Supporting Information for:

Synthesis of new photosensitive $H_2BBQ^{2+}[ZnCl_4]^{2-}$/$[(ZnCl)_2(\mu\text{-BBH})]$ complexes, through the selective oxidation of H_2O to H_2O_2

M. Stylianou,[a,b] I. Hadjiadamou,[a] C. Drouza,[b] S. C. Hayes,[a] E. Lariou,[a] I. Tantis,[c] P. Lianos,[c] A. C. Tsipis[d] and A. D. Keramidas,[a]

a. Anastasios D. Keramidas, Ioanna Hadjiadamou, Marios Stylianou, Sophia C. Hayes, Eirini Lariou
Department of Chemistry
University of Cyprus
Nicosia 1678, Cyprus
e.mail:akeramid@ucy.ac.cy
e.mail: shayes@ucy.ac.cy

b. Chryssoula Drouza
Department of Agricultural ProductionBiotechnology and Food Science
Cyprus University of Technology
Limassol 3036, Cyprus
e.mail:chryssoula.drouza@cut.ac.cy

c. Iosif Tantis, Panagiotis Lianos
Department of Chemical Engineering
University of Patras
26500 Patras, Greece
e.mail: lianos@upatras.gr

d. Athanassios C. Tsipis
Laboratory of Inorganic and General Chemistry
University of Ioannina
45110 Ioannina, Greece
e.mail:attsipis@uoi.gr

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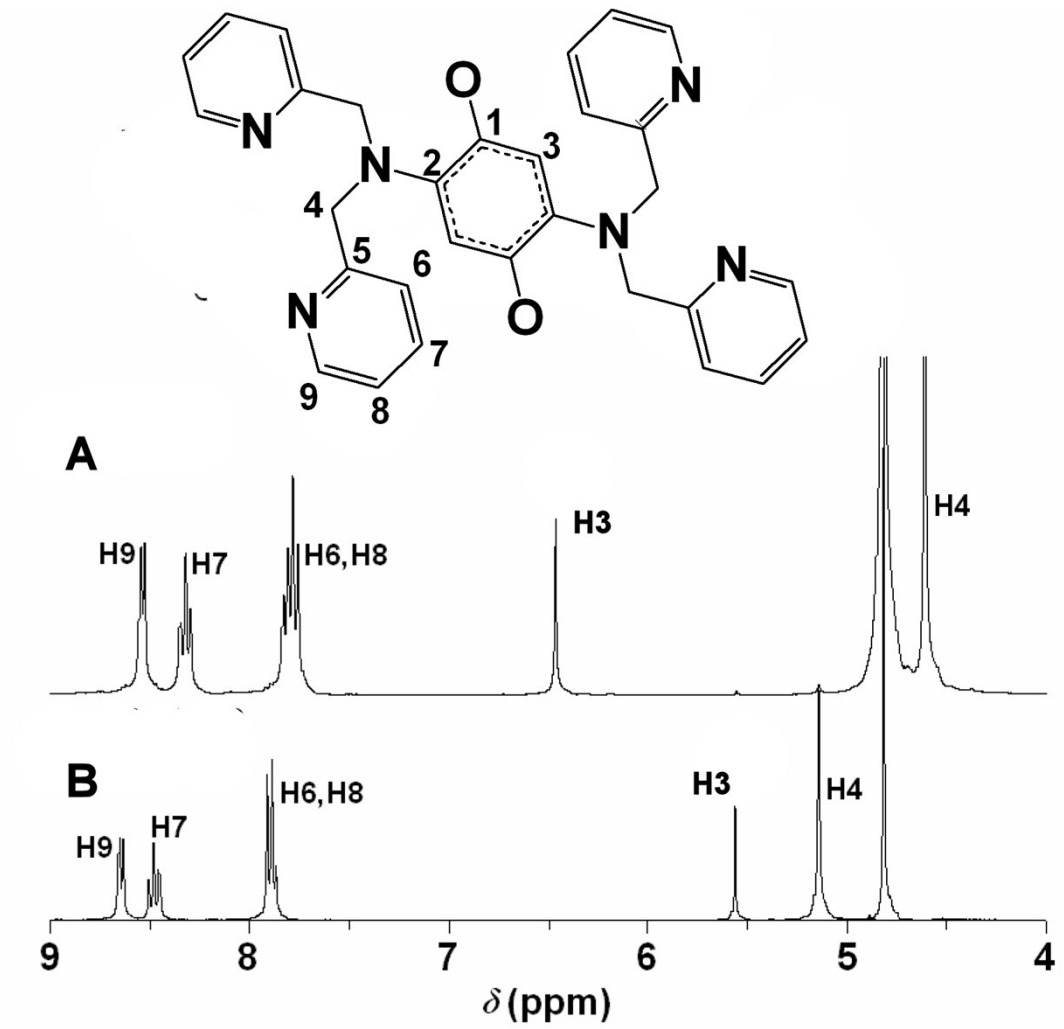

Figure S1. ^{1}H NMR spectra in D_2O and assignments (A) for **4** and (B) for compound **1** at pD=2.5.

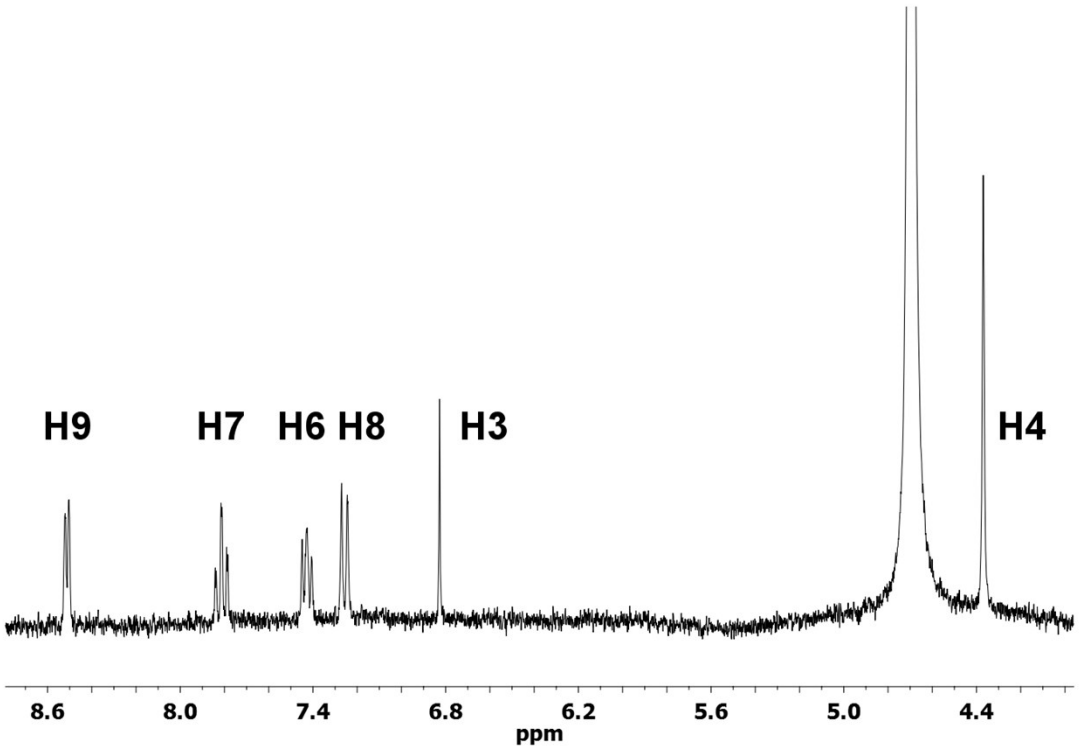

Figure S2. ^{1}H NMR spectra in D_2O at pD=6.0 and assignments of **2**.

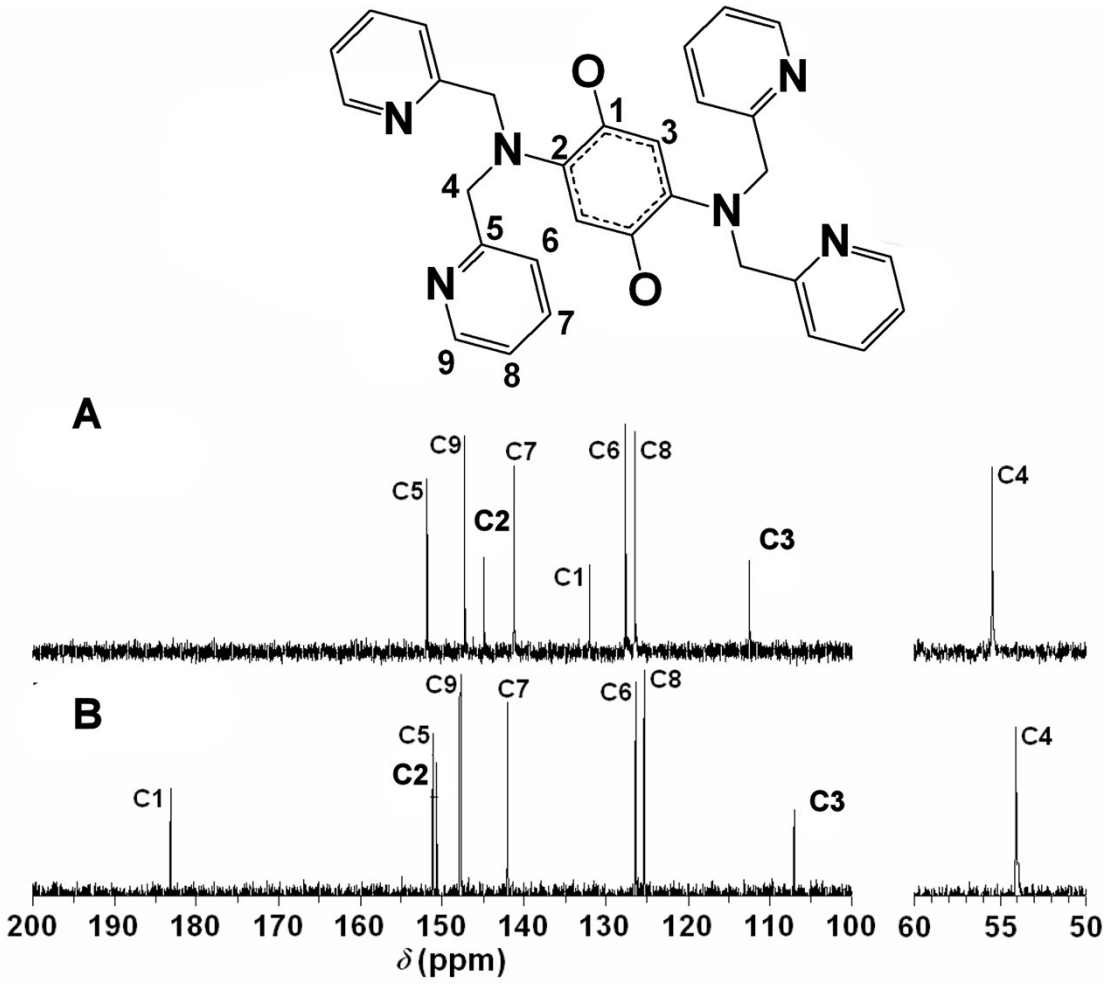

Figure S3. ^{13}C NMR spectra in D_2O and assignments (A) for **4** and (B) for compound **1** at pD=2.5.

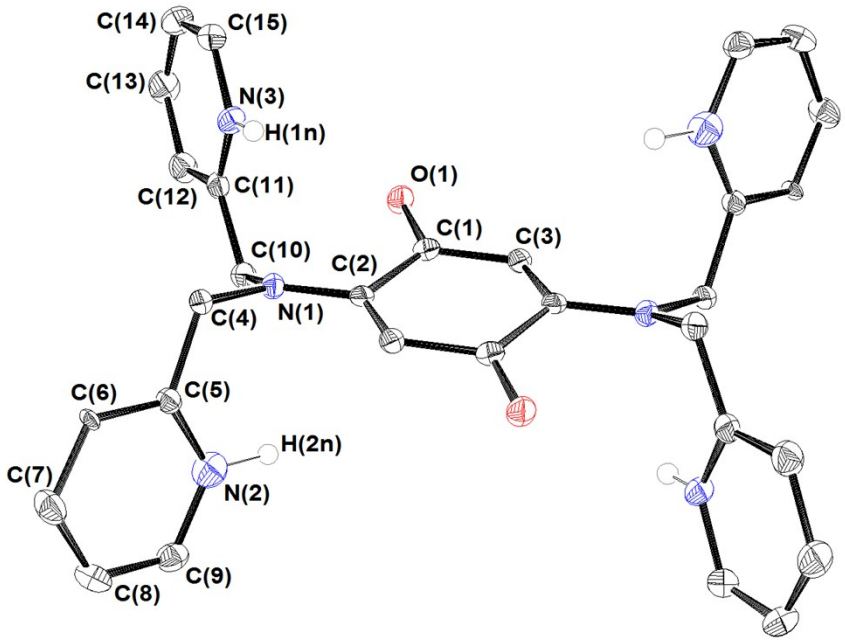

Figure S4. ORTEP diagrams of the cation of $H_4BBQ^{4+}Cl_4^{4-}$ (**3**) with atomic numbering scheme and thermal ellipsoids at 50% probability level. The hydrogen atoms except the N-H have been omitted for clarity

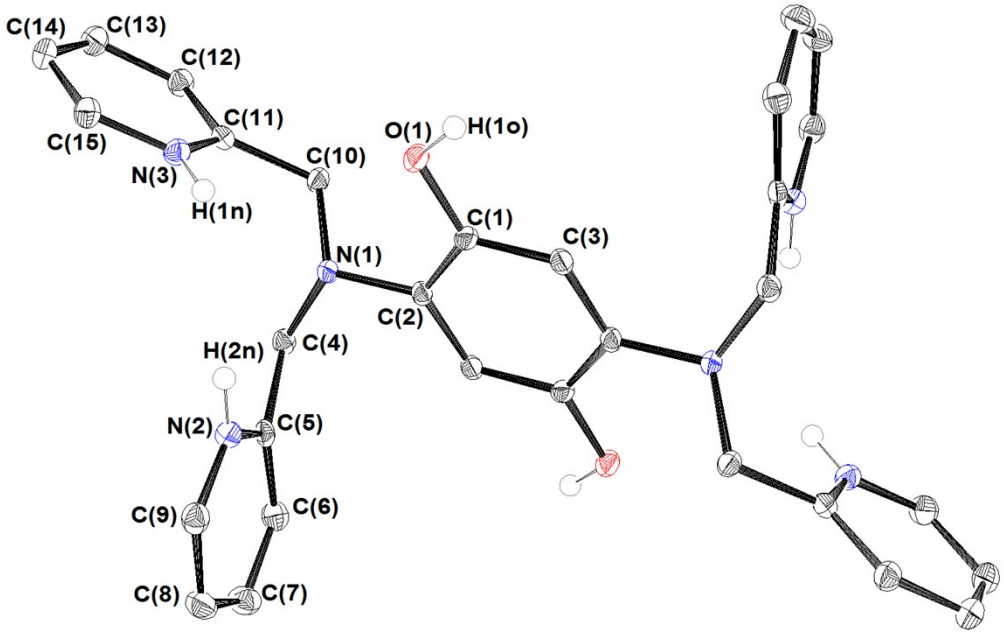

Figure S5. ORTEP diagrams of the cation of $H_6BBH^{4+}Cl_4^{4-}$ (**4**) with atomic numbering scheme and thermal ellipsoids at 50% probability level. The hydrogen atoms except the N-H and O-H have been omitted for clarity

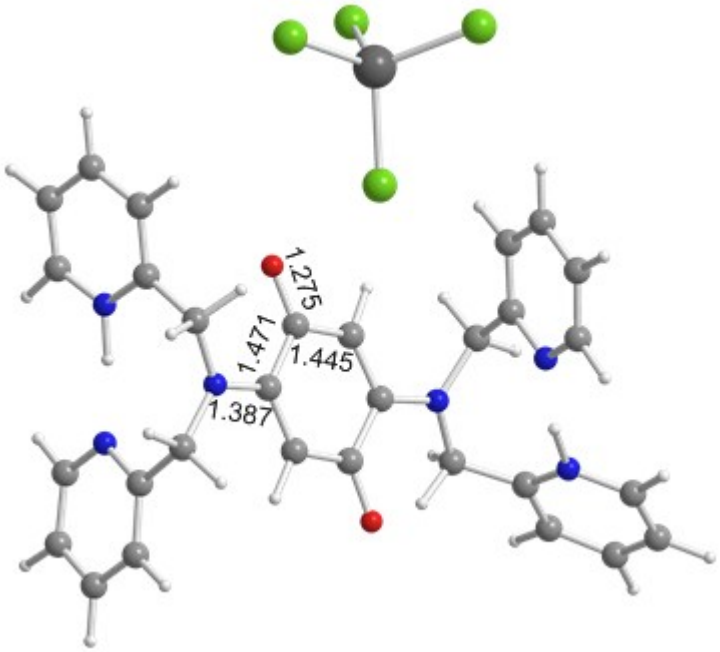

Figure S6. Equilibrium geometry of **1** optimized at the BP86/6-31G(d,p)/PCM level of theory in aqueous solution.

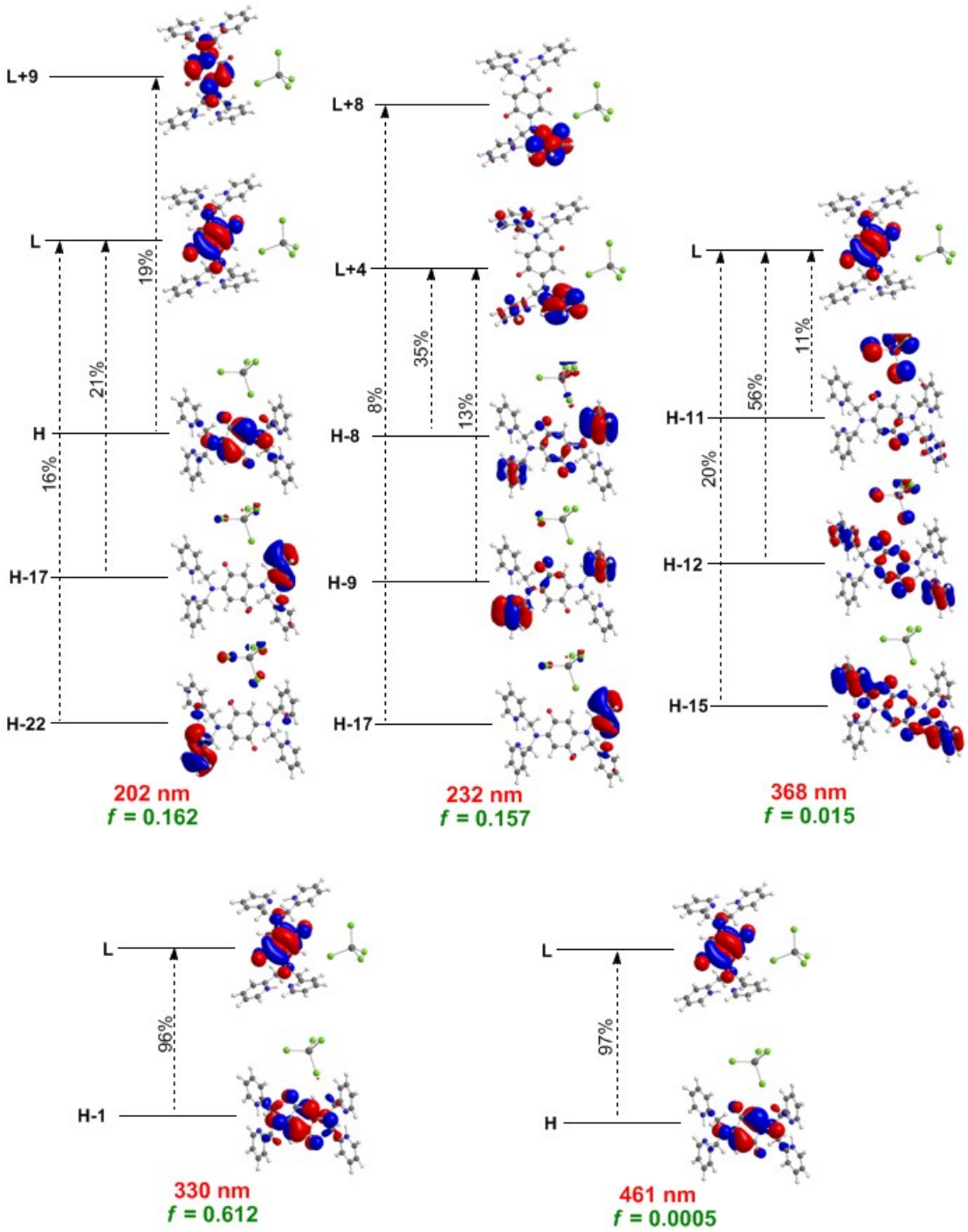

Figure S7. 3D contour plots of the Molecular Orbitals (MOs) involved in the principal electronic transitions in the TD-DFT simulated absorption spectrum of **1.**

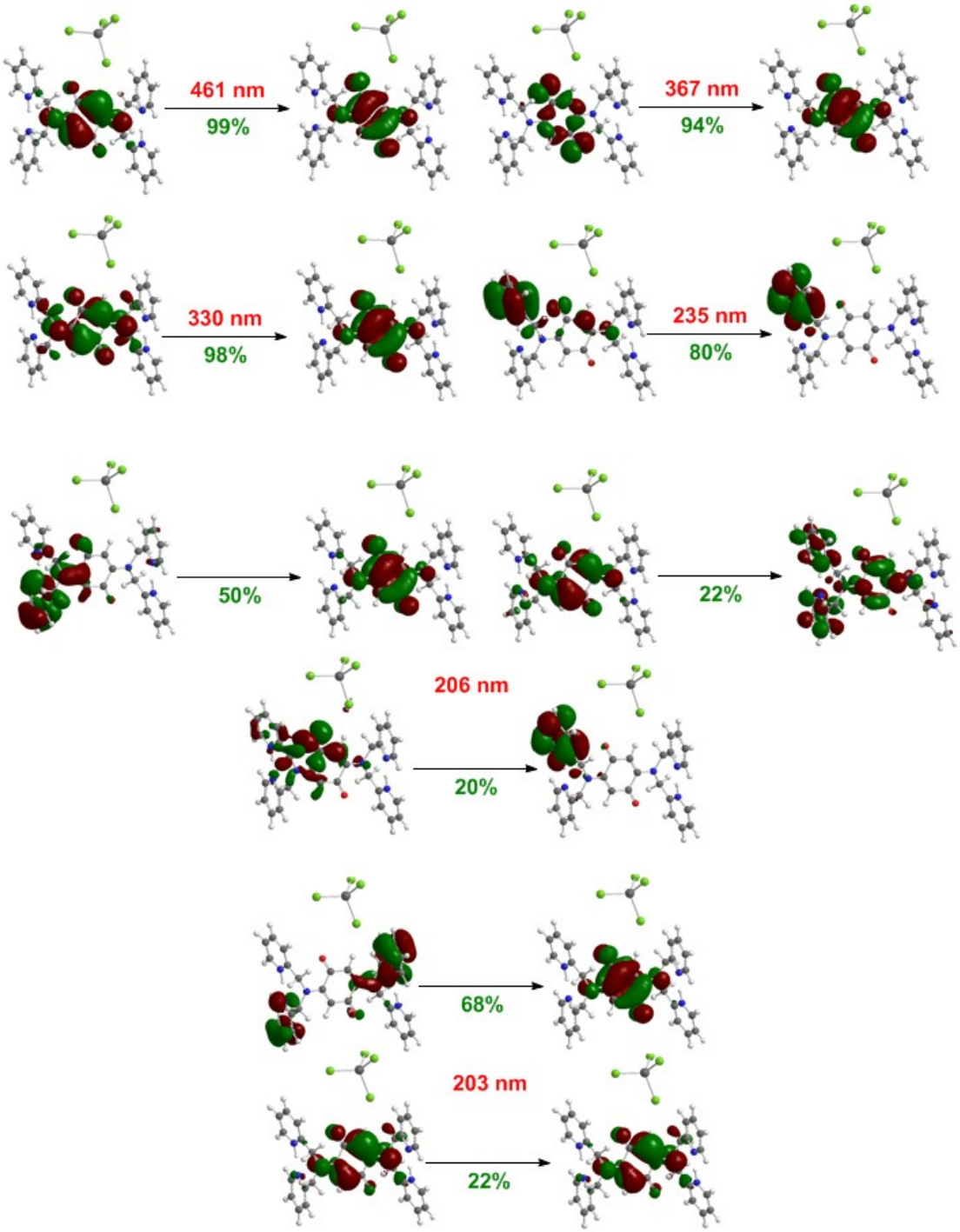

Figure S8. Dominant NTO pairs ("hole" on the left, "particle" on the right) for the principal electronic excitations in the absorption spectrum of **1**.

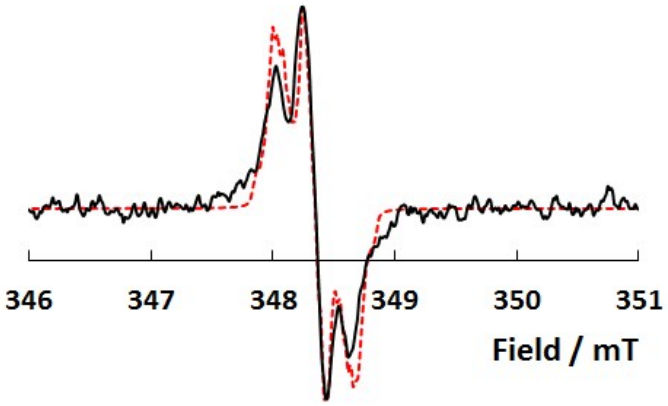

Figure S9. X-band cw EPR spectrum of a heated solution of BBQ (1.00 mM) and $ZnCl_2$ (2.00 mM) in H_2O at pH =5.0 at R.T. (black line). The signal is assigned to the diradical of BBQ. The spectrum was simulated using the following parameters g=2.00468, A_{14N}=1.04, A_{14N}=0.45, A_{1H}=6.51 and A_{1H}=2.64 MHz D=0.00020 E=0.00011 cm^{-1} and J_{dip}=21 x 10^{-4} cm^{-1} (red dashed line).

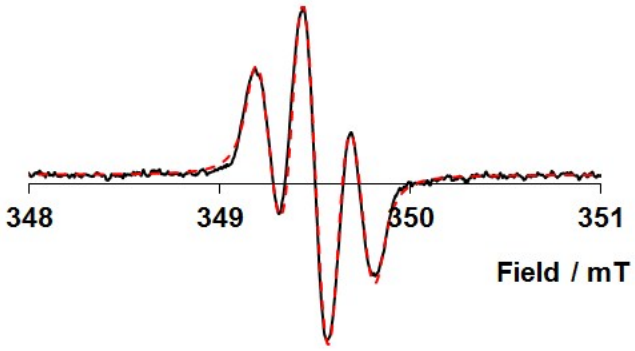

Figure S10. X-band cw EPR spectrum of a solution of BBQ (1.00 mM) and $ZnCl_2$ (2.00 mM) in H_2O exposed to the light of a 15 W mercury lamp for four hours at pH =4 at R.T. (black line). The signal is assigned to the p-semiquinone single radical, 2,5-bis(bis(pyridin-2-ylmethyl)amino)-1,4-semiquinone (BBS). The spectrum was simulated using the following parameters g=2.00510, A_{14N}=1.23, A_{14N}=0.79, A_{1H}=6.77 and A_{1H}=6.69 MHz (red dashed line).

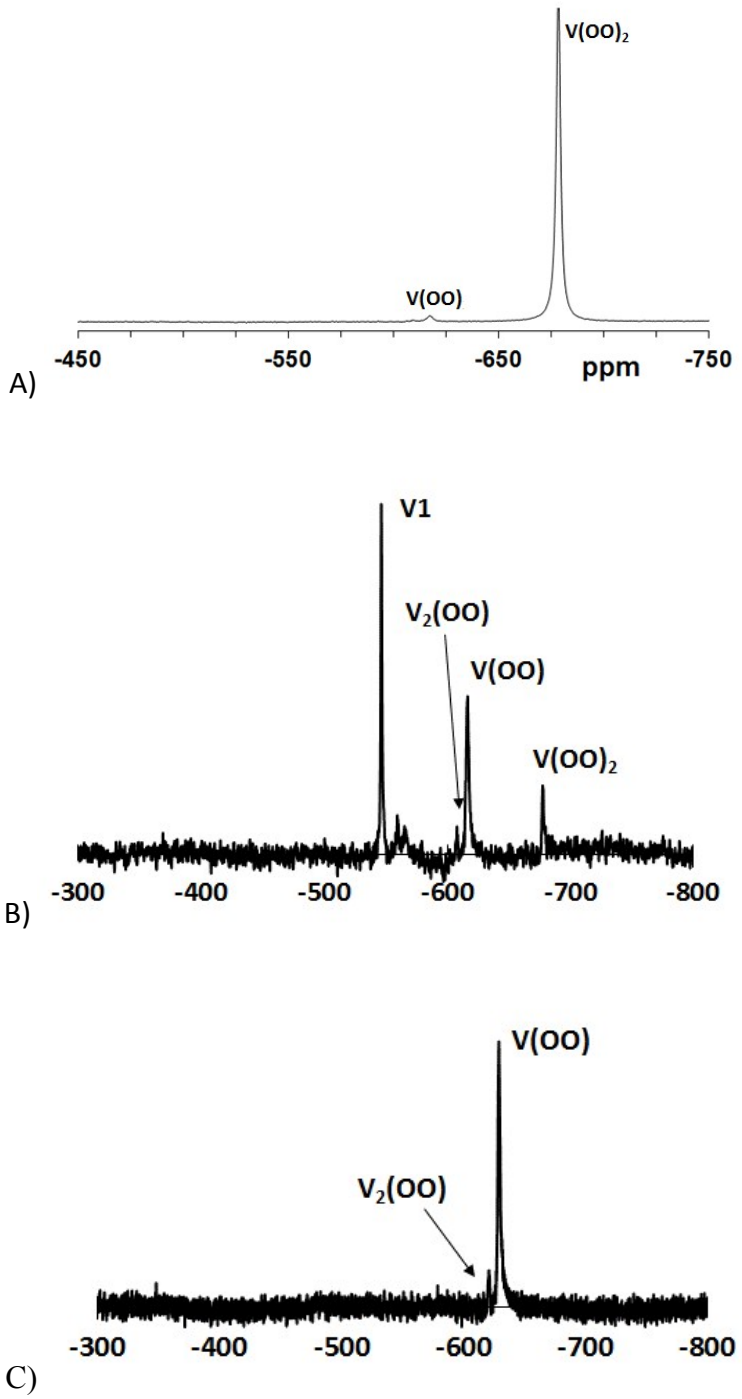

Figure S11. A) NaOH was added in an aqueous solution of 10 mM BBQ and 20 mM $ZnCl_2$ (pH=2.5) up to pH=5.5. The mixture was steered under the light of a mercury lamb (15 W) for 3 hours. To the filtrate, an aqueous solution of $NaVO_3$ (5 mM) was added and the spectrum was recorded. B) Aqueous solution of 5 mM BBQ and 10 mM $ZnCl_2$ at pH=2.5 illuminated under the light of a mercury lamb (15 W) for 3 hours. An aqueous solution of $NaVO_3$ (5 mM) was added and the spectrum were recorded. C) Aqueous mixture of 5 mM and 10 mM $ZnCl_2$ were heated to dissolve (pH=5.0). The suspension was filtered and an aqueous solution of $NaVO_3$ (5 mM) was added and the spectrum were recorded. V1=VO_4^{3-}, V(OO)=monoperoxovanadate, $V(OO)_2$=bisperoxovanadate.

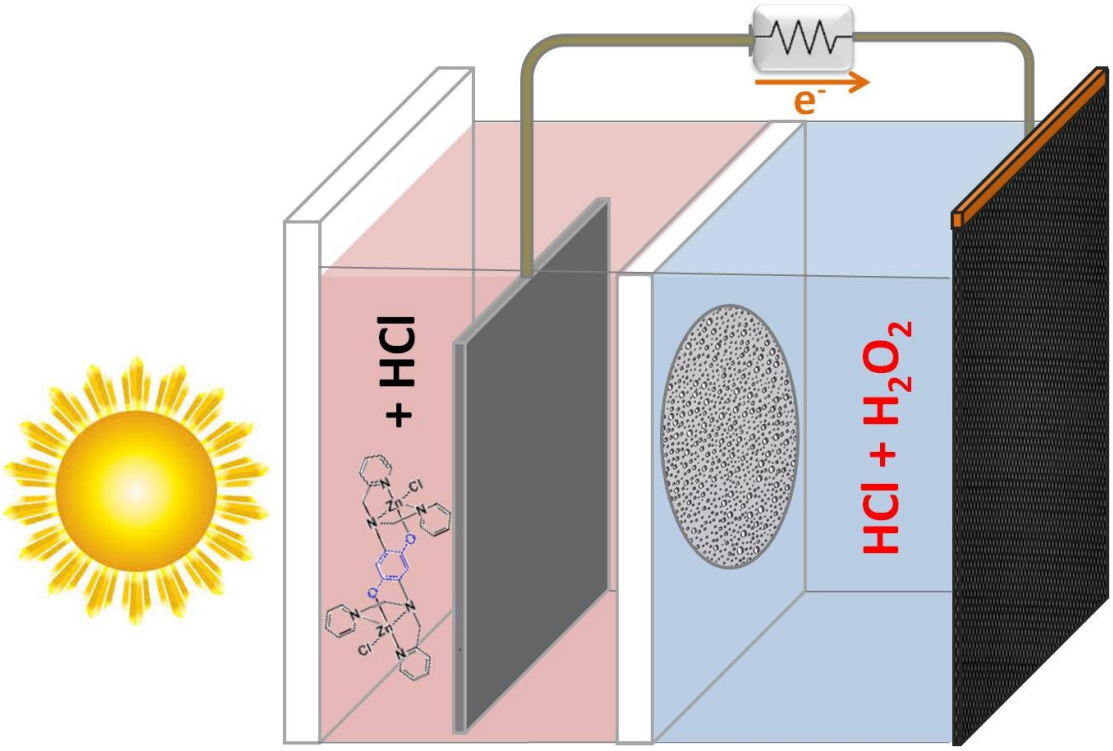

Figure S12. Schematic illustration of the solar battery.

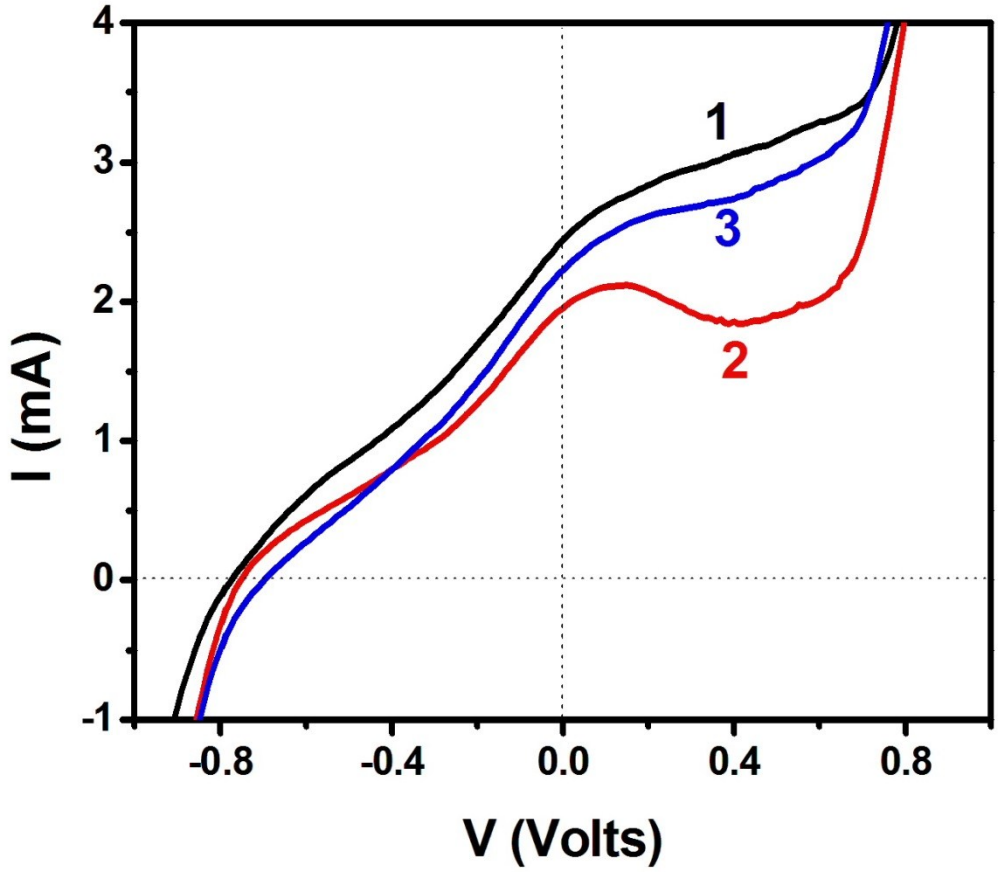

Figure S13. IV curves recorded during one discharge-recharge cycle: (1) Initial curve; (2) Curve traced after the first discharge; (3) Curve traced after the first recharge.

Table S1. Bond lengths [Å] and angles [°] of **1.**

Zn(1)-Cl(3)	2.2570(6)	N(2A)-C(5A)	1.344(4)	C(7)-C(8)	1.390(4)
Zn(1)-Cl(1)	2.2642(7)	C(10A)-C(11A)	1.497(4)	C(7)-C(6)	1.393(4)
Zn(1)-Cl(4)	2.2840(7)	N(1)-C(2)	1.374(3)	C(1)-C(3)	1.444(4)
Zn(1)-Cl(2)	2.2981(6)	N(1)-C(4)	1.457(3)	C(1)-C(2)	1.510(3)
O(1)-C(1)	1.231(3)	N(1)-C(10)	1.462(3)	C(9)-C(8)	1.383(4)
N(3)-C(11)	1.342(3)	C(10)-C(11)	1.503(4)	C(1A)-C(2A)	1.513(3)
N(3)-C(15)	1.350(4)	C(11A)-C(12A)	1.395(4)	C(3)-C(2)#2	1.363(3)
N(3)-H(1N)	0.91(5)	C(5A)-C(6A)	1.386(4)	C(13)-C(12)	1.380(4)
O(1A)-C(1A)	1.225(3)	C(5A)-C(4A)	1.510(4)	C(13)-C(14)	1.397(4)
N(2)-C(5)	1.343(3)	C(9A)-C(8A)	1.388(4)	C(5)-C(6)	1.382(4)
N(2)-C(9)	1.350(3)	C(12A)-C(13A)	1.388(4)	C(7A)-C(6A)	1.391(5)
N(1A)-C(2A)	1.372(3)	C(13A)-C(14A)	1.387(4)	C(14)-C(15)	1.370(4)
N(1A)-C(10A)	1.457(3)	C(11)-C(12)	1.393(4)	C(2)-C(3)#2	1.363(3)
N(1A)-C(4A)	1.468(3)	C(4)-C(5)	1.518(3)	C(2A)-C(3A)#1	1.361(4)
N(3A)-C(11A)	1.339(4)	C(15A)-C(14A)	1.376(4)		
N(3A)-C(15A)	1.347(4)	C(8A)-C(7A)	1.378(5)		
N(3A)-H(2N)	0.81(4)	C(3A)-C(2A)#1	1.361(4)		
N(2A)-C(9A)	1.336(4)	C(3A)-C(1A)	1.446(3)		

Cl(3)-Zn(1)-Cl(1)	112.09(3)	C(12)-C(11)-C(10)	121.5(2)
Cl(3)-Zn(1)-Cl(4)	108.27(3)	N(1)-C(4)-C(5)	112.24(19)
Cl(1)-Zn(1)-Cl(4)	107.73(3)	N(3A)-C(15A)-C(14A)	120.2(3)
Cl(3)-Zn(1)-Cl(2)	108.08(2)	C(7A)-C(8A)-C(9A)	118.5(3)
Cl(1)-Zn(1)-Cl(2)	109.08(2)	C(15A)-C(14A)-C(13A)	118.6(3)
Cl(4)-Zn(1)-Cl(2)	111.62(3)	C(2A)#1-C(3A)-C(1A)	122.3(2)
C(11)-N(3)-C(15)	122.5(2)	C(8)-C(7)-C(6)	119.3(2)
C(11)-N(3)-H(1N)	112(3)	O(1)-C(1)-C(3)	120.6(2)
C(15)-N(3)-H(1N)	125(3)	O(1)-C(1)-C(2)	120.5(2)
C(5)-N(2)-C(9)	118.2(2)	C(3)-C(1)-C(2)	118.8(2)
C(2A)-N(1A)-C(10A)	122.8(2)	N(2)-C(9)-C(8)	123.0(2)
C(2A)-N(1A)-C(4A)	117.8(2)	O(1A)-C(1A)-C(3A)	121.3(2)
C(10A)-N(1A)-C(4A)	117.46(18)	O(1A)-C(1A)-C(2A)	120.4(2)
C(11A)-N(3A)-C(15A)	123.1(2)	C(3A)-C(1A)-C(2A)	117.9(2)
C(11A)-N(3A)-H(2N)	120(3)	N(1A)-C(4A)-C(5A)	110.6(2)
C(15A)-N(3A)-H(2N)	117(3)	C(2)#2-C(3)-C(1)	122.4(2)
C(9A)-N(2A)-C(5A)	118.6(2)	C(12)-C(13)-C(14)	119.9(3)
N(1A)-C(10A)-C(11A)	115.1(2)	N(2)-C(5)-C(6)	122.6(2)

C(2)-N(1)-C(4)	117.7(2)	N(2)-C(5)-C(4)	116.2(2)
C(2)-N(1)-C(10)	124.3(2)	C(6)-C(5)-C(4)	121.1(2)
C(4)-N(1)-C(10)	117.3(2)	C(8A)-C(7A)-C(6A)	119.4(3)
N(1)-C(10)-C(11)	114.8(2)	C(13)-C(12)-C(11)	119.4(3)
N(3A)-C(11A)-C(12A)	118.6(2)	C(15)-C(14)-C(13)	118.9(3)
N(3A)-C(11A)-C(10A)	119.8(2)	C(9)-C(8)-C(7)	118.2(2)
C(12A)-C(11A)-C(10A)	121.6(2)	C(3)#2-C(2)-N(1)	122.8(2)
N(2A)-C(5A)-C(6A)	122.2(3)	C(3)#2-C(2)-C(1)	118.2(2)
N(2A)-C(5A)-C(4A)	115.7(2)	N(1)-C(2)-C(1)	119.0(2)
C(6A)-C(5A)-C(4A)	122.1(2)	N(3)-C(15)-C(14)	120.2(3)
N(2A)-C(9A)-C(8A)	122.8(3)	C(3A)#1-C(2A)-N(1A)	123.3(2)
C(13A)-C(12A)-C(11A)	119.3(3)	C(3A)#1-C(2A)-C(1A)	118.8(2)
C(14A)-C(13A)-C(12A)	120.2(3)	N(1A)-C(2A)-C(1A)	117.7(2)
N(3)-C(11)-C(12)	119.1(2)	C(5A)-C(6A)-C(7A)	118.6(3)
N(3)-C(11)-C(10)	119.4(2)	C(5)-C(6)-C(7)	118.7(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z+1 #2 -x,-y+1,-z+1

Table S2. Bond lengths [Å] and angles [°] of **2.**

Zn(1')-O(1')	1.955(4)	N(1)-C(4)	1.478(7)	C(2)-C(3)	1.389(7)
Zn(1')-N(3')	2.089(5)	C(1A)-C(3A)	1.401(7)	C(10A)-C(11A)	1.505(7)
Zn(1')-N(2')	2.090(5)	C(1A)-C(2A)	1.403(7)	C(5B)-C(6B)	1.387(8)
Zn(1')-N(1')	2.240(4)	N(3B)-C(11B)	1.352(7)	C(5B)-C(4B)	1.515(8)
Zn(1')-Cl(1')	2.3227(14)	N(3B)-C(15B)	1.352(7)	C(12)-C(13)	1.383(8)
Zn(1B)-O(1B)	1.961(4)	N(2')-C(9')	1.348(7)	C(12)-C(11)	1.390(7)
Zn(1B)-N(3B)	2.088(5)	N(2')-C(5')	1.349(7)	C(12A)-C(11A)	1.392(7)
Zn(1B)-N(2B)	2.095(5)	N(3A)-C(11A)	1.343(7)	C(5)-C(6)	1.379(8)
Zn(1B)-N(1B)	2.268(4)	N(3A)-C(15A)	1.344(7)	C(5)-C(4)	1.517(8)
Zn(1B)-Cl(1B)	2.3131(14)	C(1)-C(3')	1.391(7)	C(15B)-C(14B)	1.376(8)
Zn(1A)-O(1A)	1.957(4)	C(1)-C(2)	1.408(7)	C(5')-C(6')	1.383(8)
Zn(1A)-N(2A)	2.091(5)	C(15')-C(14')	1.381(8)	C(5')-C(4')	1.507(8)
Zn(1A)-N(3A)	2.096(5)	C(11')-C(12')	1.401(8)	C(9')-C(8')	1.384(9)
Zn(1A)-N(1A)	2.244(4)	C(11')-C(10')	1.507(8)	C(4A)-C(5A)	1.522(7)
Zn(1A)-Cl(1A)	2.3203(14)	N(2B)-C(5B)	1.339(7)	C(7B)-C(6B)	1.379(8)
Zn(1)-O(1)	1.971(4)	N(2B)-C(9B)	1.355(7)	C(7B)-C(8B)	1.393(9)
Zn(1)-N(2)	2.076(5)	C(3A)-C(2A)#1	1.376(7)	C(11)-C(10)	1.511(7)
Zn(1)-N(3)	2.092(4)	N(2A)-C(9A)	1.343(7)	C(14B)-C(13B)	1.398(9)
Zn(1)-N(1)	2.260(4)	N(2A)-C(5A)	1.350(7)	C(5A)-C(6A)	1.382(8)
Zn(1)-Cl(1)	2.3041(15)	C(1')-C(3)	1.395(7)	C(12')-C(13')	1.378(8)
N(1A)-C(2A)	1.466(6)	C(1')-C(2')	1.404(7)	C(14')-C(13')	1.389(9)
N(1A)-C(10A)	1.468(6)	N(3)-C(15)	1.340(7)	C(12B)-C(13B)	1.379(9)
N(1A)-C(4A)	1.477(6)	N(3)-C(11)	1.349(7)	C(8')-C(7')	1.382(11)
O(1)-C(1)	1.350(6)	C(2B)-C(3B)	1.388(7)	C(6')-C(7')	1.381(10)
O(1')-C(1')	1.348(6)	C(2B)-C(1B)	1.408(7)	C(8)-C(7)	1.373(9)
N(1B)-C(2B)	1.449(6)	C(3B)-C(1B)#2	1.391(7)	C(8)-C(9)	1.373(8)
N(1B)-C(4B)	1.469(7)	C(2A)-C(3A)#1	1.376(7)	C(14)-C(15)	1.379(8)
N(1B)-C(10B)	1.479(7)	C(9B)-C(8B)	1.369(8)	C(14)-C(13)	1.387(8)
O(1B)-C(1B)	1.356(6)	N(2)-C(5)	1.346(7)	C(14A)-C(15A)	1.382(8)
O(1A)-C(1A)	1.349(6)	N(2)-C(9)	1.347(7)	C(8A)-C(7A)	1.382(9)
N(1')-C(2')	1.451(6)	C(3')-C(2')	1.386(7)	C(6A)-C(7A)	1.389(8)
N(1')-C(10')	1.473(7)	C(1B)-C(3B)#2	1.391(7)	C(6)-C(7)	1.408(9)
N(1')-C(4')	1.474(7)	C(9A)-C(8A)	1.387(8)		
N(3')-C(11')	1.334(7)	C(11B)-C(12B)	1.383(8)		
N(3')-C(15')	1.341(7)	C(11B)-C(10B)	1.509(8)		
N(1)-C(2)	1.463(6)	C(13A)-C(14A)	1.373(8)		
N(1)-C(10)	1.472(7)	C(13A)-C(12A)	1.392(8)		

O(1')-Zn(1')-N(3')	125.25(17)	C(11)-N(3)-Zn(1)	117.4(4)
O(1')-Zn(1')-N(2')	104.67(17)	C(3B)-C(2B)-C(1B)	121.2(5)
N(3')-Zn(1')-N(2')	120.37(18)	C(3B)-C(2B)-N(1B)	121.8(5)
O(1')-Zn(1')-N(1')	82.13(15)	C(1B)-C(2B)-N(1B)	116.9(4)
N(3')-Zn(1')-N(1')	78.90(16)	C(2B)-C(3B)-C(1B)#2	121.1(5)
N(2')-Zn(1')-N(1')	77.86(17)	C(3A)#1-C(2A)-C(1A)	121.8(5)
O(1')-Zn(1')-Cl(1')	99.57(12)	C(3A)#1-C(2A)-N(1A)	121.2(5)
N(3')-Zn(1')-Cl(1')	99.49(13)	C(1A)-C(2A)-N(1A)	116.8(4)
N(2')-Zn(1')-Cl(1')	102.31(14)	N(2B)-C(9B)-C(8B)	122.2(6)
N(1')-Zn(1')-Cl(1')	178.16(11)	C(5)-N(2)-C(9)	118.8(5)
O(1B)-Zn(1B)-N(3B)	101.02(17)	C(5)-N(2)-Zn(1)	116.9(4)
O(1B)-Zn(1B)-N(2B)	125.77(17)	C(9)-N(2)-Zn(1)	122.1(4)
N(3B)-Zn(1B)-N(2B)	122.88(18)	C(2')-C(3')-C(1)	121.3(5)
O(1B)-Zn(1B)-N(1B)	81.79(15)	O(1B)-C(1B)-C(3B)#2	120.6(5)
N(3B)-Zn(1B)-N(1B)	78.29(17)	O(1B)-C(1B)-C(2B)	121.7(5)
N(2B)-Zn(1B)-N(1B)	78.20(17)	C(3B)#2-C(1B)-C(2B)	117.7(5)
O(1B)-Zn(1B)-Cl(1B)	101.95(11)	N(2A)-C(9A)-C(8A)	122.7(6)
N(3B)-Zn(1B)-Cl(1B)	100.14(13)	N(3B)-C(11B)-C(12B)	121.5(5)
N(2B)-Zn(1B)-Cl(1B)	99.97(14)	N(3B)-C(11B)-C(10B)	115.8(5)
N(1B)-Zn(1B)-Cl(1B)	176.19(11)	C(12B)-C(11B)-C(10B)	122.6(5)
O(1A)-Zn(1A)-N(2A)	101.49(17)	C(14A)-C(13A)-C(12A)	118.9(5)
O(1A)-Zn(1A)-N(3A)	128.69(17)	C(3)-C(2)-C(1)	121.5(5)
N(2A)-Zn(1A)-N(3A)	120.44(17)	C(3)-C(2)-N(1)	121.1(5)
O(1A)-Zn(1A)-N(1A)	82.75(15)	C(1)-C(2)-N(1)	117.3(4)
N(2A)-Zn(1A)-N(1A)	78.99(16)	N(1B)-C(10B)-C(11B)	110.9(4)
N(3A)-Zn(1A)-N(1A)	78.14(16)	N(1A)-C(10A)-C(11A)	111.2(4)
O(1A)-Zn(1A)-Cl(1A)	100.09(11)	N(2B)-C(5B)-C(6B)	121.1(5)
N(2A)-Zn(1A)-Cl(1A)	101.06(13)	N(2B)-C(5B)-C(4B)	117.9(5)
N(3A)-Zn(1A)-Cl(1A)	99.40(13)	C(6B)-C(5B)-C(4B)	120.9(5)
N(1A)-Zn(1A)-Cl(1A)	177.06(12)	C(13)-C(12)-C(11)	119.8(5)
O(1)-Zn(1)-N(2)	96.25(17)	C(11A)-C(12A)-C(13A)	119.1(5)
O(1)-Zn(1)-N(3)	136.62(16)	C(2)-C(3)-C(1')	120.9(5)
N(2)-Zn(1)-N(3)	116.97(18)	N(2)-C(5)-C(6)	122.4(5)
O(1)-Zn(1)-N(1)	82.41(14)	N(2)-C(5)-C(4)	115.7(5)
N(2)-Zn(1)-N(1)	79.57(17)	C(6)-C(5)-C(4)	121.9(5)
N(3)-Zn(1)-N(1)	77.53(16)	N(3B)-C(15B)-C(14B)	123.0(6)
O(1)-Zn(1)-Cl(1)	100.62(11)	C(3')-C(2')-C(1')	121.5(5)

N(2)-Zn(1)-Cl(1)	103.27(14)	C(3')-C(2')-N(1')	121.9(5)
N(3)-Zn(1)-Cl(1)	98.03(13)	C(1')-C(2')-N(1')	116.5(4)
N(1)-Zn(1)-Cl(1)	175.50(12)	N(2')-C(5')-C(6')	121.0(6)
C(2A)-N(1A)-C(10A)	113.0(4)	N(2')-C(5')-C(4')	116.3(5)
C(2A)-N(1A)-C(4A)	114.1(4)	C(6')-C(5')-C(4')	122.7(6)
C(10A)-N(1A)-C(4A)	110.8(4)	N(3A)-C(11A)-C(12A)	121.5(5)
C(2A)-N(1A)-Zn(1A)	103.7(3)	N(3A)-C(11A)-C(10A)	117.3(5)
C(10A)-N(1A)-Zn(1A)	108.7(3)	C(12A)-C(11A)-C(10A)	121.1(5)
C(4A)-N(1A)-Zn(1A)	106.0(3)	N(2')-C(9')-C(8')	122.1(6)
C(1)-O(1)-Zn(1)	114.4(3)	N(1')-C(10')-C(11')	111.4(4)
C(1')-O(1')-Zn(1')	114.1(3)	N(1A)-C(4A)-C(5A)	111.0(4)
C(2B)-N(1B)-C(4B)	112.9(4)	C(6B)-C(7B)-C(8B)	119.0(5)
C(2B)-N(1B)-C(10B)	112.9(4)	N(3)-C(11)-C(12)	121.0(5)
C(4B)-N(1B)-C(10B)	110.7(4)	N(3)-C(11)-C(10)	117.8(5)
C(2B)-N(1B)-Zn(1B)	104.4(3)	C(12)-C(11)-C(10)	121.1(5)
C(4B)-N(1B)-Zn(1B)	109.2(3)	C(7B)-C(6B)-C(5B)	119.6(6)
C(10B)-N(1B)-Zn(1B)	106.3(3)	C(15B)-C(14B)-C(13B)	117.8(6)
C(1B)-O(1B)-Zn(1B)	114.9(3)	N(2A)-C(5A)-C(6A)	122.2(5)
C(1A)-O(1A)-Zn(1A)	114.1(3)	N(2A)-C(5A)-C(4A)	116.1(5)
C(2')-N(1')-C(10')	112.6(4)	C(6A)-C(5A)-C(4A)	121.6(5)
C(2')-N(1')-C(4')	114.4(4)	C(13')-C(12')-C(11')	118.2(6)
C(10')-N(1')-C(4')	111.7(4)	C(15')-C(14')-C(13')	118.7(5)
C(2')-N(1')-Zn(1')	103.9(3)	C(13B)-C(12B)-C(11B)	119.3(6)
C(10')-N(1')-Zn(1')	106.8(3)	N(1)-C(10)-C(11)	110.0(4)
C(4')-N(1')-Zn(1')	106.6(3)	C(7')-C(8')-C(9')	118.2(6)
C(11')-N(3')-C(15')	119.5(5)	C(7')-C(6')-C(5')	119.4(6)
C(11')-N(3')-Zn(1')	116.1(4)	C(7)-C(8)-C(9)	119.2(6)
C(15')-N(3')-Zn(1')	124.1(4)	C(15)-C(14)-C(13)	118.8(5)
C(2)-N(1)-C(10)	113.0(4)	C(13A)-C(14A)-C(15A)	119.3(5)
C(2)-N(1)-C(4)	112.4(4)	N(1B)-C(4B)-C(5B)	111.8(4)
C(10)-N(1)-C(4)	111.1(4)	C(7A)-C(8A)-C(9A)	118.7(5)
C(2)-N(1)-Zn(1)	103.8(3)	N(1)-C(4)-C(5)	112.7(4)
C(10)-N(1)-Zn(1)	110.0(3)	C(9B)-C(8B)-C(7B)	118.7(5)
C(4)-N(1)-Zn(1)	106.1(3)	N(3)-C(15)-C(14)	122.6(5)
O(1A)-C(1A)-C(3A)	121.0(5)	C(5A)-C(6A)-C(7A)	118.9(6)
O(1A)-C(1A)-C(2A)	122.0(5)	C(12')-C(13')-C(14')	119.7(5)
C(3A)-C(1A)-C(2A)	116.9(5)	C(5)-C(6)-C(7)	118.0(6)
C(11B)-N(3B)-C(15B)	118.6(5)	N(3A)-C(15A)-C(14A)	122.2(5)

C(11B)-N(3B)-Zn(1B)	117.0(4)	C(8A)-C(7A)-C(6A)	119.2(6)
C(15B)-N(3B)-Zn(1B)	122.6(4)	N(2)-C(9)-C(8)	122.3(6)
C(9')-N(2')-C(5')	119.4(5)	N(1')-C(4')-C(5')	109.2(4)
C(9')-N(2')-Zn(1')	122.8(4)	C(12B)-C(13B)-C(14B)	119.7(6)
C(5')-N(2')-Zn(1')	116.3(4)	C(8)-C(7)-C(6)	119.4(6)
C(11A)-N(3A)-C(15A)	118.9(5)	C(12)-C(13)-C(14)	118.6(5)
C(11A)-N(3A)-Zn(1A)	116.8(3)	C(6')-C(7')-C(8')	119.8(6)
C(15A)-N(3A)-Zn(1A)	124.0(4)	C(2A)#1-C(3A)-C(1A)	121.2(5)
O(1)-C(1)-C(3')	120.9(5)	C(9A)-N(2A)-C(5A)	118.3(5)
O(1)-C(1)-C(2)	121.9(4)	C(9A)-N(2A)-Zn(1A)	124.5(4)
C(3')-C(1)-C(2)	117.2(5)	C(5A)-N(2A)-Zn(1A)	116.2(3)
N(3')-C(15')-C(14')	121.9(6)	O(1')-C(1')-C(3)	121.0(5)
N(3')-C(11')-C(12')	121.8(5)	O(1')-C(1')-C(2')	121.6(5)
N(3')-C(11')-C(10')	117.3(5)	C(3)-C(1')-C(2')	117.4(5)
C(12')-C(11')-C(10')	120.8(5)	C(15)-N(3)-C(11)	119.0(5)
C(5B)-N(2B)-C(9B)	119.3(5)	C(15)-N(3)-Zn(1)	122.8(4)
C(5B)-N(2B)-Zn(1B)	117.3(4)		
C(9B)-N(2B)-Zn(1B)	122.8(4)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 -x+1,-y,-z

Table S3. Bond lengths [Å] and angles [°] of **3.**

O(1)-C(1)	1.230(4)	N(2)-H(2N)	1.07(4)	C(6)-C(7)	1.349(5)
C(1)-C(3)	1.443(5)	C(10)-C(11)	1.511(5)	C(6)-C(5)	1.349(5)
C(1)-C(2)	1.508(5)	C(14)-C(15)	1.370(6)	C(4)-C(5)	1.511(4)
N(1)-C(2)	1.375(4)	C(14)-C(13)	1.382(6)	C(12)-C(11)	1.375(5)
N(1)-C(4)	1.451(4)	C(8)-C(7)	1.372(6)	C(12)-C(13)	1.390(5)
N(1)-C(10)	1.462(4)	C(3)-C(2)#1	1.355(5)		
N(3)-C(11)	1.338(5)	C(9)-C(8)	1.379(6)		
N(3)-C(15)	1.345(5)	C(9)-N(2)	1.393(5)		

O(1)-C(1)-C(3)	120.8(3)	N(1)-C(2)-C(1)	117.5(3)
O(1)-C(1)-C(2)	120.2(3)	C(6)-C(5)-N(2)	119.1(3)
C(3)-C(1)-C(2)	118.8(3)	C(6)-C(5)-C(4)	115.4(3)
C(2)-N(1)-C(4)	119.9(3)	N(2)-C(5)-C(4)	125.5(3)
C(2)-N(1)-C(10)	123.7(3)	C(5)-N(2)-C(9)	118.7(3)
C(4)-N(1)-C(10)	115.6(3)	C(5)-N(2)-H(2N)	119(2)
C(11)-N(3)-C(15)	123.2(3)	C(9)-N(2)-H(2N)	123(2)
C(7)-C(6)-C(5)	123.0(3)	N(1)-C(10)-C(11)	113.3(3)
N(1)-C(4)-C(5)	113.7(3)	C(15)-C(14)-C(13)	118.7(4)
C(11)-C(12)-C(13)	119.0(4)	N(3)-C(15)-C(14)	119.6(4)
C(2)#1-C(3)-C(1)	121.5(3)	N(3)-C(11)-C(12)	119.0(3)
C(8)-C(9)-N(2)	120.6(3)	N(3)-C(11)-C(10)	118.7(3)
C(3)#1-C(2)-N(1)	123.0(3)	C(12)-C(11)-C(10)	122.3(3)
C(3)#1-C(2)-C(1)	119.1(3)	C(7)-C(8)-C(9)	119.2(3)
C(14)-C(13)-C(12)	120.4(4)	C(6)-C(7)-C(8)	119.3(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z

Table S4. Bond lengths [Å] and angles [°] of **4.**

O(1)-C(1)	1.3665(17)	N(2)-C(9)	1.3441(19)	O(2W)-H(3W)	0.89(3)
O(1)-H(1O)	0.86(3)	N(2)-C(5)	1.3450(18)	O(2W)-H(4W)	0.90(3)
O(1W)-H(1W)	0.76(2)	N(2)-H(2N)	0.90(2)	C(2)-C(3)#1	1.3973(19)
O(1W)-H(2W)	0.83(3)	C(6)-C(5)	1.381(2)	C(9)-C(8)	1.371(2)
N(1)-C(2)	1.4312(17)	C(6)-C(7)	1.387(2)	C(15)-C(14)	1.375(2)
N(1)-C(4)	1.4621(17)	C(1)-C(3)	1.3905(19)	C(13)-C(12)	1.388(2)
N(1)-C(10)	1.4750(17)	C(1)-C(2)	1.3995(19)	C(13)-C(14)	1.391(2)
N(3)-C(11)	1.3441(18)	C(4)-C(5)	1.5032(18)	C(11)-C(12)	1.383(2)
N(3)-C(15)	1.3470(19)	C(3)-C(2)#1	1.3974(19)	C(8)-C(7)	1.392(2)
N(3)-H(1N)	0.89(2)	C(10)-C(11)	1.5065(18)		

C(1)-O(1)-H(1O)	107.7(16)	N(1)-C(10)-C(11)	111.30(11)
H(1W)-O(1W)-H(2W)	105(2)	H(3W)-O(2W)-H(4W)	100(2)
C(2)-N(1)-C(4)	115.41(11)	C(3)#1-C(2)-C(1)	118.12(12)
C(2)-N(1)-C(10)	114.63(10)	C(3)#1-C(2)-N(1)	122.65(12)
C(4)-N(1)-C(10)	110.10(11)	C(1)-C(2)-N(1)	119.19(12)
C(11)-N(3)-C(15)	123.52(13)	N(2)-C(5)-C(6)	118.37(13)
C(11)-N(3)-H(1N)	120.7(13)	N(2)-C(5)-C(4)	118.37(13)
C(15)-N(3)-H(1N)	115.8(13)	C(6)-C(5)-C(4)	123.09(13)
C(9)-N(2)-C(5)	123.05(13)	N(2)-C(9)-C(8)	120.22(14)
C(9)-N(2)-H(2N)	116.5(12)	N(3)-C(15)-C(14)	119.81(13)
C(5)-N(2)-H(2N)	120.4(12)	C(12)-C(13)-C(14)	120.22(14)
C(5)-C(6)-C(7)	119.83(14)	N(3)-C(11)-C(12)	118.24(13)
O(1)-C(1)-C(3)	121.60(13)	N(3)-C(11)-C(10)	117.67(12)
O(1)-C(1)-C(2)	118.46(12)	C(12)-C(11)-C(10)	124.02(12)
C(3)-C(1)-C(2)	119.93(13)	C(9)-C(8)-C(7)	118.45(14)
N(1)-C(4)-C(5)	113.39(11)	C(6)-C(7)-C(8)	119.90(14)
C(1)-C(3)-C(2)#1	121.95(13)	C(15)-C(14)-C(13)	118.43(14)
C(11)-C(12)-C(13)	119.74(13)		

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z+1

Table S5. Principal singlet-singlet excitations, absorption maxima, λ, oscillator strengths, f, of the principal electronic transitions in the simulated absorption spectra of $[H_2BBQ]^{2+}[ZnCl_4]^{2-}$, $[H_2BBQ]^{2+}$ and [BBQ] molecules calculated by the TDDFT/CAM-B3LYP/6-31G(d,p)/PCM computational protocol.

Excitation (% composition)	λ(nm)	f (au)
$[H_2BBQ]^{2+}[ZnCl_4]^{2-}$		
HOMO-22 → LUMO (16%) HOMO-17 → LUMO+(21%) HOMO→ LUMO+9 (19%)	202	0.162
HOMO-9 → LUMO+4 (13%) HOMO-8 → LUMO+4 (35%) HOMO-17 → LUMO+8 (8%)	232	0.157
HOMO-1 → LUMO (96%)	330	0.612
HOMO-15 → LUMO (20%) HOMO-12 → LUMO (56%) HOMO-11 → LUMO (11%)	368	0.0015
HOMO → LUMO (97%)	461	0.0005
$[H_2BBQ]^{2+}$		
HOMO-14 → LUMO (12%) HOMO-1 → LUMO+6 (20%) HOMO → LUMO+9 (10%)	192	0.197
HOMO-14 → LUMO (13%) HOMO-11 → LUMO (24%) HOMO-9 → LUMO (19%) HOMO → LUMO+9 (27%)	203	0.274
HOMO-7 → LUMO+2 (13%) HOMO-6 → LUMO+1 (22%) HOMO-5 → LUMO+1 (10%) HOMO-4 → LUMO+2 (20%)	232	0.209
HOMO-1 → LUMO (97%)	329	0.647
HOMO-4 → LUMO (67%) HOMO-7 → LUMO (21%)	366	0.0006
HOMO → LUMO (98%)	456	0.0000
[BBQ]		
HOMO-16 → LUMO (11%) HOMO-1 → LUMO+2 (10%) HOMO → LUMO+9 (12%)	196	0.175
HOMO-4 → LUMO+2 (29%) HOMO-3 → LUMO+2 (24%)	226	0.109
HOMO-4 → LUMO (45%) HOMO-3 → LUMO (22%)	340	0.745
HOMO-11 → LUMO (10%) HOMO-6→ LUMO (24%) HOMO-2 → LUMO (40%)	380	0.004
HOMO → $LUMO^{\beta}$ (98%)	493	0.0007

Table S6. Cartesian Coordinates and energies of [BBQ], $[H_2BBQ]^{2+}$ and $[H_2BBQ]^{2+}[ZnCl_4]^{2-}$ molecules in their singlet ground and triplet excited states calculated by the BP86/6-31G(d,p)/PCM computational protocol at the /6-31G(d,p)/PCM level of theory in aqueous solution.

[BBQ] (singlet)

O,0,0.6812195932,-1.3057063314,1.0180767125
O,0,2.5350415298,3.3264618367,-1.1160158576
N,0,-0.374794012,2.922227076,-0.849716535
N,0,0.2575238557,5.7607697233,0.2477825722
N,0,3.5099250833,-0.6772932206,1.2282432045
N,0,-1.855717537,3.2663475674,1.6101912591
C,0,1.1063063691,-0.1800619554,0.6496999759
C,0,-0.0648196931,6.88349351,0.9197986709
C,0,-0.5076941792,5.4310341906,-0.8212522025
C,0,2.0736646394,2.3030432603,-0.5504753612
N,0,4.802626827,-3.565521357,2.160933934
N,0,4.9438153997,-1.4627307525,-1.1389244859
C,0,0.1990472508,0.8198791968,0.1618710905
C,0,2.5949639463,0.1647364954,0.6635724184
C,0,2.7248481072,-3.8896856231,0.9475696222
C,0,2.9748838414,1.3329070572,0.012317478
C,0,5.4895136801,-0.5180519475,-0.3427227113
C,0,0.5680671997,2.0357538748,-0.4100596666
C,0,-2.3950190048,2.4871573932,0.6505237221
C,0,-2.4305119735,3.2348895343,2.8322210748
C,0,-0.0988843701,4.179456301,-1.5848109767
C,0,3.5884323334,-3.1232936211,1.7543008927
C,0,-1.5956384522,6.2163585738,-1.2474662543
C,0,-1.1341139441,7.7273819337,0.5742832643
C,0,3.1915388096,-1.7309916868,2.2234166471
C,0,-3.5501025096,2.4530269955,3.1519505319
C,0,-3.5136013402,1.6592046985,0.8736560472
C,0,6.5431095374,-0.8568002396,-2.8667773147
C,0,4.3889216451,-5.6384959826,0.964449983
C,0,4.9462951972,-0.3991127655,1.0803697135
C,0,5.1822576737,-4.7993153716,1.7601860178
C,0,-1.9143221832,7.3842004861,-0.5375286237
C,0,6.5651489078,0.2964897666,-0.7475278016
C,0,5.4685509302,-1.6125118181,-2.3741612687
C,0,-1.7980625347,2.563613021,-0.7561692025
C,0,7.1030327626,0.1194317836,-2.0295074719
C,0,3.1316025662,-5.1700786653,0.5510989543
C,0,-4.1028200219,1.6476563559,2.144718327
H,0,0.57155611,7.1277225214,1.7805538237
H,0,-0.848456387,0.5290590626,0.2511697027
H,0,1.7594502903,-3.4684982938,0.652699927
H,0,4.0248684188,1.6097985376,-0.0941263988
H,0,-1.966677309,3.8732590132,3.5951313348
H,0,-0.6481131963,4.1316549987,-2.54219086
H,0,0.981454707,4.2074510669,-1.7797795722
H,0,-2.1781820232,5.920473582,-2.1260076446
H,0,-1.3403981224,8.6274897901,1.1604540693
H,0,2.1173617233,-1.6904714114,2.4301559967
H,0,3.7639235291,-1.5000849995,3.1394266037
H,0,-3.9707177098,2.4732577067,4.1612646694
H,0,-3.9111313627,1.0363873281,0.0655688462
H,0,6.9239795303,-1.0280809627,-3.877553311
H,0,4.7485264235,-6.6316646315,0.6802064983
H,0,5.470047036,-1.140677135,1.7084088241
H,0,5.1835332561,0.6014129969,1.4903258357
H,0,6.1708675249,-5.1319133061,2.1013666119
H,0,-2.755262405,8.0116954934,-0.8490120336
H,0,6.9691901751,1.0554027572,-0.0696012488
H,0,5.0020704297,-2.3827668792,-3.0018391325
H,0,-1.9697585324,1.6034636762,-1.2789429486
H,0,-2.3537087494,3.3303069492,-1.3216679916
H,0,7.9388540838,0.7384195281,-2.3701178101
H,0,2.4793615273,-5.7939707769,-0.0683283864
H,0,-4.9731748986,1.0155040939,2.3463182146

Sum of electronic and zero-point Energies= -1637.325134
Sum of electronic and thermal Energies= -1637.292487
Sum of electronic and thermal Enthalpies= -1637.291543
Sum of electronic and thermal Free Energies= -1637.396305

[BBQ] (triplet)

```
O,0,1.1226320432,-0.9872795543,1.784881249
 O,0,2.4500139103,3.188297672,-1.5550364988
 N,0,-0.3567357754,2.6272426307,-0.9599178717
 N,0,0.2629155993,4.8085724019,0.9481086645
 N,0,3.9417341185,-0.4156818744,1.1886846335
 N,0,-2.5669493014,1.9479522779,1.1242898243
 C,0,1.4814660479,0.0097441194,1.0669313608
 C,0,0.1019944131,5.6753287167,1.9694690487
 C,0,-0.4749044029,5.0068041805,-0.1659045292
 C,0,2.1005810663,2.2824642055,-0.7191109305
 N,0,5.5002647124,-3.0137431383,2.5470220684
 N,0,4.6609878683,-1.6780356448,-1.3216568638
 C,0,0.4736379928,0.8761279911,0.5017185958
 C,0,2.8788273639,0.3393720597,0.7291001867
 C,0,3.2351634116,-3.5451999935,1.8494633151
 C,0,3.1085233716,1.4599417963,-0.1003541018
 C,0,5.374073839,-0.6157852068,-0.8843057624
 C,0,0.705723311,1.9475740234,-0.3871481076
 C,0,-2.7451263672,2.3873290857,-0.143005068
 C,0,-3.5144582725,2.2529227954,2.0335161374
 C,0,-0.2373204173,4.0412137535,-1.3257062054
 C,0,4.2257853433,-2.640916752,2.2798183847
 C,0,-1.3839655408,6.0742517186,-0.2977905288
 C,0,-0.7727659303,6.7724250083,1.9310809099
 C,0,3.8911667822,-1.1676964971,2.4620646062
 C,0,-4.6699485943,2.9932144793,1.7344974488
 C,0,-3.8693649238,3.1348618947,-0.5377999443
 C,0,5.6177480514,-1.3436986928,-3.5316727055
 C,0,4.8923001247,-5.2955036902,1.9750893433
 C,0,5.2819075412,-0.2805930401,0.601979076
 C,0,5.8115270607,-4.3199438508,2.3875814376
 C,0,-1.5295270301,6.9740785631,0.7677404452
 C,0,6.2285893838,0.128088626,-1.7205121885
 C,0,4.7879387015,-2.0173158396,-2.6219242471
 C,0,-1.6703924951,1.9922591291,-1.1546531016
 C,0,6.3557324406,-0.2462348676,-3.0654980153
 C,0,3.5743489927,-4.8959212188,1.7009894033
 C,0,-4.849136971,3.4411929116,0.41873117
 H,0,0.7102351496,5.4839711831,2.8628684448
 H,0,-0.5509561157,0.6828067313,0.8375049602
 H,0,2.2280800556,-3.1674989375,1.6470126957
 H,0,4.1297455228,1.7443640531,-0.3655744033
 H,0,-3.3418297877,1.8822669924,3.0515946395
 H,0,-0.9464929597,4.250505133,-2.142424002
 H,0,0.8041904598,4.1727949424,-1.6908015178
 H,0,-1.9646501269,6.193695563,-1.2176215013
 H,0,-0.855220638,7.4450461203,2.7894697291
 H,0,2.8774413582,-1.0599141171,2.8671854829
 H,0,4.6260923303,-0.7202500756,3.1569607881
 H,0,-5.4051846332,3.2076930172,2.5150593258
 H,0,-3.9757248504,3.4643842829,-1.575928402
 H,0,5.6778395601,-1.6706528901,-4.5735850272
 H,0,5.2040079259,-6.3389846498,1.8726287961
 H,0,5.9282921718,-0.9831895817,1.1577267933
 H,0,5.690739785,0.7321065746,0.7862474184
 H,0,6.8507433607,-4.5958461931,2.6069714118
 H,0,-2.2272586299,7.8139758056,0.6916805024
 H,0,6.7816376509,0.9849566997,-1.3221543646
 H,0,4.1935750235,-2.8792026029,-2.9518296932
 H,0,-1.5254636263,0.9008116358,-1.1320736703
 H,0,-2.0140515864,2.2613758791,-2.1694931331
 H,0,7.0129965295,0.3144429769,-3.7373753465
 H,0,2.8252880664,-5.6259612031,1.3779591213
 H,0,-5.7353594658,4.0190924807,0.1392303125


Sum of electronic and zero-point Energies=          -1637.285652
 Sum of electronic and thermal Energies=            -1637.253014
 Sum of electronic and thermal Enthalpies=          -1637.252070
 Sum of electronic and thermal Free Energies=       -1637.357335
```

$[BBQH_2]^{2+}$ (singlet)

O,0,-0.2332241621,1.4203493421,-1.3084760589
O,0,4.0521561062,-1.1603998047,0.7323296455
N,0,1.4973505022,-2.4050385266,0.9408922916
N,0,3.3080362116,-4.4008042403,-0.027156381
N,0,2.3216374701,2.6647323855,-1.5175261761
N,0,0.868965462,-4.1046435333,-1.2602340142
C,0,0.7679371737,0.8042041038,-0.8775675953
C,0,4.1999042228,-5.2095695692,-0.6573341861
C,0,3.5555537007,-3.8497684298,1.1869915959
C,0,3.0510262232,-0.5444031671,0.3011394424
N,0,0.5109321858,4.6606402684,-0.5500035039
N,0,2.9498895598,4.3642233829,0.6836593432
C,0,0.6342467251,-0.5098052571,-0.294117765
C,0,2.1510708999,1.4395608426,-0.9114822981
C,0,-0.9496482268,4.3990182874,-2.4049004426
C,0,3.1847331593,0.7695680253,-0.2824075305
C,0,3.9707255806,3.8342442578,-0.0298538696
C,0,1.6679248127,-1.1798252677,0.3349120545
C,0,-0.1518106847,-3.5745425038,-0.5467252606
C,0,0.6111052763,-4.6069925518,-2.4886178229
C,0,2.4826169104,-3.0054139681,1.8528638951
C,0,0.2636556095,4.1096287339,-1.7642127279
C,0,4.7691452773,-4.1388088988,1.8272869579
C,0,5.4176498286,-5.5164811704,-0.0626086294
C,0,1.3364769807,3.2648805006,-2.4297248868
C,0,-0.6708192014,-4.6155069426,-3.0513768805
C,0,-1.46624128,-3.5434640728,-1.0377931481
C,0,4.4896070571,4.8750317666,2.4748736861
C,0,-1.5983427112,5.7769423829,-0.5152457266
C,0,3.63827695,3.3184013778,-1.4265126631
C,0,-0.3808836971,5.4696999337,0.0798765878
C,0,5.7017080898,-4.9737276384,1.2037891287
C,0,5.2851497677,3.8032162365,0.4612304184
C,0,3.2076889223,4.8664794772,1.9120755147
C,0,0.1806787004,-3.0586227047,0.8498919586
C,0,5.5490103674,4.3368450941,1.7304458947
C,0,-1.8821578453,5.2342272467,-1.7817161792
C,0,-1.7301639395,-4.0771711867,-2.3069587962
H,0,2.346956918,-4.2145546841,-0.5287832045
H,0,3.8965314007,-5.5918985077,-1.6331837654
H,0,1.4717111713,4.4742277739,-0.0481688579
H,0,-0.3817982967,-0.9045814957,-0.3347815541
H,0,-1.1534497652,3.9586368748,-3.3835391507
H,0,4.2007649039,1.1643715842,-0.2417056863
H,0,1.4674010477,-5.0166774102,-3.0336656618
H,0,1.9244820034,-3.6505671728,2.5541838196
H,0,2.9828701475,-2.2319975239,2.44981342
H,0,4.973127714,-3.6983971783,2.8058827183
H,0,6.1255317818,-6.1667304051,-0.5792534927
H,0,0.8361233546,2.4912934423,-3.0263723664
H,0,1.8946783913,3.9096574124,-3.1313646451
H,0,-0.8281574507,-5.0336311115,-4.0484601781
H,0,-2.2654384741,-3.1044177997,-0.4336856393
H,0,4.6468781114,5.2930953619,3.4719955516
H,0,-2.3061935582,6.4274166598,0.0011457467
H,0,3.6348093288,4.1702529298,-2.1256343886
H,0,4.4315494932,2.631192,-1.771894505
H,0,-0.0776865744,5.8519384379,1.055813859
H,0,6.6507537942,-5.1975596955,1.6981595096
H,0,6.0843948297,3.3642895678,-0.1428992673
H,0,2.3513681403,5.2760542008,2.4571617155
H,0,-0.612542915,-2.371318629,1.1952082591
H,0,0.1840337135,-3.9104303749,1.5490665804
H,0,6.5652299055,4.3228068163,2.1346027144
H,0,-2.8309743939,5.4583480804,-2.2763952162
H,0,-2.7463937079,-4.0630863655,-2.7110951871

Sum of electronic and zero-point Energies= -1638.237996
Sum of electronic and thermal Energies= -1638.206272
Sum of electronic and thermal Enthalpies= -1638.205328
Sum of electronic and thermal Free Energies= -1638.303617

$[BBQH_2]^{2+}$ (triplet)

```
O,0,-0.3348596916,1.5156681789,-1.0803683337
 O,0,4.1543953906,-1.2558315314,0.502015675
 N,0,1.5483977005,-2.3689190645,1.0086376561
 N,0,3.3512581845,-4.3820743222,0.0278011243
 N,0,2.2709909629,2.6292374511,-1.5860527247
 N,0,0.9311129484,-4.00548364,-1.2522791133
 C,0,0.7213133419,0.875653742,-0.7672561299
 C,0,4.2277868177,-5.2180106168,-0.5896493338
 C,0,3.6089801293,-3.8212534344,1.2352418306
 C,0,3.0982228787,-0.6158572857,0.1888375685
 N,0,0.4676310705,4.6415522422,-0.6045040412
 N,0,2.8874922902,4.2644496025,0.6761434743
 C,0,0.6406989282,-0.3940229016,-0.084982381
 C,0,2.0789997761,1.4008197409,-0.9756498567
 C,0,-0.9903828586,4.3988544567,-2.4647792561
 C,0,3.1788271315,0.6538042974,-0.4934461453
 C,0,3.9043635009,3.7436944682,-0.0515040739
 C,0,1.7404735583,-1.1407753367,0.3976742304
 C,0,-0.085493106,-3.4838521105,-0.5249172878
 C,0,0.6778881579,-4.4259694241,-2.5111481188
 C,0,2.5590209032,-2.9488598538,1.9030786336
 C,0,0.2103385674,4.0815448928,-1.8123901954
 C,0,4.8100387706,-4.1379731202,1.887298458
 C,0,5.4346432999,-5.547589589,0.0136842544
 C,0,1.2604068111,3.2093265637,-2.480376602
 C,0,-0.5946781615,-4.3576278253,-3.0927307618
 C,0,-1.388949966,-3.3770360728,-1.0323325605
 C,0,4.4128824857,4.6160284773,2.5169737889
 C,0,-1.6156657305,5.8072546973,-0.5904712096
 C,0,3.5666971536,3.3235081853,-1.4771067879
 C,0,-0.4090723273,5.4771746757,0.0131216622
 C,0,5.7251428463,-5.0001313765,1.2770623237
 C,0,5.2077960217,3.6370775026,0.4560045908
 C,0,3.1403431453,4.6842271287,1.935323838
 C,0,0.2524355587,-3.0627661856,0.900357471
 C,0,5.4663705801,4.0860377086,1.759443454
 C,0,-1.9056813127,5.2606923011,-1.8543440708
 C,0,-1.6478701738,-3.8267289416,-2.3354413864
 H,0,2.4070183626,-4.1731718974,-0.4865809045
 H,0,3.9209369122,-5.6036147152,-1.5628241799
 H,0,1.4117996612,4.4323404496,-0.0898940426
 H,0,-0.3826391327,-0.7157113446,0.1225031861
 H,0,-1.1970796159,3.9577809688,-3.4424937223
 H,0,4.2021320289,0.9753321818,-0.7013483397
 H,0,1.5288644136,-4.8317420301,-3.0672512636
 H,0,2.0206461914,-3.5627974116,2.647394432
 H,0,3.0786102464,-2.1545665005,2.4533102729
 H,0,5.0171523719,-3.6961776876,2.8646008859
 H,0,6.1286785214,-6.2200383949,-0.4931657475
 H,0,0.7408870503,2.4151238012,-3.0308149904
 H,0,1.7988066216,3.823451554,-3.2245180294
 H,0,-0.7483779685,-4.7114005855,-4.1150054558
 H,0,-2.1848358873,-2.9476954061,-0.4170139722
 H,0,4.566336702,4.9692275705,3.5394847333
 H,0,-2.3098469097,6.4794101146,-0.0834271796
 H,0,3.5088932804,4.2229421584,-2.1117192869
 H,0,4.3787531874,2.7029175527,-1.8956827969
 H,0,-0.1026119809,5.862129903,0.986678101
 H,0,6.6647431178,-5.2438610048,1.7800062098
 H,0,6.003947838,3.2085249843,-0.1595223744
 H,0,2.2891275908,5.0892865076,2.4915819698
 H,0,-0.559341386,-2.4414578842,1.3184212052
 H,0,0.3097922798,-3.9617681594,1.5356255377
 H,0,6.4742216919,4.0133357019,2.1779294727
 H,0,-2.8450464191,5.5048516593,-2.3575166375
 H,0,-2.6557353534,-3.753858766,-2.7538697466
```

```
Sum of electronic and zero-point Energies=          -1638.186835
 Sum of electronic and thermal Energies=            -1638.154789
 Sum of electronic and thermal Enthalpies=          -1638.153845
 Sum of electronic and thermal Free Energies=       -1638.253840
```

$[BBQH_2][ZnCl_4]^{2-}$ (singlet)

```
O,0,1.1226320432,-0.9872795543,1.784881249
 O,0,2.4500139103,3.188297672,-1.5550364988
 N,0,-0.3567357754,2.6272426307,-0.9599178717
 N,0,0.2629155993,4.8085724019,0.9481086645
 N,0,3.9417341185,-0.4156818744,1.1886846335
 N,0,-2.5669493014,1.9479522779,1.1242898243
 C,0,1.4814660479,0.0097441194,1.0669313608
 C,0,0.1019944131,5.6753287167,1.9694690487
 C,0,-0.4749044029,5.0068041805,-0.1659045292
 C,0,2.1005810663,2.2824642055,-0.7191109305
 N,0,5.5002647124,-3.0137431383,2.5470220684
 N,0,4.6609878683,-1.6780356448,-1.3216568638
 C,0,0.4736379928,0.8761279911,0.5017185958
 C,0,2.8788273639,0.3393720597,0.7291001867
 C,0,3.2351634116,-3.5451999935,1.8494633151
 C,0,3.1085233716,1.4599417963,-0.1003541018
 C,0,5.374073839,-0.6157852068,-0.8843057624
 C,0,0.705723311,1.9475740234,-0.3871481076
 C,0,-2.7451263672,2.3873290857,-0.143005068
 C,0,-3.5144582725,2.2529227954,2.0335161374
 C,0,-0.2373204173,4.0412137535,-1.3257062054
 C,0,4.2257853433,-2.640916752,2.2798183847
 C,0,-1.3839655408,6.0742517186,-0.2977905288
 C,0,-0.7727659303,6.7724250083,1.9310809099
 C,0,3.8911667822,-1.1676964971,2.4620646062
 C,0,-4.6699485943,2.9932144793,1.7344974488
 C,0,-3.8693649238,3.1348618947,-0.5377999443
 C,0,5.6177480514,-1.3436986928,-3.5316727055
 C,0,4.8923001247,-5.2955036902,1.9750893433
 C,0,5.2819075412,-0.2805930401,0.601979076
 C,0,5.8115270607,-4.3199438508,2.3875814376
 C,0,-1.5295270301,6.9740785631,0.7677404452
 C,0,6.2285893838,0.128088626,-1.7205121885
 C,0,4.7879387015,-2.0173158396,-2.6219242471
 C,0,-1.6703924951,1.9922591291,-1.1546531016
 C,0,6.3557324406,-0.2462348676,-3.0654980153
 C,0,3.5743489927,-4.8959212188,1.7009894033
 C,0,-4.849136971,3.4411929116,0.41873117
 H,0,0.7102351496,5.4839711831,2.8628684448
 H,0,-0.5509561157,0.6828067313,0.8375049602
 H,0,2.2280800556,-3.1674989375,1.6470126957
 H,0,4.1297455228,1.7443640531,-0.3655744033
 H,0,-3.3418297877,1.8822669924,3.0515946395
 H,0,-0.9464929597,4.250505133,-2.142424002
 H,0,0.8041904598,4.1727949424,-1.6908015178
 H,0,-1.9646501269,6.193695563,-1.2176215013
 H,0,-0.855220638,7.4450461203,2.7894697291
 H,0,2.8774413582,-1.0599141171,2.8671854829
 H,0,4.6260923303,-0.7202500756,3.1569607881
 H,0,-5.4051846332,3.2076930172,2.5150593258
 H,0,-3.9757248504,3.4643842829,-1.575928402
 H,0,5.6778395601,-1.6706528901,-4.5735850272
 H,0,5.2040079259,-6.3389846498,1.8726287961
 H,0,5.9282921718,-0.9831895817,1.1577267933
 H,0,5.690739785,0.7321065746,0.7862474184
 H,0,6.8507433607,-4.5958461931,2.6069714118
 H,0,-2.2272586299,7.8139758056,0.6916805024
 H,0,6.7816376509,0.9849566997,-1.3221543646
 H,0,4.1935750235,-2.8792026029,-2.9518296932
 H,0,-1.5254636263,0.9008116358,-1.1320736703
 H,0,-2.0140515864,2.2613758791,-2.1694931331
 H,0,7.0129965295,0.3144429769,-3.7373753465
 H,0,2.8252880664,-5.6259612031,1.3779591213
 H,0,-5.7353594658,4.0190924807,0.1392303125
```

$[BBQH_2][ZnCl_4]^{2-}$ (singlet)

Zn	5.187955000	-0.316720000	-0.745070000
Cl	3.044486000	-1.164924000	-1.120072000
Cl	6.459493000	-0.728628000	-2.637429000
Cl	6.090381000	-1.449233000	1.080342000

Cl	5.093639000	1.951513000	-0.320205000
O	0.327090000	1.453245000	1.209456000
O	-3.968029000	-1.188294000	-0.729255000
N	-1.421257000	-2.434890000	-0.918157000
N	-3.296549000	-4.419761000	-0.031821000
N	-2.242953000	2.652658000	1.497721000
N	-0.927742000	-4.184885000	1.291228000
C	-0.676637000	0.812661000	0.819638000
C	-4.227520000	-5.214882000	0.557331000
C	-3.493011000	-3.848195000	-1.245499000
C	-2.967542000	-0.565734000	-0.304682000
N	-0.535836000	4.704590000	0.444606000
N	-3.034738000	4.359562000	-0.649435000
C	-0.541426000	-0.510634000	0.259659000
C	-2.066630000	1.431740000	0.884172000
C	1.033883000	4.453232000	2.209010000
C	-3.104632000	0.749937000	0.274392000
C	-4.001513000	3.793398000	0.109096000
C	-1.583048000	-1.194574000	-0.341515000
C	0.125264000	-3.623147000	0.650112000
C	-0.742100000	-4.687814000	2.532053000
C	-2.383565000	-3.015932000	-1.865338000
C	-0.209773000	4.148000000	1.637547000
C	-4.689620000	-4.104302000	-1.930747000
C	-5.431206000	-5.488685000	-0.081109000
C	-1.232611000	3.287354000	2.358725000
C	0.497840000	-4.661920000	3.181950000
C	1.399876000	-3.550656000	1.233152000
C	-4.679979000	4.857736000	-2.347680000
C	1.548564000	5.857690000	0.297643000
C	-3.583568000	3.259960000	1.476421000
C	0.304026000	5.533897000	-0.228714000
C	-5.660287000	-4.926319000	-1.350227000
C	-5.339890000	3.737496000	-0.311259000
C	-3.370134000	4.873161000	-1.854299000
C	-0.123962000	-3.119184000	-0.767098000
C	-5.684501000	4.282853000	-1.555665000
C	1.914410000	5.309534000	1.540488000
C	1.588193000	-4.082610000	2.517024000
H	-2.340677000	-4.264764000	0.507823000
H	-3.966119000	-5.613200000	1.539240000
H	-1.519919000	4.502885000	-0.002689000
H	0.484231000	-0.887242000	0.259296000
H	1.301508000	4.008372000	3.170008000
H	-4.123861000	1.137198000	0.241499000
H	-1.621308000	-5.126929000	3.014403000
H	-1.811564000	-3.665138000	-2.552202000
H	-2.850399000	-2.230804000	-2.474451000
H	-4.850026000	-3.647336000	-2.909913000
H	-6.170706000	-6.128040000	0.403901000
H	-0.688200000	2.533113000	2.941633000
H	-1.776030000	3.930023000	3.073667000
H	0.598037000	-5.082937000	4.185294000
H	2.215164000	-3.066865000	0.684420000
H	-4.900813000	5.285283000	-3.328593000
H	2.214362000	6.524298000	-0.252941000
H	-3.582330000	4.093475000	2.197469000
H	-4.333331000	2.533610000	1.838265000
H	-0.062299000	5.918143000	-1.182002000
H	-6.596249000	-5.123818000	-1.879655000
H	-6.095106000	3.270427000	0.327613000

H	-2.554355000	5.311392000	-2.437692000
H	0.708335000	-2.462042000	-1.081492000
H	-0.122574000	-3.980539000	-1.454800000
H	-6.720407000	4.249857000	-1.905040000
H	2.886441000	5.545386000	1.981551000
H	2.571179000	-4.035486000	2.994607000

Sum of electronic and zero-point Energies= -5259.000831
Sum of electronic and thermal Energies= -5258.958982
Sum of electronic and thermal Enthalpies= -5258.958038
Sum of electronic and thermal Free Energies= -5259.085160

$[BBQH_2][ZnCl_4]^{2-}$ (triplet)

Zn,0,11.0555338478,6.9302728363,8.7545296255
Cl,0,9.9408309076,6.1063505359,6.8724746898
Cl,0,11.5489056406,9.1580948378,8.3608530218
Cl,0,13.015023087,5.730707281,9.0649629
Cl,0,9.6979320413,6.7109415073,10.6168487587
O,0,6.6726686571,3.6054139912,8.4342105131
O,0,5.8472661163,1.6397361877,3.3566015599
N,0,8.3912463138,2.9335875307,4.0205033997
N,0,9.7653723643,1.0724521502,2.2576641416
N,0,4.2579287064,2.1140532074,7.8434281094
N,0,10.25140355,0.937233322,4.8992176964
C,0,6.4717010591,3.1008067429,7.2810410606
C,0,10.5402787417,0.2500949454,1.5035061809
C,0,9.1027977419,2.1363314568,1.7296745615
C,0,6.0772267065,2.1267091199,4.5195005206
N,0,3.5001270068,4.5479471495,9.1627771318
N,0,2.1413415585,3.7780329542,6.8955831952
C,0,7.4459350225,3.2831342354,6.2295600264
C,0,5.2582260226,2.3561539526,6.9129930468
C,0,4.8704879203,4.0791869366,11.0457458131
C,0,5.1059894205,1.9578997523,5.5677168508
C,0,2.1223800279,2.4655894024,6.56503197
C,0,7.3314836005,2.7961045909,4.9032606131
C,0,10.3264127372,2.1956138093,5.3968424345
C,0,10.7589424385,-0.0848870347,5.6206205747
C,0,8.1525378749,2.94148894,2.5767736682
C,0,4.2996524042,3.6784800959,9.8286911537
C,0,9.2295808409,2.3950571989,0.3548928517
C,0,10.6701579277,0.4544421878,0.1348457582
C,0,4.4773542545,2.2702070775,9.2893598987
C,0,11.3692570394,0.1056665288,6.8674025909
C,0,10.9225300749,2.4730224084,6.6350001647
C,0,0.542526592,4.2253939487,5.1390755183
C,0,3.8023303627,6.2459008176,10.8119534621
C,0,2.9791018863,1.5284103435,7.4118770505
C,0,3.2501334168,5.8048966656,9.616082206
C,0,10.0071262635,1.5513230548,-0.4446582656
C,0,1.3209098289,1.9710119266,5.5239843568
C,0,1.370995403,4.6362924383,6.1902511963
C,0,9.735339464,3.2926117316,4.5192732336
C,0,0.5147829385,2.8640646417,4.8043224977
C,0,4.6214863413,5.3626614225,11.5398109115
C,0,11.4563782141,1.4085884141,7.3779752986
H,0,9.8048021925,0.9202944739,3.355655949
H,0,11.0431930409,-0.5564544506,2.0401147085
H,0,3.0160704206,4.2363604082,8.2283110532
H,0,8.2894972986,3.9196410575,6.517341498

H,0,5.512335622,3.3808398611,11.5873001676
H,0,4.2138217087,1.4204542122,5.2407627298
H,0,10.670689476,-1.0811803381,5.1758110334
H,0,8.1216679526,3.9820731183,2.20172323
H,0,7.1333356686,2.4978792814,2.4446192211
H,0,8.7083739589,3.2538490586,-0.0746404742
H,0,11.2877883043,-0.2212973349,-0.4591071909
H,0,5.4836223429,1.9293647139,9.5630766773
H,0,3.7532751625,1.6113733791,9.8004881506
H,0,11.7648333715,-0.7508143196,7.4186947604
H,0,10.9522543864,3.5045419411,7.001542427
H,0,-0.0610975669,4.9588214779,4.5991493022
H,0,3.5942478545,7.2571090665,11.1654254183
H,0,2.4175163471,1.2606259699,8.321537259
H,0,3.1507494941,0.5833177356,6.8665787525
H,0,2.6003190957,6.4211129698,8.9929881223
H,0,10.1022077793,1.7502042022,-1.5153859446
H,0,1.3342864596,0.9042281583,5.2821740568
H,0,1.4246849591,5.6890632469,6.4846418608
H,0,9.7115945732,4.2512730284,5.0715171289
H,0,10.3750743812,3.4573472108,3.636396882
H,0,-0.1173219052,2.5021773978,3.9883600779
H,0,5.0680162401,5.6799416718,12.485923145
H,0,11.9266820166,1.5964185588,8.3474700504

Sum of electronic and zero-point Energies= -5258.950648
Sum of electronic and thermal Energies= -5258.907941
Sum of electronic and thermal Enthalpies= -5258.906996
Sum of electronic and thermal Free Energies= -5259.036149