Suppporting Information

Mono- and dinuclear zinc complexes bearing identical bis(thiosemicarbazone) ligand that exhibit alkaline phosphatase-like catalytic reactivity

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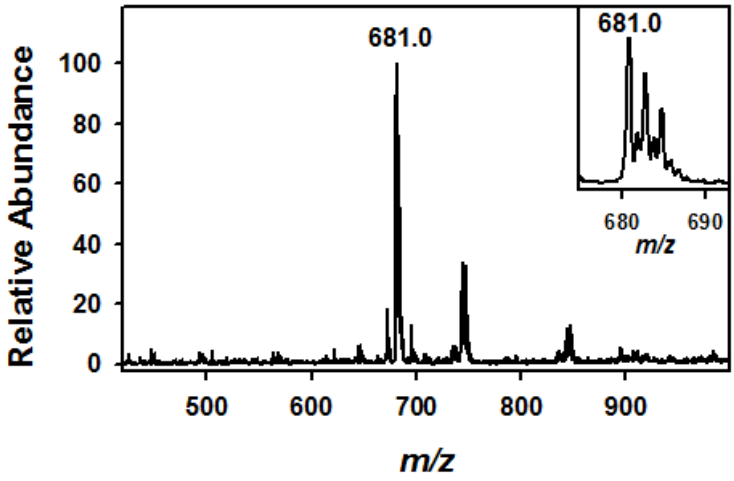

Fig. S1. Negative mode ESI MS spectrum obtained in the reaction of **1** (0.020 mM) with 4-NPP in DMSO at 40 ºC. A prominent peak at *m/z* of 681.0, whose mass and isotopic distribution pattern correspond to $\{Na[Zn(bTSC)(NO_2PO_4C_6H_5)(CH_3CN)_2(CH_3O)]\}^-$ (calculated *m/z* of 681.1). Insets show the observed isotopic distribution patterns of the peak at 681.0.

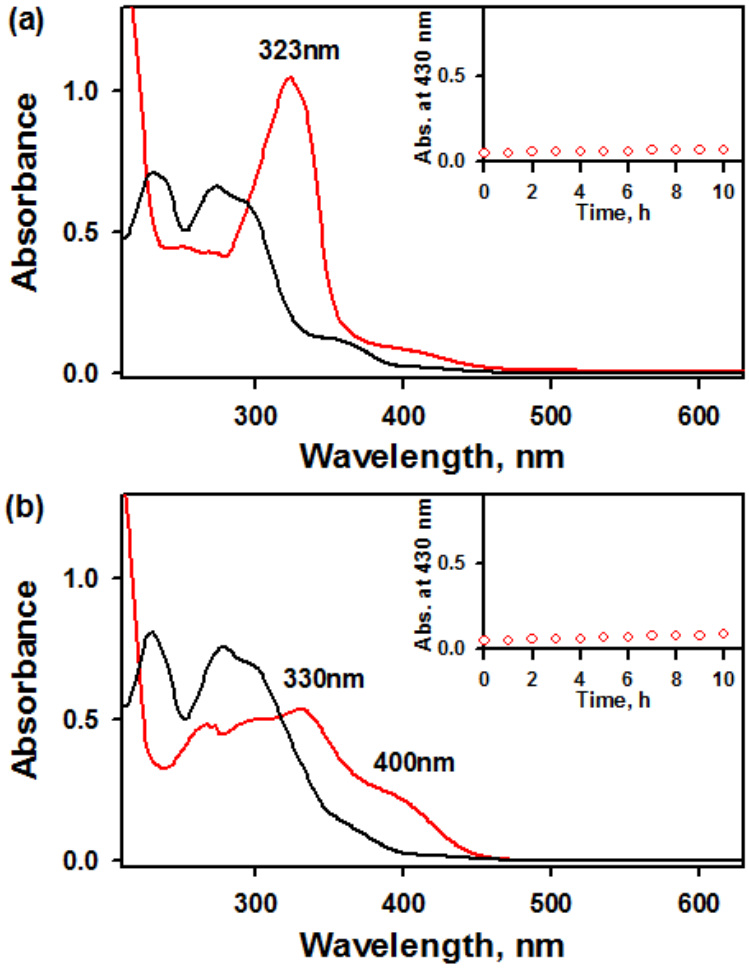

Fig. S2. UV-vis spectra of the reaction of **1** (black line, 2.0 x 10^{-2} mM) with 4-NPP (blue line, 2.0 x 10^{-1} mM) in (a) CH_3CN and (b) CH_3OH at 40 °C. Inset shows the time course monitored at 430 nm. In CH_3OH, the formation of **2** was observed upon addition of 4-NPP suggesting that 4-NPP acts as base in CH_3OH.

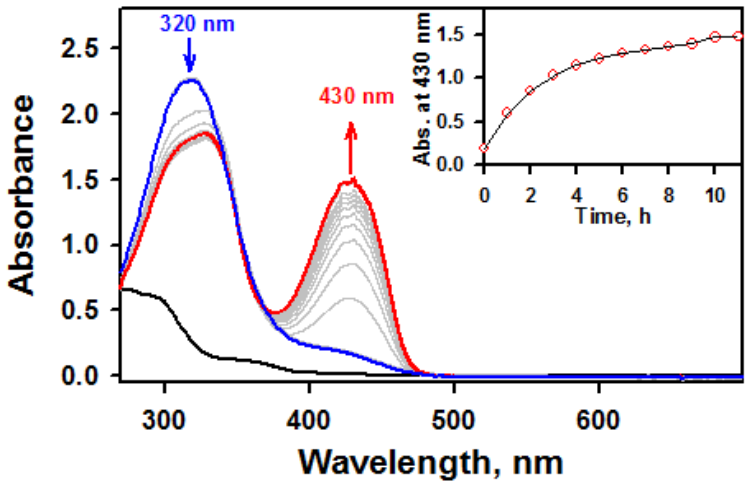

Fig S3. UV-vis spectral changes obtained in the reaction of **1** (black line, 2.0 x 10^{-2} mM) with 4-NPP (blue line, 2.0 x 10^{-1} mM) in DMF at 40 °C. The formation of 4-NP (red line) was detected at 430 nm. Inset shows the time course monitored at 430 nm due to 4-NP (red dot).

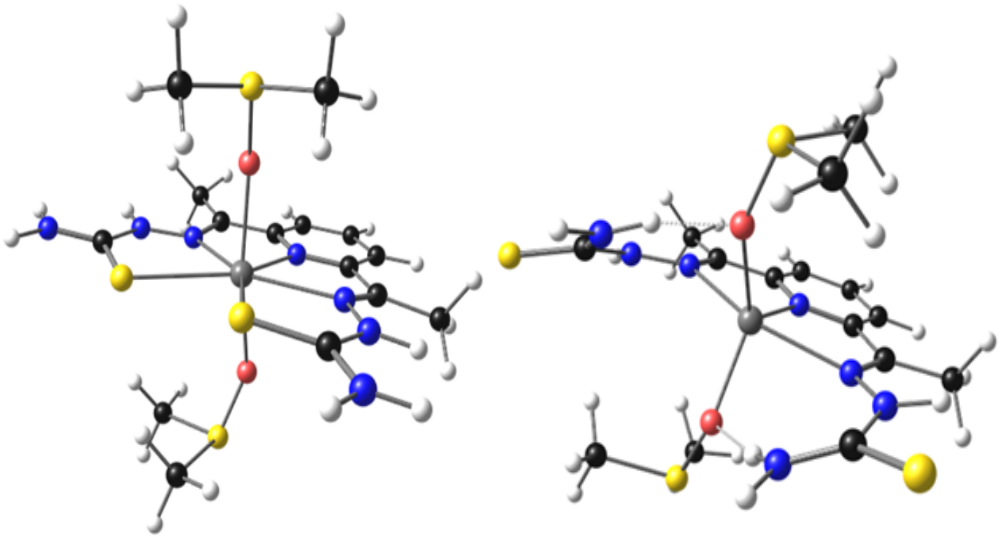

Fig. S4. Two conformations for **1** in DMSO. Left, $\mathbf{1}_{A}$; right, $\mathbf{1}_{B}$,

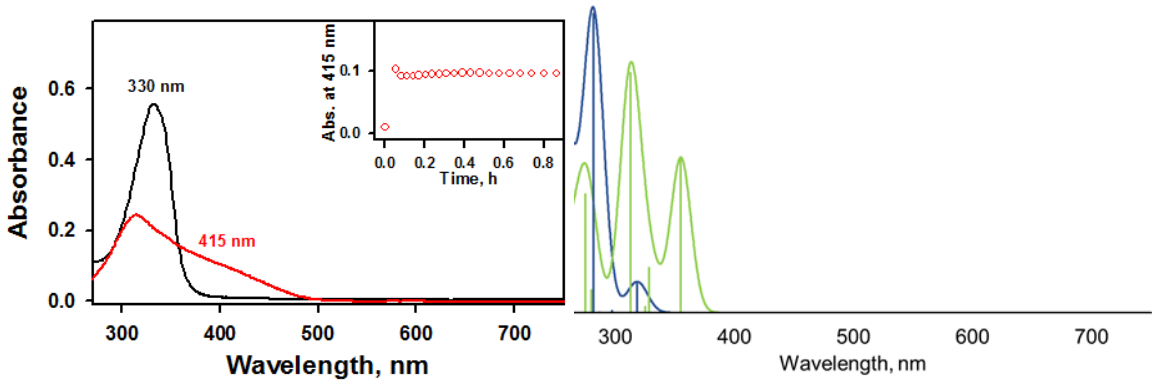

Fig. S5. UV-vis absortion spectra simulation with TDDFT of conformers $\mathbf{1_A}$ and $\mathbf{1_B}$. Left, experimental data from Fig. S15 presented as comparison. Right simulation with conformer $\mathbf{1_A}$ (blue) and conformer $\mathbf{1_B}$, (green).

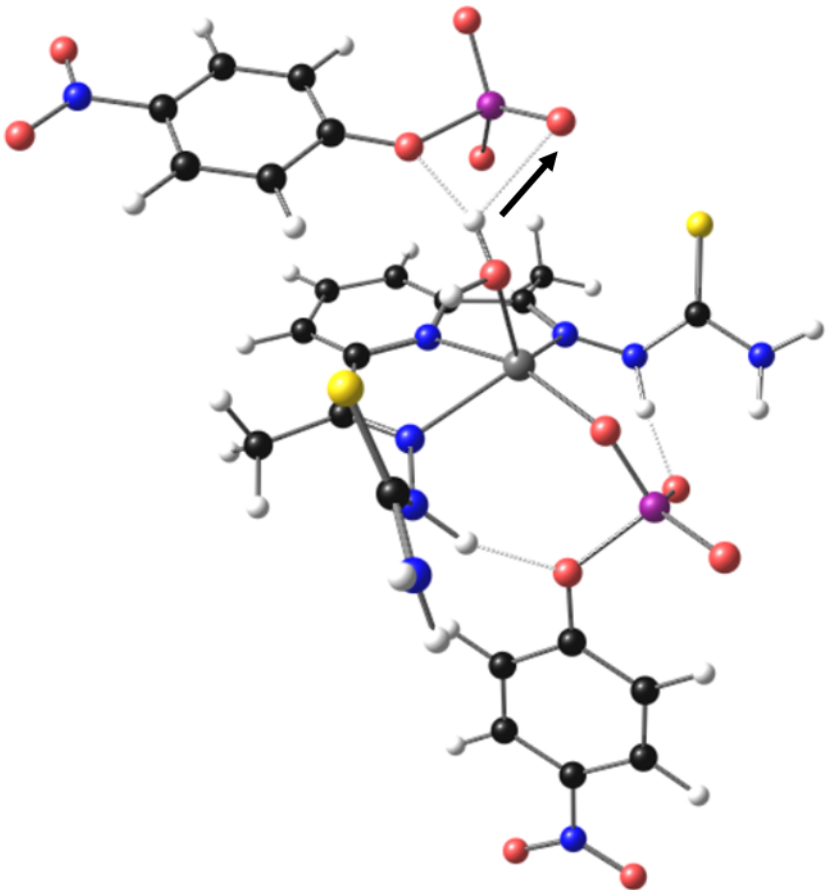

Fig. S6. Deprotonation of water molecule coordinated to Zn. DFT-optimized transition state structure of $[Zn(bTSC)(PO_4C_6H_4NO_2)_2(H_2O)]^{2-}$. Arrows indicate the atom movements in the forward reaction direction. Zn, silver; S, yellow; N, blue; O, red; P, purple; C, black; H.

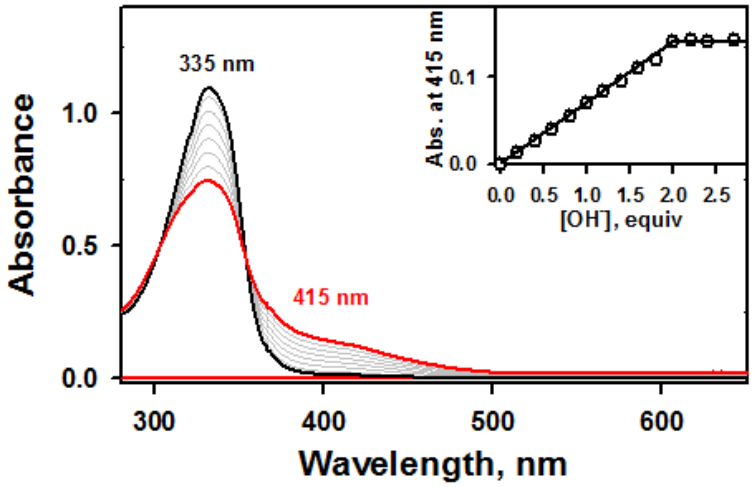

Fig. S7. UV-vis spectral changes showing the formation of **2** (red line, 2.0 x 10^{-2} mM) and disappearance of **1** (black line, 1.0 x 10^{-2} mM) upon addition of KOH to **1** in increment of 0.20 equiv in DMSO at 40 °C. Inset shows the plot of absorbance changes at 415 nm due to **2** (black dot) and against the equivalents of KOH added to **1** in DMSO at 40 °C.

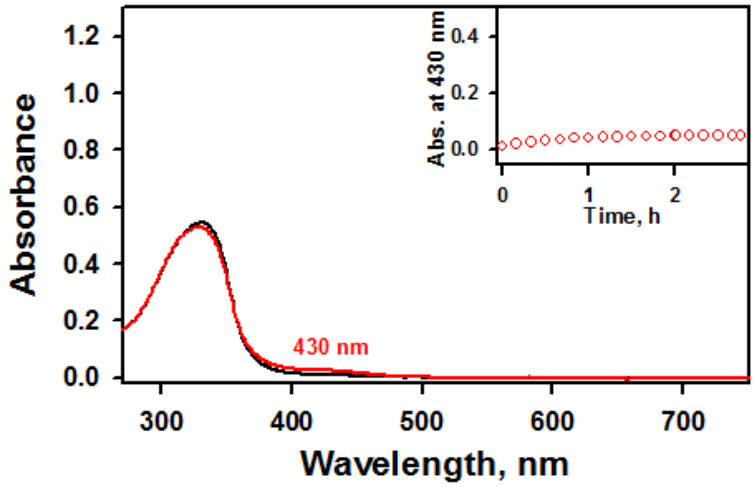

Fig. S8. Overlayed UV-vis spectra of 4-NPP (1.0×10^{-1} mM) in the absence (black line) and presence (red line) of KOH (1.0×10^{-2} mM) in DMSO at 40 °C. Inset shows the plot of absorbance changes at 430 nm due to the formation of 4-NP.

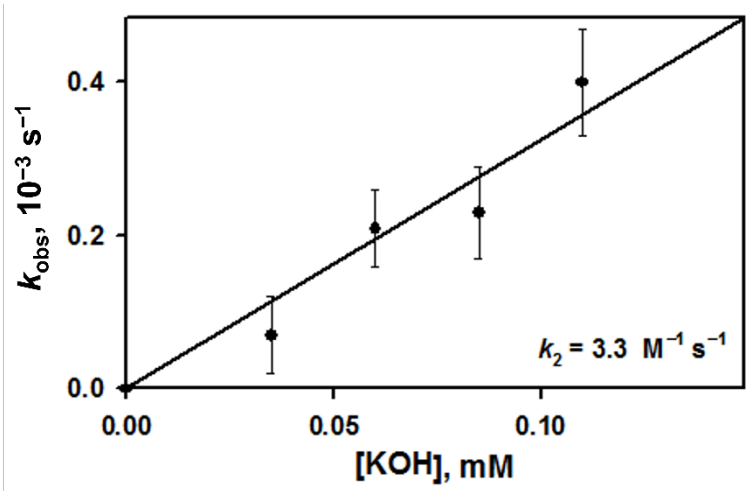

Fig. S9. Plot of pseudo-first-order rate constants (k_{obs}) against the concentrations of KOH to determine the k_2 value for **2** in DMSO at 40 °C.

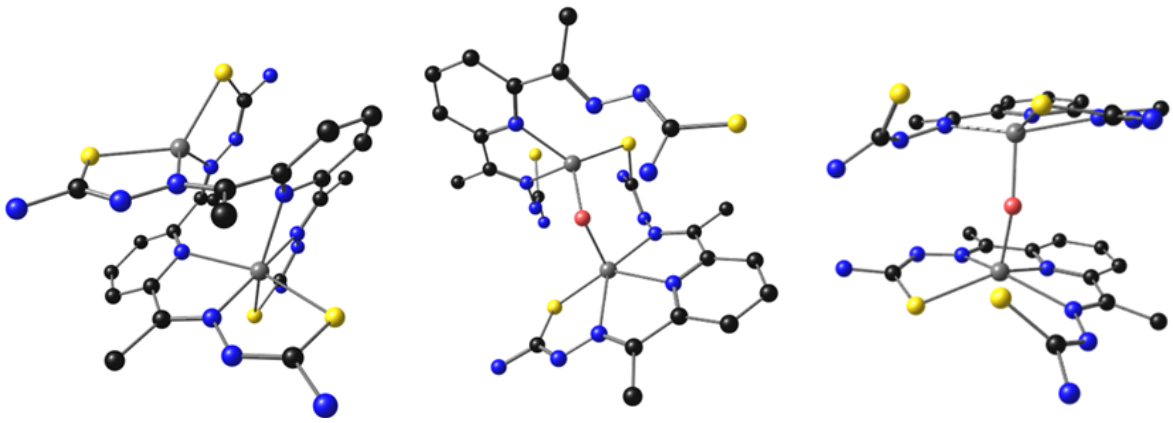

Fig. S10. Three conformations for **2** in DMSO. Left, $\mathbf{2}_{A}$; middle, $\mathbf{2}_{B}$; right, $\mathbf{2}_{C}$. Hydrogens omitted for clarity.

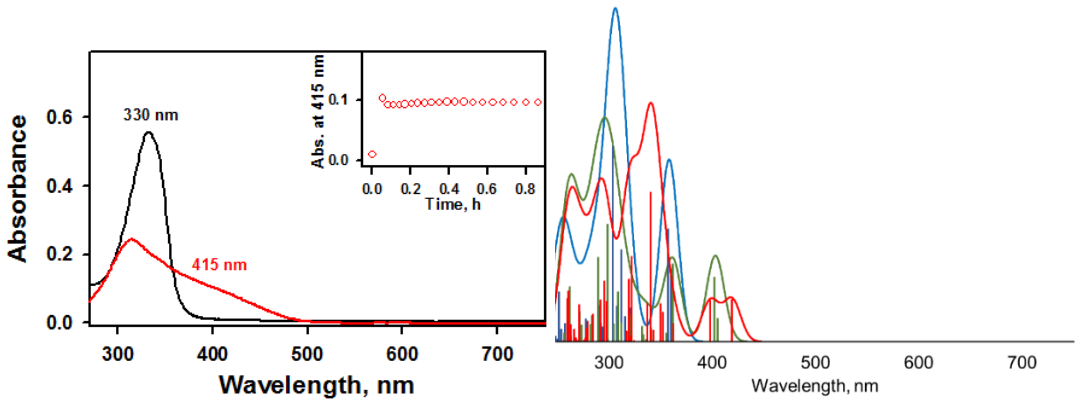

Fig. S11. UV-vis absortion spectra simulation with TDDFT of conformers $\mathbf{2_A}$, $\mathbf{2_B}$, and $\mathbf{2_C}$. Left, experimental data from Fig. S15 is presented as comparison. Right simulation of $\mathbf{2_A}$ (blue), $\mathbf{2_B}$ (green), and $\mathbf{2_C}$ (red).

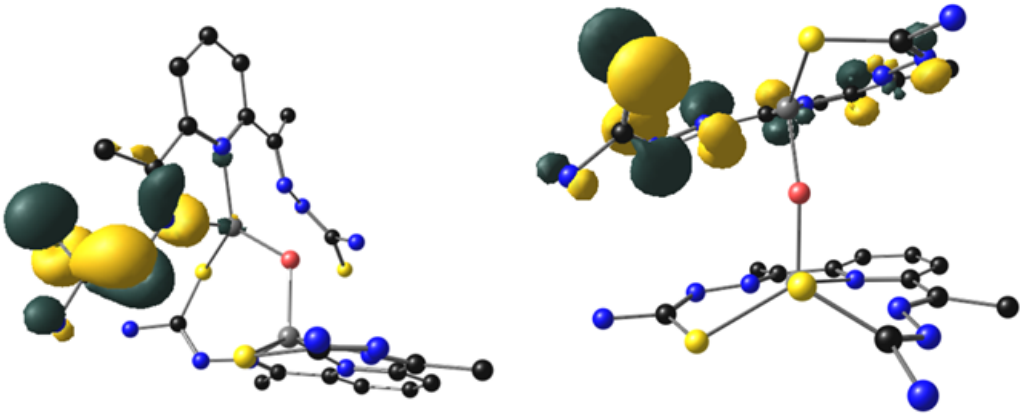

Fig. S12. Occupied NTO with the highest contribution to the lowest energy electronic transition of $\mathbf{2_B}$ (left) and $\mathbf{2_C}$ (right). Hydrogens are omitted for clarity.

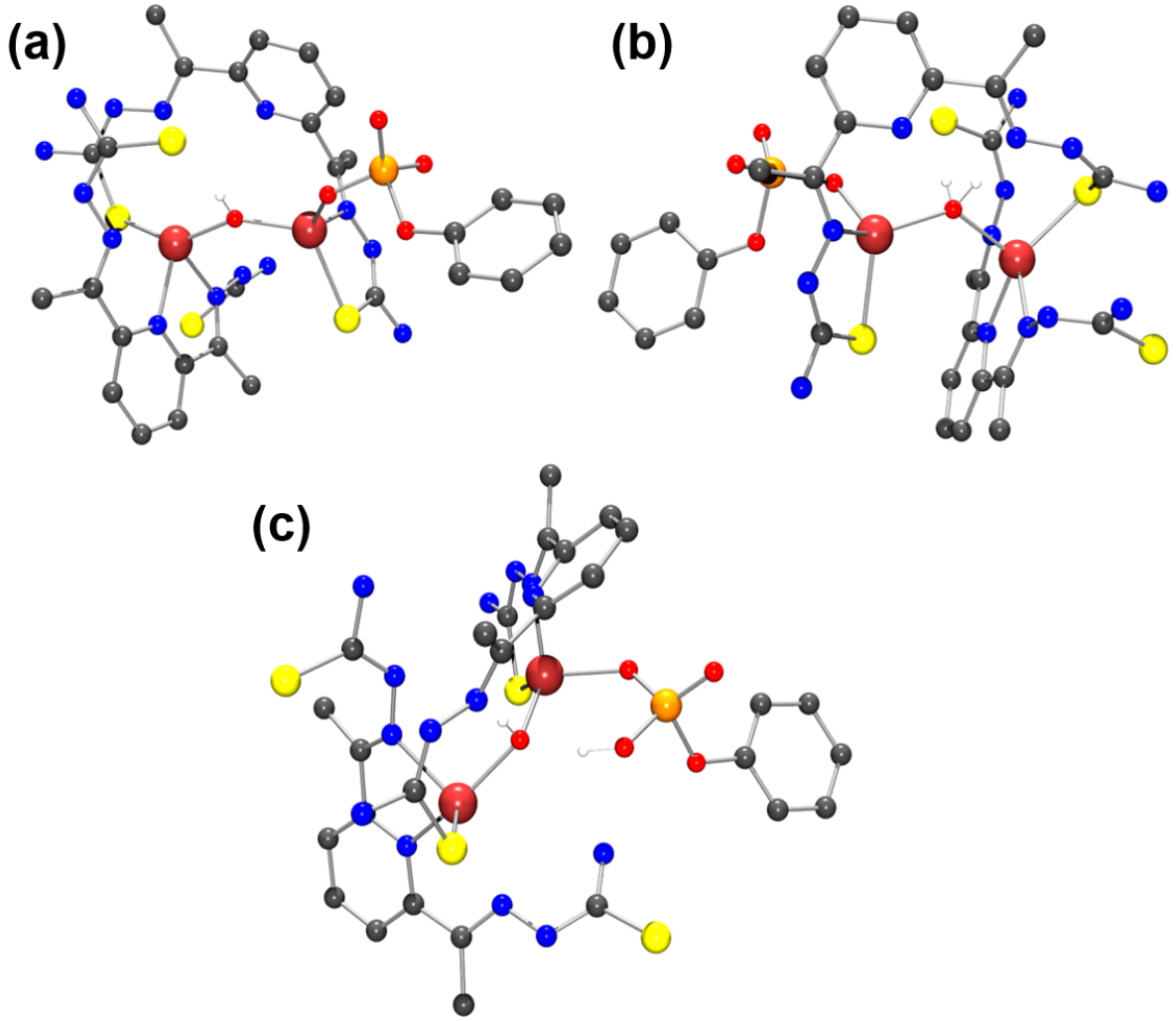

Fig. S13. Alternative structures of **2** found using DFT. Zn, dark red; S, yellow; N, blue; O, red; P, orange; C, gray; H, white. Hydrogens are omitted for clarity except for in H_2O, OH^-, and 4-NPPH.

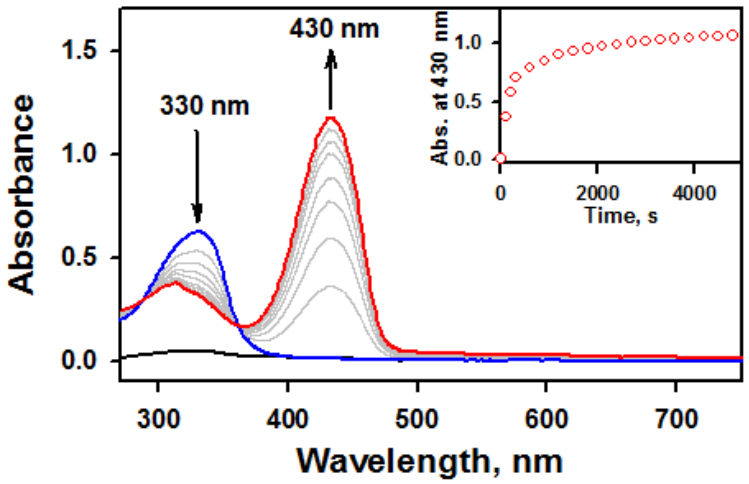

Fig. S14. UV-vis spectral changes obtained in the reaction of **2** (black line, 1.0 x 10^{-4} mM) with 4-NPP (1.0 x 10^{-1} mM) in the presence of KOH (1.0 x 10^{-1} mM) in DMSO at 40 °C. Inset shows the plot of absorbance changes at 430 nm due to 4-NP (red dot) with respect to the time (s) in DMSO at 40 °C.

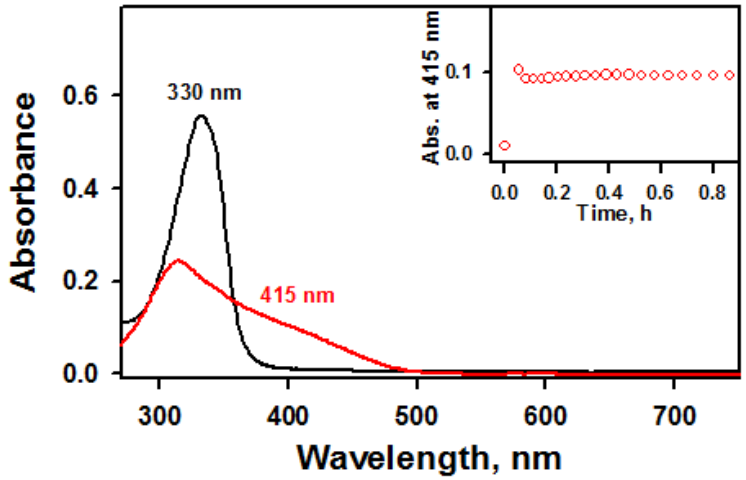

Fig. S15. UV-vis spectral changes showing the conversion from **1** (black line, 1.0 x 10^{-2} mM) to **2** (red line, 1.0 x 10^{-2} mM) upon addition of KOH (3.0 x 10^{-1} mM) in DMSO at 40 ^{o}C. Inset shows the plot of absorbance changes at 415 nm due to **2** (red dot) with respect to time in DMSO at 40 ^{o}C.

Table S1. Relative energies in kcal mol^{-1} for the monomeric species

	ΔDef2-SVP	**ΔΔ Def2-TZVPP**	**Δ*E*[a]**	**ΔΔ*Z*$_0$**	**ΔΔ*E*$_{thermal}$[b]**	**-TΔΔ*S*[b]**	**ΔΔDisp**	**Δ*G*[c]**
Deprotonation of one Zn-OH$_2$ proton by external 4-NPP								
	[Zn(bTSC)(PO$_4$C$_6$H$_4$NO$_2$)$_2$(H$_2$O)]$^{2-}$							
Reactants	0.0	+0.0	**0.0**	+0.0	+0.0	+0.0	0.0	**0.0**
Transition state	0.1	-0.6	**-0.4**	-0.4	-0.3	0.2	-0.1	**-1.1**
Products	-12.7	-1.3	**-14.1**	-1.2	+0.0	-2.2	+7.3	**-6.9**
	[Zn(bTSC)(PO$_4$C$_6$H$_4$NO$_2$)$_2$(H$_2$O) $_3$]$^{2-}$							
Reactants	0.0	+0.0	**0.0**	+0.0	+0.0	+0.0	0.0	**0.0**
Transition state	3.7	-0.8	**3.0**	-4.5	-0.1	+0.0	-0.2	**-1.9**
Products	0.5	-1.4	**-1.0**	-0.9	+0.4	-1.4	0.2	**-2.7**
Direct hydroxyl migration of Zn-OH to the phosphor in 4-NPP								
	[Zn(bTSC)(PO$_4$C$_6$H$_4$NO$_2$)(OH)]$^-$ + DMSO							
Reactants	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	**0.00**
Transition state	18.14	+7.23	**25.38**	-0.36	-0.54	+1.16	-2.47	**23.17**
Products	2.16	-1.07	**1.09**	-0.56	+0.18	-2.92	+2.44	**0.24**
Water splitting and formation of Zn-OH$_2$, HPO$_4^{2-}$ and 4-NP through intermediary waters								
	[Zn(bTSC)(PO$_4$C$_6$H$_4$NO$_2$)(OH)]$^-$ + H$_2$O							
Reactants	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	**0.00**
Transition state	29.53	+2.62	**32.15**	-1.83	+0.07	+0.13	-2.25	**28.29**
Products	8.53	-2.43	**6.10**	-1.22	+0.27	-1.62	+0.25	**3.78**
	[Zn(bTSC)(PO$_4$C$_6$H$_4$NO$_2$)(OH)]$^-$ + 6 H$_2$O							
Reactants	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	**0.00**
Transition state	24.32	+2.63	**26.95**	-1.63	0.46	-1.44	+0.21	**24.54**
Products	-14.78	+3.71	**-11.07**	-0.76	0.09	-0.55	+1.29	**-10.99**
	[Zn(bTSC)(PO$_4$C$_6$H$_4$NO$_2$)(OH)]$^-$ + 10 H$_2$O							
Reactants	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	**0.00**
Transition state	12.11	+3.85	**15.97**	-0.17	-0.59	+0.95	+0.30	**16.46**
Products	-10.65	-3.76	**-14.41**	-0.19	-0.50	-0.77	+5.65	**-10.21**

[a] Electronic energy, sum of the previous two columns. [b] T = 298 K. [c] Sum of the five previous columns, $\Delta G = \Delta E + \Delta\Delta Z_0 + \Delta\Delta E_{thermal} - T\Delta\Delta S + \Delta\Delta Disp$.

Table S2. Relative energies in kcal mol^{-1} for the dimeric species

	ΔDef2-SVP	**ΔΔ Def2-TZVPP**	**Δ*E*[a]**	**ΔΔZ_0**	**ΔΔ$E_{thermal}$[b]**	**-TΔΔ*S*[b]**	**ΔΔDisp**	**Δ*G*[c]**
$[Zn_2(bTSC)_2(PO_4C_6H_5)(OH)]^{3-}$ (**A**)	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	**0.00**
$[Zn_2(bTSC)_2(PO_4C_6H_5)(OH)]^{3-}$ (**B**)	20.14	-18.58	**1.56**	-0.57	+0.40	-0.80	+1.52	**2.10**
$[Zn_2(bTSC)_2(HPO_4C_6H_5)(OH)]^{2-}$	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	**0.00**
$[Zn_2(bTSC)_2(PO_4C_6H_5)(H_2O)]^{2-}$	4.97	+5.18	**10.15**	-1.20	+0.18	-1.06	-1.17	**6.89**
$[Zn_2(bTSC)_2(HPO_4)]^{2-}$	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	**0.00**

[a] Electronic energy, sum of the previous two columns. [b] T = 298 K. [c] Sum of the five previous columns, $\Delta G = \Delta E + \Delta\Delta Z_0 + \Delta\Delta E_{thermal} - T\Delta\Delta S + \Delta\Delta Disp$.

Table S3. Selected geometries in Å for the monomeric species.

Deprotonation of one Zn-OH_2 proton by external 4-NPP				
	Zn-OH_2	**ZnOH_2-$O_3POC_6H_4NO_2$**	**ZnHO-$HO_3POC_6H_4NO_2$**	**Zn-N(average)**
	$[Zn(bTSC)(PO_4C_6H_4NO_2)_2(H_2O)]^{2-}$			
Reactants	2.07	2.65	1.00	2.17
Transition state	2.07	2.39	0.99	2.18
Products	1.94	1.06	1.43	2.19
	$[Zn(bTSC)(PO_4C_6H_4NO_2)_2(H_2O)_3]^{2-}$			
Reactants	2.00	1.70	1.03	2.16
Transition state	1.93	1.17	1.16	2.18
Products	1.92	1.02	1.53	2.19
Direct hydroxyl migration of Zn-OH to the phosphor in 4-NPP				
	Zn-OH	**$H_{(2)}O$-$PO_4C_6H_4NO_2$**	**O_3P-$OC_6H_4NO_2$**	**Zn-N(average)**
	$[Zn(bTSC)(PO_4C_6\ H_4NO_2)(OH)]^{-}$ + DMSO			
Reactants	1.91	3.66	1.73	2.16
Transition state	1.94	2.10	2.01	2.13
Products	2.10	1.70	4.08	2.11
Water splitting and formation of Zn-OH_2, HPO_4^{2-} and 4-NP through intermediary waters				
	Zn-OH	**$H_{(2)}O$-$PO_4C_6H_4NO_2$**	**O_3P-$OC_6H_4NO_2$**	**Zn-N(average)**
	$[Zn(bTSC)(PO_4C_6\ H_4NO_2)(OH)]^{-}$ + H_2O			
Reactants	1.93	3.47	1.72	2.21
Transition state	1.96	2.28	2.62	2.18
Products	2.08	1.74	4.92	2.16
	$[Zn(bTSC)(PO_4C_6\ H_4NO_2)(OH)]^{-}$ + 6 H_2O			
Reactants	1.90	3.78	1.74	2.35
Transition state	1.92	2.22	2.25	2.29
Products	2.05	1.67	5.81	2.23
	$[Zn(bTSC)(PO_4C_6\ H_4NO_2)(OH)]^{-}$ + 10 H_2O			
Reactants	1.98	3.25	1.75	2.32
Transition state	1.96	2.17	2.27	2.22
Products	2.10	1.67	4.81	2.20

Table S4. Selected geometries in Å for the dimeric species.

	Zn-OH_2	**Zn-OPO_3**	**Zn-N(average)**
$[Zn_2(bTSC)_2(PO_4C_6H_5)(OH)]^{3-}$ (**A**)	1.95/1.96	1.96	2.25
$[Zn_2(bTSC)_2(PO_4C_6H_5)(OH)]^{3-}$ (**B**)	1.96/1.96	1.93	2.24
$[Zn_2(bTSC)_2(HPO_4C_6H_5)(OH)]^{2-}$	1.97/2.02	2.01	2.15
$[Zn_2(bTSC)_2(PO_4C_6H_5)(H_2O)]^{2-}$	2.10/2.14	1.92	2.13
$[Zn_2(bTSC)_2(HPO_4)]^{2-}$	-	1.99/2.00[a]	2.28

[a] This PO_4 binds to Zn in a bidentate fashion.

Table S5. Relative energies in kcal mol^{-1} for diiferent conformations of monomeric and dimeric species in DMSO.

	ΔDef2-SVP	**ΔΔ Def2-TZVPP**	**Δ*E*[a]**	**ΔΔ*Z*$_0$**	**ΔΔ*E*$_{thermal}$[b]**	**-TΔΔ*S*[b]**	**ΔΔDisp**	**Δ*G*[c]**
	Monomer $[Zn(bTSC)(DMSO)_2]^{2+}$							
$\mathbf{1_A}$	0.0	0.0	**0.0**	0.0	0.0	0.0	0.0	**0.0**
$\mathbf{1_B}$	-0.5	0.9	**0.3**	1.9	-1.0	2.7	4.5	**8.4**
$\mathbf{1_{TS}}$	10.2	1.1	**11.2**	0.2	-0.9	2.7	0.9	**14.0**
	Dimer $\{[Zn(bTSC)]_2(OH)\}^-$							
$\mathbf{2_A}$ + OH^-	0.0	0.0	**0.0**	0.0	0.0	0.0	0.0	**0.0**
$\mathbf{2_B}$	-47.8	27.5	**-20.3**	4.1	-0.8	9.2	12.5	**4.8**
$\mathbf{2_C}$	-61.2	28.0	**-33.2**	2.6	0.0	5.8	15.9	**-9.0**

[a] Electronic energy, sum of the previous two columns. [b] T = 298 K. [c] Free energy, sum of the previous five columns.

Coordinates

The coordinates are provided in .xyz-format, with charge/multiplicity in parenthesis in the comment row.

First proton abstraction step [Zn(bTSC)($PO_4C_6H_4NO_2$)$_2$(H_2O)]$^{2-}$ Reactant

```
75
(-2/1)
Zn -0.26794 -0.17284 -0.72895
O 0.4476 -0.59943 -2.48276
O -0.69289 1.82648 -1.03904
H -1.33291 2.27822 -0.42447
P 0.93178 -1.98089 -3.01917
O 2.29453 -2.17583 -1.90287
O -0.0081 -3.14202 -2.65056
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C 1.63615 0.73543 1.46741
C 2.76574 1.36224 2.21382
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H 3.71674 1.18391 1.69639
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H 4.44633 2.36764 -2.53537
H 4.66958 0.67965 -2.16089
O 5.70435 -7.41503 -2.43379
O 6.20756 -6.82113 -0.41884
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O -3.90535 2.22082 -1.05865
P -4.07735 2.27877 0.4463
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O -3.99625 0.9627 1.22353
O -2.3185 2.97966 0.81037
C -2.79138 4.2605 2.79608
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H -3.85079 4.01681 2.70508
C -0.53576 4.10499 1.86952
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C -0.94089 5.39547 3.86449
C -2.30639 5.06685 3.81256
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O 0.75543 6.51806 4.94575
```

First proton abstraction step [Zn(bTSC)($PO_4C_6H_4NO_2$)$_2$(H_2O)]$^{2-}$ Transition state

```
75
(-2/1)
Zn -3.26182 3.20135 -3.80007
O -2.55267 2.71652 -5.54178
O -3.60266 5.20654 -4.20704
H -4.30607 5.65044 -3.67328
P -2.06547 1.33217 -6.06522
O -0.69968 1.15192 -4.95143
O -2.99807 0.16877 -5.684
O -1.48798 1.34347 -7.45572
C 0.0631 0.05317 -4.8727
C 0.74602 -0.18798 -3.65923
C 1.55375 -1.30645 -3.51188
C 1.68312 -2.20173 -4.58252
C 1.02096 -1.97783 -5.79665
C 0.21854 -0.85422 -5.94617
H 0.61816 0.51946 -2.83774
H 2.07977 -1.50378 -2.57842
N 2.52182 -3.38229 -4.43084
H 1.1508 -2.6859 -6.61476
H -0.28363 -0.63888 -6.88965
S -7.6968 1.66786 -4.96637
S -0.54118 6.51808 -3.9164
N -5.93427 0.15565 -6.2853
N -5.19008 0.83253 -4.27307
N -4.87735 1.80182 -3.33829
N -3.54978 3.27815 -1.70514
N -1.30154 3.71725 -2.85585
N -0.16954 3.8378 -3.6392
N 1.19647 4.9076 -5.11711
C -6.2241 0.87426 -5.17707
C -6.63948 1.17003 -1.69929
H -6.98341 0.43833 -2.43655
H -6.40284 0.66927 -0.74731
H -7.44059 1.90211 -1.51562
C -5.45546 1.92898 -2.19245
C -4.70005 2.81088 -1.23562
C -5.03319 3.00654 0.11597
H -5.98524 2.66045 0.51431
C -4.11315 3.65999 0.93287
H -4.34596 3.82966 1.98605
C -2.87646 4.07994 0.4197
H -2.14022 4.55244 1.0692
C -2.62356 3.8605 -0.93673
C -1.32282 4.13164 -1.63327
C -0.18182 4.75538 -0.90112
H -0.11315 4.35884 0.12141
H 0.76303 4.5698 -1.42702
H -0.32944 5.84528 -0.83563
C 0.1931 5.02333 -4.23501
H -6.61722 0.12733 -7.0309
H -4.95824 -0.09157 -6.47218
H -4.28707 0.51637 -4.71955
H -0.0973 2.99743 -4.22999
H 1.50048 5.73012 -5.62308
H 1.69598 4.03558 -5.26311
O 2.60989 -4.15997 -5.37598
O 3.10475 -3.54955 -3.36391
H -2.7774 5.72477 -4.08664
O -6.63383 5.45252 -4.15385
P -6.92445 5.62575 -2.67242
O -7.89823 6.7196 -2.25828
O -6.90146 4.36966 -1.79618
O -5.23516 6.38028 -2.25716
C -5.81662 7.53575 -0.22484
C -4.89093 7.10542 -1.21905
H -6.86718 7.28167 -0.37015
C -3.52522 7.48621 -1.07457
H -2.8132 7.16376 -1.83708
H -2.05574 8.52807 0.11536
C -3.10137 8.24088 0.0055
C -4.03256 8.63966 0.97967
C -5.38771 8.28765 0.85662
H -6.09164 8.61997 1.61993
N -3.5935 9.4221 2.11166
O -4.42488 9.75753 2.95561
O -2.40273 9.72535 2.19281
H -0.51590 -4.10880 0.70140
```

First proton abstraction step [Zn(bTSC)($PO_4C_6H_4NO_2$)($PO_3OHC_6H_4NO_2$)(OH)]$^{2-}$ Product

```
75
(-2/1)
Zn 0.20828 -0.29475 -0.23481
O 1.6023 -1.28586 -1.23011
O -0.65435 1.08698 -1.2881
H -2.00641 1.5433 -1.20075
P 1.52896 -2.43644 -2.2856
O 2.82509 -3.4106 -1.64231
O 0.29492 -3.34162 -2.11142
O 1.9155 -2.0472 -3.69069
C 3.2662 -4.55055 -2.17248
C 4.02882 -5.40147 -1.33614
C 4.52905 -6.60399 -1.81087
C 4.26885 -6.97771 -3.13754
C 3.52098 -6.14968 -3.98576
C 3.02442 -4.94277 -3.51209
H 4.21004 -5.08803 -0.30616
H 5.11372 -7.26421 -1.17104
N 4.78666 -8.23937 -3.6402
H 3.34326 -6.46146 -5.01481
H 2.46787 -4.26635 -4.16096
S -4.25142 -1.88967 -1.00238
S 2.35701 3.76534 -0.64879
N -2.58826 -3.44378 -2.40137
N -1.6976 -2.70713 -0.46783
N -1.34824 -1.69408 0.40187
N -0.15573 0.09071 1.84885
N 1.89658 0.92713 0.56485
N 2.94873 1.13076 -0.29095
N 4.16916 2.24353 -1.85684
C -2.79936 -2.69571 -1.29504
C -3.01695 -2.31954 2.13192
H -3.23411 -3.19456 1.51027
H -2.76022 -2.63951 3.1536
H -3.92611 -1.70158 2.18383
C -1.90221 -1.51419 1.55185
C -1.24146 -0.45585 2.38744
C -1.65766 -0.08418 3.67476
H -2.55081 -0.51458 4.1262
C -0.90506 0.86882 4.3609
H -1.20877 1.1865 5.36045
C 0.24191 1.41815 3.77547
H 0.83705 2.15744 4.31124
C 0.5954 0.99068 2.48977
C 1.81825 1.44032 1.74283
C 2.83373 2.31672 2.39987
H 2.97262 2.02291 3.45038
H 3.79584 2.24934 1.87574
H 2.50998 3.36918 2.37423
C 3.19594 2.33256 -0.93355
H -3.32009 -3.46903 -3.09968
H -1.61914 -3.64955 -2.6688
H -0.82883 -3.01118 -0.98922
H 2.9946 0.29958 -0.898
H 4.391 3.06003 -2.41245
H 4.73112 1.40623 -1.97614
O 4.54158 -8.55052 -4.80256
O 5.44845 -8.94264 -2.8814
H -0.14578 1.9049 -1.18281
O -2.98213 1.95781 -1.17649
P -3.49203 2.39011 0.26857
O -4.8199 3.09895 0.17169
O -3.24225 1.36195 1.3485
O -2.26222 3.61826 0.54263
C -3.37744 4.83865 2.31051
C -2.23197 4.4727 1.55947
H -4.3394 4.40857 2.02984
C -0.98205 5.05539 1.88665
H -0.1081 4.76242 1.30075
H 0.0849 6.41694 3.18319
C -0.87327 5.96675 2.92527
C -2.01826 6.30815 3.66148
C -3.26593 5.74661 3.35432
H -4.13925 6.03818 3.93754
N -1.90956 7.25939 4.75317
O -2.92251 7.53882 5.38972
O -0.80831 7.74688 4.9966
```

First proton abstraction step through H_2O [Zn(bTSC)($PO_4C_6H_4NO_2$)$_2$(H_2O)$_3$]$^{2-}$ Reactant

```
81
(-2/1)
Zn 0.196792 -1.296684 0.890045
O 1.736597 -2.327389 0.221026
O -0.599078 -0.387526 -0.698210
H -1.047688 0.488004 -0.405762
P 1.684450 -3.376615 -0.941601
O 3.096468 -4.261337 -0.544268
O 0.535262 -4.381911 -0.800456
O 1.909845 -2.771250 -2.321492
C 3.570572 -5.314197 -1.225857
C 4.474899 -6.160917 -0.546806
C 5.018973 -7.268857 -1.179820
C 4.657430 -7.543240 -2.505860
C 3.766800 -6.714348 -3.198856
C 3.225921 -5.601787 -2.566043
H 4.731830 -5.924510 0.487399
H 5.714675 -7.929143 -0.663202
N 5.221230 -8.707885 -3.175296
H 3.512180 -6.947827 -4.232319
H 2.554911 -4.927392 -3.097995
S -4.076060 -2.820613 -0.282972
S 2.360220 2.939906 0.198224
N -2.307123 -4.500639 -1.379255
N -1.668127 -3.713742 0.640078
N -1.429247 -2.627484 1.453676
N -0.579488 -0.543644 2.718700
N 1.603129 0.224636 1.609136
N 2.756265 0.337359 0.870057
N 3.935118 1.112913 -0.920992
C -2.644708 -3.702034 -0.345960
C -3.332165 -3.095389 2.982832
H -3.407190 -4.061405 2.471159
H -3.208071 -3.257371 4.065324
H -4.274767 -2.551244 2.823734
C -2.172730 -2.313311 2.458924
C -1.696767 -1.092366 3.196519
C -2.321373 -0.546752 4.327032
H -3.241752 -0.972047 4.726569
C -1.730887 0.566276 4.933126
H -2.198490 1.018988 5.809598
C -0.536057 1.093455 4.432519
H -0.064479 1.949798 4.914316
C 0.027504 0.492841 3.298690
C 1.337149 0.896194 2.673999
C 2.220077 1.886618 3.357886
H 2.256055 1.669875 4.436545
H 3.234495 1.853246 2.943756
H 1.833570 2.908582 3.225060
C 3.047502 1.420489 0.061871
H -2.936019 -4.536264 -2.171706
H -1.315167 -4.730965 -1.510047
H -0.751350 -4.046650 0.252523
H 2.899049 -0.582185 0.428043
H 4.324919 1.888179 -1.445747
H 4.506993 0.273275 -0.864959
O 4.887502 -8.931754 -4.334422
O 6.005751 -9.414747 -2.550568
H 1.604620 -1.159389 -2.499859
O 1.351429 -0.190611 -2.527340
H 2.160587 0.278467 -2.269874
H 0.093904 -0.194910 -1.389361
O -1.704827 1.692779 0.280391
P -2.873398 4.010773 -1.490349
O -1.402044 3.969324 -1.023114
O -3.144586 4.635098 -2.842844
O -3.639581 5.194358 -0.350406
C -1.975670 6.938409 -0.539048
C -3.253672 6.437312 -0.160842
H -1.265698 6.240763 -0.983781
C -4.165410 7.330491 0.468825
H -5.144433 6.942914 0.759087
H -4.529029 9.335467 1.186873
C -3.829085 8.652081 0.706572
C -2.564316 9.122696 0.315041
C -1.642191 8.262777 -0.304282
H -0.663665 8.651015 -0.587471
N -2.207548 10.502629 0.558668
O -1.097359 10.896496 0.202222
O -3.027529 11.233453 1.114260
O -3.676583 2.760423 -1.099604
H -2.604206 1.867495 -0.128563
H -1.297709 2.536699 -0.068720
```

First proton abstraction step through H_2O [Zn(bTSC)($PO_4C_6H_4NO_2$)$_2$(H_2O)$_3$]$^{2-}$ Transition state

```
81
(-2/1)
Zn -0.645531 2.303789 -4.832815
O 0.906511 1.179184 -5.323705
O -1.350922 3.238189 -6.403640
H -1.560880 4.333946 -6.076074
P 0.892581 0.003798 -6.355452
O 2.300347 -0.817034 -5.813502
O -0.250128 -0.995159 -6.131787
O 1.156161 0.439151 -7.791062
C 2.786775 -1.949074 -6.338693
C 3.683970 -2.692985 -5.539471
C 4.238213 -3.874607 -6.008986
C 3.894884 -4.328282 -7.290022
C 3.012192 -3.604015 -8.100829
C 2.461291 -2.417781 -7.632155
H 3.926796 -2.317669 -4.543608
H 4.928046 -4.456290 -5.398515
N 4.469203 -5.571016 -7.786740
H 2.771776 -3.976638 -9.096199
H 1.796381 -1.824283 -8.259485
S -4.890398 0.536416 -5.784194
S 1.607384 6.387080 -5.902737
N -3.107733 -1.244551 -6.681818
N -2.450732 -0.184415 -4.799160
N -2.230937 0.991231 -4.114958
N 0.812851 3.838457 -4.180324
N 1.968283 3.872320 -4.919901
```

```
N 3.230415 4.453033 -6.723886
C -3.441907 -0.320729 -5.755863
C -4.089974 0.621936 -2.509158
H -4.131935 -0.396932 -2.910845
H -3.961935 0.585080 -1.416153
H -5.050803 1.111709 -2.726648
C -2.959445 1.379542 -3.124540
C -2.496203 2.669150 -2.506585
C -3.126612 3.310419 -1.430955
H -4.043801 2.915886 -0.994141
C -2.546803 4.480221 -0.930856
H -3.018833 5.007812 -0.099758
C -1.357188 4.969362 -1.479357
H -0.893886 5.870510 -1.078007
C -0.786672 4.272020 -2.553402
C 0.522113 4.627420 -3.207704
C 1.372770 5.716228 -2.641804
H 1.397386 5.639692 -1.544171
H 2.394622 5.656535 -3.033971
H 0.965286 6.703589 -2.908517
C 2.295018 4.857656 -5.827250
H -3.745564 -1.388867 -7.454429
H -2.115414 -1.477849 -6.796771
H -1.528126 -0.543525 -5.155271
H 2.114230 2.909903 -5.257591
H 3.626156 5.162329 -7.330758
H 3.802979 3.630251 -6.550999
O 4.149497 -5.953834 -8.907777
O 5.248545 -6.182144 -7.062217
H 0.887943 2.051201 -8.135947
O 0.679482 3.017014 -8.281196
H 1.506182 3.473000 -8.061225
H -0.656955 3.245208 -7.106010
O -1.777455 5.486271 -5.610917
P -3.115741 8.294080 -7.044370
O -1.636625 8.620490 -6.957275
O -3.977915 8.924189 -8.110572
O -3.821917 8.906449 -5.519469
C -2.860146 11.124549 -5.620537
C -3.779154 10.164181 -5.117118
H -2.129036 10.797975 -6.360467
C -4.702086 10.571015 -4.116877
H -5.404619 9.828413 -3.732771
H -5.427424 12.186464 -2.878387
C -4.717409 11.872340 -3.643017
C -3.806008 12.804932 -4.164191
C -2.879587 12.428379 -5.149008
H -2.176504 13.170089 -5.528068
N -3.819225 14.168659 -3.675460
O -3.015425 14.970389 -4.148069
O -4.634153 14.472647 -2.805940
O -3.438248 6.773832 -6.805459
H -2.622766 6.163147 -6.222714
H -0.929355 5.951769 -5.701818
```

First proton abstraction step through H_2O
$[Zn(bTSC)(PO_4C_6H_4NO_2)(PO_3OHC_6H_5NO_2)(OH)(H_2O)_2]^{2-}$
Product

```
81
(-2/1)
Zn 0.049188 -1.302579 0.492816
O 1.630546 -2.443332 0.060795
O -0.693179 -0.406565 -1.029043
H -0.896947 1.036709 -0.559953
P 1.626754 -3.619033 -0.967426
O 3.043559 -4.430612 -0.421523
O 0.494191 -4.630247 -0.740076
O 1.889616 -3.194330 -2.405926
C 3.549264 -5.549608 -0.952893
C 4.470640 -6.275321 -0.163454
C 5.046355 -7.443773 -0.639524
C 4.701162 -7.903963 -1.917939
C 3.794666 -7.198292 -2.719111
C 3.222050 -6.025164 -2.244027
H 4.715001 -5.895564 0.830385
H 5.755021 -8.010388 -0.036470
N 5.298337 -9.132289 -2.421788
H 3.553049 -7.575192 -3.712606
H 2.538897 -5.445418 -2.864431
S -4.163888 -3.161163 -0.341490
S 2.317516 2.769032 -0.578277
N -2.364056 -4.918849 -1.251221
N -1.697745 -3.832706 0.612807
N -1.483771 -2.648918 1.284534
N -0.643564 -0.444691 2.336476
N 1.532619 0.221010 1.165403
N 2.674099 0.252532 0.407985
N 3.955302 0.839637 -1.378334
C -2.699616 -3.993072 -0.327130
C -3.312521 -3.030474 2.922750
H -3.348570 -4.052414 2.528258
H -3.166722 -3.059381 4.013771
H -4.282839 -2.554077 2.718046
C -2.200729 -2.263497 2.284027
C -1.740325 -0.966290 2.887909
C -2.355696 -0.331311 3.976258
H -3.259881 -0.735164 4.431382
C -1.777429 0.843653 4.465882
H -2.238056 1.366632 5.306296
C -0.602292 1.342382 3.895674
H -0.137977 2.246323 4.289614
C -0.046041 0.650023 2.810505
C 1.249911 1.014099 2.136750
C 2.098293 2.114624 2.684628
H 2.134255 2.049354 3.782628
H 3.117211 2.058683 2.284257
H 1.681871 3.096816 2.412180
C 3.007631 1.238524 -0.492577
H -3.010254 -5.078045 -2.013830
H -1.369315 -5.135375 -1.378893
H -0.774787 -4.182109 0.246540
H 2.812052 -0.711527 0.069143
H 4.346762 1.548609 -1.988281
H 4.535548 0.024775 -1.194138
O 4.977005 -9.520933 -3.540570
O 6.098138 -9.727062 -1.705667
H 1.638305 -1.567056 -2.780610
O 1.456925 -0.604775 -2.960322
H 2.285340 -0.163407 -2.719989
H 0.005867 -0.392695 -1.714105
O -1.006078 1.996258 -0.195385
P -2.294050 4.911491 -1.813225
O -0.812627 5.164240 -1.668204
O -3.116914 5.535662 -2.903926
O -3.040256 5.438643 -0.314760
C -2.044352 7.646826 -0.240340
C -2.999650 6.679548 0.161653
H -1.279179 7.357045 -0.960674
C -3.966841 7.037185 1.133456
H -4.696704 6.284265 1.437506
H -4.733986 8.591011 2.425725
C -3.990115 8.310312 1.680685
C -3.042365 9.255065 1.259019
C -2.071940 8.923682 0.303154
H -1.341934 9.674884 0.002197
N -3.064576 10.592909 1.824085
O -2.231934 11.407116 1.433478
O -3.915539 10.856064 2.670097
O -2.665849 3.357038 -1.652972
H -2.000405 2.841370 -1.083763
H -0.109458 2.367314 -0.282204
```

Direct Zn-OH$^-$ migration
$[Zn(bTSC)(PO_4C_6H_4NO_2)(OH)]^-$ + DMSO
Reactants

```
66
(-1/1)
Zn -1.37149 0.71146 0.98238
O 0.60941 0.38766 1.11766
O -2.08020 0.91122 -0.77523
H -2.83408 0.31131 -0.87690
P 1.34964 -0.19495 -0.12963
O 2.85541 -0.57961 0.62859
O 0.79688 -1.55020 -0.57763
O 1.65180 0.86414 -1.18540
C 3.93092 -1.07319 0.00867
C 4.92844 -1.66087 0.82155
C 6.07998 -2.19184 0.26061
C 6.24714 -2.14477 -1.13078
C 5.27459 -1.56415 -1.95498
C 4.12339 -1.02775 -1.39269
H 4.76783 -1.68815 1.90098
N 7.45136 -2.70331 -1.72651
H 5.43629 -1.53346 -3.03221
H 3.37012 -0.54351 -2.01396
S -4.07012 -2.09458 -0.91624
S -0.92705 5.27832 0.05617
N -1.55888 -2.67517 -1.65243
N -1.79102 -2.25132 0.57317
N -2.19246 -1.25306 1.44964
N -2.71400 0.96052 2.64286
N -0.95205 2.62773 1.87252
N 0.21192 3.19012 1.35220
N 1.05967 3.65351 -0.71636
C -2.41670 -2.34566 -0.67839
C -4.05337 -2.55873 2.46331
H -3.63852 -3.42039 1.92818
H -4.08428 -2.77524 3.54368
H -5.08612 -2.40079 2.11981
C -3.21783 -1.34327 2.22296
C -3.48356 -0.07104 2.99003
C -4.44094 0.08350 4.00417
H -5.08928 -0.73994 4.30417
C -4.54227 1.33096 4.62923
H -5.28310 1.48250 5.41680
C -3.69192 2.38238 4.26485
H -3.76136 3.34963 4.76317
C -2.75633 2.14875 3.24843
C -1.69453 3.12588 2.79094
C -1.52781 4.44833 3.46318
H -1.50189 4.31633 4.55631
H -0.60979 4.93808 3.11939
H -2.37766 5.10762 3.22679
C 0.14903 3.99589 0.21245
H -1.87684 -2.58006 -2.62894
H -0.56919 -2.43659 -1.47749
H -0.77141 -2.13248 0.42814
H 0.81623 2.36687 1.20368
H 1.10283 4.24175 -1.54133
H 1.38838 2.66901 -0.81772
O -1.94996 -1.82192 -4.33432
S -0.72945 -0.88957 -4.44993
C -0.57835 -0.55145 -6.23166
C -1.28644 0.75068 -3.89966
H 0.21465 0.19101 -6.39955
H -0.31350 -1.50478 -6.70836
H -1.54939 -0.19357 -6.60273
H -1.49629 0.68944 -2.81430
H -0.47661 1.47308 -4.08165
H -2.19237 1.01813 -4.46368
O 7.57455 -2.65666 -2.94687
O 8.29380 -3.19783 -0.98312
```

Direct Zn-OH$^-$ migration
$[Zn(bTSC)(PO_4C_6H_4NO_2)(OH)]^-$ + DMSO
Transition state

```
66
(-1/1)
Zn -1.56994 0.84426 1.02291
O 0.45710 0.79397 1.08496
O -1.08886 0.78460 -0.85414
H -1.46038 0.30909 -1.62078
P 0.86939 0.24115 -0.33254
O 2.65173 -0.20257 0.47950
O 0.58035 -1.24151 -0.63245
O 1.46905 1.22858 -1.33988
C 3.63771 -0.78675 -0.10920
C 4.75862 -1.22182 0.67768
C 5.84269 -1.86351 0.11352
C 5.86626 -2.10435 -1.27505
C 4.78991 -1.68484 -2.08235
C 3.70320 -1.04212 -1.52121
H 4.72177 -1.03111 1.75316
H 6.68387 -2.19325 0.72361
N 6.98762 -2.77565 -1.86619
H 4.83364 -1.87434 -3.15530
H 2.87841 -0.70115 -2.14415
S -4.19327 -2.32939 -0.79492
S -1.64302 5.31708 -0.54615
N -1.63490 -2.62435 -1.53780
N -1.89765 -2.11214 0.66354
N -2.38429 -1.08709 1.45879
N -3.12152 1.18684 2.41803
N -1.44894 2.91354 1.56685
N -0.33627 3.50736 0.99635
N 0.59960 3.93336 -1.03650
C -2.52849 -2.35964 -0.56953
C -4.16821 -2.43094 2.55990
H -3.68946 -3.30367 2.10262
H -4.18172 -2.54778 3.65652
H -5.20975 -2.38308 2.21154
C -3.42568 -1.18209 2.21203
C -3.81788 0.13208 2.84263
C -4.83247 0.30654 3.79487
H -5.42385 -0.53446 4.15689
C -5.07111 1.60033 4.27139
H -5.86040 1.76813 5.00684
C -4.30091 2.68034 3.82316
H -4.48217 3.68581 4.20342
C -3.29629 2.42685 2.88001
C -2.31374 3.44930 2.34732
C -2.35102 4.86328 2.82543
H -2.39245 4.88490 3.92612
H -1.47092 5.41076 2.47079
H -3.24841 5.37627 2.44652
C -0.42082 4.21181 -0.20409
H -2.00466 -2.58365 -2.48304
H -0.70066 -2.18088 -1.41209
H -0.89745 -1.90786 0.48245
H 0.34739 2.73092 0.94808
H 0.60545 4.45238 -1.90784
H 1.01941 2.97434 -1.06517
O -1.86925 -0.35956 -3.41833
S -0.87947 0.05584 -4.52040
C -1.92726 0.52924 -5.93545
C -0.27531 1.71028 -4.06594
H -1.29738 0.92532 -6.74484
H -2.43748 -0.38577 -6.26535
H -2.65945 1.27514 -5.59449
H 0.32907 1.57688 -3.15294
H 0.33612 2.10092 -4.89269
H -1.14232 2.35759 -3.86906
O 6.98548 -2.98166 -3.08398
O 7.92198 -3.12820 -1.13925
```

Direct Zn-OH$^-$ migration
$[Zn(bTSC)(PO_4C_6H_4NO_2)(OH)]^-$ + DMSO
Products

```
66
(-1/1)
Zn -1.50752 0.36583 1.25755
O 0.39403 -0.20072 0.97164
O -1.16662 0.26888 -0.81006
H -1.59570 0.15732 -1.72094
P 0.33109 -0.50830 -0.57935
O 3.67755 -2.26086 0.96011
O 0.10422 -1.98900 -0.89399
O 1.38131 0.26103 -1.38151
C 4.72618 -1.92310 0.36203
C 6.03989 -2.44332 0.72725
C 7.19056 -2.07432 0.07108
C 7.13563 -1.15447 -1.00640
C 5.88414 -0.61691 -1.40352
C 4.72882 -0.98053 -0.75258
H 6.07789 -3.15294 1.55953
H 8.16203 -2.47663 0.36200
N 8.32241 -0.77411 -1.67991
H 5.86456 0.08948 -2.23493
H 3.76164 -0.56668 -1.05388
S -4.85144 -2.33144 -0.72817
S -0.66974 4.90463 -0.08899
N -2.40002 -3.11002 -1.47991
N -2.51942 -2.41646 0.67616
N -2.79123 -1.31802 1.47362
N -2.93078 0.98156 2.64311
N -0.92587 2.33241 1.79654
N 0.27089 2.72069 1.21473
N 1.18766 3.12646 -0.83508
C -3.21309 -2.62655 -0.52505
C -4.75271 -2.31522 2.63609
H -4.46023 -3.25967 2.16463
H -4.77662 -2.43535 3.73146
H -5.76914 -2.06283 2.30032
C -3.79026 -1.23025 2.28467
C -3.87463 0.10720 2.98681
C -4.84030 0.47500 3.93404
H -5.63139 -0.21008 4.23869
C -4.76468 1.76145 4.48182
H -5.50734 2.07812 5.21669
C -3.74626 2.64587 4.10411
H -3.69117 3.64455 4.53761
C -2.81197 2.20514 3.15774
C -1.61427 2.98995 2.65964
C -1.28893 4.32242 3.24575
H -1.31749 4.25992 4.34525
H -0.30092 4.65803 2.91219
H -2.02903 5.07425 2.93167
C 0.29236 3.53967 0.08142
H -2.81907 -3.29105 -2.38460
H -1.39311 -2.85374 -1.43590
H -1.50471 -2.43847 0.50173
H 0.78648 1.83909 1.07217
H 1.27750 3.70881 -1.66062
H 1.40682 2.11634 -0.95438
O -2.13758 0.02892 -3.19449
S -1.28632 -0.74962 -4.22695
C -2.16468 -0.48172 -5.79180
C 0.17366 0.29043 -4.52633
H -1.57584 -0.91100 -6.61458
H -3.12759 -1.00174 -5.70194
H -2.31951 0.59804 -5.92603
H 0.73406 0.29881 -3.57738
H 0.77469 -0.15706 -5.33108
H -0.16531 1.30191 -4.79248
O 8.25457 0.03575 -2.62062
O 9.40921 -1.25698 -1.31753
```

Water splitting and OH$^-$ coordination to P
$[Zn(bTSC)(PO_4C_6H_4NO_2)(OH)]^-$ + H_2O
Reactant

```
59
(-1/1)
Zn -1.22187 0.50381 -0.23920
O 0.53154 -0.43455 -0.39794
O -1.85114 0.82275 -2.04057
H -1.79374 -0.04822 -2.46423
P 0.81629 -1.22069 -1.71377
O 1.87985 -2.46597 -1.17229
O -0.38721 -2.04573 -2.19653
O 1.57538 -0.43090 -2.77329
C 3.06802 -2.28645 -0.58519
C 3.58620 -3.36940 0.16216
C 4.81229 -3.26780 0.80249
C 5.53806 -2.07251 0.70310
C 5.04808 -0.99001 -0.03888
C 3.82200 -1.09374 -0.68317
H 2.99508 -4.28484 0.22745
H 5.21570 -4.09580 1.38444
N 6.82162 -1.95601 1.37932
H 5.63952 -0.07726 -0.10675
H 3.43432 -0.27526 -1.28899
S -5.07094 -2.60562 -0.49885
S -1.66165 5.50700 -0.40788
N -3.21345 -3.69662 -2.07204
N -2.35158 -2.39319 -0.44296
N -2.30940 -1.34013 0.42989
N -1.81904 0.82576 1.78590
N -0.60228 2.58765 0.30356
N 0.00215 3.34976 -0.66060
N -0.03202 4.79452 -2.39889
C -3.49073 -2.90657 -1.00831
C -3.27966 -2.60847 2.33418
H -3.06872 -3.50972 1.74562
H -2.83473 -2.71494 3.33484
H -4.37211 -2.53116 2.44349
C -2.72456 -1.40165 1.64786
C -2.48980 -0.13934 2.42510
C -2.91198 0.04840 3.74945
```

H -3.47708 -0.72139 4.27404
C -2.59620 1.25188 4.38388
H -2.91551 1.42578 5.41332
C -1.86937 2.23149 3.70369
H -1.61516 3.17140 4.19255
C -1.49255 1.98022 2.37634
C -0.73703 2.96255 1.52984
C -0.13534 4.17419 2.16871
H 0.38410 3.87530 3.09335
H 0.57893 4.65281 1.48899
H -0.90295 4.91747 2.42761
C -0.52830 4.52537 -1.16988
H -3.98669 -4.03763 -2.62830
H -2.28129 -3.69499 -2.48105
H -1.52477 -2.31785 -1.11470
H 0.32810 2.72838 -1.43959
H -0.43249 5.58110 -2.89505
H 0.35376 4.01614 -2.94303
H -0.56363 1.57087 -2.74656
O 0.33319 1.96809 -2.99619
H 0.91286 1.16141 -2.98570
O 7.43761 -0.89878 1.28363
O 7.23362 -2.92021 2.01742

Water splitting and OH- coordination to P [Zn(bTSC)(PO4C6H4NO2)(OH)]- + H2O Transition state

59
(-1/1)
Zn -0.68800 0.83988 0.52061
O 1.10069 0.71833 -0.38252
O -1.78073 1.24240 -1.05965
H -1.94140 0.38821 -1.48928
P 1.23046 0.10994 -1.79665
O 1.87454 -2.05699 -0.46987
O 0.13726 -0.79293 -2.31179
O 2.52457 0.31435 -2.51906
C 2.95722 -2.28267 0.16604
C 3.01607 -3.18489 1.29136
C 4.19345 -3.42767 1.96857
C 5.38487 -2.78429 1.56940
C 5.37163 -1.89003 0.47558
C 4.19823 -1.64435 -0.20526
H 2.09116 -3.68117 1.59712
H 4.22494 -4.11260 2.81656
N 6.60293 -3.03526 2.27382
H 6.30294 -1.40120 0.18726
H 4.16466 -0.94935 -1.04728
S -3.32328 -2.77839 0.02974
S -1.77529 5.60903 0.07570
N -1.17633 -3.19804 -1.53212
N -0.70560 -2.25918 0.47815
N -0.95409 -1.17487 1.30975
N -1.17684 1.05639 2.59375
N -0.31584 2.95000 1.08562
N 0.19951 3.73803 0.08243
N -0.13264 4.82848 -1.88216
C -1.68218 -2.73850 -0.36058
C -1.75381 -2.62099 3.15854
H -1.44291 -3.46116 2.52822
H -1.25294 -2.68242 4.13722
H -2.83873 -2.69674 3.32852
C -1.42742 -1.32327 2.49769
C -1.55160 -0.03482 3.26336
C -1.96918 0.06139 4.59744
H -2.29418 -0.81724 5.15412
C -1.95315 1.32149 5.20370
H -2.27707 1.43004 6.24053
C -1.50693 2.43917 4.49299
H -1.47201 3.41946 4.96793
C -1.11209 2.26369 3.15884
C -0.56817 3.35778 2.27918
C -0.25625 4.69580 2.86763
H 0.31503 4.55546 3.79954
H 0.32587 5.30260 2.16585
H -1.17588 5.24737 3.11136
C -0.53887 4.69951 -0.59936
H -1.86730 -3.54416 -2.18890
H -0.42972 -2.61158 -1.93506
H 0.26778 -2.19617 0.07922
H 0.74043 3.12544 -0.53529
H -0.64750 5.49140 -2.45040
H 0.22660 3.99065 -2.35464
H -0.77077 1.71446 -1.96491
O 0.10530 1.95378 -2.53968
H -0.13347 1.79573 -3.46574
O 7.63611 -2.46113 1.90802
O 6.59167 -3.81960 3.23077

Water splitting and OH- coordination to P [Zn(bTSC)(PO4C6H4NO2)(OH)]- + H2O Products

59
(-1/1)
Zn -1.16232 1.22009 -0.00708
O 0.31170 1.82305 -1.14454
O -2.47502 0.74452 -1.55228
H -2.73650 -0.20381 -1.51770
P 0.84515 1.21911 -2.50939
O 2.10496 -2.03638 0.96288
O 1.14431 -0.27756 -2.43586
O 1.84875 2.11083 -3.19425
C 2.91932 -2.98751 0.70602
C 2.65149 -4.00223 -0.28439
C 3.54413 -5.02367 -0.53813
C 4.75878 -5.09890 0.17592
C 5.06498 -4.12452 1.15032
C 4.17529 -3.10216 1.40688
H 1.71523 -3.93742 -0.84413
H 3.32817 -5.78430 -1.28911
N 5.67993 -6.16117 -0.08878
H 6.00972 -4.19851 1.68973
H 4.40403 -2.34259 2.15909
S -2.77170 -2.36253 -0.83614
S -4.09801 4.83314 -1.40833
N -0.26731 -2.49600 -1.82844
N -0.42576 -1.72573 0.31226
N -0.98618 -0.69917 1.02108
N -1.53335 1.63232 2.03572
N -1.74849 3.31313 0.12539
N -1.54531 3.99708 -1.06175
N -2.24607 4.17117 -3.21980
C -1.07751 -2.18183 -0.80137
C -0.22669 -1.71724 3.12928
H -0.58813 -2.69737 2.78009
H 0.86420 -1.71141 2.96372
H -0.43138 -1.60829 4.20006
C -0.85023 -0.63604 2.30942
C -1.36588 0.63465 2.90756
C -1.68330 0.83148 4.26151
H -1.55893 0.03502 4.99457
C -2.18285 2.07704 4.64915
H -2.44563 2.25354 5.69402
C -2.34477 3.10271 3.70935
H -2.72220 4.07932 4.01274
C -1.99921 2.83723 2.37988
C -2.04369 3.84303 1.25527
C -2.30046 5.28658 1.53315
H -1.69665 5.61821 2.39193
H -2.06697 5.89314 0.65072
H -3.36083 5.44612 1.78315
C -2.58869 4.30649 -1.92030
H -0.74085 -2.90246 -2.62977
H 0.44935 -1.75618 -2.05445
H 0.62963 -1.90621 0.46561
H -0.75640 3.50040 -1.50534
H -2.95245 4.39677 -3.91044
H -1.52541 3.49743 -3.49086
H -1.92855 0.87097 -2.37497
O -0.65005 1.37724 -3.38581
H -0.56851 1.00388 -4.27719
O 6.73878 -6.20769 0.54834
O 5.39153 -7.00334 -0.94707

Water splitting and OH- coordination to P [Zn(bTSC)(PO4C6H4NO2)(OH)]- + 6 H2O Reactant

74
(-1/1)
Zn 1.03610 -0.73987 0.47182
S 2.34424 -1.74131 5.09146
S 3.74489 -0.55430 -2.77425
N 1.34494 0.69268 5.53596
N 0.77906 -0.14671 3.51408
N 0.54692 -1.08188 2.55920
N 0.02548 -2.59718 0.41791
N 0.97685 -1.80611 -2.08354
N 1.15325 -1.18449 -3.26862
N 2.17458 0.18577 -4.77682
O -0.03924 0.77805 -0.16208
C 1.43702 -0.36536 4.71758
C -0.71919 -2.53668 4.11750
H -0.05377 -3.15992 4.73571
H -0.92662 -1.62019 4.68705
H -1.66496 -3.07131 3.95476
C -0.08290 -2.18402 2.80981
C -0.26054 -3.09231 1.64025
C -0.73714 -4.40066 1.79554
H -0.95008 -4.80088 2.78556
C -0.92791 -5.18653 0.65972
H -1.27710 -6.21651 0.75473
C -0.68452 -4.64091 -0.59700
H -0.84207 -5.23706 -1.49487
C -0.20529 -3.32234 -0.68934
C 0.03392 -2.68891 -2.01559
C -0.82111 -3.08403 -3.19235
H -1.41042 -2.21849 -3.54298
H -0.20122 -3.43437 -4.03435
H -1.54054 -3.87003 -2.94226
C 2.29450 -0.50121 -3.62612
H 1.87795 0.67107 6.39657
H 0.66185 1.45089 5.37580
H 0.96630 0.81390 3.10916
H 0.42535 -1.27492 -3.97665
H 2.99654 0.66614 -5.12243
H 1.30229 0.31399 -5.29234
O 2.90567 -0.39935 0.40983
H 3.19477 -0.65588 -0.48385
P -1.33385 1.45422 0.40033
O -2.49595 1.06005 -0.83520
O -1.93498 0.76864 1.61349
O -1.22819 2.97591 0.38666
C -2.25753 1.12390 -2.14433
C -3.08602 0.35911 -2.99978
C -2.83843 0.30462 -4.36395
C -1.74036 1.00524 -4.88433
C -0.94867 1.82459 -4.06665
C -1.22068 1.90525 -2.70994
H -3.90205 -0.21434 -2.55619
H -3.45280 -0.30563 -5.02622
N -1.38638 0.84049 -6.27863
H -0.12962 2.39605 -4.50341
H -0.63630 2.55810 -2.06362
H -2.44894 1.60995 2.94909
O -2.72292 2.23344 3.67963
H -2.85513 3.07246 3.17228
H -1.47823 2.48717 4.59741
O -0.66514 2.72943 5.16679
H -1.03128 3.02488 6.01332
H 0.00428 4.00180 4.20495
O 0.44727 4.57261 3.52834
H 1.22290 4.91842 3.99361
H 1.16555 3.08937 2.80186
O 1.62609 2.24049 2.61795
H 1.92400 2.28421 1.67125
O 2.38732 2.16519 0.03205
H 1.46775 1.95106 -0.22608
H 2.74389 1.23066 0.15714
H -2.19325 3.88282 1.35417
O -2.84088 4.35439 1.95755
H -3.68085 4.27023 1.48359
O -0.22026 1.08119 -6.61037
O -2.23982 0.45538 -7.06545

Water splitting and OH- coordination to P [Zn(bTSC)(PO4C6H4NO2)(OH)]- + 6 H2O Transition state

74
(-1/1)
Zn 0.51814 0.16296 0.22885
S 1.58463 -0.12194 4.69433
S 3.11492 0.93922 -2.51806
N 0.22752 2.16167 4.88338
N -0.47074 0.81761 3.18648
N -0.36565 -0.18461 2.24662
N -0.39900 -1.77928 0.16205
N 0.49524 -0.67051 -2.10703
N 0.62958 0.12874 -3.18890
N 1.37608 2.01766 -4.21752
O -0.15971 1.87717 -0.44703
C 0.39667 0.99666 4.23134
C -1.21203 -1.87464 3.84464
H -0.40031 -2.34490 4.42162
H -1.57980 -1.02198 4.42983
H -2.02330 -2.60366 3.71363
C -0.69949 -1.39891 2.52394
C -0.64755 -2.33692 1.35807
C -0.90668 -3.70843 1.47168
H -1.09671 -4.16545 2.44191
C -0.92221 -4.48306 0.30935
H -1.10989 -5.55680 0.36919
C -0.71163 -3.87775 -0.92766
H -0.73295 -4.47152 -1.84078
C -0.44321 -2.49872 -0.96681
C -0.20845 -1.74929 -2.23167
C -0.80160 -2.21481 -3.53067
H -1.65730 -1.57505 -3.81224
H -0.05857 -2.15699 -4.34195
H -1.17911 -3.24113 -3.47395
C 1.63719 1.05506 -3.31752
H 0.87765 2.36463 5.63199
H -0.41513 2.90856 4.58560
H -0.84894 1.66795 2.69897
H -0.10106 0.11106 -3.90024
H 2.10216 2.69173 -4.42792
O 0.43554 2.20652 -4.55439
O 2.39280 -0.06440 0.57900
H 2.76092 -0.22755 -0.30524
P -0.84590 3.01853 0.33863
O -2.72626 2.75388 -0.86128
O -1.65495 2.59875 1.56730
O -0.69588 4.44137 -0.10778
C -2.74342 2.72920 -2.15253
C -3.68341 1.89845 -2.85011
C -3.73869 1.85746 -4.23102
C -2.85447 2.64990 -4.98835
C -1.92136 3.48657 -4.34201
C -1.86002 3.52338 -2.96137
H -4.36238 1.28920 -2.24816
H -4.45485 1.21965 -4.74967
N -2.90649 2.61032 -6.42383
H -1.26470 4.10979 -4.95108
H -1.14726 4.16590 -2.44276
H -2.86174 3.45215 2.30445
O -3.42388 4.14382 2.74591
H -3.67168 4.68587 1.96329
H -2.17191 4.52239 3.70640
O -1.36100 4.56857 4.30452
H -1.66913 4.97575 5.12698
H 0.05883 5.23902 3.57865
O 0.92092 5.44837 3.13944
H 1.57497 5.26426 3.82960
H 0.98411 4.01802 2.10787
O 0.93561 3.14120 1.65453
H 1.81140 2.97908 1.20212
O 3.24160 2.39681 0.57232
H 3.20581 2.50559 -0.39248
H 2.97124 1.41911 0.66826
H -3.46793 4.26203 -0.19734
O -4.03844 4.97834 0.17259
H -4.92530 4.59298 0.11739
O -2.10478 3.29472 -7.06597
O -3.74814 1.89117 -6.96884

Water splitting and OH- coordination to P [Zn(bTSC)(PO4C6H4NO2)(OH)]- + 6 H2O Products

74
(-1/1)
Zn 1.05788 -1.00276 0.27820
S 1.92260 -1.38744 4.76360
S 4.16393 -0.48279 -2.10985
N 0.68941 0.96945 4.91714
N 0.04555 -0.28296 3.13335
N 0.13094 -1.30724 2.22030
N 0.16396 -2.91252 0.15561
N 1.38937 -1.86068 -1.94897
N 1.67494 -1.04599 -3.00264
N 2.60630 0.86496 -3.80237
O 0.91929 0.78794 -0.38321
C 0.83310 -0.19057 4.25186
C -0.96105 -2.90891 3.75570
H -0.22213 -3.40317 4.40647
H -1.32965 -2.02430 4.29189
H -1.79566 -3.59925 3.57361
C -0.31826 -2.49035 2.47517
C -0.24006 -3.44118 1.32089
C -0.60667 -4.78984 1.40270
H -0.92895 -5.22845 2.34621
C -0.55456 -5.56600 0.24164
H -0.82658 -6.62255 0.27864
C -0.16279 -4.98820 -0.96510
H -0.12349 -5.58547 -1.87519
C 0.20588 -3.63321 -0.97245
C 0.65251 -2.89854 -2.18928
C 0.23734 -3.32995 -3.56344
H -0.56907 -2.68193 -3.95242
H 1.08820 -3.23714 -4.25645
H -0.13186 -4.36134 -3.58178
C 2.73828 -0.18708 -2.98260
H 1.27664 1.10916 5.72946
H 0.03309 1.71826 4.64845
H -0.20206 0.61259 5.28855
H 0.87841 -0.78711 -3.61287
H 3.38816 1.49636 -3.92395
H 1.71706 1.08418 -4.24684
O 3.01169 -1.44825 0.71644
H 3.40117 -1.56244 -0.17993
P 0.45194 2.05302 0.43435
O -5.09612 2.95570 -1.02978
O -0.61529 1.64113 1.49581
O 0.10084 3.24078 -0.43095
C -4.29782 2.32000 -1.77719
C -4.76831 1.30899 -2.70933
C -3.90420 0.58142 -3.49072
C -2.50540 0.82216 -3.42120
C -2.00324 1.81482 -2.53940
C -2.86434 2.53534 -1.75001
H -5.84647 1.13401 -2.75712
H -4.27093 -0.18649 -4.17292
N -1.62343 0.04153 -4.18417
H -0.93127 1.98149 -2.44516
H -2.45498 3.26973 -1.05483
H -2.03426 2.29671 2.02255
O -2.76714 2.70978 2.55720
H -3.15558 3.39925 1.96592
H -1.72632 3.13704 3.67229
O -0.96238 3.27086 4.32938
H -1.34461 3.70647 5.10449
H 0.43781 3.95976 3.62092
O 1.30251 4.23051 3.21649
H 1.94131 4.10429 3.93325
H 1.64396 3.09398 2.01669
O 1.82011 2.39762 1.32323
H 3.24974 1.51362 1.17240
O 4.04612 0.93772 1.02729
H 4.19352 0.99153 0.06601
H 3.43996 -0.57942 1.00209
H -4.35434 3.93288 0.09799
O -3.83295 4.48360 0.75366
H -4.46278 5.13634 1.08881
O -0.39894 0.33838 -4.19505
O -2.04268 -0.93157 -4.82796

Water splitting and OH- coordination to P [Zn(bTSC)(PO4C6H4NO2)(OH)]- + 10 H2O Reactant

86
(-1/1)
Zn 0.85339 -0.81686 0.66084

S 1.38962 -1.18829 5.30552
S 3.86322 -2.77170 -2.82524
N 0.09383 1.12423 5.18565
N -0.45345 -0.32089 3.50607
N -0.18474 -1.31692 2.57987
N 0.09463 -2.91499 0.50828
N 1.15567 -1.75553 -1.63593
N 1.74327 -1.05318 -2.65290
N 3.31296 -0.58526 -4.23005
O -0.48894 0.35815 -0.22633
C 0.29672 -0.07965 4.61529
C -1.21874 -3.02887 4.03793
H -0.49912 -3.58545 4.65843
H -1.59477 -2.18832 4.63234
H -2.05078 -3.70060 3.78332
C -0.54277 -2.53278 2.80077
C -0.31961 -3.46904 1.65318
C -0.58470 -4.84242 1.74680
H -0.90280 -5.29134 2.68678
C -0.42698 -5.62855 0.60555
H -0.62050 -6.70227 0.64571
C -0.02481 -5.03202 -0.58812
H 0.09794 -5.63259 -1.48842
C 0.23919 -3.65150 -0.60076
C 0.73456 -2.95872 -1.82985
C 0.66955 -3.67183 -3.14708
H -0.27758 -4.22450 -3.23253
H 0.73405 -2.95112 -3.97291
H 1.50265 -4.38302 -3.26007
C 2.92756 -1.44289 -3.26555
H 0.62517 1.32557 6.02352
H -0.44459 1.89405 4.76676
H -0.89762 0.47333 2.98751
H 1.74892 -0.03454 -2.45334
H 4.20308 -0.73023 -4.68977
H 2.69685 0.14538 -4.57150
O 2.78819 -1.25110 0.74957
H 2.99753 -1.82017 -0.00711
P -1.21720 1.57910 0.39302
O -2.70184 1.68782 -0.52852
O -1.79316 1.29283 1.78859
O -0.56791 2.93379 0.18233
C -2.78231 1.89707 -1.85830
C -1.80046 1.45091 -2.76985
C -1.96254 1.67571 -4.13187
C -3.10293 2.34246 -4.59443
C -4.08765 2.79235 -3.70582
C -3.92337 2.57307 -2.34523
H -0.93144 0.91499 -2.39038
H -1.21501 1.33285 -4.84667
N -3.26889 2.57244 -6.02463
H -4.96340 3.31452 -4.08966
H -4.66378 2.93231 -1.62899
H -2.81226 2.19812 2.71301
O -3.29933 2.89125 3.23776
H -3.84984 3.30051 2.53904
H -1.90386 3.50506 3.74933
O -0.98863 3.65110 4.14659
H -1.12108 4.24884 4.89646
H 0.52582 3.67279 3.35045
O 1.45424 3.46288 3.07081
H 1.88243 3.17531 3.89097
H 1.31056 1.82920 2.21076
O 1.61069 0.95868 1.87636
H 2.41101 1.16464 1.34288
O 3.82842 1.09311 0.28532
H 3.40916 1.23549 -0.59405
H 3.59098 0.12822 0.48880
H -4.03676 2.63286 0.44476
O -4.72472 3.19810 0.85453
H -5.43795 2.57242 1.05251
H 0.74252 3.46920 -0.63168
O 1.57385 3.77124 -1.09543
H 2.22748 3.87320 -0.36133
O 3.35752 3.78345 1.00472
H 2.72246 3.75551 1.74969
H 3.66679 2.85827 0.90428
H 2.78619 -2.42733 2.07091
O 2.67603 -3.10013 2.78868
H 2.30201 -2.57166 3.51664
O 2.50056 1.60207 -2.13053
H 3.18455 1.88372 -2.75516
H 2.08460 2.46758 -1.78391
O -4.28090 3.15064 -6.40658
O -2.38964 2.17763 -6.78314

Water splitting and OH$^-$ coordination to P
[Zn(bTSC)(PO$_4$C$_6$H$_4$NO$_2$)(OH)]$^-$ + 10 H$_2$O
Transition state
86
(-1/1)
Zn 0.38314 0.39450 0.21428
S 0.97860 -0.17045 4.92580
S 3.61110 -1.08734 -2.69287
N -0.19298 2.20964 4.93027
N -0.81841 0.89499 3.17740
N -0.63424 -0.05842 2.19063
N -0.37394 -1.57640 0.05974
N 0.71789 -0.26420 -1.93459
N 1.39804 0.50811 -2.83886
N 3.14111 1.05350 -4.19595
O -0.44636 2.11265 -0.30997
C -0.05442 1.02785 4.29800
C -1.70168 -1.80825 3.58062
H -0.99565 -2.42466 4.15853
H -2.03428 -0.98607 4.22474
H -2.56524 -2.43122 3.30729
C -1.03170 -1.27313 2.35752
C -0.86481 -2.15746 1.15844
C -1.22992 -3.51091 1.14630
H -1.61516 -3.99934 2.04025
C -1.08072 -4.22934 -0.04118
H -1.35427 -5.28548 -0.07891
C -0.58017 -3.59655 -1.17980
H -0.45810 -4.15130 -2.10910
C -0.22417 -2.24222 -1.09109
C 0.38305 -1.47836 -2.22531
C 0.52690 -2.13188 -3.56265
H -0.37664 -2.71140 -3.80073
H 0.67974 -1.37708 -4.34464
H 1.39193 -2.81351 -3.57660
C 2.68080 0.18655 -3.27851
H 0.37517 2.35068 5.75625
H -0.66171 3.03604 4.54046
H -1.19303 1.76653 2.72777
H 1.31793 1.51825 -2.62235
H 4.09595 0.96607 -4.52168
H 2.53966 1.75483 -4.61682
O 2.29861 0.30771 0.62171
H 2.72748 -0.12923 -0.13393
P -1.04171 3.26431 0.52150
O -2.95499 3.35500 -0.68943
O -1.89251 2.88989 1.73040
O -0.80477 4.69833 0.12776
C -3.16899 3.19435 -1.95206
C -2.44891 2.23981 -2.74805
C -2.72438 2.06960 -4.09135
C -3.72512 2.84152 -4.71461
C -4.44599 3.79659 -3.97051
C -4.17328 3.97110 -2.62813
H -1.67335 1.65279 -2.25740
H -2.17575 1.33919 -4.68676
N -4.00861 2.65757 -6.10933
H -5.21047 4.39125 -4.47120
H -4.71410 4.71902 -2.04433
H -2.91254 3.96040 2.52611
O -3.33239 4.74518 2.96296
H -3.64945 5.24248 2.17525
H -1.96322 5.04770 3.76158
O -1.10917 5.00268 4.29676
H -1.32293 5.39957 5.15369
H 0.35532 5.44777 3.60215
O 1.27137 5.44198 3.20846
H 1.83705 5.14605 3.93795
H 0.90253 3.99856 2.29408
O 0.74603 3.18694 1.75381
H 1.55906 3.09495 1.18112
O 2.97825 2.79800 0.34699
H 2.70957 2.88911 -0.59726
H 2.85059 1.80816 0.52937
H -3.76957 4.67331 0.04256
O -4.30384 5.40538 0.46007
H -5.16334 4.98421 0.60896
H 0.46484 5.24162 -0.81503
O 1.29680 5.49793 -1.29451
H 1.93910 5.61926 -0.55400
O 2.99146 5.53941 0.89563
H 2.38982 5.63388 1.65968
H 3.17533 4.57760 0.85210
H 2.30054 -1.10524 1.72972
O 2.17551 -1.90245 2.29812
H 1.80769 -1.50701 3.10940
O 2.10327 3.21656 -2.26371
H 2.89903 3.43355 -2.77100
H 1.73625 4.11350 -1.96422
O -4.88980 3.34565 -6.63370
O -3.36311 1.81672 -6.74273

Water splitting and OH$^-$ coordination to P
[Zn(bTSC)(PO$_4$C$_6$H$_4$NO$_2$)(OH)]$^-$ + 10 H$_2$O
Products
86
(-1/1)
Zn 0.94263 -1.46132 0.60669
S 1.79235 -1.20768 5.29826
S 4.53285 -2.48427 -1.83170
N 0.16321 0.86855 5.03989
N -0.21751 -0.77984 3.51001
N 0.16147 -1.81645 2.67070
N 0.69367 -3.54310 0.76800
N 1.48981 -2.31972 -1.40666
N 2.02910 -1.56181 -2.41836
N 3.70971 -0.91094 -3.81026
O -0.07272 0.02593 -0.05287
C 0.52243 -0.33796 4.56286
C -0.58766 -3.51193 4.30990
H 0.22061 -3.88130 4.96065
H -1.08326 -2.68228 4.82761
H -1.30609 -4.32806 4.14913
C -0.01679 -3.04652 3.01207
C 0.32498 -4.04713 1.94846
C 0.24210 -5.43358 2.13448
H -0.04123 -5.85736 3.09701
C 0.54504 -6.26724 1.05637
H 0.49315 -7.35129 1.17300
C 0.91848 -5.71514 -0.17054
H 1.16133 -6.36041 -1.01357
C 0.98935 -4.31906 -0.28055
C 1.44629 -3.60684 -1.51550
C 1.80962 -4.39271 -2.73338
H 1.08997 -5.20782 -2.89305
H 1.81820 -3.74636 -3.62024
H 2.81319 -4.83434 -2.62308
C 3.38216 -1.63792 -2.73475
H 0.70625 1.22711 5.81552
H -0.47065 1.52996 4.57322
H -0.79941 -0.07960 2.95170
H 1.71342 -0.57315 -2.38032
H 4.68566 -0.81147 -4.06384
H 3.00147 -0.50917 -4.41722
O 3.01354 -1.19522 0.84241
H 3.51380 -1.65218 0.12413
P -0.62630 1.24222 0.76624
O -4.89928 2.44470 -1.07706
O -1.60234 0.78542 1.88073
O -1.14386 2.37600 -0.10576
C -4.50779 2.76324 -2.24244
C -4.70210 1.88282 -3.37428
C -4.27985 2.21710 -4.64253
C -3.63490 3.45380 -4.87263
C -3.42393 4.34835 -3.79854
C -3.84578 4.01921 -2.52878
H -5.20089 0.92807 -3.18629
H -4.43265 1.54137 -5.48477
N -3.19672 3.79689 -6.18577
H -2.92408 5.29698 -3.99772
H -3.68439 4.70039 -1.68975
H -2.80900 1.82862 2.41673
O -3.35526 2.52799 2.86545
H -3.69508 3.10457 2.13526
H -2.13556 3.08815 3.66125
O -1.27733 3.29882 4.17151
H -1.55524 3.75927 4.97651
H -0.03341 3.96492 3.29642
O 0.81252 4.11383 2.78266
H 1.50768 4.01713 3.45180
H 0.70452 2.60939 2.01390
O 0.76009 1.73182 1.55177
H 2.22600 1.51017 0.78624
O 3.09675 1.38809 0.32239
H 2.82884 1.32554 -0.63012
H 3.20990 -0.21230 0.71680
H -4.53753 3.47734 0.10821
O -4.29420 4.12112 0.84790
H -5.14043 4.52048 1.09523
H -0.07849 3.01432 -1.16640
O 0.67592 3.36215 -1.72818
H 1.26075 3.78997 -1.06065
O 2.36048 4.27011 0.30764
H 1.79351 4.32655 1.10083
H 2.84034 3.42696 0.41537
H 3.31633 -2.45330 2.34719
O 3.23142 -3.15117 3.02035
H 2.79231 -2.66923 3.74848
O 2.11751 1.26809 -2.25118
H 2.78363 1.59145 -2.87567
H 1.49275 2.06026 -2.10977
O -2.63353 4.88497 -6.36681
O -3.39033 2.99786 -7.11217

[Zn$_2$(bTSC)$_2$(PO$_4$C$_6$H$_5$)(OH)]$^{3-}$ (A)
86
(-3/1)
Zn 1.63880 -0.13210 0.79100
Zn -1.57170 1.00640 -0.66350
S 4.49910 3.86490 0.60550
S 4.02270 -0.49880 0.71590
S 2.25150 -5.31720 0.28360
S -2.17000 3.12720 0.24990
N 1.88310 2.12290 0.70020
N 2.21150 2.74160 -0.45170
N 3.37940 4.14910 -1.80510
N 3.06570 -1.54880 -2.01520
N 4.24280 -2.07290 -1.59660
N 5.92940 -2.12480 -0.07930
N 1.21290 0.57050 2.74610
N 1.28280 -2.10520 2.22200
N 1.65120 -3.37200 1.99490
N 0.33910 -3.46740 0.04540
N -1.10940 2.14720 -2.40380
N -1.28280 3.49800 -2.35320
N -2.01360 5.32670 -1.22130
N 0.95190 -0.32280 -3.33990
C 3.26090 3.53010 -0.56440
C 4.70930 -1.63010 -0.45060
C 2.93450 -3.50050 -3.53670
H 4.02320 -3.45740 -3.68330
H 2.44460 -3.73410 -4.49220
H 2.74780 -4.33010 -2.83170
C 2.44940 -2.19560 -2.95460
C 1.11980 -1.65370 -3.34070
C 0.04130 -2.52940 -3.58980
H 0.20200 -3.60840 -3.62200
C -1.24020 -2.00330 -3.73080
H -2.09910 -2.66280 -3.87050
C -1.41900 -0.62140 -3.64050
H -2.40940 -0.17170 -3.70710
C -0.28200 0.17860 -3.45700
C -0.39410 1.66580 -3.37290
C 0.33680 2.49910 -4.38170
H 0.54590 3.50000 -3.98360
H -0.27190 2.61900 -5.29590
H 1.26840 1.98950 -4.66750
C 1.35550 -3.93160 0.81500
C -1.77340 3.98880 -1.23280
C 1.18850 -2.70100 4.62560
H 0.17760 -2.91770 5.01530
H 1.78550 -2.31390 5.46600
H 1.62330 -3.64420 4.27320
C 1.14330 -1.73110 3.47370
C 0.95620 -0.29980 3.74120
C 0.55050 0.18230 5.00690
H 0.33190 -0.51070 5.81840
C 0.42880 1.55380 5.19860
H 0.11770 1.94460 6.17050
C 0.70820 2.43510 4.14930
H 0.63560 3.51150 4.29700
C 1.09950 1.90110 2.91200
C 1.45080 2.75670 1.74580
C 1.26580 4.24330 1.81750
H 2.15390 4.72940 2.25270
H 0.37860 4.50990 2.40810
H 1.14500 4.64370 0.80170
H 4.32800 4.41090 -2.04970
H 2.86220 3.70210 -2.55860
H 6.48620 -2.58070 -0.79490
H 6.41230 -1.69660 0.69970
H 0.13050 -4.01160 -0.78270
H -0.43750 -2.89380 0.41400
H -1.68780 5.88350 -2.00390
H -2.22050 5.79200 -0.34790
P -3.16180 -1.63780 -0.11910
O -3.09300 -0.22250 -0.79510
O -1.91970 -1.94560 0.73570
O -3.67550 -2.72960 -1.03530
C -5.62860 -1.06550 0.93350
C -6.35420 -1.37570 -0.23460
C -6.28550 -0.39530 1.98450
C -7.70050 -1.01220 -0.33610
H -5.84170 -1.91450 -1.03260
C -7.63260 -0.04470 1.87260
H -5.71460 -0.15920 2.88610
C -8.35160 -0.34680 0.70930
H -8.25050 -1.26030 -1.24900
H -8.12310 0.47430 2.70120
H -9.40480 -0.06920 0.62030
O -4.33080 -1.39490 1.12270
O -0.08060 -0.14930 -0.13590
H -0.61400 -0.89560 0.22820

[Zn$_2$(bTSC)$_2$(PO$_4$C$_6$H$_5$)(OH)]$^{3-}$ (B)
86
(-3/1)
Zn -2.17860 -0.07130 0.56310
Zn 1.46950 -0.41830 -0.19900
S -4.47590 -3.88080 -1.57300
S -4.40210 0.32780 -0.25450
S -0.20390 3.31140 1.61920
S 1.96440 -2.71530 0.27220
N -2.19400 -2.18050 -0.23220
N -2.14020 -2.41260 -1.55510
N -2.72460 -3.38270 -3.52780
N -2.83050 2.44560 -1.78220
N -4.05730 2.86620 -1.39310
N -6.03960 2.38640 -0.39730
N -2.32550 -1.33700 2.26860
N -2.41790 1.34700 2.52410
N -2.71940 2.65860 2.53390
N -2.42120 4.77930 1.77420
N 1.36650 -1.11480 -2.22060
N 1.56540 -2.44130 -2.46130
N 2.11390 -4.50240 -1.68110
N -0.47480 1.58410 -2.89040
C -3.01700 -3.17120 -2.18620
C -4.78380 1.98450 -0.73800
C -2.37690 4.80870 -2.36490
H -3.43560 4.91770 -2.63690
H -1.75190 5.33520 -3.09960
H -2.25310 5.30490 -1.38550
C -2.02840 3.34380 -2.26350
C -0.64960 2.87680 -2.56800
C 0.45320 3.73980 -2.39140
H 0.29890 4.79400 -2.15780
C 1.74160 3.21200 -2.43850
H 2.61000 3.84810 -2.24900
C 1.91280 1.84560 -2.66930
H 2.89840 1.37490 -2.62490
C 0.76120 1.07880 -2.90620
C 0.87440 -0.38760 -3.17360
C 0.40510 -0.91240 -4.49640

H 0.25860 -1.99830 -4.45630
H 1.14510 -0.68970 -5.28560
H -0.52910 -0.40000 -4.77380
C -1.88260 3.52800 1.99610
C 1.85440 -3.19230 -1.41910
C -3.21540 1.24240 4.86800
H -2.42180 1.27490 5.63480
H -4.04860 0.65570 5.28480
H -3.54820 2.27030 4.68120
C -2.70660 0.64620 3.58350
C -2.50130 -0.81530 3.49250
C -2.49930 -1.65130 4.62640
H -2.63960 -1.23710 5.62410
C -2.30540 -3.01950 4.44830
H -2.29690 -3.68760 5.31260
C -2.12860 -3.53880 3.16400
H -1.99800 -4.60960 3.01420
C -2.14490 -2.65470 2.07250
C -2.02920 -3.10850 0.66210
C -1.71140 -4.53980 0.35150
H -2.63070 -5.14490 0.29080
H -1.03750 -4.97200 1.10450
H -1.22390 -4.59880 -0.63200
H -3.53030 -3.59810 -4.10440
H -2.07730 -2.71540 -3.94030
H -6.40430 3.23860 -0.80920
H -6.67990 1.72690 0.02300
H -1.76750 5.55210 1.74060
H -3.31500 4.97140 2.21810
H 1.93750 -4.85170 -2.61670
H 2.16650 -5.16410 -0.91870
P 4.26330 1.09780 -0.09530
O 2.79540 0.84780 0.40710
O 4.57900 0.42610 -1.43010
O 4.73230 2.52150 0.12880
C 6.42470 0.04350 1.21420
C 7.29740 0.18240 0.11280
C 6.97840 -0.24050 2.48030
C 8.67720 0.04820 0.29040
H 6.86140 0.37590 -0.86830
C 8.35830 -0.38100 2.64200
H 6.29830 -0.34720 3.32950
C 9.22210 -0.23330 1.54930
H 9.33790 0.15980 -0.57500
H 8.76310 -0.60230 3.63410
H 10.30240 -0.33840 1.67680
O 5.08640 0.14790 1.12210
O -0.28270 0.33010 0.27460
H -0.15880 1.21820 0.67420

[Zn$_2$(bTSC)$_2$(HPO$_4$C$_6$H$_5$)(OH)]$^{2-}$
87
(-2/1)
Zn 1.82060 1.04100 0.25030
Zn -0.86960 -0.93060 -1.04380
S 4.93960 -2.65440 0.56240
S 2.19040 1.35480 2.59830
S -1.82080 4.59870 2.15770
S -0.27000 -0.27350 -3.25490
N 2.93650 -0.62290 -0.72440
N 2.54610 -1.90360 -0.57120
N 2.73950 -4.08810 0.01470
N 0.89420 -1.57490 2.58250
N 2.03270 -1.36360 3.28950
N 3.87660 -0.20710 3.89930
N 3.23270 1.99380 -0.99910
N 1.37990 3.54960 0.23840
N 0.56180 4.26450 1.02660
N -1.21300 3.09590 0.03310
N -1.10760 -2.83330 -1.89500
N -0.86450 -2.98350 -3.21690
N -0.13440 -2.09650 -5.17290
N -0.92610 -3.07870 0.90820
C 3.32150 -2.82640 -0.04750
C 2.68000 -0.22750 3.24040
C 0.43040 -3.20720 4.35790
H 1.50240 -3.45180 4.39710
H -0.15930 -4.12120 4.49830
H 0.24240 -2.53130 5.20970
C 0.13310 -2.52200 3.04480
C -1.03040 -3.01050 2.24770
C -2.16930 -3.50630 2.91560
H -2.25750 -3.41620 3.99890
C -3.17850 -4.11920 2.17760
H -4.07360 -4.50050 2.67440
C -3.02290 -4.25580 0.80000
H -3.78350 -4.75810 0.20110
C -1.88080 -3.70090 0.19570
C -1.67630 -3.82310 -1.27280
C -2.11100 -5.06190 -2.00440
H -2.88830 -4.82160 -2.74880
H -2.48770 -5.83520 -1.32440
H -1.26090 -5.46770 -2.57460
C -0.73350 3.91370 1.00740
C -0.44980 -1.90910 -3.87080
C 2.80900 5.57110 0.13460
H 2.61270 6.21630 -0.74030
H 3.86680 5.70360 0.40860
H 2.16830 5.91650 0.95420
C 2.48510 4.13040 -0.15980
C 3.40810 3.32910 -0.96940
C 4.45000 3.92090 -1.71780
H 4.59440 5.00020 -1.70160
C 5.27440 3.11060 -2.48900
H 6.08270 3.55190 -3.07670
C 5.06720 1.72800 -2.51050
H 5.71600 1.07800 -3.09570
C 4.02510 1.19540 -1.73990
C 3.76040 -0.26190 -1.65770
C 4.39270 -1.21910 -2.62160
H 5.30950 -1.65290 -2.18980
H 4.63030 -0.74200 -3.58160
H 3.69910 -2.05570 -2.79510
H 3.15000 -4.69610 0.71460
H 1.72080 -4.07940 0.01700
H 4.28140 -1.09850 4.16880
H 4.50220 0.56990 3.73190
H -2.13630 2.68620 0.15150
H -0.53910 2.58660 -0.53030
H -0.26620 -3.01200 -5.58820
H 0.11300 -1.31280 -5.76100
P -3.32880 0.04460 0.77470
O -2.77620 -0.66160 -0.48140
O -2.10690 0.45870 1.72560
O -4.47240 -0.56480 1.51780
C -4.97930 1.92710 -0.29500
C -5.72210 1.04280 -1.09240
C -5.45030 3.22900 -0.06470
C -6.93610 1.46670 -1.64270
H -5.34540 0.03690 -1.28290
C -6.65910 3.64240 -0.62900
H -4.84810 3.89650 0.55630
C -7.41170 2.76310 -1.41720
H -7.51220 0.77310 -2.26120
H -7.01750 4.65910 -0.44630
H -8.35970 3.08640 -1.85360
O -3.77570 1.59410 0.26140
O 0.09360 0.00700 0.39010
H -1.21390 0.40970 1.24680
H 0.39730 -0.64980 1.07790

[Zn$_2$(bTSC)$_2$(PO$_4$C$_6$H$_5$)(H$_2$O)]$^{2-}$
87
(-2/1)
Zn 2.36440 0.85380 0.63390
Zn -1.05300 -0.37170 -0.67630
S 5.76030 1.34510 -1.96280
S 3.99610 -0.57190 1.53420
S 0.29310 -1.16840 3.32580
S -1.18050 1.50300 -2.14660
N 2.74550 1.30580 -1.49040
N 3.21790 0.39850 -2.38530
N 4.89170 -0.67150 -3.49720
N 2.22180 -2.71000 0.02770
N 3.55650 -2.68100 -0.22690
N 5.62150 -1.72010 -0.23590
N 1.69700 2.81100 0.40410
N 1.63750 1.58500 2.78370
N 1.89280 0.99320 3.95950
N 2.06740 -0.84520 5.27180
N -1.87290 -1.42420 -2.30730
N -2.32990 -0.70670 -3.36380
N -2.34420 1.25340 -4.51860
N -0.43640 -3.22720 -0.78080
C 4.50910 0.31520 -2.60330
C 4.32830 -1.73460 0.22660
C 2.51900 -5.12220 0.32110
H 3.24840 -5.15130 -0.50460
H 1.91550 -6.03770 0.30700
H 3.11140 -5.09660 1.25070
C 1.68190 -3.87890 0.18620
C 0.19650 -3.99630 0.12060
C -0.49140 -4.95570 0.88490
H 0.03640 -5.56330 1.62170
C -1.86370 -5.11430 0.68430
H -2.42760 -5.83610 1.28000
C -2.50170 -4.35580 -0.29420
H -3.57010 -4.45710 -0.47850
C -1.74480 -3.41100 -1.01030
C -2.35250 -2.61350 -2.10850
C -3.48410 -3.18240 -2.90930
H -3.47310 -2.77290 -3.92700
H -4.42030 -2.86190 -2.42060
H -3.45900 -4.28000 -2.94080
C 1.50120 -0.25380 4.17570
C -2.00800 0.57020 -3.39300
C 1.21010 3.68320 4.03510
H 0.14740 3.93340 4.19810
H 1.76470 4.63260 3.97920
H 1.56110 3.10490 4.89770
C 1.38750 2.86660 2.78610
C 1.28260 3.51850 1.46680
C 0.79840 4.82920 1.28920
H 0.44910 5.41270 2.14030
C 0.76980 5.36470 0.00350
H 0.39870 6.37940 -0.15620
C 1.22120 4.60870 -1.08270
H 1.22140 5.02640 -2.08850
C 1.68530 3.30880 -0.84210
C 2.23890 2.42360 -1.90130
C 2.23310 2.85290 -3.33690
H 3.09120 3.51390 -3.54590
H 1.31090 3.39090 -3.59340
H 2.32850 1.96650 -3.97730
H 5.87000 -0.93060 -3.46400
H 4.23860 -1.43950 -3.62820
H 5.75810 -2.28470 -1.07240
H 6.02650 -0.78570 -0.32050
H 1.61140 -1.65950 5.66240
H 2.60240 -0.25750 5.90340
H -2.92780 0.78650 -5.20470
H -2.32720 2.26460 -4.51330
P -3.77460 -0.85500 0.93690
O -2.20770 -0.76910 0.80500
O -4.46810 -1.65810 -0.15160
O -4.20480 -1.06870 2.37700
C -5.34700 1.35500 0.50140
C -6.42520 0.90650 1.29450
C -5.55540 2.44250 -0.37250
C -7.67060 1.53400 1.20010
H -6.24610 0.07910 1.98330
C -6.80260 3.06560 -0.45030
H -4.71330 2.77890 -0.98330
C -7.87330 2.61460 0.33260
H -8.49630 1.17500 1.82230
H -6.94070 3.90860 -1.13380
H -8.85040 3.10010 0.26880
O -4.11530 0.81730 0.55100
O 0.75890 -0.53390 0.37290
H 0.51070 -0.67470 1.35470
H 1.30040 -1.40000 0.15090

[Zn$_2$(bTSC)$_2$(HPO$_4$)]$^{2-}$
74
(-2/1)
Zn -2.38360 0.07070 -0.31160
Zn 2.39850 0.08390 0.32400
S -4.02700 -0.60360 -2.19430
S -3.80390 2.05970 0.35010
S 3.80290 2.09380 -0.29690
S 4.03660 -0.63440 2.18320
N -3.77640 -1.25330 0.75430
N -4.89530 -1.73330 0.18350
N -6.27500 -1.87780 -1.60540
N -1.24990 1.82940 -1.31760
N -1.71180 3.09910 -1.11530
N -3.29410 4.55220 -0.39650
N -1.60050 -0.07150 1.94420
N 1.24920 1.79060 1.35730
N 1.70360 3.06940 1.20220
N 3.20190 4.57620 0.41690
N 3.76390 -1.23100 -0.77880
N 4.87310 -1.74550 -0.21510
N 6.25850 -1.94070 1.56530
N 1.60060 -0.00490 -1.94970
C -5.08220 -1.44530 -1.10340
C -2.83600 3.25980 -0.44370
C 0.70230 3.01180 -2.24850
H 0.24720 3.50840 -3.12450
H 1.74190 2.75210 -2.48320
H 0.68390 3.73390 -1.42320
C -0.08740 1.77730 -1.89380
C 0.46830 0.50340 -2.45510
C -0.10210 0.01990 -3.64390
H -1.02760 0.45850 -4.01980
C 0.55970 -0.99000 -4.33910
H 0.15580 -1.37510 -5.27900
C 1.74680 -1.49920 -3.82300
H 2.27740 -2.28840 -4.35320
C 2.23260 -1.00700 -2.59640
C 3.45580 -1.58550 -1.99260
C 4.26180 -2.58460 -2.77820
H 5.19910 -2.79160 -2.25140
H 4.48340 -2.22320 -3.79430
H 3.70450 -3.53190 -2.88050
C 2.81460 3.26310 0.51770
C 5.07090 -1.48020 1.07350
C -0.70770 2.92690 2.33040
H -0.25870 3.39160 3.22690
H -1.74770 2.65500 2.54900
H -0.68540 3.67910 1.53240
C 0.08840 1.70910 1.93360
C -0.46170 0.41540 2.45520
C 0.11260 -0.10580 3.62660
H 1.04340 0.31580 4.00870
C -0.55000 -1.13140 4.29630
H -0.14080 -1.54760 5.22050
C -1.74830 -1.61400 3.77800
H -2.28360 -2.41070 4.29230
C -2.24140 -1.08060 2.57190
C -3.48160 -1.62170 1.96780
C -4.31930 -2.59750 2.75040
H -4.52020 -2.23530 3.77060
H -3.80300 -3.56880 2.84420
H -5.26720 -2.76330 2.22760
H -6.41040 -1.88490 -2.60750
H -6.83050 -2.51010 -1.03850
H -2.64660 5.28020 -0.68250
H -3.97180 4.78930 0.31680
H 4.15730 4.76420 0.14010
H 2.77070 5.23100 1.06250
H 6.79680 -2.57850 0.98810
H 6.39040 -1.97470 2.56750
P 0.07820 -2.22470 -0.12920
O -1.07420 -1.37190 -0.73490
O 0.71320 -3.20280 -1.10720
O 1.04860 -1.33580 0.70300
O -0.63880 -3.20890 1.03410
H -0.51590 -4.10880 0.70140

1A [Zn(bTSC)(DMSO)$_2$]$^{2+}$
56
(0/1)
Zn 0.00000 0.00000 0.22821
S -1.66432 0.04817 2.33955
S 1.66432 -0.04817 2.33955
N -4.25473 0.62991 2.27652
N -3.26654 0.47067 0.22150
N -2.22026 0.28396 -0.60096
N 0.00000 0.00000 -2.02560
N 2.22026 -0.28396 -0.60096
N 3.26654 -0.47067 0.22150
N 4.25473 -0.62991 2.27652
C -3.13746 0.40320 1.58086
C -3.67429 0.82165 -2.51629
H -4.19062 1.59922 -1.93181
H -4.34692 -0.05007 -2.59149
H -3.53733 1.22701 -3.52371
C -2.37009 0.43874 -1.87371
C -1.14607 0.20696 -2.68951
C -1.18504 0.20117 -4.09407
H -2.11937 0.34596 -4.63298
C 0.00000 0.00000 -4.79708
H 0.00000 0.00000 -5.88863
C 1.18504 -0.20117 -4.09407
H 2.11937 -0.34596 -4.63298
C 1.14607 -0.20696 -2.68951
C 2.37009 -0.43874 -1.87371
C 3.67429 -0.82165 -2.51629
H 3.53733 -1.22701 -3.52371
H 4.19062 -1.59922 -1.93181
H 4.34692 0.05007 -2.59149
C 3.13746 -0.40320 1.58086
H -4.22025 0.59048 3.28853
H -5.14694 -0.84185 1.83847
S 0.45018 3.45009 0.53283
O 0.00000 2.07503 -0.00667
C 2.26612 3.41209 0.58140
C 0.12528 3.46309 2.32101
H 2.60088 3.27891 -0.45557
H -0.95946 3.34980 2.44228
H 2.59556 2.57793 1.21403
H 2.61974 4.37708 0.97148
H 0.45295 4.43680 2.71239
H 0.65934 2.63351 2.80231
S -0.45018 -3.45009 0.53283
O 0.00000 -2.07503 -0.00667
C -0.12528 -3.46309 2.32101
C -2.26612 -3.41209 0.58140
H 0.95946 -3.34980 2.44228
H -2.60088 -3.27891 -0.45557
H -0.45295 -4.43680 2.71239
H -0.65934 -2.63351 2.80231
H -2.59556 -2.57793 1.21403
H -2.61974 -4.37708 0.97148

1B [Zn(bTSC)(DMSO)$_2$]$^{2+}$
56
(0/1)
Zn 0.00000 0.00000 0.03371
S 4.08373 -2.45725 -2.34433
S -4.08373 2.45725 -2.34433
N 2.66833 -0.20982 -2.01595
N 2.96439 -1.55405 -0.14351
N 2.04598 -0.93492 0.63498
N 0.00000 0.00000 2.09959
N -2.04598 0.93492 0.63498
N -2.96439 1.55405 -0.14351
N -2.66833 0.20982 -2.01595
C 3.17924 -1.31978 -1.48862
C 3.28833 -1.83911 2.54848
H 4.24250 -1.53236 2.09215
H 3.17395 -2.92735 2.39525
H 3.36560 -1.67257 3.62604
C 2.14713 -1.09225 1.92317
C 1.05086 -0.52675 2.75182
C 1.07926 -0.53760 4.15494
H 1.92428 -0.95104 4.70036
C 0.00000 0.00000 4.85262
H 0.00000 0.00000 5.94402
C -1.07926 0.53760 4.15494
H -1.92428 0.95104 4.70036
C -1.05086 0.52675 2.75182
C -2.14713 1.09225 1.92317
C -3.28833 1.83911 2.54848
H -3.36560 1.67257 3.62604

H -4.24250 1.53236 2.09215
H -3.17395 2.92735 2.39525
C -3.17924 1.31978 -1.48862
H 2.79969 -0.06255 -3.00995
H 2.19914 0.52183 -1.46757
H 3.50968 -2.32656 0.23502
H -3.50968 2.32656 0.23502
H -2.79969 0.06255 -3.00995
H -2.19914 -0.52183 -1.46757
S 1.03678 3.10516 -1.09187
O 1.00501 1.60199 -0.65490
C 0.01442 3.99543 0.10271
C 0.00000 3.23063 -2.57029
H 0.48166 3.84961 1.08514
H 0.43447 2.54573 -3.31018
H -1.01262 3.61176 0.08411
H 0.04337 5.05892 -0.17454
H 0.08362 4.26653 -2.93007
H -1.04610 2.97546 -2.35332
S -1.03678 -3.10516 -1.09187
O -1.00501 -1.60199 -0.65490
C 0.00000 -3.23063 -2.57029
C -0.01442 -3.99543 0.10271
H -0.43447 -2.54573 -3.31018
H -0.48166 -3.84961 1.08514
H -0.08362 -4.26653 -2.93007
H 1.04610 -2.97546 -2.35332
H 1.01262 -3.61176 0.08411
H -0.04337 -5.05892 -0.17454

1TS [Zn(bTSC)(DMSO)$_2$]$^{2+}$

56
(0/1)
Zn 0.00000 0.00000 0.00000
S 3.18724 3.15224 -0.79883
S -1.45619 1.50196 1.55049
N 2.75363 1.89325 1.52063
N 3.29226 0.51572 -0.25329
N 2.26187 -0.18218 -0.78278
N 0.12816 -1.74331 -1.24736
N -2.11987 -0.79575 -0.26718
N -3.16551 -0.19065 0.32120
N -4.10096 1.39000 1.68509
C 3.04168 1.84504 0.21735
C 3.88830 -1.93107 -1.33728
H 4.24045 -2.20267 -0.32544
H 4.59022 -1.17814 -1.73186
H 3.94965 -2.83517 -1.95190
C 2.50463 -1.35640 -1.27566
C 1.31653 -2.10168 -1.75953
C 1.40024 -3.12863 -2.71782
H 2.36081 -3.42109 -3.13939
C 0.22906 -3.74564 -3.14495
H 0.26763 -4.53413 -3.89896
C -0.99960 -3.34682 -2.61198
H -1.92039 -3.82225 -2.94521
C -1.01391 -2.32723 -1.65322
C -2.27513 -1.81830 -1.04154
C -3.59986 -2.44511 -1.36222
H -3.49311 -3.50404 -1.62314
H -4.07421 -1.93273 -2.21687
H -4.29070 -2.39449 -0.50793
C -2.98884 0.87245 1.16481
H 2.59293 2.79652 1.95619
H 2.36372 1.05187 1.96174
H 3.95782 -0.01786 0.31008
H -4.11215 -0.50931 0.11344
H -4.02844 2.18171 2.31413
H -5.02821 1.02491 1.48673
S 1.06514 -1.49766 2.90986
O 1.14451 -0.46758 1.73827
C 1.29748 -3.12768 2.15349
C -0.68052 -1.64537 3.37308
H 2.32786 -3.16062 1.77731
H -1.00107 -0.65491 3.71923
H 0.57286 -3.26473 1.33973
H 1.16129 -3.88425 2.93931
H -0.73864 -2.37693 4.19156
H -1.27396 -1.96901 2.50799
S -1.37236 2.28761 -1.82794
O -0.19412 1.29524 -1.58182
C -0.72247 3.91233 -1.35426
C -1.35444 2.47175 -3.62766
H -0.65112 3.90837 -0.25927
H -1.64054 1.49662 -4.04267
H -1.43107 4.68416 -1.68681
H 0.26982 4.04165 -1.80713
H -0.33986 2.74833 -3.94522
H -2.08963 3.23718 -3.91257

2A [Zn(bTSC)]$_2$

68
(0/1)
Zn 0.00000 0.00000 2.34705
Zn 0.00000 0.00000 -1.67856
S 1.95638 -0.10998 -3.23918
S -0.95185 -1.87856 3.41816
S -1.95638 0.10998 -3.23918
S 0.95185 1.87856 3.41816
N 0.00000 -4.30410 2.93593
N 1.18531 -2.69926 1.85652
N -1.53902 -0.95236 -0.12624
N 1.34636 -1.39782 1.52293
N 0.37620 -2.12067 -1.67160
N 1.42302 -2.65880 -2.31705
N -1.34636 1.39782 1.52293
N -1.18531 2.69926 1.85652
N 3.25766 -2.38791 -3.61686
N -3.25766 2.38791 -3.61686
N 1.53902 0.95236 -0.12624
N -0.37620 2.12067 -1.67160
N 0.00000 4.30410 2.93593
N -1.42302 2.65880 -2.31705
C 2.78590 3.00696 -0.11620
C 3.88623 2.35095 0.42961
C 0.47762 2.91135 -1.08531
C 1.62468 2.26943 -0.41107
C 3.79387 0.98944 0.70822
C -3.88623 -2.35095 0.42961
C -2.78590 -3.00696 -0.11620
C 0.17918 -2.99065 2.66540
C -3.79387 -0.98944 0.70822
C -1.62468 -2.26943 -0.41107
C -0.47762 -2.91135 -1.08531
C -2.58240 -0.32889 0.44672
C -2.41849 1.09064 0.85275
C 2.41849 -1.09064 0.85275
C 2.18484 -1.81898 -3.01752
C -0.17918 2.99065 2.66540
C -2.18484 1.81898 -3.01752
C 2.58240 0.32889 0.44672
H -4.80603 -2.89961 0.64385
H -4.62772 -0.45192 1.16136
H -2.83809 -4.07081 -0.34394
H 4.80603 2.89961 0.64385
H 4.62772 0.45192 1.16136
H 2.83809 4.07081 -0.34394
H -3.84145 1.84591 -4.23902
H 3.37361 -3.39446 -3.57345
H 0.69032 4.60088 3.61240
H 0.67450 -4.97592 2.58639
H -3.37361 3.39446 -3.57345
H -0.67450 4.97592 2.58639
H 3.84145 -1.84591 -4.23902
H -0.69032 -4.60088 3.61240
C -3.47443 2.10356 0.52389
H -3.75784 2.67678 1.41950
H -3.06484 2.82496 -0.20277
H -4.36124 1.63557 0.07879
C 0.37358 4.40943 -1.11697
H 0.57078 4.83977 -0.12372
H 1.10772 4.84237 -1.81866
H -0.62622 4.70224 -1.45437
C 3.47443 -2.10356 0.52389
H 3.06484 -2.82496 -0.20277
H 4.36124 -1.63557 0.07879
H 3.75784 -2.67678 1.41950
C -0.37358 -4.40943 -1.11697
H -1.10772 -4.84237 -1.81866
H 0.62622 -4.70224 -1.45437
H -0.57078 -4.83977 -0.12372

2B {[Zn(bTSC)]$_2$(OH)}$^-$

70
(-1/1)
Zn 2.86275 1.96559 0.05619
Zn 0.00000 0.00000 0.00000
S 6.03154 -0.37627 2.43497
S 2.63123 2.57875 2.34326
S -0.66396 5.78579 0.87355
S 0.73505 -2.23452 -0.53803
N 4.16018 0.19008 0.03998
N 3.89826 -0.91034 0.77925
N 4.33013 -2.44143 2.40646
N 0.07673 0.81150 2.09101
N 1.03034 0.41828 2.97317
N 3.05459 0.54229 4.03201
N 4.47501 2.49052 -1.22069
N 2.59502 4.32595 -0.65555
N 1.76875 5.21909 -0.06990
N -0.00567 4.03257 -1.05063
N -1.41540 -0.56210 -1.64663
N -1.09116 -1.52979 -2.50731
N 0.26618 -3.30524 -2.91745
N -1.82510 1.08338 0.30971
C 4.66676 -1.24868 1.79003
C 2.16041 1.04101 3.11058
C -0.95955 2.31750 3.75705
H -0.25976 1.86966 4.47318
H -1.97800 2.27464 4.17055
H -0.69400 3.38026 3.62849
C -0.87682 1.61651 2.43536
C -1.94955 1.81547 1.41829
C -3.03917 2.68503 1.57795
H -3.14802 3.29724 2.47192
C -3.98374 2.75260 0.54890
H -4.84053 3.42366 0.64209
C -3.84077 1.96373 -0.59371
H -4.58112 2.00339 -1.39281
C -2.72422 1.11250 -0.68474
C -2.47904 0.16776 -1.80057
C -3.43999 0.05160 -2.94629
H -3.07363 -0.69783 -3.65772
H -3.55480 1.01601 -3.46821
H -4.44288 -0.24948 -2.59948
C 0.47117 4.96962 -0.12801
C -0.10404 -2.31727 -2.07693
C 3.96740 6.21828 -1.47529
H 3.79173 6.50416 -2.52709
H 5.01541 6.46047 -1.24097
H 3.30147 6.82014 -0.84474
C 3.66985 4.76172 -1.24922
C 4.61991 3.73218 -1.71414
C 5.66158 4.01768 -2.61914
H 5.78288 5.02142 -3.02505
C 6.52898 2.99375 -2.98920
H 7.34046 3.19099 -3.69325
C 6.36962 1.71513 -2.44815
H 7.06192 0.91576 -2.70763
C 5.31752 1.49444 -1.54698
C 5.11544 0.20358 -0.83759
C 5.99229 -0.97778 -1.12241 - H -1.25337 1.89781 5.31448
0.96177 -0.47388
H 6.31657 -1.00595 -2.17130
H 5.43971 -1.89921 -0.88937
H 4.64847 -2.54162 3.36296
H 3.39634 -2.79566 2.21616
H 2.83227 -0.40353 4.33741
H 4.03762 0.63487 3.76180
H -1.00918 4.08438 -1.19798
H 0.51933 3.97790 -1.92201
H -0.20770 -3.40326 -3.80872
H 1.00312 -3.95014 -2.66690
O 1.20292 1.34745 -0.81028
H 0.68195 2.17357 -0.85614

2C {[Zn(bTSC)]$_2$(OH)}$^-$

70
(-1/1)
Zn 0.00000 0.00000 0.00000
S 0.88935 -0.87887 -2.13391
S 0.06852 2.44337 -2.39505
N 1.98889 -3.29539 -2.32237
N 0.60798 -3.10511 -0.52740
N -0.17098 -2.28749 0.18675
N -1.56565 -0.43877 1.39758
N -1.00037 1.98735 0.45879
N -0.53388 3.19957 0.17544
N 0.88570 4.53507 -0.96295
C 1.16325 -2.51700 -1.58896
C -1.07571 -4.19299 1.49193
H -0.35703 -4.78102 0.90925
H -2.09025 -4.57647 1.29091
H -0.87936 -4.34558 2.56597
C -0.95307 -2.74407 1.11649
C -1.78867 -1.71200 1.76929
C -2.78864 -2.01796 2.70732
H -2.96254 -3.04553 3.02506
C -3.56390 -0.97124 3.21305
H -4.35800 -1.18012 3.93397
C -3.33273 0.33819 2.79809
H -3.94565 1.15028 3.18515
C -2.29473 0.58712 1.87246
C -1.92552 1.92539 1.39153
C -2.51621 3.17829 1.97223
H -3.33870 2.98526 2.67020
H -2.87963 3.83594 1.16680
H -1.73419 3.75019 2.49938
C 0.14440 3.38946 -0.96805
H 2.44687 -2.92900 -3.14532
H 2.15501 -4.25446 -2.03734
H 1.48460 4.72245 -1.75568
H 1.09718 4.97517 -0.06978
Zn 2.82616 1.09503 2.36952
S 4.72307 0.81692 -0.18688
S 3.57570 3.38810 1.98451
N 7.04267 -0.34050 0.35945
N 5.43258 -0.94797 1.82003
N 4.27840 -0.71874 2.45242
N 2.19124 -0.13851 4.00883
N 1.43962 2.33302 3.68524
N 1.26756 3.64461 3.47633
N 1.95678 5.47460 2.30486
C 5.74264 -0.20937 0.74756
C 4.64373 -2.95103 3.39829
H 5.68452 -2.73974 3.69360
H 4.70772 -3.45518 2.42033
C 3.88096 -1.66271 3.27305
C 2.68540 -1.38337 4.08875
C 2.07337 -2.32290 4.94646
H 2.44712 -3.34250 5.02312
C 0.97289 -1.92453 5.70363
H 0.48519 -2.64012 6.36975
C 0.49853 -0.61260 5.62195
H -0.35060 -0.28737 6.22249
C 1.14567 0.27220 4.74425
C 0.77405 1.70055 4.60165
C -0.25330 2.32474 5.50036
H -0.29389 3.40520 5.31977
H -0.01731 2.14631 6.56190
C 2.17246 4.17663 2.66050
H 7.32511 0.00388 -0.54805
H 7.62771 -1.01982 0.83419
H 2.72747 6.00801 1.92084
H 1.24225 5.98646 2.81460
O 1.70209 0.37956 0.91156
H 2.40593 0.23372 0.25409