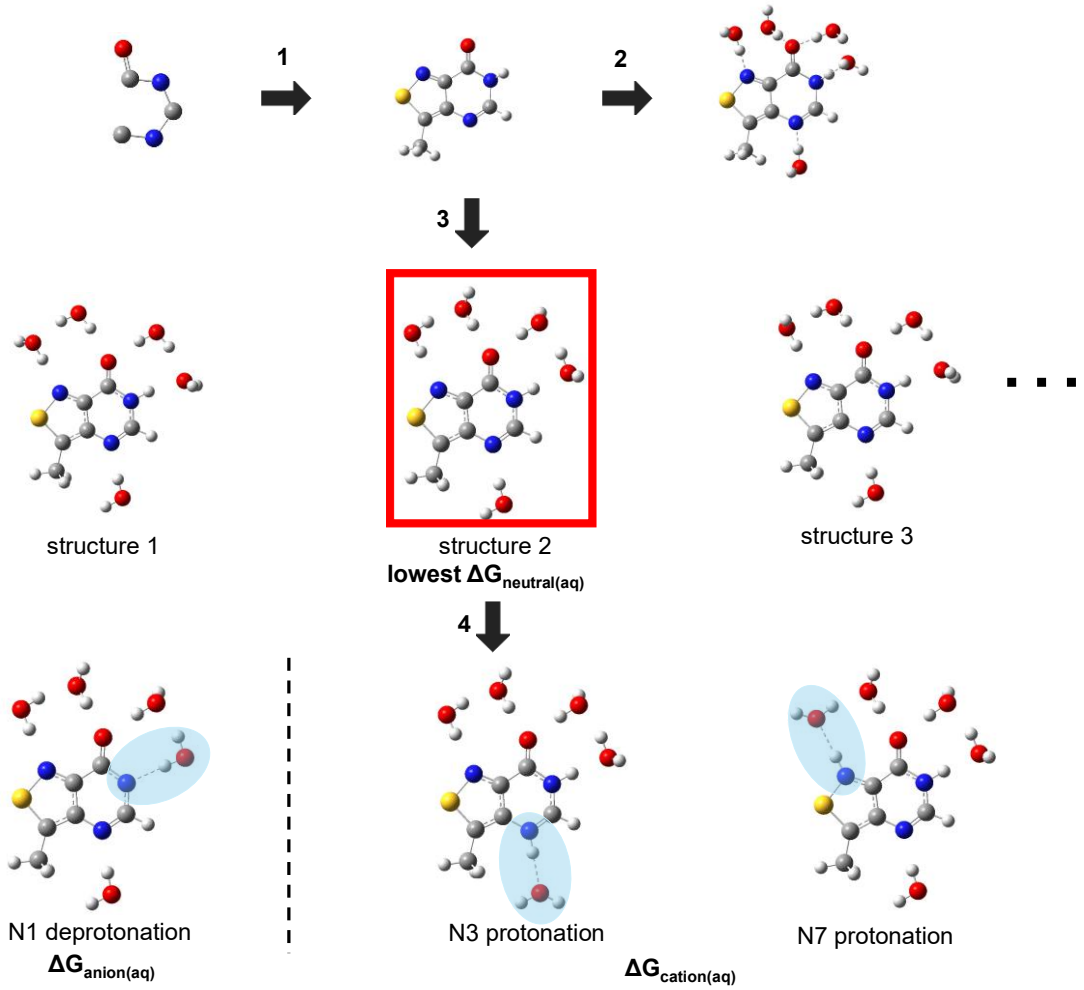
Calculations of pK_a Values for a Series of Fluorescent Nucleobase Analogues

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Figure of Contents

Figure S1	**Methodological Diagram of pK_a Calculations for the Fluorescent Analogues**	**S2**
Figure S2	**Images of Optimized Structures of Adenosine Fluorescent Analogues**	**S3-S5**
Figure S3	**Images of Optimized Structures of Guanosine Fluorescent Analogues**	**S6-S7**
Figure S4	**Images of Optimized Structures of Cytidine Fluorescent Analogues**	**S8-S10**
Figure S5	**Images of Optimized Structures of Uridine Fluorescent Analogues**	**S11-S12**
Figure S6	**Images of Optimized Structures of Non-natural Modifications**	**S13**
Figure S7	**Cartesian Coordinates of Optimized Structures**	**S14-S66**



$$pK_a = \frac{\Delta G_{dissoc(aq)}}{2.303RT} \quad \text{Equation 1}$$

$$\text{adjusted } pK_a = \frac{(\text{calculated } pK_a + 0.70)}{1.22} \quad \text{Equation 2}$$

$$\text{adjusted } pK_a = \frac{(\text{calculated } pK_a + 0.94)}{1.24} \quad \text{Equation 3}$$

Figure S1. Methodological Diagram of p*K*ₐ Calculations for the Fluorescent Analogues. Step 1. The neutral form of the fluorescent analogue (^{tz}I is shown in this example) is built using Gaussview 6.1.1. Graphical Interface. Step 2. The water molecules are placed at every proton donor/acceptor site of the fluorescent analogue. Step 3. Varied arrangements of the explicit water molecules surrounding the fluorescent analogue are designed and calculated with geometry optimization to determine the lowest energy neutral structure ($\Delta G_{neutral(aq)}$). This optimization requires an average CPU time of 10 hours. The bulkier structures need longer CPU time for the optimization. Step 4. The selected neutral structure with the lowest free energy is either protonated ($\Delta G_{cation(aq)}$) or deprotonated ($\Delta G_{anion(aq)}$), depending on the site of the interest. The protonated/deprotonated structures also undergo geometry optimization, which is accomplished on average in 2 hours of CPU time. Step 5. The differences in free energies of the neutral structure and (de)protonated structure are used to calculate $\Delta G_{dissoc(aq)}$, followed by the p*K*ₐ calculation by using Equation 1. The calculated p*K*ₐ value is then adjusted by Equation 2 for purines and Equation 3 for pyrimidines. Note that other chemically reasonable placements of the explicit water molecules could change the p*K*ₐ values by a fraction of a p*K*ₐ unit.

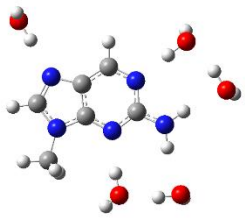
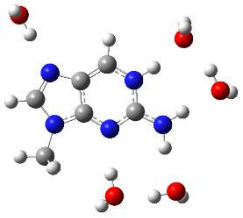
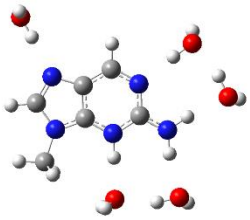
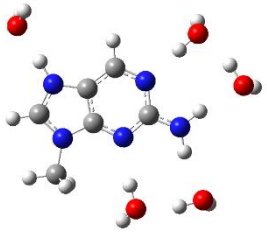
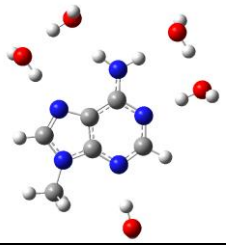
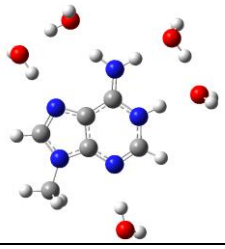
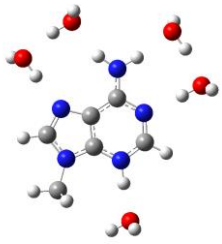
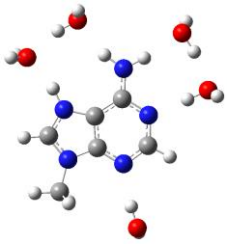
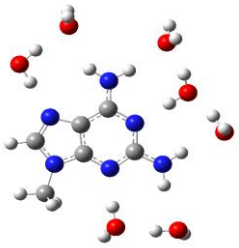
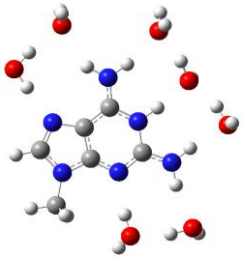
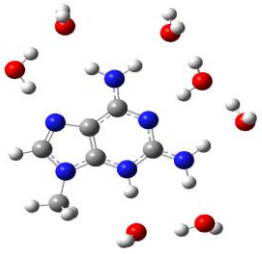
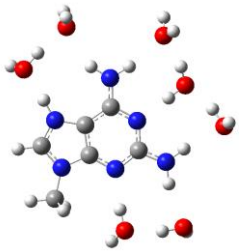
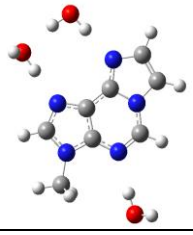
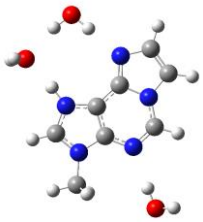
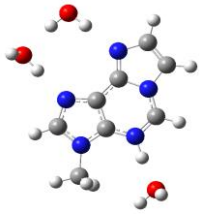
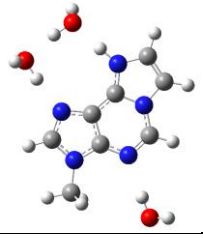
2-aminopurine (2AP)			
			
neutral	N1 cation	N3 cation	N7 cation
adenosine (A)			
			
neutral	N1 cation	N3 cation	N7 cation
2,6-diaminopurine (DAP)			
			
neutral	N1 cation	N3 cation	N7 cation
1,N^6-ethenoadenosine (εA)			
			
neutral	N1 cation	N4 cation	N9 cation

Figure S2. Images of optimized structures of adenosine fluorescent analogues. Geometry optimization was performed on the neutral and protonated structures of the analogues.

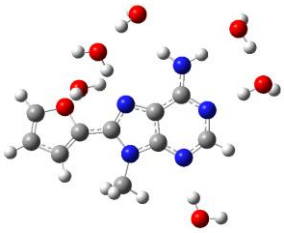
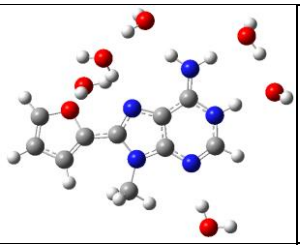
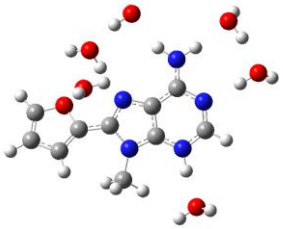
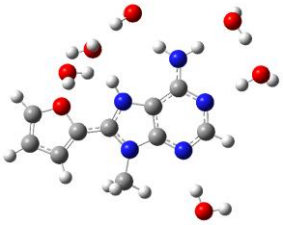
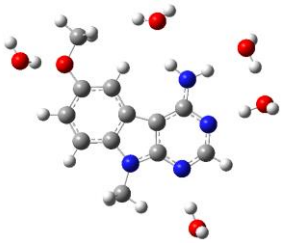
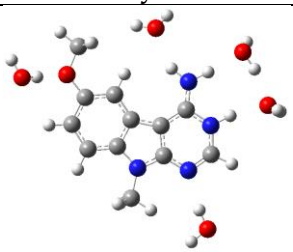
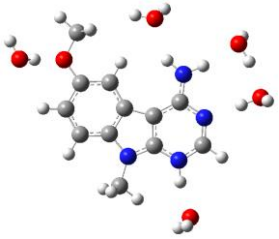
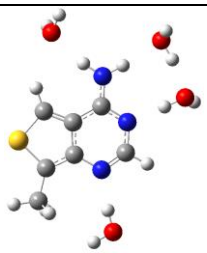
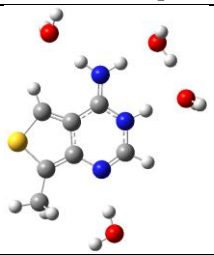
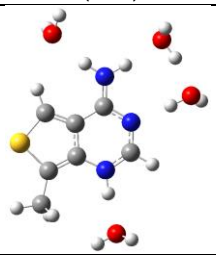
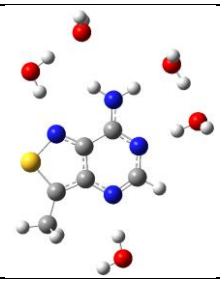
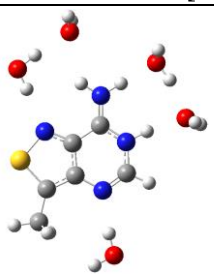
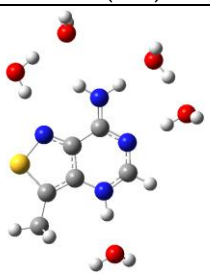
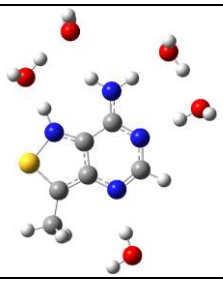
8-furan-adenosine (8-Furan-A)			
			
neutral	N1 cation	N3 cation	N7 cation
methoxybenzodeeza-adenosine (^{MD}A)			
			
neutral	N1 cation	N3 cation	
thieno[3,4,*d*]adenosine (thA)			
			
neutral	N1 cation	N3 cation	
isothiazolo[4,3,*d*]adenosine (^{tz}A)			
			
neutral	N1 cation	N3 cation	N7 cation

Figure S2. continued.

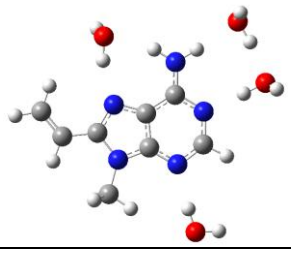
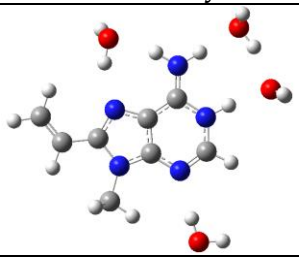
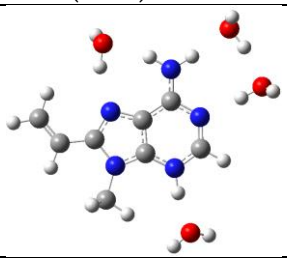
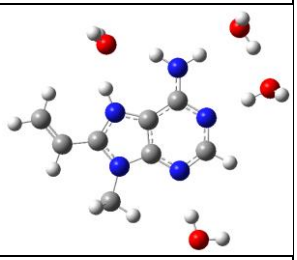
8-vinyladenosine (8vA)			
			
neutral	N1 cation	N3 cation	N7 cation

Figure S2. continued.

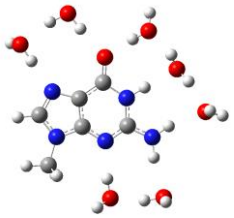
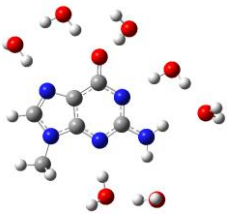
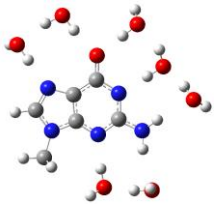
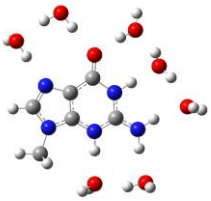
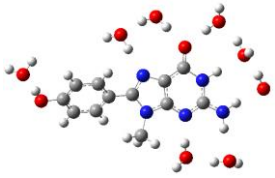
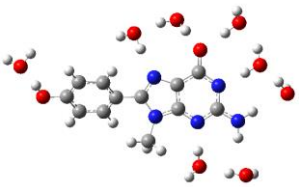
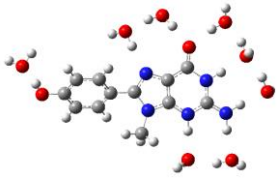
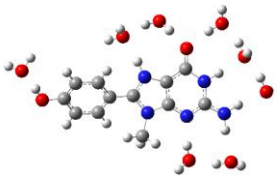
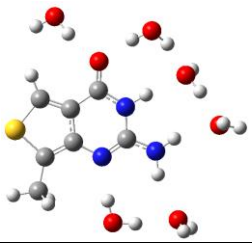
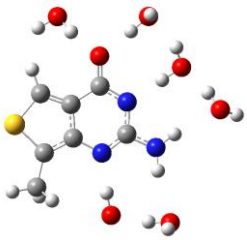
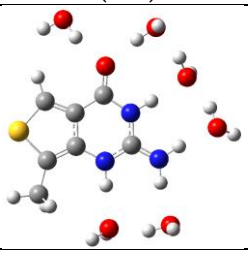
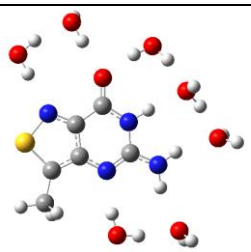
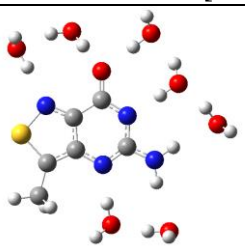
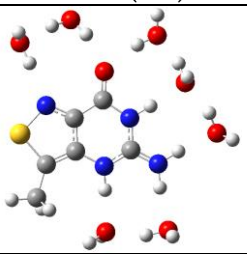
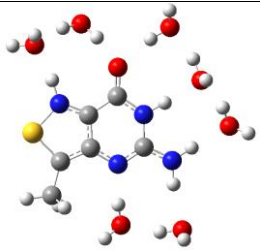
guanosine (G)				
				
neutral	N1 cation_1	N1 cation_2	N3 cation	N7 cation
8-phenol-guanosine (8-Phenol-G)				
				
neutral	N1 anion	N3 cation	N7 cation	
thieno[3,4,*d*]guanosine (thG)				
				
neutral	N1 cation	N3 cation		
isothiazolo[4,3,*d*]guanosine (^{tz}G)				
				
neutral	N1 anion	N3 cation	N7 cation	

Figure S3. Images of optimized structures of guanosine fluorescent analogues. Geometry optimization was performed on the neutral, protonated, and deprotonated structures of the analogues.

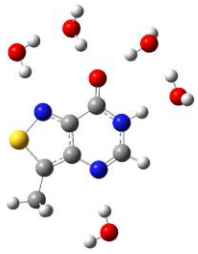
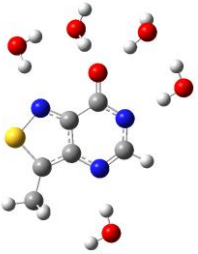
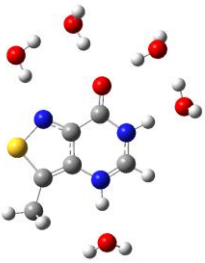
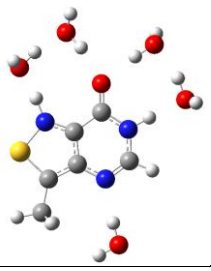
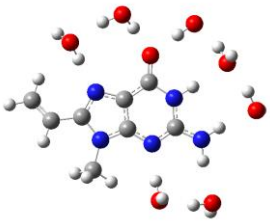
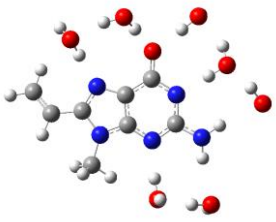
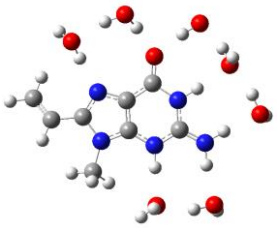
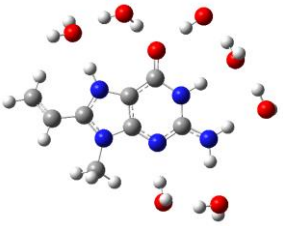
isothiazolo[4,3,*d*]inosine (^{tz}I)			
			
neutral	N1 anion	N3 cation	N7 cation
8-vinylguanosine (8vG)			
			
neutral	N1 anion	N3 cation	N7 cation

Figure S3. continued.

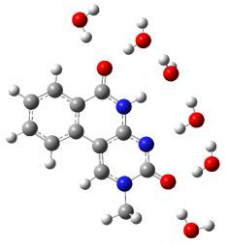
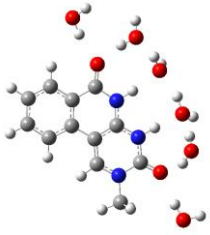
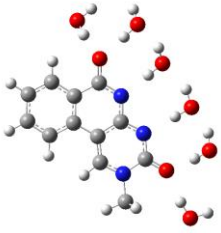
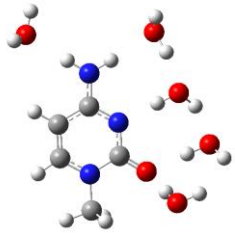
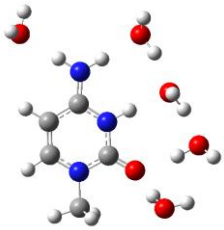
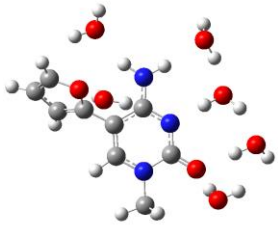
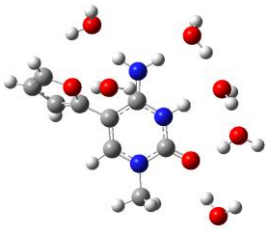
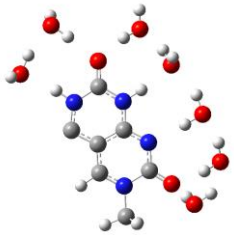
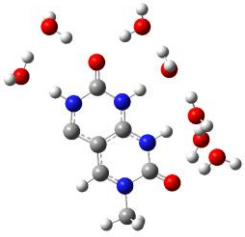
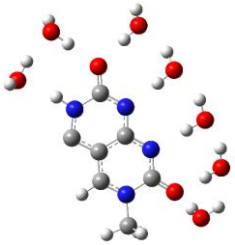
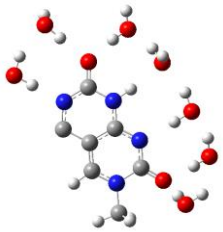
benzopyridopyrimidine (BPP)			
			
neutral	N3 cation	N7 anion	
cytidine (C)			
			
neutral	N3 cation		
5-furan-cytidine (C^{FU})			
			
neutral	N3 cation		
locked bicyclic 4-*N*-carbamoyldeoxycytidine (C^{hpp})			
			
neutral	N3 cation	N7 anion	N9 anion

Figure S4. Images of optimized structures of cytidine fluorescent analogues. Geometry optimization was performed on the neutral, protonated, and deprotonated structures of the analogues.

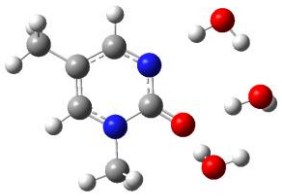
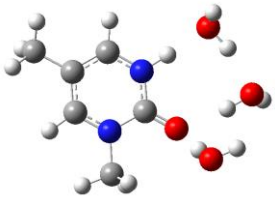
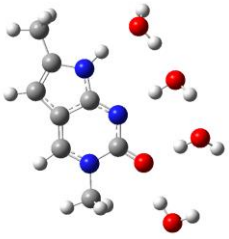
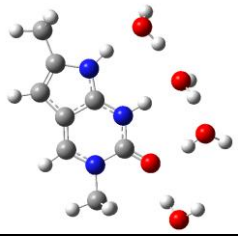
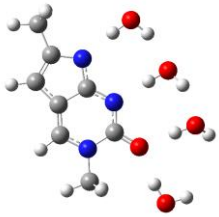
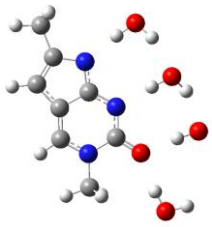
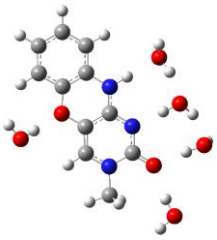
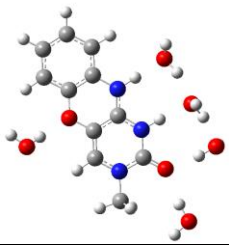
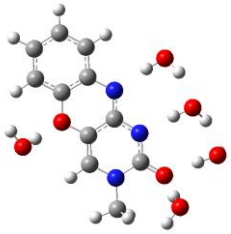
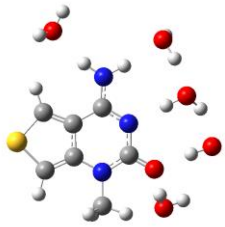
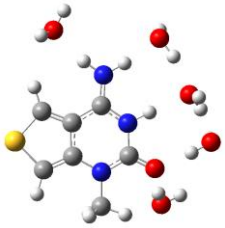
5-methyl-2-pyrimidinone (m^5K)			
			
neutral	N3 cation		
pyrrolocytidine (pC)			
			
neutral	N3 cation	N7 anion_1	N7 anion_2
1,3-diaza-2-oxophenoxazine (tC°)			
			
neutral	N3 cation	N7 anion	
thieno[3,4,*d*]cytidine (^{th}C)			
			
neutral	N3 cation		

Figure S4. continued.

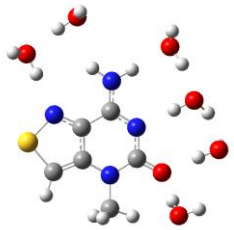
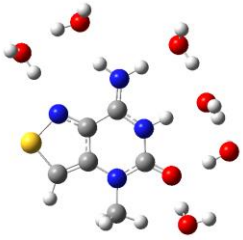
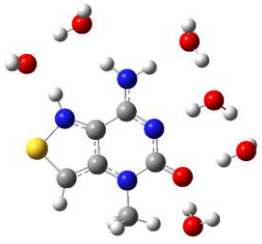
isothiazolo[4,3,*d*]cytidine (^{tz}C)			
			
neutral	N3 cation	N7 cation	

Figure S4. continued.

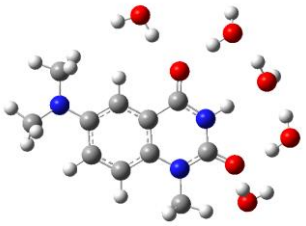
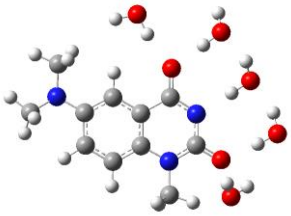
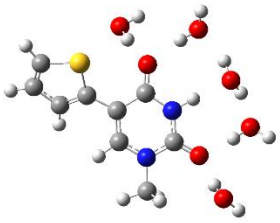
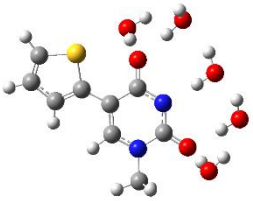
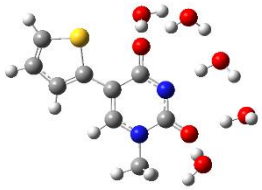
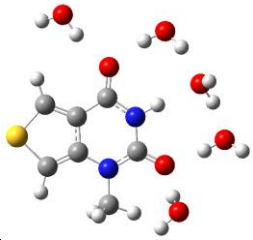
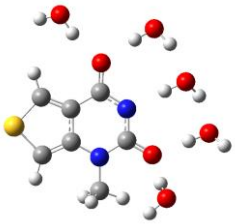
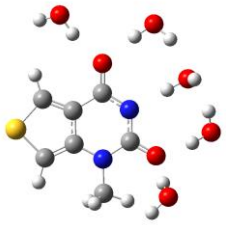
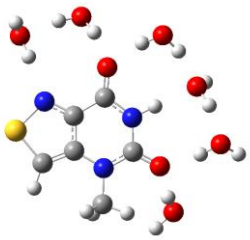
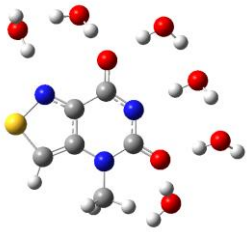
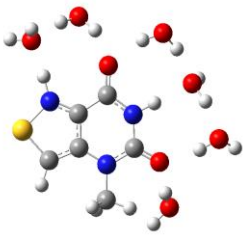
N,N-dimethylaniline-2-deoxythymidine (^{DMA}T)			
			
neutral	N3 anion		
5-thiophene-uridine (5-thU)			
			
neutral	N3 anion_1	N3 anion_2	
thieno[3,4,*d*]uridine (thU)			
			
neutral	N3 anion_1	N3 anion_2	
isothiazolo[4,3,*d*]uridine (^{tz}U)			
			
neutral	N3 anion	N7 cation	

Figure S5. Images of optimized structures of uridine fluorescent analogues. Geometry optimization was performed on the neutral, protonated, and deprotonated structures of the analogues.

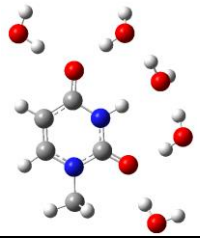
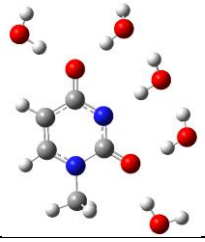
Uridine (U)			
			
neutral	N3 anion		

Figure S5. continued.

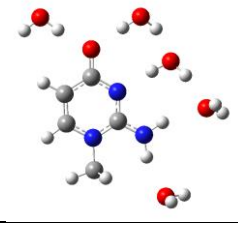
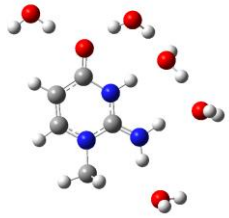
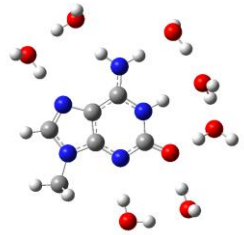
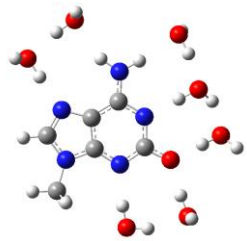
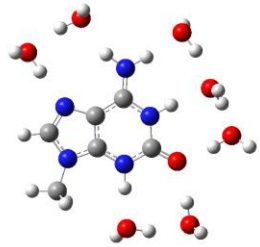
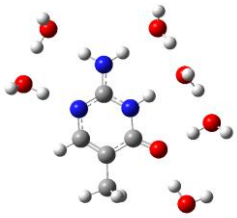
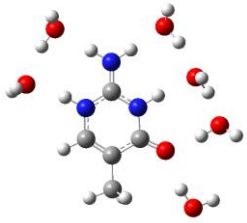
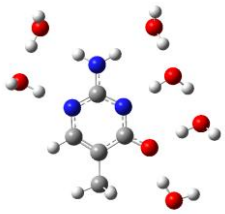
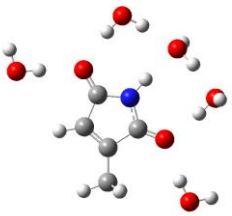
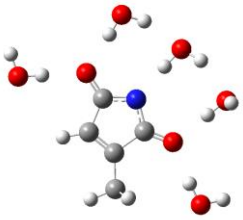
isocytidine (iC)			
			
neutral	N3 cation		
isoguanosine (iG)			
			
neutral	N1 anion	N3 cation	
pseudoisocytidine, NH3 tautomer (piC)			
			
neutral	N1 cation	N3 anion	
showdomycin (Show)			
			
neutral	N3 anion		

Figure S6. Images of optimized structures of non-natural modifications. Geometry optimization was performed on the neutral, protonated, and deprotonated structures of the analogues.

2AP 5H2O B3LYP Neutral

Enthalpy (Hartrees) = -888.671958

Free Energy (Hartrees) = -888.756511

Charge = 0 Multiplicity = 1

N	2.07687000	-1.58488300	0.05715900
C	3.23706100	-0.84308000	0.11175500
H	4.20216400	-1.32824500	0.16739300
N	3.04161800	0.45720700	0.08987000
C	1.65879200	0.59378000	0.01557600
C	0.79878600	1.68174900	-0.03490900
N	-0.52432100	1.49191200	-0.09781100
C	-1.01430700	0.21614000	-0.11446500
N	-2.35770200	0.08083200	-0.20321900
H	-2.95293000	0.89979500	-0.11003900
H	-2.78579700	-0.82936100	-0.06111100
N	-0.26234500	-0.91014200	-0.07298500
C	1.04990500	-0.67689300	-0.00590700
C	1.97797600	-3.04252400	0.07153500
H	1.38944500	-3.37015200	0.93119400
H	1.51244300	-3.39777700	-0.84968300
H	2.98577600	-3.45087700	0.14874500
O	-3.99589300	-2.56816200	0.23753500
H	-3.12765900	-3.00924600	0.08159500
H	-4.14590900	-2.62718700	1.19162300
O	-2.06534100	3.83647500	-0.10710000
H	-1.86221400	4.30770000	0.71409700
H	-1.50827600	3.01182000	-0.08721400
O	-4.42008700	2.39637500	0.01432900
H	-4.76896800	2.39680400	0.91693900
H	-3.64423200	3.00517800	0.03307800
O	-1.48449400	-3.50126900	-0.38164700
H	-1.06570300	-4.11524200	0.23904400
H	-1.01117500	-2.64248100	-0.25875700
O	5.18984700	2.31816500	0.11409100
H	5.34218400	2.57844300	-0.80525500
H	4.42810400	1.68919800	0.08147000
H	1.15238400	2.70944600	-0.02339100

2AP 5H2O B3LYP N1 Cation

Enthalpy (Hartrees) = -889.111318

Free Energy (Hartrees) = -889.194664

Charge = 1 Multiplicity = 1

N	-2.01621100	1.65011700	0.05595700
C	-3.19770300	0.93045500	0.07562900
H	-4.15114900	1.44106200	0.09547800
N	-3.03742800	-0.37045500	0.06805200
C	-1.65810900	-0.53917400	0.04187500
C	-0.84676100	-1.64079900	0.02442900
N	0.49153600	-1.42626400	0.00482300
C	1.06155500	-0.16867000	-0.00158900
N	2.38994800	-0.08474400	-0.01984400
H	2.98382700	-0.92078800	-0.00823700
H	2.84705200	0.82952800	0.00638900
N	0.30144500	0.94424200	0.00815600
C	-1.01109200	0.72846600	0.03326700
C	-1.89033600	3.10810200	0.06331000
H	-1.32270800	3.42719900	0.93945000
H	-1.38980200	3.44352600	-0.84644500
H	-2.89280000	3.53351400	0.10580400
O	4.01536300	2.41784600	0.03109000
H	3.20875600	2.98091100	-0.03360100
H	4.35907600	2.55915700	0.92479100
O	1.84499800	-3.92880000	-0.06660400
H	1.62865900	-4.56102000	0.63557900
H	1.09609500	-2.26702100	-0.01100800
O	4.17578700	-2.40625700	-0.03436300
H	4.65979700	-2.49168200	0.79971400
H	3.45533000	-3.07085400	0.01181300
O	1.56994900	3.60583200	-0.34532500
H	1.22805200	4.21669700	0.32394200
H	1.08244900	2.76595800	-0.20217000
O	-5.23106300	-2.23476900	0.01493700
H	-5.48898900	-2.33431800	-0.91234900
H	-4.47174200	-1.60826000	0.00449000
H	-1.17774900	-2.67217600	0.02589900
H	1.69521400	-4.40280700	-0.89896000

Figure S7. Cartesian coordinates, enthalpies, and free energies of optimized structures of fluorescent nucleobases used in this study are given.

2AP 5H2O B3LYP N3 Cation

Enthalpy (Hartrees) = -889.104658

Free Energy (Hartrees) = -889.187425

Charge = 1 Multiplicity = 1

N	-2.10334600	1.55319300	0.02558000
C	-3.24942300	0.77206600	0.04926800
H	-4.22672400	1.23415700	0.06576200
N	-3.00998400	-0.51694000	0.04840900
C	-1.62508400	-0.61247300	0.02270000
C	-0.73767800	-1.68530400	0.00648200
N	0.58125400	-1.48861500	-0.01693500
C	1.08445400	-0.22711000	-0.02618800
N	2.40088400	-0.05502800	-0.04544500
H	3.01629600	-0.87437400	-0.04985000
H	2.83696000	0.87261100	-0.02794100
N	0.26552300	0.87667100	-0.01776700
C	-1.07281800	0.67360800	0.00833400
C	-2.06024000	3.01857400	0.02382000
H	-1.53417100	3.37550800	0.91088300
H	-1.55854700	3.37382800	-0.87766600
H	-3.08730400	3.38051000	0.03772900
O	3.87445000	2.48934900	-0.01945400
H	3.04474800	3.01179000	0.01691700
H	4.30738200	2.63141600	0.83479700
O	2.13263500	-3.90244600	-0.05887400
H	1.99338900	-4.35818000	0.78428200
H	1.57568600	-3.08852900	-0.01369600
O	4.36346400	-2.26775100	-0.10662900
H	4.85953300	-2.30283600	0.72379300
H	3.67525500	-2.96904000	-0.03210200
O	1.30177700	3.50682200	-0.07652500
H	0.92304700	4.03583400	0.64259400
H	0.66319300	1.84039600	-0.03696700
O	-5.13967800	-2.46143500	0.04794900
H	-5.28253800	-2.72069600	-0.87329500
H	-4.39447600	-1.81919800	0.02061600
H	-1.08164200	-2.71577300	0.01249000
H	1.03313100	3.95512500	-0.89347600

2AP 5H2O B3LYP N7 Cation

Enthalpy (Hartrees) = -889.109301

Free Energy (Hartrees) = -889.192457

Charge = 1 Multiplicity = 1

N	2.04268300	-1.64143000	0.04276800
C	3.21206400	-0.96918400	0.05001400
H	4.18196400	-1.44324300	0.08092900
N	3.00742000	0.34116700	0.01445500
C	1.63623300	0.55606600	-0.01740000
C	0.80212100	1.66793600	-0.05683900
N	-0.51606800	1.49166900	-0.07283100
C	-1.02875000	0.21815500	-0.05289900
N	-2.36612300	0.10599200	-0.07150600
H	-2.95584100	0.93663700	-0.06734900
H	-2.81497300	-0.80443600	-0.00298100
N	-0.28690600	-0.91927300	-0.02166200
C	1.02256100	-0.70150500	-0.00047100
C	1.89106300	-3.09981700	0.08283100
H	1.32253300	-3.38054500	0.97060300
H	1.37360900	-3.43642800	-0.81609200
H	2.88491000	-3.54401500	0.12598900
O	-4.06739800	-2.45647700	0.15262300
H	-3.22847200	-2.96312500	0.04848800
H	-4.31788300	-2.56172400	1.08138500
O	-2.02044000	3.90533900	-0.07956600
H	-1.84924900	4.35162800	0.76268200
H	-1.48072800	3.07541400	-0.05418400
O	-4.35564300	2.42013600	-0.06596700
H	-4.77812000	2.44643600	0.80435100
H	-3.60307600	3.05421500	-0.01081100
O	-1.58179500	-3.53323800	-0.33405400
H	-1.20189100	-4.15155300	0.30718000
H	-1.08756600	-2.69197300	-0.20722000
O	5.05206300	2.18340700	0.02270500
H	4.93840400	2.86216600	-0.66026000
H	3.76515900	1.06248900	0.01555300
H	1.17811600	2.68643300	-0.07407800
H	5.08002200	2.67150600	0.85990300

Figure S7. continued.

A 5H2O B3LYP Neutral

Enthalpy (Hartrees) = -888.676864

Free Energy (Hartrees) = -888.760606

Charge = 0 Multiplicity = 1

C	1.58439800	0.19654000	-0.03145700
C	1.00298400	-1.95039100	0.00442200
C	-0.74231800	-0.39250000	0.00957700
C	0.25180800	0.61709200	-0.01525600
H	1.27005300	-3.00333500	0.01467000
C	1.45812000	2.38510700	-0.05324300
H	1.79790500	3.41155000	-0.06883500
N	0.19400000	2.00264700	-0.02905200
N	-0.31202500	-1.68475200	0.02027600
N	2.01555800	-1.08150000	-0.02282800
N	-2.06004700	-0.15179800	0.02558200
H	-2.72181900	-0.92734300	0.03170900
H	-2.44183800	0.79144300	-0.00811200
C	3.80232000	1.42947500	-0.08240300
H	4.22246400	0.96679000	0.81276000
H	4.19210600	0.92790600	-0.97025900
H	4.07993700	2.48291600	-0.11008100
N	2.34392000	1.34160000	-0.05652700
O	-1.97346100	-3.94337000	0.03506200
H	-1.36686100	-3.15408900	0.00279600
H	-1.85812300	-4.39564900	-0.81339500
O	-1.72101000	4.05262700	0.10708000
H	-1.04373100	3.32651900	0.09433000
H	-1.68577500	4.42672100	0.99953100
O	4.62584600	-2.24753500	0.01650100
H	4.87136400	-2.33763000	0.94805800
H	3.74759200	-1.79627000	0.02473400
O	-4.21509100	-2.33133300	-0.02562400
H	-4.66138300	-2.38208900	0.83161500
H	-3.49224100	-3.00157000	0.01561100
O	-3.83804600	2.29714800	-0.05294800
H	-4.21073800	2.34786300	-0.94463000
H	-3.14489300	2.99875300	-0.01853700

A 5H2O B3LYP N1 Cation

Enthalpy (Hartrees) = -889.116294

Free Energy (Hartrees) = -889.198964

Charge = 1 Multiplicity = 1

C	1.56920600	0.26321600	0.01753800
C	1.06249900	-1.88544700	0.28372400
C	-0.76905100	-0.33319300	-0.01609100
C	0.23468200	0.66294000	-0.09691100
H	1.29801300	-2.93184700	0.43815800
C	1.42390900	2.42501300	-0.27874900
H	1.75506400	3.44702900	-0.39945000
N	0.16377800	2.02834900	-0.28274400
N	-0.26522500	-1.59948300	0.18150000
N	2.02474500	-1.00082400	0.20821100
N	-2.07292400	-0.14831500	-0.11059900
H	-2.72944200	-0.93991100	-0.05780500
H	-2.47650400	0.78201000	-0.26850900
C	3.77583600	1.50886800	-0.05413200
H	4.14246800	1.16460800	0.91416100
H	4.21794500	0.90944800	-0.85156800
H	4.04220000	2.55579400	-0.19420900
N	2.31660000	1.40182100	-0.10190800
O	-1.80285800	-3.98118600	0.49927300
H	-0.90812500	-2.40699300	0.26752900
H	-1.60114900	-4.71616100	-0.09983800
O	-1.76698800	4.10483200	-0.49168100
H	-1.08589600	3.39672800	-0.38162800
H	-1.77431400	4.59175000	0.34537600
O	4.74921000	-2.04740000	0.52281600
H	4.74101400	-2.51905500	1.36782900
H	3.84964800	-1.66580300	0.43680500
O	-3.97408900	-2.33711400	-0.06565300
H	-4.58417200	-2.27277100	0.68331100
H	-3.32682100	-3.03274800	0.18015000
O	-3.74896200	2.19783400	-0.49578900
H	-4.14954000	2.15368100	-1.37588900
H	-3.12497500	2.96162000	-0.52848500
H	-1.74566100	-4.35152600	1.39338400

Figure S7. continued.

A 5H2O B3LYP N3 Cation

Enthalpy (Hartrees) = -889.113116

Free Energy (Hartrees) = -889.193165

Charge = 1 Multiplicity = 1

C	1.59978300	0.17072100	-0.00368500
C	0.95306900	-2.03558600	0.00328300
C	-0.73949200	-0.42287200	-0.00666000
C	0.26972100	0.57890600	-0.00992700
H	1.24793800	-3.07886200	0.00792300
C	1.48266000	2.34185300	-0.00891100
H	1.83140400	3.36509200	-0.00937900
N	0.22102100	1.96196100	-0.01378100
N	-0.32757500	-1.73581000	-0.00066000
N	1.96086000	-1.13953900	0.00193800
N	-2.04107000	-0.17782200	-0.00854400
H	-2.71140300	-0.95287900	0.00123700
H	-2.42497100	0.77105900	-0.01269500
C	3.83298300	1.38096200	0.00519400
H	4.23047800	0.86174900	0.87923300
H	4.23657400	0.93996200	-0.90791200
H	4.10286600	2.43515500	0.05343600
N	2.37001400	1.29175900	-0.00170000
O	-2.03954200	-4.05019700	0.01347500
H	-1.42177400	-3.28216600	-0.03033200
H	-1.94698900	-4.50579100	-0.83611100
O	-1.67223400	4.08604500	-0.01897200
H	-1.00568800	3.35734700	0.01858800
H	-1.60458000	4.54409800	0.83160700
O	4.56610300	-2.08950900	0.05655900
H	5.13616800	-1.35714800	0.33801300
H	2.95533200	-1.46499400	0.00486900
O	-4.16232000	-2.27677000	-0.02626800
H	-4.61501000	-2.29468900	0.82907700
H	-3.50741700	-3.01256200	0.00763100
O	-3.71817100	2.24549900	0.04022300
H	-4.21351100	2.29014100	-0.79010400
H	-3.07047100	2.98835600	0.00025400
H	4.87533800	-2.31830500	-0.83332200

A 5H2O B3LYP N7 Cation

Enthalpy (Hartrees) = -889.111815

Free Energy (Hartrees) = -889.193371

Charge = 1 Multiplicity = 1

C	1.55618500	0.16456900	-0.03734800
C	0.96477700	-1.97417600	-0.01553600
C	-0.78296900	-0.41428000	0.00299000
C	0.22958200	0.58217800	-0.01538600
H	1.22903300	-3.02738700	-0.01199200
C	1.52195000	2.36579000	-0.03801300
H	1.84823100	3.39507600	-0.04134800
N	0.25088000	1.97034000	-0.01662600
N	-0.34597900	-1.70340400	0.00407600
N	1.98200400	-1.10785500	-0.03918700
N	-2.09308000	-0.17250900	0.02027500
H	-2.75179300	-0.95462600	0.02880100
H	-2.48606300	0.77176400	-0.00127300
C	3.80894200	1.34748600	-0.08208100
H	4.20344000	0.86310600	0.81179900
H	4.16737200	0.83309500	-0.97439800
H	4.11687900	2.39154400	-0.10618500
N	2.34342500	1.30562200	-0.05287400
O	-2.00591700	-4.00530700	0.03419200
H	-1.40425200	-3.21871800	-0.00776700
H	-1.89272900	-4.46472700	-0.81077800
O	-1.60492100	4.07066700	0.13633600
H	-0.53570000	2.64535500	0.01980900
H	-1.55812700	4.54654200	0.97984700
O	4.60472900	-2.33468900	0.03885900
H	4.83429000	-2.43094900	0.97395000
H	3.74246300	-1.86150300	0.03519300
O	-4.20071900	-2.32768300	-0.02762700
H	-4.67117000	-2.38071400	0.81653300
H	-3.51015300	-3.03039200	0.01251100
O	-3.71331500	2.26836500	-0.00747700
H	-4.17451900	2.33236400	-0.85611100
H	-3.05883600	2.99916700	-0.01005800
H	-1.48878100	4.74542200	-0.55020400

Figure S7. continued.

DAP 7H2O B3LYP Neutral

Enthalpy (Hartrees) = -1096.890572

Free Energy (Hartrees) = -1096.993185

Charge = 0 Multiplicity = 1

N	0.50746300	-2.98751700	-0.05564800
C	-0.82477300	-3.32750300	-0.03036800
H	-1.13848500	-4.36226500	-0.02635000
N	-1.63017600	-2.28531500	-0.01467200
C	-0.77580800	-1.18977100	-0.03218900
C	-0.99329600	0.20782700	-0.02847200
N	0.08639800	1.01923100	-0.06595400
C	1.33643000	0.48832100	-0.08335100
N	2.36360400	1.37826000	-0.15087800
H	2.17969500	2.35537800	0.05550900
H	3.31274900	1.04874400	-0.01342600
N	1.64663300	-0.82634600	-0.07096900
C	0.55411500	-1.61272500	-0.05629600
O	-4.47445100	-2.53822200	0.02950900
H	-3.49282600	-2.43917300	0.01315300
H	-4.81325400	-1.62175500	0.08629800
O	4.31662900	-1.66710000	0.36962200
H	4.54916100	-2.32937400	-0.29709900
H	3.37228200	-1.42366900	0.18240100
O	5.51702200	0.79290300	0.12365300
H	5.81737000	0.92463500	-0.78666900
H	5.17291100	-0.13140700	0.15433700
O	-0.31033000	3.70363400	-0.88152400
H	-1.20083600	3.90525600	-0.52612900
H	-0.16420900	2.75794700	-0.61987400
O	1.98753000	4.49912500	0.39989600
H	1.81762900	4.58939500	1.34818100
H	1.10462200	4.32831600	-0.00793600
N	-2.21729700	0.76609300	0.00474600
H	-3.05541400	0.20072700	0.05432500
H	-2.32329700	1.77491700	0.05514900
O	-5.31176400	0.17349800	0.19952500
H	-5.76616700	0.33269800	1.04038800
H	-5.97038900	0.37690600	-0.48142500
O	-2.90889100	3.82216300	0.21637500
H	-2.96568800	4.28661500	1.06484600
H	-3.59793800	4.22163700	-0.33543700
C	1.63654100	-3.91264700	-0.08155500
H	2.25944500	-3.72143700	-0.95801200
H	2.23732600	-3.80575500	0.82383100
H	1.24372300	-4.92819100	-0.13550700

DAP 7H2O B3LYP N1 Cation

Enthalpy (Hartrees) = -1097.335241

Free Energy (Hartrees) = -1097.434385

Charge = 1 Multiplicity = 1

N	-0.54401200	-2.95898200	0.01309600
C	0.78561700	-3.31744000	0.00383300
H	1.08405400	-4.35653300	-0.01019000
N	1.60557100	-2.28954300	0.01460300
C	0.76632600	-1.18619000	0.03447700
C	1.02788200	0.19393800	0.05297600
N	-0.09135400	0.99010900	0.08022400
C	-1.38868200	0.50520000	0.05825800
N	-2.37154700	1.41222900	0.07910900
H	-2.19116100	2.41063100	-0.04862200
H	-3.34295200	1.10163200	0.06331300
N	-1.66540800	-0.80036400	0.03015300
C	-0.57341200	-1.58989500	0.03119300
O	4.46701700	-2.64091000	0.01409600
H	3.48975000	-2.52794800	0.01652600
H	4.80997700	-1.72450200	-0.01336300
O	-4.40178000	-1.69168300	-0.36795400
H	-4.61195900	-2.37572400	0.28423200
H	-3.45774300	-1.45826500	-0.20662500
O	-5.35028700	0.84435500	0.06667400
H	-5.67499000	0.95099600	0.97209200
H	-5.14100400	-0.11508700	-0.02748200
O	0.45988600	3.76043500	0.62030000
H	1.38238000	3.86163700	0.28649300
H	0.04838800	2.00858200	0.21419800
O	-2.05778800	4.33708300	-0.33837000
H	-2.07131500	4.53649900	-1.28537400
H	-1.10835300	4.28827100	-0.09217100
N	2.23153400	0.75671800	0.05429300
H	3.07281100	0.18714400	0.02774700
H	2.35922800	1.76510600	-0.01974600
O	5.20647000	0.09226200	-0.06157100
H	5.65495900	0.33212200	-0.88630600
H	5.83046100	0.32838400	0.64112600
O	3.01345100	3.66120700	-0.35359300
H	3.12083000	4.01901500	-1.24788100
H	3.69916600	4.09150900	0.17914600
C	-1.68646600	-3.87101300	-0.00409400
H	-2.32376700	-3.68763800	0.86296800
H	-2.26274300	-3.73590600	-0.92108700
H	-1.30532800	-4.89116200	0.03787500
H	0.50249300	3.91048400	1.57625500

Figure S7. continued.

DAP 7H2O B3LYP N3 Cation

Enthalpy (Hartrees) = -1097.330604

Free Energy (Hartrees) = -1097.429428

Charge = 1 Multiplicity = 1

N	0.65478900	-2.93801400	-0.03610800
C	-0.66617400	-3.33891300	-0.04663900
H	-0.92785500	-4.38748600	-0.06597400
N	-1.51300700	-2.33304200	-0.03162400
C	-0.71254400	-1.20211200	-0.01055300
C	-1.00396900	0.19012400	0.01467500
N	0.02676600	1.06887500	0.01833300
C	1.30210300	0.65091400	0.02263200
N	2.28382000	1.55566100	0.04075800
H	2.04892300	2.54698600	0.11272800
H	3.27145800	1.29131800	0.04266000
N	1.64505200	-0.67904500	0.00815300
C	0.62031800	-1.57739600	-0.01366200
O	-4.36902700	-2.74584200	-0.04835600
H	-3.39543100	-2.60731800	-0.04477500
H	-4.73990100	-1.84140400	0.00753900
O	4.36853300	-1.59142300	0.10526500
H	4.54163100	-2.24718600	-0.58755700
H	2.63448800	-0.98270800	0.03282700
O	5.21217800	1.04572800	0.09168500
H	5.62469000	1.30831500	-0.74369000
H	5.08229800	0.07526100	0.02722800
O	-0.57950100	3.74792900	-0.88985600
H	-1.46928200	3.88624300	-0.50324100
H	-0.35738100	2.82737200	-0.61894000
O	1.80295100	4.53279300	0.24273000
H	1.69960400	4.79896600	1.16749400
H	0.88623500	4.41294800	-0.10000900
N	-2.24744400	0.67049800	0.03289000
H	-3.05627900	0.05846700	0.03889500
H	-2.41671600	1.67352600	0.08566700
O	-5.25965800	-0.06019500	0.12535700
H	-5.72066500	0.09357200	0.96366300
H	-5.91258400	0.14619800	-0.56018500
O	-3.13303600	3.61327500	0.28174800
H	-3.23742100	4.00760300	1.16067800
H	-3.89208600	3.93180900	-0.22947400
C	1.82632400	-3.81672000	-0.04559600
H	2.44557300	-3.60250700	-0.91850600
H	2.40770300	-3.67614700	0.86733600
H	1.47089000	-4.84530400	-0.09616200
H	4.52640300	-2.05655700	0.94126100

DAP 7H2O B3LYP N7 Cation

Enthalpy (Hartrees) = -1097.332371

Free Energy (Hartrees) = -1097.430609

Charge = 1 Multiplicity = 1

N	-0.41315200	-2.97392500	0.09017900
C	0.89289100	-3.30576300	0.07921100
H	1.26374000	-4.31924900	0.10519500
N	1.64906700	-2.21602500	0.03417100
C	0.80686000	-1.11146200	0.01516900
C	0.98556800	0.29464300	-0.02965900
N	-0.12689900	1.05316400	-0.02233800
C	-1.35914500	0.47786300	0.00316000
N	-2.41288000	1.31931300	0.00003000
H	-2.26966300	2.32117200	-0.09353600
H	-3.36371600	0.96261100	0.01641900
N	-1.61554100	-0.85376400	0.03549500
C	-0.49866500	-1.58860900	0.04874200
O	4.37732900	-2.37442600	-0.05860200
H	2.69852500	-2.23631500	0.01815800
H	4.74129100	-1.45699400	-0.05255800
O	-4.26983300	-1.80519100	-0.52463100
H	-4.46834500	-2.55765100	0.05131800
H	-3.34246400	-1.54435600	-0.30401400
O	-5.44976400	0.60640800	0.06562900
H	-5.73874700	0.63261700	0.98873200
H	-5.13638000	-0.31654700	-0.08515400
O	0.20606900	3.74207700	0.89260000
H	1.07835300	3.97635100	0.51215800
H	0.07331100	2.80700300	0.60116400
O	-2.20159700	4.42352200	-0.24643500
H	-2.09388100	4.68061800	-1.17306700
H	-1.28554300	4.32175800	0.10556100
N	2.18265100	0.89575800	-0.07696300
H	3.05323400	0.37495900	-0.07322600
H	2.24161800	1.90995600	-0.12695600
O	5.18684700	0.24956900	-0.15000900
H	5.63967400	0.43660000	-0.98635800
H	5.82671100	0.47999500	0.54052300
O	2.76369500	3.94916400	-0.27698800
H	2.79241700	4.43192500	-1.11660800
H	3.45714300	4.35012100	0.26818500
C	-1.53317900	-3.91647800	0.14317900
H	-2.14518500	-3.70553600	1.02139000
H	-2.13485600	-3.82353000	-0.76162600
H	-1.12564200	-4.92420900	0.21282600
H	4.72773200	-2.80310300	0.73613200

Figure S7. continued.

ethenoA 3H2O B3LYP Neutral

Enthalpy (Hartrees) = -811.998606

Free Energy (Hartrees) = -812.066277

Charge = 0 Multiplicity = 1

C	-1.16609900	-0.45550400	0.01393900
C	0.22812900	-0.37217000	0.00666200
C	0.79388400	0.92616700	-0.00587500
C	-1.51099200	1.76954100	-0.00562100
C	-0.26903900	-2.45160900	0.02826600
H	-2.13177600	2.65783000	-0.01114000
H	-0.21230300	-3.53112000	0.03806600
C	0.57102900	3.16072800	-0.02399400
H	0.08262900	4.12248600	-0.03058100
C	1.88591900	2.78576500	-0.02286800
H	2.75034400	3.43471900	-0.02898700
N	0.77760300	-1.63504700	0.01572700
N	-1.46516800	-1.79991100	0.02819800
N	-2.04850700	0.57820700	0.00827800
N	-0.15253300	1.97085100	-0.01286000
N	2.02819500	1.40845700	-0.01191100
C	-2.79616300	-2.40510900	0.04310200
H	-3.34138400	-2.08590100	0.93335000
H	-3.34960300	-2.11332600	-0.85140900
H	-2.67716600	-3.48823100	0.05953300
O	3.42205900	-2.64238000	-0.05748300
H	2.49318600	-2.29697300	-0.05767900
H	3.56998600	-2.98149200	-0.95217800
O	4.51323900	-0.02591400	0.13956700
H	3.66624100	0.47580500	0.08313000
H	4.23662700	-0.96413300	0.07004500
O	-4.97120200	0.59648200	0.02396700
H	-5.20669200	1.37833200	-0.49534500
H	-3.98999300	0.56175000	0.00109300

ethenoA 3H2O B3LYP N1 Cation

Enthalpy (Hartrees) = -812.434025

Free Energy (Hartrees) = -812.502396

Charge = 1 Multiplicity = 1

C	1.15893700	-0.44633000	-0.00468200
C	-0.22444000	-0.32662900	0.01235600
C	-0.78088500	0.97216100	0.01894400
C	1.54130000	1.76968700	-0.00601900
C	0.28586800	-2.46436800	0.00637000
H	2.17923900	2.64584500	-0.01217300
H	0.18808300	-3.53941300	0.00760200
C	-0.51514100	3.19636800	0.01712600
H	-0.01006800	4.14949200	0.01237300
C	-1.83730400	2.84495200	0.02949000
H	-2.69039400	3.50819200	0.03727700
N	-0.73894800	-1.60443400	0.01978200
N	1.44872500	-1.80228100	-0.00923800
N	2.05668800	0.56931800	-0.01437800
N	0.18737000	1.99747700	0.00968500
N	-2.00335400	1.47094300	0.03078100
C	2.78731500	-2.40353000	-0.03186400
H	3.31334900	-2.07814400	-0.92993600
H	3.33690900	-2.09510100	0.85799700
H	2.67106800	-3.48602200	-0.04106600
O	-3.35434500	-2.55603000	0.06993200
H	-1.73758100	-1.90231000	0.03676800
H	-3.55651000	-3.01032800	0.90254100
O	-4.50804500	0.05627600	-0.13574900
H	-3.66129900	0.55411400	-0.07315700
H	-4.23398800	-0.87945300	-0.08265800
O	5.02008600	0.52962900	-0.06069300
H	5.27738300	1.31590800	0.44143200
H	4.04171400	0.51481500	-0.02438200
H	-3.52675000	-3.20762900	-0.62727000

Figure S7. continued.

ethenoA 3H2O B3LYP N4 Cation

Enthalpy (Hartrees) = -812.424228

Free Energy (Hartrees) = -812.489996

Charge = 1 Multiplicity = 1

C	1.17383600	-0.43083700	-0.00596800
C	-0.21784100	-0.36423600	0.00125800
C	-0.82369100	0.91577100	0.01334900
C	1.43360300	1.87523700	0.01289200
C	0.32591600	-2.43079700	-0.01951200
H	2.06412900	2.75492100	0.01647300
H	0.29684800	-3.51134000	-0.02873900
C	-0.67833400	3.17017300	0.03199500
H	-0.22680300	4.14964600	0.03875100
C	-1.97287200	2.74042200	0.02934600
H	-2.86229900	3.35398400	0.03435800
N	-0.73503400	-1.63770300	-0.00751300
N	1.51415800	-1.75498600	-0.01976700
N	1.98178700	0.67336100	-0.00090300
N	0.09410800	2.00794800	0.02144300
N	-2.06280900	1.35566200	0.01807000
C	2.85817100	-2.34293600	-0.02965900
H	3.40251600	-2.00418000	-0.91311400
H	3.39434800	-2.05486900	0.87621300
H	2.74826000	-3.42595800	-0.06160900
O	-3.38428000	-2.72986700	0.04889800
H	-2.46807800	-2.36320300	0.05786200
H	-3.53045900	-3.07523200	0.94158000
O	-4.54831200	-0.14991100	-0.16778900
H	-3.71988800	0.37349300	-0.09982700
H	-4.24554500	-1.07970900	-0.09211100
O	4.67183200	0.66637500	-0.07650100
H	5.05359000	0.89993800	0.78422300
H	3.04424700	0.61142800	-0.00905400
H	4.99700500	-0.22845100	-0.26339200

ethenoA 3H2O B3LYP N9 Cation

Enthalpy (Hartrees) = -812.441846

Free Energy (Hartrees) = -812.509836

Charge = 1 Multiplicity = 1

C	1.21198500	-0.44696000	-0.01663000
C	-0.18932600	-0.42032800	-0.01302000
C	-0.77410000	0.85619800	-0.00205400
C	1.46691900	1.78844800	0.00255100
C	0.38669100	-2.47172900	-0.03049900
H	2.04538700	2.70420400	0.00960600
H	0.37348300	-3.55278000	-0.03866800
C	-0.65992700	3.11297600	0.01646600
H	-0.19330100	4.08470500	0.02409000
C	-1.96136200	2.73046500	0.01360700
H	-2.85816900	3.32981400	0.01835100
N	-0.69140700	-1.70002100	-0.02172800
N	1.55916900	-1.77406100	-0.02826200
N	2.04671100	0.61956200	-0.00932800
N	0.09698200	1.93541000	0.00628200
N	-2.02125500	1.34604300	0.00242400
C	2.91444000	-2.32790200	-0.03686200
H	3.44649200	-1.98974000	-0.92758700
H	3.45017600	-2.00922800	0.85874000
H	2.83588200	-3.41427400	-0.04874900
O	-3.37136600	-2.61758000	0.03351600
H	-2.42080400	-2.34231200	0.04500800
H	-3.53507900	-3.02790600	0.89538300
O	-4.37551000	-0.07812900	0.00682200
H	-2.90241800	0.77875700	-0.01078000
H	-4.09819000	-1.02939800	0.00187700
O	5.01596000	0.73225000	-0.00959800
H	5.22223500	1.53477400	0.49038800
H	4.03948200	0.66683200	0.00931300
H	-4.86116600	0.05867000	-0.81997700

Figure S7. continued.

8furanA 6H2O B3LYP Neutral

Enthalpy (Hartrees) = -1193.89071

Free Energy (Hartrees) = -1193.993283

Charge = 0 Multiplicity = 1

N	-0.62390200	-0.47557600	-0.23382400
C	-1.51179400	0.51652800	-0.19441500
C	0.60442600	0.14225500	-0.12854900
N	-0.91397600	1.75742900	-0.06585700
C	-2.94144100	0.32142900	-0.28307200
H	-1.08829400	-2.11343600	-0.96446900
C	0.44093400	1.52605900	-0.03358100
C	1.93143500	-0.35512500	-0.10126400
C	-1.55664500	3.06571700	0.05190900
C	-4.01186000	1.11539000	-0.61231500
O	-3.38475900	-0.95885700	-0.02453100
O	-1.27932200	-2.98815200	-1.38759000
N	1.43038000	2.43462300	0.06924100
N	2.93500700	0.55954500	-0.00339200
N	2.24589200	-1.65635500	-0.16915300
H	-1.93015800	3.40220600	-0.91790200
H	-0.81651800	3.77592600	0.41694400
H	-2.37910900	3.00888100	0.76624300
C	-5.17330300	0.28272200	-0.55539000
H	-3.98147800	2.15892600	-0.88631200
C	-4.74258100	-0.95855500	-0.19585500
H	-2.92198300	-1.56297200	1.94643300
H	-2.18458000	-3.20366900	-1.12060600
H	-1.86814000	-1.82649500	3.02965300
C	2.63783500	1.86512400	0.07322200
H	1.47938000	4.32087200	0.14097300
H	4.71003000	0.19814900	0.03707000
H	1.53405100	-2.38154300	-0.17785700
H	3.22068700	-1.95318000	-0.12357300
H	-6.19389500	0.57405900	-0.75943400
H	-5.23740300	-1.90171100	-0.01936600
O	-2.82386900	-1.82651600	2.87584300
O	0.74731200	-4.35478500	-0.13556200
H	3.48786700	2.53753500	0.14809800
O	1.56885300	5.30263300	0.17574700
O	5.67795200	-0.03206200	0.00440100
O	5.10678400	-2.73089200	-0.10641500
H	0.47864800	-4.59135200	0.76328700
H	-0.05422300	-3.95811400	-0.55215600
H	2.52226400	5.46686500	0.15678700
H	5.43167300	-1.80516900	-0.00364800
H	6.04482400	0.25313000	0.85370800
H	5.26691100	-3.15675800	0.74775900

8furanA 6H2O B3LYP N1 Cation

Enthalpy (Hartrees) = -1194.330431

Free Energy (Hartrees) = -1194.432777

Charge = 1 Multiplicity = 1

N	-0.67319200	-0.49048100	-0.20541700
C	-1.52042000	0.53851300	-0.18257600
C	0.57318100	0.07851200	-0.12065300
N	-0.86871600	1.75689100	-0.08880500
C	-2.95581900	0.39639100	-0.24203300
H	-1.24028500	-2.07145600	-1.08939700
C	0.46850000	1.47015700	-0.05563400
C	1.86683900	-0.49642400	-0.07588700
C	-1.45740700	3.09501100	-0.00756600
C	-4.00991400	1.23679000	-0.50650300
O	-3.43280500	-0.87692700	-0.01196200
O	-1.44847500	-2.90360700	-1.57563700
N	1.49223000	2.35464800	0.02842100
N	2.87643100	0.43531500	0.00888200
N	2.15842400	-1.78501900	-0.10148900
H	-1.87721600	3.38486900	-0.97276400
H	-0.67170500	3.79533500	0.26882400
H	-2.23445700	3.10646700	0.75815900
C	-5.19461400	0.44093300	-0.43838900
H	-3.95757800	2.28851400	-0.74210400
C	-4.79319800	-0.82582500	-0.13621300
H	-2.96679600	-1.53409900	1.96985000
H	-2.36052800	-3.11609000	-1.32967600
H	-1.91790600	-1.82604500	3.05027900
C	2.66875700	1.77924500	0.05530900
H	1.63782100	4.32118100	0.08409900
H	3.86514800	0.12798100	0.04511100
H	1.42748600	-2.50270200	-0.14272200
H	3.13338200	-2.11239300	-0.05964100
H	-6.21109200	0.77231000	-0.59617800
H	-5.31369900	-1.75790300	0.02482800
O	-2.87337700	-1.81076600	2.89556700
O	0.56342900	-4.22945100	-0.25886200
H	3.56601700	2.38330500	0.11952000
O	1.76262900	5.29271900	0.11281100
O	5.66661800	-0.13266500	0.14733500
O	4.88018900	-2.79672200	-0.04214700
H	0.25841500	-4.52489400	0.61081300
H	-0.23871700	-3.87773600	-0.71247200
H	2.72180100	5.42106000	0.11903100
H	5.30498200	-1.91939900	0.07307500
H	6.08682400	0.18810400	0.95990800
H	5.06649100	-3.28335000	0.77395400
H	6.20426100	0.21701300	-0.57960800

Figure S7. continued.

8furanA 6H2O B3LYP N3 Cation

Enthalpy (Hartrees) = -1194.326319

Free Energy (Hartrees) = -1194.427846

Charge = 0 Multiplicity = 1

N	-0.60859500	-0.50530300	-0.21612200
C	-1.51074900	0.47036800	-0.18536400
C	0.61023400	0.12509500	-0.10830600
N	-0.92842700	1.72682300	-0.05372100
C	-2.93546800	0.25857900	-0.28911100
H	-1.11000600	-2.14519200	-1.01821800
C	0.41251300	1.49904800	-0.02298700
C	1.94389200	-0.36706300	-0.07150300
C	-1.60166200	3.02377000	0.07956800
C	-4.00406600	1.02063900	-0.69257200
O	-3.37081600	-1.01035100	0.02839700
O	-1.30221300	-3.00505200	-1.46143700
N	1.44719600	2.37448900	0.07022500
N	2.95920800	0.55638000	0.01548300
N	2.26897700	-1.65135300	-0.11215000
H	-1.86633100	3.41942900	-0.90291600
H	-0.93584600	3.71939200	0.58835500
H	-2.49766300	2.89628400	0.68602500
C	-5.15661600	0.17892700	-0.61925100
H	-3.97605600	2.04623100	-1.02915900
C	-4.72198700	-1.03515800	-0.17812600
H	-2.91310700	-1.56213100	2.02009100
H	-2.19939900	-3.23647800	-1.18033400
H	-1.85533800	-1.81490000	3.10211300
C	2.68679800	1.84079000	0.07845100
H	1.33708900	3.41417700	0.11289900
H	4.82964900	0.21187000	0.00639700
H	1.56804600	-2.39489200	-0.14028400
H	3.25275800	-1.93689300	-0.07528300
H	-6.17417300	0.44530900	-0.86733800
H	-5.21227500	-1.97217100	0.03934800
O	-2.81211100	-1.80204100	2.95546200
O	0.79279200	-4.22982300	-0.17204000
H	3.50460800	2.54977900	0.14329500
O	1.35575800	5.13722300	0.22279200
O	5.78250900	-0.03026000	-0.06992400
O	5.05547300	-2.70310500	-0.06736400
H	0.52707900	-4.50521300	0.71680800
H	-0.03390400	-3.91331300	-0.60645100
H	2.03748200	5.51144000	-0.35626700
H	5.45579300	-1.80509300	-0.00517600
H	6.19535700	0.27405000	0.75141100
H	5.23233600	-3.12458200	0.78589500
H	0.51692100	5.47294100	-0.12908600

8furanA 6H2O B3LYP N7 Cation

Enthalpy (Hartrees) = -1194.32496

Free Energy (Hartrees) = -1194.426107

Charge = 1 Multiplicity = 1

N	-0.64800800	-0.36862400	-0.24783000
C	-1.53283100	0.64473100	-0.16314800
C	0.63108900	0.15232400	-0.13605100
N	-0.86006200	1.81359500	0.01405100
C	-2.95395700	0.49169000	-0.24869100
H	-0.91011800	-1.34175800	-0.50193100
C	0.49563800	1.52699900	0.01719400
C	1.94041400	-0.39363500	-0.13515400
C	-1.44175300	3.14717900	0.18989400
C	-4.01380900	1.35571900	-0.40673700
O	-3.41842700	-0.80439700	-0.19957700
O	-1.42458300	-2.93780500	-1.10935200
N	1.50254600	2.40398600	0.13699000
N	2.96038300	0.50239500	-0.03848500
N	2.22755000	-1.69478500	-0.22989300
H	-1.87076700	3.49749100	-0.75058000
H	-0.64525400	3.81971500	0.49948900
H	-2.20665400	3.11059500	0.96669400
C	-5.18655400	0.54888400	-0.45706000
H	-3.96918800	2.43006600	-0.49567500
C	-4.77433200	-0.74576100	-0.32644500
H	-2.93211400	-1.93445100	1.55731600
H	-2.37271800	-3.01625200	-0.92183400
H	-2.01519700	-2.31497500	2.72821600
C	2.69802400	1.80787900	0.08624000
H	1.64917200	4.32597100	0.27511500
H	4.76933800	0.11649200	-0.07588600
H	1.51352800	-2.41929500	-0.15538500
H	3.20240500	-2.00065600	-0.18259700
H	-6.20499800	0.88927400	-0.57645900
H	-5.28911000	-1.69434300	-0.29900300
O	-2.89007800	-2.48929600	2.35230000
O	0.68198500	-4.23383800	0.13528200
H	3.56392900	2.45922700	0.15896000
O	1.77571000	5.29844400	0.33614100
O	5.72461200	-0.13484600	-0.15556600
O	5.02447800	-2.80837500	-0.17413600
H	0.49878100	-4.40827300	1.06937700
H	-0.15981300	-3.89677100	-0.23792900
H	2.73485900	5.42650900	0.32906000
H	5.40731800	-1.90262600	-0.10370600
H	6.14325800	0.16416200	0.66468500
H	5.19788100	-3.22925700	0.68001200
H	-1.34255600	-3.01198600	-2.07276300

Figure S7. continued.

MDA 5H2O B3LYP Neutral

Enthalpy (Hartrees) = -1140.710514

Free Energy (Hartrees) = -1140.809089

Charge = 0 Multiplicity = 1

N	0.31754800	2.49397300	0.09134400
C	0.70324900	0.24638500	0.08131100
C	1.59905500	-0.84735700	0.03127600
N	1.22939700	-2.14040200	0.06025000
H	1.93668300	-2.87025200	0.00191800
H	0.26238100	-2.44263800	0.08436300
N	2.93933800	-0.59470800	-0.04705800
C	3.35743300	0.67413400	-0.07762700
H	4.43321100	0.81578600	-0.14097900
N	2.61619700	1.78238800	-0.04075000
C	1.29062600	1.53546500	0.03851800
C	-0.91879400	1.85312700	0.17286000
C	-2.19063100	2.42600900	0.25133800
C	-0.72776600	0.44626000	0.16959600
C	-3.28655700	1.57325600	0.33038200
H	-2.32824600	3.50210800	0.25329200
C	-1.84681500	-0.40517800	0.24780300
C	-3.11335500	0.17417200	0.32870000
H	-4.29246800	1.97522100	0.39559600
H	-1.72842900	-1.47985900	0.24744300
O	-4.28642900	-0.55619500	0.41505500
C	-4.19986000	-1.98877500	0.44502000
H	-3.75065800	-2.37351700	-0.47653900
H	-3.62382500	-2.32280600	1.31454600
H	-5.22727400	-2.34414400	0.52873600
O	-1.11236800	-4.08071800	0.04567400
H	-1.96018100	-3.83627900	0.44506000
H	-0.76033600	-4.77500900	0.62216900
O	3.16954500	-4.54573800	-0.18994500
H	3.90700300	-3.88993200	-0.20768200
H	3.26729400	-5.01910700	0.64841000
O	4.98936800	-2.47804200	-0.26579500
H	4.26278100	-1.79614500	-0.21360900
H	5.36591800	-2.39099000	-1.15365800
O	4.35592200	4.05395600	-0.09551800
H	4.59740700	4.18500400	-1.02328900
H	3.70371300	3.31245300	-0.10190100
O	-6.33497000	0.19911200	-1.45874900
H	-5.64093400	-0.04216900	-0.81392500
H	-7.06465000	-0.40935800	-1.27549200
C	0.50254400	3.93826800	0.07883600
H	0.11559900	4.37931200	1.00210600
H	1.56475500	4.16046300	-0.00244000
H	-0.02044100	4.37950700	-0.77446300

MDA 5H2O B3LYP N1 Cation

Enthalpy (Hartrees) = -1141.152705

Free Energy (Hartrees) = -1141.248362

Charge = 1 Multiplicity = 1

N	0.28446300	-2.46232600	-0.08266500
C	0.65802200	-0.21790900	-0.05284300
C	1.52965600	0.88852000	0.01194200
N	1.20000600	2.17548100	-0.00769200
H	1.91654400	2.91061500	0.03080400
H	0.23457900	2.49114900	-0.06953500
N	2.86956400	0.57093100	0.10615800
C	3.33301400	-0.70320400	0.13955400
H	4.40934000	-0.80426500	0.21881600
N	2.57850200	-1.76988600	0.08377100
C	1.24714900	-1.50866400	-0.01144100
C	-0.95473100	-1.82453900	-0.17341100
C	-2.22305600	-2.40364600	-0.26844100
C	-0.76958800	-0.41890700	-0.15826100
C	-3.31839600	-1.55406000	-0.35070900
H	-2.35588400	-3.47997200	-0.27941300
C	-1.88877300	0.43131000	-0.24006900
C	-3.15094300	-0.15245700	-0.33640800
H	-4.32258700	-1.95784500	-0.42789000
H	-1.77197800	1.50563100	-0.22962000
O	-4.32350300	0.57096500	-0.42619600
C	-4.24463400	2.00534100	-0.44224700
H	-3.80599500	2.38267200	0.48720500
H	-3.66236700	2.34943500	-1.30343600
H	-5.27335400	2.35482900	-0.53213700
O	-1.10061300	4.04115800	-0.07865000
H	-1.98016900	3.84348400	-0.43285300
H	-0.76982600	4.76528500	-0.63079600
O	3.14542700	4.34931900	0.12117800
H	3.93611800	3.76806300	0.14535300
H	3.20067400	4.82633200	-0.71936900
O	5.09305700	2.37529400	0.31867900
H	3.58175300	1.31621900	0.17129600
H	5.56483900	2.33336000	1.16443100
O	4.35667700	-4.09099700	0.09261200
H	3.83930900	-4.90710200	0.03830900
H	3.68911000	-3.37166100	0.08731700
O	-6.37467300	-0.19882100	1.45290600
H	-5.68346000	0.04515800	0.80686200
H	-7.10512300	0.41028100	1.27473000
C	0.47046000	-3.90929100	-0.07666600
H	0.09425300	-4.33816400	-1.00910300
H	1.53049000	-4.13489400	0.01885000
H	-0.06787100	-4.34965200	0.76642100
H	5.77379700	2.27132700	-0.36346900

Figure S7. continued.

MDA 5H2O B3LYP N3 Cation

Enthalpy (Hartrees) = -1141.149207

Free Energy (Hartrees) = -1141.245522

Charge = 1 Multiplicity = 1

N	0.30839400	-2.47602500	-0.14077600
C	0.69106900	-0.22543500	-0.06623400
C	1.58244900	0.87368400	0.00889400
N	1.22029300	2.15520400	-0.00653000
H	1.93143800	2.88949000	0.03112600
H	0.25516800	2.46423400	-0.08049200
N	2.93855600	0.63329700	0.10673700
C	3.37932700	-0.59972400	0.13048300
H	4.44535300	-0.78015600	0.21309000
N	2.60231400	-1.70050800	0.06087800
C	1.25635800	-1.51817700	-0.04433400
C	-0.93364600	-1.82718600	-0.20638100
C	-2.20346400	-2.40072900	-0.29289700
C	-0.74056000	-0.42438900	-0.17052300
C	-3.29662100	-1.54551200	-0.35155200
H	-2.34167600	-3.47614900	-0.31306800
C	-1.85641600	0.43165800	-0.23189300
C	-3.12276400	-0.14587700	-0.32198800
H	-4.30315500	-1.94480100	-0.42019900
H	-1.73709200	1.50569800	-0.20964600
O	-4.29352000	0.58288500	-0.38744800
C	-4.21132400	2.01689600	-0.38942100
H	-3.75385800	2.38361600	0.53541000
H	-3.64543200	2.36845600	-1.25844000
H	-5.24067700	2.36978800	-0.45539200
O	-1.06177900	4.06861200	-0.15368600
H	-1.98381800	3.85338900	-0.35699000
H	-0.78828900	4.66814700	-0.86364300
O	3.08764400	4.50927700	0.08607400
H	3.87883400	3.92591800	0.15907200
H	3.14149400	4.90581100	-0.79526900
O	5.04133500	2.56884600	0.33687500
H	4.33290400	1.88134800	0.29862800
H	5.37684900	2.54581900	1.24506000
O	4.16782600	-4.00709000	0.14643900
H	4.14622600	-4.43109300	1.01793400
H	3.06705700	-2.63160200	0.09223600
O	-6.33218300	-0.20897300	1.49530300
H	-5.64442000	0.04186300	0.84817300
H	-7.06555500	0.39857500	1.32389600
C	0.47988900	-3.92763300	-0.13752100
H	-0.14757600	-4.36113700	-0.91857600
H	1.51753800	-4.18264600	-0.34625100
H	0.19250900	-4.34315400	0.83224700
H	3.85891200	-4.68909200	-0.46933900

thA 4H2O B3LYP Neutral

Enthalpy (Hartrees) = -1139.017221

Free Energy (Hartrees) = -1139.095814

Charge = 0 Multiplicity = 1

C	-3.99423900	-0.16070700	0.01168100
H	-4.21384500	0.38905300	0.93414700
C	-0.21370400	-0.70677400	-0.01534300
C	1.05531800	-0.01047200	-0.02600600
N	2.21506200	-0.67269300	-0.03104800
H	3.09938500	-0.16281800	-0.03062200
H	2.25131300	-1.69217300	-0.01828500
N	1.06170700	1.33286900	-0.03172700
C	-0.13020600	1.99030700	-0.02592500
H	-0.04957000	3.07480400	-0.03002800
N	-1.34289900	1.48675700	-0.01584500
C	-1.40728400	0.10348500	-0.01129100
H	-4.70068800	-0.99218900	-0.05733200
H	-4.18534500	0.51255900	-0.83103200
S	-2.17652600	-2.33301100	0.00253800
C	-0.47845900	-2.06036100	-0.00804600
C	-2.57559800	-0.64269500	-0.00212200
O	-3.42294800	3.38886100	0.02121100
H	-4.26180300	2.90910600	-0.02759800
H	-2.72792400	2.67984000	0.00575900
O	3.34118400	2.93310600	-0.03054600
H	3.36111000	3.41492100	0.80898100
H	2.51140100	2.37815300	-0.00484300
O	4.93958000	0.69305700	0.07162800
H	4.47386000	1.56220500	0.02056200
H	5.43115700	0.61482500	-0.75833900
H	0.21141000	-2.89392100	-0.01211500
O	2.66989300	-3.62675600	-0.00191900
H	2.80099600	-3.90813000	0.91591500
H	3.52921200	-3.76943400	-0.42612500

Figure S7. continued.

thA 4H2O B3LYP N1 Cation

Enthalpy (Hartrees) = -1139.460291

Free Energy (Hartrees) = -1139.53784

Charge = 1 Multiplicity = 1

C	3.98253400	0.05945900	0.01013600
H	4.20848900	-0.41227400	0.97320300
C	0.22935100	0.75898300	-0.01018700
C	-1.07455300	0.14559500	-0.01442900
N	-2.21003400	0.80996900	-0.01433100
H	-3.11731400	0.31960900	-0.02815800
H	-2.22182200	1.83759900	-0.00513200
N	-1.07255400	-1.21484700	-0.01727900
C	0.08458000	-1.96679400	-0.01844000
H	-0.07919100	-3.03866200	-0.02049400
N	1.28467200	-1.48612200	-0.01704900
C	1.39001900	-0.10064200	-0.01213800
H	4.71674800	0.85188200	-0.15566500
H	4.11519000	-0.69390800	-0.77252900
S	2.25325700	2.30126000	0.00262400
C	0.54900600	2.09906000	-0.00197200
C	2.58453300	0.59556000	-0.00672400
O	3.36570000	-3.48654100	-0.00753300
H	4.21517900	-3.02591000	-0.06049200
H	2.69456700	-2.76547700	-0.01303000
O	-3.36385100	-2.94953200	0.10411100
H	-3.42966400	-3.43393000	0.94117900
H	-1.96004500	-1.74261200	-0.00273800
O	-4.76057300	-0.54809700	-0.01027100
H	-4.40297100	-1.46258200	-0.01588900
H	-5.23506500	-0.44995300	-0.84852500
H	-0.10935700	2.95750400	-0.00309600
O	-2.54370200	3.69399300	0.00530300
H	-2.66559200	3.99606000	0.91808100
H	-3.39221400	3.87240900	-0.42766000
H	-3.45706100	-3.61882600	-0.59078000

thA 4H2O B3LYP N3 Cation

Enthalpy (Hartrees) = -1139.462147

Free Energy (Hartrees) = -1139.538193

Charge = 1 Multiplicity = 1

C	3.98312200	0.19924300	0.00339100
H	4.20792900	-0.33883100	0.93115900
C	0.19435000	0.73380500	-0.01151500
C	-1.07645700	0.03919000	-0.01706000
N	-2.22820200	0.68377500	-0.01918300
H	-3.11550600	0.16700000	-0.01730400
H	-2.27410300	1.70775700	-0.01020700
N	-1.09494700	-1.32327400	-0.02045400
C	0.05541300	-1.98419500	-0.01169400
H	0.02165400	-3.06848200	-0.00999800
N	1.26835000	-1.43638600	-0.00417700
C	1.39628200	-0.05324100	-0.00686900
H	4.68376100	1.03362800	-0.07874600
H	4.16865900	-0.48008300	-0.83569900
S	2.15146900	2.36768700	-0.00791800
C	0.45866700	2.08751900	-0.01139400
C	2.56374500	0.67746400	-0.00606200
O	3.42403400	-3.26669100	0.11408100
H	4.23056500	-2.79524300	-0.14538600
H	2.09595400	-2.06237500	0.00999700
O	-3.42576200	-2.97778300	-0.06287500
H	-3.46375500	-3.47026300	0.77000200
H	-2.59929900	-2.43766700	-0.01509600
O	-4.87785500	-0.63470200	0.07807700
H	-4.49323000	-1.54031500	0.01125700
H	-5.37447700	-0.50345300	-0.74246600
H	-0.23818000	2.91538800	-0.01744100
O	-2.66415000	3.58719000	-0.00199000
H	-2.79120800	3.88559400	0.91120200
H	-3.51964100	3.73962100	-0.43091700
H	3.32010600	-3.96689600	-0.54807600

Figure S7. continued.

tzA 5H2O B3LYP Neutral

Enthalpy (Hartrees) = -1231.497224

Free Energy (Hartrees) = -1231.582095

Charge = 0 Multiplicity = 1

N	0.11063400	1.81132400	-0.01106100
C	0.30739400	0.49280800	0.00205700
C	-0.73791200	-0.51406400	0.01882200
N	-2.02727100	-0.17693900	0.02494600
H	-2.75987600	-0.89207300	0.02539600
H	-2.31052500	0.79460900	0.01732600
N	-0.37365900	-1.80401300	0.02835100
C	0.94881400	-2.11962600	0.02435800
H	1.16263700	-3.18513600	0.03331800
N	1.98275400	-1.30669000	0.01163400
C	1.65795200	0.03241200	0.00024900
S	1.61243400	2.54542000	-0.02524400
C	4.04085500	1.08294200	-0.02079900
H	4.41383300	0.55848900	0.86547200
H	4.40633500	0.55010000	-0.90517800
H	4.46460800	2.08991700	-0.02735900
C	2.54765900	1.10666900	-0.01443400
O	-2.21535900	3.64728100	-0.06327400
H	-1.46725800	3.01788900	-0.04333900
H	-3.01849700	3.08814800	-0.00668600
O	-4.48835000	1.97723100	0.09069900
H	-5.14924400	2.21876300	-0.57539000
H	-4.93927300	2.09348200	0.94045100
O	-4.23502100	-2.19635500	0.03043000
H	-3.58190800	-2.93433500	-0.02065600
H	-4.67165900	-2.17810300	-0.83317300
O	-2.14269100	-3.99320500	0.04751000
H	-2.03323600	-4.47233000	-0.78680500
H	-1.49240300	-3.24185200	0.01210300
O	4.56179400	-2.50407100	0.03798200
H	5.21291700	-1.79040000	0.09391300
H	3.68584600	-2.04354700	0.02913500

tzA 5H2O B3LYP N1 Cation

Enthalpy (Hartrees) = -1231.934907

Free Energy (Hartrees) = -1232.019048

Charge = 1 Multiplicity = 1

N	0.10137900	-1.85465600	0.00607900
C	0.28883300	-0.53903200	-0.00021600
C	-0.78281200	0.43623700	-0.00616300
N	-2.05884700	0.12999700	-0.00856200
H	-2.79979800	0.85477900	-0.02611600
H	-2.35239200	-0.84234000	-0.00395400
N	-0.36419400	1.72711100	-0.00960800
C	0.96345900	2.09734100	-0.01119500
H	1.12962400	3.16855700	-0.01399100
N	1.96484600	1.27669400	-0.00985400
C	1.63477800	-0.06647300	-0.00383600
S	1.60527200	-2.57585200	0.00809700
C	4.02408800	-1.09523800	-0.00162200
H	4.38474200	-0.56605100	-0.88984500
H	4.38648600	-0.55937300	0.88184900
H	4.45579800	-2.09844100	0.00177400
C	2.53219700	-1.13162200	-0.00001700
O	-2.26221700	-3.71038800	0.08109800
H	-1.50217700	-3.09934800	0.05383700
H	-3.04850100	-3.12672400	0.03179000
O	-4.42543600	-1.90928800	-0.05509400
H	-5.08782300	-2.11063900	0.62289000
H	-4.89513100	-2.00380900	-0.89738800
O	-4.08121100	2.11692600	-0.13730600
H	-3.49813500	2.89904100	-0.02681100
H	-4.65262900	2.10457400	0.64440000
O	-2.05602700	4.01184200	0.08158900
H	-1.98262900	4.50005200	0.91593200
H	-1.05221000	2.50342800	-0.00002200
O	4.61193800	2.48562700	-0.02412300
H	5.26191800	1.76956300	-0.06318000
H	3.74158800	2.02924700	-0.02010300
H	-1.93500000	4.67205800	-0.61800000

F Figure S7. continued.

tzA 5H2O B3LYP N3 Cation

Enthalpy (Hartrees) =			-1231.936922
Free Energy (Hartrees) =			-1232.019218
Charge = 1 Multiplicity = 1			
N	0.10549300	-1.83243200	0.01839800
C	0.29481600	-0.51633200	0.01007000
C	-0.76118300	0.48563700	-0.00259800
N	-2.03493200	0.15205400	-0.01210100
H	-2.77694700	0.86923100	-0.01824500
H	-2.32064400	-0.82155700	-0.01283600
N	-0.41319600	1.79761800	-0.00482500
C	0.87003700	2.13627600	-0.00225300
H	1.12118300	3.19129900	-0.00640900
N	1.89760900	1.28892100	0.00428500
C	1.64467700	-0.07076800	0.01091800
S	1.60167500	-2.56542600	0.02668700
C	4.03722600	-1.10584500	0.02444300
H	4.40939900	-0.58356900	-0.86334900
H	4.40282100	-0.57532600	0.91007200
H	4.45404300	-2.11522000	0.03057500
C	2.54396700	-1.12650200	0.01940100
O	-2.27653000	-3.68308600	0.01848500
H	-1.51405400	-3.07513600	0.01798800
H	-3.06135700	-3.09604400	-0.01660400
O	-4.45379100	-1.89910400	-0.07507400
H	-5.11729900	-2.12140500	0.59516800
H	-4.92009800	-1.97603100	-0.92102300
O	-4.18766300	2.08619100	-0.07148000
H	-3.61536900	2.88573400	0.00004100
H	-4.69833500	2.05627200	0.75042000
O	-2.23396900	4.03804000	-0.03298700
H	-2.15961200	4.51131900	0.80864400
H	-1.57183500	3.30951900	0.01525900
O	4.46884700	2.39603200	0.00977700
H	5.10440600	1.69855900	-0.21288400
H	2.86904900	1.66660600	-0.00484000
H	4.57065300	3.06005700	-0.68892100

tzA 5H2O B3LYP N7Cation

Enthalpy (Hartrees) =			-1231.922137
Free Energy (Hartrees) =			-1232.004548
Charge = 1 Multiplicity = 1			
N	0.21475300	-1.79458800	0.02625700
C	0.26770200	-0.45366500	0.01824600
C	-0.83310900	0.49150000	0.01129200
N	-2.10673100	0.11102800	0.00134300
H	-2.85690100	0.81295800	-0.00090700
H	-2.38673000	-0.86287300	-0.03611800
N	-0.51469700	1.79411900	0.01555000
C	0.78552500	2.17299500	0.01232800
H	0.95178500	3.24634400	0.01292400
N	1.85630700	1.40488500	0.00508000
C	1.58560100	0.06271900	0.00954200
S	1.75402800	-2.47310900	0.02210100
C	4.02714400	-0.83956600	-0.00029700
H	4.34141000	-0.28690500	-0.89200500
H	4.35146100	-0.27415600	0.87969400
H	4.52351100	-1.81190700	0.00380400
C	2.54364500	-0.96538200	0.00960500
O	-1.72117700	-3.57295000	0.09686000
H	-0.64038700	-2.45561900	0.06887200
H	-2.62163900	-3.17711900	-0.01811600
O	-4.07849600	-2.26668500	-0.26919300
H	-4.74072400	-2.46850200	0.40914500
H	-4.50162200	-2.49398400	-1.11110500
O	-4.35384800	2.01558400	-0.02389800
H	-3.76512200	2.80493500	0.03089500
H	-4.82881700	1.98714200	0.81901800
O	-2.38604800	3.95086300	-0.03037400
H	-2.30618000	4.44263400	0.79997400
H	-1.70740200	3.23294900	0.02031300
O	4.39206000	2.76380400	-0.11458300
H	5.08012100	2.08866400	-0.20033300
H	3.54895600	2.25536400	-0.07176900
H	-1.73257900	-4.01481500	0.95969000

Figure S7. continued.

8vA 4H2O B3LYP Neutral

Enthalpy (Hartrees) = -889.621824

Free Energy (Hartrees) = -889.703536

Charge = 0 Multiplicity = 1

C	0.80187300	0.90939900	0.00238800
C	-1.19099400	1.90474700	-0.01595400
C	-1.19439600	-0.42928000	-0.01167300
C	0.22063600	-0.36093100	-0.00073800
H	-1.79659800	2.80664600	-0.02315300
N	-1.87411700	0.74825800	-0.01991500
N	-1.87408800	-1.58600400	-0.01501000
H	-2.89363800	-1.59666800	-0.00746700
H	-1.37029400	-2.46894400	-0.01189700
C	3.19353600	1.73687500	0.02166800
H	2.70370400	2.70900900	0.03380400
H	3.81830800	1.64120300	0.91170900
H	3.81302000	1.66007900	-0.87406400
N	2.15887000	0.70231000	0.01464200
O	-4.66514600	0.98945700	-0.12397000
H	-3.67337400	0.92988700	-0.05627300
H	-4.95608900	1.43747400	0.68360500
O	-4.92360800	-1.75557400	-0.00076700
H	-4.95440500	-0.76925200	0.00570200
H	-5.21498300	-2.02671100	0.88145200
N	0.13196400	2.08015500	-0.00489300
O	0.86196000	4.85829400	-0.00896600
H	0.00553400	5.30336300	-0.07866300
H	0.64887200	3.89504700	-0.01029000
N	1.19507600	-1.33319100	0.00980100
H	0.68062300	-3.12069900	-0.01708600
O	0.16436600	-3.96310400	0.01717200
H	0.27062900	-4.36488600	-0.85699500
C	2.34918300	-0.67063900	0.01761500
C	3.68051000	-1.26118100	0.02689800
H	4.51280900	-0.56375000	0.03624900
C	3.92013400	-2.58161400	0.02309300
H	3.11916400	-3.31513000	0.01318100
H	4.93931500	-2.95421000	0.03028700

8vA 4H2O B3LYP N1 Cation

Enthalpy (Hartrees) = -890.061784

Free Energy (Hartrees) = -890.143022

Charge = 1 Multiplicity = 1

C	-0.81085700	0.89129900	-0.01520500
C	1.17732600	1.89464500	-0.01738100
C	1.15096200	-0.51841200	-0.00984400
C	-0.25860300	-0.39225400	-0.01394600
H	1.83298100	2.75744700	-0.01970700
N	1.80992500	0.68732500	-0.01668500
N	1.82108600	-1.65901900	-0.00051000
H	2.84969000	-1.69372500	0.01930400
H	1.29434900	-2.53622800	0.01208000
C	-3.17935700	1.77400300	-0.01773800
H	-2.67014300	2.73577100	-0.03151700
H	-3.80788400	1.68693600	-0.90546600
H	-3.79372800	1.70426300	0.88150400
N	-2.16547800	0.71638700	-0.01610900
O	4.63948700	0.96553200	-0.06776200
H	2.84620100	0.71458200	-0.02488600
H	4.97986900	1.37627000	-0.87730700
O	4.70281000	-1.80952600	0.14137200
H	4.85206300	-0.84617100	0.02664000
H	5.08910300	-2.22804700	-0.64148100
N	-0.12203300	2.06028800	-0.01482500
O	-0.83110600	4.91914800	0.09734500
H	0.03479600	5.35136600	0.09972700
H	-0.63322100	3.95996200	0.05725200
N	-1.24793300	-1.34075600	-0.01454700
H	-0.70885000	-3.17034100	0.02261000
O	-0.10577600	-3.94809000	-0.01872500
H	-0.18589100	-4.38362000	0.84226600
C	-2.38738000	-0.65292800	-0.01615800
C	-3.72989100	-1.21525500	-0.01806300
H	-4.54848700	-0.50227900	-0.01004700
C	-3.98750600	-2.53187000	-0.02911900
H	-3.19651200	-3.27623100	-0.03876300
H	-5.01169300	-2.89025600	-0.02958400
H	5.01690900	1.47884400	0.66298300

Figure S7. continued.

8vA 4H2O B3LYP N3 Cation

Enthalpy (Hartrees) = -890.057655

Free Energy (Hartrees) = -890.136123

Charge = 1 Multiplicity = 1

C	0.85831300	0.85368400	0.01416100
C	-1.17640400	1.93587400	0.00547400
C	-1.21218800	-0.39429200	0.00376900
C	0.20843000	-0.37658600	0.01177800
H	-1.71087800	2.87890700	0.00272400
N	-1.86436600	0.81412500	0.00224300
N	-1.93114500	-1.50944400	-0.00280000
H	-2.95584600	-1.47985800	-0.01451300
H	-1.46245000	-2.41675700	-0.00974100
C	3.28671700	1.58446600	0.02330700
H	2.86433400	2.58747200	0.01453700
H	3.89098500	1.45965400	0.92307100
H	3.90568700	1.45089000	-0.86508700
N	2.19375900	0.60488400	0.01879000
O	-4.72707700	1.15439500	-0.04876800
H	-3.74495800	1.08248900	0.00817400
H	-5.00679800	1.55497400	0.78733300
O	-4.89097200	-1.60628100	-0.09919500
H	-4.98581500	-0.62845100	-0.01956300
H	-5.24281300	-1.97004800	0.72587900
N	0.17005000	2.02665000	0.01144000
O	1.07572400	4.64829500	0.02146100
H	0.48936800	5.16416100	-0.55312700
H	0.61024400	2.97459300	0.00446800
N	1.13839200	-1.38795300	0.01591100
H	0.49868300	-3.18967600	-0.02387200
O	-0.13194800	-3.94454500	0.01704800
H	-0.07395200	-4.37608700	-0.84760900
C	2.32038400	-0.78347000	0.01954900
C	3.62233600	-1.43357400	0.02350100
H	4.48897300	-0.78018200	0.03002200
C	3.78990400	-2.76481800	0.01899500
H	2.95060300	-3.45411900	0.01222800
H	4.78781400	-3.19092000	0.02244300
H	1.95921900	4.75252000	-0.36403400

8vA 4H2O B3LYP N7 Cation

Enthalpy (Hartrees) = -890.058933

Free Energy (Hartrees) = -890.139427

Charge = 1 Multiplicity = 1

C	0.78034400	0.91638900	-0.01580600
C	-1.21235400	1.90287800	-0.02411300
C	-1.21974200	-0.43221500	-0.01659900
C	0.19404900	-0.34160600	-0.01505200
H	-1.81781300	2.80428700	-0.02876400
N	-1.89294800	0.74772200	-0.02336100
N	-1.88791400	-1.58875300	-0.01099000
H	-2.91076600	-1.60460600	0.00748200
H	-1.37726600	-2.46868300	-0.00704600
C	3.16807100	1.78141400	-0.00430600
H	2.65307100	2.73929500	-0.00777300
H	3.78122600	1.70058500	0.89408000
H	3.79111000	1.70039700	-0.89592500
N	2.15118000	0.72239800	-0.00982600
O	-4.71977500	0.98902000	-0.14261700
H	-3.73274400	0.94371700	-0.06710200
H	-5.02179000	1.44606000	0.65588300
O	-4.87091000	-1.76541600	0.03151100
H	-4.95511500	-0.78277900	0.01661300
H	-5.17138700	-2.03482600	0.91137000
N	0.11223800	2.08105700	-0.01963500
O	0.82753800	4.89995900	0.05546900
H	-0.02924000	5.34270000	-0.02473000
H	0.62020500	3.93971000	0.02412200
N	1.21764900	-1.26773500	-0.00795300
H	1.07475300	-2.29336200	-0.01954300
O	0.16113300	-3.84182600	-0.07029400
H	0.26343100	-4.32393500	-0.90493600
C	2.39371000	-0.61731300	-0.00316100
C	3.71797700	-1.20363700	0.00916800
H	4.53934700	-0.49740400	-0.04821800
C	3.95979200	-2.52117600	0.09093600
H	3.17232600	-3.26656800	0.15962900
H	4.98238800	-2.88330900	0.09321300
H	0.36185400	-4.48640200	0.62504800

Figure S7. continued.

G 7H2O B3LYP Neutral

Enthalpy (Hartrees) = -1116.780951

Free Energy (Hartrees) = -1116.878709

Charge = 0 Multiplicity = 1

N	0.53135200	2.86824000	0.11832500
C	1.90313200	2.78493600	0.16141400
H	2.51507100	3.67092700	0.25952200
N	2.35373400	1.55151400	0.07389200
C	1.21040000	0.77238800	-0.03510900
C	1.03443800	-0.63107400	-0.15438700
O	1.92126800	-1.52249400	-0.19174100
N	-0.30869300	-0.99590800	-0.23532900
H	-0.50202100	-2.00148300	-0.39823100
C	-1.37588800	-0.12807500	-0.18077600
N	-2.60670200	-0.66873100	-0.26856800
H	-2.73695000	-1.66623600	-0.11885600
H	-3.41670100	-0.07515300	-0.09150000
N	-1.22178300	1.19178400	-0.07282900
C	0.07090400	1.58199400	-0.00823600
C	-0.26239100	4.09243500	0.20291000
H	-0.82950700	4.24007200	-0.71801300
H	-0.94687300	4.03794300	1.05184100
H	0.42106500	4.92947800	0.34488400
O	1.46724300	-4.12483800	0.73638700
H	2.10070200	-4.71644600	0.30521500
H	1.68004800	-3.22434100	0.40122800
O	4.75846000	-1.57540900	-0.14740700
H	5.02272500	-0.63497300	-0.05507900
H	3.78092500	-1.53742100	-0.16534900
O	-0.87024100	-3.77392400	-0.76197400
H	-1.71636100	-3.85946900	-0.27500300
H	-0.15637600	-4.09930200	-0.17241100
O	-3.40607900	-3.57755400	0.40716000
H	-3.51724400	-3.87229800	1.32339000
H	-4.09896200	-4.03564800	-0.09163100
O	-3.51712000	2.91663100	-0.33400300
H	-3.44310500	3.63971300	0.30567600
H	-2.69243500	2.38463200	-0.22264300
O	5.15664700	1.19959600	0.16253300
H	4.17542900	1.32883600	0.10021100
H	5.52164700	1.59456200	-0.64240800
O	-5.22224000	0.82920400	0.18414000
H	-5.47199800	0.79673900	1.11846700
H	-4.71150800	1.66625800	0.07658300

G 7H2O B3LYP N1 Anion_1

Enthalpy (Hartrees) = -1116.322942

Free Energy (Hartrees) = -1116.421651

Charge = -1 Multiplicity = 1

N	-0.61326600	-2.81870700	0.06902300
C	-1.98026600	-2.68792100	0.09496900
H	-2.62517300	-3.55209400	0.17708600
N	-2.38547800	-1.43665900	0.01001600
C	-1.21265800	-0.69163900	-0.07952400
C	-0.95962600	0.71078100	-0.17894900
O	-1.87356000	1.60922200	-0.20813400
N	0.35388000	1.08107300	-0.24186700
H	0.73922900	2.85586500	-0.64967500
C	1.34132100	0.15701200	-0.20652300
N	2.62238200	0.62762800	-0.32758200
H	2.77407700	1.61704800	-0.17036700
H	3.37847700	0.01775500	-0.03553800
N	1.18879800	-1.18097000	-0.10467000
C	-0.10788300	-1.54281700	-0.04453300
C	0.13988000	-4.06634300	0.14745600
H	0.71779400	-4.22045600	-0.76636800
H	0.81466200	-4.04741000	1.00630000
H	-0.56873600	-4.88632600	0.26709100
O	-1.84050000	3.80834200	1.44139800
H	-2.74784000	3.80734300	1.77715900
H	-1.79770800	3.03022900	0.83445500
O	-4.64357600	1.72167600	-0.15964900
H	-4.96128700	0.79475500	-0.14431400
H	-3.66382700	1.63060500	-0.17791500
O	1.01232000	3.77833800	-0.88773100
H	1.95881500	3.81481000	-0.64528100
O	3.76264000	3.63711900	-0.09817000
H	3.96084600	4.26214800	0.61499100
H	4.37200900	3.87453900	-0.81300500
O	3.44027800	-2.86011500	-0.21684700
H	3.28887500	-3.61624200	0.36838400
H	2.60930200	-2.31386100	-0.16362800
O	-5.15900800	-1.06417700	-0.07869500
H	-4.17133600	-1.18774600	-0.06631500
H	-5.44503900	-1.37188200	-0.95085900
O	5.29547000	-1.00799200	0.62360600
H	5.25513700	-0.93373100	1.58745500
H	4.67039800	-1.73563600	0.39230900

Figure S7. continued.

G 7H2O B3LYP N1 Anion_2

Enthalpy (Hartrees) = -1116.327612

Free Energy (Hartrees) = -1116.423779

Charge = -1 Multiplicity = 1

N	-0.21845200	-2.90212800	0.02774100
C	-1.58893000	-2.94170800	0.10826700
H	-2.12072700	-3.88150000	0.16573500
N	-2.14521900	-1.74681400	0.10521100
C	-1.07574600	-0.86023400	0.01521500
C	-0.99957300	0.56599500	-0.02310300
O	-2.01806100	1.34164000	0.02862900
N	0.25779200	1.09499600	-0.11819900
H	0.39273700	2.82108100	-0.58964000
C	1.35172200	0.29878900	-0.15349300
N	2.56110200	0.93233100	-0.28090800
H	2.59375000	1.91644400	-0.03299200
H	3.39135300	0.40025700	-0.04235300
N	1.36524300	-1.05000600	-0.11462600
C	0.12412800	-1.57000000	-0.03335700
C	0.68343500	-4.04937400	0.01258200
H	1.25471900	-4.07103100	-0.91776700
H	1.37005000	-4.00295600	0.86099100
H	0.08357800	-4.95686900	0.08687700
O	-2.06593600	4.03914700	0.47200300
H	-2.78326800	4.37431700	-0.08458500
H	-2.03914100	3.06158000	0.30446300
O	-4.78933200	1.10875300	0.06156000
H	-4.97940600	0.14712000	0.07423100
H	-3.80680000	1.14969800	0.05065800
O	0.45842500	3.79117400	-0.81831500
H	-0.35280600	4.16052200	-0.41446300
O	2.87831200	4.10558500	0.42909400
H	3.51488300	4.38469400	-0.24391600
H	2.00077300	4.10120300	-0.02605600
O	3.78956300	-2.44444100	-0.42979700
H	3.75359100	-3.25360600	0.10049400
H	2.90488500	-2.00574700	-0.30382400
O	-4.94534900	-1.71692300	0.12523600
H	-3.95041400	-1.72062900	0.09818700
H	-5.22726600	-2.05323700	-0.73763600
O	5.44259200	-0.45771300	0.51222200
H	5.38919300	-0.43704800	1.47802200
H	4.89513300	-1.23152300	0.23732500

G 7H2O B3LYP N3 Cation

Enthalpy (Hartrees) = -1117.213258

Free Energy (Hartrees) = -1117.310705

Charge = 1 Multiplicity = 1

N	-0.46315900	-2.87316200	0.11237400
C	-1.84127200	-2.80999000	0.13725800
H	-2.43640300	-3.70922100	0.21087900
N	-2.30523400	-1.58271000	0.06413700
C	-1.17665600	-0.78551400	-0.01536200
C	-1.03181200	0.63110300	-0.11123300
O	-1.93484000	1.48722600	-0.14365100
N	0.30770600	1.04466200	-0.17271100
H	0.46281200	2.06943200	-0.33257400
C	1.40601800	0.24332100	-0.12522500
N	2.61832500	0.77186800	-0.17244900
H	2.74354900	1.78583300	-0.13265200
H	3.46310600	0.19032700	-0.07896000
N	1.23695800	-1.10002900	-0.03394300
C	-0.04334400	-1.58371900	0.01380500
C	0.34205800	-4.09560300	0.18985300
H	0.93146700	-4.21344400	-0.72065000
H	1.00016700	-4.05319700	1.05940000
H	-0.34271200	-4.93643200	0.29310700
O	-1.58659000	4.13084400	0.86070700
H	-2.23491800	4.71835200	0.44605700
H	-1.78645200	3.23667500	0.51210800
O	-4.81673000	1.49317600	-0.20605500
H	-5.05243500	0.54262200	-0.14237100
H	-3.84111700	1.48855000	-0.18647400
O	0.70655900	3.75309400	-0.69037600
H	1.58862700	3.90827700	-0.29214900
H	0.02984100	4.11717000	-0.08023100
O	3.34983900	3.64921600	0.17112400
H	3.60253800	3.94879900	1.05725200
H	3.97374800	4.07956300	-0.43264000
O	3.43525800	-2.87276900	-0.12750900
H	3.33354800	-3.56433400	0.54466100
H	2.06032900	-1.73709100	-0.04165000
O	-5.14825800	-1.29742000	0.03858000
H	-4.16639600	-1.40424300	0.02348800
H	-5.46225100	-1.69114000	-0.78839700
O	5.10276900	-0.68375400	0.08268800
H	5.45868900	-0.56966000	0.97588600
H	4.67003600	-1.56460500	0.08198400
H	3.44804700	-3.34112400	-0.97656600

Figure S7. continued.

G 7H2O B3LYP N7 Cation

Enthalpy (Hartrees) = -1117.218849

Free Energy (Hartrees) = -1117.313002

Charge = 1 Multiplicity = 1

N	-0.55560500	-2.85688000	0.10163900
C	-1.90127300	-2.79518500	0.12333400
H	-2.55076300	-3.65417200	0.20088800
N	-2.30807600	-1.53526100	0.03747300
C	-1.18466900	-0.72736500	-0.04477900
C	-0.99800700	0.67937400	-0.15039900
O	-1.87796100	1.56641100	-0.19848800
N	0.34927500	1.01498600	-0.20073400
H	0.56432100	2.02263700	-0.36373700
C	1.40042400	0.12625600	-0.12966900
N	2.63522800	0.63934000	-0.16569600
H	2.79056400	1.64097500	-0.07202100
H	3.44373600	0.02825300	-0.03741400
N	1.21854100	-1.19766900	-0.04085000
C	-0.07329400	-1.56126300	-0.00435900
C	0.24124400	-4.08519400	0.18616000
H	0.81987500	-4.20927600	-0.72972600
H	0.90887600	-4.02565700	1.04658400
H	-0.44330600	-4.92321400	0.30842600
O	-1.40698000	4.21576800	0.69909200
H	-2.01688500	4.81759500	0.24838700
H	-1.63861500	3.31913600	0.37456200
O	-4.71696800	1.66370900	-0.15660300
H	-4.98179900	0.72698900	-0.07053200
H	-3.74080000	1.62371700	-0.17449800
O	0.94160400	3.72664600	-0.74358300
H	1.79821600	3.83017100	-0.27825700
H	0.24305900	4.11404700	-0.17417700
O	3.49491800	3.52741800	0.36029300
H	3.63453200	3.82680900	1.27111800
H	4.19249200	3.95621700	-0.15776200
O	3.52199100	-2.98231600	-0.33885800
H	3.45589100	-3.70399800	0.30341300
H	2.70592800	-2.44744800	-0.21248000
O	-5.08229300	-1.13241700	0.09900600
H	-3.31156600	-1.26742800	0.04318900
H	-5.53753300	-1.60016800	-0.61787100
O	5.20620000	-0.87320200	0.15796200
H	5.49412100	-0.84908600	1.08161400
H	4.71753600	-1.72362400	0.05606600
H	-5.47405600	-1.46995500	0.91911300

8-phenol-G 8H2O B3LYP Neutral

Enthalpy (Hartrees) = -1499.425219

Free Energy (Hartrees) = -1499.542905

Charge = 0 Multiplicity = 1

C	-0.78126400	-0.90185600	-0.14111200
C	-0.61577100	0.48382300	-0.13940100
C	-1.77341000	1.29999400	-0.21193300
C	-3.02567200	-0.82284300	-0.27480200
C	1.36527700	-0.35980600	-0.04050400
H	-3.81919400	1.08729900	-0.44856700
C	2.82492200	-0.50647000	0.04008500
C	3.43040500	-1.42051100	0.92304900
C	3.65384700	0.31320600	-0.74632200
C	4.81584300	-1.51267300	1.01702200
H	2.81925800	-2.04971600	1.56183600
C	5.04163500	0.22600800	-0.66084900
H	3.20848600	1.01696600	-1.44165300
C	5.62952800	-0.68974200	0.22519400
H	5.27696100	-2.21222700	1.70727200
H	5.66872400	0.85882600	-1.28162500
O	6.98494300	-0.82013900	0.35443700
H	7.46823300	-0.17604000	-0.22403500
O	-1.82725000	2.55752300	-0.22485700
N	-2.95228300	0.55420200	-0.29260300
N	-1.94017000	-1.59371500	-0.18839900
N	0.72965100	0.80246500	-0.07480700
N	0.48036400	-1.43478400	-0.08436400
N	-4.24618600	-1.37638000	-0.37210300
H	-5.09170000	-0.82459300	-0.22039700
H	-4.33319300	-2.39036000	-0.31060200
C	0.79483400	-2.86058100	-0.18397200
H	0.80630200	-3.33030200	0.80188600
H	0.03868900	-3.34024400	-0.80589500
H	1.76854900	-2.98093400	-0.65673900
O	8.46057500	0.87557500	-1.18129200
H	9.23271600	1.16447100	-0.67139200
H	7.95669700	1.68624300	-1.35164000
O	-2.24784800	-4.25148400	0.87727600
H	-1.59040200	-4.83477800	0.47073100
H	-2.07627200	-3.35962400	0.48923300
O	-5.41397400	2.13348900	-0.90762800
H	-5.51433700	2.33084900	-1.84992000
H	-5.05291300	2.95212200	-0.48756300
O	-0.31546800	4.31545400	1.44702700
H	-0.87881300	3.71609400	0.91842200
H	0.59247800	4.04795200	1.18657000
O	-4.04969600	4.10249900	0.38875500
H	-3.22549100	3.60462700	0.17841600
H	-3.97017200	4.94725700	-0.07768800
O	2.07090300	3.25844100	0.42061000
H	2.78351500	3.05171300	1.04241100
H	1.63213200	2.38973400	0.22966900
O	-4.74934100	-4.38471200	-0.26661400
H	-3.87796000	-4.47428900	0.18614100
H	-5.41397600	-4.56322900	0.41383200
O	-6.86015500	0.02775400	0.09734000
H	-7.04142400	0.14073800	1.04129600
H	-6.44907400	0.87243400	-0.19324700

Figure S7. continued.

8-phenol-G 8H2O B3LYP N1 Anion

Enthalpy (Hartrees) = -1498.970879

Free Energy (Hartrees) = -1499.088584

Charge = -1 Multiplicity = 1

C	-0.79924500	-0.90485300	-0.19502300
C	-0.63620000	0.47751800	-0.15561900
C	-1.81472400	1.28282000	-0.20335200
C	-3.03007200	-0.74545800	-0.32687900
C	1.34978500	-0.37409300	-0.07658300
H	-4.44993300	1.51532800	-0.84225800
C	2.81013300	-0.51956600	0.00727400
C	3.41610300	-1.46772300	0.85350500
C	3.64188900	0.33696700	-0.73609500
C	4.80188700	-1.55789000	0.95275900
H	2.80456800	-2.12728500	1.46062100
C	5.02983400	0.25406100	-0.64370400
H	3.19813900	1.06864100	-1.40316100
C	5.61677200	-0.69685400	0.20458300
H	5.26155000	-2.28527500	1.61478800
H	5.65759000	0.91781900	-1.23065900
O	6.97347300	-0.82540400	0.33754100
H	7.45559500	-0.15316400	-0.20823500
O	-1.80333600	2.56570000	-0.16464000
N	-2.99885300	0.60784900	-0.30487600
N	-1.96672100	-1.57490300	-0.26665100
N	0.71331900	0.79022100	-0.08008500
N	0.46601600	-1.44521700	-0.15084300
N	-4.26611900	-1.32085100	-0.46186000
H	-5.07185800	-0.75147200	-0.22489100
H	-4.35390600	-2.31057300	-0.25712600
C	0.77654400	-2.86587200	-0.30170900
H	0.77458600	-3.37741200	0.66366500
H	0.02609300	-3.31941400	-0.95025500
H	1.75517900	-2.97496400	-0.76756300
O	8.45245300	0.94761900	-1.11118900
H	9.20862200	1.23385500	-0.57648600
H	7.93926500	1.75481200	-1.26973600
O	-2.30627500	-4.20678100	0.67114000
H	-1.74364400	-4.80068500	0.15343300
H	-2.14080200	-3.29840600	0.30037600
O	-5.26039900	2.03442000	-1.10936500
H	-5.05299000	2.93344900	-0.78193200
O	-0.41611000	4.01813400	1.77096300
H	-0.93835900	3.49518900	1.12194700
H	0.50920000	3.82315100	1.51201300
O	-3.92506200	4.27422700	0.00504800
H	-3.16308500	3.64165800	-0.06795500
H	-3.72224500	4.99231800	-0.61113400
O	2.02570700	3.17208500	0.64765300
H	2.75851200	2.90160000	1.21934300
H	1.58948400	2.32370500	0.36372200
O	-4.98946200	-4.45562900	0.12178300
H	-4.02851200	-4.44364000	0.34720000
H	-5.45012700	-4.42453600	0.97218200
O	-7.00734800	0.38955700	0.21659700
H	-6.95002600	0.57055100	1.16534300
H	-6.43175000	1.06932100	-0.21223300

8-phenol-G 8H2O B3LYP N3 Cation

Enthalpy (Hartrees) = -1499.857037

Free Energy (Hartrees) = -1499.972711

Charge = 1 Multiplicity = 1

C	-0.76027500	-0.90706500	-0.07208300
C	-0.61950400	0.46902200	-0.10891600
C	-1.78204800	1.29082600	-0.18939400
C	-3.09576000	-0.80478800	-0.17339800
C	1.36782000	-0.35871100	-0.01092900
H	-3.83954200	1.09998500	-0.42812500
C	2.82676400	-0.49978800	0.06516000
C	3.43672000	-1.36966800	0.98864300
C	3.64802800	0.28358700	-0.76480300
C	4.82219300	-1.45584900	1.07820600
H	2.82886700	-1.96727200	1.66022200
C	5.03597400	0.20096300	-0.68378900
H	3.19705800	0.95329900	-1.48954500
C	5.62998100	-0.67138600	0.24180500
H	5.28868600	-2.12051900	1.79852100
H	5.65898900	0.80367500	-1.33764600
O	6.98465200	-0.79541900	0.36865800
H	7.46571100	-0.17603400	-0.23875200
O	-1.82675600	2.53424500	-0.22962600
N	-2.97815300	0.55092000	-0.24755700
N	-1.96647500	-1.55471000	-0.08668700
N	0.72152200	0.79480300	-0.06768300
N	0.48541500	-1.44473600	-0.02134600
N	-4.28693700	-1.37534500	-0.18585700
H	-5.14677400	-0.81080500	-0.13618300
H	-4.38985500	-2.39892100	-0.21147100
C	0.81364900	-2.87278900	-0.10330900
H	0.75053800	-3.34086400	0.88051200
H	0.11895800	-3.35695900	-0.79059300
H	1.82279000	-2.97689700	-0.49679300
O	8.44732300	0.83724400	-1.23944700
H	9.23119800	1.13114000	-0.75073400
H	7.94802600	1.64826300	-1.42130200
O	-2.17745300	-4.31623300	0.54828900
H	-1.51027200	-4.85822700	0.09982500
H	-2.03863900	-2.57599200	0.09454300
O	-5.29316900	2.16086200	-0.89940800
H	-5.34681300	2.33895800	-1.84970500
H	-4.98226900	2.99777100	-0.47551200
O	-0.25902400	4.40282900	1.36410100
H	-0.84981700	3.79439800	0.88347000
H	0.63414200	4.11686200	1.07271400
O	-4.03354100	4.18452100	0.42296400
H	-3.20534200	3.70080100	0.21814900
H	-3.96027100	5.03216400	-0.03952900
O	2.08068900	3.30104400	0.28490500
H	2.81579600	3.12189200	0.88894200
H	1.64455900	2.42598500	0.14195200
O	-4.77536300	-4.22913600	-0.36930200
H	-3.89862600	-4.45510900	0.01020000
H	-5.42618400	-4.50180200	0.29349200
O	-6.78644600	0.06109300	0.01089100
H	-7.04796900	0.16143600	0.93763900
H	-6.38656200	0.92238700	-0.24584700
H	-2.03252700	-4.46068200	1.49612000

Figure S7. continued.

8-phenol-G 8H2O B3LYP N7 Cation

Enthalpy (Hartrees) = -1499.864415

Free Energy (Hartrees) = -1499.982533

Charge = 1 Multiplicity = 1

C	-0.80506900	-0.90141300	-0.12959600
C	-0.65206000	0.47676400	-0.12758900
C	-1.79905100	1.30978300	-0.20076600
C	-3.04818400	-0.81390800	-0.25108100
C	1.37249900	-0.42506100	-0.03510800
H	-3.84230500	1.10292900	-0.43274100
C	2.82264000	-0.54913800	0.03840600
C	3.43211200	-1.49662900	0.88551100
C	3.63946200	0.31431900	-0.71736900
C	4.81523500	-1.57701300	0.97377400
H	2.82655200	-2.15332300	1.50057300
C	5.02483300	0.23197600	-0.63771600
H	3.18989400	1.03922300	-1.38798000
C	5.62125700	-0.71512900	0.21231300
H	5.28455400	-2.29777400	1.63547600
H	5.64649700	0.89133200	-1.23521700
O	6.96998400	-0.83976600	0.33468700
H	7.45464200	-0.17457200	-0.22267900
O	-1.82737800	2.56141300	-0.21695400
N	-2.97416700	0.56479500	-0.27446400
N	-1.95712300	-1.58789200	-0.17373000
N	0.70603300	0.73767400	-0.06854800
N	0.46586600	-1.44793500	-0.08172000
N	-4.26152700	-1.36794500	-0.32107200
H	-5.11441300	-0.81185700	-0.22597300
H	-4.35253700	-2.38506300	-0.29605100
C	0.75696700	-2.88220700	-0.18951100
H	0.75537700	-3.34840900	0.79680000
H	-0.01040400	-3.33737100	-0.81442900
H	1.72833100	-3.01298300	-0.66292900
O	8.42955700	0.89770300	-1.13610900
H	9.20419400	1.17264800	-0.62212000
H	7.92681300	1.71309900	-1.28620200
O	-2.27780900	-4.29165200	0.88265000
H	-1.62424100	-4.87533900	0.47024400
H	-2.09657000	-3.39945000	0.50888200
O	-5.36373700	2.15763900	-0.88321300
H	-5.43684000	2.35047200	-1.82919500
H	-5.02962000	2.98373900	-0.45621700
O	-0.27362900	4.20238900	1.55074500
H	-0.85704600	3.65072800	0.99472700
H	0.62000900	3.96592900	1.23441000
O	-4.04690200	4.15575000	0.42860000
H	-3.22092800	3.66785900	0.21581700
H	-3.97680400	5.00164900	-0.03742200
O	2.07720400	3.18640400	0.33933000
H	2.90315800	2.95708500	0.79264900
H	1.16376900	1.66355500	0.02533900
O	-4.76721900	-4.33623200	-0.29943200
H	-3.90635500	-4.46781600	0.16217700
H	-5.44736700	-4.52597900	0.36255900
O	-6.86180500	0.03820600	0.01018900
H	-7.09630100	0.12231800	0.94549500
H	-6.44624500	0.89490600	-0.23409600
H	2.35066000	3.63268500	-0.47672700

thG 6H2O B3LYP Neutral

Enthalpy (Hartrees) = -1367.121686

Free Energy (Hartrees) = -1367.214859

Charge = 0 Multiplicity = 1

C	1.92937100	3.65155500	0.11119400
H	1.43968800	3.98723600	-0.80960100
C	1.66896900	-0.15099100	0.08425300
C	0.76878200	-1.28227300	0.00021500
N	-0.55682800	-0.93806500	-0.11027300
C	-1.02399100	0.37561600	-0.13976700
N	-0.24108700	1.42456100	-0.07026000
C	1.12033100	1.18231600	0.03594900
H	2.89471000	4.16038600	0.17943500
H	1.31570400	3.98616500	0.95522200
S	3.66492800	1.41660400	0.26260100
C	3.04024200	-0.18134500	0.20810600
C	2.09348700	2.16213500	0.12134000
O	-1.53509800	4.03105900	-0.27461600
H	-2.47600500	3.77042700	-0.21560300
H	-1.04404800	3.18064400	-0.19961400
O	-2.61050000	-3.00518700	-0.53848800
H	-2.75847600	-3.21300700	-1.47242000
H	-3.42459500	-2.54570700	-0.22743900
O	-0.69199200	-4.53568400	0.83408900
H	0.00067000	-3.88547300	0.60068400
H	-1.48860900	-4.14884700	0.41900000
H	3.69453400	-1.04018200	0.26957600
O	1.11468300	-2.48506800	0.02062100
H	-1.23723600	-1.70348100	-0.23400900
N	-2.36550500	0.50651100	-0.28820400
H	-2.97816500	-0.27313100	-0.07151200
H	-2.76825800	1.43057700	-0.16884800
O	-4.18826700	3.02349200	-0.05269700
H	-4.78842900	3.27845200	-0.76933100
H	-4.61171700	3.34677400	0.75654500
O	3.54894100	-3.67819500	-0.72533500
H	2.75518900	-3.17321800	-0.44842600
H	4.19570900	-3.00525000	-0.98035700
O	-4.68749900	-1.47833700	0.43827500
H	-4.86409300	-1.69131800	1.36715700
H	-5.53677200	-1.59647200	-0.01344600

Figure S7. continued.

thG 6H2O B3LYP N1 Anion

Enthalpy (Hartrees) = -1366.673291

Free Energy (Hartrees) = -1366.762058

Charge = -1 Multiplicity = 1

C	-4.10085200	-0.34623200	-0.15507100
H	-4.36379500	-0.01989300	0.85873000
C	-0.45316400	-1.47392500	-0.16345600
C	0.93050600	-1.01806000	-0.08538000
N	1.14937100	0.30163300	0.04694900
C	0.08533300	1.16765700	0.10018800
N	-1.20769300	0.86384200	0.05037500
C	-1.49845700	-0.48289000	-0.08950100
H	-4.89886200	-1.00734700	-0.50581700
H	-4.09812500	0.54094700	-0.79657700
S	-2.64507500	-2.76402700	-0.36393200
C	-0.92413700	-2.75851400	-0.31465100
C	-2.76785400	-1.03113100	-0.19027000
O	-3.02245600	2.84654700	0.76333500
H	-2.99990900	2.88779800	1.73039600
H	-2.40082700	2.10092500	0.51184000
O	3.74861700	1.13793200	0.63114900
H	4.27508800	0.43391400	0.20045500
O	4.55492800	-1.30732500	-0.56747300
H	3.58604200	-1.48180300	-0.45196300
H	4.69774400	-1.26923500	-1.52384800
H	-0.36723800	-3.68095700	-0.40592400
O	1.90478700	-1.84491200	-0.14592300
H	2.80947500	0.84840800	0.45233900
N	0.43691800	2.48263800	0.26384800
H	1.38934500	2.73864900	0.02751900
H	-0.26473100	3.18709500	0.06533600
O	-1.61547500	5.00702800	-0.19010800
H	-1.85013000	5.12607200	-1.12094500
H	-2.18964400	4.27160800	0.13510500
O	2.01022800	-4.32110500	1.04823600
H	1.89472100	-3.44651500	0.60583700
H	1.11038300	-4.64812600	1.18631300
O	3.46086300	3.58101800	-0.56757400
H	3.66464400	2.71529500	-0.13501600
H	3.71665700	4.25590900	0.07665100

thG 6H2O B3LYP N3 Cation

Enthalpy (Hartrees) = -1367.568624

Free Energy (Hartrees) = -1367.658875

Charge = 1 Multiplicity = 1

C	3.84517500	1.48549400	-0.10205400
H	4.16727000	1.08216600	0.86410800
C	0.02621300	1.54727700	-0.08103500
C	-1.18494500	0.75368500	-0.02478400
N	-0.97902900	-0.61597300	0.05040700
C	0.24461700	-1.23753900	0.06328300
N	1.36194800	-0.49303600	0.03385100
C	1.30649600	0.90277100	-0.04433100
H	4.42049400	2.39468800	-0.29389800
H	4.10367600	0.75640100	-0.87728400
S	1.76221600	3.40298700	-0.20737700
C	0.11945500	2.91775800	-0.16897000
C	2.37332800	1.76733800	-0.10761400
O	3.90433900	-1.84456400	0.42171000
H	4.15497700	-1.75733400	1.35416200
H	2.27550200	-0.96841000	0.10706800
O	-3.39181400	-2.12508600	0.58038900
H	-4.01761100	-1.50986700	0.12677600
H	-3.61094900	-2.08560800	1.52293100
O	-4.76739000	-0.11690700	-0.67495300
H	-3.94733100	0.41031300	-0.57851600
H	-4.87566300	-0.25907500	-1.62672500
H	-0.68230100	3.64236200	-0.21260300
O	-2.34097100	1.20628000	-0.04050900
H	-1.82411500	-1.20261800	0.18317200
N	0.28962700	-2.55821400	0.11354400
H	-0.56738500	-3.11982700	0.02377900
H	1.18254600	-3.06253000	0.03486600
O	2.64970100	-4.23056300	-0.14847600
H	2.75158300	-4.49354500	-1.07467400
H	3.26439600	-3.47591600	-0.01973300
O	-3.37234100	3.77013500	0.63602900
H	-2.91629800	2.93946000	0.39415000
H	-2.66245200	4.38520300	0.86873200
O	-1.99015900	-4.30619900	-0.31508000
H	-2.63577500	-3.63653200	0.00285700
H	-2.02489700	-5.02703900	0.33040300
H	4.62809100	-1.43499500	-0.07600000

Figure S7. continued.

tzG 7H2O B3LYP Neutral

Enthalpy (Hartrees) = -1459.600127

Free Energy (Hartrees) = -1459.700354

Charge = 0 Multiplicity = 1

C	0.12321700	-4.20226000	-0.08680900
H	0.74289500	-4.23118900	-0.98964400
C	-1.23160900	-0.68357400	0.09649300
C	-0.92273900	0.74209400	0.18535200
N	0.42609000	1.00331700	0.21330300
C	1.42674900	0.03634200	0.13812800
N	1.17802400	-1.25204600	0.05836500
C	-0.15130800	-1.61637600	0.04911900
H	-0.54176800	-5.06933200	-0.10123000
H	0.78816100	-4.29526100	0.77838300
S	-2.35713200	-2.83156400	-0.01956900
C	-0.63926000	-2.91934200	-0.01984700
O	3.47442100	-3.05093600	-0.05317900
H	4.19824200	-2.39490500	-0.10877500
H	2.65851400	-2.50267100	-0.01593700
O	1.37725200	3.73162500	0.68803900
H	1.44836800	3.96123600	1.62593700
H	2.29946200	3.70029900	0.34294300
O	-1.04892500	4.36132600	-0.56971700
H	-1.40855300	3.48154500	-0.34900000
H	-0.14738900	4.31902000	-0.19166000
O	-1.75933200	1.66176300	0.24165000
H	0.70803500	1.98909100	0.34599800
N	2.69289600	0.50126200	0.18272100
H	2.89657300	1.48373800	0.02929800
H	3.45617100	-0.15010300	0.02677500
O	5.39419800	-0.96020300	-0.21199400
H	6.07979400	-1.02488900	0.46975200
H	5.87479200	-0.97024600	-1.05321900
N	-2.47128400	-1.17014500	0.06778300
O	-5.23917800	-0.12103900	-0.08976200
H	-4.32726600	-0.46983400	-0.02689500
H	-5.10826800	0.84935000	-0.13004500
O	-4.44385500	2.59846100	-0.12935300
H	-3.52269800	2.28352600	-0.04729900
H	-4.50563100	2.96991400	-1.02144100
O	3.88433800	3.31495100	-0.37268900
H	4.62161000	3.68280300	0.13752100
H	3.98134000	3.68731700	-1.26213100

tzG 7H2O B3LYP N1 Anion

Enthalpy (Hartrees) = -1459.152953

Free Energy (Hartrees) = -1459.25122

Charge = -1 Multiplicity = 1

C	-0.40556000	-4.12008300	-0.13252700
H	-0.86098500	-4.27279400	0.85255700
C	1.08275400	-0.64264600	-0.17123500
C	0.80151900	0.80067000	-0.17489400
N	-0.49202100	1.16378300	-0.17947200
C	-1.48628200	0.21945900	-0.13562600
N	-1.33476100	-1.10387500	-0.09619300
C	-0.03006400	-1.53895400	-0.13734500
H	0.20315000	-4.99859800	-0.36242000
H	-1.21395100	-4.06368000	-0.86906500
S	2.12517300	-2.84902000	-0.20703600
C	0.40375400	-2.86292800	-0.15461000
O	-3.44409600	-2.67192900	0.82830700
H	-3.43025500	-3.52105100	0.36385500
H	-2.66824400	-2.15773200	0.46321400
O	-1.07294700	3.81508700	-0.91966200
H	-0.27548400	4.28015400	-0.59296900
O	1.49619900	4.39616500	0.12282200
H	1.58441500	3.41851100	0.00023900
H	2.11964200	4.79140800	-0.50314200
O	1.73896700	1.66128100	-0.18788700
H	-0.88315900	2.86775600	-0.67916700
N	-2.75229200	0.72275100	-0.16603200
H	-2.89216300	1.70522200	0.04489800
H	-3.53428000	0.09937500	0.00269400
O	-5.49199100	-0.95904300	0.19841500
H	-5.75196300	-1.10246300	-0.72244100
H	-4.81519300	-1.65257800	0.38927100
N	2.30083200	-1.18371400	-0.21083800
O	5.07082200	-0.43298200	-0.06060700
H	4.11536300	-0.64105800	-0.18616100
H	5.37982800	-0.11844400	-0.92257000
O	4.09387900	1.83129700	1.35854600
H	3.23760600	1.78033900	0.88398700
H	4.60356800	1.09851700	0.95614500
O	-3.44486900	3.83046900	0.46113400
H	-4.14086300	4.04229900	-0.17676100
H	-2.59653900	3.94063400	-0.03295900

Figure S7. continued.

tzG 7H2O B3LYP N3 Cation

Enthalpy (Hartrees) = -1460.041359

Free Energy (Hartrees) = -1460.13793

Charge = 1 Multiplicity = 1

C	-1.15933600	-4.01222200	-0.01872800
H	-1.63155100	-4.02987800	0.96906900
C	0.93130300	-0.86317000	-0.18515200
C	0.95835400	0.60286700	-0.22738900
N	-0.29975100	1.18635600	-0.21417500
C	-1.49517900	0.52412900	-0.08147300
N	-1.49740900	-0.81971400	-0.00886000
C	-0.31074600	-1.54274700	-0.09064700
H	-0.70244400	-4.98844300	-0.19685700
H	-1.94163700	-3.85605200	-0.76841200
S	1.55091500	-3.21069400	-0.20813100
C	-0.14612700	-2.91656200	-0.09357600
O	-3.92199600	-2.20031800	0.70026100
H	-3.99131200	-3.06133800	0.26023900
H	-2.38522100	-1.31171500	0.19277100
O	-0.25593600	3.99976100	-0.77626600
H	0.62182200	4.20447000	-0.37039700
H	-0.15626600	4.15400800	-1.72720400
O	2.18017700	4.07170400	0.44154100
H	2.25359500	3.12673000	0.20126100
H	2.90033400	4.51555100	-0.02989000
O	1.98209600	1.28673000	-0.29142400
H	-0.32842200	2.21442300	-0.37072600
N	-2.61419200	1.22007400	-0.03044300
H	-2.60323900	2.24764700	0.03567300
H	-3.53205800	0.75434600	0.00786700
O	-5.28229400	0.11293100	0.06647300
H	-5.66578200	0.09648200	-0.82232800
H	-4.97087500	-0.80245400	0.23685000
N	2.02308300	-1.61499200	-0.25632800
O	4.92109800	-1.17529500	-0.16624100
H	3.95252800	-1.27938500	-0.28004900
H	5.27121300	-1.03332300	-1.05784300
O	4.72371500	1.26987800	1.19326300
H	3.82294300	1.50186000	0.91904700
H	4.88755500	0.41848000	0.73023000
O	-2.76601200	4.08525100	0.31659300
H	-3.40098300	4.49250900	-0.29014400
H	-1.88114400	4.24286200	-0.08191600
H	-3.93219700	-2.39664100	1.64968700

tzG 7H2O B3LYP N7 Cation

Enthalpy (Hartrees) = -1460.026079

Free Energy (Hartrees) = -1460.123472

Charge = 1 Multiplicity = 1

C	-0.57166900	-4.07733500	-0.16698500
H	-1.14943600	-4.11159300	0.76292900
C	1.02532200	-0.66512700	-0.19259600
C	0.84426000	0.78339200	-0.22215900
N	-0.47736700	1.14438100	-0.23151500
C	-1.55084500	0.25477100	-0.17161400
N	-1.39088600	-1.05917000	-0.13672800
C	-0.10118300	-1.51349400	-0.17008300
H	0.00906900	-4.99807800	-0.25164900
H	-1.27914400	-4.02991200	-1.00155900
S	1.99640300	-2.97047200	-0.20457200
C	0.29229600	-2.86431300	-0.17721100
O	-3.52858600	-2.61372600	1.01993800
H	-3.50512400	-3.51166500	0.65863500
H	-2.76355700	-2.14919700	0.60447900
O	-0.92046700	3.94926800	-0.79109700
H	-0.02708900	4.28340100	-0.53092100
H	-0.99422300	4.08367600	-1.74726600
O	1.61438700	4.41436800	0.09603200
H	1.77166300	3.45478800	-0.02537500
H	2.21257500	4.85652900	-0.52408000
O	1.77452700	1.60298200	-0.25666400
H	-0.67438800	2.15454100	-0.36618100
N	-2.77054300	0.80447700	-0.17158400
H	-2.90718100	1.80021400	0.01706300
H	-3.58850200	0.19585800	-0.10413300
O	-5.32770100	-0.76997700	0.05478500
H	-5.64231600	-1.00885500	-0.82872000
H	-4.80177600	-1.54399900	0.36465600
N	2.20145300	-1.30430500	-0.21093800
O	4.80559200	-0.49243600	-0.17447500
H	3.17334300	-0.89344900	-0.22182800
H	5.17062700	-0.24102700	-1.03723100
O	4.09741800	1.65355900	1.57225300
H	3.24500700	1.78305500	1.12242100
H	4.50294200	0.92995900	1.05653200
O	-3.28247300	3.64448900	0.58285000
H	-4.01825200	4.05428800	0.10598900
H	-2.47045900	3.92472900	0.10605600
H	5.36451100	-1.21897600	0.14360300

Figure S7. continued.

tzl 5H2O B3LYP Neutral

Enthalpy (Hartrees) =			-1251.385086
Free Energy (Hartrees) =			-1251.468691
Charge = 0 Multiplicity = 1			
C	-4.03867100	0.80720100	-0.07191400
H	-4.31365100	0.31184600	-1.00901700
C	-0.27352000	0.50843300	0.12790800
C	0.88586700	-0.38523600	0.14610700
N	0.53106200	-1.71202200	0.05664000
C	-0.76072700	-2.16630200	-0.05054500
N	-1.81804500	-1.41515600	-0.07638100
C	-1.58290700	-0.05366900	0.01740000
H	-4.53771000	1.77827900	-0.03668800
H	-4.41423600	0.19611700	0.75555700
S	-1.73840900	2.44676600	0.16250800
C	-2.55460800	0.94307500	0.02163500
O	-4.34731700	-2.78937200	-0.32877900
H	-5.03986600	-2.11563600	-0.27158600
H	-3.50561300	-2.28543000	-0.24294000
O	2.50633000	-3.77305600	0.03694200
H	3.27676500	-3.16386800	0.13164700
H	2.47762900	-4.28745600	0.85682300
O	4.33586900	-1.72622200	0.24583400
H	3.58427100	-1.09606500	0.20618200
H	4.82235900	-1.59955700	-0.58196900
O	2.07367500	-0.02599000	0.23821100
H	1.28224200	-2.42925700	0.07036600
N	-0.18632500	1.83253100	0.21623700
O	1.99089500	3.86649000	0.14031500
H	1.27180100	3.20853000	0.21437400
H	2.74029700	3.34067300	-0.20863400
H	-0.85985000	-3.24450500	-0.11737900
O	3.85868200	1.97024700	-0.84412100
H	3.27668500	1.27675800	-0.47747500
H	4.66891000	1.92605700	-0.31563300

tzl 5H2O B3LYP N1 Anion

Enthalpy (Hartrees) =			-1250.934214
Free Energy (Hartrees) =			-1251.01743
Charge = -1 Multiplicity = 1			
C	-4.04713200	-0.70740500	0.09640700
H	-4.28505600	-0.25151500	1.06359000
C	-0.28035900	-0.47137900	-0.20458300
C	0.88335500	0.42172400	-0.21689200
N	0.62966200	1.74035600	-0.05048800
C	-0.64688800	2.17070600	0.11136100
N	-1.75954700	1.46459300	0.13447900
C	-1.57524500	0.10783300	-0.02914500
H	-4.56984600	-1.66476800	0.03198800
H	-4.43736700	-0.05033500	-0.68839800
S	-1.79197000	-2.38283900	-0.28505500
C	-2.56900800	-0.86960300	-0.05007300
O	-4.18774400	2.88330000	0.41980800
H	-4.90020300	2.23502500	0.32676900
H	-3.35419500	2.35421100	0.32110100
O	2.75004100	3.63943900	-0.03942400
H	3.50590300	3.04114100	-0.20165000
O	4.43784200	1.37781900	-0.56874000
H	3.57406000	0.90362300	-0.49262100
H	4.95408700	1.08207300	0.19506500
O	2.06246700	-0.02066000	-0.38545600
H	1.98140400	3.01406500	-0.03424700
N	-0.22655000	-1.79579900	-0.35792500
O	1.95042400	-3.72705900	0.00656300
H	1.22281500	-3.09442200	-0.17147600
H	2.61877000	-3.17590100	0.46246200
H	-0.75538300	3.24584500	0.23794700
O	3.55426300	-1.72266900	1.25958100
H	3.02559600	-1.09335500	0.72053800
H	4.45930500	-1.63692200	0.92625000

Figure S7. continued.

tzl 5H2O B3LYP N3 Cation

Enthalpy (Hartrees) = -1251.8164

Free Energy (Hartrees) = -1251.8977

Charge = 1 Multiplicity = 1

C	-4.03459700	-0.96190400	-0.00506700
H	-4.37892000	-0.41083500	0.87639200
C	-0.26927500	-0.51460700	-0.02782600
C	0.86378500	0.41811500	-0.03245700
N	0.46825100	1.75937000	-0.02773000
C	-0.80363500	2.18040600	-0.01253400
N	-1.82436500	1.35604500	-0.00615400
C	-1.60312300	-0.01731300	-0.01476600
H	-4.48533200	-1.95615400	0.01081800
H	-4.38879700	-0.43492100	-0.89719000
S	-1.65601800	-2.50876900	-0.02712400
C	-2.54322500	-1.03483300	-0.01297300
O	-4.31819400	2.49232400	0.02027100
H	-4.94296500	1.89758500	0.46381500
H	-2.79645200	1.75981500	0.01422700
O	2.34266100	3.77346700	0.03790000
H	3.17055000	3.23772200	-0.01852500
H	2.31776100	4.30566300	-0.77120900
O	4.33423600	1.89051300	-0.09781300
H	3.63402600	1.21170700	-0.03224900
H	4.84728600	1.80956700	0.71972100
O	2.05354500	0.10653900	-0.03945500
H	1.21310400	2.50546600	-0.02850200
N	-0.13259700	-1.83408900	-0.03593500
O	2.11735300	-3.84272600	-0.05166000
H	1.40044000	-3.18106300	-0.05656000
H	2.92851400	-3.30097500	0.04248500
H	-0.98944900	3.24783000	-0.00461000
O	4.18813300	-1.93546600	0.26424800
H	3.52784500	-1.23456500	0.12190000
H	4.77780600	-1.88634400	-0.50239900
H	-4.31959800	3.30413300	0.55041600

tzl 5H2O B3LYP N7 Cation

Enthalpy (Hartrees) = -1251.8093

Free Energy (Hartrees) = -1251.8896

Charge = 1 Multiplicity = 1

C	-4.01710800	-0.72032100	0.07394500
H	-4.27834000	-0.17599800	0.98749200
C	-0.25441100	-0.46307400	-0.08545600
C	0.92468800	0.40502900	-0.10786300
N	0.57734500	1.73447800	-0.06247600
C	-0.70978700	2.20040900	0.00718400
N	-1.77619000	1.45825800	0.03480300
C	-1.54861200	0.09952600	-0.01257600
H	-4.54337400	-1.67672600	0.07167600
H	-4.35705400	-0.12849300	-0.78239700
S	-1.79829100	-2.42623500	-0.07266800
C	-2.54007200	-0.89228000	0.00324800
O	-4.31585600	2.88669400	0.22735600
H	-5.01466100	2.21971400	0.28799400
H	-3.48491700	2.36753000	0.16425900
O	2.57269700	3.70333000	-0.03333500
H	3.35408300	3.10386400	-0.09884600
H	2.57008800	4.22196900	-0.85124700
O	4.42438500	1.67187100	-0.17373400
H	3.67442500	1.04366400	-0.12738000
H	4.90602100	1.56053700	0.65919700
O	2.09768700	0.01145400	-0.16409700
H	1.34230200	2.44738900	-0.07601000
N	-0.23976300	-1.79789500	-0.12534900
O	1.65996200	-3.57872100	-0.23884100
H	0.61305100	-2.48003500	-0.19335600
H	2.50330400	-3.17728600	0.09732500
H	-0.80330100	3.28042400	0.04109800
O	3.74973000	-2.18332600	0.77847800
H	3.32200200	-1.34924800	0.50957800
H	4.56908800	-2.22852600	0.26366100
H	1.83316100	-3.83906200	-1.15671100

Figure S7. continued.

8vG 7H2O B3LYP Neutral

Enthalpy (Hartrees) = -1194.15248

Free Energy (Hartrees) = -1194.254773

Charge = 0 Multiplicity = 1

C	1.43709800	3.53885200	-0.27954700
H	2.12403700	3.91503600	-1.03796200
N	1.52107400	2.07937700	-0.21824200
C	2.67365500	1.30148300	-0.29218600
N	2.39776200	0.00424900	-0.25359800
C	1.02281000	-0.06996200	-0.15395800
C	0.14666900	-1.18536400	-0.11056800
O	0.45477500	-2.40418300	-0.15740300
N	-1.19504600	-0.81211700	-0.01833800
H	-1.87197100	-1.58078000	0.08691800
C	-1.66029000	0.48618400	0.01010900
N	-2.98847500	0.66162500	0.10963900
H	-3.63772800	-0.11225500	-0.04126200
H	-3.36609400	1.60522000	0.02922500
N	-0.84187400	1.53934700	-0.03702800
C	0.46570900	1.21235400	-0.12281300
H	1.67956400	3.98240500	0.68926800
H	0.42224700	3.81556900	-0.55927300
O	-1.14878900	-4.47266900	-1.03495300
H	-0.54149400	-3.73253400	-0.79981800
H	-1.27635400	-4.41143900	-1.99283900
O	-3.06240200	-3.11607900	0.37546500
H	-3.08021000	-3.46910300	1.27672500
H	-2.48213800	-3.72173200	-0.14664300
O	-4.37192400	3.37141700	0.04759300
H	-4.47992200	3.75537200	-0.83410800
H	-3.52273800	3.73557300	0.39154400
O	-1.87794100	4.02970200	1.03272800
H	-1.90117300	3.93435600	1.99616900
H	-1.46672000	3.19864400	0.69633400
O	4.31927700	-1.84250800	0.78524900
H	3.68293300	-1.21445300	0.36153400
H	4.94984900	-2.07466600	0.08850100
C	3.99735400	1.90292400	-0.39188500
H	4.06201200	2.95902500	-0.14669400
C	5.10719000	1.24390900	-0.75948400
H	5.09586700	0.19420500	-1.03585200
H	6.06286200	1.75734400	-0.79241100
O	2.41295400	-3.79899700	1.37544900
H	1.68335300	-3.36819900	0.88901000
H	3.17053100	-3.19642800	1.20667900
O	-5.09274800	-1.41856300	-0.34405500
H	-5.32269200	-1.51047300	-1.27963400
H	-4.44490500	-2.13529400	-0.16103100

8vG 7H2O B3LYP N1 Anion

Enthalpy (Hartrees) = -1193.698509

Free Energy (Hartrees) = -1193.801025

Charge = -1 Multiplicity = 1

C	-1.44289000	-3.53018000	-0.20641900
H	-2.09930100	-3.92654300	-0.98208400
N	-1.51947600	-2.07053600	-0.18679000
C	-2.66145700	-1.28758000	-0.31258300
N	-2.37481000	0.01019500	-0.29751200
C	-1.00005400	0.08072400	-0.16041800
C	-0.09087300	1.18342700	-0.12410500
O	-0.45548300	2.40889300	-0.22741700
N	1.23067000	0.86797400	0.01148200
H	2.37070800	2.21261800	0.34866900
C	1.63506100	-0.42213300	0.08900800
N	2.97775600	-0.62665800	0.26282400
H	3.59893800	0.14173500	0.03264800
H	3.34136000	-1.55604600	0.07837500
N	0.84593400	-1.51707900	0.04815400
C	-0.45828600	-1.20363300	-0.08309800
H	-1.72639200	-3.94997900	0.76238300
H	-0.41861000	-3.81968700	-0.43522200
O	1.07054400	4.56678600	-0.87965700
H	0.53346300	3.75556600	-0.68162400
H	1.17706000	4.57834800	-1.84137300
O	3.00084900	2.97565600	0.48475900
H	2.56133100	3.70371500	0.00057600
O	4.41116600	-3.50713900	-0.09554600
H	4.35238800	-3.81807800	-1.00993800
H	3.54629200	-3.74531300	0.31456400
O	1.93063800	-3.93564800	1.05252600
H	2.01293900	-3.82113800	2.01051300
H	1.50276900	-3.10236900	0.72141400
O	-4.29154100	1.82559000	0.74894100
H	-3.64983300	1.20581800	0.31503400
H	-4.89768600	2.09883700	0.04561700
C	-3.98625500	-1.88057800	-0.43796600
H	-4.06434600	-2.93221700	-0.17655700
C	-5.08499000	-1.22564300	-0.84681900
H	-5.06293300	-0.18118200	-1.14213900
H	-6.04141600	-1.73658700	-0.89514000
O	-2.29669100	3.68403900	1.41934400
H	-1.60663700	3.24792700	0.87149100
H	-3.08984000	3.13352000	1.24417000
O	5.19419200	1.68918100	-0.53105700
H	5.13856600	1.67793800	-1.49684300
H	4.42972400	2.24055400	-0.23239100

Figure S7. continued.

8vG 7H2O B3LYP N3 Cation

Enthalpy (Hartrees) = -1194.583922

Free Energy (Hartrees) = -1194.684062

Charge = 1 Multiplicity = 1

C	-1.37708300	-3.55477600	-0.23549400
H	-2.24420700	-3.95282400	-0.75812000
N	-1.48797000	-2.09332900	-0.16780300
C	-2.64975700	-1.32034500	-0.26213600
N	-2.37851500	-0.02383500	-0.23470000
C	-1.00847800	0.06292800	-0.12102700
C	-0.14448100	1.19705200	-0.08933800
O	-0.47164000	2.39619300	-0.15447900
N	1.21520400	0.85376100	0.01051000
H	1.87261500	1.65161600	0.10204500
C	1.73014900	-0.40655800	0.07260900
N	3.03358700	-0.59287800	0.17049600
H	3.68699700	0.19949000	0.09209600
H	3.44053300	-1.53789100	0.13523400
N	0.87780400	-1.46398000	0.03706500
C	-0.46329700	-1.20996800	-0.06863200
H	-1.31983500	-3.98115200	0.76784200
H	-0.48398700	-3.81521300	-0.80407500
O	1.06075800	4.50255800	-1.22634500
H	0.45538900	3.77645300	-0.96502800
H	1.19682200	4.39728100	-2.17934400
O	2.91279300	3.17560600	0.29578600
H	2.88307900	3.55388300	1.18691300
H	2.37196000	3.77423900	-0.27427900
O	4.39181400	-3.14938800	0.09484700
H	4.65630700	-3.36796100	-0.81046200
H	3.56742000	-3.65646000	0.25769900
O	1.85646300	-4.05291100	0.70737900
H	1.74299700	-4.20492200	1.65841100
H	1.23893300	-2.42452600	0.20040000
O	-4.35678200	1.79969200	0.82399100
H	-3.71827200	1.18733200	0.38870300
H	-4.99966200	2.02771700	0.13709500
C	-3.97343800	-1.92152100	-0.36536400
H	-4.06547900	-2.95296700	-0.03954500
C	-5.05337400	-1.27117600	-0.82353600
H	-5.00525700	-0.24708100	-1.18068600
H	-6.01917800	-1.76537800	-0.85193100
O	-2.48201100	3.79706100	1.39094400
H	-1.74016900	3.39031800	0.90729000
H	-3.22171100	3.17171300	1.22540100
O	5.01699600	1.48499400	-0.14221900
H	5.34078800	1.49205300	-1.05451700
H	4.36874700	2.22221100	-0.08453500
H	1.38581900	-4.78036500	0.27269300

8vG 7H2O B3LYP N7 Cation

Enthalpy (Hartrees) = -1194.590166

Free Energy (Hartrees) = -1194.692584

Charge = 1 Multiplicity = 1

C	-1.37531100	-3.54400100	-0.25254200
H	-2.13812900	-3.93635800	-0.92332900
N	-1.48877100	-2.08242700	-0.18636500
C	-2.64875700	-1.36158000	-0.22181300
N	-2.34505100	-0.05638600	-0.19072700
C	-0.97059400	0.07807400	-0.12866900
C	-0.10995100	1.20685100	-0.08770900
O	-0.44555900	2.41261500	-0.09477900
N	1.23018500	0.83323400	-0.04078600
H	1.90951800	1.60475000	0.06872000
C	1.69733200	-0.46734800	-0.04688600
N	3.01947900	-0.64870000	-0.01214200
H	3.67442000	0.12932200	-0.12445800
H	3.39695400	-1.59679700	-0.06440700
N	0.87357300	-1.52437200	-0.07579900
C	-0.42709300	-1.19942400	-0.12005200
H	-1.48889000	-3.97752500	0.74289100
H	-0.39291500	-3.78908700	-0.65110500
O	1.13113500	4.57466500	-0.88279900
H	0.52466800	3.82314300	-0.69979200
H	1.23790600	4.59785200	-1.84491900
O	3.05425800	3.09763500	0.37990300
H	3.08209000	3.37352500	1.30764100
H	2.47390900	3.74861900	-0.08502100
O	4.37939300	-3.31326600	0.00679600
H	4.50730400	-3.72781000	-0.85833500
H	3.55492600	-3.71163800	0.37075400
O	1.91853800	-4.04383100	1.03626800
H	1.94931500	-3.94230400	1.99893400
H	1.49884600	-3.22105600	0.70032200
O	-4.28965800	1.98022300	0.17125100
H	-3.04428200	0.70790400	-0.12858000
H	-4.57142400	2.43684200	-0.63636300
C	-3.97277900	-1.95255500	-0.26829500
H	-4.03236600	-2.98703600	0.05386000
C	-5.07551000	-1.30924900	-0.68119200
H	-5.06098400	-0.28580200	-1.04221600
H	-6.03291300	-1.81966800	-0.67224100
O	-2.41417700	3.45838000	1.70976500
H	-1.67408500	3.14501300	1.15541500
H	-3.18892800	3.03065800	1.29577900
O	5.09194600	1.43352200	-0.39676600
H	5.31985000	1.53907300	-1.33149600
H	4.44868100	2.15016600	-0.20004200
H	-5.09040600	1.55462400	0.51454900

Figure S7. continued.

BPP 6H2O B3LYP Neutral

Enthalpy (Hartrees) = -1235.882878

Free Energy (Hartrees) = -1235.984029

Charge = 0 Multiplicity = 1

C	0.29360300	-0.13124400	-0.13049900
N	1.50592600	0.41373700	-0.19299400
C	2.60539500	-0.37703300	-0.14359000
C	1.19891100	-2.30992600	0.01287700
H	1.16518100	-3.38945500	0.08756100
C	3.63458500	-2.61590700	0.00140200
H	4.23945100	-2.34378500	0.86743100
H	3.32323500	-3.65612900	0.08077300
H	4.21675500	-2.47179300	-0.90976700
O	3.76790700	0.08535100	-0.18457600
N	2.43098000	-1.76789600	-0.04402500
N	-0.78136300	0.72322200	-0.17463900
H	-0.60876700	1.73282400	-0.28797100
H	1.95954100	2.30012600	-0.41077000
H	4.29142400	1.68815000	0.69173200
H	5.56710800	-0.40846100	-0.14655200
O	-0.61464500	3.72096000	-0.61955200
H	-1.42139200	3.92024100	-0.09050500
H	-0.86176400	3.87412400	-1.54311600
O	2.13396000	3.26581000	-0.46329300
O	4.43456800	2.58000900	1.06647700
O	6.53500400	-0.54834100	-0.13518700
H	1.23519600	3.64885600	-0.42956100
H	3.68478700	3.08243700	0.69336500
H	6.91172800	0.34129800	-0.08077000
C	0.06064900	-1.52964800	-0.02117000
C	-2.10002500	0.32809700	-0.11363900
O	-2.99553000	1.19590400	-0.14716300
C	-1.30530600	-2.03996500	0.03698100
H	-3.02251600	2.87858400	0.60772200
H	-4.87655300	1.45962300	-0.19485100
O	-2.90069400	3.79500300	0.93482100
H	-3.65108500	4.29356700	0.57926500
O	-5.80591800	1.75794500	-0.21535600
H	-5.77125200	2.67963000	0.07843800
C	-2.37203800	-1.11007000	-0.01429000
C	-1.61457500	-3.41002800	0.14299500
C	-3.70682900	-1.55202400	0.03496600
C	-2.93715000	-3.83313300	0.18935600
H	-3.15380600	-4.89400100	0.27008700
C	-3.99080800	-2.90598700	0.13376100
H	-5.02054600	-3.24621300	0.17011200
H	-0.82383700	-4.15008700	0.19033000
H	-4.50736400	-0.82288600	-0.00560600

BPP 6H2O B3LYP N3 Cation

Enthalpy (Hartrees) = -1236.314747

Free Energy (Hartrees) = -1236.415137

Charge = 1 Multiplicity = 1

C	0.26339800	-0.10462500	-0.22186900
N	1.50672100	0.42087000	-0.31675700
C	2.66704500	-0.32231200	-0.27365900
C	1.26823300	-2.24829900	-0.04377900
H	1.25264100	-3.32598500	0.05761500
C	3.71505300	-2.52835400	-0.10223500
H	4.32284900	-2.23027600	0.75272600
H	3.41782600	-3.57027400	-0.00322100
H	4.27730000	-2.38464100	-1.02542300
O	3.77820400	0.20112300	-0.34683600
N	2.49361700	-1.69905100	-0.14284100
N	-0.80353000	0.72278000	-0.27359800
H	-0.67966400	1.74222800	-0.43548900
H	1.65827500	1.46097300	-0.38033200
H	4.09155000	1.63771800	1.31502700
H	5.64871500	-0.23839600	-0.16674900
O	-0.64303700	3.57371500	-0.76596000
H	-1.43551100	3.84546100	-0.24248200
H	-0.85185400	3.76738700	-1.69177900
O	1.99076700	3.14288500	-0.32783500
O	3.83652700	2.47323300	1.73779000
O	6.61012700	-0.38662700	-0.10375900
H	1.07336100	3.48506900	-0.44579400
H	3.16459400	2.83317500	1.12597400
H	6.99855400	0.49963600	-0.09699300
C	0.10437700	-1.49967400	-0.06892900
C	-2.12195300	0.28246900	-0.16076100
O	-3.02911300	1.12639100	-0.20238300
C	-1.24346000	-2.05039400	0.04346300
H	-3.07016100	2.88322100	0.47354200
H	-4.93979400	1.35635400	-0.11675100
O	-2.91226100	3.80925200	0.74846100
H	-3.64540300	4.31628700	0.36938100
O	-5.87356700	1.63508100	-0.08390800
H	-5.84151500	2.55686900	0.21001700
C	-2.34000000	-1.15577900	-0.00281400
C	-1.50247500	-3.42394500	0.20220900
C	-3.65805600	-1.63611500	0.10388100
C	-2.80927200	-3.88534200	0.30508400
H	-2.98880200	-4.94906400	0.42643500
C	-3.89329400	-2.99419900	0.25526000
H	-4.90950700	-3.36552200	0.33652100
H	-0.68801300	-4.13752800	0.24860000
H	-4.48178000	-0.93302200	0.06650800
H	2.48993200	3.43711600	-1.10461800

Figure S7. continued.

BPP 6H2O B3LYP N7 Anion

Enthalpy (Hartrees) = -1235.430329

Free Energy (Hartrees) = -1235.52992

Charge = -1 Multiplicity = 1

C	0.24019800	-0.06695400	0.00506900
N	1.48965100	0.44462000	-0.07842700
C	2.56886200	-0.35716900	-0.13394900
C	1.15150200	-2.28055000	-0.05526700
H	1.10757500	-3.36267100	-0.05748800
C	3.58205000	-2.61213400	-0.18911400
H	4.22949000	-2.41071400	0.66564500
H	3.25883600	-3.65188000	-0.16666200
H	4.13073600	-2.41875800	-1.11228200
O	3.74629900	0.09291700	-0.19278500
N	2.39203800	-1.75001500	-0.12627800
N	-0.77511700	0.82638400	0.08028400
H	-0.68031800	2.62792500	-0.41993400
H	1.89894800	2.28336400	-0.23907100
H	4.26062500	1.63128400	0.69185100
H	5.49629500	-0.42847000	-0.34660700
O	-0.66098500	3.58568900	-0.67912000
H	-1.41144900	3.96885400	-0.18393500
O	2.08710900	3.25215600	-0.30499800
O	4.45032200	2.49969000	1.10721100
O	6.46117500	-0.58535900	-0.41895100
H	1.19114700	3.64342500	-0.35606300
H	3.70370600	3.04470700	0.79545100
H	6.85826700	0.29548800	-0.36811900
C	0.02844800	-1.48871200	0.01658600
C	-2.05110800	0.39301900	0.19348300
O	-2.99316400	1.24123100	0.30768400
C	-1.33331800	-1.99906300	0.10064600
H	-3.01925200	2.95847200	0.68652300
H	-4.50337600	1.42098200	-0.66472500
O	-3.04674800	3.92940400	0.86933900
H	-3.79483300	4.26178200	0.35237100
O	-5.30617400	1.64262300	-1.18647600
H	-5.28742700	2.60715600	-1.26321800
C	-2.37615900	-1.04935600	0.19090100
C	-1.66130300	-3.37143900	0.10297500
C	-3.71384200	-1.47826800	0.28295000
C	-2.98605500	-3.77873900	0.19002700
H	-3.22022900	-4.83924200	0.18897000
C	-4.02086100	-2.83183700	0.28084800
H	-5.05401600	-3.15789100	0.35018700
H	-0.88271500	-4.12345400	0.03569500
H	-4.50117700	-0.73687900	0.35620900

C 5H2O B3LYP Neutral

Enthalpy (Hartrees) = -816.304766

Free Energy (Hartrees) = -816.388919

Charge = 0 Multiplicity = 1

C	2.03856200	-2.93252800	-0.37545900
H	2.52818700	-2.74881400	-1.33378100
N	0.83518900	-2.09804200	-0.25490900
C	-0.40054100	-2.65732000	-0.09152100
H	-0.43203700	-3.73967800	-0.05202400
C	-1.51864100	-1.89073200	0.00862200
H	-2.49577900	-2.33935400	0.13220200
C	-1.34982200	-0.47258500	-0.05848800
N	-2.40646900	0.34511500	0.02725100
H	-2.29023900	1.35412400	-0.05929000
H	-3.34629400	-0.03782000	0.13351600
N	-0.12537000	0.07378700	-0.20753500
C	0.96780600	-0.71125300	-0.31644900
O	2.12625200	-0.23131800	-0.47852600
O	-5.17643800	-0.73339100	0.32812600
H	-5.80850100	-0.00160300	0.38801900
H	-5.26301700	-1.20103100	1.17224400
O	-2.15670800	3.41312300	-0.29621000
H	-1.21112200	3.33235800	-0.02662500
H	-2.59399400	3.87261000	0.43465700
O	0.39701500	2.77063200	0.49475900
H	1.21924000	2.94985800	-0.00424200
H	0.21067900	1.82272700	0.27122300
O	2.78523800	2.42203700	-1.02968400
H	3.58169700	2.58428400	-0.50367000
H	2.54730000	1.48254200	-0.84922500
O	3.89083700	0.11746100	1.68810700
H	4.13499300	1.05193400	1.62565400
H	3.26516700	-0.02602500	0.94698200
H	1.73982300	-3.97825100	-0.31454900
H	2.73669800	-2.70574300	0.43245200

Figure S7. continued.

C 5H2O B3LYP N3 Cation

Enthalpy (Hartrees) = -816.746278

Free Energy (Hartrees) = -816.828538

Charge = 1 Multiplicity = 1

C	2.01715300	-2.92420800	-0.45865600
H	2.50188000	-2.67382100	-1.40354400
N	0.81558200	-2.08969600	-0.28075500
C	-0.42653700	-2.64544300	-0.12747700
H	-0.46045600	-3.72797200	-0.13631200
C	-1.54940300	-1.89336500	0.01459500
H	-2.52148300	-2.35461300	0.12073800
C	-1.42412700	-0.47577900	0.00861200
N	-2.45489500	0.33979000	0.11813500
H	-2.35939700	1.36133500	0.03465900
H	-3.39760600	-0.05920400	0.20913100
N	-0.16030900	0.03565400	-0.11654300
C	0.98086900	-0.72177400	-0.27494600
O	2.09777300	-0.19872300	-0.40811500
O	-5.13316200	-0.75936400	0.35225900
H	-5.78960400	-0.10363700	0.07329000
H	-5.34557900	-0.94084800	1.28013000
O	-2.27739200	3.20438800	-0.30970600
H	-1.31784900	3.24653400	-0.10407300
H	-2.71227700	3.73716500	0.37164200
O	0.37723800	2.83533700	0.32828100
H	1.25374100	2.88599700	-0.12575700
H	-0.00394700	1.05818900	-0.02207500
O	2.75021800	2.48946400	-0.98884500
H	3.52906200	2.72915300	-0.46511200
H	2.60936900	1.53411500	-0.82143100
O	4.18932500	-0.03007800	1.58355800
H	4.53698100	0.85750000	1.41451000
H	3.47523400	-0.14241800	0.92889800
H	1.70676100	-3.96715300	-0.47026500
H	2.71244200	-2.75429800	0.36484000
H	0.56035500	2.94897000	1.27264700

CFU 6H2O B3LYP Neutral

Enthalpy (Hartrees) = -1121.515152

Free Energy (Hartrees) = -1121.619488

Charge = 0 Multiplicity = 1

C	1.86102100	-3.13728200	-1.06053700
H	2.49434800	-2.99400400	-1.93780500
N	1.12349600	-1.89924300	-0.76788400
C	-0.23493800	-1.88528900	-0.73441500
H	-0.72709400	-2.83242400	-0.92069100
C	-0.94733500	-0.74644900	-0.47312100
C	-0.17463200	0.45251700	-0.25209700
N	-0.76390400	1.63416900	-0.04047900
H	-0.19441900	2.46654900	0.11396600
H	-1.77101800	1.76169600	-0.12577100
N	1.17172400	0.41619000	-0.25688300
C	1.83978100	-0.73142300	-0.49467700
O	3.09947600	-0.79284300	-0.49133100
H	1.13786900	-3.92772600	-1.25691600
H	2.48377100	-3.41425800	-0.20829600
C	-2.41080300	-0.77956400	-0.45388400
C	-3.35748600	-1.14789200	-1.36665600
O	-3.03654700	-0.40586800	0.72445500
C	-4.63559800	-0.99795700	-0.72938900
H	-3.16416900	-1.47110500	-2.38003400
C	-4.38882500	-0.54492000	0.53056400
H	-5.60791600	-1.19523200	-1.15906400
H	-5.01387100	-0.28647300	1.37198100
O	4.89834100	1.26256300	0.12228600
H	5.61712000	1.17426300	-0.52007500
H	4.26707600	0.53810600	-0.09442000
O	2.67442000	2.77630600	-0.80944900
H	3.56583900	2.52895000	-0.49008600
H	2.14677600	1.95650800	-0.63804700
O	0.80279500	4.20071100	0.61230100
H	0.49365000	4.94630700	0.07826700
H	1.57046200	3.82491500	0.11992700
O	-1.97919600	-1.01849100	3.43394200
H	-2.22685600	-0.77682200	2.52486700
H	-1.06373900	-0.71922900	3.52998400
O	-3.56938000	2.63867900	-0.55114200
H	-4.21354600	1.92086400	-0.44905900
H	-3.81509500	3.28634500	0.12572600
O	4.47723000	-2.11299400	1.60805400
H	5.08432000	-1.42120300	1.90712700
H	3.97305300	-1.69878100	0.87747700

Figure S7. continued.

CFU 6H2O B3LYP N3 Cation

Enthalpy (Hartrees) = -1121.954805

Free Energy (Hartrees) = -1122.053912

Charge = 1 Multiplicity = 1

C	2.03136200	-3.15381800	-0.41217500
H	2.67524100	-3.14930700	-1.29239300
N	1.19881400	-1.93691600	-0.40462900
C	-0.16033400	-2.00528700	-0.33104900
H	-0.57903100	-3.00278900	-0.27638400
C	-0.96910100	-0.90176000	-0.31990700
C	-0.33305600	0.38453900	-0.39535700
N	-0.98806100	1.52625100	-0.43845100
H	-0.50231000	2.43508900	-0.45157200
H	-2.01297400	1.55345300	-0.46729300
N	1.03338500	0.39882500	-0.43909700
C	1.84323900	-0.71681000	-0.43165800
O	3.07687200	-0.62106100	-0.45900100
H	1.37100200	-4.01823200	-0.44498400
H	2.64238600	-3.18919600	0.49093700
C	-2.42436100	-1.05211500	-0.25040100
C	-3.34483700	-1.65762800	-1.05573900
O	-3.05926600	-0.53591900	0.86501900
C	-4.61997300	-1.51064800	-0.41310200
H	-3.13720400	-2.13980400	-2.00080000
C	-4.39456000	-0.82343300	0.74077800
H	-5.57657100	-1.86595300	-0.76977300
H	-5.02706800	-0.47574700	1.54354600
O	4.36292900	1.51159400	0.97892300
H	5.30400600	1.58191700	0.76096700
H	4.05594500	0.69027200	0.54593500
O	2.59572500	2.79437400	-0.68308200
H	3.31992200	2.49780100	-0.08050700
H	1.54110300	1.30219600	-0.53181100
O	0.23710800	4.14404500	-0.27268500
H	0.03326300	4.71328600	-1.02868700
H	1.15180200	3.81856400	-0.42446900
O	-1.57975600	0.42156600	3.25932700
H	-2.05864700	0.11858700	2.46876800
H	-0.78981100	0.86004600	2.91149600
O	-3.81232900	2.18698300	-0.80940700
H	-4.37123600	1.39416500	-0.80493200
H	-4.12322600	2.70728600	-0.05336900
O	5.44345400	-2.03091000	0.45099500
H	5.90089900	-1.28649500	0.86767300
H	4.59444200	-1.65833000	0.14942100
H	2.99093100	2.85245100	-1.56559600

Chpp 7H2O B3LYP Neutral

Enthalpy (Hartrees) = -1174.707022

Free Energy (Hartrees) = -1174.80622

Charge = 0 Multiplicity = 1

C	-3.50136900	-2.88214200	0.58049600
H	-4.01731500	-2.56979800	1.48938300
N	-2.30323500	-2.04614700	0.38449500
C	-1.07858400	-2.57758400	0.36033900
H	-0.99322100	-3.65137300	0.48854500
C	0.04773300	-1.78278100	0.17911900
C	-0.20466200	-0.38945200	0.02028300
N	0.88225600	0.42565800	-0.15659500
H	0.75966000	1.44716200	-0.29197800
N	-1.41447500	0.15504200	0.03319700
C	-2.49461400	-0.64472700	0.22919600
O	-3.65850800	-0.20817500	0.27998200
H	-3.18430200	-3.91974900	0.66773600
H	-4.16836600	-2.76537000	-0.27428500
C	2.16972700	-0.04773000	-0.16379900
C	1.35811200	-2.35930000	0.15764100
O	3.14542200	0.70365900	-0.29527300
O	3.18635200	3.32971600	0.84188200
H	3.31127100	2.42892300	0.48143700
H	3.89315200	3.86359800	0.45026300
O	0.78948500	3.30989300	-0.52433100
H	0.96798500	3.51289400	-1.45451200
H	1.63379400	3.49034100	-0.04735200
O	-1.99317800	3.01775500	-0.25127900
H	-1.08303200	3.37179800	-0.23807600
H	-1.84733900	2.04767000	-0.20480200
O	-4.19348400	2.38841800	1.44127200
H	-3.46088400	2.85925600	0.99844800
H	-4.09278100	1.47792100	1.10262200
N	2.32163900	-1.42865000	-0.01685300
H	3.30161600	-1.75233100	-0.04464800
O	4.99643800	-2.59571800	-0.04564400
H	5.46219400	-1.74184900	-0.20267400
H	5.10109300	-3.10252700	-0.86397800
O	5.89077700	0.00085100	-0.40341200
H	6.34474100	0.32758400	0.38709400
H	4.96157300	0.29850200	-0.31370500
O	-5.28225300	-0.17659100	-2.09472100
H	-4.72379700	-0.17962100	-1.29389800
H	-5.39580100	0.75948400	-2.31277900

Figure S7. continued.

Chpp 7H2O B3LYP N3 Cation

Enthalpy (Hartrees) = -1175.138931

Free Energy (Hartrees) = -1175.235208

Charge = 1 Multiplicity = 1

C	3.38370700	-3.32925100	-0.08249300
H	3.98304700	-3.10861900	-0.96644800
N	2.25217100	-2.38173000	-0.01582500
C	0.98222400	-2.79655100	-0.03475300
H	0.81022100	-3.86566200	-0.10198400
C	-0.09096900	-1.91102500	0.03216600
C	0.22817000	-0.53651500	0.11450400
N	-0.76638900	0.37027900	0.19940100
H	-0.56701300	1.38589100	0.36208800
N	1.51214200	-0.13475900	0.10971600
C	2.57965100	-1.01178400	0.06243400
O	3.74292200	-0.63308300	0.08644100
H	2.97662200	-4.33621100	-0.14379700
H	3.99415900	-3.22188900	0.81458200
C	-2.09767100	-0.00933100	0.17217900
C	-1.44538800	-2.38666100	0.00437000
O	-3.00442500	0.82111100	0.23683900
O	-2.66882400	3.58399000	-0.54706400
H	-2.92761400	2.67635100	-0.29371800
H	-3.29331300	4.16854800	-0.09271400
O	-0.32016600	3.10471300	0.75356200
H	-0.45264800	3.25660500	1.70131400
H	-1.12655800	3.46208700	0.30530700
O	2.22944200	2.46328100	-0.04618900
H	1.42283500	2.91684800	0.28170300
H	1.77349500	0.89855100	0.08386000
O	3.30719200	1.78822700	-2.57703700
H	2.91242100	2.07998200	-1.73029000
H	3.62872900	0.89306700	-2.39584800
N	-2.34121300	-1.38019200	0.07097200
H	-3.34630800	-1.63242900	0.04224900
O	-5.05458700	-2.29608000	-0.13662300
H	-5.49314400	-1.41550400	-0.09219000
H	-5.33910300	-2.76949600	0.65863600
O	-5.82550700	0.36693100	-0.04035500
H	-6.10470000	0.68324300	-0.91217800
H	-4.87525900	0.58967600	0.02243200
O	4.31596600	1.82432000	1.65026500
H	4.31130200	0.98451900	1.15436900
H	5.17405900	2.23019100	1.45839600
H	2.92734500	2.50849400	0.64521600

Chpp 7H2O B3LYP N7 Anion

Enthalpy (Hartrees) = -1174.261938

Free Energy (Hartrees) = -1174.360616

Charge = -1 Multiplicity = 1

C	3.54121100	-2.83461000	-0.40377600
H	4.07729800	-2.57797900	-1.31874000
N	2.33254200	-2.00211200	-0.28819100
C	1.11115800	-2.54606300	-0.24823500
H	1.04379600	-3.62780300	-0.29995500
C	-0.02462300	-1.75767900	-0.14906500
C	0.17270400	-0.33613900	-0.08801800
N	-0.87830200	0.50610200	0.00671400
H	-0.81138400	2.33564700	0.48743300
N	1.41062800	0.20334000	-0.12489000
C	2.49300200	-0.58911900	-0.23163600
O	3.66610100	-0.14652400	-0.28820100
H	3.23667200	-3.87970800	-0.43313000
H	4.19039800	-2.66142100	0.45539000
C	-2.11689900	-0.02231400	0.02846500
C	-1.32367900	-2.35907900	-0.11387800
O	-3.15523000	0.68944200	0.09711800
O	-3.44535700	3.41081700	-0.43068600
H	-3.35583800	2.44840100	-0.24257300
H	-4.11750900	3.72900700	0.18901600
O	-0.82443200	3.29818600	0.71333100
H	-1.67463400	3.60304000	0.33861600
O	1.92433100	3.03405500	0.11826900
H	1.02852000	3.41032000	0.22318500
H	1.75629200	2.06266600	0.05347100
O	4.18655800	2.37804800	-1.48930300
H	3.44779000	2.87684300	-1.09209400
H	4.06074400	1.48198500	-1.11367300
N	-2.28748700	-1.42433600	-0.02584700
H	-3.26283600	-1.74281400	0.00478600
O	-5.01679800	-2.68541000	0.02795000
H	-5.43423200	-1.80275300	0.16301400
H	-5.11997900	-3.15124400	0.87020700
O	-5.80503100	-0.05329200	0.32137700
H	-6.26588200	0.25843200	-0.47101400
H	-4.86529800	0.22301000	0.20617000
O	5.31426600	-0.16351000	2.02373000
H	4.73624800	-0.16052900	1.23381300
H	5.41566700	0.76946100	2.25974900

Figure S7. continued.

Chpp 7H2O B3LYP N9 Anion

Enthalpy (Hartrees) =			-1174.245623
Free Energy (Hartrees) =			-1174.345194
Charge = -1 Multiplicity = 1			
C	3.56243300	-2.79226500	-0.54920800
H	4.08096900	-2.46630500	-1.45204400
N	2.34218400	-1.98883100	-0.36227300
C	1.12683800	-2.56138500	-0.33825100
H	1.08293400	-3.63916700	-0.45496900
C	-0.02184400	-1.80773300	-0.17529100
C	0.18824000	-0.40998800	-0.03211600
N	-0.92848700	0.35526300	0.12549200
H	-0.84461300	1.37228400	0.25965400
N	1.38531800	0.17825800	-0.04188200
C	2.48761200	-0.58861300	-0.21951900
O	3.64466500	-0.11282900	-0.26550600
H	3.27270000	-3.83733900	-0.64486500
H	4.22072100	-2.66633000	0.31132300
C	-2.20253000	-0.19730000	0.12392400
C	-1.34140700	-2.41726900	-0.14871900
O	-3.18213600	0.58035700	0.24280000
O	-3.27852700	3.14203400	-0.84409800
H	-3.32695000	2.22990500	-0.47855200
H	-4.03374800	3.61420400	-0.46449000
O	-0.92800200	3.36947400	0.56396000
H	-1.14455700	3.52171700	1.49518100
H	-1.78043200	3.45012300	0.07363400
O	1.83728100	3.04059600	0.22810200
H	0.91593200	3.36581500	0.25172700
H	1.72440800	2.06457200	0.17437600
O	4.07965700	2.45631100	-1.43751500
H	3.33407600	2.92502800	-1.01621900
H	3.98882700	1.55056800	-1.07783400
N	-2.36963600	-1.55753500	0.00035500
H	-3.97400400	-2.28674600	0.07477000
O	-4.88784700	-2.69402200	0.12398300
H	-5.46173400	-1.91307300	0.23772000
O	-5.91195600	-0.00094400	0.46821400
H	-6.33782400	0.31863700	-0.34007900
H	-4.95446300	0.19109800	0.34978400
O	5.29129400	-0.12440700	2.06059000
H	4.71709300	-0.11905000	1.26888900
H	5.40352500	0.80876200	2.29099400

m5K 3H2O B3LYP Neutral

Enthalpy (Hartrees) =			-647.372782
Free Energy (Hartrees) =			-647.440474
Charge = 0 Multiplicity = 1			
C	0.52360500	2.58215000	-0.63943200
H	0.02062700	2.61810200	-1.60725400
N	0.90954500	1.19403200	-0.33503900
C	2.21256900	0.86005300	-0.14306700
H	2.92996000	1.66841500	-0.22828600
C	2.58655700	-0.43323500	0.14346200
C	1.52518200	-1.35669500	0.21882900
N	0.24809800	-1.04920900	0.03357500
C	-0.10010100	0.23834000	-0.25043600
O	-1.29313000	0.59086000	-0.44053400
H	1.42227500	3.19605700	-0.66561500
H	-0.15407400	2.95135500	0.13163100
O	-1.81909200	-3.06952400	0.20885800
H	-2.58643900	-2.52230000	-0.05292000
H	-1.07611100	-2.42437400	0.17065100
O	-3.60923900	-0.96662100	-0.55803500
H	-3.85898500	-1.03685900	-1.49066400
H	-2.78366600	-0.43064100	-0.55016000
C	4.01979000	-0.83727200	0.35851800
H	4.68163400	0.03024000	0.29736200
H	4.15245600	-1.30125500	1.34160800
H	4.33925900	-1.56505600	-0.39527300
H	1.73581100	-2.40087200	0.44298200
O	-2.74701300	2.24812100	1.34168700
H	-3.57319200	1.75505200	1.44561500
H	-2.21086200	1.70564800	0.72752300

Figure S7. continued.

m5K 3H2O B3LYP N3 Cation

Enthalpy (Hartrees) =			-647.810795
Free Energy (Hartrees) =			-647.878583
Charge = 1 Multiplicity = 1			
C	-0.66677300	-2.63989000	-0.66191500
H	-0.20332900	-2.69427700	-1.64771400
N	-0.97899200	-1.22980300	-0.35116400
C	-2.24279300	-0.82574300	-0.11212600
H	-3.00372300	-1.59684000	-0.16206600
C	-2.56353200	0.49482200	0.18359200
C	-1.48925500	1.37203300	0.22774200
N	-0.23542200	0.95314800	-0.00871000
C	0.09753000	-0.34574700	-0.31298000
O	1.25587700	-0.71720800	-0.53580300
H	-1.59408500	-3.20822100	-0.65015100
H	0.02246000	-3.02703100	0.08945600
O	1.75609700	2.84335700	0.05755100
H	2.53367500	2.27814300	-0.16926000
H	0.55013600	1.65520300	0.03779600
O	3.59746400	0.91568300	-0.61792000
H	3.91701900	1.00572100	-1.52774700
H	2.84289300	0.29395100	-0.66612900
C	-3.98232300	0.93589300	0.41818800
H	-4.55712200	0.14612900	0.90826500
H	-4.00766600	1.82929200	1.04656700
H	-4.47481300	1.17375400	-0.53102900
H	-1.59893000	2.42703900	0.45526000
O	2.80881500	-2.07355900	1.53615600
H	3.62311200	-1.55089500	1.56302300
H	2.27164600	-1.65349400	0.84020300
H	1.91649500	3.16372100	0.95776600

pC 4H2O B3LYP Neutral

Enthalpy (Hartrees) =			-855.363161
Free Energy (Hartrees) =			-855.440471
Charge = 0 Multiplicity = 1			
C	-1.27293200	-1.72168300	0.01767900
C	-1.07881200	-0.30362200	-0.01512300
C	1.20955800	-0.45339600	-0.07316500
C	-2.69656200	-1.94566600	0.06842200
C	-3.29100000	-0.71157500	0.06746800
H	-3.20830500	-2.89695500	0.10239400
C	-4.73074000	-0.33218300	0.11057000
H	-5.35386300	-1.22842100	0.14563700
H	-4.95215500	0.28037200	0.99261100
H	-5.01159800	0.25254500	-0.77346200
N	-2.29876900	0.28331900	0.01379000
N	0.09908300	0.31689300	-0.06654500
O	2.37073100	0.04623900	-0.10127600
N	1.08355600	-1.85409200	-0.04933900
C	-0.12782800	-2.47647700	-0.00532800
C	2.32014200	-2.65193000	-0.06933900
H	2.04940700	-3.70662700	-0.07082100
H	2.89597100	-2.42047000	-0.96677800
H	2.92143500	-2.42851100	0.81343300
H	-0.11266200	-3.55981300	0.01146700
H	-2.46173900	1.29770900	0.02872600
O	-2.43039400	3.22030000	0.15056400
H	-2.90353900	3.63205000	-0.58681900
H	-1.47620800	3.34578700	-0.05124300
O	0.27354900	3.09589600	-0.53926000
H	0.21658800	2.11564800	-0.40933800
H	1.14447200	3.30923600	-0.15126400
O	2.91437100	2.71344000	0.54666200
H	2.71871300	1.77964800	0.29924700
H	3.67039400	2.96723100	-0.00189500
O	5.13658500	-0.39268900	0.00583800
H	4.15814300	-0.35077700	-0.02942000
H	5.40816000	0.50220800	0.25486000

Figure S7. continued.

pC 4H2O B3LYP N3 Cation

Enthalpy (Hartrees) = -855.800843

Free Energy (Hartrees) = -855.87631

Charge = 1 Multiplicity = 1

C	1.28406100	-1.70181000	-0.02973100
C	1.11205500	-0.29429900	0.08158900
C	-1.24566500	-0.50678100	0.29677900
C	2.69999100	-1.91677000	-0.19970300
C	3.29385200	-0.68540100	-0.18828400
H	3.20083800	-2.86638900	-0.31809300
C	4.72095300	-0.28835600	-0.32705800
H	5.34178700	-1.17575300	-0.46563900
H	4.86250300	0.37583900	-1.18752200
H	5.06933500	0.24683800	0.56396500
N	2.29989500	0.30679300	-0.00896300
N	-0.10757100	0.26195700	0.24976500
O	-2.37243800	-0.00252400	0.43130900
N	-1.07069200	-1.88731400	0.19287400
C	0.14918500	-2.47173900	0.03469700
C	-2.29486400	-2.71064900	0.25254800
H	-2.00297300	-3.75772500	0.20898400
H	-2.82237100	-2.51083600	1.18587700
H	-2.93999900	-2.46912400	-0.59308600
H	0.15598400	-3.55286400	-0.03773600
H	2.45148100	1.33223900	-0.01250000
O	2.36364400	3.13140200	-0.15097200
H	2.83456500	3.57589200	0.56906300
H	1.41042900	3.24830100	0.04958000
O	-0.36185400	3.05568300	0.52047600
H	-0.21894300	1.29375600	0.36713900
H	-1.26027600	3.10115400	0.10838300
O	-2.82736900	2.64120900	-0.58740700
H	-2.79539300	1.72924500	-0.23174700
H	-3.56743500	3.07005500	-0.13331600
O	-5.05840800	-0.37677400	-0.57935900
H	-4.13928200	-0.36566300	-0.25324700
H	-5.21068200	0.52229200	-0.90422600
H	-0.48700400	3.29555100	1.45098900

pC 4H2O B3LYP N7 Anion_1

Enthalpy (Hartrees) = -854.899948

Free Energy (Hartrees) = -854.977162

Charge = -1 Multiplicity = 1

C	1.35661900	-1.65966100	-0.00829100
C	1.16042000	-0.22267900	0.02203600
C	-1.14630600	-0.44068100	0.04007700
C	2.78152700	-1.84441800	-0.03069700
C	3.31333700	-0.56934600	-0.01543700
H	3.32790200	-2.77824900	-0.05614100
C	4.75832300	-0.18440700	-0.03065400
H	5.39917200	-1.07015600	-0.05563600
H	4.99366900	0.43513100	-0.90518300
H	5.02018800	0.40444400	0.85743400
N	2.33180700	0.42938000	0.01762900
N	-0.06369400	0.35301700	0.05143800
O	-2.33408500	0.02996100	0.05597100
N	-1.00030600	-1.83623700	0.01100600
C	0.23148500	-2.43538100	-0.01060700
C	-2.21510200	-2.66290800	0.00203400
H	-1.91853600	-3.71103800	-0.01578700
H	-2.80983900	-2.47070900	0.89699600
H	-2.81617400	-2.44206100	-0.88202700
H	0.23199800	-3.51935100	-0.03083000
H	2.42393000	2.21206900	-0.13625500
O	2.38830700	3.20701400	-0.22301600
H	1.45123100	3.41438500	-0.04992600
O	-0.41693300	3.10612000	0.52710800
H	-0.27405200	2.13340800	0.37431900
H	-1.33129500	3.23960300	0.20902400
O	-3.08218100	2.62760900	-0.43763400
H	-2.79854600	1.69816400	-0.24961000
H	-3.79476400	2.80786100	0.19195100
O	-5.04854200	-0.56378600	0.01812200
H	-4.07285000	-0.44799000	0.02659600
H	-5.40104800	0.33291700	-0.07061700

Figure S7. continued.

pC 4H2O B3LYP N7 Anion_2

Enthalpy (Hartrees) = -854.899857

Free Energy (Hartrees) = -854.975102

Charge = -1 Multiplicity = 1

C	1.33664400	-1.66667900	0.02386400
C	1.15375500	-0.22885700	-0.03329900
C	-1.15488100	-0.42644800	-0.06730500
C	2.75956500	-1.86372500	0.06233800
C	3.30299400	-0.59385400	0.02982000
H	3.29710700	-2.80186300	0.10877000
C	4.75117400	-0.22139400	0.05114800
H	5.38389000	-1.11216000	0.09648800
H	5.02569900	0.35007500	-0.84442700
H	4.98457100	0.41074000	0.91714400
N	2.33084400	0.41282000	-0.02956500
N	-0.06487700	0.35696200	-0.08406000
O	-2.33821400	0.05514900	-0.09997900
N	-1.02153300	-1.82255500	-0.01360300
C	0.20455700	-2.43217700	0.02910200
C	-2.24304100	-2.63910400	-0.00083300
H	-1.95487500	-3.68920600	0.03200200
H	-2.84717300	-2.40252500	0.87706800
H	-2.83104800	-2.45377400	-0.90156900
H	0.19492600	-3.51554900	0.06752500
H	2.43357800	2.19723300	0.11431600
O	2.40040700	3.19255400	0.19549300
H	1.46583500	3.40156400	0.00958900
O	-0.39593100	3.10611200	-0.57787200
H	-0.25810200	2.13258500	-0.42373600
H	-1.29855400	3.24823200	-0.23105400
O	-3.06511100	2.65898600	0.39456200
H	-2.77447800	1.72290800	0.25636500
H	-3.10784300	2.77515300	1.35436100
O	-5.05054800	-0.55881200	-0.04010700
H	-4.07666600	-0.42890500	-0.05847500
H	-5.41734500	0.33641200	-0.02956100

tC° 5H2O B3LYP Neutral

Enthalpy (Hartrees) = -1121.300722

Free Energy (Hartrees) = -1121.393278

Charge = 0 Multiplicity = 1

N	1.72318800	-1.78663300	-0.29124500
C	0.39129200	-2.11650700	-0.33149700
H	0.14348600	-3.16563500	-0.43047400
C	-0.12289100	0.20458000	-0.13130600
N	1.17339700	0.51016900	-0.07632200
C	2.11979200	-0.46358800	-0.15825700
O	3.34892800	-0.18849900	-0.11800400
C	-0.55624600	-1.14876700	-0.25362000
C	-2.42272500	0.88147000	-0.11778900
H	-0.75523900	2.16955800	-0.01697400
N	-1.05008200	1.18408100	-0.06991400
C	-2.83121800	-0.45464800	-0.22908700
C	-4.17591600	-0.79534400	-0.27808700
C	-3.39340300	1.88395800	-0.05631700
C	-5.14315500	0.21495300	-0.21451100
C	-4.75059600	1.55085800	-0.10464100
H	-3.07798500	2.91919600	0.02964200
H	-6.19509500	-0.04869400	-0.25289700
H	-5.49502200	2.33906700	-0.05574300
O	-1.89951400	-1.48979900	-0.29788100
H	-4.45376700	-1.84077400	-0.36584900
O	-2.63863200	-3.94265500	1.23594700
H	-3.58139500	-3.84641900	1.43342800
H	-2.41261600	-3.14367600	0.72891900
O	-0.23816600	4.01336100	0.01654100
H	0.64714800	3.82345500	0.40720800
H	-0.73817500	4.46339900	0.71287800
O	2.09326400	2.98136800	1.06032700
H	1.77038200	2.11568600	0.71287100
H	2.97835900	3.05544600	0.64882700
O	5.87849000	-1.36141900	0.27675000
H	4.96499000	-1.03639600	0.13612900
H	5.79279500	-2.32466100	0.30865900
C	2.74852900	-2.83528600	-0.39581800
H	3.39794600	-2.63530800	-1.24981500
H	3.34723300	-2.86748600	0.51640200
H	2.24692300	-3.79159300	-0.53629700
O	4.53601900	2.34308100	-0.24891800
H	4.10054200	1.46010700	-0.26372600
H	4.57007100	2.62783700	-1.17334600

Figure S7. continued.

tC° 5H2O B3LYP N3 Cation

Enthalpy (Hartrees) = -1121.735999

Free Energy (Hartrees) = -1121.827727

Charge = 1 Multiplicity = 1

N	1.70504300	-1.79019700	-0.25420300
C	0.36590100	-2.09618100	-0.31248700
H	0.10828200	-3.13887700	-0.44585600
C	-0.17857300	0.22235400	-0.05161300
N	1.15290100	0.46852900	0.03071900
C	2.13973300	-0.50053800	-0.07704600
O	3.34050900	-0.19987700	-0.01306800
C	-0.58342400	-1.13062100	-0.21538500
C	-2.45466900	0.89606700	-0.05678400
H	-0.78743100	2.20242000	0.06237000
N	-1.07461100	1.19891800	0.01918600
C	-2.85631600	-0.43560000	-0.20637200
C	-4.19858100	-0.77639700	-0.28317700
C	-3.41828100	1.90162200	0.01415500
C	-5.16287600	0.23568800	-0.21070400
C	-4.77390700	1.56911200	-0.06341800
H	-3.10266100	2.93352600	0.12940100
H	-6.21430600	-0.02541300	-0.27163200
H	-5.51988700	2.35498400	-0.00821800
O	-1.91973600	-1.46499200	-0.28641500
H	-4.47613000	-1.81883100	-0.39993300
O	-2.61052300	-4.08646200	1.01586100
H	-3.57440000	-4.17152900	0.98907600
H	-2.42756400	-3.23378000	0.58651400
O	-0.32042300	3.88911500	-0.01584700
H	0.60854100	3.76067200	0.28049600
H	-0.75487600	4.39242600	0.68862900
O	2.14946500	3.01567000	0.78180800
H	1.49073000	1.42988800	0.25963100
H	3.04125400	2.95428700	0.35819900
O	5.93201500	-1.42371000	0.29843300
H	5.02176800	-1.09250100	0.18161700
H	5.84023800	-2.38694000	0.31789400
C	2.72090800	-2.85130300	-0.38243100
H	3.37122900	-2.63466400	-1.23104000
H	3.31251800	-2.90822500	0.53248800
H	2.20355600	-3.79451900	-0.54689800
O	4.51678400	2.36376100	-0.40392400
H	4.18658300	1.44228400	-0.39472300
H	4.57890300	2.60852500	-1.33888600
H	2.30610400	3.03226200	1.73774200

tC° 5H2O B3LYP N7 Anion

Enthalpy (Hartrees) = -1120.841822

Free Energy (Hartrees) = -1120.933226

Charge = -1 Multiplicity = 1

N	1.69019500	-1.79187000	-0.61979600
C	0.33894400	-2.08234100	-0.63010800
H	0.05636400	-3.10856700	-0.82764200
C	-0.12212700	0.24642000	-0.15058400
N	1.22101700	0.48167800	-0.12402400
C	2.11520500	-0.49839900	-0.35874700
O	3.37060100	-0.27833700	-0.35169300
C	-0.56499200	-1.10543800	-0.39891800
C	-2.33123200	0.94169900	-0.00152200
H	-0.45692700	3.01200100	0.05611300
N	-0.96645600	1.24965100	0.04551100
C	-2.81279000	-0.36421000	-0.21934100
C	-4.16729400	-0.66336900	-0.26325900
C	-3.29092600	1.95344000	0.16892700
C	-5.10411100	0.36439000	-0.08602000
C	-4.66048800	1.67180200	0.12915000
H	-2.94241800	2.96840300	0.33677100
H	-6.16499000	0.13686200	-0.11827500
H	-5.37695700	2.47629500	0.26652800
O	-1.91900000	-1.42158600	-0.39305800
H	-4.47966800	-1.68935800	-0.43381000
O	-2.55054100	-3.75615800	1.28708100
H	-3.44901300	-3.59461400	1.60890700
H	-2.35186200	-2.98909400	0.72039300
O	-0.11223500	3.94459300	0.06251300
H	0.82489800	3.82112100	0.31323600
O	2.38640400	2.86515700	0.88950800
H	1.94788200	2.03307100	0.56886700
H	3.23622800	2.85950900	0.40570900
O	4.92255500	-1.26325700	1.73716600
H	4.35721300	-0.95431600	0.99381900
H	4.93549700	-2.22692300	1.65017700
C	2.67625900	-2.84112600	-0.90098800
H	3.26560200	-2.58348300	-1.78430000
H	3.34931800	-2.97295100	-0.05080000
H	2.14335100	-3.77364900	-1.08434400
O	4.68299100	2.11022600	-0.64436100
H	4.18152400	1.25886700	-0.60016700
H	4.60577400	2.40831900	-1.56181200

Figure S7. continued.

thC 5H2O B3LYP Neutral

Enthalpy (Hartrees) =			-1290.687022
Free Energy (Hartrees) =			-1290.774434
Charge = 0 Multiplicity = 1			
C	1.57760400	-0.16283100	-0.00991600
C	0.54857400	0.86037800	-0.04096800
N	0.85603900	2.14957800	0.09457500
H	0.11618600	2.85375600	0.11514800
H	1.81836400	2.46965000	0.21249400
N	-0.73201800	0.51355800	-0.20247600
C	-1.11910200	-0.79024300	-0.34432000
N	-0.18811000	-1.80996000	-0.37841000
C	1.15930800	-1.52338100	-0.18922600
S	3.69928600	-1.58675800	0.12274000
C	2.93893600	-0.04824100	0.17216800
C	2.20014100	-2.41966000	-0.14205600
O	-2.70837000	2.42158200	-0.93569800
H	-3.52210500	2.00784900	-0.58407400
H	-2.01021100	1.75432500	-0.71225200
O	-1.21309100	4.38832100	0.24566200
H	-1.88937300	3.75989600	-0.10379100
H	-1.43650900	4.51631800	1.17852000
H	3.52474500	0.84660100	0.33463000
O	-2.34529700	-1.07097000	-0.45757000
C	-0.58753200	-3.20771700	-0.56700300
H	-0.43247600	-3.77522000	0.35559300
H	-1.63656000	-3.24348300	-0.84570300
H	0.01301800	-3.64988000	-1.36616400
H	2.18303100	-3.49527800	-0.23838900
O	-4.58472800	0.50923800	0.03287400
H	-3.77664300	-0.04226400	-0.08249100
H	-4.74443900	0.53200300	0.98724400
O	3.50908800	3.44685200	0.45770700
H	3.35315500	4.38807500	0.28918800
H	4.13880300	3.17583700	-0.22695600
O	-3.56818600	-2.75627500	1.45200100
H	-4.34099600	-2.23833500	1.71891400
H	-3.12085000	-2.20377700	0.77653200

thC 5H2O B3LYP N3 Cation

Enthalpy (Hartrees) =			-1291.129096
Free Energy (Hartrees) =			-1291.214451
Charge = 1 Multiplicity = 1			
C	1.59665400	-0.15674000	-0.01655000
C	0.60316500	0.88574500	-0.07851900
N	0.87008900	2.16296800	0.05888800
H	0.12671500	2.87944400	0.08909100
H	1.83533600	2.49289700	0.18959400
N	-0.67644200	0.47492900	-0.28868400
C	-1.11056500	-0.84559600	-0.42704000
N	-0.16793800	-1.82757700	-0.39834800
C	1.17729600	-1.51971700	-0.18614400
S	3.70685500	-1.58011300	0.18509600
C	2.95490800	-0.04329300	0.19784200
C	2.21384000	-2.41350500	-0.10297300
O	-2.78405600	2.40748900	-0.74316600
H	-3.53410200	1.86690600	-0.39559700
H	-1.42319700	1.18366700	-0.41523300
O	-1.06862500	4.27638300	0.26858700
H	-1.82300600	3.70784800	-0.00574200
H	-1.22281500	4.48328800	1.20175600
H	3.53653900	0.85363500	0.36354200
O	-2.32440800	-1.07061200	-0.57714300
C	-0.55426900	-3.23493300	-0.57007800
H	-0.35731000	-3.78736900	0.35203900
H	-1.61189000	-3.28499500	-0.81172100
H	0.02680700	-3.66720400	-1.38793700
H	2.19663700	-3.49021600	-0.18715000
O	-4.55162500	0.53313300	0.17783500
H	-3.82332100	-0.09921100	0.00989700
H	-4.67338700	0.53749700	1.13869200
O	3.45435900	3.42861200	0.41251900
H	3.30080000	4.37359000	0.26243600
H	4.08977500	3.17003900	-0.27203100
O	-3.59617300	-2.78517000	1.42010200
H	-4.34592900	-2.23656200	1.69218100
H	-3.14844700	-2.26227700	0.72898200
H	-2.96079500	2.53816100	-1.68641600

Figure S7. continued.

tzC 6H2O B3LYP Neutral

Enthalpy (Hartrees) =			-1383.164601
Free Energy (Hartrees) =			-1383.254618
Charge = 0 Multiplicity = 1			
N	2.41995400	-0.99283400	-0.00478200
C	1.11330400	-0.76856200	0.07589400
C	0.46592700	0.53950400	0.07663900
N	-0.86249200	0.60343600	0.13593800
C	-1.65532300	-0.50990300	0.22894100
N	-1.09802400	-1.77578600	0.26892300
C	0.27425700	-1.91514000	0.16600500
N	1.18327300	1.65609100	0.01508600
H	2.19507100	1.63765600	-0.04651600
H	0.72741900	2.57343800	0.05647700
O	-2.90607400	-0.38454000	0.28477500
S	2.67953900	-2.64083300	0.02207000
C	-1.92581500	-2.98116000	0.39314200
H	-1.92447600	-3.54024700	-0.54688600
H	-1.52557900	-3.61126600	1.19114900
H	-2.94102000	-2.68632600	0.64253500
C	1.02537200	-3.07180100	0.14420300
H	0.70376100	-4.10352000	0.18839700
O	-0.06184500	4.35974200	0.25955800
H	-0.93913200	4.01877600	-0.03760200
H	0.24068400	4.94686000	-0.44794400
O	4.02091800	3.09905500	-0.33723100
H	4.02294100	3.31754400	-1.27970100
H	4.41182000	2.19725800	-0.27717700
O	4.93288000	0.50753500	-0.00527700
H	4.07668400	0.02942900	-0.03420900
H	5.42766100	0.19246600	-0.77613600
O	-2.28303600	2.99168200	-0.58180800
H	-3.09452600	2.90155700	-0.04256600
H	-1.79432400	2.15707000	-0.37820500
O	-4.38478100	1.88336000	0.99754700
H	-4.26162000	2.07081000	1.93914700
H	-3.83617600	1.08706900	0.81630700
O	-4.62113500	-1.59054000	-1.60646900
H	-5.20172400	-0.86727500	-1.88202000
H	-4.02079900	-1.19231000	-0.94201800

tzC 6H2O B3LYP N3 Cation

Enthalpy (Hartrees) =			-1383.600112
Free Energy (Hartrees) =			-1383.689395
Charge = 1 Multiplicity = 1			
N	-2.48876800	-0.80304900	-0.02243700
C	-1.17049500	-0.64694400	-0.05676100
C	-0.48432700	0.63284100	0.02346700
N	0.87133900	0.55911500	0.01368100
C	1.64918600	-0.59518000	-0.12498700
N	0.99605500	-1.78790600	-0.23456300
C	-0.39039700	-1.83231600	-0.17889200
N	-1.09348500	1.78514500	0.10380100
H	-2.11786600	1.87445200	0.11594900
H	-0.56636900	2.67812900	0.10548500
O	2.88448300	-0.49051400	-0.14528800
S	-2.82982700	-2.42644500	-0.13868400
C	1.74799800	-3.04153400	-0.39908800
H	1.63736500	-3.65804500	0.49608500
H	1.36030100	-3.57710200	-1.26799800
H	2.79580400	-2.80340700	-0.55744300
C	-1.20292300	-2.94373800	-0.23790000
H	-0.93538300	-3.98792300	-0.32892000
O	0.24873100	4.29279200	-0.06229700
H	1.15164000	3.94227200	0.10876200
H	0.04961000	4.88168600	0.67994300
O	-3.74256800	2.91924400	0.11254300
H	-3.81609800	3.42054800	0.93748300
H	-4.37612000	2.17144300	0.20224100
O	-5.13686200	0.54319800	0.19627200
H	-4.25788200	0.11509200	0.19309300
H	-5.51358900	0.34995300	1.06752600
O	2.53471800	2.85516600	0.37666700
H	3.25235100	2.58611800	-0.24678900
H	1.43220900	1.42753700	0.14162200
O	4.33752300	1.66061300	-1.31149000
H	4.13581700	1.80809800	-2.24724200
H	3.87404400	0.83324600	-1.07029700
O	4.62851500	-1.91946300	1.64977400
H	5.27759700	-1.24668800	1.89964100
H	4.02962400	-1.46840600	1.02464900
H	2.93762200	2.87591800	1.25730900

Figure S7. continued.

tzC 6H2O B3LYP N7 Cation

Enthalpy (Hartrees) = -1383.577285

Free Energy (Hartrees) = -1383.668912

Charge = 1 Multiplicity = 1

N	-2.49013000	-0.66293800	0.01327500
C	-1.16397000	-0.52001500	-0.08044600
C	-0.35845100	0.70267500	-0.06643100
N	0.96394000	0.56922200	-0.12080000
C	1.60367500	-0.63396900	-0.24262400
N	0.87341100	-1.81340300	-0.31936600
C	-0.49511400	-1.75920800	-0.20684800
N	-0.90359600	1.90745800	0.00068700
H	-1.91192900	2.08919000	0.03857600
H	-0.29428600	2.73520000	-0.03015900
O	2.85394800	-0.68246800	-0.29348900
S	-2.98449400	-2.26706700	-0.04173500
C	1.52743700	-3.11974300	-0.47815800
H	1.45269500	-3.69409600	0.44907000
H	1.04470700	-3.66693400	-1.29088400
H	2.57202700	-2.95496700	-0.72532700
C	-1.38868000	-2.82058400	-0.20032800
H	-1.18555500	-3.88125800	-0.27495200
O	0.70465400	4.38476200	-0.18390600
H	1.53595200	3.94223000	0.10908900
H	0.47306200	4.99841000	0.52798800
O	-3.54678500	3.10253700	0.04709400
H	-3.59861800	3.65684500	0.83905000
H	-4.13697200	2.33983000	0.22098000
O	-4.83804100	0.66443000	0.33786800
H	-3.24770500	0.05473200	0.13309100
H	-5.27041200	0.45227500	1.17984000
O	2.74522200	2.73341700	0.64071300
H	3.52549300	2.52235000	0.08792100
H	2.13420000	1.98682700	0.44238000
O	4.66244400	1.37079800	-0.95690600
H	4.58385000	1.58112600	-1.89850500
H	4.01668400	0.64810200	-0.79698800
O	4.33012100	-2.18167200	1.62188900
H	4.97384500	-1.55401000	1.97948400
H	3.82399700	-1.67253600	0.95687600
H	-5.48640100	0.45801700	-0.35344100

DMAT 5H2O B3LYP Neutral

Enthalpy (Hartrees) = -1123.700813

Free Energy (Hartrees) = -1123.797112

Charge = 0 Multiplicity = 1

N	-0.91490800	-1.87990800	-0.25981400
C	0.43403500	-1.49600000	-0.15271000
C	0.77928400	-0.14233900	0.02680900
C	-0.28524800	0.85087000	0.10494100
N	-1.56437200	0.35264100	0.02285300
C	-1.92507100	-0.97213800	-0.15265900
O	-3.13540700	-1.27970500	-0.20824800
C	-1.25311900	-3.29256100	-0.49086300
H	-0.94691100	-3.89873500	0.36493300
H	-2.32707000	-3.37395400	-0.62741600
H	-0.74889600	-3.64750500	-1.39183600
H	-2.34727400	1.01698600	0.12023600
O	1.97816700	4.04016800	0.49513300
H	1.32595100	3.31805800	0.40523900
H	2.83926200	3.59882400	0.45657000
O	-3.77121400	2.33371000	0.29153500
H	-3.19979900	3.11787700	0.11012700
H	-4.12257200	2.45466000	1.18542400
O	-0.10175300	2.07768600	0.24594900
O	-1.85569000	4.18653400	-0.34393600
H	-1.19229300	3.49610300	-0.12560100
H	-1.71065000	4.89643400	0.29833200
O	-4.23518200	-3.06377300	1.71890700
H	-4.99112000	-2.57992400	2.08065200
H	-3.84948800	-2.46321800	1.04950700
O	-5.00025000	0.50481100	-1.45946500
H	-4.41240900	-0.20532600	-1.13679100
H	-4.70502700	1.27244400	-0.92987400
C	1.47575800	-2.43457700	-0.22960500
C	2.79991100	-2.03429600	-0.12612500
H	3.55978800	-2.80253500	-0.19267800
C	2.12072700	0.25585400	0.12617400
C	3.16822300	-0.67628800	0.07025900
H	1.26520300	-3.48650900	-0.37257600
H	2.31866100	1.30897600	0.25514200
N	4.50236600	-0.29692100	0.23152400
C	4.80763300	1.13013200	0.10740700
H	5.87704600	1.27299300	0.26617900
H	4.54367000	1.53283500	-0.88284500
H	4.28125300	1.70972300	0.87038600
C	5.52993200	-1.17959200	-0.33027500
H	6.51023300	-0.75351200	-0.11337900
H	5.49684200	-2.16914400	0.12974100
H	5.43222700	-1.29607500	-1.42051800

Figure S7. continued.

DMAT 5H2O B3LYP N3 Anion

Enthalpy (Hartrees) = -1123.24664

Free Energy (Hartrees) = -1123.339634

Charge = -1 Multiplicity = 1

N	-0.94763600	-1.85046400	-0.31691300
C	0.39828100	-1.49593100	-0.17641900
C	0.74330600	-0.14348700	-0.00214400
C	-0.34426700	0.84295300	0.03133100
N	-1.62207600	0.41801800	-0.04989900
C	-1.93776300	-0.89292200	-0.21662100
O	-3.15492700	-1.25079800	-0.28900000
C	-1.30020700	-3.25340600	-0.56283900
H	-1.06053000	-3.87112100	0.30747800
H	-2.36525300	-3.31385800	-0.76364800
H	-0.75181500	-3.62681900	-1.43104700
H	-2.95038200	1.63388500	0.33649300
O	1.92195100	4.00037600	0.45478700
H	1.27975600	3.26530400	0.34566800
H	2.79122400	3.57431800	0.44854900
O	-3.64212000	2.33091800	0.49475300
H	-3.20046300	3.14506000	0.18036800
O	-0.09513200	2.08685500	0.14751500
O	-1.73666600	4.21159900	-0.48467900
H	-1.14795300	3.45178500	-0.25230600
H	-1.48344900	4.92409200	0.11945400
O	-4.22557800	-2.94404600	1.63591800
H	-4.87465800	-2.39503100	2.09772700
H	-3.83051300	-2.35138600	0.95691500
O	-5.16918100	0.52441300	-1.05883500
H	-4.47947300	-0.14000000	-0.83398700
H	-4.82827100	1.32768800	-0.61512800
C	1.43393100	-2.44757700	-0.21235800
C	2.75872500	-2.05759100	-0.07720600
H	3.51460200	-2.83236200	-0.10926500
C	2.08777600	0.23969300	0.12716800
C	3.12901800	-0.69987000	0.10898400
H	1.21681600	-3.50009500	-0.34411100
H	2.29367700	1.29183900	0.24890000
N	4.46955400	-0.32735700	0.30414900
C	4.77922500	1.09705300	0.16189500
H	5.84452200	1.24276500	0.34617200
H	4.54227000	1.48317900	-0.84241600
H	4.23366000	1.69127300	0.89934400
C	5.49266700	-1.20169300	-0.27990200
H	6.47603600	-0.78947700	-0.04863100
H	5.45245700	-2.20372100	0.15104700
H	5.39791400	-1.28656400	-1.37393600

5-thU 5H2O B3LYP Neutral

Enthalpy (Hartrees) = -1387.958893

Free Energy (Hartrees) = -1388.051394

Charge = 0 Multiplicity = 1

C	-1.83104400	-3.18230600	0.79348100
H	-2.39517900	-3.03250600	1.71564100
N	-1.11921900	-1.94249600	0.43754200
C	0.24552700	-1.91374700	0.34606400
H	0.73591600	-2.86148300	0.53010800
C	0.96246100	-0.78553600	0.04845500
C	0.21551600	0.42922800	-0.21277200
O	0.72694600	1.53762600	-0.48525000
N	-1.16226300	0.30995000	-0.15124300
H	-1.73108900	1.14883200	-0.38377500
C	-1.86869500	-0.81576200	0.18554200
O	-3.11219800	-0.82079400	0.25814900
H	-1.09141200	-3.96761700	0.93825200
H	-2.51299500	-3.46257400	-0.01031400
C	2.42809100	-0.82322800	0.02018300
C	3.25054500	-1.61375000	0.79593400
S	3.38132800	0.08581400	-1.14076500
C	4.63178600	-1.50169700	0.45971500
H	2.87314800	-2.24782000	1.59084900
C	4.85662500	-0.62469200	-0.56942600
H	5.42297100	-2.03775100	0.97186700
H	5.80071600	-0.32915100	-1.00928900
O	-0.54531400	4.04115400	-0.01965000
H	-0.26809800	4.67630600	-0.69577400
H	-0.06524700	3.21104000	-0.22755000
O	-2.79627600	2.57817000	-0.81070700
H	-2.16631800	3.24993000	-0.47254300
H	-3.45989200	2.41932800	-0.10618600
O	-4.53782000	1.48689400	1.10549300
H	-5.45198200	1.41603100	0.79458200
H	-4.10769300	0.64827700	0.83596600
O	2.50213300	2.80138200	1.42191100
H	1.95972200	2.32239300	0.76598200
H	1.98799500	3.59584000	1.62552100
O	-4.86739300	-2.30874000	-1.46740400
H	-5.70569600	-2.37511000	-0.98859700
H	-4.26123500	-1.85575900	-0.84998400

Figure S7. continued.

5-thU 5H2O B3LYP N3 Anion_1

Enthalpy (Hartrees) = -1387.507784

Free Energy (Hartrees) = -1387.598807

Charge = -1 Multiplicity = 1

C	1.73333000	-3.37495500	-0.61052000
H	2.28115100	-3.36192100	-1.55464100
N	1.06041900	-2.08576100	-0.39992200
C	-0.29312700	-2.02009900	-0.25387700
H	-0.80932200	-2.97138800	-0.29197100
C	-0.95399200	-0.83417500	-0.06810500
C	-0.12627700	0.36243200	0.01589700
O	-0.65750900	1.50392500	0.21682100
N	1.22230000	0.25784300	-0.11624400
H	2.29864400	1.66879700	0.40214200
C	1.82738100	-0.92516400	-0.33223200
O	3.08305200	-1.03333000	-0.47580900
H	0.97608500	-4.15754600	-0.64090500
H	2.43104800	-3.57421600	0.20506100
C	-2.41560700	-0.80648800	0.04155900
C	-3.30509900	-1.77616800	-0.38225600
S	-3.28660300	0.49043200	0.84834700
C	-4.66246300	-1.49805800	-0.04844300
H	-2.99659900	-2.66184900	-0.92647200
C	-4.80890500	-0.31299700	0.62521200
H	-5.49196700	-2.14480600	-0.31302500
H	-5.72129700	0.15462400	0.97338300
O	0.44962200	3.99472000	0.61729900
H	0.19493300	4.25627400	1.51374800
H	0.06753700	3.09120600	0.49074400
O	2.84176000	2.45410700	0.67420800
H	2.18257800	3.17737800	0.68817300
O	4.64375800	1.19971700	-1.14228000
H	4.18379700	1.88163200	-0.61536700
H	4.11337800	0.39384700	-0.95111000
O	-1.87039800	2.75790600	-1.98325800
H	-1.48133800	2.28898400	-1.21303400
H	-1.33595800	3.55923600	-2.07549300
O	4.59874100	-1.76510100	1.75918000
H	4.97065400	-0.94359600	2.10981900
H	4.05963300	-1.48966000	0.98586500

5-thU 5H2O B3LYP N3 Anion_2

Enthalpy (Hartrees) = -1387.507685

Free Energy (Hartrees) = -1387.59645

Charge = -1 Multiplicity = 1

C	1.73439100	-3.25989300	-0.65546300
H	2.28358500	-3.22748200	-1.59826700
N	1.03141700	-1.98761000	-0.43799500
C	-0.32281300	-1.95900000	-0.28381100
H	-0.81100300	-2.92491400	-0.32116300
C	-1.01470800	-0.79273200	-0.08680400
C	-0.21766700	0.42392100	-0.00154900
O	-0.77022500	1.54582900	0.24074900
N	1.12946900	0.36104100	-0.17625400
H	2.10012700	1.93532900	-0.34045500
C	1.76620500	-0.80481200	-0.38868100
O	3.02366900	-0.88147100	-0.54464000
H	0.99517400	-4.05919500	-0.69332400
H	2.43490600	-3.45002900	0.16009500
C	-2.47562000	-0.79978700	0.03165000
C	-3.34133900	-1.81032900	-0.34464600
S	-3.37943300	0.51677200	0.76886000
C	-4.70576700	-1.54701200	-0.02974500
H	-3.01174300	-2.71529100	-0.84279400
C	-4.88176700	-0.33250700	0.58187600
H	-5.51867100	-2.22635600	-0.26234100
H	-5.80605900	0.12989500	0.90485800
O	0.64971500	3.62963000	1.43460200
H	1.49664000	3.54189100	0.95529000
H	0.11561200	2.89854500	1.04673700
O	2.65662000	2.75559200	-0.39396400
H	3.56571200	2.40695000	-0.29837900
O	4.95615100	1.08141800	-0.27770200
H	5.34177900	0.96581200	0.60264800
H	4.25359500	0.39104800	-0.34425700
O	-1.76450300	3.06326400	-1.86888500
H	-1.40525500	2.52063900	-1.13204200
H	-1.05342700	3.67995700	-2.09279100
O	4.55126400	-2.04233100	1.52463900
H	4.30841400	-2.97606100	1.59923200
H	3.98830700	-1.69564800	0.79956400

Figure S7. continued.

thU 5H2O B3LYP Neutral

Enthalpy (Hartrees) = -1310.577179

Free Energy (Hartrees) = -1310.664497

Charge = 0 Multiplicity = 1

C	-1.59876400	-0.10542900	0.01249300
C	-0.60416400	0.94243500	0.14679000
N	0.69919100	0.49816400	0.05580600
C	1.12877500	-0.80602600	-0.16327800
N	0.17753300	-1.77051300	-0.32232400
C	-1.18075600	-1.45905600	-0.21597400
S	-3.73811200	-1.49326400	-0.12419400
C	-2.96769200	0.02430200	0.08449900
C	-2.23158000	-2.33584300	-0.31306300
O	2.91061600	2.45071200	0.37723400
H	3.25088600	2.55836500	1.27711900
H	3.57937900	1.91063900	-0.10683300
O	0.94094500	4.22838100	-0.54568200
H	0.23934100	3.60182100	-0.28515000
H	1.75375100	3.74742200	-0.29047500
H	-3.54315300	0.92502300	0.25080600
O	-0.85016900	2.14694100	0.33515600
H	1.45100100	1.19308900	0.18737500
O	3.45821300	-2.90903200	1.67308300
H	3.04928500	-2.31987100	1.00908300
H	2.94569700	-3.72844300	1.62158400
H	-2.22035500	-3.40302200	-0.48026700
C	0.56552300	-3.16254300	-0.58191300
H	1.63428000	-3.20400200	-0.77092600
H	0.31665700	-3.78646100	0.28069000
H	0.02755000	-3.52453300	-1.46096000
O	2.35070300	-1.05267900	-0.20803600
O	-3.21108800	3.67945200	0.63886700
H	-2.46669800	3.05853600	0.50217200
H	-3.97021200	3.25804600	0.21184800
O	4.40055800	0.65312700	-1.07501600
H	5.22906800	0.36157000	-0.66727100
H	3.72998600	-0.01177100	-0.80823400

thU 5H2O B3LYP N3 Anion_1

Enthalpy (Hartrees) = -1310.124464

Free Energy (Hartrees) = -1310.209711

Charge = -1 Multiplicity = 1

C	-1.57318700	-0.11958500	-0.02230100
C	-0.56261800	0.93557700	0.05665400
N	0.73750500	0.57706400	-0.01697600
C	1.13623400	-0.71530800	-0.19019800
N	0.21935700	-1.74541200	-0.31154500
C	-1.13998600	-1.47421100	-0.20350400
S	-3.69697500	-1.54963800	-0.08412900
C	-2.94244100	-0.01027700	0.05851300
C	-2.17743100	-2.37503000	-0.25675500
O	2.83481700	2.42270900	0.49637800
H	3.56713000	2.02252600	-0.01277100
O	0.87524900	4.24903000	-0.40826000
H	0.21500900	3.54599400	-0.21688300
H	1.71785800	3.80589300	-0.17972100
H	-3.53511600	0.88376100	0.19521200
O	-0.89283900	2.15270500	0.19601800
H	2.08943600	1.78078200	0.35312400
O	3.48744200	-2.68010400	1.67854100
H	3.06665800	-2.11819500	0.99092500
H	2.97661000	-3.50188700	1.66846500
H	-2.15029200	-3.44766400	-0.38190900
C	0.64141600	-3.13202700	-0.52257000
H	1.70487800	-3.15167600	-0.74208200
H	0.43862600	-3.73297200	0.36963200
H	0.09116000	-3.55321200	-1.36832300
O	2.37115500	-0.99505100	-0.24702000
O	-3.19781600	3.61813800	0.61421900
H	-2.45009900	3.00254300	0.43734600
H	-3.96816000	3.20630600	0.19870000
O	4.45214000	0.63716800	-1.05519800
H	5.24048800	0.29498500	-0.60994700
H	3.71627000	0.04386400	-0.77252500

Figure S7. continued.

thU 5H2O B3LYP N3 Anion_2

Enthalpy (Hartrees) = -1310.124344

Free Energy (Hartrees) = -1310.209141

Charge = -1 Multiplicity = 1

C	-1.53830100	-0.13090700	-0.03774800
C	-0.51762000	0.91438000	0.04717400
N	0.78128900	0.54315900	-0.00690900
C	1.16650200	-0.76004300	-0.15229700
N	0.23740500	-1.77840700	-0.28609900
C	-1.11992900	-1.49132300	-0.20390700
S	-3.67903100	-1.53431600	-0.12324500
C	-2.90709600	-0.00373700	0.02153400
C	-2.16740600	-2.37980900	-0.26715700
O	2.85405400	2.45052500	0.25188000
H	3.17184900	2.43534600	1.16655500
O	0.81602500	4.36149200	-0.16338700
H	0.17757900	3.62124400	-0.06340100
H	1.66992900	3.90184000	-0.02950700
H	-3.49033900	0.89855900	0.14310800
O	-0.84370500	2.13327900	0.17461700
H	2.12654600	1.76667800	0.20800900
O	3.44950000	-2.75595100	1.77411700
H	3.04901000	-2.19203400	1.07577300
H	2.94946700	-3.58354900	1.73657700
H	-2.15148500	-3.45357500	-0.38415900
C	0.64664000	-3.17163500	-0.47726800
H	1.71126900	-3.20502300	-0.68941700
H	0.43157000	-3.76075800	0.42002500
H	0.09768100	-3.59635400	-1.32199600
O	2.39641300	-1.05789900	-0.17062400
O	-3.13227300	3.62691500	0.60587600
H	-2.39480600	3.00166000	0.42203200
H	-3.91401400	3.22082100	0.20630000
O	4.35683500	0.60823700	-1.30009000
H	4.03667000	1.40883400	-0.83733800
H	3.71116500	-0.06224000	-0.99068500

tzU 6H2O B3LYP Neutral

Enthalpy (Hartrees) = -1403.049177

Free Energy (Hartrees) = -1403.141401

Charge = 0 Multiplicity = 1

C	-1.23573400	-0.58662200	0.23318200
C	-0.52994100	0.69528900	0.13057100
N	0.83916600	0.55917800	0.07617200
C	1.58269000	-0.61713700	0.13073600
N	0.89983000	-1.79328400	0.27113200
C	-0.49030500	-1.79795800	0.29908100
S	-2.94951700	-2.31155600	0.38458500
C	-1.33378100	-2.88394400	0.38824100
O	2.44662800	2.98466200	-0.15038400
H	3.29479500	2.60437100	0.18146700
H	2.61381600	3.26361200	-1.06241800
O	0.25682600	4.15017800	1.16838000
H	-0.31899700	3.42481100	0.86385700
H	1.12394000	3.89944900	0.79079600
O	-1.07924500	1.80232000	0.09388200
H	1.39622700	1.42612000	-0.03212600
N	-2.55708000	-0.69751400	0.26934700
O	-4.81966600	1.05239200	-0.44261400
H	-4.06195500	0.51771100	-0.12519000
H	-5.19381300	1.46059600	0.35191800
O	-3.13560600	2.92017500	-1.72345000
H	-2.33283300	2.67132200	-1.23498700
H	-3.81774700	2.33017000	-1.33571900
O	2.82313200	-0.56748400	0.05366900
H	-1.09758500	-3.93777300	0.45075500
C	1.61883300	-3.07145900	0.36887900
H	2.68191700	-2.87068300	0.46568900
H	1.26881000	-3.60987800	1.25236600
H	1.43309200	-3.67180900	-0.52538500
O	4.14011000	-2.01413100	-2.05175700
H	3.86848800	-2.94003800	-1.97569300
H	3.68416000	-1.56406700	-1.31443100
O	4.53491300	1.52454000	0.87088100
H	5.34143000	1.51810900	0.33495500
H	4.02781700	0.73399500	0.59124000

Figure S7. continued.

tzU 6H2O B3LYP N3 Anion

Enthalpy (Hartrees) = -1402.600397

Free Energy (Hartrees) = -1402.691273

Charge = -1 Multiplicity = 1

C	1.21523800	-0.53696800	-0.23919300
C	0.46037400	0.72779600	-0.14628800
N	-0.88103200	0.63698400	-0.06726800
C	-1.56038800	-0.54655000	-0.11112700
N	-0.89435500	-1.75338500	-0.26117100
C	0.48895400	-1.76133700	-0.29504200
S	2.95524300	-2.25013300	-0.39217800
C	1.34342200	-2.83981600	-0.38283300
O	-2.52315100	2.96396200	0.21773500
H	-3.34191500	2.65767200	-0.22030700
O	-0.26162400	4.19439300	-0.96297300
H	0.24097600	3.39456700	-0.69382100
H	-1.16759000	3.98070500	-0.66002000
O	1.05712200	1.84058800	-0.14270300
H	-1.93580400	2.16682800	0.16962800
N	2.53879400	-0.63451400	-0.28349300
O	4.81833600	1.05836300	0.37933700
H	4.03901700	0.54178000	0.07734700
H	5.13701400	1.52237000	-0.40855800
O	2.99237400	2.76841300	1.72632000
H	2.25363300	2.48734800	1.15042800
H	3.74897000	2.26511400	1.35994000
O	-2.82034800	-0.55829900	-0.01806800
H	1.11898600	-3.89646500	-0.43696700
C	-1.60952000	-3.03045000	-0.34834000
H	-2.67032500	-2.83389100	-0.47357200
H	-1.24249600	-3.59113900	-1.21198600
H	-1.44817200	-3.62011400	0.55922100
O	-4.03654000	-1.94777000	2.09368800
H	-3.75987400	-2.87208900	2.01870900
H	-3.59400600	-1.49628200	1.34287200
O	-4.56266400	1.36763900	-1.01082300
H	-5.37456800	1.30805300	-0.48717500
H	-3.96812600	0.66970200	-0.65052000

tzU 6H2O B3LYP N7 Cation

Enthalpy (Hartrees) = -1403.463868

Free Energy (Hartrees) = -1403.554513

Charge = -1 Multiplicity = 1

C	1.21124500	-0.55549300	-0.18623100
C	0.49885700	0.72710800	-0.09246000
N	-0.86352200	0.56511700	-0.06613800
C	-1.58656600	-0.62519900	-0.14790900
N	-0.87700100	-1.79375000	-0.28759800
C	0.50571700	-1.77172400	-0.27862500
S	2.99205200	-2.31237400	-0.30740200
C	1.37842200	-2.84622600	-0.35323400
O	-2.46974800	2.93021000	0.15501000
H	-3.32458300	2.56399400	-0.17760000
H	-2.62976600	3.20302300	1.07041300
O	-0.31561300	4.18523600	-1.14211100
H	0.29914300	3.49260900	-0.84307500
H	-1.16866300	3.88477300	-0.76810000
O	1.05829500	1.82193800	-0.04085300
H	-1.43996100	1.42616300	0.03826800
N	2.53400800	-0.70243600	-0.19279600
O	4.45874100	1.11493400	0.07575700
H	3.27572700	0.07173700	-0.10605600
H	4.69943300	1.54755900	-0.75948000
O	3.11456500	2.90917300	1.88271000
H	2.23269400	2.77086500	1.50284100
H	3.68487100	2.34983600	1.32073100
O	-2.82303000	-0.60177200	-0.09751200
H	1.15708900	-3.90359900	-0.43153300
C	-1.57343700	-3.08425200	-0.41784900
H	-2.63401100	-2.89380700	-0.55423500
H	-1.18390100	-3.61088200	-1.29144100
H	-1.41355600	-3.68437100	0.48111700
O	-4.16859800	-2.11420400	1.97453600
H	-3.90765700	-3.04184500	1.88343900
H	-3.70623700	-1.65692500	1.24733400
O	-4.57762200	1.50776300	-0.86704400
H	-5.38144100	1.50248400	-0.32689600
H	-4.08091200	0.70667200	-0.60496900
H	5.27315000	0.69566500	0.39730700

Figure S7. continued.

U 5H2O B3LYP Neutral

Enthalpy (Hartrees) = -836.191735

Free Energy (Hartrees) = -836.272044

Charge = 0 Multiplicity = 1

N	-1.19878600	-1.61479900	0.54608400
C	-0.44780100	-2.56068700	-0.10362200
H	-0.71903300	-3.58892800	0.10280500
C	0.56638900	-2.23768200	-0.94734500
C	0.87118800	-0.85691400	-1.17990500
N	0.07937400	0.04911200	-0.48877700
C	-0.95209300	-0.26979200	0.36435200
O	-1.61736500	0.60686200	0.94183800
C	-2.29082500	-2.00004400	1.45553400
H	-2.11510300	-1.57698400	2.44580000
H	-3.24487700	-1.63969400	1.06762700
H	-2.30877800	-3.08653000	1.51985500
H	0.26898200	1.05698900	-0.61531000
O	3.56056900	-2.23509500	-3.16962800
H	2.92490500	-1.61791700	-2.74657900
H	4.07211100	-1.68755100	-3.78167500
O	0.62654700	2.90755900	-0.99303100
H	1.13105500	2.74634700	-1.82653900
O	1.77711100	-0.44079100	-1.94054300
O	1.89587800	2.01744700	-3.25174000
H	1.91106400	1.13276300	-2.82273300
H	2.82366000	2.28306900	-3.33190700
O	-4.30434700	1.00281400	1.88033500
H	-4.38972800	1.94956800	1.69862400
H	-3.40691200	0.77317300	1.57153500
H	1.14237100	-3.00288900	-1.44932700
O	-2.13333900	3.08985300	-0.47930200
H	-2.11328400	2.25741600	0.02835300
H	-1.20094900	3.18723800	-0.75980200
H	1.24292500	3.33810000	-0.38329600

U 5H2O B3LYP N3 Anion

Enthalpy (Hartrees) = -835.739619

Free Energy (Hartrees) = -835.817429

Charge = -1 Multiplicity = 1

N	1.15937200	-1.82699900	0.03823600
C	0.03658800	-2.60723000	0.08188000
H	0.20509800	-3.67569600	0.15098900
C	-1.20595900	-2.06042700	0.04325600
C	-1.31929700	-0.62676400	-0.04527000
N	-0.18779700	0.12665200	-0.10300800
C	1.03661800	-0.44061700	-0.05659900
O	2.09620400	0.25190300	-0.09753000
C	2.49861600	-2.42652100	0.08364300
H	3.05499100	-2.18039200	-0.82296100
H	3.04807100	-2.06026600	0.95299300
H	2.38766200	-3.50786800	0.15603600
H	-0.33187900	1.93304400	-0.43420500
O	-4.80062000	-1.46878100	0.09532900
H	-3.94267500	-0.97737800	0.04176300
H	-5.46008700	-0.80091800	0.32917900
O	-0.45090500	2.91167700	-0.56287500
H	-1.36183800	3.06024400	-0.23798000
O	-2.46504300	-0.05568200	-0.07161400
O	-3.11743400	2.56858900	0.38693800
H	-2.87801400	1.62532900	0.20309600
H	-3.76597100	2.80524200	-0.29133100
O	4.89050900	0.20081500	-0.12275600
H	5.05970900	1.15340400	-0.11064100
H	3.91250100	0.12252700	-0.10961400
H	-2.09090900	-2.68245500	0.08130100
O	2.07080900	2.93612700	0.73356600
H	2.13343200	1.99011100	0.47476700
H	1.18530400	3.18266600	0.39804300

Figure S7. continued.

iC 5H2O B3LYP Neutral

Enthalpy (Hartrees) =			-816.294341
Free Energy (Hartrees) =			-816.377134
Charge = 0 Multiplicity = 1			
C	1.54979000	-0.48153800	0.04162100
N	0.33750200	0.14472000	0.06790200
C	-0.79407200	-0.56529900	0.03842900
C	0.40796700	-2.59775500	-0.01498300
H	0.34700300	-3.67851400	-0.04355800
C	-2.05809800	-2.69998300	-0.02902400
H	-2.63604900	-2.44436100	-0.92011100
H	-1.81553400	-3.76083600	-0.05584700
H	-2.64552300	-2.49128500	0.86782800
N	-0.79872400	-1.94039800	-0.00210600
H	2.66022700	1.96957600	-0.40950900
H	4.18822700	-0.57385100	0.04744200
H	0.23982700	1.96768000	0.55919800
H	-1.96130100	1.09802000	0.02289700
H	-2.87606100	-0.37540800	-0.00528500
O	2.63154600	2.93160700	-0.61492000
O	5.10764800	-0.93733700	0.05435100
H	1.77724100	3.20239000	-0.22453300
H	5.01004300	-1.86590300	-0.19933300
O	0.14222400	2.92637900	0.77696500
O	-2.51322400	3.13853700	-0.18087000
O	-4.86330200	-0.63339000	-0.07759800
H	-0.75507100	3.14418500	0.45097600
H	-3.12176600	3.61790200	0.40098900
H	-5.18325700	-0.54060500	-0.98721100
C	1.58315900	-1.92333100	0.00280700
O	2.61700600	0.21166100	0.05203800
N	-1.96797000	0.08252100	0.05343200
H	-2.58675600	3.57913500	-1.04064900
H	-5.27287400	0.10269300	0.40063900
H	2.52832600	-2.45094600	-0.01137600

iC 5H2O B3LYP N3 Cation

Enthalpy (Hartrees) =			-816.735969
Free Energy (Hartrees) =			-816.817674
Charge = 1 Multiplicity = 1			
C	1.58262900	-0.50272400	0.18371700
N	0.32413800	0.09500100	0.20324500
C	-0.85273900	-0.57085100	0.07372300
C	0.39348400	-2.58142200	-0.05272500
H	0.32892400	-3.65754400	-0.15122200
C	-2.07393900	-2.68780500	-0.20257100
H	-2.60940200	-2.35456400	-1.09371300
H	-1.81570200	-3.73865200	-0.31221500
H	-2.69617200	-2.55831700	0.68454200
N	-0.81893100	-1.92562900	-0.05512900
H	2.69608800	1.91968500	-0.63428900
H	4.26419000	-0.56408500	0.14430900
H	0.28802600	1.12716500	0.33959500
H	-1.99937100	1.11561600	0.11198400
H	-2.91194200	-0.35697700	-0.00763200
O	2.52988500	2.81334900	-0.98975500
O	5.18263800	-0.90399100	0.08864100
H	1.68907900	3.05515400	-0.55456700
H	5.08924600	-1.82624300	-0.18931300
O	0.16669900	2.91927600	0.56472600
O	-2.51086000	3.02398300	-0.02426900
O	-4.78992600	-0.63962500	-0.07895300
H	-0.78718800	3.10170900	0.39853200
H	-3.10005500	3.46787600	0.60414900
H	-5.11617500	-0.56576900	-0.98831100
C	1.57673800	-1.93180300	0.05715800
O	2.59957200	0.21317300	0.27820300
N	-1.99351400	0.09477100	0.07292600
H	-2.70821700	3.41913000	-0.88699500
H	-5.22873400	0.08056900	0.39799200
H	2.51461300	-2.47028700	0.04831400
H	0.33984000	3.19484800	1.47699300

Figure S7. continued.

iG 7H2O B3LYP Neutral			
Enthalpy (Hartrees) =			-1116.782093
Free Energy (Hartrees) =			-1116.878021
Charge = 0 Multiplicity = 1			
N	0.51099100	-2.89345100	0.10108700
C	1.16403300	-0.78870800	-0.01386400
C	0.95337700	0.60132300	-0.08965100
N	-0.36898300	0.96559100	-0.11977000
C	-1.46264100	0.08596100	-0.06677900
H	-3.04514400	2.08418700	0.78840400
H	-4.19345800	-0.12664100	-0.39927900
C	0.03104600	-1.60978100	0.02349900
C	-0.27612800	-4.12223200	0.17363600
H	-0.91375500	-4.10825000	1.05978000
H	-0.89382100	-4.22690100	-0.72043800
H	0.41275800	-4.96433000	0.23788900
H	-0.60775800	1.95987900	-0.22712400
O	-5.08827800	-0.52739800	-0.51087600
H	-5.29158500	-0.44442600	-1.45353200
O	-1.21948800	3.84589000	-0.46619400
H	-1.59623400	4.04061800	-1.33630200
H	-1.98572400	3.69568400	0.13914800
O	-3.18660900	2.96299500	1.21572300
H	-4.09274400	3.21861100	0.99015500
O	1.42366900	4.43501400	-0.02416300
H	1.66503100	2.53494000	-0.11886200
H	0.44759600	4.35100100	-0.10894200
O	4.85485900	1.48644200	-0.12097200
H	5.05551300	0.52351700	-0.03737200
H	2.88924500	1.29254500	-0.12291100
N	-1.26309800	-1.24069900	0.00300300
O	-3.65035800	-2.93717500	-0.00573900
H	-2.80022900	-2.44374900	0.01765900
H	-4.30461200	-2.23436400	-0.19590900
H	4.12593300	-1.35840800	0.12722600
N	2.31915100	-1.55795600	0.04424300
O	5.10504700	-1.22971600	0.22536200
H	5.50485300	-1.66947200	-0.53899100
C	1.88198200	-2.79747800	0.11041300
H	2.50634900	-3.67834300	0.16866400
N	1.89603800	1.53577000	-0.13477400
O	-2.61606900	0.61290300	-0.09016200
H	1.57980900	4.75094100	0.87736400
H	5.14708500	1.73203000	-1.01051300

iG 7H2O B3LYP N1 Anion			
Enthalpy (Hartrees) =			-1116.327006
Free Energy (Hartrees) =			-1116.422488
Charge = -1 Multiplicity = 1			
N	0.41779700	-2.91611000	0.05538600
C	1.11713300	-0.81986300	-0.00783100
C	0.90721700	0.57892800	-0.05078900
N	-0.36497700	1.02942400	-0.06384000
C	-1.43110800	0.16344900	-0.02175000
H	-3.02691100	2.23774500	0.59541400
H	-4.13016800	-0.00914400	-0.34504200
C	-0.03175800	-1.61286800	0.01708100
C	-0.39713700	-4.12543200	0.09946900
H	-1.01615800	-4.13329400	0.99934900
H	-1.03877000	-4.18206100	-0.78247600
H	0.26962800	-4.98785100	0.11455500
H	-0.74280900	2.71881900	-0.48154500
O	-5.04810500	-0.37099800	-0.47651700
H	-5.20791300	-0.33101600	-1.43007100
O	-0.96925800	3.67330200	-0.67998200
H	-1.78704100	3.80882100	-0.16190400
O	-3.26395900	3.14147800	0.93573300
H	-4.14434600	3.32744300	0.57968400
O	1.47340300	4.59634500	0.11022300
H	1.70084700	2.47348000	-0.04112500
H	0.53440200	4.37040300	-0.10369700
O	4.98704300	1.42876900	-0.04846000
H	5.08090000	0.44645800	-0.01151500
H	2.88760200	1.20451400	-0.05526600
N	-1.30750000	-1.19371400	0.01562800
O	-3.68719700	-2.78810900	0.16367800
H	-2.82651000	-2.30144500	0.12672000
H	-4.33589700	-2.09002600	-0.05886300
H	4.02819300	-1.42173000	0.08441500
N	2.25526500	-1.62149200	0.01847400
O	5.01489300	-1.31063000	0.17303400
H	5.39825700	-1.73409100	-0.60863200
C	1.78946900	-2.85394200	0.05535200
H	2.39335700	-3.75056200	0.08413100
N	1.91032600	1.47957600	-0.08740200
O	-2.61442900	0.68347600	-0.01839300
H	1.47602900	4.82259300	1.05096000
H	5.24890100	1.67644700	-0.94654400

Figure S7. continued.

iG 7H2O B3LYP N3 Cation

Enthalpy (Hartrees) = -1117.222402

Free Energy (Hartrees) = -1117.317591

Charge = 1 Multiplicity = 1

N	0.54174100	-2.87946200	0.03632700
C	1.17517300	-0.76489400	-0.03014500
C	0.95876700	0.63451100	-0.07534700
N	-0.36428500	1.01321100	-0.13264600
C	-1.46524100	0.17043300	-0.12468300
H	-3.25347800	2.25511500	0.52259000
H	-4.26848700	-0.18932700	-0.10183500
C	0.07141800	-1.60690000	-0.03032400
C	-0.22870000	-4.12582500	0.06483400
H	-0.91414300	-4.11798900	0.91405400
H	-0.78734400	-4.24028600	-0.86549400
H	0.47460900	-4.95059100	0.17316600
H	-0.59512500	2.01820200	-0.24591900
O	-5.08666800	-0.71961800	0.00279900
H	-5.57646800	-0.60667200	-0.82505000
O	-1.11545100	3.77625800	-0.53600800
H	-1.30982800	3.94289600	-1.47005200
H	-1.98860200	3.73502900	-0.07586100
O	-3.41508000	3.17426100	0.82040100
H	-4.24387200	3.44146900	0.39643900
O	1.45937400	4.41921100	0.14377200
H	1.67375900	2.56107200	-0.02463500
H	0.48955600	4.35422400	-0.00162100
O	4.79963800	1.50076300	-0.03833200
H	5.04895600	0.54923000	0.03851800
H	2.89640300	1.31233100	-0.04917800
N	-1.22071000	-1.17513600	-0.07296700
O	-3.41267600	-2.90468000	-0.11550600
H	-2.03530800	-1.83281300	-0.06689300
H	-4.14209200	-2.24548500	-0.03690100
H	4.18210000	-1.34128200	0.16263600
N	2.33426400	-1.52070400	0.03992300
O	5.15353500	-1.20942200	0.28423200
H	5.57180900	-1.62988800	-0.48120100
C	1.91626500	-2.76577900	0.07515400
H	2.54615000	-3.64243800	0.13032200
N	1.89858200	1.55680400	-0.06417500
O	-2.61754100	0.63649000	-0.16826000
H	1.56788800	4.69263500	1.06604600
H	5.09449800	1.77252900	-0.91951500
H	-3.44524600	-3.43633000	0.69343400

piC, NH3 tautomer 6H2O B3LYP Neutral

Enthalpy (Hartrees) = -892.741936

Free Energy (Hartrees) = -892.82951

Charge = 0 Multiplicity = 1

C	-0.58228100	-2.26128100	0.01235300
H	-0.95364900	-3.28239900	-0.03251500
H	-3.25507800	-1.86103600	-0.08042800
C	-1.14144200	-0.03517400	0.09562900
N	-2.03029000	0.96989300	0.13693000
H	-3.02094500	0.75167500	0.02817500
N	0.19154400	0.27618300	0.13931700
C	1.20139900	-0.67455200	0.09596800
O	2.40334900	-0.28813700	0.12465000
C	1.79299800	-3.14341000	-0.01298700
H	2.43840100	-3.06040400	-0.89503600
H	2.44540600	-3.12380500	0.86760100
H	1.29446700	-4.11606400	-0.04649500
H	0.47683000	1.25948700	0.25852800
O	-5.01768100	0.51085100	-0.17689500
H	-4.85762300	-0.46200700	-0.13703600
H	-5.45603800	0.73431700	0.65651300
O	3.38329500	2.19328600	-0.57173900
H	4.20467900	2.32396200	-0.07603100
H	3.07451700	1.28649100	-0.33499100
O	1.09247700	3.07159800	0.63812000
H	1.98204100	2.92035900	0.23592700
O	4.99625600	-1.32432500	-0.08435600
H	5.45795600	-0.48495900	-0.22216400
H	4.04932000	-1.07604600	-0.02155500
H	-1.73948700	1.93779900	-0.01176900
O	-1.31556400	3.81734600	-0.47050800
H	-0.42433000	3.69377700	-0.07507900
H	-1.76953700	4.44759000	0.10684800
H	1.24396500	3.22275100	1.58220200
O	-4.20768700	-2.12753900	-0.19944900
H	-4.44715100	-2.61114800	0.60442300
C	0.77591100	-2.03852700	0.03078000
N	-1.54679600	-1.30426300	0.03573000

Figure S7. continued.

piC, NH3 tautomer 6H2O B3LYP N1 Cation

Enthalpy (Hartrees) = -893.182655

Free Energy (Hartrees) = -893.268892

Charge = 1 Multiplicity = 1

C	-0.67485700	-2.20978500	0.01373300
H	-1.14030500	-3.18748200	-0.02108900
H	-2.56786100	-1.37364400	-0.02427300
C	-1.13665000	0.12579900	0.05820200
N	-1.98817800	1.13410500	0.05083100
H	-3.00018100	0.95788000	-0.02493100
N	0.20458400	0.33401700	0.11728300
C	1.16342400	-0.67897900	0.09828100
O	2.37015700	-0.36661300	0.13357800
C	1.64617000	-3.17879300	0.03861500
H	2.30541300	-3.12523400	-0.83437900
H	2.28193500	-3.15952700	0.93030800
H	1.11370500	-4.13255400	0.01268800
H	0.55358600	1.30378500	0.23409700
O	-4.82704000	0.68350500	-0.25426100
H	-4.79338800	-0.29359500	-0.16808600
H	-5.33631100	0.99349600	0.50869300
O	3.57219900	2.05949300	-0.62256500
H	4.39576200	2.15592000	-0.12232400
H	3.22686500	1.17174300	-0.38616600
O	1.29545500	2.97799300	0.60320700
H	2.17968700	2.82396000	0.19118700
O	4.95883300	-1.53038400	-0.08018900
H	5.43951500	-0.70764200	-0.25038400
H	4.02290900	-1.25612200	-0.01254500
H	-1.65590400	2.10642300	-0.01769200
O	-1.14019500	3.87259400	-0.31467500
H	-0.22528600	3.71952700	0.00922200
H	-1.53899800	4.49296700	0.31244800
H	1.45554800	3.07470900	1.55345800
O	-4.26691000	-2.03840800	-0.05021100
H	-4.54984300	-2.49089800	0.75904500
C	0.67189900	-2.03847300	0.04777100
N	-1.55810600	-1.15658600	0.01311900
H	-4.49485700	-2.63851000	-0.77658000

piC, NH3 tautomer 6H2O B3LYP N3 Anion

Enthalpy (Hartrees) = -892.287667

Free Energy (Hartrees) = -892.374388

Charge = -1 Multiplicity = 1

C	-0.52035300	-2.27557400	0.01526300
H	-0.86673000	-3.30641700	-0.03286100
H	-3.15388400	-1.85436000	0.06068400
C	-1.07700900	-0.06024900	0.14150400
N	-2.02940900	0.92083700	0.25284500
H	-2.98111200	0.67531400	-0.00274300
N	0.21057700	0.33168100	0.14566400
C	1.19108700	-0.61158200	0.06570700
O	2.42149700	-0.23048000	0.05044900
C	1.87526700	-3.07799300	-0.07599100
H	2.49795900	-2.97206700	-0.97247700
H	2.55175300	-3.04970900	0.78671300
H	1.40679900	-4.06674200	-0.10557800
H	0.65790500	2.01011500	0.55894700
O	-5.14014100	0.38330700	-0.44740800
H	-4.86056000	-0.54229400	-0.24667800
H	-5.56741100	0.70268300	0.35983200
O	3.42347900	2.25282200	-0.40637000
H	4.20804100	2.30409600	0.15806000
H	3.03623200	1.35338100	-0.23372800
O	0.91992800	2.95290300	0.76469900
H	1.82352600	3.01028800	0.39449900
O	4.95097000	-1.24824400	-0.17392900
H	5.42319500	-0.41055300	-0.28162600
H	4.00041800	-0.98945700	-0.10261300
H	-1.74523800	1.86544200	0.01309100
O	-1.26796400	4.04838300	-0.48145000
H	-0.43878100	3.75040100	-0.03437400
H	-1.72721300	4.59760800	0.16930100
O	-4.11696600	-2.13925900	-0.00500900
H	-4.35075300	-2.47907000	0.87083800
C	0.82802600	-2.00243000	0.00365000
N	-1.49869500	-1.33639700	0.07749800

Figure S7. continued.

Show 5H2O B3LYP Neutral

Enthalpy (Hartrees) =			-780.824347
Free Energy (Hartrees) =			-780.904129
Charge = 0 Multiplicity = 1			
C	0.84365600	-1.89554100	-0.01857700
C	1.33976200	-0.49962300	0.07985200
N	0.23025600	0.33262800	0.11872400
C	-0.91813400	-0.42741500	0.05818700
O	-2.06598100	0.01419400	0.06938800
C	-1.48766500	-2.98202300	-0.12396500
H	-2.15040400	-2.97755900	0.74877900
H	-2.12216100	-2.85717800	-1.00885400
H	-0.98200300	-3.94780300	-0.18234600
H	0.25636400	1.35660100	0.23828700
O	4.60307900	-2.08631000	-0.03337300
H	3.90457800	-1.40464500	0.02106700
H	5.43566900	-1.59481600	0.00529500
O	0.12394800	3.22952600	0.41670500
H	0.10670400	3.49319300	1.34834900
H	-0.82021100	3.21941700	0.12339500
O	2.50798900	-0.11274900	0.11542800
O	2.84282700	2.76563400	-0.35492700
H	2.85249000	1.80437800	-0.19264600
H	1.92052500	3.02065600	-0.16075900
O	-4.66065700	-1.26623800	0.05603700
H	-5.24051600	-0.54255500	0.33249900
H	-3.76126500	-0.88691800	0.06839000
H	1.50861700	-2.74748100	-0.07174800
O	-2.49052200	2.82831000	-0.31777700
H	-2.41801600	1.85577500	-0.22982600
H	-2.65206900	2.99032700	-1.25891200
C	-0.50021100	-1.87685100	-0.03281000

Show 5H2O B3LYP N3 Anion

Enthalpy (Hartrees) =			-780.371739
Free Energy (Hartrees) =			-780.450726
Charge = -1 Multiplicity = 1			
C	-0.83948900	-1.87548100	0.01799700
C	-1.29929200	-0.44950500	-0.05963900
N	-0.23634900	0.40771100	-0.10792300
C	0.87418100	-0.37418700	-0.05299800
O	2.05061100	0.04897400	-0.05648000
C	1.50056100	-2.95172600	0.09580700
H	2.15677500	-2.93751500	-0.78215100
H	2.14464200	-2.83348600	0.97501500
H	1.00820600	-3.92564900	0.15031700
H	-0.22101900	2.17217900	-0.37935700
O	-4.53241000	-2.01221600	0.03540700
H	-3.82055700	-1.33505400	-0.00419100
H	-5.35894000	-1.51250000	-0.01955000
O	-0.16035800	3.16232400	-0.47745100
H	0.75119100	3.34428100	-0.17712400
O	-2.49792800	-0.09072800	-0.07020000
O	-2.94919000	2.71217100	0.28225800
H	-2.80303200	1.75102200	0.15128700
H	-2.06856800	3.10234800	0.13270600
O	4.58885800	-1.18140100	-0.04970300
H	5.15762500	-0.44733400	-0.32119400
H	3.67947000	-0.81414400	-0.05851400
H	-1.50970000	-2.72494400	0.06440800
O	2.61243800	2.80454900	0.27136600
H	2.40608900	1.84701400	0.18038300
H	2.81527100	2.93306500	1.20899400
C	0.50084500	-1.85287500	0.02430900

Figure S7. continued.