SUPPORTING INFORMATION OR MATERIAL

Polyoxometalate Cluster-Based Single-Atom Catalyst for NH_3 Synthesis *via* an Enzymatic Mechanism

Shamraiz Hussain Talib[‖†], Xiaohu Yu[‡*], Zhansheng Lu[‖], Khalil Ahmad[¶], Tongtong Yang[†], Hai Xiao[†] and Jun Li[†§*]

[‖]School of Physics, Henan Normal University, Xinxiang 453007, China

[‡]Shaanxi Key Laboratory of Catalysis and School of Chemical & Environment Sciences, Shaanxi University of Technology, Hanzhong 723000, China

[¶]Department of Chemistry, Mirpur University of Science and Technology (MUST), Mirpur 10250, AJK, Pakistan

[†]Department of Chemistry and Key Laboratory of Organic Optoelectronics & Molecular Engineering of Ministry of Education, Tsinghua University, Beijing 100084, China

[§]Department of Chemistry, Southern University of Science and Technology, Shenzhen 518055, China

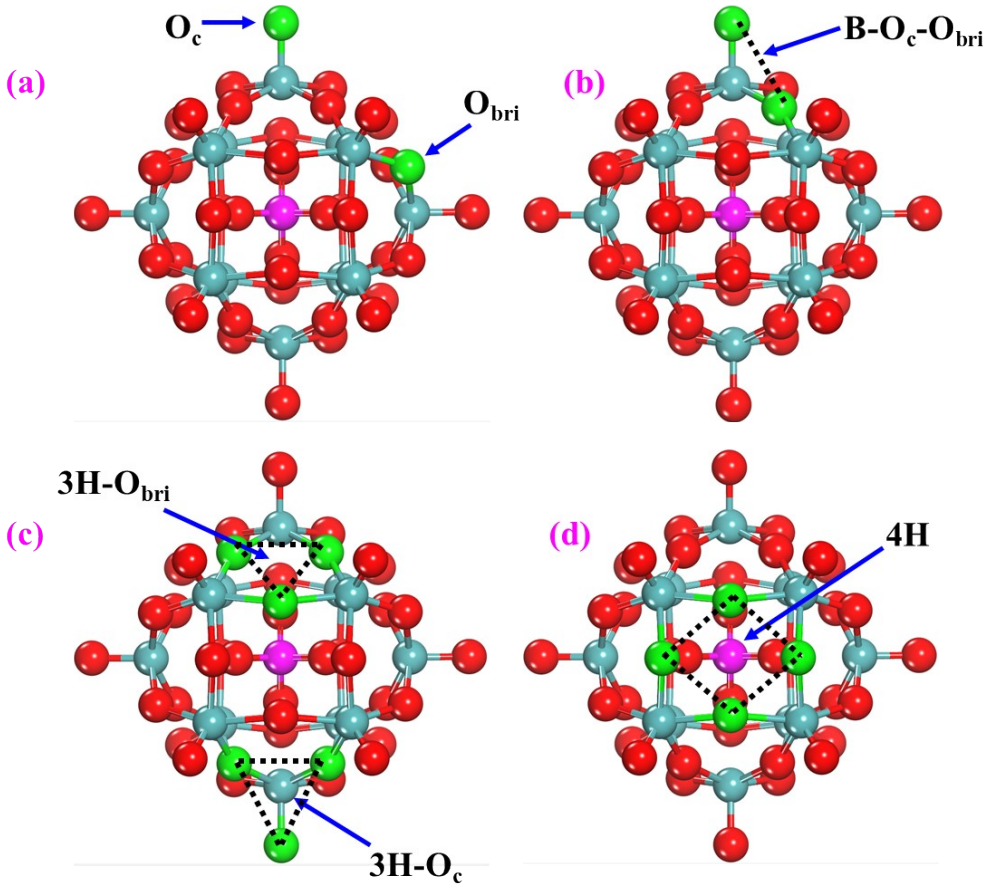

Fig. S1 Optimized geometry of PMA cluster with various possible coordination sites. Color pattern: P, pink; O, red and green; and Mo, dark cyan.

A vacuum space of 20 Å in the *z*-direction was used to avoid the interlayer interaction with the periodic systems. All the geometry optimization and energy calculation were performed by means of spin-polarized density functional theory (DFT) methods using the Vienna ab initio simulation package (VASP-5.3). To improve the calculation efficiency, the projector augmented wave (PAW) pseudo-potentials are employed to define the interaction between the valence and core electrons. In this work, the generalized gradient approximation (GGA) using the Perdew, Burke and Ernzerhof (PBE) exchange-correlation functional was employed. The valence electrons are described by Sc [$3d^1$ $4s^2$], Ti [$3d^2$ $4s^2$], V [$3d^3$ $4s^2$], Cr [$3d^4$ $4s^2$], Mn [$3d^5$ $4s^2$], Fe [$3d^6$ $4s^2$], Co [$3d^7$ $4s^2$], Ni [$3d^8$ $4s^2$], Cu [$3d^9$ $4s^2$], Zn [$3d^{10}$ $4s^2$], for 3d, Zr [$4d^2$ $5s^2$], Nb [$4d^3$ $5s^2$], Mo [$4d^4$ $5s^2$], Tc [$4d^5$ $5s^2$], Ru [$4d^7$ $5s^1$], Rh [$4d^8$ $5s^1$], Pd [$4d^8$ $5s^2$], Ag [$4d^9$ $5s^2$], for 4d, and W [$5d^4$ $6s^2$], Re [$5d^5$ $6s^2$], Os [$5d^6$ $6s^2$], Ir [$5d^7$ $6s^2$], Pt [$5d^8$ $6s^2$], Au [$5d^9$ $6s^2$], for 5d transition metal atoms, [$2s^2$ $2p^4$] for O, [$2s^2$ $2p^3$] for P and [$1s^1$] for H. The Kohn-Sham orbitals are extended by using plane wave basis sets with an energy cutoff of 400 eV and the geometry optimization were done with a convergence criterion of 10^{-5} eV for a total energy. All the ions are permitted to relax until the maximum force is less than 0.02 eV/Å. The Brillouin zone interrogation was sampled using a 1 x 1 x 1 Γ point. The Bader charge analysis was performed to compute the electron charge transfer. The PMA cluster was generated in a cubic unit cell (with 12 Mo atoms, one P atom and 40 O atoms), which has been verified to be sufficient for inspecting the reaction mechanisms. By using the standard hydrogen electrode (SHE), the Gibbs free energy change (ΔG) of every elemental step was calculated.

The formation energy of transition metal atoms on the phosphomolybdic acid (PMA) cluster was defined as:

$$E_{for} = E_{tol}^{M_1-PMA} - E^{PMA} - E_{tol}^{M_1} / (nM_1) \qquad (S1)$$

where, $E_{tol}^{M_1-PMA}$, E^{PMA}, and $E_{tol}^{M_1} / (nM_1)$ are corresponding to the total energies of a single metal atom bonded to PMA, the energy of PMA cluster and the energy of single metal atom, respectively. Where the nM_1 is the number of atoms in the bulk unit cells.

The binding energy of transition metal atoms (TM) on the PMA cluster was defined as:

$$E_b(TM) = E_{tot}(TM_1/PMA) - E(PMA) - E(TM) \qquad (S2)$$

where $E_{tot}(TM_1/PMA)$ is the energy of PMA cluster containing one TM atom, E(PMA) corresponds to the energy of PMA cluster and E(TM) is the energy of the transition metal atom.

Under standard conditions, the Gibbs free energy of hydrogen adsorption (ΔG_H) is used to define the HER catalytic properties, obtained from the following equation:

$$\Delta G_H = \Delta E_H + \Delta E_{ZPE} - T\Delta S_H \qquad (S3)$$

ΔE_H is the hydrogen adsorption energy, ΔE_{ZPE} corresponds to the zero-point energy of adsorbed hydrogen and gas phase hydrogen, and ΔS_H is the entropy difference between the gas phase and adsorbed state. T indicates a temperature of 298.15 K. Furthermore, the ΔE_{ZPE} and $T\Delta S_H$ values can be measured through the vibrational frequencies of the system.

ΔE_H define as:

$$\Delta E_H = E_{(catalyst + H)} - E\ (catalyst) - 1/2\ E_{H2} \qquad (S4)$$

where $E_{(catalyst + H)}$ represents the calculated adsorption energies of M_1/PMA systems with adsorption of one H atom and E (catalyst), which signifies the energy of M_1/PMA system rather than the adsorption of the H atom. The optimal value of ΔE_H=0 indicates the best performance of HER.

The Gibbs free energy change (ΔG) of every elemental step is calculated as follows.

$$\Delta G = \Delta E + \Delta ZPE - T\Delta S + \Delta G_U + \Delta Gp_H \qquad (S5)$$

where ΔE corresponds to the electronic energy difference directly obtained from DFT calculations, ΔZPE is the adjustment from the zero-point energies, T is the temperature (T=298.15 k), ΔS is the entropy change, ΔG_U corresponds to the free energy contribution associated to electrode potential (U), and ΔGp_H is the free energy contribution of the H^+ ions, respectively. ΔGp_H value can be determined by as follows:

$$\Delta Gp_H = \ln(10) \times k_B T \times pH \text{ (or } 0.059 \text{ eV} \times pH)$$

where k_B is the Boltzmann constant, and the pH value was assumed to be zero because the overpotential is pH independent in this case. The entropies and zero-point energies of the eNRR species were computed from the vibrational frequencies, in which just the adsorbate vibrational modes were explicitly considered, while the catalyst cluster was fixed. The vibrational frequencies and entropies of molecules in the gas phase were taken from the NIST database.

The Gibbs free energy (ΔG) of an adsorbate was calculated of every elemental step of eNRR by using the following equations:

$$\Delta G = G(N_2 \ldots M_1/PMA) - G(M_1/PMA) - G(N_2) \qquad (Step1)$$

$$\Delta G = G(N_2H \ldots M_1/PMA) - G(M_1/PMA) - G(N_2) - G(H) \qquad (Step2)$$

$$\Delta G = G(N_2H_2 \ldots M_1/PMA) - G(M_1/PMA) - G(N_2) - G(2H) \qquad (Step3)$$

$$\Delta G = G(N_2H_3 \ldots M_1/PMA) - G(M_1/PMA) - G(N_2) - G(3H) \qquad (Step4)$$

$$\Delta G = G(N_2H_4 \ldots M_1/PMA) - G(M_1/PMA) - G(N_2) - G(4H) \qquad (Step5)$$

In the Distal pathway, the first NH_3 molecule is desorbed from the surface in the fourth step, so the ΔG value of the fifth step is calculated by using the following equation.

$$\Delta G = G(NH \ldots M_1/PMA) + G(NH_3) - G(M_1/PMA) - G(N_2) - G(4H) \qquad (Step5\text{-}Distal)$$

$$\Delta G = G(N_2H_5 \ldots M_1/PMA) - G(M_1/PMA) - G(N_2) - G(5H) \qquad (Step6)$$

$$\Delta G = G(NH_2 \ldots M_1/PMA) + G(NH_3) - G(M_1/PMA) - G(N_2) - G(5H) \qquad (Step6\text{-}Distal)$$

In the case of Alternating and Enzymatic pathways, the first NH_3 molecule desorbed from the surface in the sixth step, so the ΔG value of the seventh step is calculated by using the following equation.

$$\Delta G = G(NH_3 \ldots M_1/PMA) + G(NH_3) - G(M_1/PMA) - G(N_2) - G(6H) \qquad \text{(Step7)}$$

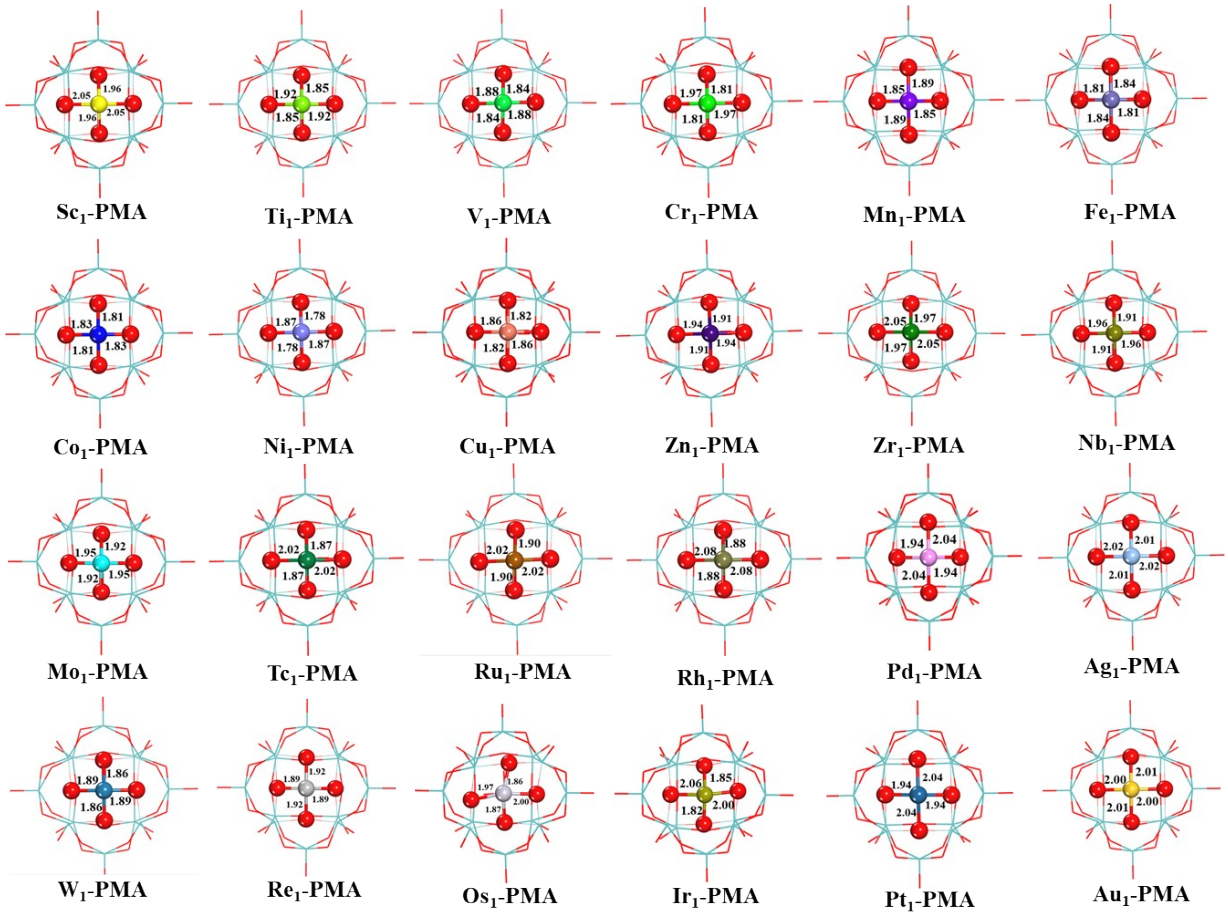

Fig. S2 Top view of the optimized structure of transition metal atoms supported on the PMA cluster. All bond lengths are given in Å.

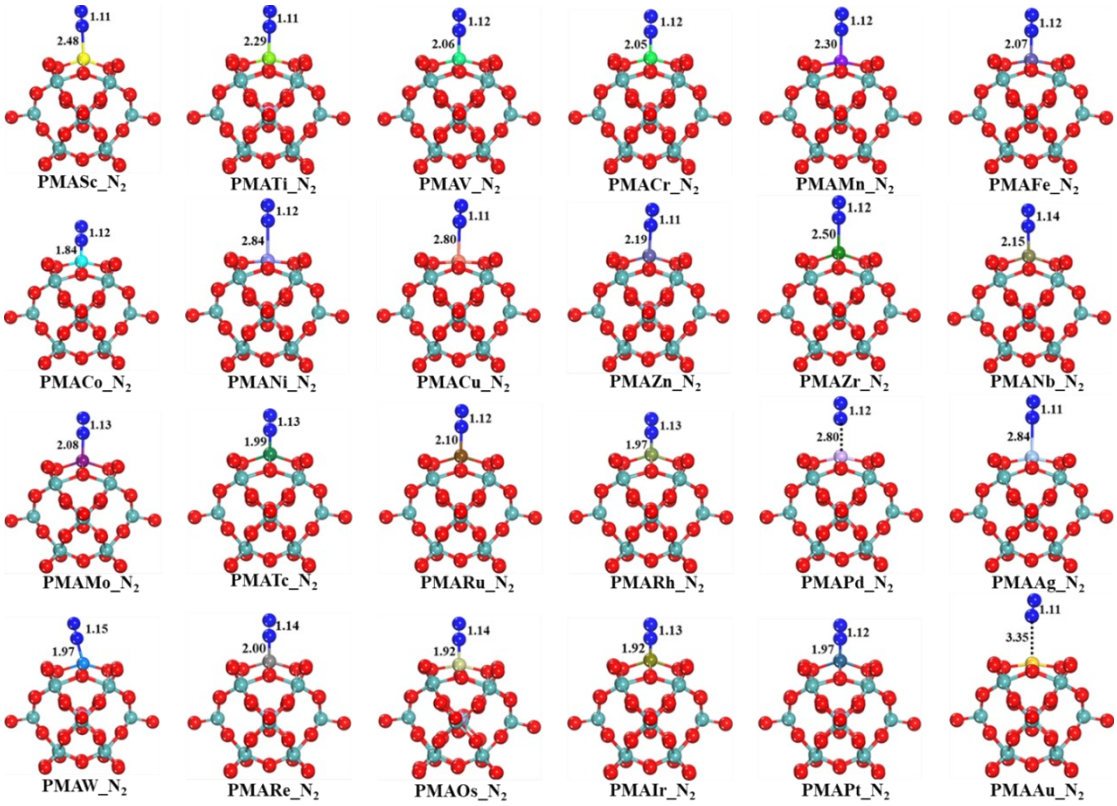

Fig. S3 Optimized structure of N_2 adsorption *via* end-on configurations on various transition metal atoms supported on the PMA cluster. All bond lengths are given in Å.

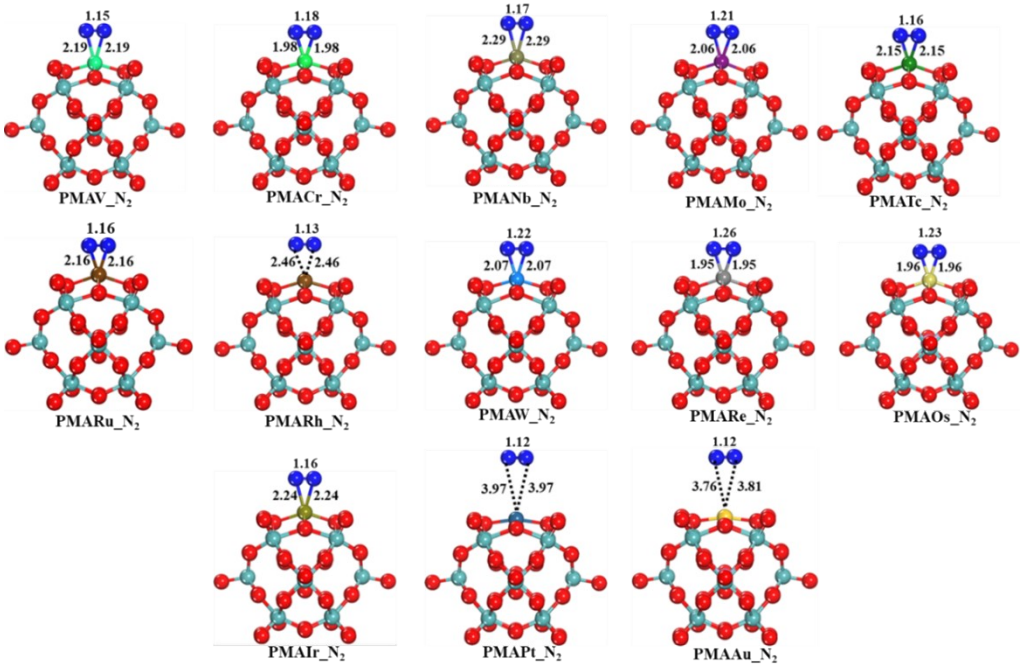

Fig. S4 Optimized structure of N_2 adsorption *via* side-on configurations on various transition metal atoms supported on the PMA cluster. All bond lengths are given in Å.

Table S1. Calculated P-O, Mo-O_C, Mo-O_{bri} and O_{bri}-O_{bri} (fourfold binding sites) bond lengths (Å) in isolated PMA and results from past theories and experimental works.

Bond	This work	Past theories	Past experiments
P-O	1.55	1.54 ,1.55,1.58	1.54
Mo-O_C	1.70	1.69,1.70	1.68
Mo-O_{bri}	1.93	1.94,1.94,1.93	1.92
O_{bri}-O_{bri}	2.72	2.68 2.72	-

Table S2. Binding site, calculated binding energies (eV), formation energies (eV), average bond lengths between the between the metal atoms and neighboring oxygen atoms (Å) and Bader charge [q(e)] of transition metal atoms (3d= Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn: 4d= Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag: 5d= W, Re, Os, Ir, Pt, Au) anchored over Phosphomolybdic (PMA) cluster.

Systems	Binding Site	E_{bin}/eV	Formation energies (eV)	Average Bond Length (Å)	q (e)
Sc_PMA	4H_site	-15.122	-10.92	2.01	2.78
Ti_PMA	4H-site	-14.73	-9.33	1.88	2.55
V_PMA	4H-site	-12.90	-7.74	1.86	2.17
Cr_PMA	4H-site	-10.77	-7.11	1.89	1.82
Mn_PMA	4H-site	-10.72	-6.92	1.87	1.82
Fe_PMA	4H-site	-10.47	-5.68	1.83	1.67
Co_PMA	4H-site	-10.44	-4.84	1.82	1.38
Ni_PMA	4H-site	-9.40	-4.51	1.83	1.35
Cu_PMA	4H-site	-7.44	-3.90	1.84	0.61
Zn_PMA	4H-site	-5.46	-4.50	1.93	0.84
Zr_PMA	4H-site	-16.34	-9.92	2.01	3.09
Nb_PMA	4H-site	-14.06	-7.34	1.94	2.87
Mo_PMA	4H-site	-11.47	-5.56	1.94	2.49
Tc_PMA	4H-site	-10.83	-4.21	1.95	1.57
Ru_PMA	4H-site	-10.17	-3.03	1.96	1.55

Rh_PMA	4H-site	-9.05	-2.97	1.98	1.35
Pd_PMA	4H-site	-6.35	-2.60	1.99	1.19
Ag_PMA	4H-site	-4.62	-2.11	2.01	1.03
W_PMA	4H-site	-13.59	-5.60	1.88	3.69
Re_PMA	4H-site	-11.14	-3.32	1.91	2.28
Os_PMA	4H-site	-11.06	-2.77	1.93	1.90
Ir_PMA	4H-site	-9.48	-2.35	1.96	1.67
Pt_PMA	4H-site	-7.83	-2.27	1.99	1.23
Au_PMA	4H-site	-5.01	-1.98	2.00	0.15

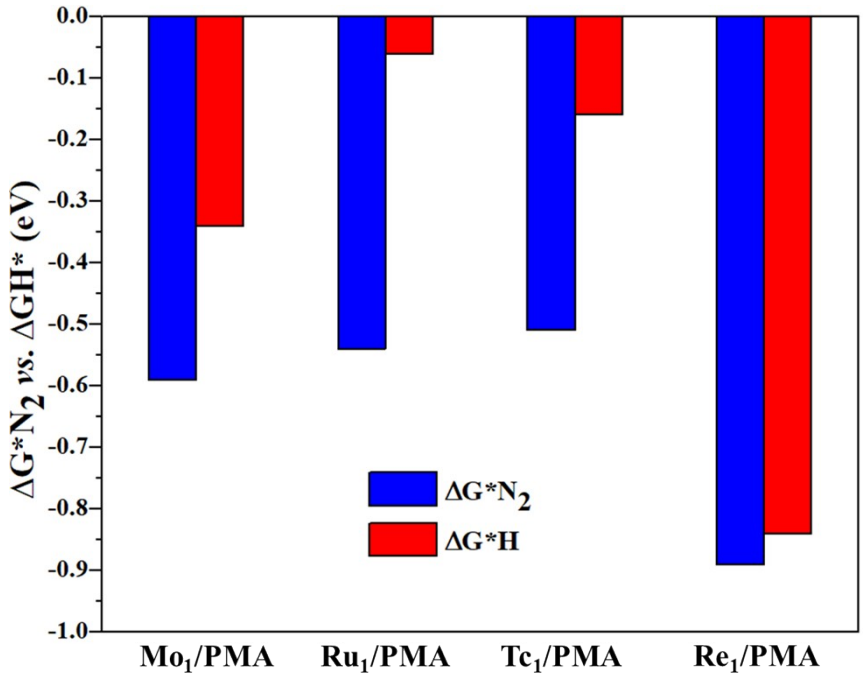

Fig S5. Gibbs free energy changes of the N_2 molecule (ΔG^*N_2) and the H atom (ΔG^*H) anchored on the Mo_1/PMA, Ru_1/PMA, Tc_1/PMA, and Re_1/PMA, catalysts.

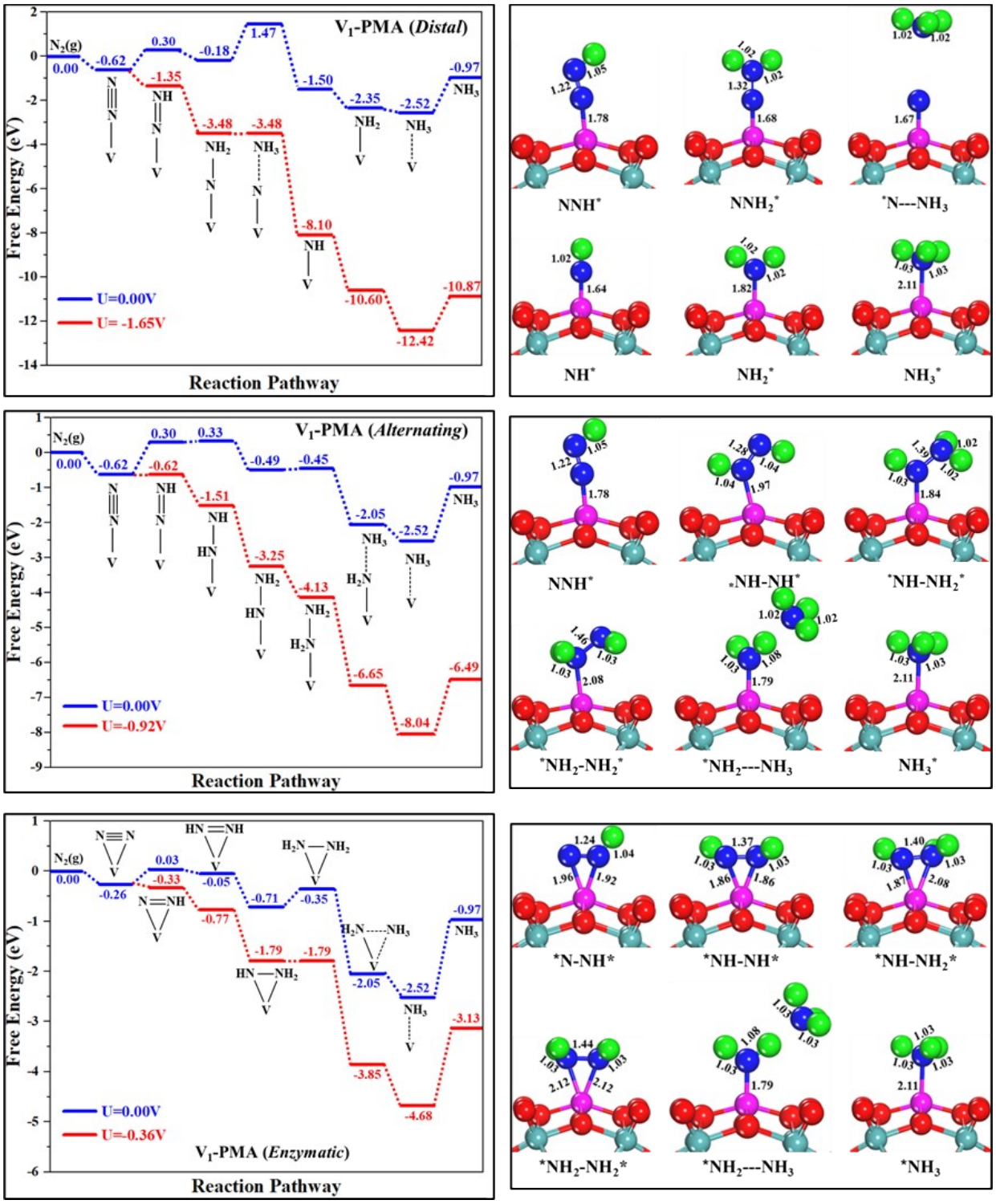

Fig. S6 (a) Free energy profiles for the eNRR on the V_1/PMA cluster at zero and applied potential (limiting potential) *via* distal, alternating and enzymatic pathways. (b) Optimized geometric structures of various elementary steps of the eNRR pathway using the V_1/PMA cluster *via* distal, alternating and enzymatic pathways. All bond lengths are given in Å.

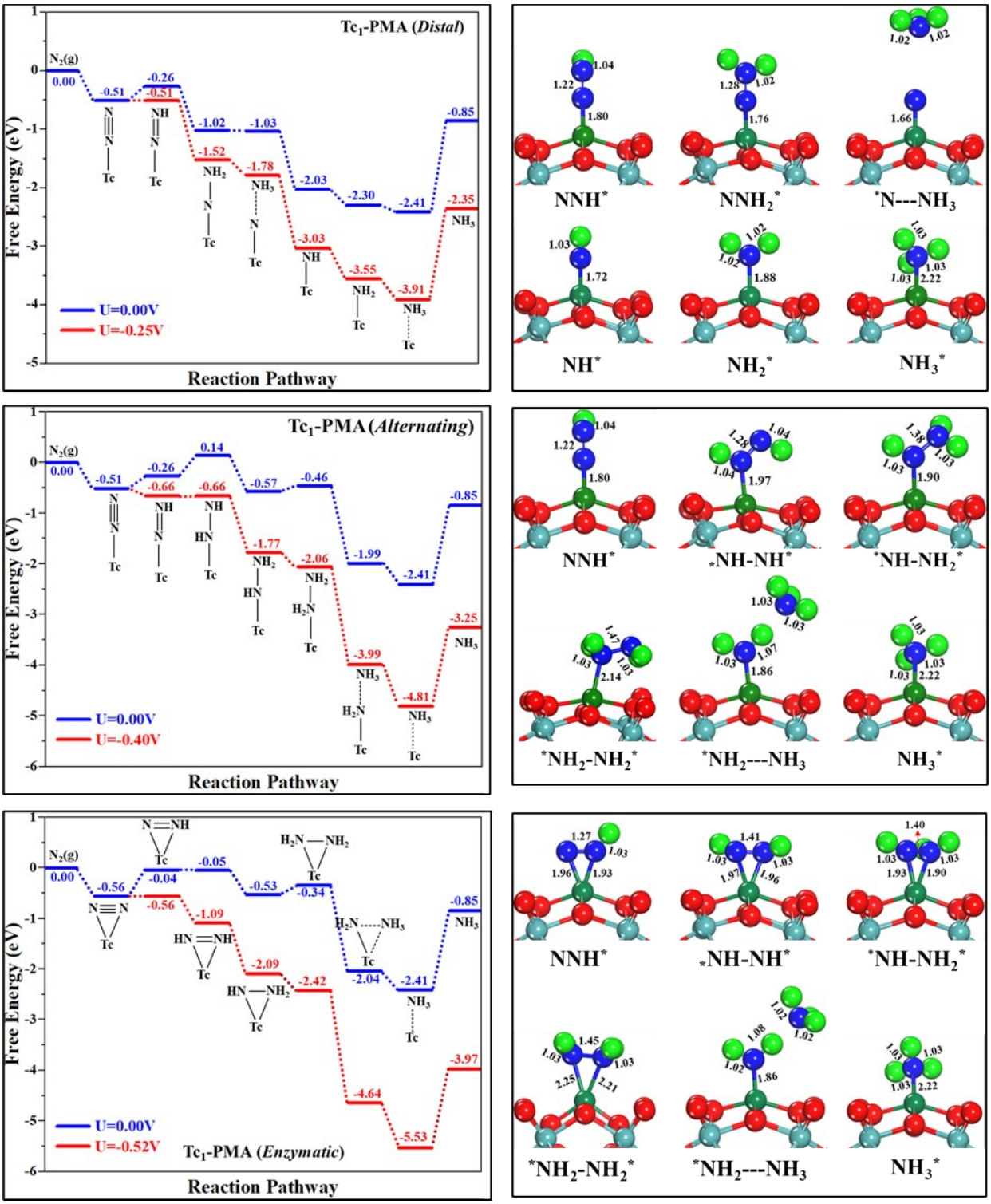

Fig. S7 (a) Free energy profiles for the eNRR on the Tc_1/PMA cluster at zero and applied potential (limiting potential) *via* distal, alternating and enzymatic pathways. (b) Optimized geometric structures of various elementary steps of the eNRR pathway using the Tc_1/PMA cluster *via* distal, alternating and enzymatic pathways. All bond lengths are given in Å.

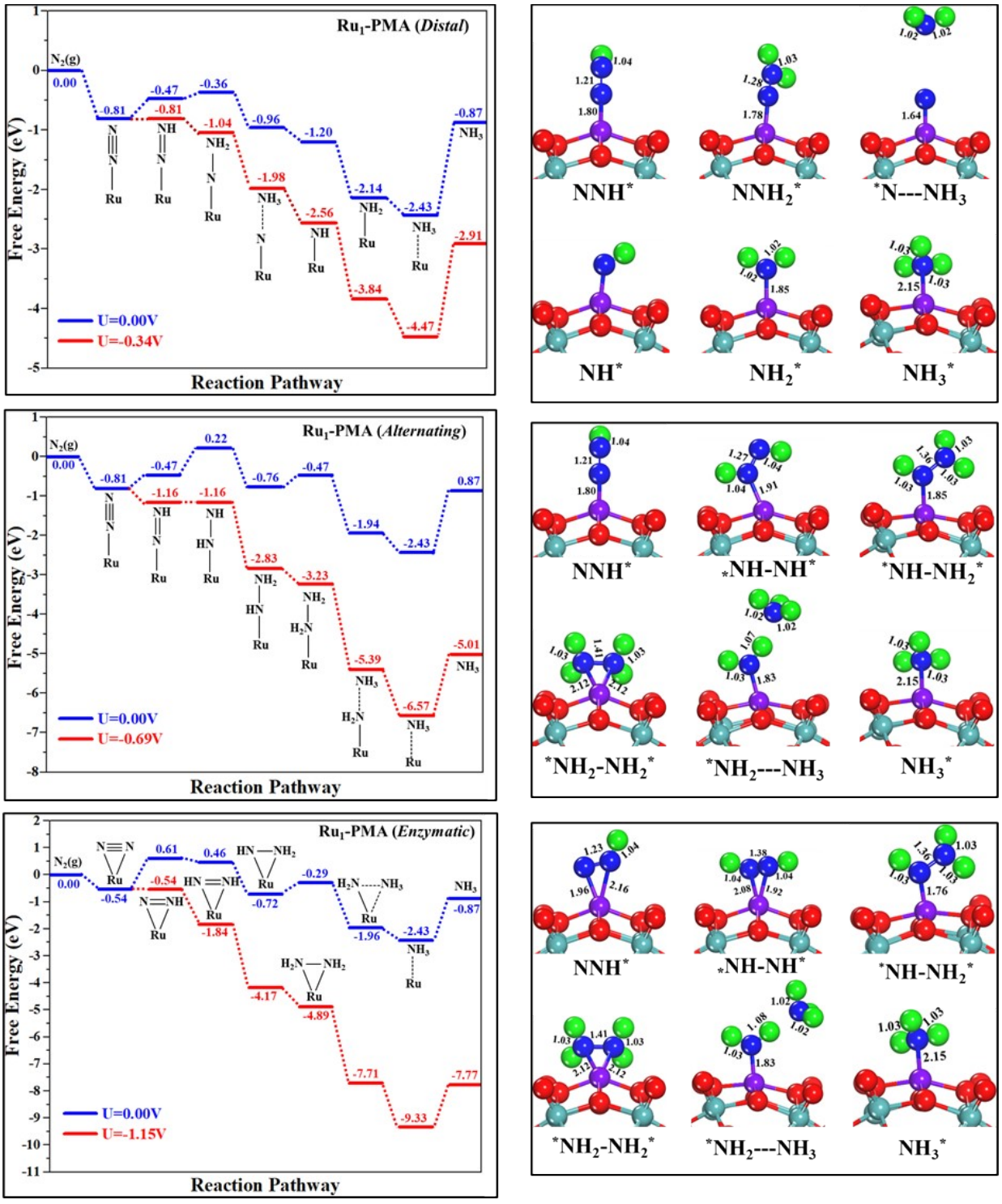

Fig. S8 (a) Free energy profiles for the eNRR on the Ru_1/PMA cluster at zero and applied potential (limiting potential) *via* distal, alternating and enzymatic pathways. (b) Optimized geometric structures of various elementary steps of the eNRR pathway using the Ru_1/PMA cluster *via* distal, alternating and enzymatic pathways. All bond lengths are given in Å.

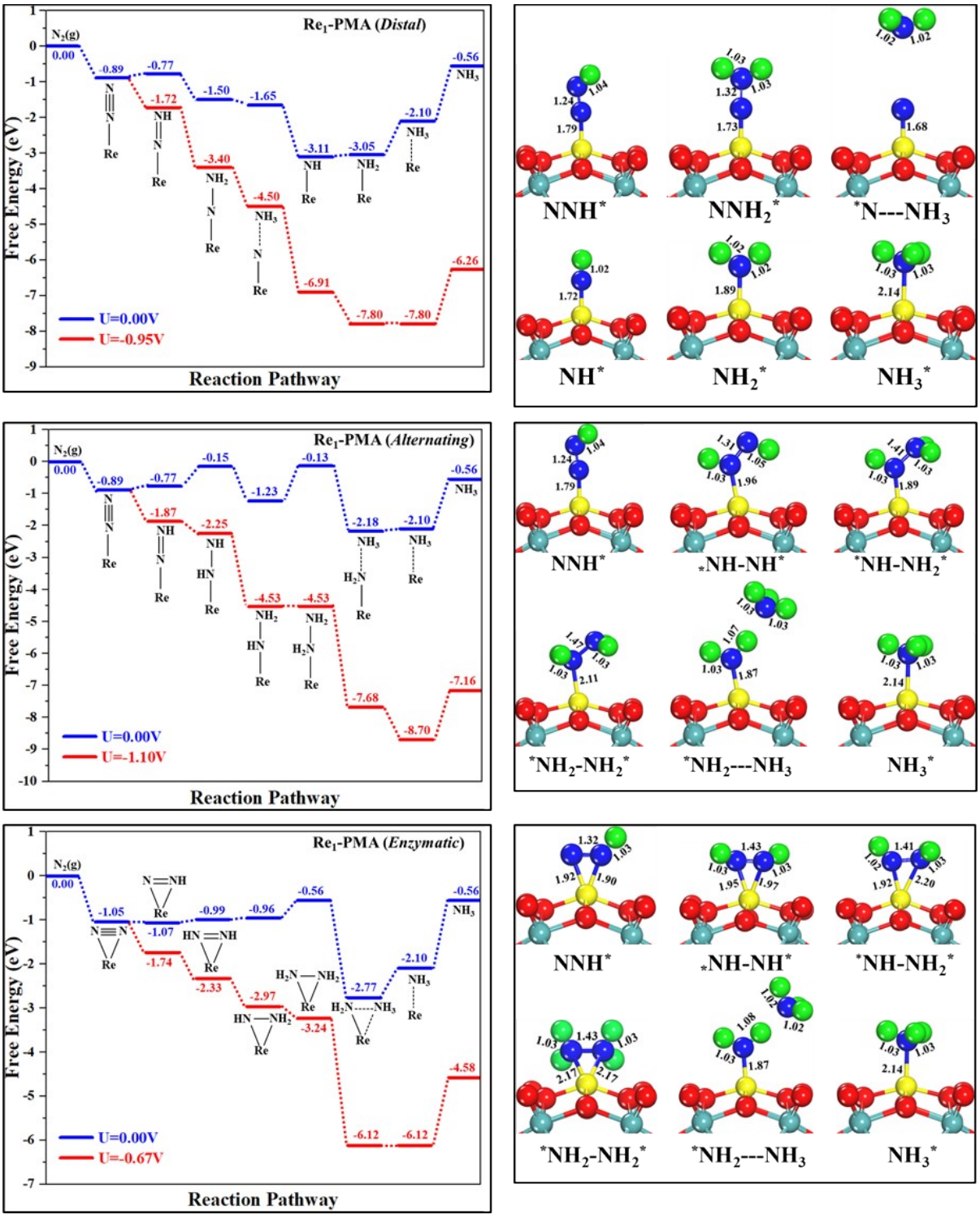

Fig. S9 (a) Free energy profiles for the eNRR on the Re_1/PMA cluster at zero and applied potential (limiting potential) *via* distal, alternating and enzymatic pathways. (b) Optimized geometric structures of various elementary steps of the eNRR pathway using the Re_1/PMA cluster *via* distal, alternating and enzymatic pathways. All bond lengths are given in Å.

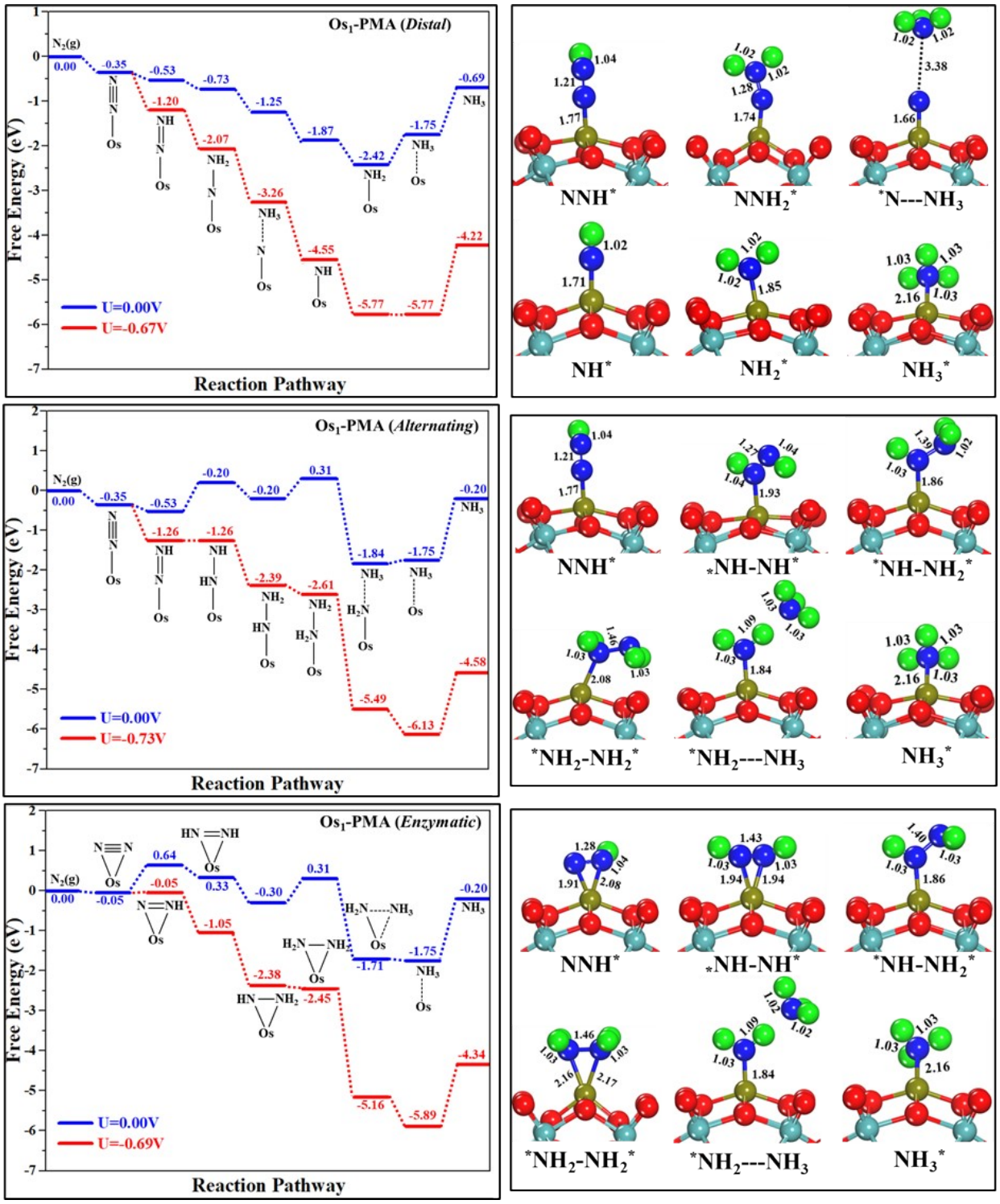

Fig. S10 (a) Free energy profiles for the eNRR on the Os_1/PMA cluster at zero and applied potential (limiting potential) *via* distal, alternating and enzymatic pathways. (b) Optimized geometric structures of various elementary steps of the eNRR pathway using the Os_1/PMA cluster *via* distal, alternating and enzymatic pathways. All bond lengths are given in Å.

Table S3. Free energy (ΔG) for the electrocatalytic nitrogen reduction reaction (eNRR) in each elementary step on the Mo_1/PMA cluster through distal, alternating and enzymatic pathways, respectively. All energies in eV.

S. No:	System	Distal (eV)	Alternating (eV)	Enzymatic (eV)
1	PMAMo-N≡N	-0.64	-0.64	-0.59
2	PMAMo-N-NH,	-0.19	-0.19	-0.56
3	PMAMo-N-NH_2, PMAMo-NH-NH	-0.99	0.15	-0.78
4	PMAMo-N-NH_3, PMAMo-NH-NH_2	-0.56	-0.89	-1.18
5	PMAMo-NH, PMAMo-NH_2-NH_2	-2.35	-0.25	-0.83
6	PMAMo-NH_2, PMAMo-NH_2-NH_3	-2.86	-2.56	-2.56
7	PMAMo-NH_3	-2.38	-2.38	-2.38

Table S4. Bader charge variation of the three moieties (shown in Figure 12) along distal, alternating and enzymatic pathways respectively. The numbers 1, 2 and 3 represent the moiety 1, moiety 2 and moiety 3 respectively.

System	Distal Pathway			Alternating Pathway			Enzymatic Pathway		
	1	2	3	1	2	3	1	2	3
PMAMo-N≡N	-1.85	2.69	-0.25	-1.85	2.69	-0.25	-1.85	2.68	-0.66
PMAMo-N-NH,	-1.85	2.95	-0.80	-1.85	2.95	-0.80	-1.85	2.95	-0.91
PMAMo-N-NH_2, PMAMo-NH-NH	-1.85	3.09	-1.32	-1.85	2.83	-1.09	-1.85	3.32	-1.38
PMAMo-N-NH_3, PMAMo-NH-NH_2	-1.85	3.63	-2.03	-1.85	2.95	-1.68	-1.85	2.96	-1.68
PMAMo-NH, PMAMo-NH_2-NH_2	-1.85	3.20	-2.03	-1.85	2.57	-1.92	-1.85	2.56	-1.88
PMAMo-NH_2, PMAMo-NH_2-NH_3	-1.85	3.13	-2.57	-1.85	3.12	-2.74	-1.85	3.08	-2.71
PMAMo-NH_3	-1.85	2.61	-2.89	-1.85	2.61	-2.89	-1.85	2.61	-2.89

Table S5. The calculated bond length of the adsorbed N_2 molecule in the distal, alternating, and enzymatic pathway, respectively. All bond lengths are given in Å.

S. No:	System	Distal (Å)	Alternating (Å)	Enzymatic (Å)
1	Free N_2	1.11	1.11	1.11
2	Mo-N≡N	1.13	1.13	1.21
3	Mo-N-NH,	1.23	1.23	1.29
4	Mo-N-NH_2, Mo-NH-NH	1.30	1.31	1.38
5	Mo-N-NH_3, Mo-NH-NH_2	3.60	1.40	1.40
6	Mo-NH_2-NH_2	--	1.47	1.43
7	Mo-NH_2-NH_3	--	2.77	2.77

Table S6. Calculated magnetic moments (in μ_B) of Mo_1/PMA, side-on and end-on N_2 adsorption and all the elementary steps involved in the distal, alternating, and enzymatic reaction pathways for the Mo_1/PMA cluster.

S. No:	System	(μ_B)	Distal (μ_B)	Alternating (μ_B)	Enzymatic (μ_B)
1	PMA-Mo	1.54	---	---	---
2	Mo-N≡N(side-on)	0.61	---	---	---
3	Mo-N≡N(end-on)	0.58	---	---	---
4	Mo-N-NH,	---	0.59	0.59	0.013
5	Mo-N-NH_2, Mo-NH-NH	---	0.30	1.10	0.052
6	Mo-N-NH_3, Mo-NH-NH_2	---	-0.00	0.00	0.00
7	Mo-NH_2-NH_2, Mo-NH	---	0.39	1.32	0.68
8	Mo-NH_2-NH_3, Mo-NH_2	---	0.80	0.75	0.75
9	Mo-----NH_3	---	1.37	1.37	1.37

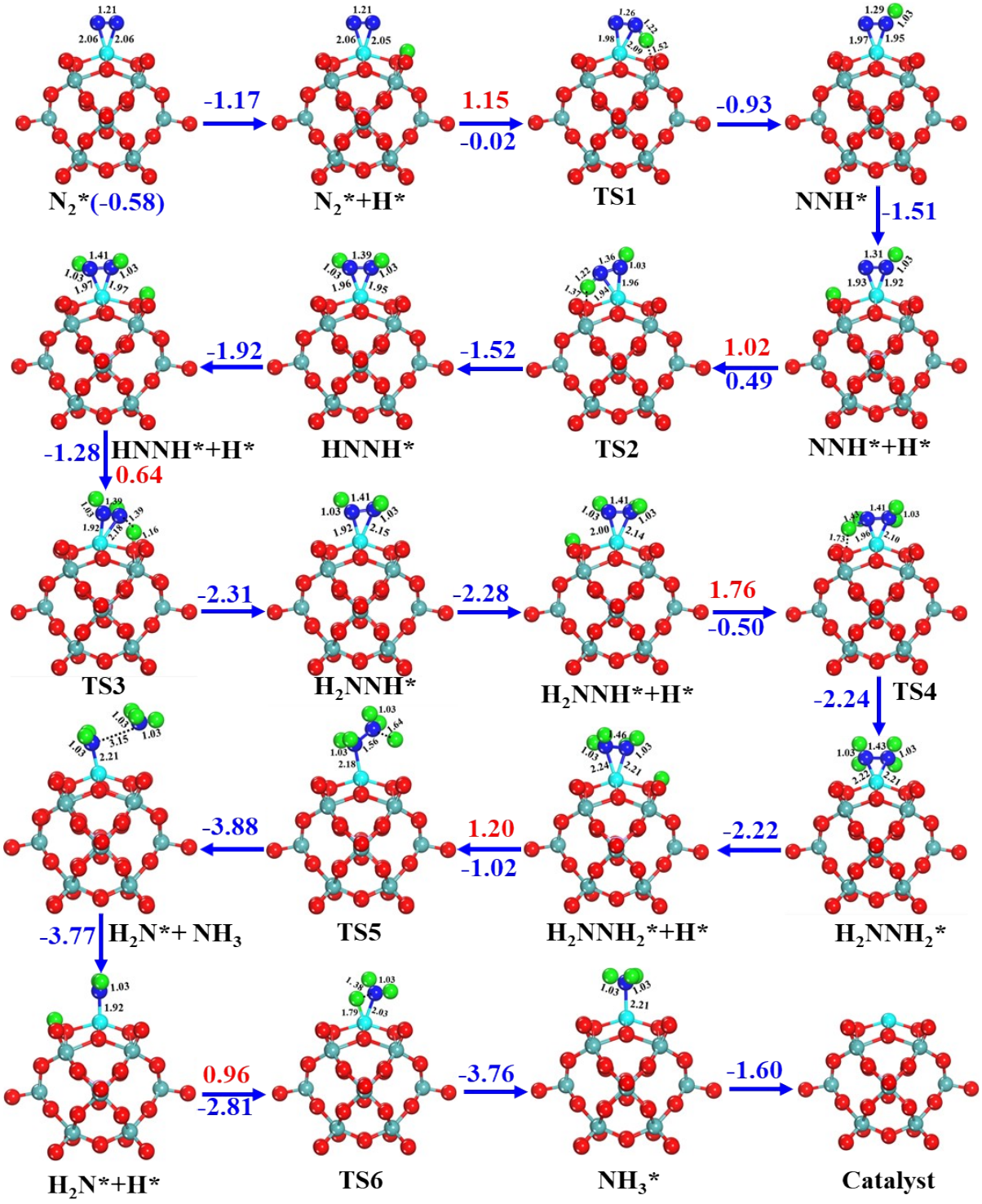

Fig S11. Minimum kinetic reaction energy profile along the six-repeated proton coupled electron transfer steps on the Mo_1/PMA cluster for eNRR. The arrows represent the total energy difference between the prior and latter configurations. All the energies are measured in eV.

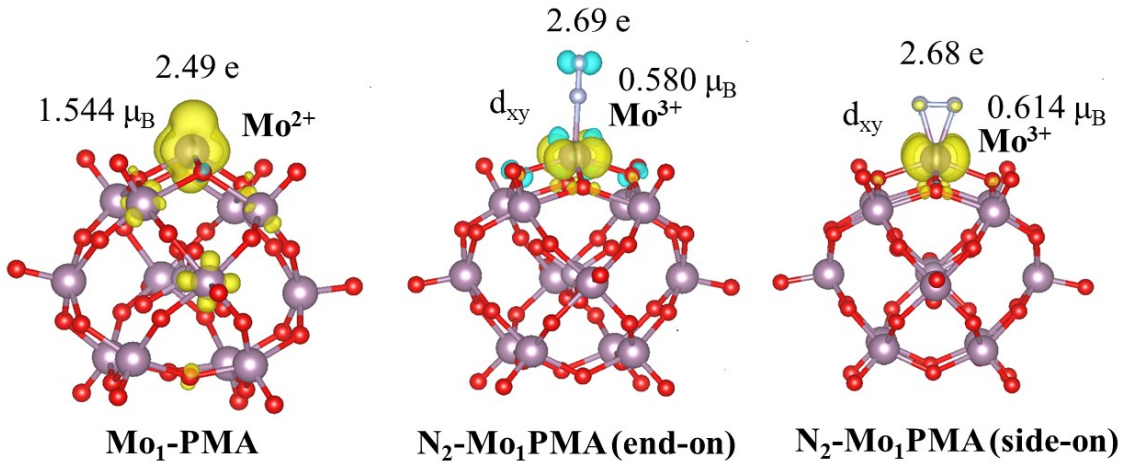

Fig. S12 Spin density localizations, oxidation states and magnetic moments of the Mo atom in the Mo_1/PMA cluster, end-on and side-on N_2 in Mo_1/PMA with the spin density population displayed in yellow and aqua.

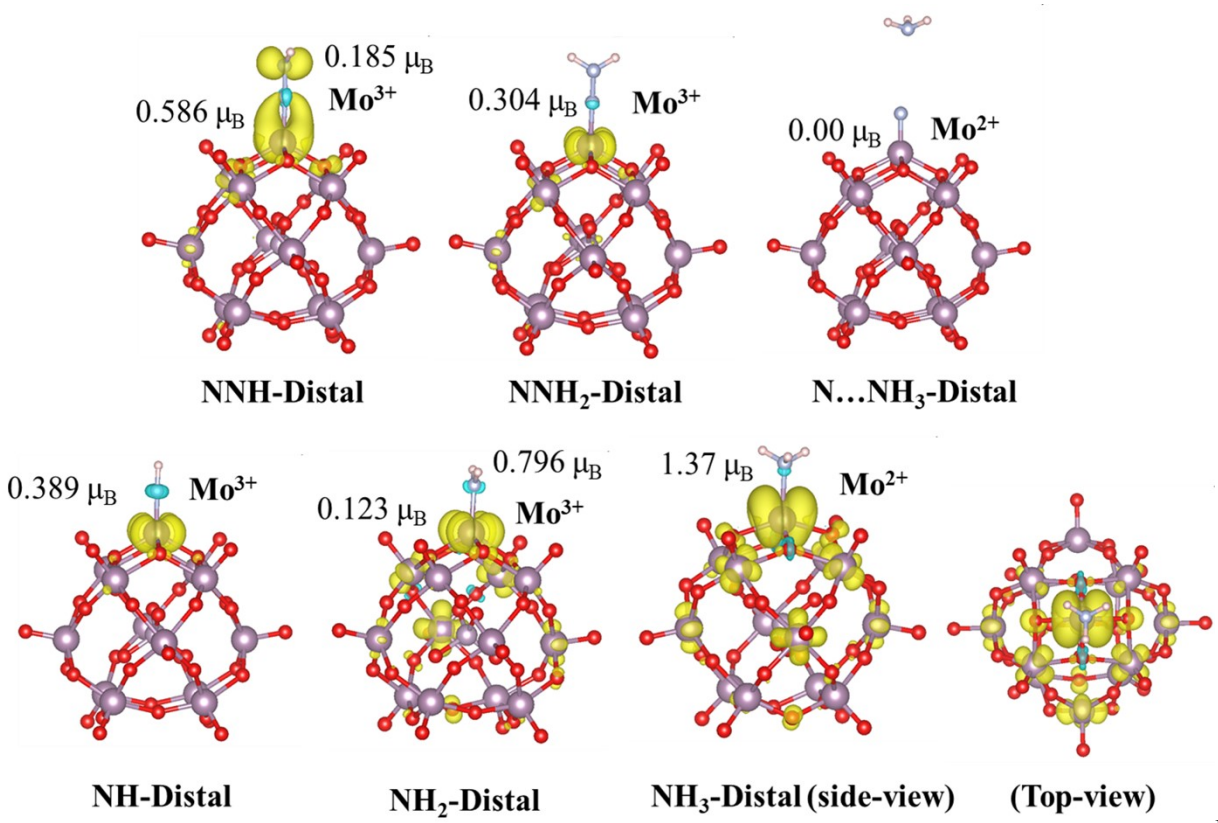

Fig. S13 Spin density localizations, oxidation states and magnetic moments of all the elementary steps involved in the eNRR *via* distal pathway in the Mo_1/PMA cluster, with the spin density population displayed in yellow and aqua.

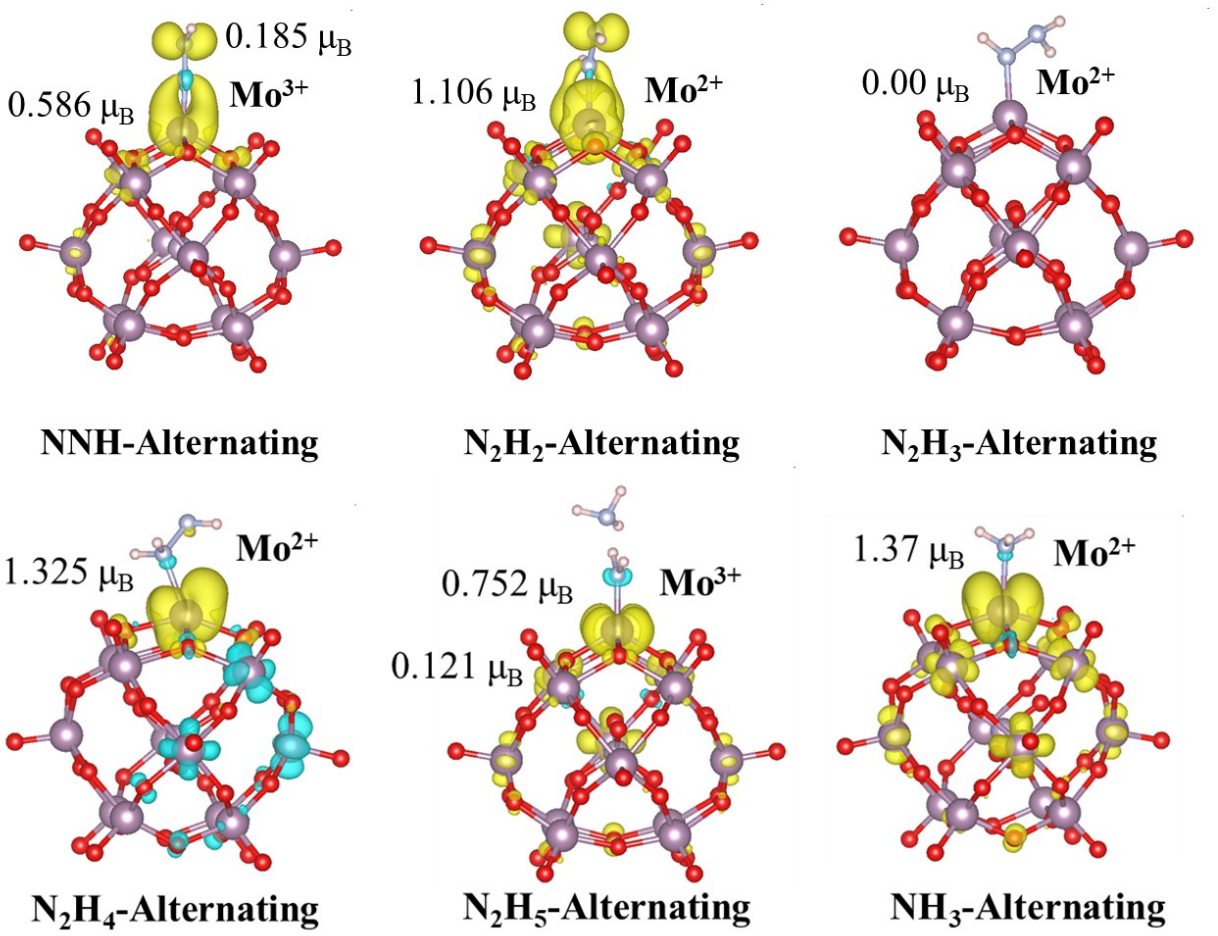

Fig. S14 Spin density localizations, oxidation states and magnetic moments of all the elementary steps involved in the eNRR *via* the alternating pathway in the Mo_1/PMA cluster with the spin density population displayed in yellow and aqua.

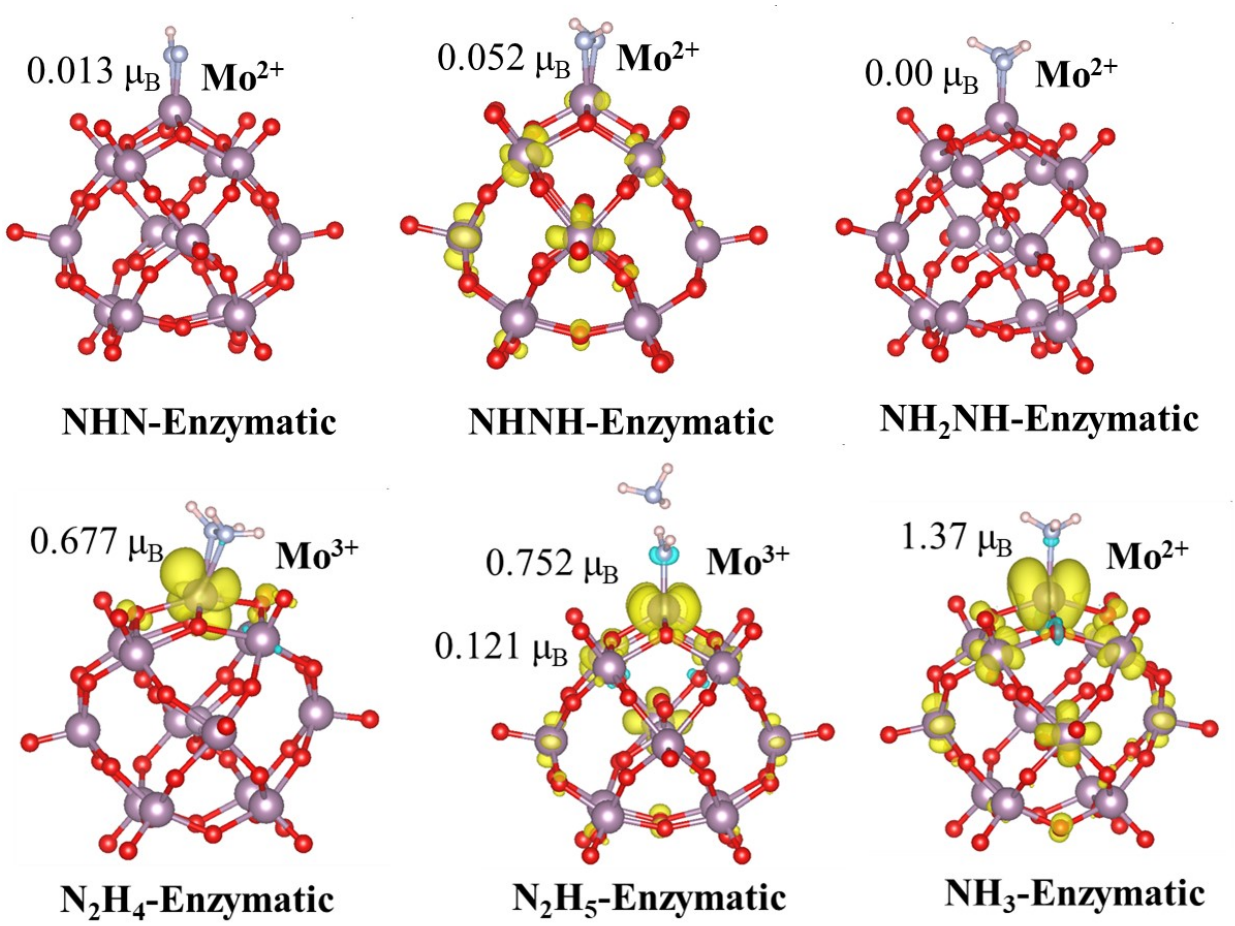

Fig. S15 Spin density localizations, oxidation states and magnetic moments of all the elementary steps involved in the eNRR *via* enzymatic pathway in the Mo_1/PMA cluster with the spin density population displayed in yellow and aqua.

Table S7. Cartesian coordinates of the optimized structures of PMA, Mo embedded on PMA, N_2 adsorption on end on and side on configuration on Mo_1/PMA, and some important intermediate of distal, alternating, and enzymatic pathway electronic structure calculations, respectively.

PMA

Atoms	X	Y	Z
Mo1	0.6004507782000912	0.5910690247711883	0.4773146750859993
Mo2	0.3955550096480173	0.3849516739404045	0.4735129248016574
Mo3	0.3952866656660536	0.5889338103694035	0.4661073138055101
Mo4	0.5975822570313800	0.3824943691773601	0.4637237251079169
Mo5	0.4985789300477186	0.5901658876976242	0.5722196566684188
Mo6	0.4986580909488713	0.3844739957058120	0.3665530424062711

Mo7	0.4924152656901493	0.3845650828580297	0.5720457271695932
Mo8	0.4901321380974201	0.5912285242220230	0.3655462556163796
Mo9	0.5976552169307480	0.4931371514030048	0.5740907198111178
Mo10	0.3953396365506542	0.4906167638740593	0.3677800305479547
Mo11	0.6004891275131676	0.4794260353927905	0.3658491153948285
Mo12	0.3955157174734014	0.4831299410612743	0.5717014312251146
O1	0.4391150335796674	0.4276438886853522	0.6055789494585937
O2	0.5592041887286991	0.5508832494929561	0.6041424050539496
O3	0.5575145322601843	0.4279731280697559	0.3327990246658185
O4	0.4396939052034403	0.5467719692637045	0.3321176321201884
O5	0.6349658022676639	0.4306392107550304	0.4127691259622212
O6	0.6349779457650994	0.5441895314787014	0.5260986975689819
O7	0.3642131616814516	0.5488995255720753	0.4077841268669524
O8	0.3635353089871834	0.4258483916048135	0.5308264154454798
O9	0.4396026231648273	0.6245949790622509	0.4099055726418995
O10	0.5574301193634568	0.6240270465093607	0.5287512222685201
O11	0.4389908788620250	0.3510806596176604	0.5291370959554936
O12	0.5592856963749936	0.3525359794223559	0.4058419917600669
O13	0.4503443582479147	0.4399440367193620	0.3478798333401341
O14	0.6483875663417178	0.6378476890684973	0.4656046324590285
O15	0.5465591871746568	0.5359852837969107	0.3506792359878689
O16	0.3480929091806671	0.3377202267901231	0.4622431342989803
O17	0.6463619355840358	0.3364667214361743	0.4747939065251625
O18	0.4507131285098858	0.5348935570293660	0.5910114842437901
O19	0.3478676513397422	0.6363242857085700	0.4769743710012189
O20	0.5454403195061561	0.4407866102354066	0.5902633549476214
O21	0.6484470997452638	0.4910791297408959	0.3190812190815028
O22	0.4502776605189021	0.6088843648101689	0.5167148403905679
O23	0.5465062919813707	0.6061564306471616	0.4207640436777172
O24	0.3480481681057644	0.4943775110845605	0.6189338198165443
O25	0.3479345904670321	0.4797362172429768	0.3203778264651084
O26	0.5453418152771827	0.3661922427552254	0.5159028478912019
O27	0.4507983592691726	0.3656244043434518	0.4218598385160821
O28	0.6463947629001847	0.4820741092825604	0.6201670683680642
O29	0.5030901319930547	0.6384077771417600	0.3183345327040095
O30	0.6145571167117171	0.4394733176536457	0.5172710380270460
O31	0.6147524802940234	0.5374041522753926	0.4194091476230505
O32	0.5051392203270151	0.3374792621918672	0.6192879618061529
O33	0.3776641933160077	0.4401430058975733	0.4225028206980664
O34	0.4874124882055464	0.6379340149755591	0.6192423696524919
O35	0.4875453996242676	0.3374737910134870	0.3187578654304770
O36	0.3776085893737375	0.5341864240923097	0.5165291720999001

O37	0.5329468315667212	0.5233786473504605	0.5055058218337452
O38	0.4621682169281225	0.4514840890357925	0.5051814172150718
O39	0.4618885828273691	0.5230685153606842	0.4336362675303894
O40	0.5329701015465651	0.4512080718469431	0.4333613926415694
P1	0.4978225760998276	0.4873661694661157	0.4693318393185339

Mo_1/PMA

Atoms	X	Y	Z
Mo1	0.5835306770456872	0.3975168103016311	0.4892474994014851
Mo2	0.4124783432643419	0.5357558102607152	0.2999369394560001
Mo3	0.4253773595662391	0.5484532811706462	0.4983994951583136
Mo4	0.5707290489355487	0.4057617513438647	0.2915775155351183
Mo5	0.4354426057871273	0.3879781789379958	0.4986486479521874
Mo6	0.5625476362862163	0.5451017397663871	0.2903459820110121
Mo7	0.4224124857101655	0.3965755950407630	0.3008090593271617
Mo8	0.5736764577217318	0.5580089218482475	0.4891042790145365
Mo9	0.5078394977724952	0.3247952499795244	0.3994648954171086
Mo10	0.4892256177497126	0.6184066241335120	0.3969800656368679
Mo11	0.6448103412640330	0.4813907177972892	0.3806380565533699
Mo12	0.3512896812012332	0.4626496801251463	0.3993321425041563
Mo13	0.5087638816733102	0.4731481063880657	0.5619778612729143
O1	0.3594789868901899	0.4101881360560836	0.3457354066872450
O2	0.4582599016345656	0.3282836813726110	0.4616015390345159
O3	0.6297107996864278	0.5351895004539460	0.3298951353038209
O4	0.5453324219520587	0.6170153489339788	0.4564648995498736
O5	0.6366818333118826	0.4275601298415682	0.3286114604059743
O6	0.5640684575901942	0.3350617599576145	0.4550996515537773
O7	0.4416115357773456	0.6103879925545279	0.4630247208720414
O8	0.3529194020827994	0.5176955601283842	0.3473066063753655
O9	0.5026813875005499	0.5468308168081185	0.5373993390358678
O10	0.5117724169700245	0.3990600514314044	0.5373452157613758
O11	0.4055332661976188	0.4668135792395879	0.2694334289713876
O12	0.5749416647594657	0.4773170199415180	0.2589379627355640
O13	0.5410028349822558	0.5946899183881804	0.3490445152222040
O14	0.6267449305926626	0.3758755820318875	0.5372558037025619
O15	0.6189910246643369	0.5331367570972005	0.4377765055358927
O16	0.3823270557812297	0.5758797302387919	0.2541513600167189
O17	0.5951039074063751	0.3660263791166440	0.2421669374061061
O18	0.3837845676248545	0.4127004245395094	0.4526533901735161
O19	0.3886934635868635	0.5698857554306394	0.5517538070133955

O20	0.4512887464030001	0.3494714896919298	0.3537598572078842
O21	0.7121740895491973	0.4856445084244345	0.3883219825114855
O22	0.4402397612955282	0.4685788937225792	0.5274273647523416
O23	0.5724547313502197	0.4771749073957173	0.5191289507028528
O24	0.2854298855598103	0.4584613586287241	0.4153901586091190
O25	0.4842092552777980	0.6851577537213082	0.3851027007869337
O26	0.4951666891510860	0.4071236575060208	0.2777679640465357
O27	0.4867859955716495	0.5393672202151836	0.2802602616884095
O28	0.5113809296882164	0.2581286937211351	0.3875800579401654
O29	0.6139365221759883	0.5845959116019834	0.5373049867063920
O30	0.5550508937710594	0.3560617688169996	0.3475234738053848
O31	0.6256205973312836	0.4282127598889476	0.4376131139419562
O32	0.3973600013983616	0.3538598902982384	0.2543258721688997
O33	0.4352316315071073	0.5880223271827187	0.3556894266324626
O34	0.4013330329545182	0.3611358955257677	0.5511269228575248
O35	0.5814359563282593	0.5882341419728840	0.2413756293558849
O36	0.3773558918213403	0.5177894775101183	0.4529761197747064
O37	0.5041630591739128	0.4217933003797302	0.4369391210473382
O38	0.4458232079444134	0.4685602172329343	0.3686732605457663
O39	0.4976801958410060	0.5230005074227299	0.4366505662820199
O40	0.5470746492124817	0.4750719784321852	0.3622611373657887
P1	0.4986306197242234	0.4721626510517455	0.4002611736726880

PMAMo$_1$_N$_2$ end-on configuration

Atoms	X	Y	Z
Mo1	0.4336277683097793	0.5765236631911772	0.4316040271470972
Mo2	0.5663482101268017	0.4132347554594825	0.2325419575906164
Mo3	0.5657257540120162	0.4023810898849734	0.4317581771692494
Mo4	0.4264419806937162	0.5628007270828675	0.2327857628144439
Mo5	0.5783008908198644	0.5668615521048299	0.4298215686589712
Mo6	0.4161441532619631	0.4244039857897037	0.2341181471907055
Mo7	0.5766518546152591	0.5521519531730285	0.2314903587291136
Mo8	0.4217334838386679	0.4135019881944672	0.4331017066648913
Mo9	0.5089835381100665	0.6366436676413402	0.3326498323670212
Mo10	0.4874823323548570	0.3413783012810091	0.3354042947981739
Mo11	0.3534485270883841	0.4995968223821197	0.3315281221567173
Mo12	0.6440816458824375	0.4779776532680477	0.3263843626374457
Mo13	0.5003488469539384	0.4912465273083180	0.4994909230648498
O1	0.6402558692606986	0.5321965839463647	0.2748303478676061

O2	0.5619478309170322	0.6286235297942785	0.3943638866554373
O3	0.3560201472154145	0.4454303170538586	0.2761095479634986
O4	0.4369073066957895	0.3508739248148560	0.3972500371708789
O5	0.3638230084863201	0.5515935195183016	0.2750263623491097
O6	0.4575913523968145	0.6356072066796057	0.3944705770702748
O7	0.5410190125363358	0.3429333405160824	0.3972702182562138
O8	0.6322576511772435	0.4241377784157104	0.2757790864638188
O9	0.4944496478296334	0.4128937604407816	0.4755623270727961
O10	0.5061413506960193	0.5683023482973486	0.4743038244879149
O11	0.5831883049360018	0.4814918137277066	0.2011358439524496
O12	0.4148625447426917	0.4937271513594330	0.2005105206735564
O13	0.4371614399306438	0.3723370375604371	0.2893093614106884
O14	0.3960027675867522	0.6026643605382529	0.4820355722236374
O15	0.3764014409751384	0.4448523128400366	0.3837640680806696
O16	0.5881857312925922	0.3696470974167966	0.1852085798402854
O17	0.4046986158425878	0.6053486738729497	0.1845059318546324
O18	0.6216766055030665	0.5331853865030278	0.3817114033586361
O19	0.6043721776957279	0.3777652331927326	0.4822971257821936
O20	0.5600976248101892	0.6043841957744926	0.2879706205885076
O21	0.2870244223201504	0.5045878115534921	0.3444547048817164
O22	0.5638861008603702	0.4856653614917192	0.4598926409182612
O23	0.4360129301832305	0.4946408849771267	0.4597661699895437
O24	0.7106785579603674	0.4731159899204379	0.3392142750619673
O25	0.4828213152914476	0.2747260310270957	0.3231202212104809
O26	0.5027962935020183	0.5548354130686493	0.2161095488435931
O27	0.4928579426631457	0.4208536773930329	0.2173758718899204
O28	0.5138692244572711	0.7030204994097394	0.3190690942684119
O29	0.3807720619604918	0.3941687231745422	0.4840063105528052
O30	0.4547843784294376	0.6123253901143342	0.2869708353503558
O31	0.3841247897922757	0.5513635524223369	0.3827912820759019
O32	0.6046225600510570	0.5911979201758535	0.1834222268563062
O33	0.5425774850055585	0.3650004580831800	0.2901866862396787
O34	0.6201523887568452	0.5867081989375329	0.4799105073777148
O35	0.3883511023707847	0.3845382510039085	0.1866608722260551
O36	0.6135742904481013	0.4284888233347985	0.3829242514929561
O37	0.5027648651316550	0.5400091593880932	0.3735732096711890
O38	0.5486368052484086	0.4850619029166845	0.3019132694942135
O39	0.4952438579679156	0.4385583156368846	0.3742986452594429
O40	0.4475123649660329	0.4925397193421446	0.3032129530871419
N1	0.5078046527971317	0.4871866594988168	0.5821526742394828
N2	0.5106892221307078	0.4857105759584099	0.6273911260083019
P1	0.4985627731111358	0.4890282571467534	0.3375581668924664

PMAMo_N_2 Side-on configuration

Atoms	X	Y	Z
Mo1	0.4347194987915273	0.5764939406817842	0.4326529202867770
Mo2	0.5673560190648803	0.4134164726288191	0.2325878541873153
Mo3	0.5647260395849067	0.4028595351083218	0.4326991973231598
Mo4	0.4279094037587692	0.5627336171747712	0.2329212524992320
Mo5	0.5771279556531167	0.5663023567426482	0.4309007965950196
Mo6	0.4175063542000587	0.4244495814594870	0.2341644010010745
Mo7	0.5777868754568126	0.5516868730142257	0.2315680147183142
Mo8	0.4225409699098581	0.4132389265891770	0.4339495775460894
Mo9	0.5094414751968506	0.6360752379223057	0.3330481898791166
Mo10	0.4879031793451801	0.3417361013845316	0.3355996972434616
Mo11	0.3541425402005772	0.4996059373800726	0.3307926386647951
Mo12	0.6431568622869258	0.4779714579532987	0.3279075073501846
Mo13	0.5007665501752657	0.4905190346213978	0.5018976649895722
O1	0.6400078924350258	0.5319437799003724	0.2744423884062651
O2	0.5618376522007419	0.6282176606681601	0.3940127145457517
O3	0.3562137977949683	0.4448325534564282	0.2781678586382754
O4	0.4369789658766040	0.3507514173545480	0.3975939258018381
O5	0.3640777758573068	0.5522355342486743	0.2771161792879843
O6	0.4576000537202762	0.6355764784483035	0.3951148966469172
O7	0.5411272492872968	0.3432406692831294	0.3965219520132022
O8	0.6321065242750342	0.4245777752157728	0.2751885604839521
O9	0.4943013416647808	0.4102078679097208	0.4739894984375402
O10	0.5062439623605426	0.5700820394359021	0.4723910929062621
O11	0.5824096987134313	0.4815963229833991	0.2000131069024970
O12	0.4120874570028146	0.4940731723250998	0.2017305020870618
O13	0.4368103020980767	0.3725673207156402	0.2901815920142795
O14	0.3960953620146526	0.6022038623863279	0.4824567431635781
O15	0.3778387729235616	0.4457336301767348	0.3847943449534582
O16	0.5889109322467018	0.3699526870015271	0.1850861611517854
O17	0.4053256219321961	0.6055021532258912	0.1852707604539816
O18	0.6207252678471651	0.5329423284004363	0.3813480043174832
O19	0.6044462281351441	0.3779546528641530	0.4820480658221251
O20	0.5595974281944701	0.6044864879045090	0.2870996951582597
O21	0.2877907614376818	0.5045651260115837	0.3444938868760493
O22	0.5633130008841795	0.4855595907718573	0.4596875919004832
O23	0.4369444973430585	0.4944051605843727	0.4612868033813126
O24	0.7097738080731990	0.4731554655562836	0.3403055086104880
O25	0.4829717199487035	0.2751201691968375	0.3233423373644597

O26	0.5024296930402340	0.5550858691575992	0.2160129266420198
O27	0.4924502286859082	0.4208388736736603	0.2170921590158912
O28	0.5140783708406272	0.7024897523867598	0.3196184491242162
O29	0.3807622137892845	0.3941298419362158	0.4841678914344576
O30	0.4542746483304479	0.6121729848762939	0.2881854945970819
O31	0.3856010752408313	0.5499104036762361	0.3839417443119912
O32	0.6054374153173813	0.5907828278697231	0.1834378505197050
O33	0.5421056764463921	0.3649308700946441	0.2891655033688439
O34	0.6200011189400113	0.5860600135045808	0.4799347958658042
O35	0.3888631941168947	0.3846666348036487	0.1871858288808169
O36	0.6128402888778463	0.4286551842000834	0.3824543048873686
O37	0.5029076539169259	0.5400824252018404	0.3718771984973421
O38	0.5487891765452231	0.4848845129869022	0.3006057823270702
O39	0.4953601570166158	0.4384257342909904	0.3728694535727908
O40	0.4479553709961128	0.4923470210527475	0.3016122374020335
N1	0.5044729208400776	0.5159465856020190	0.5801891381169632
N2	0.5011020064854116	0.4677633890527831	0.5811293258519832
P1	0.4987488286814264	0.4889339419467602	0.3366160999742144

PMAMo_N-NH (Distal)

Atoms	X	Y	Z
Mo1	0.4340847270356570	0.5747192369270054	0.4347304052518348
Mo2	0.5667116724856389	0.4138239002409624	0.2331206663736690
Mo3	0.5655290916453234	0.4051077626206891	0.4345403754182196
Mo4	0.4279688722594533	0.5623522673134408	0.2330350974323582
Mo5	0.5800526693930709	0.5666351684770394	0.4307901428094063
Mo6	0.4165108545145884	0.4241838842105490	0.2359818704139842
Mo7	0.5777025448859271	0.5523459848853983	0.2330373101899166
Mo8	0.4199137909823077	0.4135149444874796	0.4338568222231515
Mo9	0.5083340222660893	0.6355286916340565	0.3347369049532774
Mo10	0.4887401095312194	0.3424702986039991	0.3373159275359179
Mo11	0.3534185459591308	0.5011190489724027	0.3316885314395294
Mo12	0.6443036110990946	0.4772629993974818	0.3277880995614254
Mo13	0.4997665965144077	0.4915728542102132	0.4988308731903340
O1	0.6405717507300960	0.5315318138559693	0.2750822599940184
O2	0.5617569498764302	0.6281182655079446	0.3948148438064244
O3	0.3559165661850291	0.4452881260173962	0.2786543893041637
O4	0.4373163744928547	0.3510394883197497	0.3992444131007607
O5	0.3639100235004856	0.5519666377662383	0.2761732827189063
O6	0.4570503196441285	0.6336449718717476	0.3961027638279340
O7	0.5413813186471532	0.3453987330769398	0.3992594555893830

O8	0.6322430563593617	0.4240273100425289	0.2760741163312128
O9	0.4929791016669537	0.4135390840623889	0.4762378285877903
O10	0.5078168937270794	0.5687279378968895	0.4739162391882269
O11	0.5826718211223814	0.4816648016832312	0.2013647876286482
O12	0.4132050866407891	0.4932155088909702	0.2021413991736160
O13	0.4371524957442355	0.3725894494245248	0.2919530426631416
O14	0.3963645660639504	0.6024239683571040	0.4840762998890944
O15	0.3753082827318751	0.4448939569255359	0.3846612653514599
O16	0.5879818893601337	0.3700175596407435	0.1857453304401892
O17	0.4060289217849724	0.6049073893417896	0.1848595414236465
O18	0.6230769799137238	0.5334308275403451	0.3816597538604460
O19	0.6040303428657895	0.3794091951726228	0.4845094127868297
O20	0.5594433133990552	0.6040281068900694	0.2885089594469658
O21	0.2869685987763211	0.5066863677794351	0.3445200100677575
O22	0.5674799897557041	0.4873670061639090	0.4625704337275404
O23	0.4317980489604279	0.4938751301129908	0.4624826584987303
O24	0.7109456756929943	0.4717692057741379	0.3398510487533944
O25	0.4845791645527445	0.2756258026734968	0.3258111711616402
O26	0.5029103053367207	0.5544064581381181	0.2164726262433898
O27	0.4923116036722051	0.4205104352060072	0.2187417136468204
O28	0.5124063488682961	0.7020340998878613	0.3215822456732621
O29	0.3789547185299005	0.3929981323967951	0.4842474890472891
O30	0.4543856926647278	0.6112846474346724	0.2883320113017044
O31	0.3845807757204516	0.5504309545724521	0.3842816514740786
O32	0.6054660667741916	0.5914953874186846	0.1849635195941636
O33	0.5427125069405916	0.3654936764041081	0.2911668401187392
O34	0.6225090224694088	0.5886718301436151	0.4792343517433540
O35	0.3881984960135802	0.3837968063933938	0.1892724381732863
O36	0.6136679809490277	0.4291164259697649	0.3840310105255928
O37	0.5032222749549580	0.5397294964408897	0.3738093097825727
O38	0.5488442243117631	0.4847749499386682	0.3021419647592455
O39	0.4950062232359131	0.4389443429477032	0.3748823973021480
O40	0.4478109425742318	0.4925392307811607	0.3031972033035636
N1	0.5039681419190528	0.4948248556667598	0.5716330934195990
N2	0.5035716436300969	0.5045431251433883	0.6201311080569500
P1	0.4987294815782344	0.4890268996627337	0.3378809344071717
H1	0.5066888010900581	0.4704743626838008	0.6439004293121481

PMAMo_N-NH_2 (Distal)

Atoms	X	Y	Z
Mo1	0.4354822184234035	0.5756182223688409	0.4344579233186187

Mo2	0.5667666123873522	0.4135849250614608	0.2330703932799047
Mo3	0.5669812277723019	0.4060036403253932	0.4343023183053441
Mo4	0.4274339622039970	0.5620031396574676	0.2333549026297027
Mo5	0.5806542706979159	0.5678725113584450	0.4296701199633156
Mo6	0.4168080160252104	0.4235837273132445	0.2370362039602067
Mo7	0.5773137954783970	0.5520910740894062	0.2317243004732829
Mo8	0.4215501743119978	0.4139512323336519	0.4349999888780902
Mo9	0.5086470828465340	0.6361243531618825	0.3333941748614550
Mo10	0.4896820402709205	0.3426037401087766	0.3383490367098237
Mo11	0.3538094550745222	0.5007189959395723	0.3325937965914468
Mo12	0.6444437019615180	0.4781575057737291	0.3270026621536368
Mo13	0.5023657759094886	0.4919697379802362	0.4983687408065317
O1	0.6400985701407308	0.5321382093231040	0.2733927180044442
O2	0.5621428153019546	0.6291730204023714	0.3933807663673151
O3	0.3560184962033727	0.4448906492149628	0.2802481228580385
O4	0.4387353678678914	0.3513591951769625	0.4002180907748852
O5	0.3636703530127778	0.5518550760851892	0.2775675155008286
O6	0.4577068854009119	0.6343944277353862	0.3957607291779562
O7	0.5431980678375855	0.3460230936738359	0.3988697573463986
O8	0.6323709057184005	0.4249167104349657	0.2747673435514861
O9	0.4949900220769099	0.4133267482968206	0.4760576532799062
O10	0.5090820986321709	0.5700458791342932	0.4739313113043643
O11	0.5815123462613978	0.4815823338936340	0.2003451907384000
O12	0.4120343871964447	0.4927978152368999	0.2032365688550122
O13	0.4376301869724319	0.3726335142574139	0.2929969698765192
O14	0.3980196106282329	0.6029548918043152	0.4843195118808586
O15	0.3766086530267837	0.4452143651957933	0.3861229820975184
O16	0.5877061913381358	0.3697286722290364	0.1855931911041463
O17	0.4047321386298899	0.6042473188771008	0.1852251325962373
O18	0.6236042813841549	0.5349127915624492	0.3801484423814905
O19	0.6063805969487224	0.3805469567899571	0.4836849881937478
O20	0.5590139589655813	0.6045772043588131	0.2869185369389108
O21	0.2874913269225280	0.5061725945772090	0.3463148874153710
O22	0.5693992001523972	0.4883422138912014	0.4611436939039975
O23	0.4338247483695102	0.4942350673653226	0.4636085448210057
O24	0.7112512707207355	0.4731720924294331	0.3384164862162659
O25	0.4855579163897212	0.2757193461633766	0.3271108097653753
O26	0.5019260142446397	0.5542810423266324	0.2161927307286928
O27	0.4919328440248313	0.4205411422079047	0.2188151907720025
O28	0.5123677502046589	0.7025953270185091	0.3198615816430728
O29	0.3808459399452072	0.3933519164374474	0.4855904507450109
O30	0.4538473522514377	0.6115050916740485	0.2883050169496652

O31	0.3856570286542282	0.5503670109221326	0.3852519407988182
O32	0.6043064911522433	0.5910170437466656	0.1830151171160630
O33	0.5429259711592452	0.3657500553488583	0.2908747669381487
O34	0.6233854111743464	0.5901841830016160	0.4778006206749758
O35	0.3881123297493683	0.3829699094544832	0.1907412912692388
O36	0.6146712155354594	0.4300221830918826	0.3828053204136109
O37	0.5038188982642001	0.5402786325757365	0.3736484971412223
O38	0.5490313125005136	0.4852793851024458	0.3017487661392851
O39	0.4960125324350630	0.4394009957526082	0.3750070317867051
O40	0.4479978801529808	0.4926265355648677	0.3036328636887108
N1	0.5049841136523177	0.4893892721344669	0.5690552067649650
N2	0.5059752966183875	0.4835595254267964	0.6206774386807172
P1	0.4992090260590989	0.4893870704130157	0.3378961767621231
H1	0.4713644275126821	0.4885305856314551	0.6417261098082082
H2	0.5415092512461633	0.4882599895865166	0.6402094312968798

PMAMo_N…. NH_3 (Distal)

Atoms	X	Y	Z
Mo1	0.4319871855635158	0.5739823754903547	0.4338575748857871
Mo2	0.5673869609366099	0.4135779498465558	0.2332170225057446
Mo3	0.5675489167845795	0.4049529344371137	0.4335970838954202
Mo4	0.4279234063601779	0.5627184340411182	0.2336671877644836
Mo5	0.5791193051866288	0.5632436987111005	0.4323610341466709
Mo6	0.4176707196830912	0.4245261150692491	0.2347566648880298
Mo7	0.5776502768472317	0.5517894090036728	0.2322762316731732
Mo8	0.4204418213270646	0.4157505746863505	0.4349879360686515
Mo9	0.5093052850871700	0.6340238617695394	0.3355212393681842
Mo10	0.4881333190436093	0.3436326460387286	0.3376380146179773
Mo11	0.3523907096049948	0.4995506533196376	0.3302256284098211
Mo12	0.6449340701965728	0.4780251709433066	0.3273378458400230
Mo13	0.5004752701203197	0.4899341457647751	0.4987747094201636
O1	0.6406682550041118	0.5319205108263400	0.2742848131527820
O2	0.5617079119807149	0.6251582001012598	0.3958806914004837
O3	0.3555669985366593	0.4449180000458026	0.2778648924817245
O4	0.4370613885009410	0.3533329236441466	0.3990193481001120
O5	0.3634323586246653	0.5521976737639626	0.2770061603187857
O6	0.4574382032914813	0.6327915835739223	0.3969765781881969
O7	0.5413207426077261	0.3457291861541675	0.3979681616968115
O8	0.6327535771323592	0.4246655927884032	0.2750539140782849
O9	0.4945824696025291	0.4126702473238265	0.4750341222176175
O10	0.5058377589720207	0.5668490869292291	0.4737905423103883

O11	0.5824091728458759	0.4817272297344049	0.2004255402101642
O12	0.4121791134336651	0.4941403715657636	0.2021141506655935
O13	0.4369398004455096	0.3735797851980532	0.2913220004817531
O14	0.3946034849682540	0.6027414334762528	0.4828326731436210
O15	0.3754774586797849	0.4457578479493416	0.3847664487230094
O16	0.5886615299438523	0.3698009932975161	0.1858465484743796
O17	0.4056668541121656	0.6058804799408470	0.1861918626123900
O18	0.6230140554019866	0.5325497924052383	0.3815739284474634
O19	0.6059953567689160	0.3767538195962364	0.4820639281091520
O20	0.5595076785309910	0.6034409176969912	0.2885177741849228
O21	0.2858452796892680	0.5045075589837934	0.3428522631809299
O22	0.5710842407594846	0.4845074105764128	0.4625212961963002
O23	0.4291494984625737	0.4948842852513836	0.4638440599346644
O24	0.7117210762868121	0.4732054263385804	0.3386701488562013
O25	0.4831514700348442	0.2767991116103990	0.3264551629488185
O26	0.5024084229309084	0.5551236252533502	0.2165590972253409
O27	0.4925357770250296	0.4209555600428116	0.2175708408807376
O28	0.5140321204304245	0.7006934703337163	0.3233176985801531
O29	0.3793136075734847	0.3934351003296240	0.4843193962748604
O30	0.4542709651899651	0.6111309323033087	0.2895744301916330
O31	0.3830547400138852	0.5501287085025605	0.3840088576652441
O32	0.6050239371656495	0.5913090928586360	0.1843035402364253
O33	0.5421847024204418	0.3659108672538234	0.2902763298053838
O34	0.6213017878341685	0.5862670157434737	0.4804589674843018
O35	0.3893261983652024	0.3843500616325781	0.1879064712703483
O36	0.6153915715245060	0.4281920675393611	0.3824081603414924
O37	0.5027760701926466	0.5393516008422671	0.3728343844891430
O38	0.5489523484968406	0.4849155819716904	0.3009732808934619
O39	0.4954457249412959	0.4388485416444704	0.3736029011230417
O40	0.4478020255452220	0.4923115566058936	0.3019569599770799
N1	0.5010427333539678	0.4906860081153669	0.5656971032376066
N2	0.5101257229358866	0.4754818094231367	0.7093238254540084
P1	0.4987335297559659	0.4888503400880106	0.3368086662840419
H1	0.5151809723062396	0.5138272473665727	0.7224069146678040
H2	0.5394650194994167	0.4518660127205330	0.7250888190006789
H3	0.4736889301400672	0.4617572065350642	0.7215882333185478

PMAMo_NH (Distal)

Atoms	X	Y	Z
Mo1	0.4339512379060630	0.5744792993948624	0.4340320259667035
Mo2	0.5668076560424670	0.4134720256869532	0.2328695684691968

Mo3	0.5670016684675525	0.4070440701643098	0.4345133223514674
Mo4	0.4279885312897314	0.5621033982061154	0.2327472263771951
Mo5	0.5809410124269464	0.5659730807240467	0.4299319997398464
Mo6	0.4170711573776865	0.4239249564104340	0.2360123688189779
Mo7	0.5778093423910953	0.5516608245263733	0.2317402153158192
Mo8	0.4201164169421390	0.4157264799644831	0.4348232642097322
Mo9	0.5088976251319340	0.6348099048075061	0.3339148911984856
Mo10	0.4889208771823315	0.3439348798366108	0.3386040390446223
Mo11	0.3527409818959887	0.5008671119937934	0.3307596063956517
Mo12	0.6449983225045355	0.4774570287884348	0.3266954129751571
Mo13	0.5017841440335072	0.4918395575667777	0.5002771561722995
O1	0.6406363396391722	0.5315753388520177	0.2733794756701728
O2	0.5620756344205180	0.6275250352162128	0.3939578004497234
O3	0.3554511306543309	0.4452034111413285	0.2790898582501262
O4	0.4378357460501790	0.3530841971787460	0.4001011278696428
O5	0.3635741129306043	0.5525257662394725	0.2768623142343965
O6	0.4577563609727107	0.6332520763172547	0.3961165919218228
O7	0.5421411676533771	0.3472253681334658	0.3990658882151927
O8	0.6325537465014929	0.4243183548349911	0.2745649604013118
O9	0.4941974144723770	0.4151562289785804	0.4752617762740211
O10	0.5081920451930223	0.5676409514218462	0.4726015025427208
O11	0.5819469878517533	0.4813451757379064	0.1999686906149865
O12	0.4117044343658310	0.4932989537875079	0.2024165917228270
O13	0.4370324734584858	0.3734325871030920	0.2925226169983809
O14	0.3967748788254897	0.6027576224062821	0.4834946827523290
O15	0.3752497746639495	0.4462056978258270	0.3853836680181470
O16	0.5877550326269134	0.3693676188306156	0.1856539801523643
O17	0.4055743063190601	0.6048028321946809	0.1849166911742409
O18	0.6242692409229912	0.5339685301079646	0.3801011162375296
O19	0.6057866505485031	0.3802608999871031	0.4835760141771667
O20	0.5594232248463710	0.6038516166696637	0.2872084948230940
O21	0.2863241705237506	0.5064738935559128	0.3438405289622944
O22	0.5695123810450871	0.4878276256206379	0.4607596260645048
O23	0.4325502083998529	0.4946755898461238	0.4630322300069123
O24	0.7117880491520864	0.4722082487967970	0.3378616677650692
O25	0.4845289895690092	0.2769812754158935	0.3279316081241299
O26	0.5023258049609818	0.5545541970765522	0.2159008045879167
O27	0.4918920206598451	0.4205678718008583	0.2179794300360808
O28	0.5129600943239332	0.7014123082153598	0.3211223050127217
O29	0.3793179521814490	0.3943570322635604	0.4849190115088456
O30	0.4540897592706742	0.6111882028328014	0.2884224096497572
O31	0.3844225010850873	0.5503301552585114	0.3845007353863753

O32	0.6050288071206100	0.5908263461681396	0.1833855836659368
O33	0.5423189418920999	0.3661440102195105	0.2907094880534277
O34	0.6231858429399070	0.5887688507005557	0.4781764005689399
O35	0.3883452365960609	0.3833738421359759	0.1897133389024852
O36	0.6150257608062901	0.4296513447025249	0.3826574445528949
O37	0.5036027641778900	0.5402679784364642	0.3719983769289741
O38	0.5490317114060723	0.4849358197934091	0.3006050754850068
O39	0.4955131341283879	0.4395291420762179	0.3737032204519194
O40	0.4478664566413965	0.4926264340004387	0.3020370900373743
N1	0.5029933682616984	0.4934537301475583	0.5695262737509119
P1	0.4989926638574317	0.4893398912726962	0.3365973539877324
H1	0.5055735084912787	0.4950752146282335	0.6102750779744248

PMAMo_NH_2 (Distal)

Atoms	X	Y	Z
Mo1	0.4317821407393467	0.5740341735438248	0.4327022288743165
Mo2	0.5675700047344598	0.4142606804203407	0.2320994846382718
Mo3	0.5694149999449825	0.4038725527167385	0.4313715708703019
Mo4	0.4288025254099606	0.5641131132891102	0.2342031087027852
Mo5	0.5808308208815497	0.5632419859296879	0.4303132344615588
Mo6	0.4173502842885051	0.4250965711115227	0.2342697825520614
Mo7	0.5772066487042981	0.5533898384056017	0.2322212461708534
Mo8	0.4199361166674527	0.4150066473322722	0.4337780655404956
Mo9	0.5097683318855802	0.6356756670452347	0.3365414516718266
Mo10	0.4882367257116926	0.3433925693030316	0.3362301608819279
Mo11	0.3517430779941086	0.4998152488220244	0.3294720173898089
Mo12	0.6460793339176368	0.4782386260109779	0.3255308670301489
Mo13	0.5019492233939296	0.4894680796952052	0.5008071125072827
O1	0.6408724265527931	0.5313501444008566	0.2719976449468884
O2	0.5631169416978505	0.6255129117557384	0.3944135239842855
O3	0.3553932929778438	0.4441417245346838	0.2787085556161835
O4	0.4377709273130942	0.3525876611356041	0.3999483585662952
O5	0.3631644034171052	0.5518209519551380	0.2764970358671578
O6	0.4571959518360475	0.6331243339796573	0.3963693309350476
O7	0.5415573730113070	0.3448742923150450	0.3982158893971127
O8	0.6326704978697204	0.4239854835479669	0.2743505438601841
O9	0.4959450642356724	0.4162431709298291	0.4757018900652238
O10	0.5066446558546334	0.5626300581355339	0.4744259130622701
O11	0.5814552828913588	0.4814423245771940	0.2001682889201384
O12	0.4117659125952774	0.4938020289697876	0.2029532012668625
O13	0.4364939487467062	0.3735148123191771	0.2920075210870052

O14	0.3958370756466720	0.6019731859888460	0.4833470150689774
O15	0.3746481691388817	0.4452295768529990	0.3854684293488386
O16	0.5882613714178572	0.3701314630548272	0.1847412802790122
O17	0.4062640364615989	0.6066483640979340	0.1862442484003625
O18	0.6250071600254692	0.5321672693028451	0.3803899693006732
O19	0.6068598125444099	0.3770727642212822	0.4816564954116427
O20	0.5587339270572080	0.6039541709659737	0.2864494441684902
O21	0.2851886558878781	0.5047495494127902	0.3422162614755687
O22	0.5680123884357829	0.4845298303265900	0.4602024730282365
O23	0.4341765009609158	0.4943061059718920	0.4627803360270672
O24	0.7129899660393245	0.4733639571085764	0.3361112374577053
O25	0.4830614613968097	0.2764993240123317	0.3251168398821309
O26	0.5018898542242354	0.5526728183691023	0.2147598540401525
O27	0.4921048921163094	0.4204519242393244	0.2181520195944588
O28	0.5142263038881998	0.7022647067266637	0.3244228471556108
O29	0.3805067902298144	0.3939092848110599	0.4852731619549518
O30	0.4548537723303404	0.6112429571553867	0.2885064538289291
O31	0.3821849187558458	0.5497342172440587	0.3844394138363866
O32	0.6040993708113933	0.5921966488889397	0.1833837679445826
O33	0.5423545587844327	0.3657744895651559	0.2902682743030557
O34	0.6219838608972881	0.5856671817498629	0.4797185163858577
O35	0.3889523853568198	0.3846109113145771	0.1876568289051419
O36	0.6173064939667736	0.4271413959779510	0.3816013147046916
O37	0.5033203375521250	0.5395193092578549	0.3739918812979661
O38	0.5493047713234581	0.4852134626042615	0.3020242244977442
O39	0.4959342578571962	0.4385575741081658	0.3744654314945204
O40	0.4478436541305704	0.4925675616209463	0.3034779221581534
N1	0.5045001391892767	0.4894889664518045	0.5774009429039096
P1	0.4990684935670089	0.4888826669821887	0.3376086979402145
H1	0.5136825477904741	0.5225128055921570	0.5997457744124165
H2	0.4977049709427153	0.4562598098418622	0.6002806089262419

PMAMo…. NH_3 (Distal)

Atoms	X	Y	Z
Mo1	0.4338217030226515	0.5773620567245736	0.4337349579633312
Mo2	0.5666476558062710	0.4131275839795678	0.2349075146127134
Mo3	0.5653504701885332	0.4022497382541991	0.4341046001465940
Mo4	0.4267361208726586	0.5632038458227810	0.2354400664716959
Mo5	0.5775180020853102	0.5668170608536760	0.4325043918371521
Mo6	0.4165488281215260	0.4244117033292362	0.2365867462334798
Mo7	0.5766713418186431	0.5522554827775316	0.2337457675413506

Mo8	0.4219001181806745	0.4127057466136795	0.4352752446754816
Mo9	0.5093880098240068	0.6371415451316654	0.3351629527385508
Mo10	0.4877268459072199	0.3408718720199962	0.3376321850211388
Mo11	0.3537207192966491	0.4995270952376189	0.3338485716249369
Mo12	0.6436079581341243	0.4782089425891413	0.3292167022317431
Mo13	0.4997997933799637	0.4906267593376437	0.5013094380392612
O1	0.6400035653485656	0.5320709369611734	0.2769883138700251
O2	0.5621524231098856	0.6286918065116349	0.3963963668973355
O3	0.3562058836743793	0.4452363285953935	0.2789716393049403
O4	0.4367731099214749	0.3501310124557371	0.3994615860168324
O5	0.3638805596472900	0.5516210074320590	0.2777788792920238
O6	0.4576424656267388	0.6363946288097704	0.3965250737077249
O7	0.5410948039579619	0.3426154948708040	0.3992307618557914
O8	0.6321207205098313	0.4243337356649260	0.2780925205451649
O9	0.4940759654150371	0.4115633022771430	0.4782954887702530
O10	0.5056207535936015	0.5690598316047443	0.4767804381091433
O11	0.5829502721100642	0.4814550085450852	0.2034594969319837
O12	0.4145372472438092	0.4938305246753505	0.2034623734795371
O13	0.4373275432006015	0.3723580845522225	0.2917423245655548
O14	0.3960362155695499	0.6030132081270208	0.4844915953180059
O15	0.3767209881675774	0.4446183867585443	0.3863715930619063
O16	0.5884183847212564	0.3696558362164347	0.1873768207603642
O17	0.4047740361932680	0.6056153956693268	0.1870875000774458
O18	0.6211234715868437	0.5332111583341262	0.3841523857718271
O19	0.6037801009449795	0.3779191754529302	0.4851374366135626
O20	0.5600117215061258	0.6044292493700696	0.2898095582486982
O21	0.2872943879269735	0.5044551343120411	0.3470606149633121
O22	0.5632959396971958	0.4854876365842027	0.4619043103707005
O23	0.4360324036677625	0.4948110281522737	0.4620382262779028
O24	0.7102293752078316	0.4734266523589479	0.3420861701101953
O25	0.4829098637273126	0.2742477568145733	0.3251260390893551
O26	0.5026443477941653	0.5543935034347174	0.2181116111441613
O27	0.4929288269849072	0.4210737251318986	0.2196049225346120
O28	0.5143954634234164	0.7034750042521217	0.3213618330818467
O29	0.3809901891777115	0.3940478202202449	0.4867021450377595
O30	0.4550097686691499	0.6124591571074847	0.2892140047174238
O31	0.3844773256583145	0.5514321606319964	0.3852674845711893
O32	0.6045247206945387	0.5911540402004377	0.1854299205254206
O33	0.5425465380367543	0.3647661363916395	0.2921094159876931
O34	0.6192889032370376	0.5863519703495930	0.4829403006484225
O35	0.3886403548706445	0.3846252534122668	0.1890732710718511
O36	0.6133545174566261	0.4281800175336877	0.3852438491176389

O37	0.5026806209384900	0.5401289231014387	0.3761972802192309
O38	0.5485981681302593	0.4849732349218620	0.3047018531386438
O39	0.4952061198749850	0.4385233695306971	0.3771682195093335
O40	0.4475483915857277	0.4924623683963630	0.3059434773817135
N1	0.4978136439634304	0.4878367359539884	0.5896304065104352
P1	0.4985375634693382	0.4890130470441177	0.3402865262217603
H1	0.5197660367242833	0.5178345071232824	0.6072948841232764
H2	0.5111089842290342	0.4519536348981860	0.6048061880129482
H3	0.4590195771670119	0.4924934675861524	0.6027157642976054

PMAMo_N-NH (Alternating)

Atoms	X	Y	Z
Mo1	0.4340847270356570	0.5747192369270054	0.4347304052518348
Mo2	0.5667116724856389	0.4138239002409624	0.2331206663736690
Mo3	0.5655290916453234	0.4051077626206891	0.4345403754182196
Mo4	0.4279688722594533	0.5623522673134408	0.2330350974323582
Mo5	0.5800526693930709	0.5666351684770394	0.4307901428094063
Mo6	0.4165108545145884	0.4241838842105490	0.2359818704139842
Mo7	0.5777025448859271	0.5523459848853983	0.2330373101899166
Mo8	0.4199137909823077	0.4135149444874796	0.4338568222231515
Mo9	0.5083340222660893	0.6355286916340565	0.3347369049532774
Mo10	0.4887401095312194	0.3424702986039991	0.3373159275359179
Mo11	0.3534185459591308	0.5011190489724027	0.3316885314395294
Mo12	0.6443036110990946	0.4772629993974818	0.3277880995614254
Mo13	0.4997665965144077	0.4915728542102132	0.4988308731903340
O1	0.6405717507300960	0.5315318138559693	0.2750822599940184
O2	0.5617569498764302	0.6281182655079446	0.3948148438064244
O3	0.3559165661850291	0.4452881260173962	0.2786543893041637
O4	0.4373163744928547	0.3510394883197497	0.3992444131007607
O5	0.3639100235004856	0.5519666377662383	0.2761732827189063
O6	0.4570503196441285	0.6336449718717476	0.3961027638279340
O7	0.5413813186471532	0.3453987330769398	0.3992594555893830
O8	0.6322430563593617	0.4240273100425289	0.2760741163312128
O9	0.4929791016669537	0.4135390840623889	0.4762378285877903
O10	0.5078168937270794	0.5687279378968895	0.4739162391882269
O11	0.5826718211223814	0.4816648016832312	0.2013647876286482
O12	0.4132050866407891	0.4932155088909702	0.2021413991736160
O13	0.4371524957442355	0.3725894494245248	0.2919530426631416
O14	0.3963645660639504	0.6024239683571040	0.4840762998890944
O15	0.3753082827318751	0.4448939569255359	0.3846612653514599
O16	0.5879818893601337	0.3700175596407435	0.1857453304401892

O17	0.4060289217849724	0.6049073893417896	0.1848595414236465
O18	0.6230769799137238	0.5334308275403451	0.3816597538604460
O19	0.6040303428657895	0.3794091951726228	0.4845094127868297
O20	0.5594433133990552	0.6040281068900694	0.2885089594469658
O21	0.2869685987763211	0.5066863677794351	0.3445200100677575
O22	0.5674799897557041	0.4873670061639090	0.4625704337275404
O23	0.4317980489604279	0.4938751301129908	0.4624826584987303
O24	0.7109456756929943	0.4717692057741379	0.3398510487533944
O25	0.4845791645527445	0.2756258026734968	0.3258111711616402
O26	0.5029103053367207	0.5544064581381181	0.2164726262433898
O27	0.4923116036722051	0.4205104352060072	0.2187417136468204
O28	0.5124063488682961	0.7020340998878613	0.3215822456732621
O29	0.3789547185299005	0.3929981323967951	0.4842474890472891
O30	0.4543856926647278	0.6112846474346724	0.2883320113017044
O31	0.3845807757204516	0.5504309545724521	0.3842816514740786
O32	0.6054660667741916	0.5914953874186846	0.1849635195941636
O33	0.5427125069405916	0.3654936764041081	0.2911668401187392
O34	0.6225090224694088	0.5886718301436151	0.4792343517433540
O35	0.3881984960135802	0.3837968063933938	0.1892724381732863
O36	0.6136679809490277	0.4291164259697649	0.3840310105255928
O37	0.5032222749549580	0.5397294964408897	0.3738093097825727
O38	0.5488442243117631	0.4847749499386682	0.3021419647592455
O39	0.4950062232359131	0.4389443429477032	0.3748823973021480
O40	0.4478109425742318	0.4925392307811607	0.3031972033035636
N1	0.5039681419190528	0.4948248556667598	0.5716330934195990
N2	0.5035716436300969	0.5045431251433883	0.6201311080569500
P1	0.4987294815782344	0.4890268996627337	0.3378809344071717
H1	0.5066888010900581	0.4704743626838008	0.6439004293121481

PMAMo_NH-NH (Alternating)

Atoms	X	Y	Z
Mo1	0.4159513970981988	0.5546750397970807	0.4367586413648306
Mo2	0.5854606659397787	0.4394667824718326	0.2315229283140601
Mo3	0.5758627071283531	0.4047436621321951	0.4271137976584807
Mo4	0.4230739031034315	0.5647544394480930	0.2380773501833003
Mo5	0.5595313015134876	0.5671896523073419	0.4446524896342118
Mo6	0.4355489540384516	0.4265367623208415	0.2232557162179181
Mo7	0.5718261327004005	0.5776460730851339	0.2459796938612963
Mo8	0.4300160918708055	0.3922500730787600	0.4194827570858654
Mo9	0.4859112282607019	0.6374898688904280	0.3516705324463795
Mo10	0.5131654374628917	0.3438478963323867	0.3196341042476043

Mo11	0.3548244737589422	0.4787159634815181	0.3220283229729330
Mo12	0.6448972308569845	0.5042582382675531	0.3375907673790819
Mo13	0.4928301431252706	0.4696605253565999	0.4974124487776773
O1	0.6350696681137401	0.5618071356723833	0.2895777863652328
O2	0.5361701467907782	0.6297016651722044	0.4136635877965310
O3	0.3694626894512330	0.4311674794234430	0.2643971719526519
O4	0.4581556409121217	0.3377569120648465	0.3794248242467778
O5	0.3596155063827904	0.5376919975841506	0.2745270352149252
O6	0.4314386048660685	0.6206442666660609	0.4078739055287476
O7	0.5619411783965488	0.3465526889711253	0.3850063069583625
O8	0.6450452954235772	0.4551899565485642	0.2795657966977392
O9	0.5006497976603271	0.3963359303201285	0.4690151925899319
O10	0.4862261789512773	0.5513696775745224	0.4824886286088700
O11	0.5899401009489568	0.5118288058522540	0.2080400490011678
O12	0.4213973733070761	0.4972367819314910	0.1987512204268426
O13	0.4600470738712223	0.3717209499723466	0.2753652318420376
O14	0.3720698278542131	0.5689030455296721	0.4869630469733051
O15	0.3832476620907452	0.4215721666694354	0.3716084932363937
O16	0.6161373137180078	0.4054555638727954	0.1813271664008974
O17	0.3967848813598054	0.6083453485383969	0.1931070574938185
O18	0.6108564420634072	0.5472352886380728	0.3955262538426564
O19	0.6149463412202022	0.3798114330913727	0.4771753237147600
O20	0.5427637393575439	0.6188709536728436	0.3044122407685873
O21	0.2878626057106924	0.4718515732591007	0.3311425521297801
O22	0.5598441622808190	0.4822249744455557	0.4653144462807799
O23	0.4285464384076834	0.4709038478207532	0.4579091877383169
O24	0.7106354897552177	0.5089941492855370	0.3540920486000510
O25	0.5198238973746644	0.2791612119624819	0.2998710769478963
O26	0.4988665781442877	0.5681169830631477	0.2241588030873979
O27	0.5111304818620321	0.4360951723256635	0.2123458650955749
O28	0.4804074560600508	0.7048696956003527	0.3460122231625666
O29	0.3905800713831465	0.3603713367832556	0.4650842143870453
O30	0.4386673875156511	0.6098853193534035	0.2986500923345936
O31	0.3744116718120036	0.5266753468111032	0.3825206919189987
O32	0.5949826075531327	0.6254864629386061	0.2036725808288591
O33	0.5653401561524932	0.3808453442725599	0.2812009016625905
O34	0.5945839874361688	0.5883717715557347	0.4991697583960680
O35	0.4169242638094988	0.3882343421034054	0.1703080581349252
O36	0.6216162054379506	0.4424068227152681	0.3845400650585429
O37	0.4931852696024875	0.5365216515671022	0.3802454895219552
O38	0.5515089280825610	0.4975865461940910	0.3072742290013055
O39	0.5025419684635694	0.4359336453516097	0.3713066347221332

O40	0.4506711817729679	0.4887420082157531	0.3018409466526056
P1	0.4995100963196801	0.4897992643941643	0.3392813450768672
N1	0.4898266614110173	0.4925055784535358	0.5759460695587553
N2	0.4965987132448096	0.4664996195204119	0.6194574734471955
H1	0.4825939339536210	0.5327241760711459	0.5827988946346889
H2	0.5035245728564054	0.4264599972002694	0.6102003278166082

PMAMo_NH-NH_2 (Alternating)

Atoms	X	Y	Z
Mo1	0.4318734531994437	0.5633484195972035	0.4447753829825938
Mo2	0.5675690875272698	0.4186519771089182	0.2319770970873990
Mo3	0.5622793552188878	0.4001506519030624	0.4335381459390575
Mo4	0.4292309889122177	0.5638629534744727	0.2359542443918644
Mo5	0.5794828921521348	0.5613401618833450	0.4363549737371740
Mo6	0.4164206120993252	0.4261408928386228	0.2346417429281897
Mo7	0.5777663796475803	0.5575211145019808	0.2425865426717867
Mo8	0.4157142309070892	0.4033621237822595	0.4286310327219379
Mo9	0.5018940980255184	0.6331282597301696	0.3466465938366872
Mo10	0.4902569814408054	0.3400439092784616	0.3311761888779038
Mo11	0.3535241539963978	0.5011936360191277	0.3329439797789926
Mo12	0.6447477224159722	0.4751877195820436	0.3310664677080362
Mo13	0.4899629366273898	0.4883002012524673	0.4972044372555521
O1	0.6413106919789781	0.5326842589568737	0.2828356175454594
O2	0.5607136067894055	0.6234632090332702	0.4031215577627820
O3	0.3569611844081413	0.4453197152987592	0.2769332499736809
O4	0.4371952371780634	0.3430619958529808	0.3935323040646141
O5	0.3639613735573469	0.5515436857657364	0.2773850439316017
O6	0.4541341402113468	0.6264133844949655	0.4051044283327400
O7	0.5401415953067652	0.3409204287732415	0.3969330772163702
O8	0.6329492503371557	0.4245330287619994	0.2780076203452471
O9	0.4883242196575656	0.4103507114995925	0.4739507640402665
O10	0.5081058793153318	0.5637003907573684	0.4803340823173955
O11	0.5846747166826245	0.4872637148052191	0.2061061387542338
O12	0.4152823833547433	0.4958700034203709	0.2024588590281091
O13	0.4381658765076895	0.3709949271253448	0.2878701404541026
O14	0.3936347608204218	0.5895509230705989	0.4943061241444095
O15	0.3727012686348502	0.4369838140391132	0.3805428710949191
O16	0.5900139856661498	0.3776001298625298	0.1826544635090852
O17	0.4080359145628065	0.6082433314118858	0.1890876258936477
O18	0.6233241241122718	0.5288413053255472	0.3883138632053940
O19	0.5984188046417995	0.3746092963364159	0.4854887010639050

O20	0.5568008462102427	0.6033886409682865	0.2988624607359774
O21	0.2866802930097785	0.5053871793047994	0.3443905014749583
O22	0.5589923713608739	0.4818560142361613	0.4635127914877636
O23	0.4237577317361875	0.4820955520591552	0.4609095161280639
O24	0.7111980641607104	0.4688232673081441	0.3440948243960932
O25	0.4877934453668866	0.2736772220252473	0.3164367091731730
O26	0.5041296586311944	0.5571522358505505	0.2209229881666812
O27	0.4937539405070321	0.4235540658766846	0.2187140860670024
O28	0.5057359692523866	0.7002759366447268	0.3371438483001399
O29	0.3740188690407794	0.3798061041978454	0.4772608834966249
O30	0.4529387461565763	0.6105033701315579	0.2943396449391071
O31	0.3825224902030224	0.5446936412977971	0.3875055719640349
O32	0.6066653833425459	0.5994667556410392	0.1975798706266979
O33	0.5446970783012428	0.3659351639219314	0.2887066322701849
O34	0.6205333545881710	0.5805503739934341	0.4875830747677087
O35	0.3892857046692842	0.3874465029205322	0.1858094819693703
O36	0.6123607824165012	0.4257933169852701	0.3865348484127391
O37	0.5011014094425894	0.5338855672386652	0.3808174890271057
O38	0.5488744510747199	0.4849044095017604	0.3059835673746777
O39	0.4932948668026502	0.4333558593301070	0.3734036890838345
O40	0.4477323244256281	0.4921505504314773	0.3051066794696882
P1	0.4978268217327460	0.4862595488768022	0.3405346595693463
N1	0.4859072230357417	0.4941703864711933	0.5736138267721466
N2	0.5270477167536133	0.5180269282572911	0.6027415214550842
H1	0.5530181304536349	0.4905794467748681	0.6187548530274483
H2	0.5470279067205613	0.5457802477126419	0.5800956991311952
H3	0.4544822977112331	0.4820912734980820	0.5970970061179955

PMAMo_NH_2-NH_2 (Alternating)

Atoms	X	Y	Z
Mo1	0.4225256532360933	0.5805016389778668	0.4218435750462723
Mo2	0.5815740975960397	0.4165298860215901	0.2423754629085721
Mo3	0.5774750281702200	0.4252799657267646	0.4414609674297110
Mo4	0.4244655773687064	0.5463556005450544	0.2267034495572061
Mo5	0.5676823900702531	0.5876643661080979	0.4235975627821920
Mo6	0.4308525672338043	0.4076916922059703	0.2417281313848364
Mo7	0.5733458969796893	0.5547927481405447	0.2269492077846245
Mo8	0.4329410854418951	0.4182754754465122	0.4411738298280763
Mo9	0.4933738275647778	0.6397806822036120	0.3196162975926672
Mo10	0.5090619746667406	0.3453348751612652	0.3514821194340185
Mo11	0.3553033004383320	0.4830658553251760	0.3285245745569104

Mo12	0.6464090508862774	0.5003154257913287	0.3307325865539084
Mo13	0.4997331671568503	0.5112492144014994	0.4986612995200855
O1	0.6370820570368485	0.5453804477916965	0.2698995508944990
O2	0.5452928704320138	0.6427546627671680	0.3791528992433273
O3	0.3662424300393756	0.4231438617598676	0.2841014595874425
O4	0.4561375717877071	0.3546675879265620	0.4140064362730651
O5	0.3600755711890382	0.5300895987639790	0.2702576862875563
O6	0.4395588655569452	0.6378991001652542	0.3791551122373362
O7	0.5600124254833191	0.3598036771147157	0.4138424127769545
O8	0.6423437735537297	0.4392206010380877	0.2842644215857735
O9	0.5048840326785773	0.4306028148257301	0.4838330212998164
O10	0.4947796604154108	0.5856462293389384	0.4658813799950816
O11	0.5861397663057600	0.4808783190079026	0.2028792228347035
O12	0.4167116566327426	0.4714522630109871	0.2034691006135079
O13	0.4546259464712260	0.3645784103790024	0.3048190793171217
O14	0.3811276473960977	0.6068451941500419	0.4693576493494969
O15	0.3848977726464735	0.4385898296977627	0.3899848618276555
O16	0.6089029127069249	0.3708400977850497	0.2001068658458024
O17	0.3973667422494990	0.5799313646017669	0.1741628625163903
O18	0.6167386229248870	0.5562798390308158	0.3774549792619148
O19	0.6175467198649349	0.4110375282163675	0.4950331567058668
O20	0.5465171630270586	0.6086894311604679	0.2743275246781609
O21	0.2885988660385347	0.4804795829910853	0.3415536531214665
O22	0.5653890404936622	0.5096343791721035	0.4607767662821542
O23	0.4351578171716470	0.5039136467006325	0.4600519125684667
O24	0.7129614267174961	0.5053530791790173	0.3433697800980289
O25	0.5126230070027491	0.2775596364635504	0.3466927512960072
O26	0.4983315545742473	0.5425566151060573	0.2093300084929716
O27	0.5056593323148073	0.4111811143977738	0.2274053231882566
O28	0.4898862840697744	0.7044332653212365	0.2993369730293323
O29	0.3952092292659653	0.4011986647186715	0.4958234447766540
O30	0.4423330079077686	0.6025106218651691	0.2756585134118156
O31	0.3780168989719808	0.5429982217441526	0.3770645897811697
O32	0.5962300834033109	0.5909797069346844	0.1741961047191170
O33	0.5607268278889236	0.3703463745023725	0.3045549903175758
O34	0.6060705559823173	0.6192451990171144	0.4702204886787000
O35	0.4087813152845089	0.3593031552423989	0.1993764841729651
O36	0.6227527129010039	0.4508563788427387	0.3899982713412120
O37	0.4974678893074863	0.5469400799703655	0.3692942449933078
O38	0.5518556909380591	0.4915889026645562	0.3043286456713415
O39	0.5033748056584779	0.4460578429099986	0.3807469682200192
O40	0.4506084839613005	0.4855990458723801	0.3038127833057697

P1	0.5008327517288402	0.4924554505545199	0.3388011354422663
N1	0.4920315293216885	0.4864734472915851	0.5818727070245381
N2	0.4640654484592821	0.5214789323334265	0.6191631202785602
H1	0.4817978594013689	0.5584746587270714	0.6166069913217170
H2	0.4256448657825791	0.5257821189948760	0.6052537673075028
H3	0.4723330561814020	0.4501428999241848	0.5823313844241904
H4	0.5287220310625413	0.4781387429708191	0.5987793662243516

PMAMo_NH_2…. NH_3 (Alternating)

Atoms	X	Y	Z
Mo1	0.4217057548781461	0.5683991043312877	0.4349349095031507
Mo2	0.5798603375309171	0.4471380010849154	0.2241227395792731
Mo3	0.5756818184840884	0.4140805874443473	0.4208298049223059
Mo4	0.4262370763306740	0.5819004742618771	0.2365125839908120
Mo5	0.5708802813077157	0.5721798722409116	0.4385216340100753
Mo6	0.4293272374336454	0.4434953539865168	0.2203744324796643
Mo7	0.5750122376277071	0.5855251041083951	0.2401033057764349
Mo8	0.4257897970854902	0.4104075242916607	0.4172811188945727
Mo9	0.4964108960478595	0.6480308472556292	0.3500153278353914
Mo10	0.5044912602272026	0.3575656281255578	0.3158127027624489
Mo11	0.3532353196978322	0.4998160673351103	0.3204897436263901
Mo12	0.6482662607323975	0.5072496045125506	0.3275080051673253
Mo13	0.4971088402220641	0.4835104545284152	0.4961458352656077
O1	0.6395460502592680	0.5655298021063090	0.2806771450123890
O2	0.5483655374301669	0.6362363651324617	0.4091463900782230
O3	0.3643670626109179	0.4513333659384803	0.2633502321392984
O4	0.4510210403276990	0.3544041546218267	0.3771905678777351
O5	0.3611998385746010	0.5585089478974178	0.2736955053345625
O6	0.4423983288880499	0.6335734688679624	0.4064589577616873
O7	0.5552093372937144	0.3569959724291171	0.3796769123719816
O8	0.6423825171565971	0.4582599596346765	0.2702526323791312
O9	0.4996924803336323	0.4135490894787504	0.4619412546439371
O10	0.4955400087122497	0.5597746568677789	0.4784464245108867
O11	0.5886449706062395	0.5187947958749728	0.2007398795317451
O12	0.4184543700797954	0.5145912105190837	0.1964057506095273
O13	0.4518178228873195	0.3876393354748777	0.2724316104194348
O14	0.3814350982807328	0.5871156782868003	0.4866713328743046
O15	0.3794269341963911	0.4414046174804822	0.3702680724145071
O16	0.6066152617108131	0.4110654484155857	0.1730767835245706
O17	0.4014261597724406	0.6274862616060051	0.1926242007410656
O18	0.6197753460307237	0.5518087316552920	0.3876291524083236

O19	0.6139322611419376	0.3850362909862531	0.4692820666796431
O20	0.5503757640200151	0.6271503102232689	0.2993957829020193
O21	0.2860908478266118	0.4968548731774021	0.3304921420880086
O22	0.5654737051139384	0.4898801291792040	0.4586225853465565
O23	0.4302494489668491	0.4865386590561976	0.4554308959650848
O24	0.7149065483386194	0.5077240263720316	0.3408461292825687
O25	0.5065392546983850	0.2922104651653382	0.2970453483357210
O26	0.5013372681844442	0.5799921541974140	0.2191896886206876
O27	0.5049784035156155	0.4481278288675377	0.2072968143685713
O28	0.4948991375850074	0.7157638997817437	0.3458927086352018
O29	0.3866869900441548	0.3794974257745741	0.4638322760865327
O30	0.4462748397351010	0.6247556588396012	0.2966174599158423
O31	0.3764049853695456	0.5457758142405496	0.3816099702615882
O32	0.5997648989764801	0.6324151375886021	0.1975672241597114
O33	0.5578487578742981	0.3902286858158787	0.2751209932429946
O34	0.6075678662625786	0.5927046459054270	0.4921905547381776
O35	0.4070051210173818	0.4061476289905855	0.1681268945301585
O36	0.6226670895502661	0.4475357319543573	0.3762449226639810
O37	0.4983415916813282	0.5482523909686569	0.3758380787230512
O38	0.5520793177139757	0.5075830827575284	0.3002680077413177
O39	0.5011097046296902	0.4477986436920152	0.3642361260070351
O40	0.4503936339843113	0.5051121435979246	0.2978246588670870
P1	0.5004947675496418	0.5021767119291108	0.3336856106743211
N1	0.4955422888335447	0.4750070451402702	0.5709777454892712
N2	0.4809107271584500	0.5524628444274829	0.6491691245533389
H1	0.4891631102650498	0.5063415020084602	0.6006087284159392
H2	0.4987639199507976	0.5410129416006121	0.6842115052568430
H3	0.4413346954907768	0.5591591989639436	0.6573715787877475
H4	0.5024254764035053	0.4382827285960288	0.5879620377400846
H5	0.4973524243606207	0.5884708704069762	0.6385675454741330

PMAMo…. NH_3 (Alternating)

Atoms	X	Y	Z
Mo1	0.4338217030226515	0.5773620567245736	0.4337349579633312
Mo2	0.5666476558062710	0.4131275839795678	0.2349075146127134
Mo3	0.5653504701885332	0.4022497382541991	0.4341046001465940
Mo4	0.4267361208726586	0.5632038458227810	0.2354400664716959
Mo5	0.5775180020853102	0.5668170608536760	0.4325043918371521
Mo6	0.4165488281215260	0.4244117033292362	0.2365867462334798
Mo7	0.5766713418186431	0.5522554827775316	0.2337457675413506
Mo8	0.4219001181806745	0.4127057466136795	0.4352752446754816

Mo9	0.5093880098240068	0.6371415451316654	0.3351629527385508
Mo10	0.4877268459072199	0.3408718720199962	0.3376321850211388
Mo11	0.3537207192966491	0.4995270952376189	0.3338485716249369
Mo12	0.6436079581341243	0.4782089425891413	0.3292167022317431
Mo13	0.4997997933799637	0.4906267593376437	0.5013094380392612
O1	0.6400035653485656	0.5320709369611734	0.2769883138700251
O2	0.5621524231098856	0.6286918065116349	0.3963963668973355
O3	0.3562058836743793	0.4452363285953935	0.2789716393049403
O4	0.4367731099214749	0.3501310124557371	0.3994615860168324
O5	0.3638805596472900	0.5516210074320590	0.2777788792920238
O6	0.4576424656267388	0.6363946288097704	0.3965250737077249
O7	0.5410948039579619	0.3426154948708040	0.3992307618557914
O8	0.6321207205098313	0.4243337356649260	0.2780925205451649
O9	0.4940759654150371	0.4115633022771430	0.4782954887702530
O10	0.5056207535936015	0.5690598316047443	0.4767804381091433
O11	0.5829502721100642	0.4814550085450852	0.2034594969319837
O12	0.4145372472438092	0.4938305246753505	0.2034623734795371
O13	0.4373275432006015	0.3723580845522225	0.2917423245655548
O14	0.3960362155695499	0.6030132081270208	0.4844915953180059
O15	0.3767209881675774	0.4446183867585443	0.3863715930619063
O16	0.5884183847212564	0.3696558362164347	0.1873768207603642
O17	0.4047740361932680	0.6056153956693268	0.1870875000774458
O18	0.6211234715868437	0.5332111583341262	0.3841523857718271
O19	0.6037801009449795	0.3779191754529302	0.4851374366135626
O20	0.5600117215061258	0.6044292493700696	0.2898095582486982
O21	0.2872943879269735	0.5044551343120411	0.3470606149633121
O22	0.5632959396971958	0.4854876365842027	0.4619043103707005
O23	0.4360324036677625	0.4948110281522737	0.4620382262779028
O24	0.7102293752078316	0.4734266523589479	0.3420861701101953
O25	0.4829098637273126	0.2742477568145733	0.3251260390893551
O26	0.5026443477941653	0.5543935034347174	0.2181116111441613
O27	0.4929288269849072	0.4210737251318986	0.2196049225346120
O28	0.5143954634234164	0.7034750042521217	0.3213618330818467
O29	0.3809901891777115	0.3940478202202449	0.4867021450377595
O30	0.4550097686691499	0.6124591571074847	0.2892140047174238
O31	0.3844773256583145	0.5514321606319964	0.3852674845711893
O32	0.6045247206945387	0.5911540402004377	0.1854299205254206
O33	0.5425465380367543	0.3647661363916395	0.2921094159876931
O34	0.6192889032370376	0.5863519703495930	0.4829403006484225
O35	0.3886403548706445	0.3846252534122668	0.1890732710718511
O36	0.6133545174566261	0.4281800175336877	0.3852438491176389
O37	0.5026806209384900	0.5401289231014387	0.3761972802192309

O38	0.5485981681302593	0.4849732349218620	0.3047018531386438
O39	0.4952061198749850	0.4385233695306971	0.3771682195093335
O40	0.4475483915857277	0.4924623683963630	0.3059434773817135
N1	0.4978136439634304	0.4878367359539884	0.5896304065104352
P1	0.4985375634693382	0.4890130470441177	0.3402865262217603
H1	0.5197660367242833	0.5178345071232824	0.6072948841232764
H2	0.5111089842290342	0.4519536348981860	0.6048061880129482
H3	0.4590195771670119	0.4924934675861524	0.6027157642976054

PMAMo_N-NH (Enzymatic)

Atoms	X	Y	Z
Mo1	0.4340116001701780	0.5748236421125359	0.4326173807741722
Mo2	0.5674282738264396	0.4134376415954824	0.2330022012928802
Mo3	0.5649345551022970	0.4043622452942167	0.4334443955341792
Mo4	0.4277825649978014	0.5626659549356292	0.2337031627796144
Mo5	0.5790331300328831	0.5657993407883932	0.4298515498903609
Mo6	0.4175946066331770	0.4246613735892590	0.2346565248776194
Mo7	0.5778274216747157	0.5513166802323721	0.2321664218243863
Mo8	0.4208124278686985	0.4134278517314782	0.4330712309874959
Mo9	0.5094457707729539	0.6352595077411289	0.3340498962286985
Mo10	0.4881455802170908	0.3424204126520965	0.3366699177696162
Mo11	0.3525975575849999	0.4998245483870378	0.3305388461696641
Mo12	0.6445376230171330	0.4772462046639513	0.3279281847106340
Mo13	0.5008244549633178	0.4913590499835370	0.5007570376333028
O1	0.6403539456361212	0.5316063374655917	0.2747510709283342
O2	0.5622649268523811	0.6283072125725797	0.3947179894277039
O3	0.3555600559602498	0.4450084527789924	0.2780732225405285
O4	0.4365074321757285	0.3506272728256344	0.3980212713660439
O5	0.3632407815501510	0.5521100616379703	0.2770324195056482
O6	0.4568112800451001	0.6344329853144338	0.3958637829812000
O7	0.5419358885663431	0.3444341336412312	0.3971295518242705
O8	0.6327578677677532	0.4244745880363364	0.2749030362483613
O9	0.4931648404123888	0.4116273789688931	0.4730089942865044
O10	0.5071130161741967	0.5686049963833295	0.4709924471254422
O11	0.5826809757320061	0.4815930045373538	0.2000790392626815
O12	0.4120245444258137	0.4940861847901603	0.2018768420922176
O13	0.4369643297518742	0.3729801503006408	0.2908734057461769
O14	0.3959291053830912	0.6012840233972213	0.4826448757965674
O15	0.3759260304841852	0.4454957403613390	0.3845775994724835
O16	0.5889645445853245	0.3697939453858862	0.1856528646944130
O17	0.4053544012491967	0.6058555581457835	0.1862881584191945

O18	0.6233023451953116	0.5331828606378513	0.3814338244765774
O19	0.6047911212127305	0.3782933491104071	0.4821141959486173
O20	0.5595706766640312	0.6039815292192059	0.2881417680601717
O21	0.2861321730696069	0.5046326966930003	0.3436756175833471
O22	0.5641689610576103	0.4867606811783737	0.4574556690451205
O23	0.4360398816356059	0.4930557190384643	0.4593929507188098
O24	0.7114110144096013	0.4726907108364152	0.3392457623862773
O25	0.4833906082328693	0.2756705868947685	0.3251708623346813
O26	0.5024853128211884	0.5550858418275887	0.2166240206343780
O27	0.4924807749985086	0.4208783832780066	0.2175278827209524
O28	0.5141336668054456	0.7016634947872066	0.3215218023842909
O29	0.3799863890410109	0.3943251564655667	0.4840891848056603
O30	0.4543050099491859	0.6117212528863960	0.2890851684118381
O31	0.3841040529897921	0.5498777492740977	0.3840595794368185
O32	0.6051785243489854	0.5912144043545600	0.1844776819444126
O33	0.5422361395177530	0.3652258274258586	0.2896302645826627
O34	0.6202113280019264	0.5856212194709652	0.4805319267052906
O35	0.3888710574743768	0.3846245115559692	0.1879209895212465
O36	0.6139326751535008	0.4286957922022875	0.3828095608221122
O37	0.5029688985900336	0.5400553297606497	0.3707104765722553
O38	0.5489216227027203	0.4846352841727616	0.3001168231513634
O39	0.4950553364771206	0.4379641903101971	0.3716610128877535
O40	0.4475223830662394	0.4922743313920880	0.3012014188905541
N1	0.5042577363921320	0.5204545196221557	0.5722672400302447
N2	0.5019014619204338	0.4688188815007802	0.5762635494920055
P1	0.4986249916510363	0.4887405682348846	0.3357296132805332
H1	0.5088461100076554	0.5481184776189922	0.6022378449816190

PMAMo_NH-NH (Enzymatic)

Atoms	X	Y	Z
Mo1	0.4340774629503566	0.5783108191020626	0.4316480010285240
Mo2	0.5664495317959418	0.4125774087617400	0.2333094562443528
Mo3	0.5669076020837733	0.4013993159500083	0.4312691258079038
Mo4	0.4268886498990458	0.5625303414533956	0.2333854098637012
Mo5	0.5775091767921414	0.5665360143000715	0.4304570361353997
Mo6	0.4169615205068219	0.4237840797332956	0.2350368628739069
Mo7	0.5772836138511604	0.5514899670549426	0.2310289997065052
Mo8	0.4234304847530030	0.4138776503397664	0.4344937989687538
Mo9	0.5100148410541572	0.6367420902765640	0.3322181714979154
Mo10	0.4873787410158579	0.3407147993953623	0.3364948613357082
Mo11	0.3540457085923845	0.4991842554899972	0.3319708293153223

Mo12	0.6439391556548634	0.4784418857488272	0.3268931536319216
Mo13	0.5014690256811966	0.4903293646198435	0.4997798027763830
O1	0.6401300021670328	0.5325180776768456	0.2743607108701325
O2	0.5626314562301135	0.6283529694377757	0.3945532316020570
O3	0.3560601503245632	0.4455835647350565	0.2775388125063249
O4	0.4368750678117514	0.3513553999278065	0.3976658067241880
O5	0.3642624565557661	0.5523826587676304	0.2774266840213954
O6	0.4588408592583793	0.6369846663905361	0.3954167342132902
O7	0.5415348118419853	0.3421105517634443	0.3963489632124215
O8	0.6322763324636564	0.4249790692828244	0.2749038619858665
O9	0.4964994180401469	0.4115226596403276	0.4753861649440253
O10	0.5057592318750421	0.5686451250075270	0.4738216550135755
O11	0.5822861114109357	0.4816172298360514	0.2007733007376013
O12	0.4132745608928957	0.4942750425470895	0.2020634254004478
O13	0.4372061453988718	0.3725286727777780	0.2896759324895706
O14	0.3965181802164892	0.6045517787395998	0.4821825043858794
O15	0.3782273281387675	0.4461713398912855	0.3854343409051564
O16	0.5879376494020184	0.3692703252572181	0.1855711295369365
O17	0.4047490348160657	0.6054626360424956	0.1856126580677269
O18	0.6208377650383331	0.5328617022760694	0.3816740141815999
O19	0.6058961912868006	0.3757450932773163	0.4810166693125587
O20	0.5603515637836507	0.6045792309546639	0.2876129414893818
O21	0.2877141405951997	0.5039263755668049	0.3456846767459468
O22	0.5652669139573288	0.4837849530781229	0.4614923818624314
O23	0.4362042378006721	0.4963180901605561	0.4633577974337514
O24	0.7106099645058047	0.4739716249233835	0.3393282117851434
O25	0.4819485223446234	0.2742258427326575	0.3240449548610218
O26	0.5023663632153489	0.5552568973477184	0.2170028477542659
O27	0.4926071991676997	0.4220951686417884	0.2169923134665599
O28	0.5151394678322795	0.7031243612355432	0.3185762058488964
O29	0.3821526026745643	0.3942030105011032	0.4848847910739942
O30	0.4546924813987801	0.6126434408443900	0.2884716081426114
O31	0.3850434433786659	0.5518736122303732	0.3839615060102449
O32	0.6045783876554109	0.5906618126929019	0.1826811863727057
O33	0.5419016857520021	0.3648705202006915	0.2894728270310250
O34	0.6198771649448421	0.5860190225843687	0.4801504469218213
O35	0.3886949935129664	0.3842544197099939	0.1875922305856680
O36	0.6144313134397139	0.4277719158167647	0.3820814634778682
O37	0.5029672596713742	0.5401004567963731	0.3737065526471851
O38	0.5488875883390336	0.4849541082857883	0.3020980831693468
O39	0.4960056553694425	0.4388452723859201	0.3749967462951969
O40	0.4478662396596480	0.4922253414299246	0.3035910048565287

N1	0.5122602161442678	0.5171208833218812	0.5723932759692169
N2	0.4952806972865921	0.4643068426392397	0.5733338203582390
P1	0.4989347620234403	0.4890259559891833	0.3378819535985692
H1	0.4880878304074560	0.5448156608837819	0.5910715468184701
H2	0.5210908263388916	0.4369684655455544	0.5903465381268487

PMAMo_NH-NH_2 (Enzymatic)

Atoms	X	Y	Z
Mo1	0.4371046542033906	0.5699729345348286	0.4400542155836111
Mo2	0.5655713016178168	0.4156715413539828	0.2290178433198989
Mo3	0.5653217902692749	0.4042866540043233	0.4313668065404381
Mo4	0.4284711092775191	0.5615393135011529	0.2307952742801068
Mo5	0.5833307409471086	0.5662341574925094	0.4274080727619083
Mo6	0.4145261659322134	0.4241999566904439	0.2357033217254112
Mo7	0.5772746541103938	0.5545221939647017	0.2338370920385089
Mo8	0.4200975105275986	0.4094646063245082	0.4299344786247255
Mo9	0.5045448883621068	0.6344577714038377	0.3366856112261789
Mo10	0.4906014090583614	0.3411651148125622	0.3331097778178745
Mo11	0.3553895279739861	0.5039102139737657	0.3327838790027578
Mo12	0.6454056085165016	0.4753353952112212	0.3239920990293005
Mo13	0.4968017322735261	0.4945238970511851	0.4963779276940239
O1	0.6415209105025845	0.5309157028481901	0.2734698749652952
O2	0.5645163275050321	0.6273200761556410	0.3923871283751876
O3	0.3565961094876516	0.4456825768875584	0.2787270769931910
O4	0.4391641415329840	0.3473455301927798	0.3966346506379016
O5	0.3644916256834023	0.5517183449599536	0.2747556731093370
O6	0.4583770507264650	0.6307308329790708	0.3971662507310039
O7	0.5422353971125830	0.3438634118296149	0.3974624610544063
O8	0.6322348709548623	0.4227318599892088	0.2731740129484205
O9	0.4933760509930311	0.4156968904127356	0.4729967255589723
O10	0.5132986164977495	0.5701046919816012	0.4720448296573641
O11	0.5827335760807196	0.4829745652342753	0.1997950150472530
O12	0.4130910909849235	0.4925363919781110	0.2004717503066368
O13	0.4375375774975572	0.3708590861255973	0.2900840056346835
O14	0.3999541131516064	0.5980505296946388	0.4896642200778979
O15	0.3756734040582878	0.4417132737271470	0.3820429296672174
O16	0.5864595967281782	0.3724219148648668	0.1808698673870419
O17	0.4063117918036903	0.6041740029546037	0.1827336213742854
O18	0.6253680051689722	0.5312156057971053	0.3793792527189533
O19	0.6031852039218305	0.3807832279803262	0.4831395678737015
O20	0.5581114944034349	0.6029520388719813	0.2887369021437678

O21	0.2888961083298233	0.5090923851405232	0.3458247416671533
O22	0.5634851687751160	0.4875317610507781	0.4595212174777274
O23	0.4319239118743142	0.4897070889392657	0.4573072326098758
O24	0.7120663312232953	0.4690079794077096	0.3359876707352130
O25	0.4873955162065683	0.2742789185795074	0.3210550893298957
O26	0.5029850807853404	0.5539138135891654	0.2142892101774982
O27	0.4914836646400896	0.4205376744536388	0.2175858262820642
O28	0.5082904829730247	0.7011790083629962	0.3244246470746948
O29	0.3796166156280401	0.3891499842907300	0.4809688980552409
O30	0.4540003111647066	0.6103494318866134	0.2867954597761788
O31	0.3860360471998135	0.5492301448563374	0.3849048379549070
O32	0.6052395046519045	0.5943984469383120	0.1864058848846215
O33	0.5439997977075879	0.3650513985018122	0.2883005678871362
O34	0.6263472092730815	0.5868300595431973	0.4763981901871288
O35	0.3856873762366048	0.3837727956205951	0.1892911181775707
O36	0.6139176900647493	0.4284148433644839	0.3820128237387284
O37	0.5046084539980032	0.5375287317044537	0.3736491412421264
O38	0.5494592719291675	0.4843690190278334	0.3001514120274894
O39	0.4957562929912998	0.4364818870786759	0.3715390939040344
O40	0.4483949500354630	0.4925109296503776	0.3021689877505798
N1	0.5012963465091094	0.5279295209440761	0.5768596015796116
N2	0.4882992889060642	0.4735115928308655	0.5713566179125545
P1	0.4995818326387587	0.4879316527721077	0.3362881316154392
H1	0.4716140580062121	0.5513759455702492	0.5926559833761065
H2	0.5071987233606104	0.4465571046547424	0.5957911423351893
H3	0.5387717250259139	0.5380734204569245	0.5903642663339712

PMAMo_NH_2-NH_2 (Enzymatic)

Atoms	X	Y	Z
Mo1	0.4189999866587467	0.5836246633502166	0.4216268075487527
Mo2	0.5715221244339070	0.4122411951995715	0.2416201211840833
Mo3	0.5636279213003855	0.4082045299057517	0.4356121289916101
Mo4	0.4265071306648102	0.5608509421965973	0.2264538717028889
Mo5	0.5640015832119117	0.5701158399760229	0.4322171496243311
Mo6	0.4235035870540969	0.4225038609218907	0.2281136260522423
Mo7	0.5774216200834482	0.5514304639195705	0.2310837573054706
Mo8	0.4185935381910325	0.4236920476507627	0.4357575978049333
Mo9	0.5045042928954921	0.6379981293859347	0.3271583901202856
Mo10	0.4830174835749460	0.3452732952152648	0.3414414025225910
Mo11	0.3513202308137582	0.4938258834844877	0.3217960966005946
Mo12	0.6426535678102312	0.4866681055139594	0.3337881962778897

Mo13	0.4799614789745411	0.4896862818143528	0.4900771482476613
O1	0.6391830162640113	0.5380330099853793	0.2800158828030944
O2	0.5510650005555355	0.6316116230716509	0.3947317811823555
O3	0.3583675372074501	0.4422401451735811	0.2665706959275520
O4	0.4338740850399683	0.3572059138479671	0.3975719560146684
O5	0.3633148562243962	0.5485112925330330	0.2658689119727740
O6	0.4489118603123934	0.6406593870556095	0.3868574267385557
O7	0.5400558862016829	0.3485980464630568	0.4007552843530084
O8	0.6353031234822403	0.4299814842843447	0.2846306209042008
O9	0.4911185415363346	0.4106944180152153	0.4779444386921560
O10	0.4881491827787497	0.5697856414529032	0.4693515252665218
O11	0.5876073370866727	0.4813132006254507	0.2056620313796104
O12	0.4189598111530264	0.4915757138121528	0.1942003722268311
O13	0.4392859539627194	0.3731652253430754	0.2870801490330634
O14	0.3773275170718054	0.6127018803429333	0.4672241457477791
O15	0.3729828973316774	0.4470063693038667	0.3770296968876424
O16	0.5975843002702131	0.3674612352920379	0.1975637095072453
O17	0.4061857283978808	0.6022354474146270	0.1764797948446448
O18	0.6137026071893782	0.5394622645785734	0.3872047493782266
O19	0.6005488510247651	0.3851563528821031	0.4885923210503348
O20	0.5576352871970630	0.6060990076421600	0.2869375706642208
O21	0.2839742373234273	0.4970977900736843	0.3305213398205721
O22	0.5507652610939009	0.4894179880722388	0.4586232177857986
O23	0.4149700295766174	0.5053128051730951	0.4535457433750018
O24	0.7087550850799683	0.4854441785712577	0.3498839958939778
O25	0.4800525992807242	0.2780298696012086	0.3319442386591884
O26	0.5041138117615580	0.5546976958329318	0.2142336416463651
O27	0.4992960023650936	0.4207387280357901	0.2166781414884902
O28	0.5101287915766550	0.7042563449836243	0.3126923917986936
O29	0.3777710237271996	0.4027019635944087	0.4864015661057769
O30	0.4514784829494228	0.6130658236346499	0.2810556986768140
O31	0.3754143809065631	0.5552729529752042	0.3702978122949239
O32	0.6065717474202610	0.5897538457816736	0.1830425936065847
O33	0.5431140421128978	0.3687772527824643	0.2965647150217152
O34	0.6001066081151750	0.5908173105248343	0.4864098217365176
O35	0.3994991699557098	0.3809082252222080	0.1799940801516227
O36	0.6127808862587669	0.4351586734610431	0.3890021250947927
O37	0.4953409131711856	0.5447249906558658	0.3689101053482551
O38	0.5477644225233788	0.4870329649343826	0.3040680282833848
O39	0.4909736525978440	0.4437282941142150	0.3761036520942632
O40	0.4467319694493450	0.4916170255397834	0.2981913668145348
N1	0.5088789425073558	0.4661620257636925	0.5709598478062644

N2	0.4512367614724473	0.4607778646456223	0.5673455232697490
P1	0.4953344592746544	0.4917612060907533	0.3360459253021074
H1	0.5206712564298437	0.4905887305590123	0.6016844445222084
H2	0.4314578265972162	0.4830636142489360	0.5954886831835872
H3	0.5274496731848750	0.4295031867592214	0.5728459352041397
H4	0.4388501093326486	0.4214957697141464	0.5680159754568251

PMAMo_NH_2…. NH_3 (Enzymatic)

Atoms	X	Y	Z
Mo1	0.4147335989390727	0.5736573262988571	0.4237622082981294
Mo2	0.5730581362469237	0.4148623594929992	0.2381488422846247
Mo3	0.5630130296486987	0.4015014370817835	0.4322322065527421
Mo4	0.4269624945382334	0.5621670520335449	0.2288860400815072
Mo5	0.5623605863393348	0.5612738271532015	0.4372901926349620
Mo6	0.4255292875018553	0.4240049390795214	0.2228284203538317
Mo7	0.5779002757946174	0.5543500302903597	0.2357590783942745
Mo8	0.4140782764721878	0.4140361989041045	0.4306864134570934
Mo9	0.5022693344119554	0.6341774790471464	0.3352455888377419
Mo10	0.4839908277380139	0.3425605410521318	0.3338541654773730
Mo11	0.3498013974621270	0.4892191748171620	0.3181477497255278
Mo12	0.6431061556801432	0.4843198388453544	0.3350110041710803
Mo13	0.4760073853375522	0.4785383965006451	0.4912948575819677
O1	0.6392020252856008	0.5392648374777081	0.2851368982776485
O2	0.5475084422104667	0.6244087770808459	0.4034758563019641
O3	0.3591245372432696	0.4408858342015947	0.2606803064915878
O4	0.4330139273315469	0.3508924718468392	0.3889169342797043
O5	0.3629270741136998	0.5471864383254158	0.2661571732150609
O6	0.4453324173559282	0.6330099861180971	0.3940604789246059
O7	0.5394885652011098	0.3438952704379105	0.3937681921618109
O8	0.6367163521035807	0.4306719092723910	0.2832827154597211
O9	0.4878800539768531	0.4041254286884209	0.4711188002065113
O10	0.4843322461787609	0.5559047605870202	0.4718387828125423
O11	0.5897616736196574	0.4860015748846091	0.2066420506272273
O12	0.4206654680407134	0.4948581081379587	0.1925691880821247
O13	0.4411043097712601	0.3725950438616171	0.2795304242852982
O14	0.3733718315220923	0.5997305690165222	0.4714187583550469
O15	0.3705032128060987	0.4400931472464795	0.3718217331924165
O16	0.6004782467200268	0.3726933302030583	0.1923922761095222
O17	0.4071577592801214	0.6061476059116204	0.1809819261240199
O18	0.6130814872483199	0.5342366475160260	0.3922805291907487
O19	0.5991349055411765	0.3737848782967465	0.4829789157393683

O20	0.5565798986160767	0.6057815482538572	0.2941544272405341
O21	0.2822319502080827	0.4913440238113275	0.3250089640085824
O22	0.5492185199057694	0.4801809797189782	0.4626551543840316
O23	0.4119929755840080	0.4937971258062694	0.4514730079591686
O24	0.7090470857297204	0.4831414682401554	0.3516833083079099
O25	0.4820323143527011	0.2759106825427523	0.3208000058142643
O26	0.5049298918463396	0.5577204121205216	0.2176986810120396
O27	0.5016120199280814	0.4240943076661605	0.2121890330788722
O28	0.5074037292663505	0.7013229571925594	0.3252783549187828
O29	0.3712455453514454	0.3883944427513632	0.4767163279677314
O30	0.4503505353340844	0.6116435680065575	0.2867666489507148
O31	0.3716347854794855	0.5483997281139958	0.3710007889130686
O32	0.6074650084606120	0.5957227982166121	0.1905981464907002
O33	0.5445355092623851	0.3687625287975935	0.2904679806175962
O34	0.5957675096579415	0.5815651044887539	0.4934435538377124
O35	0.4030045159749460	0.3845503847763791	0.1722839887435827
O36	0.6127714856107838	0.4310439296471590	0.3880683558851236
O37	0.4937864780638769	0.5397769354415940	0.3709327211256794
O38	0.5478644081890461	0.4861528569773802	0.3040778049313262
O39	0.4901795340064545	0.4389741885132661	0.3729872412926087
O40	0.4466512726524506	0.4900096309502431	0.2967450292128324
N1	0.5012710947856620	0.5722826908755915	0.6148949059766041
N2	0.4674712150673057	0.4818481940358046	0.5653902749755602
P1	0.4947352502334667	0.4885225794225715	0.3353494850626603
H1	0.4741849271942624	0.5879830112447187	0.6412916719776528
H2	0.4455724236409218	0.4550061690234473	0.5873865011799604
H3	0.5370754355518802	0.5683763316874599	0.6344044734377562
H4	0.4816550621891978	0.5177239886325826	0.5879426702566145
H5	0.5066241481956747	0.5997023633366362	0.5848719107525701

PMAMo…. NH_3 (Enzymatic)

Atoms	X	Y	Z
Mo1	0.4338217030226515	0.5773620567245736	0.4337349579633312
Mo2	0.5666476558062710	0.4131275839795678	0.2349075146127134
Mo3	0.5653504701885332	0.4022497382541991	0.4341046001465940
Mo4	0.4267361208726586	0.5632038458227810	0.2354400664716959
Mo5	0.5775180020853102	0.5668170608536760	0.4325043918371521
Mo6	0.4165488281215260	0.4244117033292362	0.2365867462334798
Mo7	0.5766713418186431	0.5522554827775316	0.2337457675413506
Mo8	0.4219001181806745	0.4127057466136795	0.4352752446754816
Mo9	0.5093880098240068	0.6371415451316654	0.3351629527385508

Mo10	0.4877268459072199	0.3408718720199962	0.3376321850211388
Mo11	0.3537207192966491	0.4995270952376189	0.3338485716249369
Mo12	0.6436079581341243	0.4782089425891413	0.3292167022317431
Mo13	0.4997997933799637	0.4906267593376437	0.5013094380392612
O1	0.6400035653485656	0.5320709369611734	0.2769883138700251
O2	0.5621524231098856	0.6286918065116349	0.3963963668973355
O3	0.3562058836743793	0.4452363285953935	0.2789716393049403
O4	0.4367731099214749	0.3501310124557371	0.3994615860168324
O5	0.3638805596472900	0.5516210074320590	0.2777788792920238
O6	0.4576424656267388	0.6363946288097704	0.3965250737077249
O7	0.5410948039579619	0.3426154948708040	0.3992307618557914
O8	0.6321207205098313	0.4243337356649260	0.2780925205451649
O9	0.4940759654150371	0.4115633022771430	0.4782954887702530
O10	0.5056207535936015	0.5690598316047443	0.4767804381091433
O11	0.5829502721100642	0.4814550085450852	0.2034594969319837
O12	0.4145372472438092	0.4938305246753505	0.2034623734795371
O13	0.4373275432006015	0.3723580845522225	0.2917423245655548
O14	0.3960362155695499	0.6030132081270208	0.4844915953180059
O15	0.3767209881675774	0.4446183867585443	0.3863715930619063
O16	0.5884183847212564	0.3696558362164347	0.1873768207603642
O17	0.4047740361932680	0.6056153956693268	0.1870875000774458
O18	0.6211234715868437	0.5332111583341262	0.3841523857718271
O19	0.6037801009449795	0.3779191754529302	0.4851374366135626
O20	0.5600117215061258	0.6044292493700696	0.2898095582486982
O21	0.2872943879269735	0.5044551343120411	0.3470606149633121
O22	0.5632959396971958	0.4854876365842027	0.4619043103707005
O23	0.4360324036677625	0.4948110281522737	0.4620382262779028
O24	0.7102293752078316	0.4734266523589479	0.3420861701101953
O25	0.4829098637273126	0.2742477568145733	0.3251260390893551
O26	0.5026443477941653	0.5543935034347174	0.2181116111441613
O27	0.4929288269849072	0.4210737251318986	0.2196049225346120
O28	0.5143954634234164	0.7034750042521217	0.3213618330818467
O29	0.3809901891777115	0.3940478202202449	0.4867021450377595
O30	0.4550097686691499	0.6124591571074847	0.2892140047174238
O31	0.3844773256583145	0.5514321606319964	0.3852674845711893
O32	0.6045247206945387	0.5911540402004377	0.1854299205254206
O33	0.5425465380367543	0.3647661363916395	0.2921094159876931
O34	0.6192889032370376	0.5863519703495930	0.4829403006484225
O35	0.3886403548706445	0.3846252534122668	0.1890732710718511
O36	0.6133545174566261	0.4281800175336877	0.3852438491176389
O37	0.5026806209384900	0.5401289231014387	0.3761972802192309
O38	0.5485981681302593	0.4849732349218620	0.3047018531386438

O39	0.4952061198749850	0.4385233695306971	0.3771682195093335
O40	0.4475483915857277	0.4924623683963630	0.3059434773817135
N1	0.4978136439634304	0.4878367359539884	0.5896304065104352
P1	0.4985375634693382	0.4890130470441177	0.3402865262217603
H1	0.5197660367242833	0.5178345071232824	0.6072948841232764
H2	0.5111089842290342	0.4519536348981860	0.6048061880129482
H3	0.4590195771670119	0.4924934675861524	0.6027157642976054

References

1 H. J. van Grinsven, L. Bouwman, K. G. Cassman, H. M. van Es, M. L. McCrackin and A. H. Beusen, *J. Environ. Qual.*, 2015, **44**, 356-367.

2 D. G. Capone and J. P. Montoya, *Meth. Microbiol.*, 2001, **30**, 501-515.

3 R. Manjunatha and A. Schechter, *Electrochem. Commun.*, 2018, **90**, 96-100.

4 J. Zhao and Z. Chen, *J. Am. Chem. Soc.*, 2017, **139**, 12480-12487.

5 S. Kuriyama, K. Arashiba, K. Nakajima, Y. Matsuo, H. Tanaka, K. Ishii, K. Yoshizawa and Y. Nishibayashi, *Nat. Commun.*, 2016, **7**, 12181.

6 N. Cao and G. Zheng, *Nano Res.*, 2018, **11**, 2992-3008.

7 Y. Jia, J. Zhang, Z.-M. Zhang, Q.-Y. Li and E.-B. Wang, *Inorg. Chem. Commun.*, 2014, **43**, 5-9.

8 S. Wen, W. Guan, J. Wang, Z. Lang, L. Yan and Z. Su, *Dalton Trans.*, 2012, **41**, 4602-4607.

9 S. Wen, W. Guan, Y. Kan, G. Yang, N. Ma, L. Yan, Z. Su and G. Chen, *Phys. Chem. Chem. Phys.*, 2013, **15**, 9177-9185.

10 X. Lu, D. T. Morelli, Y. Xia and V. Ozolins, *Chem. Mater.*, 2015, **27**, 408-413.

11 S. Zhao, X. W. Liu, C. F. Huo, Y. W. Li, J. Wang and H. Jiao, *Catal. Struct. & Reactivity*, 2015, **1**, 44-60.

12 J. Nørskov, J. Rossmeisl, Logadottir, A., L. Lindqvist, J. Kitchin, T. Bligaard and H. Jónsson, *J. Phys. Chem. B,* 2004, **108**, 17886-17892.