Electrostatic Effects on Proton-Coupled Electron Transfer in Oxomanganese Complexes Inspired by the Oxygen-Evolving Complex of Photosystem II

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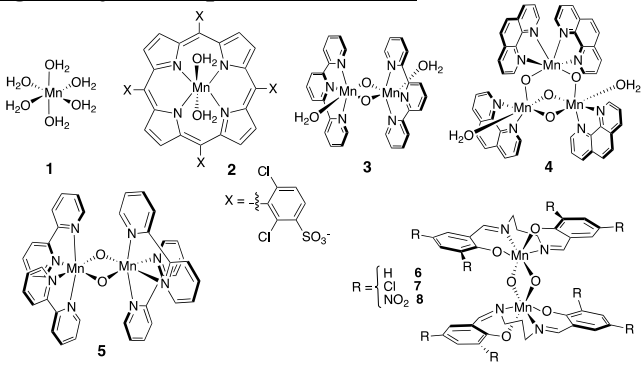
Fig 1. Key to complexes used here.



(**1**) hexa-aqua Mn(II and III);
(**2**) Mn(III) [5,10,15,20- tetrakis (2,6-dichloro-3-sulfonatophenyl) porphyrinato]$^{3-}$;
(**3**) $[Mn(IV,IV)_2(\mu\text{-}O)_2(terpy)_2(H_2O)_2]^{4+}$ (terpy = 2,2':6',2''-terpyridine);
(**4**) $[Mn(IV,IV,IV)_3(\mu\text{-}O)_4(phen)_4(H_2O)_2]^{4+}$ (phen = 1,10-phenanthroline);
(**5**) $[Mn(III,III, III,IV, and IV,IV)_2(\mu\text{-}O)_2(bpy)_4]^{2+}$ (bpy = 2,2'-bipyridyl);
(**6-8**) $[Mn(III,IV and IV,IV)_2(\mu\text{-}O)_2(3,5\text{-di(R)-salpn})_2]$, (**6**) R=H, (**7**) R=Cl or (**8**) R=NO_2
(salpn = N,N'-bis(salicylidene)-1,3-propanediamine).
Each porphyrinato and salpn unit has a charge of -2. The other ligands are neutral.

S1. ***Parameters for calculating electrostatic energies.*** The Poisson-Boltzmann solver DelPhi[1] is used to determine the electrostatic interactions between each pair of primitive objects in a microstate and the loss of solvation energy of each primitive object in the complex and isolated in water. DelPhi requires atomic coordinates, partial charges and radii. S8a-S8h gives this information for each cluster in a single redox and protonation state with deprotonated bridging oxygens and terminal waters. The net charge on each ligand is 0 for complexes **3-5** and -2 for complexes **2** and **6-8.** The ligand atomic partial charges and positions are the same for all states of a complex. Mn can have charges +2, +3 or +4. The terminal hydroxyl group has a charge of -1.2 on the oxygen and 0.2 on the proton. The bridging hydroxyl has a charge of -1.7 on the oxygen and 0.7 on the proton.

The desolvation energy ($\Delta\Delta G_{solv,i}$) that determines the destabilization of a charged group when it is moved out of a high dielectric medium is the difference between the solvation energy for the fragment in the complex and when it is isolated in the appropriate solvent (water or ACN).[2,3]

In solving the Poisson-Boltzmann equation, the internal dielectric constant of the complex is set to 4. This is chosen since the aim is to develop a method that can be used for clusters in proteins where the standard dielectric constant for cofactors is 4.[4] The external, solution dielectric constant is 80 for water and 40 for ACN. The probe radius for water or ACN solvent is 1.4 Å. The ion probe radius is 2.00 Å and the salt concentration is 0.15 mM.

S2. ***Input structures*** Coordinates for complexes **3, 5** and **6** (Fig. 1) are obtained from the Cambridge Database (reference codes SAWYEU,[5] FIQFIU[6] and SOZMUP[7], respectively). The structure of complex **4** is obtained from the published coordinates obtained by DFT.[8] For analysis of complexes **7** and **8**, the chlorine and the NO_2 groups are added to the salpn ring of complex **6** at positions 3 and 5 using MacMolPlot.[9] The structures are optimized with DFT using the B3LYP[10-12] functional and LANL2DZ[13] basis sets for Mn and 6-31G*[14] for all other atoms.

The terminal water pK_as are calculated for complexes **1-4** with their geometry optimized in the Mn oxidation state in which the pK_a is measured (Table 1 main text).

The geometries of complexes **3-8** are optimized considering the antiferromagnetic coupling between the di-Mn ions and generating the broken symmetry solution for the wavefunction with JAGUAR[15] or Gaussian09.[16]

Optimization is carried out in both the Mn(IV,IV) and the Mn(III,IV) oxidation states. In the comparison of the structure dependence of the E_ms and pK_as the ligand geometry is modified but the same ligand partial charges, optimized in the symmetric Mn(IV,IV) state are used for all calculations.

The protons on the bridging oxygen are placed in the plane of the $[Mn(\mu\text{-}O)_2Mn]$ core, bisecting the Mn-O-Mn angle using GaussView.[17] Protons are placed on terminal hydroxyo and waters within the MCCE program.[18] In addition the protons positions from the DFT optimization were added.

S3. Empirical method for assigning the partial charge distribution on the μ-oxo bridges.

To account for the charge transfer effect, atomic charges are adjusted to reproduce the experimental ΔpK_a of 8.7 pH units between the Mn(III,III) and Mn(III,IV) states of $[Mn_2(bpy)_4(\mu\text{-}O)(\mu\text{-}OH)]$.[19]

The protonated μ-oxo-bridge has a charge of -1. The DFT charges for a hydroxyl group would place -1.2 on the oxygen and +0.2 on the hydrogen using the B3LYP/6-31G level of theory. This charge distribution does not provide good results in the classical valence model. For example, the difference in the pK_a of the μ-hydroxo in the $[Mn_2(III,III)(bpy)_4(\mu\text{-}O)(\mu\text{-}OH)]^{+3}$ and $[Mn_2(III,IV)(bpy)_4(\mu\text{-}O)(\mu\text{-}OH)]^{+4}$ complexes is calculated to be 16.5 pH units, while the experimental value is 8.7. The charge distribution on the bridging μ-hydroxo was optimized to match this pK_a difference. The pK_a difference decreases linearly as the negative partial charges on the oxygen increases. The experimental ΔpK_a is recovered by a charge of -1.7 on oxygen and +0.7 on hydrogen and this charge distribution is used for all μ-hydroxo ligands. The correspondence between the experimental and calculated pK_as improves from having a slope of 0.81, y intercept of 0.72 and R^2 of 0.88 with an μ-OH oxygen charge of -1.2 to a slope 1.02, y-intercept of -68 mV and R^2 of 0.9 when the oxygen charge is -1.7 (Figure 3a).

A DFT analysis gives a $pK_{a,sol}$ for an isolated $\mu\text{-}OH^- \rightarrow \mu\text{-}O^{2-}$ of ≈78. An enhanced MCCE analysis using the ESP charges derived from DFT analysis of an OH^- in water gives a partial charge of -1.2 on the oxygen and +0.2 on the hydrogen, and bond dissociation energy of ≈91.6 kcal/mol, leading to a $pK_{a,sol}$ of ≈67. The optimal reference $pK_{a,sol}$ for $\mu\text{-}OH^-$ is only 31.1 pH units.

The question arises why a larger charge separation in the μ-hydroxo produces better results. The valence model used here requires integer charges on the assembled pieces. Thus, the μ-hydroxo bridging oxygens have a charge of -1 and the Mn charges are +3 or +4. However, as the oxygen looses its proton there will be increasing charge transfer to the Mn. As the interaction between the Mn and O^{2-} or OH^- is calculated here solely by classical electrostatics, the valence model has a much stronger stabilization of O^{2-} relative to OH^-. Since no charge transfer is allowed out of the Mn, the charges in the hydroxo state are increased to over stabilize the bridging hydroxyl by an amount that will balance the over stabilization of the O^{2-} state in the valance model. Although the degree of charge transfer is expected to increase with the Mn redox state the same OH^- charges are used in all complexes.

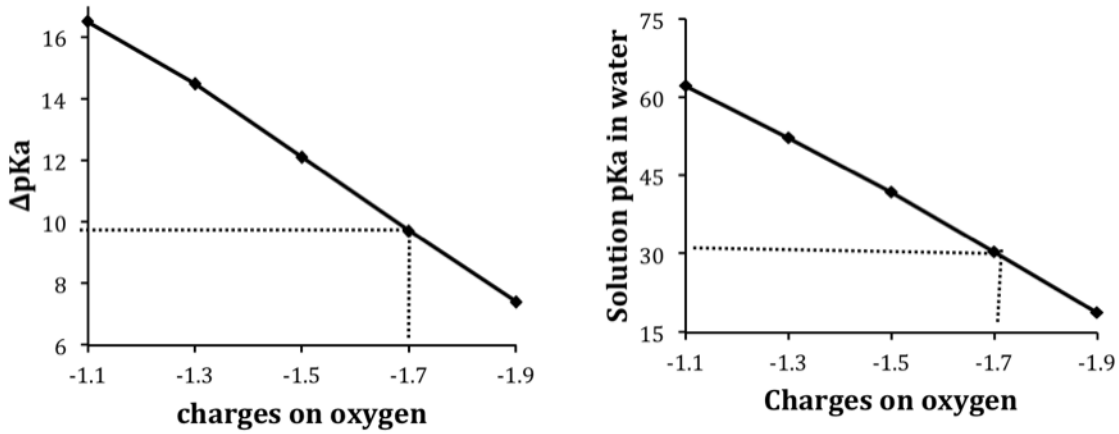


Figure S3. The influence of the charge placed on the bridging oxygen on the calculated (a) difference in the pK_as (ΔpK_a) for the μ-oxo oxygen in the Mn(III,III) and Mn(III,IV) states and (b) reference $pK_{a,sol}$ for the deprotonation of $\mu\text{-}OH^-$ in water required to obtain the experimental μ-oxo pK_a of 2.3 in the Mn(III,IV) state. In each calculation the charge on the hydrogen is adjusted so the μ-OH net charge is -1.

S4. Calculated vs. experimental terminal water pK_as complexes in complexes 1-4.

The classical MCCE valance model is used to determine the pK_a for the deprotonation of terminal waters in complexes **1**-**4** (Main text, Table 1). The reference $pK_{a,H2O}$ of a terminal water is 15.7 is used. This is the pH where 50% of the water will be OH^- given $pK_{a,H2O} = pK_w + \log[H_2O]$, with $K_w=[H^+][HO^-]=10^{-14}$, and $[H_2O]=55.5$ M. The enhanced MCCE method can capture the pK_a shifts of 15 pH units found when a water goes from being in bulk solvent to becoming a Mn ligand.

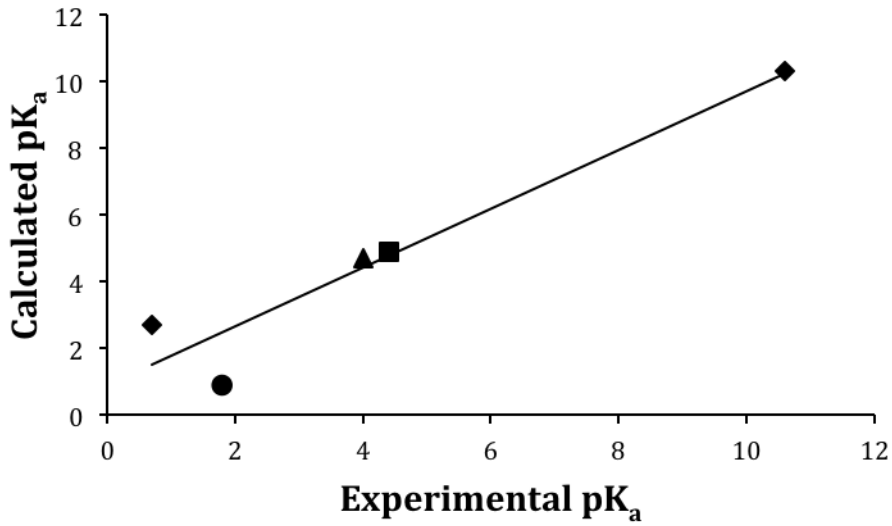


Figure S4. ◆ Complex 1 ▲ Complex 2 • Complex 3 □ Complex 4. The best-fit line has a slope of 1, y-intercept of 0.9 and R^2 of 0.91. RMSD 0.88.

S5. Table 1. Experimental vs. calculated values of redox potentials and pK_as for complexes 5-8

	pK_as				E_ms		
				$[Bpy]_4^0$(pK_as in water; E_ms in ACN)			
	EXP	III-IV	IV-IV		EXP	III-IV	IV-IV
$[Mn(III,III)(O)(OH)]^{+3}$	11.0	12.4	11	Mn(III,IV)→Mn(III,III)[(O)(OH)]	1.10	1.02	1.58
$[Mn(III,IV)(O)(OH)]^{+4}$		2.3		Mn(III,IV)→Mn(III,III)[$(O)_2$]	0.53	0.37	1.00
				Mn(IV,IV)→Mn(III,IV)[$(O)_2$]		1.51	
				$[Salpn]_2^{-2}$ (pK_as and E_ms in ACN)			
$[Mn(III,IV)(O)(OH)]^0$	24.5	21.3	23	Mn(IV,IV)→Mn(III,IV)[(OH)(OCH_3)]	0.82	0.69	0.77
$[Mn(IV,IV)(OH)_2]^{+2}$		6.5		Mn(IV,IV)→Mn(III,IV)[(O)(OH)]	0.42	0.41	0.46
$[Mn(IV,IV)(O)(OH)]^{+1}$	13.4	12.0	12.1	Mn(IV,IV)→Mn(III,IV)[$(O)_2$]	-0.24	-0.14	-0.19
				$[3,5\text{-di(Cl)salpn}]_2^{-2}$ (pK_as and E_ms in ACN)			
$[Mn(III,IV)(O)(OH)]^0$	20.2	21.1	21.3	Mn(IV,IV)→Mn(III,IV)[(O)(OH)]	0.64	0.67	0.73
$[Mn(IV,IV)(O)(OH)]^{+1}$	10.8	11.2	10.1	Mn(IV,IV)→Mn(III,IV)[$(O)_2$]	0	0.09	-0.01
				$[3,5\text{-di}(NO_2)\text{salpn}]_2^{-2}$ (pK_as and E_ms in ACN)			
$[Mn(III,IV)(O)(OH)]^0$	13.3	12.7	15.5	Mn(IV,IV)→Mn(III,IV)[(O)(OH)]	1.10	1.20	1.29
$[Mn(IV,IV)(O)(OH)]^{+1}$	5.0	2.1	3.8	Mn(IV,IV)→Mn(III,IV)[$(O)_2$]	0.51	0.59	0.54

EXP. Represents the measured values, III-IV: the calculated values based on the III-IV structures; IV-IV: the calculated values based on IV-IV structures. All Mn-bpy measured values were obtained from Ref.19,20 and Mn-salpn from Ref. 21 Entries with common value for calculated and measured are the reference values used to obtain the solution pK_a and E_m. All potentials reported vs. NHE.

The reference $E_{m,sol}$ is 1.87 V for the Mn(IV,IV) structure and 1.30 for the Mn(III,IV) structures.

The $pK_{a,sol}$ in water: 28 for the Mn(IV,IV) structures and 30.1 for the Mn(III,IV) structures.

$pK_{a,sol}$ in ACN: 45 for Mn(IV,IV) structures and 47.5 Mn(III,IV) structures.

S5. **Table 2. The predicted values of E_ms and pK_as for complexes 5-8**

	pK_a			E_m	
	$[Bpy]_4^0$(pK_as in water; E_ms in ACN)				
	III-IV	IV-IV		III-IV	IV-IV
$[Mn(III,III)(OH)_2]^{+4}$	4.3	6.1	Mn(III,IV)→Mn(III,III)[$(OH)_2$]	1.65	2.26
$[Mn(III,IV)(OH)_2]^{+5}$	-5.5	-3.6	Mn(IV,IV)→Mn(III,IV)[(O)(OH)]	2.08	2.27
$[Mn(IV,IV)(OH)_2]^{+6}$	-14.5	-13.0	Mn(IV,IV)→Mn(III,IV)[$(OH)_2$]	2.66	2.88
$[Mn(IV,IV)(O)(OH)]^{+5}$	-6.5	-7.4			
	$[Salpn]_2^{-2}$ (pK_as and E_ms in ACN)				
$[Mn(III,III)(O)(OH)]^{-1}$	32.0	33.8	Mn(III,IV)→Mn(III,III)[$(O)_2$]	-1.20	-0.74
$[Mn(III,III)(OH)_2]^0$	26.3	28.2	Mn(III,IV)→Mn(III,III)[(O)(OH)]	-0.58	-0.11
$[Mn(III,IV)(OH)_2]^{+1}$	16.0	17.3	Mn(III,IV)→Mn(III,III)[$(OH)_2$]	0.02	0.52
			Mn(IV,IV)→Mn(III,IV)[$(OH)_2$]	0.96	1.09
	$[3,5\text{-di(Cl)salpn}]_2^{-2}$ (pK_as and E_ms in ACN)				
$[Mn(III,III)(O)(OH)]^{-1}$	31.9	32.6	Mn(III,IV)→Mn(III,III)[$(O)_2$]	-1.00	-0.53
$[Mn(III,III)(OH)_2]^0$	25.6	26.8	Mn(III,IV)→Mn(III,III)[(O)(OH)	-0.37	0.12
$[Mn(III,IV)(OH)_2]^{+1}$	14.4	15.6	Mn(III,IV)→Mn(III,III)[$(OH)_2$]	0.28	0.78
$[Mn(IV,IV)(OH)_2]^{+2}$	4.6	4.3	Mn(IV,IV)→Mn(III,IV)[$(OH)_2$]	1.14	1.38
	$[3,5\text{-di}(NO_2)\text{salpn}]_2^{-2}$ (pK_as and E_ms in ACN)				
$[Mn(III,III)(O)(OH)]^{-1}$	24.3	28.5	Mn(III,IV)→Mn(III,III)[$(O)_2$]	-0.48	0.03
$[Mn(III,III)(OH)_2]^0$	18.6	22.6	Mn(III,IV)→Mn(III,III)[(O)(OH)]	0.20	0.71
$[Mn(III,IV)(OH)_2]^{+1}$	6.2	10.8	Mn(III,IV)→Mn(III,III)[$(OH)_2$]	0.91	1.39
$[Mn(IV,IV)(OH)_2]^{+2}$	-4.4	-1	Mn(IV,IV)→Mn(III,IV)[$(OH)_2$]	1.82	2.03

The E_m and pK_as are calculated using the reference $E_{m,sol}$ and $pK_{a,sol}$ in S5. Table 1.

S5. Table 3 Predicted pK_as of complex 6 in ACN and water

	ACN	WATER
$[Mn(III,III)(OH)_2]^{+4}$	26.3	18.6
$[Mn(III,III)(O)(OH)]^{+3}$	32.0	24.1
$[Mn(III,IV)(OH)_2]^{+5}$	16.0	9.3
$[Mn(III,IV)(O)(OH)]^{+4}$	21.3	14.6
$[Mn(IV,IV)(OH)_2]^{+6}$	6.5	1.0
$[Mn(IV,IV)(O)(OH)]^{+5}$	12.0	6.20

The average μ-oxo pKa in water is 6.7±0.9 lower than in ACN.

The differences between the calculations in water and ACN: $pK_{a,sol}$ for the OH^- fragment is 30.1 in water and 47.5 in ACN (S4, table 1). The electrostatic interactions are calculated with solvent dielectric constants of 80 for water and 40 for ACN.

The cluster dielectric constant is always 4. The structures optimized in the Mn(III,IV) redox state are always used.

S6. The correlation between the atomic partial charges on the individual oxygen or nitrogen directly ligating the Mn ions and the E_m and pK_a shift in complexes 6-8.

The DFT protocol for determining charges on the ligands allows the enhanced MCCE methods to be sensitive to the effects of substituent groups on the ligands. The three salpn complexes **6**–**8**, show significant polarization effects induced by the electron withdrawing groups on the salpn ligands (Main Text, Fig. 6). These charge changes are responsible for the distinct calculated values of E_ms and pK_as of the three complexes. There are 6 pK_as calculated for each complex (e.g. Main Text, Fig 6). Calculations reported in S5, Table 2 show that Cl substitution shifts the μ-O pK_a by -0.9±0.7 pH units and the E_m by +0.22±0.03 V, while NO_2 substitution shifts the pK_a by -9.1±1.3 pH units and the E_m by +0.8±0.07 mV.

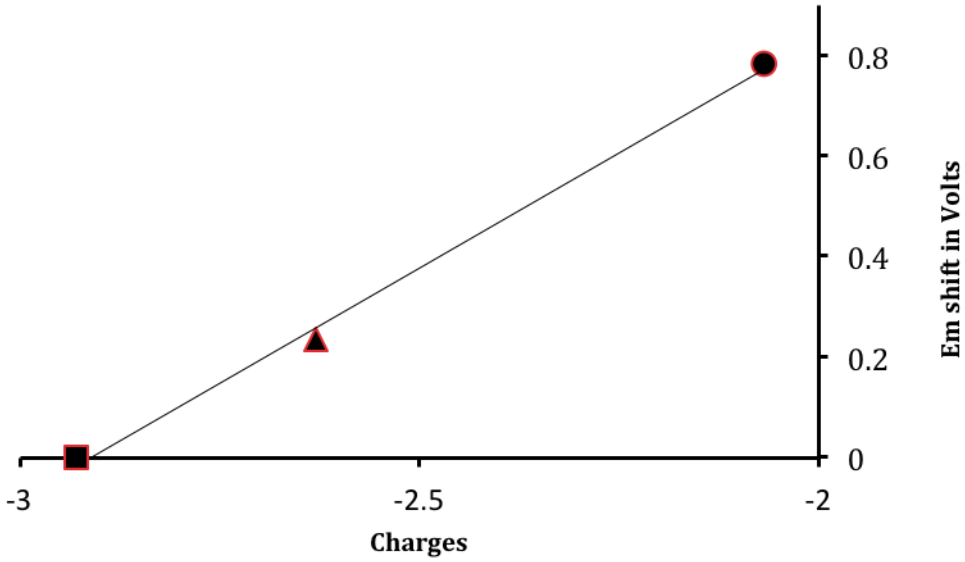


Figure S6.a. The best-fit line has a slope of -0.9 V. ■ complex 6 ▲ complex 7 ● complex 8. Data from Table S5. Table 1-2.

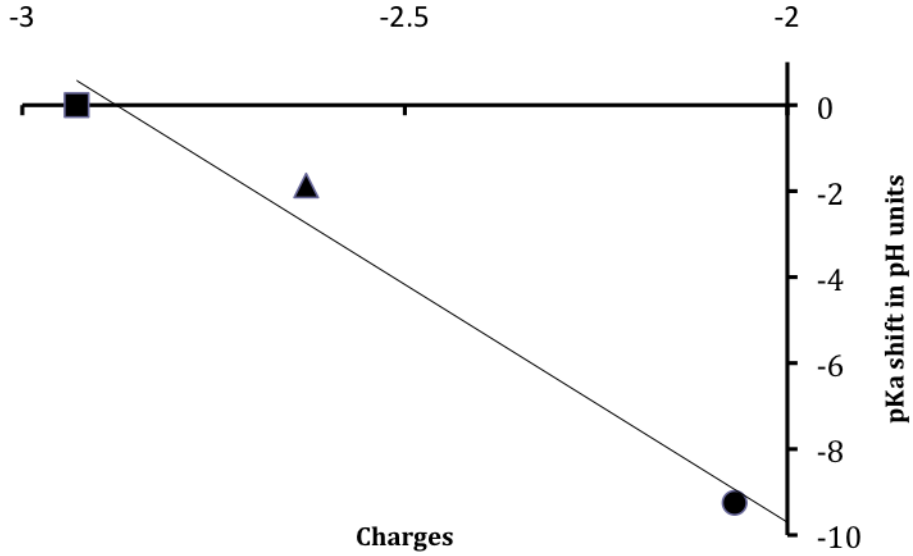


Figure S6.b. The best-fit line has a slope of -11 pH units. . ■ complex 6 ▲ complex 7 ● complex 8.

S7. The coupling between changes in E_m and pH in coupled electron/proton transfer reactions.

The reaction described is along the diagonal in Fig 4 and 5.

E_m changes in 59 mV/pH unit for the one-proton *coupled* one-electron reduction:

$[Mn^{IV}(\mu_2\text{-}O)_2Mn^{IV}]+e^-+H^+ \rightleftharpoons [Mn^{III}(\mu\text{-}O)(\mu\text{-}OH)Mn^{IV}]$ is described by the Nernst equation:

$$E_m = E_m^0 + \frac{RT}{nF}\ln\frac{[Mn^{III}(\mu\text{-}O)(\mu\text{-}OH)Mn^{IV}]}{[Mn^{IV}(\mu_2\text{-}O)_2Mn^{IV}]} + pH \times 59\text{mV}$$

$$= E_m^0 + \frac{RT}{nF}\ln\frac{[Mn^{III}(\mu_2\text{-}O)_2Mn^{IV}]}{[Mn^{IV}(\mu_2\text{-}O)_2Mn^{IV}]} + pK_a \times 59\text{mV}$$

since

$\Delta G = -nF(E_m - E_m^0) = \Delta G_m - \Delta G_a$, where

$$\Delta G_m = -RT\ln\frac{[Mn^{III}(\mu_2\text{-}O)_2Mn^{IV}]}{[Mn^{IV}(\mu_2\text{-}O)_2Mn^{IV}]}$$

is the free energy change for the reduction,

$[Mn^{IV}(\mu_2\text{-}O)_2Mn^{IV}] + e^- \rightarrow [Mn^{III}(\mu_2\text{-}O)_2Mn^{IV}]$

and

$$\Delta G_a = -RT\ln\frac{[Mn^{III}(\mu\text{-}O)_2Mn^{IV}][H^+]}{[Mn^{III}(\mu\text{-}O)(\mu\text{-}OH)Mn^{IV}]}$$

is the free energy change of the deprotonation,

$[Mn^{III}(\mu\text{-}O)(\mu\text{-}OH)Mn^{IV}] \rightarrow [Mn^{III}(\mu\text{-}O)_2Mn^{IV}] + H^+$

S8. The optimized structure and ESP (Electrostatic Potential) charges for all complexes (All the geometry optimizations were performed using JAGUAR[6] and Gaussian 09[16]):

S8.a) Optimized structure of complex 1 in the III state:

					X	Y	Z	DelPhi Radius	DelPhi Charge
ATOM	**1**	**MN**	**MNC**	**1**	**-0.974**	**-1.378**	**-1.855**	**2**	**3**
ATOM	2	O	HOH	2	-2.242	-1.623	-3.56	1.62	-0.8
ATOM	3	1H	HOH	2	-2.796	-1.069	-4.114	1	0.4
ATOM	4	2H	HOH	2	-1.688	-2.177	-4.114	1	0.4
ATOM	5	O	HOH	3	0.09	-2.957	-2.385	1.62	-0.8
ATOM	6	1H	HOH	3	-0.464	-3.511	-2.939	1	0.4
ATOM	7	2H	HOH	3	0.644	-3.511	-1.831	1	0.4
ATOM	8	O	HOH	4	-2.039	0.2	-1.326	1.62	-0.8
ATOM	9	1H	HOH	4	-1.485	0.754	-0.772	1	0.4
ATOM	10	2H	HOH	4	-2.593	0.754	-1.88	1	0.4
ATOM	11	O	HOH	5	0.294	-1.134	-0.151	1.62	-0.8
ATOM	12	1H	HOH	5	0.848	-1.688	0.403	1	0.4
ATOM	13	2H	HOH	5	-0.26	-0.58	0.403	1	0.4
ATOM	14	O	HOH	6	-2.17	-2.54	-0.791	1.62	-0.8
ATOM	15	1H	HOH	6	-2.724	-3.094	-1.345	1	0.4
ATOM	16	2H	HOH	6	-2.724	-1.986	-0.237	1	0.4
ATOM	17	O	HOH	7	0.222	-0.216	-2.92	1.62	-0.8
ATOM	18	1H	HOH	7	0.776	0.338	-2.366	1	0.4
ATOM	19	2H	HOH	7	0.776	-0.77	-3.474	1	0.4

S8.b) Optimized structure of complex 2 in the III state:

					X	Y	Z	DelPhi Radius	DelPhi Charge
ATOM	1	C1	PYR	1	-0.359	4.259	0.236	1.7	-0.356
ATOM	2	C2	PYR	1	0.967	4.166	-0.073	1.7	-0.286
ATOM	3	C3	PYR	1	1.266	2.771	-0.216	1.7	-0.039
ATOM	4	N1	PYR	1	0.135	2.019	-0.042	1.55	-0.094
ATOM	5	C4	PYR	1	-0.886	2.923	0.236	1.7	0.255
ATOM	6	C5	PYR	1	2.573	2.256	-0.421	1.7	-0.092
ATOM	7	C6	PYR	1	2.9	0.907	-0.303	1.7	0.094
ATOM	8	C7	PYR	1	4.237	0.38	-0.329	1.7	-0.321
ATOM	9	C8	PYR	1	4.148	-0.951	-0.043	1.7	-0.372
ATOM	10	C9	PYR	1	2.753	-1.252	0.108	1.7	0.432
ATOM	11	N2	PYR	1	2	-0.12	-0.043	1.55	-0.304
ATOM	12	C10	PYR	1	2.24	-2.559	0.314	1.7	-0.517
ATOM	13	C11	PYR	1	0.891	-2.89	0.193	1.7	0.233
ATOM	14	C12	PYR	1	0.367	-4.227	0.197	1.7	-0.295
ATOM	15	C13	PYR	1	-0.967	-4.135	-0.075	1.7	-0.394
ATOM	16	C14	PYR	1	-1.273	-2.737	-0.19	1.7	0.22
ATOM	17	N3	PYR	1	-0.139	-1.986	-0.04	1.55	-0.207
ATOM	18	C15	PYR	1	-2.585	-2.216	-0.346	1.7	-0.365
ATOM	19	C16	PYR	1	-2.909	-0.872	-0.178	1.7	0.218
ATOM	20	C17	PYR	1	-4.245	-0.347	-0.152	1.7	-0.326
ATOM	21	C18	PYR	1	-4.148	0.982	0.14	1.7	-0.348

ATOM	22	C19	PYR	1	-2.749	1.285	0.244	1.7	0.307
ATOM	23	N4	PYR	1	-2.001	0.152	0.068	1.55	-0.289
ATOM	24	C20	PYR	1	-2.229	2.598	0.406	1.7	-0.455
ATOM	25	C21	PYR	1	-5.619	-5.082	-1.364	1.7	-0.107
ATOM	26	C22	PYR	1	-4.891	-4.459	-2.378	1.7	-0.056
ATOM	27	C23	PYR	1	-3.926	-3.525	-2.024	1.7	-0.196
ATOM	28	C24	PYR	1	-3.671	-3.185	-0.684	1.7	0.631
ATOM	29	C25	PYR	1	-4.444	-3.821	0.303	1.7	-0.321
ATOM	30	C26	PYR	1	-5.415	-4.764	-0.022	1.7	-0.043
ATOM	31	C27	PYR	1	3.781	-4.482	-0.308	1.7	-0.139
ATOM	32	C28	PYR	1	4.633	-5.527	0.04	1.7	-0.085
ATOM	33	C29	PYR	1	4.913	-5.744	1.388	1.7	-0.088
ATOM	34	C30	PYR	1	4.387	-4.921	2.383	1.7	-0.046
ATOM	35	C31	PYR	1	3.541	-3.885	2.007	1.7	-0.288
ATOM	36	C32	PYR	1	3.203	-3.647	0.664	1.7	0.561
ATOM	37	C33	PYR	1	-5.155	5.604	1.334	1.7	-0.1
ATOM	38	C34	PYR	1	-4.572	4.872	2.367	1.7	-0.028
ATOM	39	C35	PYR	1	-3.61	3.92	2.046	1.7	-0.315
ATOM	40	C36	PYR	1	-3.208	3.683	0.72	1.7	0.607
ATOM	41	C37	PYR	1	-3.804	4.465	-0.286	1.7	-0.213
ATOM	42	C38	PYR	1	-4.77	5.423	0.006	1.7	-0.043
ATOM	43	C39	PYR	1	3.971	3.572	-2.054	1.7	-0.377
ATOM	44	C40	PYR	1	3.676	3.218	-0.726	1.7	0.747
ATOM	45	C41	PYR	1	4.483	3.769	0.286	1.7	-0.427
ATOM	46	C42	PYR	1	5.558	4.602	-0.008	1.7	0.06
ATOM	47	C43	PYR	1	5.837	4.892	-1.343	1.7	-0.156
ATOM	48	C44	PYR	1	5.042	4.399	-2.376	1.7	0.015
ATOM	49	S1	PYR	1	-6.743	-6.437	-1.795	1.8	0.754
ATOM	50	O1	PYR	1	-7.782	-6.449	-0.705	1.52	-0.584
ATOM	51	O2	PYR	1	-5.882	-7.619	-1.881	1.52	-0.544
ATOM	52	O3	PYR	1	-7.404	-6.006	-3.078	1.52	-0.581
ATOM	53	S2	PYR	1	5.858	-7.214	1.872	1.8	0.753
ATOM	54	O4	PYR	1	6.654	-6.79	3.079	1.52	-0.587
ATOM	55	O5	PYR	1	6.812	-7.463	0.735	1.52	-0.578
ATOM	56	O6	PYR	1	4.843	-8.245	2.102	1.52	-0.543
ATOM	57	S3	PYR	1	-6.552	6.698	1.703	1.8	0.745
ATOM	58	O7	PYR	1	-7.737	5.856	1.523	1.52	-0.539
ATOM	59	O8	PYR	1	-6.413	7.855	0.748	1.52	-0.579
ATOM	60	O9	PYR	1	-6.303	7.201	3.1	1.52	-0.578
ATOM	61	S6	PYR	1	7.357	5.793	-1.748	1.8	0.744
ATOM	62	O10	PYR	1	7.056	6.52	-3.033	1.52	-0.571
ATOM	63	O11	PYR	1	8.391	4.758	-1.82	1.5	-0.557
ATOM	64	O12	PYR	1	7.519	6.812	-0.651	1.5	-0.573
ATOM	65	CL1	PYR	1	-4.169	-3.438	1.994	1.7	-0.109
ATOM	66	CL2	PYR	1	-2.997	-2.75	-3.306	1.7	-0.111
ATOM	67	CL3	PYR	1	-3.35	4.211	-1.963	1.7	-0.111
ATOM	68	CL5	PYR	1	-2.882	2.987	3.347	1.7	-0.103
ATOM	69	CL6	PYR	1	4.137	3.395	1.965	1.7	-0.102
ATOM	70	CL7	PYR	1	2.978	2.933	-3.357	1.7	-0.051
ATOM	71	CL8	PYR	1	3.425	-4.205	-2.003	1.7	-0.144
ATOM	72	CL9	PYR	1	2.865	-2.854	3.269	1.7	-0.115
ATOM	73	H1	PYR	1	5.266	4.649	-3.407	1.1	0.133
ATOM	74	H2	PYR	1	6.176	5.013	0.783	1.1	0.117
ATOM	75	H3	PYR	1	5.129	0.959	-0.518	1.1	0.144

ATOM	76	H4	PYR	1	4.95	-1.67	0.034	1.1	0.15
ATOM	77	H5	PYR	1	-4.95	1.698	0.25	1.1	0.16
ATOM	78	H6	PYR	1	-5.141	-0.928	-0.312	1.1	0.138
ATOM	79	H7	PYR	1	1.686	4.966	-0.171	1.1	0.137
ATOM	80	H8	PYR	1	-0.937	5.151	0.426	1.1	0.145
ATOM	81	H9	PYR	1	0.949	-5.123	0.359	1.1	0.15
ATOM	82	H10	PYR	1	-1.683	-4.939	-0.164	1.1	0.171
ATOM	83	H11	PYR	1	4.63	-5.095	3.426	1.1	0.133
ATOM	84	H12	PYR	1	5.068	-6.167	-0.719	1.1	0.152
ATOM	85	H13	PYR	1	-5.998	-5.254	0.75	1.1	0.138
ATOM	86	H14	PYR	1	-5.073	-4.708	-3.418	1.1	0.148
ATOM	87	H15	PYR	1	-4.873	5.039	3.394	1.1	0.132
ATOM	88	H16	PYR	1	-5.227	6.009	-0.783	1.1	0.143
ATOM	**93**	**MN**	**MNC**	**1**	**0**	**0.016**	**-0.016**	**2**	**3**
ATOM	95	O	HOH	2	0.148	-0.001	2.143	1.52	-1.1
ATOM	96	1H	HOH	2	0.702	-0.555	2.697	1	0.55
ATOM	97	2H	HOH	2	-0.406	0.553	2.697	1	0.55
ATOM	135	O	HOH	3	-0.097	-0.065	-2.169	1.52	-1.1
ATOM	136	1H	HOH	3	-0.651	0.489	-2.723	1	0.55
ATOM	137	2H	HOH	3	0.457	-0.619	-2.723	1	0.55

S8.c) Optimized structure of complex 3 in the III-IV state:

					X	Y	Z	DelPhi Radius	DelPhi Charge
ATOM	1	N1	TXY	1	0.791	0.086	2.735	1.55	-0.54
ATOM	2	N2	TXY	1	-0.562	-2.083	2.11	1.55	-0.57
ATOM	3	N3	TXY	1	0.122	-2.807	-0.326	1.55	-0.54
ATOM	4	C1	TXY	1	1.666	1.078	2.985	1.7	0.05
ATOM	5	H1	TXY	1	2.231	1.449	2.138	1.1	0.2
ATOM	6	C2	TXY	1	1.847	1.588	4.271	1.7	-0.23
ATOM	7	H2	TXY	1	2.576	2.369	4.449	1.1	0.2
ATOM	8	C3	TXY	1	1.085	1.061	5.316	1.7	-0.15
ATOM	9	H3	TXY	1	1.203	1.431	6.327	1.1	0.2
ATOM	10	C4	TXY	1	0.18	0.029	5.051	1.7	-0.2
ATOM	11	H4	TXY	1	-0.395	-0.403	5.859	1.1	0.2
ATOM	12	C5	TXY	1	0.061	-0.455	3.747	1.7	0.26
ATOM	13	C6	TXY	1	-0.758	-1.625	3.372	1.7	0.27
ATOM	14	C7	TXY	1	-1.629	-2.299	4.23	1.7	-0.2
ATOM	15	H7	TXY	1	-1.804	-1.941	5.235	1.1	0.2
ATOM	16	C8	TXY	1	-2.27	-3.453	3.778	1.7	-0.15
ATOM	17	H8	TXY	1	-2.956	-3.983	4.428	1.1	0.2
ATOM	18	C9	TXY	1	-2.007	-3.939	2.496	1.7	-0.2
ATOM	19	H9	TXY	1	-2.474	-4.853	2.156	1.1	0.2
ATOM	20	C10	TXY	1	-1.129	-3.234	1.67	1.7	0.27
ATOM	21	C11	TXY	1	-0.682	-3.681	0.335	1.7	0.26
ATOM	22	C12	TXY	1	-0.964	-4.938	-0.203	1.7	-0.2
ATOM	23	H12	TXY	1	-1.6	-5.637	0.323	1.1	0.2
ATOM	24	C13	TXY	1	-0.383	-5.306	-1.419	1.7	-0.15
ATOM	25	H13	TXY	1	-0.576	-6.287	-1.837	1.1	0.2
ATOM	26	C14	TXY	1	0.464	-4.408	-2.073	1.7	-0.23
ATOM	27	H14	TXY	1	0.95	-4.673	-3.003	1.1	0.2
ATOM	28	C15	TXY	1	0.688	-3.157	-1.497	1.7	0.05
ATOM	29	H15	TXY	1	1.334	-2.421	-1.96	1.1	0.2

ATOM	30	N1	TXY	2	-0.628	0.06	-2.694	1.55	-0.54
ATOM	31	N2	TXY	2	0.596	2.279	-2.305	1.55	-0.57
ATOM	32	N3	TXY	2	0.021	2.771	0.144	1.55	-0.54
ATOM	33	C1	TXY	2	-1.457	-0.996	-2.795	1.7	0.05
ATOM	34	H1	TXY	2	-1.923	-1.33	-1.878	1.1	0.2
ATOM	35	C2	TXY	2	-1.7	-1.606	-4.027	1.7	-0.23
ATOM	36	H2	TXY	2	-2.387	-2.441	-4.086	1.1	0.2
ATOM	37	C3	TXY	2	-1.058	-1.116	-5.165	1.7	-0.15
ATOM	38	H3	TXY	2	-1.232	-1.567	-6.134	1.1	0.2
ATOM	39	C4	TXY	2	-0.201	-0.015	-5.05	1.7	-0.2
ATOM	40	H4	TXY	2	0.282	0.392	-5.929	1.1	0.2
ATOM	41	C5	TXY	2	-0.008	0.572	-3.804	1.7	0.26
ATOM	42	C6	TXY	2	0.765	1.803	-3.556	1.7	0.27
ATOM	43	C7	TXY	2	1.574	2.505	-4.451	1.7	-0.2
ATOM	44	H7	TXY	2	1.734	2.15	-5.461	1.1	0.2
ATOM	45	C8	TXY	2	2.185	3.687	-4.013	1.7	-0.15
ATOM	46	H8	TXY	2	2.822	4.243	-4.691	1.1	0.2
ATOM	47	C9	TXY	2	1.974	4.162	-2.713	1.7	-0.2
ATOM	48	H9	TXY	2	2.441	5.082	-2.386	1.1	0.2
ATOM	49	C10	TXY	2	1.154	3.422	-1.859	1.7	0.27
ATOM	50	C11	TXY	2	0.755	3.747	-0.478	1.7	0.26
ATOM	51	C12	TXY	2	0.996	4.958	0.162	1.7	-0.2
ATOM	52	H12	TXY	2	1.57	5.733	-0.33	1.1	0.2
ATOM	53	C13	TXY	2	0.456	5.183	1.433	1.7	-0.15
ATOM	54	H13	TXY	2	0.621	6.131	1.931	1.1	0.2
ATOM	55	C14	TXY	2	-0.311	4.186	2.038	1.7	-0.23
ATOM	56	H14	TXY	2	-0.761	4.338	3.011	1.1	0.2
ATOM	57	C15	TXY	2	-0.506	2.979	1.365	1.7	0.05
ATOM	58	H15	TXY	2	-1.089	2.168	1.781	1.1	0.2
ATOM	59	MN	MNC	2	0.443	-0.817	0.779	2	3
ATOM	62	MN	MNC	3	-0.342	1.143	-0.946	2	4
ATOM	79	O	OXO	4	-1.115	0.11	0.227	1.52	-2
ATOM	96	O	OXO	5	1.132	0.314	-0.496	1.52	-2
ATOM	106	O	HOH	6	2.527	-1.418	1.123	1.52	-0.8
ATOM	107	1H	HOH	6	3.133	-0.812	1.729	1	0.4
ATOM	108	2H	HOH	6	3.133	-2.024	0.517	1	0.4
ATOM	151	O	HOH	7	-2.233	2.102	-1.3	1.52	-0.8
ATOM	152	1H	HOH	7	-2.839	1.496	-0.694	1	0.4
ATOM	153	2H	HOH	7	-2.839	2.708	-1.906	1	0.4

S8.d) Optimized structure of complex 4 in the III-IV state:

					X	Y	Z	DelPhi Radius	DelPhi Charge
ATOM	1	N1	PHN	1	3.693	3.388	4.56	1.55	-0.584
ATOM	2	N2	PHN	1	6.31	3.082	5.046	1.55	-0.596
ATOM	3	C1	PHN	1	2.387	3.606	4.327	1.7	0.382
ATOM	4	C2	PHN	1	1.642	2.747	3.493	1.7	-0.405
ATOM	5	C3	PHN	1	2.259	1.655	2.892	1.7	0.091
ATOM	6	C4	PHN	1	3.644	1.417	3.11	1.7	-0.156
ATOM	7	C5	PHN	1	4.381	0.323	2.531	1.7	-0.175
ATOM	8	C6	PHN	1	5.72	0.164	2.782	1.7	-0.173
ATOM	9	C7	PHN	1	6.431	1.084	3.631	1.7	-0.183
ATOM	10	C8	PHN	1	7.817	0.99	3.929	1.7	0.102
ATOM	11	C9	PHN	1	8.407	1.937	4.758	1.7	-0.434

ATOM	12	C10	PHN	1	7.624	2.975	5.304	1.7	0.396
ATOM	13	C11	PHN	1	5.717	2.16	4.218	1.7	0.441
ATOM	14	C12	PHN	1	4.329	2.325	3.958	1.7	0.41
ATOM	15	1HA	PHN	1	1.944	4.469	4.804	1.1	0.048
ATOM	16	2HA	PHN	1	0.588	2.948	3.332	1.1	0.167
ATOM	17	3HA	PHN	1	1.69	0.981	2.257	1.1	0.096
ATOM	18	4HA	PHN	1	3.853	-0.38	1.89	1.1	0.146
ATOM	19	5HA	PHN	1	6.268	-0.666	2.341	1.1	0.136
ATOM	20	6HA	PHN	1	8.409	0.181	3.508	1.1	0.082
ATOM	21	7HA	PHN	1	9.465	1.888	4.997	1.1	0.166
ATOM	22	8HA	PHN	1	8.066	3.722	5.952	1.1	0.044
ATOM	23	N1	PHN	2	4.625	3.113	7.322	1.55	-0.584
ATOM	24	N2	PHN	2	6.288	5.19	7.078	1.55	-0.596
ATOM	25	C1	PHN	2	3.757	2.09	7.418	1.7	0.382
ATOM	26	C2	PHN	2	3.726	1.244	8.54	1.7	-0.405
ATOM	27	C3	PHN	2	4.606	1.458	9.586	1.7	0.091
ATOM	28	C4	PHN	2	5.522	2.536	9.521	1.7	-0.156
ATOM	29	C5	PHN	2	6.472	2.851	10.553	1.7	-0.175
ATOM	30	C6	PHN	2	7.321	3.914	10.43	1.7	-0.173
ATOM	31	C7	PHN	2	7.292	4.752	9.262	1.7	-0.183
ATOM	32	C8	PHN	2	8.135	5.873	9.064	1.7	0.102
ATOM	33	C9	PHN	2	8.028	6.619	7.903	1.7	-0.434
ATOM	34	C10	PHN	2	7.092	6.258	6.919	1.7	0.396
ATOM	35	C11	PHN	2	6.372	4.446	8.235	1.7	0.441
ATOM	36	C12	PHN	2	5.491	3.342	8.363	1.7	0.41
ATOM	37	1HA	PHN	2	3.08	1.941	6.59	1.1	0.048
ATOM	38	2HA	PHN	2	3.011	0.431	8.567	1.1	0.167
ATOM	39	3HA	PHN	2	4.6	0.81	10.455	1.1	0.096
ATOM	40	4HA	PHN	2	6.502	2.223	11.436	1.1	0.146
ATOM	41	5HA	PHN	2	8.036	4.141	11.212	1.1	0.136
ATOM	42	6HA	PHN	2	8.861	6.137	9.826	1.1	0.082
ATOM	43	7HA	PHN	2	8.662	7.48	7.733	1.1	0.166
ATOM	44	8HA	PHN	2	6.978	6.821	6.005	1.1	0.044
ATOM	45	N1	PHN	3	3.143	7.836	8.064	1.55	-0.584
ATOM	46	N2	PHN	3	1.998	8.968	5.958	1.55	-0.596
ATOM	47	C1	PHN	3	3.728	7.216	9.102	1.7	0.382
ATOM	48	C2	PHN	3	3.751	7.793	10.38	1.7	-0.405
ATOM	49	C3	PHN	3	3.162	9.028	10.59	1.7	0.091
ATOM	50	C4	PHN	3	2.533	9.7	9.52	1.7	-0.156
ATOM	51	C5	PHN	3	1.862	10.966	9.631	1.7	-0.175
ATOM	52	C6	PHN	3	1.239	11.531	8.555	1.7	-0.173
ATOM	53	C7	PHN	3	1.245	10.885	7.271	1.7	-0.183
ATOM	54	C8	PHN	3	0.593	11.379	6.115	1.7	0.102
ATOM	55	C9	PHN	3	0.654	10.666	4.928	1.7	-0.434
ATOM	56	C10	PHN	3	1.376	9.461	4.871	1.7	0.396
ATOM	57	C11	PHN	3	1.929	9.658	7.143	1.7	0.441
ATOM	58	C12	PHN	3	2.556	9.061	8.264	1.7	0.41
ATOM	59	1HA	PHN	3	4.167	6.251	8.892	1.1	0.048
ATOM	60	2HA	PHN	3	4.225	7.259	11.196	1.1	0.167
ATOM	61	3HA	PHN	3	3.168	9.482	11.578	1.1	0.096
ATOM	62	4HA	PHN	3	1.846	11.459	10.596	1.1	0.146
ATOM	63	5HA	PHN	3	0.72	12.478	8.657	1.1	0.136
ATOM	64	6HA	PHN	3	0.039	12.31	6.171	1.1	0.082
ATOM	65	7HA	PHN	3	0.148	11.02	4.039	1.1	0.166

ATOM	66	8HA	PHN	3	1.465	8.877	3.964	1.1	0.044
ATOM	67	N1	PHN	4	4.534	9.158	3.224	1.55	-0.584
ATOM	68	N2	PHN	4	4.667	6.825	1.972	1.55	-0.596
ATOM	69	C1	PHN	4	4.542	10.319	3.906	1.7	0.382
ATOM	70	C2	PHN	4	4.406	11.552	3.247	1.7	-0.405
ATOM	71	C3	PHN	4	4.239	11.587	1.872	1.7	0.091
ATOM	72	C4	PHN	4	4.223	10.379	1.131	1.7	-0.156
ATOM	73	C5	PHN	4	4.074	10.295	-0.297	1.7	-0.175
ATOM	74	C6	PHN	4	4.114	9.09	-0.938	1.7	-0.173
ATOM	75	C7	PHN	4	4.316	7.867	-0.209	1.7	-0.183
ATOM	76	C8	PHN	4	4.415	6.587	-0.802	1.7	0.102
ATOM	77	C9	PHN	4	4.641	5.474	-0.008	1.7	-0.434
ATOM	78	C10	PHN	4	4.762	5.621	1.383	1.7	0.396
ATOM	79	C11	PHN	4	4.446	7.934	1.192	1.7	0.441
ATOM	80	C12	PHN	4	4.388	9.182	1.859	1.7	0.41
ATOM	81	1HA	PHN	4	4.659	10.24	4.979	1.1	0.048
ATOM	82	2HA	PHN	4	4.438	12.466	3.827	1.1	0.167
ATOM	83	3HA	PHN	4	4.131	12.534	1.354	1.1	0.096
ATOM	84	4HA	PHN	4	3.938	11.211	-0.86	1.1	0.146
ATOM	85	5HA	PHN	4	4.008	9.036	-2.015	1.1	0.136
ATOM	86	6HA	PHN	4	4.323	6.487	-1.878	1.1	0.082
ATOM	87	7HA	PHN	4	4.732	4.489	-0.448	1.1	0.166
ATOM	88	8HA	PHN	4	4.944	4.785	2.044	1.1	0.044
ATOM	89	MN	MNC	5	4.907	4.518	5.76	2	3
ATOM	126	MN	MNC	8	3.08	7.204	6.081	2	4
ATOM	209	MN	MNC	2	4.744	7.248	4	2	4
ATOM	107	O	OXO	6	5.36	5.606	4.44	1.52	-2
ATOM	124	O	OXO	7	3.629	5.505	6.484	1.52	-2
ATOM	143	O	OXO	9	4.662	7.885	5.699	1.52	-2
ATOM	160	O	OXO	0	3.026	6.955	4.287	1.52	-2
ATOM	173	O	HOH	1	1.14	6.331	6.41	1.52	-0.8
ATOM	174	1H	HOH	1	0.586	5.777	6.964	1	0.4
ATOM	175	2H	HOH	1	0.586	6.885	5.856	1	0.4
ATOM	237	O	HOH	3	6.858	7.686	3.809	1.52	-0.8
ATOM	238	1H	HOH	3	7.412	8.24	3.255	1	0.4
ATOM	239	2H	HOH	3	7.412	7.132	4.363	1	0.4

S8.e) Optimized structure of complex 5 in the III-IV state:

					X	Y	Z	DelPhi Radius	DelPhi Charge
ATOM	1	N1	BXY	1	2.822	-1.465	-0.74	1.55	-0.728
ATOM	2	N2	BXY	1	1.85	0.577	-2.17	1.55	-0.296
ATOM	3	C0	BXY	1	3.365	-1.271	-1.972	1.7	0.568
ATOM	4	C1	BXY	1	4.319	-2.156	-2.486	1.7	-0.579
ATOM	5	H1	BXY	1	4.746	-1.997	-3.468	1.1	0.161
ATOM	6	C2	BXY	1	4.716	-3.261	-1.735	1.7	0.147
ATOM	7	H2	BXY	1	5.456	-3.951	-2.128	1.1	0.067
ATOM	8	C3	BXY	1	4.139	-3.465	-0.485	1.7	-0.381
ATOM	9	H3	BXY	1	4.404	-4.317	0.132	1.1	0.134
ATOM	10	C4	BXY	1	3.2	-2.544	-0.03	1.7	0.201
ATOM	11	H4	BXY	1	2.731	-2.67	0.936	1.1	0.031
ATOM	12	C5	BXY	1	2.866	-0.104	-2.742	1.7	0.67
ATOM	13	C6	BXY	1	3.384	0.28	-3.986	1.7	-0.683

ATOM	14	H6	BXY	1	4.211	-0.253	-4.439	1.1	0.203
ATOM	15	C7	BXY	1	2.831	1.378	-4.645	1.7	0.334
ATOM	16	H7	BXY	1	3.227	1.691	-5.606	1.1	0.038
ATOM	17	C8	BXY	1	1.772	2.067	-4.052	1.7	-0.602
ATOM	18	H8	BXY	1	1.318	2.927	-4.532	1.1	0.17
ATOM	19	C9	BXY	1	1.316	1.631	-2.81	1.7	0.554
ATOM	20	H9	BXY	1	0.509	2.135	-2.286	1.1	-0.007
ATOM	21	N1	BXY	2	1.873	-0.609	2.148	1.55	-0.728
ATOM	22	N2	BXY	2	2.873	1.408	0.7	1.55	-0.296
ATOM	23	C0	BXY	2	2.918	0.045	2.701	1.7	0.568
ATOM	24	C1	BXY	2	3.447	-0.353	3.935	1.7	-0.579
ATOM	25	H1	BXY	2	4.296	0.158	4.373	1.1	0.161
ATOM	26	C2	BXY	2	2.879	-1.436	4.604	1.7	0.147
ATOM	27	H2	BXY	2	3.284	-1.76	5.558	1.1	0.067
ATOM	28	C3	BXY	2	1.791	-2.097	4.03	1.7	-0.381
ATOM	29	H3	BXY	2	1.324	-2.946	4.518	1.1	0.134
ATOM	30	C4	BXY	2	1.324	-1.649	2.797	1.7	0.201
ATOM	31	H4	BXY	2	0.495	-2.131	2.288	1.1	0.031
ATOM	32	C5	BXY	2	3.433	1.199	1.923	1.7	0.67
ATOM	33	C6	BXY	2	4.418	2.059	2.418	1.7	-0.683
ATOM	34	H6	BXY	2	4.859	1.888	3.393	1.1	0.203
ATOM	35	C7	BXY	2	4.831	3.154	1.661	1.7	0.334
ATOM	36	H7	BXY	2	5.595	3.824	2.04	1.1	0.038
ATOM	37	C8	BXY	2	4.236	3.373	0.421	1.7	-0.602
ATOM	38	H8	BXY	2	4.512	4.218	-0.2	1.1	0.17
ATOM	39	C9	BXY	2	3.266	2.476	-0.016	1.7	0.554
ATOM	40	H9	BXY	2	2.783	2.615	-0.974	1.1	-0.007
ATOM	41	N1	BXY	3	-1.665	-0.136	-1.991	1.55	-0.728
ATOM	42	N2	BXY	3	-2.876	1.516	-0.333	1.55	-0.296
ATOM	43	C0	BXY	3	-2.579	0.696	-2.559	1.7	0.568
ATOM	44	C1	BXY	3	-2.874	0.599	-3.922	1.7	-0.579
ATOM	45	H1	BXY	3	-3.608	1.254	-4.374	1.1	0.161
ATOM	46	C2	BXY	3	-2.231	-0.364	-4.699	1.7	0.147
ATOM	47	H2	BXY	3	-2.462	-0.452	-5.756	1.1	0.067
ATOM	48	C3	BXY	3	-1.301	-1.214	-4.099	1.7	-0.381
ATOM	49	H3	BXY	3	-0.789	-1.984	-4.665	1.1	0.134
ATOM	50	C4	BXY	3	-1.042	-1.067	-2.74	1.7	0.201
ATOM	51	H4	BXY	3	-0.34	-1.697	-2.208	1.1	0.031
ATOM	52	C5	BXY	3	-3.227	1.651	-1.639	1.7	0.67
ATOM	53	C6	BXY	3	-4.136	2.627	-2.05	1.7	-0.683
ATOM	54	H6	BXY	3	-4.406	2.729	-3.094	1.1	0.203
ATOM	55	C7	BXY	3	-4.699	3.482	-1.103	1.7	0.334
ATOM	56	H7	BXY	3	-5.408	4.245	-1.408	1.1	0.038
ATOM	57	C8	BXY	3	-4.332	3.341	0.233	1.7	-0.602
ATOM	58	H8	BXY	3	-4.74	3.985	1.005	1.1	0.17
ATOM	59	C9	BXY	3	-3.416	2.347	0.573	1.7	0.554
ATOM	60	H9	BXY	3	-3.103	2.215	1.6	1.1	-0.007
ATOM	61	N1	BXY	4	-1.623	0.198	2.032	1.55	-0.728
ATOM	62	N2	BXY	4	-2.909	-1.419	0.397	1.55	-0.296
ATOM	63	C0	BXY	4	-2.55	-0.608	2.617	1.7	0.568
ATOM	64	C1	BXY	4	-2.816	-0.503	3.985	1.7	-0.579
ATOM	65	H1	BXY	4	-3.559	-1.139	4.45	1.1	0.161
ATOM	66	C2	BXY	4	-2.133	0.441	4.75	1.7	0.147
ATOM	67	H2	BXY	4	-2.342	0.535	5.811	1.1	0.067

ATOM	68	C3	BXY	4	-1.192	1.266	4.132	1.7	-0.381
ATOM	69	H3	BXY	4	-0.649	2.022	4.689	1.1	0.134
ATOM	70	C4	BXY	4	-0.962	1.112	2.769	1.7	0.201
ATOM	71	H4	BXY	4	-0.254	1.724	2.224	1.1	0.031
ATOM	72	C5	BXY	4	-3.239	-1.545	1.709	1.7	0.67
ATOM	73	C6	BXY	4	-4.168	-2.496	2.137	1.7	-0.683
ATOM	74	H6	BXY	4	-4.421	-2.591	3.186	1.1	0.203
ATOM	75	C7	BXY	4	-4.77	-3.336	1.2	1.7	0.334
ATOM	76	H7	BXY	4	-5.494	-4.079	1.519	1.1	0.038
ATOM	77	C8	BXY	4	-4.424	-3.204	-0.142	1.7	-0.602
ATOM	78	H8	BXY	4	-4.863	-3.837	-0.906	1.1	0.17
ATOM	79	C9	BXY	4	-3.488	-2.235	-0.499	1.7	0.554
ATOM	80	H9	BXY	4	-3.191	-2.111	-1.532	1.1	-0.007
ATOM	81	MN	MNC	5	1.364	-0.009	-0.007	2	3
ATOM	84	MN	MNC	6	-1.372	0.028	0.018	2	4
ATOM	101	O	OXO	7	-0.095	-1.175	-0.008	1.52	-2
ATOM	118	O	OXO	8	-0.062	1.196	0.021	1.52	-2

S8.f) Optimized structure of complex 6 in the III-IV state:

					X	Y	Z	DelPhi Radius	DelPhi Charge
ATOM	1	O1	SLP	1	-2.69	2.421	7.071	1.52	-0.633
ATOM	2	O3	SLP	1	-1.397	0.247	6.211	1.52	-0.733
ATOM	3	N1	SLP	1	-1.53	2.305	9.582	1.55	-0.859
ATOM	4	N2	SLP	1	0.169	2.366	7.362	1.55	-0.704
ATOM	5	C1	SLP	1	-3.713	2.957	7.669	1.7	0.104
ATOM	6	C2	SLP	1	-4.846	3.37	6.903	1.7	-0.063
ATOM	7	C3	SLP	1	-5.949	3.956	7.501	1.7	-0.194
ATOM	8	C4	SLP	1	-5.984	4.19	8.895	1.7	-0.089
ATOM	9	C5	SLP	1	-4.885	3.831	9.658	1.7	-0.025
ATOM	10	C6	SLP	1	-3.748	3.216	9.084	1.7	-0.437
ATOM	11	C7	SLP	1	-2.598	2.976	9.905	1.7	0.369
ATOM	12	C8	SLP	1	-0.368	2.288	10.496	1.7	0.522
ATOM	13	C9	SLP	1	0.954	2.499	9.722	1.7	-0.492
ATOM	14	C10	SLP	1	0.763	3.244	8.392	1.7	0.785
ATOM	15	C11	SLP	1	0.673	2.377	6.166	1.7	0.381
ATOM	16	C12	SLP	1	0.246	1.603	5.035	1.7	-0.376
ATOM	17	C13	SLP	1	0.878	1.853	3.792	1.7	-0.09
ATOM	18	C14	SLP	1	0.542	1.162	2.64	1.7	-0.29
ATOM	19	C15	SLP	1	-0.461	0.171	2.717	1.7	-0.037
ATOM	20	C16	SLP	1	-1.094	-0.107	3.916	1.7	-0.462
ATOM	21	C17	SLP	1	-0.768	0.59	5.121	1.7	0.75
ATOM	22	H1	SLP	1	-4.81	3.187	5.834	1.1	0.149
ATOM	23	H2	SLP	1	-6.803	4.239	6.888	1.1	0.128
ATOM	24	H3	SLP	1	-6.856	4.647	9.354	1.1	0.096
ATOM	25	H4	SLP	1	-4.884	4.015	10.731	1.1	0.086
ATOM	26	H5	SLP	1	-2.613	3.45	10.893	1.1	0.046
ATOM	27	H6	SLP	1	-0.372	1.324	11.009	1.1	0.036
ATOM	28	H7	SLP	1	-0.506	3.085	11.241	1.1	-0.081
ATOM	29	H8	SLP	1	1.403	1.526	9.51	1.1	0.082
ATOM	30	H9	SLP	1	1.65	3.068	10.351	1.1	0.078
ATOM	31	H10	SLP	1	0.092	4.101	8.536	1.1	-0.251
ATOM	32	H11	SLP	1	1.727	3.634	8.031	1.1	-0.139
ATOM	33	H12	SLP	1	1.52	3.048	5.97	1.1	-0.051

ATOM	34	H13	SLP	1	1.649	2.621	3.758	1.1	0.083
ATOM	35	H14	SLP	1	1.037	1.375	1.698	1.1	0.098
ATOM	36	H15	SLP	1	-0.742	-0.382	1.823	1.1	0.075
ATOM	37	H16	SLP	1	-1.865	-0.867	3.982	1.1	0.139
ATOM	38	O1	SLP	2	-0.319	-2.496	10.082	1.52	-0.633
ATOM	39	O3	SLP	2	-1.687	-0.382	11.413	1.52	-0.733
ATOM	40	N1	SLP	2	-1.692	-2.615	7.633	1.55	-0.859
ATOM	41	N2	SLP	2	-3.386	-2.299	10.017	1.55	-0.704
ATOM	42	C1	SLP	2	0.648	-3.071	9.416	1.7	0.104
ATOM	43	C2	SLP	2	1.864	-3.377	10.098	1.7	-0.063
ATOM	44	C3	SLP	2	2.921	-4.01	9.462	1.7	-0.194
ATOM	45	C4	SLP	2	2.827	-4.389	8.106	1.7	-0.089
ATOM	46	C5	SLP	2	1.649	-4.122	7.423	1.7	-0.025
ATOM	47	C6	SLP	2	0.554	-3.472	8.036	1.7	-0.437
ATOM	48	C7	SLP	2	-0.651	-3.286	7.26	1.7	0.369
ATOM	49	C8	SLP	2	-2.884	-2.537	6.782	1.7	0.522
ATOM	50	C9	SLP	2	-4.168	-2.592	7.65	1.7	-0.492
ATOM	51	C10	SLP	2	-3.954	-3.247	9.029	1.7	0.785
ATOM	52	C11	SLP	2	-4.041	-2.14	11.135	1.7	0.381
ATOM	53	C12	SLP	2	-3.737	-1.314	12.268	1.7	-0.376
ATOM	54	C13	SLP	2	-4.651	-1.346	13.352	1.7	-0.09
ATOM	55	C14	SLP	2	-4.459	-0.607	14.507	1.7	-0.29
ATOM	56	C15	SLP	2	-3.303	0.204	14.605	1.7	-0.037
ATOM	57	C16	SLP	2	-2.387	0.265	13.572	1.7	-0.462
ATOM	58	C17	SLP	2	-2.559	-0.479	12.353	1.7	0.75
ATOM	59	H1	SLP	2	1.926	-3.079	11.14	1.1	0.149
ATOM	60	H2	SLP	2	3.836	-4.213	10.016	1.1	0.128
ATOM	61	H3	SLP	2	3.659	-4.88	7.611	1.1	0.096
ATOM	62	H4	SLP	2	1.55	-4.412	6.378	1.1	0.086
ATOM	63	H5	SLP	2	-0.656	-3.786	6.278	1.1	0.046
ATOM	64	H6	SLP	2	-2.842	-1.582	6.253	1.1	0.036
ATOM	65	H7	SLP	2	-2.878	-3.352	6.037	1.1	-0.081
ATOM	66	H8	SLP	2	-4.536	-1.576	7.811	1.1	0.082
ATOM	67	H9	SLP	2	-4.944	-3.15	7.11	1.1	0.078
ATOM	68	H10	SLP	2	-3.263	-4.092	8.936	1.1	-0.251
ATOM	69	H11	SLP	2	-4.912	-3.637	9.408	1.1	-0.139
ATOM	70	H12	SLP	2	-4.97	-2.719	11.253	1.1	-0.051
ATOM	71	H13	SLP	2	-5.531	-1.982	13.257	1.1	0.083
ATOM	72	H14	SLP	2	-5.175	-0.648	15.322	1.1	0.098
ATOM	73	H15	SLP	2	-3.134	0.786	15.509	1.1	0.075
ATOM	74	H16	SLP	2	-1.495	0.88	13.646	1.1	0.139
ATOM	75	MN	MNC	3	-1.442	1.114	7.949	2	3
ATOM	78	MN	MNC	4	-1.634	-1.188	9.406	2	4
ATOM	95	O	OXO	5	-0.345	-0.019	8.73	1.52	-2
ATOM	112	O	OXO	6	-2.722	0.079	8.553	1.52	-2

S8.g) Optimized structure of complex 7 in the III-IV state:

					X	Y	Z	DelPhi Radius	DelPhi Charge
ATOM	1	O1	CLS	1	-2.886	2.566	7.351	1.52	-0.932
ATOM	2	O3	CLS	1	-1.497	0.437	5.9	1.52	-0.800
ATOM	3	N1	CLS	1	-1.441	2.6	9.72	1.55	-0.495
ATOM	4	N2	CLS	1	0.149	2.368	7.298	1.55	-0.402
ATOM	5	C1	CLS	1	-3.842	3.067	8.073	1.7	0.118

ATOM	6	C2	CLS	1	-5.101	3.391	7.481	1.7	-0.099
ATOM	7	C3	CLS	1	-6.164	3.943	8.171	1.7	0.038
ATOM	8	C4	CLS	1	-5.997	4.217	9.532	1.7	-0.065
ATOM	9	C5	CLS	1	-4.806	3.955	10.178	1.7	0.055
ATOM	10	C6	CLS	1	-3.724	3.386	9.474	1.7	-0.315
ATOM	11	C7	CLS	1	-2.477	3.205	10.194	1.7	0.317
ATOM	12	C8	CLS	1	-0.166	2.528	10.437	1.7	0.188
ATOM	13	C9	CLS	1	0.964	3.154	9.571	1.7	-0.195
ATOM	14	C10	CLS	1	0.539	3.524	8.139	1.7	0.232
ATOM	15	C11	CLS	1	0.894	2.115	6.261	1.7	0.36
ATOM	16	C12	CLS	1	0.689	1.167	5.199	1.7	-0.626
ATOM	17	C13	CLS	1	1.725	1.069	4.239	1.7	0.071
ATOM	18	C14	CLS	1	1.582	0.266	3.132	1.7	-0.165
ATOM	19	C15	CLS	1	0.401	-0.455	2.906	1.7	0.072
ATOM	20	C16	CLS	1	-0.611	-0.36	3.837	1.7	-0.352
ATOM	21	C17	CLS	1	-0.542	0.414	5.054	1.7	0.961
ATOM	22	H1	CLS	1	-7.099	4.155	7.668	1.1	0.092
ATOM	23	H2	CLS	1	-4.692	4.183	11.232	1.1	0.092
ATOM	24	H3	CLS	1	-2.44	3.645	11.201	1.1	0.032
ATOM	25	H4	CLS	1	0.033	1.47	10.61	1.1	0.08
ATOM	26	H5	CLS	1	-0.228	3.026	11.414	1.1	-0.028
ATOM	27	H6	CLS	1	1.818	2.47	9.531	1.1	0.056
ATOM	28	H7	CLS	1	1.318	4.081	10.042	1.1	0.041
ATOM	29	H8	CLS	1	-0.325	4.193	8.176	1.1	-0.009
ATOM	30	H9	CLS	1	1.365	4.068	7.655	1.1	-0.06
ATOM	31	H10	CLS	1	1.797	2.728	6.131	1.1	-0.015
ATOM	32	H11	CLS	1	2.635	1.642	4.385	1.1	0.077
ATOM	33	H12	CLS	1	0.28	-1.065	2.02	1.1	0.083
ATOM	34	CL1	CLS	1	-7.406	4.951	10.462	1.75	-0.085
ATOM	35	CL2	CLS	1	-5.325	3.045	5.702	1.75	-0.006
ATOM	36	CL3	CLS	1	-2.159	-1.278	3.48	1.75	-0.137
ATOM	37	CL4	CLS	1	2.942	0.136	1.899	1.75	-0.179
ATOM	38	O1	CLS	2	-0.532	-2.569	9.955	1.52	-0.932
ATOM	39	O3	CLS	2	-1.684	-0.408	11.145	1.52	-0.8
ATOM	40	N1	CLS	2	-1.859	-2.177	7.604	1.55	-0.495
ATOM	41	N2	CLS	2	-3.399	-2.332	9.925	1.55	-0.402
ATOM	42	C1	CLS	2	0.453	-2.994	9.234	1.7	0.118
ATOM	43	C2	CLS	2	1.655	-3.489	9.829	1.7	-0.099
ATOM	44	C3	CLS	2	2.736	-3.947	9.106	1.7	0.038
ATOM	45	C4	CLS	2	2.646	-3.963	7.706	1.7	-0.065
ATOM	46	C5	CLS	2	1.506	-3.55	7.053	1.7	0.055
ATOM	47	C6	CLS	2	0.405	-3.067	7.796	1.7	-0.315
ATOM	48	C7	CLS	2	-0.823	-2.779	7.102	1.7	0.317
ATOM	49	C8	CLS	2	-3.137	-2.127	6.871	1.7	0.188
ATOM	50	C9	CLS	2	-4.234	-2.925	7.633	1.7	-0.195
ATOM	51	C10	CLS	2	-3.808	-3.425	9.023	1.7	0.232
ATOM	52	C11	CLS	2	-4.087	-2.123	11.003	1.7	0.36
ATOM	53	C12	CLS	2	-3.784	-1.201	12.065	1.7	-0.626
ATOM	54	C13	CLS	2	-4.709	-1.137	13.133	1.7	0.071
ATOM	55	C14	CLS	2	-4.429	-0.39	14.254	1.7	-0.165
ATOM	56	C15	CLS	2	-3.21	0.288	14.382	1.7	0.072
ATOM	57	C16	CLS	2	-2.31	0.229	13.338	1.7	-0.352
ATOM	58	C17	CLS	2	-2.552	-0.457	12.102	1.7	0.961
ATOM	59	H1	CLS	2	3.632	-4.287	9.609	1.1	0.092

ATOM	60	H2	CLS	2	1.446	-3.586	5.97	1.1	0.092
ATOM	61	H3	CLS	2	-0.898	-3.148	6.075	1.1	0.032
ATOM	62	H4	CLS	2	-5.637	-1.694	13.064	1.1	0.08
ATOM	63	H5	CLS	2	-2.971	0.839	15.282	1.1	-0.028
ATOM	64	H6	CLS	2	-3.413	-1.079	6.788	1.1	0.056
ATOM	65	H7	CLS	2	-2.995	-2.525	5.863	1.1	0.041
ATOM	66	H8	CLS	2	-5.128	-2.301	7.735	1.1	-0.009
ATOM	67	H9	CLS	2	-4.524	-3.809	7.05	1.1	-0.06
ATOM	68	H10	CLS	2	-2.949	-4.097	8.931	1.1	-0.015
ATOM	69	H11	CLS	2	-4.633	-3.995	9.474	1.1	0.077
ATOM	70	H12	CLS	2	-4.979	-2.739	11.174	1.1	0.083
ATOM	71	CL1	CLS	2	4.089	-4.574	6.747	1.75	-0.085
ATOM	72	CL2	CLS	2	1.77	-3.493	11.65	1.75	-0.006
ATOM	73	CL3	CLS	2	-0.702	1.058	13.578	1.75	-0.137
ATOM	74	CL4	CLS	2	-5.641	-0.295	15.63	1.75	-0.179
ATOM	75	MN	MNC	3	-1.567	1.221	7.943	2	3
ATOM	78	MN	MNC	4	-1.78	-1.125	9.322	2	4
ATOM	95	O	OXO	5	-0.492	-0.103	8.705	1.52	-2
ATOM	112	O	OXO	6	-2.865	0.104	8.69	1.52	-2

S8.h) Optimized structure of complex 8 in the III-IV state:

					X	Y	Z	DelPhi Radius	DelPhi Charge
ATOM	1	O1	SNO	1	-2.859	2.729	7.715	1.52	-0.629
ATOM	2	O3	SNO	1	-1.564	0.683	5.939	1.52	-0.631
ATOM	3	N1	SNO	1	-1.212	2.453	9.899	1.55	-0.441
ATOM	4	N2	SNO	1	0.174	2.414	7.368	1.55	-0.368
ATOM	5	C1	SNO	1	-3.734	3.143	8.552	1.7	0.387
ATOM	6	C2	SNO	1	-5.047	3.538	8.118	1.7	-0.18
ATOM	7	C3	SNO	1	-6.039	3.923	8.991	1.7	-0.252
ATOM	8	C4	SNO	1	-5.757	4.017	10.35	1.7	0.1
ATOM	9	C5	SNO	1	-4.492	3.705	10.835	1.7	-0.259
ATOM	10	C6	SNO	1	-3.489	3.263	9.98	1.7	-0.222
ATOM	11	C7	SNO	1	-2.169	3.02	10.543	1.7	0.341
ATOM	12	C8	SNO	1	0.154	2.347	10.422	1.7	0.158
ATOM	13	C9	SNO	1	1.086	3.266	9.574	1.7	-0.233
ATOM	14	C10	SNO	1	0.527	3.606	8.171	1.7	0.459
ATOM	15	C11	SNO	1	0.944	2.102	6.378	1.7	0.221
ATOM	16	C12	SNO	1	0.733	1.07	5.385	1.7	-0.131
ATOM	17	C13	SNO	1	1.797	0.752	4.549	1.7	-0.274
ATOM	18	C14	SNO	1	1.666	-0.199	3.54	1.7	0.074
ATOM	19	C15	SNO	1	0.447	-0.841	3.324	1.7	-0.302
ATOM	20	C16	SNO	1	-0.64	-0.497	4.098	1.7	-0.056
ATOM	21	C17	SNO	1	-0.575	0.448	5.199	1.7	0.384
ATOM	22	H1	SNO	1	-7.027	4.159	8.621	1.1	0.154
ATOM	23	H2	SNO	1	-4.3	3.811	11.896	1.1	0.141
ATOM	24	H3	SNO	1	-2.019	3.368	11.573	1.1	-0.034
ATOM	25	H4	SNO	1	0.446	1.303	10.304	1.1	0.053
ATOM	26	H5	SNO	1	0.211	2.626	11.482	1.1	-0.036
ATOM	27	H6	SNO	1	2.065	2.786	9.473	1.1	0.04
ATOM	28	H7	SNO	1	1.227	4.222	10.093	1.1	0.029
ATOM	29	H8	SNO	1	-0.388	4.195	8.27	1.1	-0.072
ATOM	30	H9	SNO	1	1.275	4.206	7.632	1.1	-0.154
ATOM	31	H10	SNO	1	1.86	2.688	6.226	1.1	-0.048

ATOM	32	H11	SNO	1	2.758	1.239	4.674	1.1	0.14
ATOM	33	H12	SNO	1	0.355	-1.587	2.545	1.1	0.175
ATOM	34	N75	SNO	1	-6.794	4.466	11.27	1.55	0.644
ATOM	35	N76	SNO	1	-5.392	3.519	6.685	1.55	0.72
ATOM	36	N77	SNO	1	-1.899	-1.174	3.814	1.55	0.702
ATOM	37	N78	SNO	1	2.805	-0.509	2.687	1.55	0.716
ATOM	38	O79	SNO	1	-1.839	-2.393	3.518	1.52	-0.435
ATOM	39	O80	SNO	1	-2.952	-0.536	3.89	1.52	-0.369
ATOM	40	O81	SNO	1	2.64	-1.348	1.785	1.52	-0.409
ATOM	41	O82	SNO	1	3.875	0.087	2.908	1.52	-0.431
ATOM	42	O87	SNO	1	-4.52	3.83	5.87	1.52	-0.427
ATOM	43	O88	SNO	1	-6.567	3.228	6.397	1.52	-0.436
ATOM	44	O89	SNO	1	-7.907	4.749	10.796	1.52	-0.405
ATOM	45	O90	SNO	1	-6.5	4.543	12.476	1.7	-0.405
ATOM	46	O1	SNO	2	-0.482	-2.639	9.658	1.52	-0.629
ATOM	47	O3	SNO	2	-1.728	-0.567	11.006	1.52	-0.631
ATOM	48	N1	SNO	2	-1.865	-2.144	7.391	1.55	-0.441
ATOM	49	N2	SNO	2	-3.377	-2.401	9.699	1.55	-0.368
ATOM	50	C1	SNO	2	0.502	-2.964	8.912	1.7	0.387
ATOM	51	C2	SNO	2	2.724	-3.661	7.285	1.7	-0.18
ATOM	52	C3	SNO	2	2.847	-3.696	8.674	1.7	-0.252
ATOM	53	C4	SNO	2	1.757	-3.403	9.46	1.7	0.1
ATOM	54	C5	SNO	2	1.524	-3.305	6.684	1.7	-0.259
ATOM	55	C6	SNO	2	0.427	-2.942	7.462	1.7	-0.222
ATOM	56	C7	SNO	2	-0.841	-2.693	6.817	1.7	0.341
ATOM	57	C8	SNO	2	-3.21	-2.154	6.747	1.7	0.158
ATOM	58	C9	SNO	2	-4.109	-3.216	7.448	1.7	-0.233
ATOM	59	C10	SNO	2	-3.638	-3.593	8.871	1.7	0.459
ATOM	60	C11	SNO	2	-4.179	-2.109	10.664	1.7	0.221
ATOM	61	C12	SNO	2	-3.998	-1.055	11.634	1.7	-0.131
ATOM	62	C13	SNO	2	-5.052	-0.782	12.503	1.7	-0.274
ATOM	63	C14	SNO	2	-4.909	0.139	13.53	1.7	0.074
ATOM	64	C15	SNO	2	-3.692	0.779	13.743	1.7	-0.302
ATOM	65	C16	SNO	2	-2.621	0.489	12.927	1.7	-0.056
ATOM	66	C17	SNO	2	-2.718	-0.395	11.79	1.7	0.384
ATOM	67	H1	SNO	2	3.791	-3.964	9.128	1.1	0.154
ATOM	68	H2	SNO	2	1.46	-3.313	5.603	1.1	0.141
ATOM	69	H3	SNO	2	-0.945	-3.04	5.786	1.1	-0.034
ATOM	70	H4	SNO	2	-6.001	-1.291	12.395	1.1	0.053
ATOM	71	H5	SNO	2	-3.585	1.487	14.553	1.1	-0.036
ATOM	72	H6	SNO	2	-3.612	-1.151	6.875	1.1	0.04
ATOM	73	H7	SNO	2	-3.115	-2.389	5.685	1.1	0.029
ATOM	74	H8	SNO	2	-5.132	-2.829	7.492	1.1	-0.072
ATOM	75	H9	SNO	2	-4.119	-4.14	6.857	1.1	-0.154
ATOM	76	H10	SNO	2	-2.699	-4.15	8.824	1.1	-0.048
ATOM	77	H11	SNO	2	-4.399	-4.225	9.349	1.1	0.14
ATOM	78	H12	SNO	2	-5.072	-2.727	10.815	1.1	0.175
ATOM	79	N75	SNO	2	1.931	-3.518	10.92	1.55	0.644
ATOM	80	N76	SNO	2	3.866	-4.039	6.457	1.55	0.72
ATOM	81	N77	SNO	2	-1.35	1.149	13.246	1.55	0.702
ATOM	82	N78	SNO	2	-6.03	0.4	14.428	1.55	0.716
ATOM	83	O79	SNO	2	-1.419	2.295	13.74	1.52	-0.435
ATOM	84	O80	SNO	2	-0.297	0.546	13.025	1.52	-0.369
ATOM	85	O81	SNO	2	-5.847	1.193	15.364	1.52	-0.409

ATOM	86	O82	SNO	2	-7.095	-0.2	14.202	1.52	-0.431
ATOM	87	O87	SNO	2	4.913	-4.374	7.036	1.52	-0.427
ATOM	88	O88	SNO	2	3.716	-4.012	5.224	1.52	-0.436
ATOM	89	O89	SNO	2	3.052	-3.24	11.378	1.52	-0.405
ATOM	90	O90	SNO	2	0.97	-3.916	11.585	1.7	-0.405
ATOM	91	MN	MNC	3	-1.537	1.278	8.035	2	3
ATOM	94	MN	MNC	4	-1.77	-1.187	9.136	2	4
ATOM	111	O	OXO	5	-0.475	-0.139	8.584	1.52	-2
ATOM	128	O	OXO	6	-2.849	0.096	8.632	1.52	-2

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