

Supporting Information

Element Table of TM-substituted Polyoxotungstates for Direct Electrocatalytic Reduction of Nitric Oxide to Ammonia: A DFT Guideline for Experiments

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Computational details for the periodic POM-graphene model

Considering the low electroconductivity and specific surface area of polyoxometalates, we constructed a composite model by adsorbing the $\text{SiW}_{11}\text{Ni}^{\text{II}}$ on the graphene surface, aiming to evaluate its possibility in experiment and promote this kind of catalysts applied in NOER in a quite near future.

With regard to the size of the Keggin anion ($\sim 11 \text{ \AA}$), we built a orthogonal cell $17.33 \times 17.15 \times 30 \text{ \AA}$ with 112 carbon atoms to support the polyoxometalate $\text{SiW}_{11}\text{O}_{39}\text{Ni}^{\text{II}}(\text{H}_2\text{O})$. The c direction was set to 30 \AA by considering a vacuum space of $>15 \text{ \AA}$, which was proven to be sufficient to prevent the interactions between the replicated cells. Previous study has suggested the adsorption of POM on the graphene are thermodynamic preferable via the S4 orientation, therefore only this orientation is considered in this work.^[1] Regarding to the anion character, we introduced six hydrogen to balance the negative charge and keeps neutral for the whole system. In Figure S4, a 2×2 supercell for $\text{H}_6\text{SiW}_{11}\text{O}_{39}\text{Ni}(\text{H}_2\text{O})$ deposited on the graphene surface is displayed. The isolated POM molecule was calculated in a cubic box with a 25 \AA side.

All first-principles calculations were performed using the Vienna ab initio simulation package (VASP5.3). We set the kinetic energy cutoff to 400 eV and used the PBE functional to describe the exchange correlation potential.^[2] The van der Waals interactions were corrected by DFT-D3 method with B–J damping.^[3] The interaction between valence electrons and the corresponding pseudopotential for each atom was taken into account with the projector augmented wave (PAW) scheme.^[4] A Monkhorst–Pack k-mesh sampling of $3 \times 3 \times 1$ was used for structural optimization and density of states (DOS) calculations.^[5] All optimizations were reached until self-consistency, with thresholds of $1 \times 10^{-5} \text{ eV}$ and 0.02 eV \AA^{-1} for electronic and ionic convergence, respectively.

References

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	PCM model	HSM model
TS1	<p>$f/i = -1160.5 \text{ cm}^{-1}$</p>	<p>$f/i = -645.4 \text{ cm}^{-1}$</p>
TS2	<p>$f/i = -716.9 \text{ cm}^{-1}$</p>	<p>$f/i = -889.7 \text{ cm}^{-1}$</p>

Fig. S1. The transition state diagrams for the successive reduction of *NO to *NHO and *NHOH based on the PCM and HSM models.

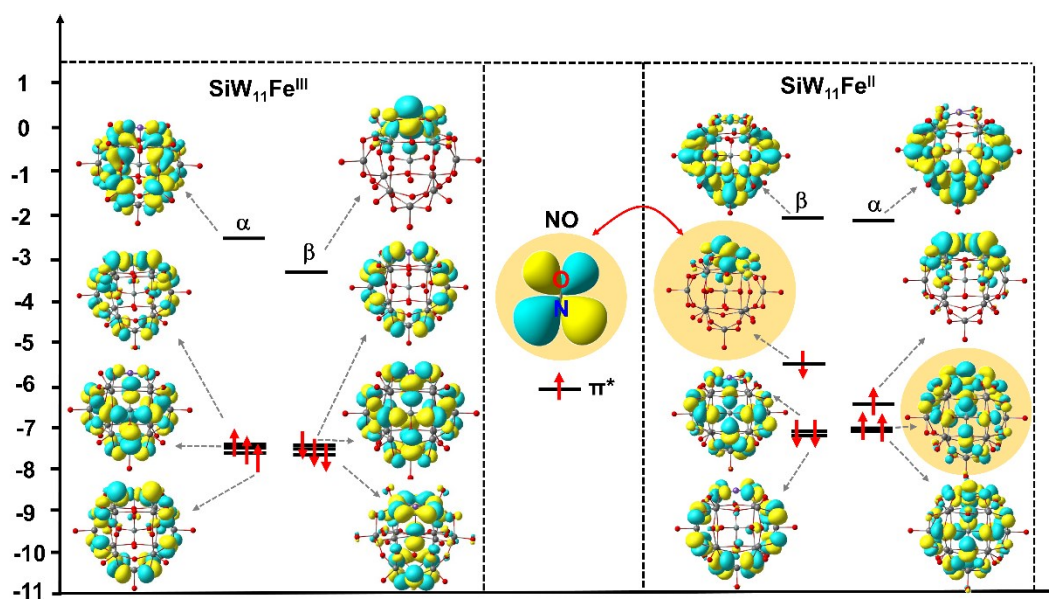


Fig. S2. Representation of the Kohn-Sham frontier molecular orbitals for the $\text{SiW}_{11}\text{Fe}^{\text{II}}$, $\text{SiW}_{11}\text{Fe}^{\text{III}}$, and the individual NO.

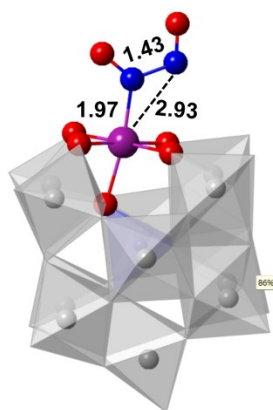


Fig. S3. The geometric representation (distance in Å) for the adsorption of two NO on $\text{SiW}_{11}\text{Fe}^{\text{II}}$.

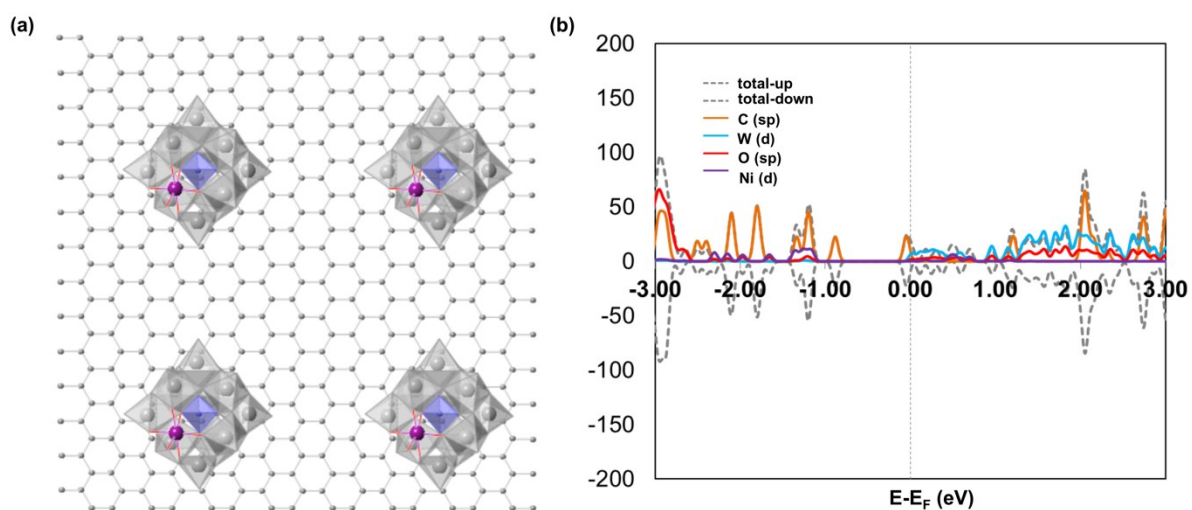


Fig. S4. (a) Ball-stick-polyhedra representation of the optimized geometries (a 2×2 supercell) for $\text{H}_6\text{SiW}_{11}\text{O}_{39}\text{Ni}(\text{H}_2\text{O})$ deposited on the graphene surface at VASP/PBE-D3/kpoint (111) level; (b) Projected density of states for $\text{H}_6\text{SiW}_{11}\text{O}_{39}\text{Ni}(\text{H}_2\text{O})$ -GO model.

Table S1. The relative electronic energies (eV) for the possible intermediates involved in each elementary electronic reduction step catalyzed by $\text{SiW}_{11}\text{Fe}^{\text{II}}$.

Reduction step	Species	Multiplicity	ΔE (eV)
NO-ads	$\text{SiW}_{11}\text{Fe}^{\text{II}}\text{-NO}$	S4	0.00
		S6	0.43
+ $1\text{H}^+/1\text{e}^-$	$\text{SiW}_{11}\text{Fe}^{\text{II}}\text{-NHO}$	S3	0.44
		S5	0.00
	$\text{SiW}_{11}\text{Fe}^{\text{II}}\text{-NOH}$	S3	---
		S5	1.04
+ $2\text{H}^+/2\text{e}^-$	$\text{SiW}_{11}\text{Fe}^{\text{II}}\text{-NHOH}$	S2	0.41
		S4	0.04
		S6	0.00
	$\text{SiW}_{11}\text{Fe}^{\text{II}}\text{-NH}_2\text{O}$	S2	1.55
		S4	1.27
+ $3\text{H}^+/3\text{e}^-$	$\text{SiW}_{11}\text{Fe}^{\text{II}}\text{-NH}_2\text{OH}$	S3	1.95
		S5	0.00
	$\text{SiW}_{11}\text{Fe}^{\text{II}}\text{-NH-H}_2\text{O}$	S3	2.61
		S5	1.49
+ $4\text{H}^+/4\text{e}^-$	$\text{SiW}_{11}\text{Fe}^{\text{II}}\text{-NH}_2\text{-H}_2\text{O}$	S4	0.58
		S6	0.00
+ $5\text{H}^+/5\text{e}^-$	$\text{SiW}_{11}\text{Fe}^{\text{II}}\text{-NH}_3\text{-H}_2\text{O}$	S5	0.00

xyz coordination for the intermediates related to $\text{SiW}_{11}\text{Fe}^{\text{II}}$

$\text{SiW}_{11}\text{Fe}^{\text{II}}$

-6 5

W	1.90486700	2.39365100	-1.92254500
W	1.95016200	2.44123100	1.48395600
W	1.02253100	-3.35223400	-0.17267800
W	-2.87059600	0.97097100	-2.08949600
W	2.91798100	-1.14567700	1.48237900
W	-2.83482000	0.97387100	1.68057700
W	-1.97401300	-2.25833500	1.67709000
W	-0.09961000	-0.03248200	3.35411000
W	2.86832100	-1.13711200	-1.93712700
W	-0.79287700	3.41800700	-0.16717100
W	-2.00110500	-2.24638600	-2.08044300
Si	-0.02782000	-0.00914100	-0.17954700
O	-4.38154500	1.70465100	-2.47674300
O	2.36950500	-2.96801900	-1.46822700
O	1.24582600	-1.04783900	-0.21363400
O	-2.01723700	0.98988400	-3.65358400
O	4.29650100	-1.42450900	-2.85824800
O	-0.31530900	-3.05986400	1.16699300
O	0.74435400	1.54173900	2.69153000
O	0.55378700	1.52935300	-0.20142500
O	-1.86261100	2.50033300	-1.42361600
O	-2.44084200	-2.27032800	-0.11275400
O	2.86707500	0.76430200	1.43253500
O	1.41570100	-0.96152500	2.68918900
O	0.83192600	1.64785900	-3.15149700
O	2.97223200	3.34390800	-2.88223200
O	-0.90924500	-0.24664500	1.18736800
O	-0.36218900	-3.07321400	-1.43109300
O	4.19188700	-1.42096500	2.60251000
O	2.89495900	0.76641200	-1.71328300
O	1.61014700	-1.04583000	-3.18917500
O	2.92514800	3.31857100	2.59402200
O	-1.78891000	2.49934900	1.18151800
O	-0.98873400	-0.24762400	-1.48471100
O	-1.22367400	-1.79214000	-3.63641300
O	2.71642400	2.92265400	-0.14322300
O	0.55580800	3.72533200	1.18059100
O	3.82460300	-1.19150700	-0.12962000
O	-3.24250700	0.75846400	-0.09838800
O	2.32859800	-2.95131100	1.18852500
O	-3.26251900	-0.87394700	2.03999000
O	1.12376700	-5.06707800	-0.16041300
O	-1.76694800	0.89890700	3.31710100
O	-2.82557800	-3.61628000	2.30080200
O	0.26280000	0.06115800	5.03292300
O	-4.24743300	1.72563300	2.31248600

O	-2.92322200	-3.63369600	-2.51770700
O	0.56462100	3.73977300	-1.47338100
O	-1.54821800	4.96063300	-0.15014100
O	-1.08030900	-1.67430000	3.31111900
O	-3.36067200	-0.89076900	-2.21734700
Fe	-0.16602000	-0.04967600	-3.45636700

SiW₁₁Fe^{II}-NO

-6 4

W	-2.23960400	-1.81282600	-2.11219500
W	-2.72650400	-1.80013100	1.25043700
W	-0.05786000	3.51015300	-0.13962400
W	2.70814100	-1.72366100	-1.64500100
W	-2.67215400	1.91109700	1.20563200
W	2.21246000	-1.68491000	2.07466000
W	2.27022100	1.65859800	2.03557400
W	-0.33296800	0.04766700	3.41192800
W	-2.17782400	1.83564500	-2.15405400
W	-0.16849000	-3.50962300	-0.06450300
W	2.75968400	1.60440800	-1.68540900
Si	0.03656100	-0.00153900	-0.10995600
O	3.98688100	-2.84618100	-1.90605000
O	-1.26999700	3.47628400	-1.61376300
O	-0.89678000	1.34625300	-0.25140900
O	2.06425600	-1.49193200	-3.31094000
O	-3.29978400	2.47739500	-3.29200400
O	0.96459900	2.87627200	1.34599100
O	-1.48253000	-1.23949500	2.61178400
O	-0.93703200	-1.32349900	-0.22150700
O	1.25733700	-2.92034000	-1.16089900
O	2.93957800	1.52526300	0.31882500
O	-3.14610200	0.06176500	1.11382800
O	-1.44372000	1.34828700	2.58313100
O	-0.85302200	-1.38418200	-3.15832900
O	-3.38566000	-2.44454300	-3.23165700
O	0.77244700	0.00433100	1.36342200
O	1.34801400	2.85496300	-1.22698600
O	-3.95790900	2.53831800	2.15575400
O	-2.77028000	0.02221500	-1.98559600
O	-0.80302300	1.33458700	-3.18527700
O	-4.02967000	-2.36492900	2.21581900
O	0.87463100	-2.87734300	1.41157700
O	1.16581200	-0.03207600	-1.29401300
O	2.11204400	1.35375600	-3.34554000
O	-3.38432800	-2.09097100	-0.46571200
O	-1.69910200	-3.41900400	1.10301700
O	-3.31828100	2.18500500	-0.51745900
O	2.88849500	-1.60759800	0.35566700
O	-1.59340800	3.49351900	1.02386400
O	3.07832800	-0.02006900	2.51985600
O	0.30449300	5.18782500	-0.10015800
O	1.01012900	-1.30507700	3.56207700
O	3.37223600	2.73998900	2.79154500
O	-0.91677800	0.07422600	5.02825600
O	3.28194500	-2.78062700	2.85604200
O	4.07444800	2.67893400	-1.96905200

O	-1.38030100	-3.47062500	-1.53605600
O	0.14286100	-5.19625700	0.01128700
O	1.05367400	1.35661200	3.53141300
O	3.70384200	-0.07567000	-1.67955500
Fe	0.62049300	-0.05141000	-3.51523500
N	0.68033600	-0.07972100	-5.37071500
O	1.42609000	-0.14269900	-6.27625100

SiW₁₁Fe^{II}-HNO

-6 5

W	-2.86223800	0.97549500	1.91335800
W	-3.01059300	1.00945100	-1.48569200
W	0.96708700	-3.37398400	0.03727400
W	1.92010600	2.32709500	1.96821500
W	-1.86368100	-2.52365500	-1.53408000
W	1.81095300	2.36540700	-1.78463400
W	2.83244400	-0.81840200	-1.84688600
W	0.00751500	0.06226300	-3.43625500
W	-1.73338900	-2.49690400	1.86186700
W	-1.19250300	3.29932000	0.13967800
W	2.97390800	-0.83251200	1.90711100
Si	0.02774300	0.01085300	0.10841200
O	2.77549400	3.75760400	2.39727400
O	-0.33406900	-3.76863200	1.37771700
O	-0.47770900	-1.55476000	0.11783000
O	1.23704500	1.80616300	3.55599300
O	-2.71091500	-3.50317300	2.85862700
O	1.88706900	-2.39806200	-1.32833600
O	-1.53991700	0.91000600	-2.73402100
O	-1.29845600	0.98437400	0.15392200
O	0.22824900	3.07025800	1.37591700
O	3.27901400	-0.58920800	-0.07333300
O	-2.86335500	-0.89790900	-1.44749300
O	-0.73864100	-1.55586400	-2.76604500
O	-1.51287000	0.92744000	3.07160000
O	-4.24266300	1.19012300	2.92321200
O	0.86444600	0.29882400	-1.27940400
O	2.01934200	-2.40410200	1.27093000
O	-2.81946500	-3.44381200	-2.62475200
O	-2.81777600	-0.92987200	1.69526800
O	-0.66194600	-1.68122900	3.05311800
O	-4.32867000	1.22468800	-2.56581800
O	0.12524100	3.07994000	-1.22853200
O	0.99011000	0.28597200	1.40448900
O	2.16250100	-0.89511300	3.50123800
O	-3.87935400	0.99420500	0.15619600
O	-2.51519400	2.84166900	-1.19000700
O	-2.56135100	-3.06312500	0.10915400
O	2.31102300	2.39229600	-0.00444000
O	-0.39568300	-3.73666500	-1.27889000
O	3.15693700	1.05346500	-2.19240400
O	1.79996000	-4.87476900	-0.00718200
O	0.90691800	1.74815400	-3.40013600
O	4.26616800	-1.48828400	-2.51948100
O	-0.38750000	-0.03813800	-5.10608700
O	2.57807700	3.76893200	-2.41531300
O	4.52426500	-1.49316100	2.26210300

O	-2.48431300	2.84057000	1.46125100
O	-1.37375200	5.00687100	0.14412400
O	1.72140800	-0.78442000	-3.44782800
O	3.36082200	1.05009300	2.04574700
Fe	0.27566600	0.02290000	3.52363600
N	-0.09288900	-0.29497100	5.44723000
O	0.37063700	0.22721900	6.46215100
H	-0.74551900	-1.07555600	5.67351800

SiW₁₁Fe^{II}-NHOH

-6 4			
W	-0.73707200	3.09538400	1.59589900
W	-1.69656000	2.58873700	-1.62894600
W	-1.72376500	-2.86234700	1.09580000
W	3.44119200	0.42886300	1.02842900
W	-3.43271300	-0.52253700	-0.57157800
W	2.37388300	-0.19027000	-2.52010200
W	0.82215600	-2.99053100	-1.56630200
W	-0.86906000	-0.63957400	-3.26490200
W	-2.44544500	0.04681900	2.65132400
W	1.53712400	3.01152100	-0.88989800
W	1.87666300	-2.35791800	1.98339200
Si	0.04334400	-0.00496700	0.10552300
O	5.12292100	0.75260000	0.86161700
O	-2.53994000	-1.90529400	2.52516000
O	-1.38636600	-0.61752200	0.64795300
O	3.14445400	0.96353700	2.72894000
O	-3.60020100	0.33409100	3.90039900
O	-0.77339500	-3.18979100	-0.53845600
O	-1.10620700	1.19771100	-2.83071600
O	-0.14779700	1.61489200	-0.12492300
O	2.65700000	2.04444700	0.29971700
O	1.74505200	-2.82464800	0.02337800
O	-2.92531700	1.27447300	-0.98691300
O	-2.30802500	-0.98133400	-2.08720400
O	0.43003100	2.27833500	2.66885300
O	-1.23927800	4.45378100	2.52998100
O	0.43168900	-0.70650300	-1.33372200
O	-0.02068800	-2.77441700	1.91794500
O	-4.98590100	-0.61006400	-1.30188900
O	-2.10549500	1.81333700	1.99151000
O	-0.91572300	-0.01570100	3.54000100
O	-2.70384000	3.50446800	-2.67736600
O	1.89861800	1.63087100	-2.16018000
O	1.23268500	-0.28003200	1.19620200
O	1.70824600	-1.47569100	3.53220700
O	-1.85549400	3.54130400	-0.03950400
O	-0.00997800	3.45542800	-1.95057100
O	-3.85957500	-0.04132100	1.15682600
O	3.18988300	-0.20827700	-0.86230700
O	-3.22069400	-2.34673300	-0.00407500
O	2.25530300	-2.11053800	-2.51625800
O	-2.21395000	-4.45697300	1.50624200
O	0.92098100	-0.22456400	-3.81299500
O	1.13376200	-4.61942000	-2.02451800
O	-1.64044600	-0.73002100	-4.79971000
O	3.70000600	0.01912800	-3.59581200

O	2.53853900	-3.86507500	2.49324100
O	0.70559100	3.92206300	0.56212700
O	2.60828600	4.24149400	-1.42907400
O	-0.31007100	-2.45747900	-3.06356500
O	3.50259100	-1.43456900	1.49413500
Fe	1.09327400	0.47304900	3.28320000
N	1.79061600	1.14550900	5.19428000
O	3.04624200	1.58767000	5.17256900
H	1.45729100	1.30484200	6.14632800
H	3.31467300	1.41473200	4.20857700

SiW₁₁Fe^{II}-NH₂OH

-6 5

W	-1.92039300	2.52365300	1.61351800
W	-1.03217400	2.89889800	-1.65096600
W	-1.50071200	-3.08939100	-0.63843700
W	2.33833700	0.22949900	2.79556800
W	-2.48557000	-0.43047500	-2.41362100
W	3.34844800	0.58370700	-0.82185000
W	2.01633100	-2.40699300	-1.49969400
W	1.06252300	0.28364200	-3.26602000
W	-3.40346000	-0.73591500	0.85587100
W	1.27636500	3.18527400	0.75653300
W	1.01921400	-2.75173300	2.11162400
Si	0.01582200	-0.02393100	0.11338900
O	3.79416900	0.63194900	3.62775300
O	-3.08449400	-2.58414600	0.29470800
O	-1.36428900	-0.80084200	-0.34022100
O	1.13343800	0.26228400	4.10259600
O	-5.05241600	-0.82996700	1.34368400
O	0.17950400	-2.92901900	-1.54904300
O	0.30548400	1.90709300	-2.62481000
O	-0.30646800	1.58899300	0.18780800
O	1.79721200	1.96360000	2.10540400
O	1.96564900	-2.66698500	0.32606200
O	-2.17720100	1.42979500	-2.07218600
O	-0.70781700	-0.41334200	-3.14629000
O	-1.36051900	1.47159200	2.94202000
O	-3.04988200	3.56059800	2.39870800
O	1.19121100	-0.28866200	-1.00919200
O	-0.49259900	-3.17975500	0.95611100
O	-3.42309600	-0.35690600	-3.85179900
O	-3.06380300	1.14323700	0.91850100
O	-2.53789200	-1.02316900	2.39415700
O	-1.50955700	4.04453800	-2.83954200
O	2.45755600	2.22914000	-0.40244100
O	0.52435300	-0.55646800	1.57637200
O	-0.06063800	-2.34047600	3.48306500
O	-2.12057300	3.37321500	-0.22147900
O	0.41869800	3.86270400	-0.83050700
O	-3.81148300	-0.45457500	-1.11038500
O	3.21353700	0.12847900	0.94616800
O	-2.30034700	-2.33130700	-2.22618100
O	3.56022500	-1.26292700	-1.33122000
O	-1.85609100	-4.74813800	-0.91173400
O	2.77010500	0.87666400	-2.67649400
O	2.78629200	-3.83603900	-2.07059500

O	1.18824700	0.60462300	-4.95135600
O	4.97954200	1.11417100	-0.96585100
O	1.56946600	-4.32788400	2.53872000
O	-0.31793600	3.63233400	1.71281700
O	2.23977400	4.55128600	1.15384900
O	1.71458000	-1.51070900	-3.21003000
O	2.48436400	-1.69686600	2.77436700
Fe	-0.76101400	-0.41165500	3.35256400
N	-1.96359500	-0.50517200	5.20776400
O	-3.30161800	-0.87746900	4.92420100
H	-2.00962900	0.39637300	5.67854900
H	-1.61559900	-1.17382500	5.89200600
H	-3.26156800	-1.00578800	3.94835300

SiW₁₁Fe^{II}-NH₂-H₂O

-6 6

W	-2.34330500	2.47663300	0.92728300
W	-1.11914200	2.42446500	-2.23669200
W	-1.04203400	-3.34849900	-0.24495500
W	1.92399000	0.97587200	2.90443800
W	-2.10156000	-1.14411300	-2.52807800
W	3.34296500	0.86840700	-0.56615600
W	2.45491000	-2.34402500	-0.81727700
W	1.42199300	-0.13759400	-3.13028500
W	-3.30165900	-1.03273400	0.63322900
W	0.82456300	3.41340000	0.29813600
W	1.02156500	-2.21107600	2.65124700
Si	0.00935500	-0.00547900	0.11091000
O	3.15364400	1.70101700	3.86621900
O	-2.76602100	-2.89379900	0.44417700
O	-1.19256800	-1.02959000	-0.35543200
O	0.50183600	1.03126300	4.00786800
O	-4.95305600	-1.23155700	1.10230800
O	0.70432400	-3.11065900	-0.97228700
O	0.42831300	1.46353000	-2.88129300
O	-0.48798700	1.54302000	-0.14186700
O	1.29489700	2.50574200	1.88922300
O	2.18445500	-2.31255500	1.01218600
O	-2.03340600	0.76410400	-2.49174700
O	-0.26202900	-1.02808200	-3.08440100
O	-1.78253700	1.72606200	2.46064600
O	-3.66637500	3.45288800	1.43449800
O	1.34023800	-0.29918300	-0.81301200
O	-0.25475400	-3.04195100	1.45057700
O	-2.88091100	-1.42367000	-4.03166200
O	-3.21754600	0.86773800	0.38937300
O	-2.47719800	-0.89811700	2.21259300
O	-1.58111800	3.27821500	-3.65263800
O	2.23326000	2.42367800	-0.53499100
O	0.37022500	-0.22611300	1.68878600
O	-0.27054600	-1.67721400	3.79484400
O	-2.42492600	2.98000000	-1.02902500
O	0.10102500	3.69255700	-1.46772900
O	-3.56155500	-1.12285700	-1.35950800
O	3.03383500	0.70507000	1.24935200
O	-1.74045300	-2.95624700	-1.99866500
O	3.82185000	-0.99607400	-0.68225400

O	-1.17645500	-5.05932100	-0.25731800
O	2.97685100	0.76203700	-2.47863200
O	3.44381500	-3.73261900	-1.03296300
O	1.73549000	-0.09219500	-4.81882300
O	4.91007000	1.57141000	-0.62212200
O	1.65841600	-3.59479900	3.45174200
O	-0.91105400	3.80283500	0.98459200
O	1.58317100	4.93423900	0.53672700
O	2.26546700	-1.79379600	-2.67648100
O	2.27243300	-0.88286900	3.26976500
Fe	-1.19306200	0.07890100	3.39797500
N	-2.28205100	0.21908100	4.98323700
O	-4.86807800	0.24681900	3.77004700
H	-2.26857600	1.10079000	5.48918500
H	-2.20641400	-0.53243200	5.66366500
H	-4.84492100	-0.28297300	2.96263900
H	-3.94659500	0.20019000	4.11458700

SiW₁₁Fe^{II}-NH₃-H₂O

-6 5			
W	-3.12145700	1.44875000	1.00602100
W	-2.04081700	1.76099100	-2.22159200
W	0.28931200	-3.48808300	-0.15175600
W	1.55423300	1.69226000	2.80700100
W	-1.62243100	-1.92459400	-2.41165900
W	2.74525900	2.03663200	-0.74968900
W	3.12863100	-1.27606400	-0.92243900
W	1.23898400	0.31101800	-3.20365200
W	-2.65396300	-2.17050400	0.81581600
W	-0.51057900	3.45179500	0.23120500
W	1.93397100	-1.61146700	2.64192100
Si	0.02427000	-0.00035900	0.12188800
O	2.48331100	2.86790200	3.65897000
O	-1.44875900	-3.69377000	0.61709300
O	-0.73156600	-1.40991400	-0.27437000
O	0.28773000	1.27436700	4.00477700
O	-4.09705300	-2.97057200	1.33049000
O	1.78941100	-2.64509400	-0.98625300
O	-0.26829200	1.43195300	-2.90849500
O	-1.04338600	1.23343300	-0.10784700
O	0.33234100	2.83623800	1.80568100
O	2.96450900	-1.27983400	0.89880500
O	-2.27125900	-0.13073900	-2.42510300
O	0.02036200	-1.14247100	-3.05909400
O	-2.43482900	0.99208700	2.58811600
O	-4.73384200	1.88743400	1.42917000
O	1.32113300	0.20104800	-0.87592000
O	0.99568200	-2.86591300	1.48777600
O	-2.28967700	-2.52802800	-3.87572800
O	-3.30832200	-0.39784500	0.51501200
O	-1.92153200	-1.71094800	2.37348600
O	-2.82241000	2.34717600	-3.63565600
O	1.12575400	3.06454800	-0.66847900
O	0.52152200	-0.03899400	1.68106500
O	0.67018600	-1.64921000	3.88613700
O	-3.41541900	1.81203900	-0.98726000
O	-1.36113100	3.40738600	-1.49998100

O	-2.92812400	-2.41998400	-1.18105700
O	2.59517500	1.81501800	1.07467100
O	-0.57462000	-3.44545900	-1.87577500
O	3.89176800	0.49937000	-0.89010700
O	0.80180200	-5.12810800	-0.13944500
O	2.35676100	1.75867500	-2.64066500
O	4.55802800	-2.19712900	-1.19089800
O	1.42654500	0.43151500	-4.90954600
O	3.92100600	3.28543500	-0.88967500
O	3.15108700	-2.62291100	3.32959800
O	-2.25315200	3.18439500	0.99400800
O	-0.38585500	5.15435500	0.42955200
O	2.66402400	-0.88094800	-2.78688200
O	2.60711000	0.12333000	3.16029700
Fe	-0.91774700	-0.26994000	3.38994300
N	-1.95120100	-0.57646500	5.29623700
O	-4.43581400	-0.75257000	3.73288600
H	-1.97369600	0.24307300	5.89479100
H	-1.53760900	-1.33322800	5.83136200
H	-4.30770300	-1.55200700	3.20496900
H	-3.81010000	-0.12781900	3.32123600
H	-2.91702000	-0.82383900	5.06703700

SiW₁₁Fe^{II}-NH₄-H₂O

-5 5

W	2.47635400	2.32229600	1.16302100
W	1.62243900	2.22151300	-2.12768600
W	-3.34810700	0.55027800	0.99324500
W	1.77619000	-2.74654100	1.57786900
W	-1.91847200	2.72400900	-1.11443400
W	0.82758200	-2.67097400	-2.04605100
W	-2.36561200	-2.30733400	-1.11985400
W	-0.99114500	-0.14331400	-3.29166700
W	-1.02419500	2.68833600	2.17432300
W	3.36668400	-0.30483800	-0.79392400
W	-1.40615600	-2.25670900	2.51743300
Si	-0.00302000	-0.02164800	0.11307500
O	2.79358600	-4.12606700	1.71173000
O	-2.81787400	1.94859800	2.19161200
O	-1.16408500	1.09514300	0.44227800
O	2.15517400	-1.86402600	3.12068100
O	-1.23597600	4.04625500	3.20954500
O	-3.22653000	-0.75069900	-0.39237400
O	0.59392000	0.90315300	-3.05821400
O	1.39118900	0.76759000	-0.25314600
O	2.95835100	-1.48020400	0.62677700
O	-1.84595200	-2.72730800	0.59128200
O	-0.08114600	2.91640600	-1.58298500
O	-1.88326700	1.23780800	-2.37012200
O	2.32285100	1.15821800	2.54383800
O	3.49730700	3.53353200	1.83222800
O	-0.46983600	-0.94779000	-1.16138800
O	-2.55995400	-0.75920500	2.12820200
O	-2.64866100	3.93378300	-2.08882900
O	0.74372100	3.02027300	1.43626500
O	-0.38424900	1.44624400	3.26674300
O	2.02747100	3.28404300	-3.41281000

O	2.27022200	-1.44185900	-1.89345100
O	0.23756700	-0.96919800	1.43495700
O	-0.64988800	-1.47062100	3.92529600
O	2.41953900	3.09783300	-0.67424700
O	3.11570600	1.02927800	-2.17715300
O	-1.66255000	3.63068900	0.47633600
O	1.12748900	-3.09493400	-0.25401000
O	-3.49250900	1.89337700	-0.37554400
O	-0.96604600	-3.37742200	-1.88084900
O	-5.00116000	0.41663300	1.43295700
O	0.16751700	-1.66318600	-3.55175400
O	-3.71122500	-3.34395000	-1.38002100
O	-1.39245900	0.20325500	-4.92533200
O	1.57579900	-3.97792500	-2.87261400
O	-2.49823400	-3.36789000	3.24695300
O	3.83673400	1.10862600	0.38558700
O	4.93810800	-0.84959200	-1.22123600
O	-2.37716200	-1.35834800	-2.83999400
O	0.12399600	-3.43228800	2.21974400
Fe	0.87473700	-0.18254100	3.26888000
N	4.40002900	-0.49551400	2.89329400
O	1.63095400	0.63039200	5.18988800
H	4.88448900	-0.74615600	2.03642000
H	3.69354700	-1.23698200	3.12657300
H	0.87926600	1.12681900	5.54092400
H	2.17880800	1.30106200	4.75113700
H	5.05654300	-0.32486400	3.64897300
H	3.78712500	0.33144200	2.70601200

SiW₁₁Fe^{II}-NHO-TS-PCM

-6 5

W	3.42635400	-0.62181500	1.01616500
W	2.66782300	-0.05140300	-2.23990900
W	-1.51176500	3.01206200	0.98424100
W	-1.04581200	-3.00848400	1.71739100
W	1.01350600	3.10390800	-1.21108500
W	-1.72724400	-2.31172400	-1.91280100
W	-3.30277700	0.50356500	-1.02572000
W	-0.82650000	0.61455500	-3.28612300
W	1.62829500	2.42080300	2.06107000
W	1.72727100	-2.92049900	-0.79163800
W	-2.57349100	-0.18777700	2.60614700
Si	-0.02016700	-0.03322200	0.11532500
O	-1.52460800	-4.64585900	1.94112900
O	-0.02595400	3.42527200	2.13172000
O	0.20767600	1.57125500	0.39840500
O	-0.09396100	-2.67763400	3.20666100
O	2.62327000	3.40374100	3.06180300
O	-2.52685400	2.13403300	-0.36837800
O	0.98580900	-0.02738200	-3.10676000
O	1.43404300	-0.69043900	-0.28701900
O	0.59908600	-3.23824500	0.67440200
O	-3.29598600	-0.12362600	0.69030600
O	2.25437700	1.73350600	-1.68604200
O	-0.18930000	2.16652700	-2.40251500
O	2.44403900	-1.17234800	2.50061600
O	5.01435100	-0.69218800	1.65740100

O	-1.07996700	-0.22264300	-1.13033900
O	-2.07198100	1.63299900	2.15200500
O	1.53117600	4.39099800	-2.22232400
O	2.92731500	1.17394800	1.33287200
O	1.03422900	1.17166600	3.19309300
O	3.72849300	0.23344800	-3.55773500
O	0.13327000	-2.72908800	-1.84241700
O	-0.63393500	-0.74463200	1.45662600
O	-1.46970500	-0.25929300	3.99785900
O	3.91783400	-0.13663900	-0.80783600
O	2.62049100	-1.95417900	-2.22678600
O	1.95802400	3.45572700	0.35205900
O	-1.81871800	-2.77644300	-0.12369200
O	-0.54833900	3.90421400	-0.42823400
O	-3.35132800	-1.27537800	-1.74915600
O	-2.57550500	4.28152100	1.43333300
O	-1.35011400	-1.21343600	-3.48006400
O	-4.93993400	0.97261300	-1.25800900
O	-0.82712400	1.11671900	-4.92900100
O	-2.35855200	-3.70294900	-2.69968400
O	-4.10422700	0.05123500	3.35860000
O	3.20872700	-2.42763100	0.30690000
O	2.20536700	-4.51559300	-1.20867700
O	-2.59648900	1.04237100	-2.78977300
O	-2.61256500	-2.10621300	2.35629300
Fe	0.49374600	-0.74477100	3.31216100
N	2.11057200	-1.14324600	4.85296600
O	2.27005200	-2.01768000	5.69119800
H	2.65231300	-1.20241200	3.67508800

SiW₁₁Fe^{II}-NHO-TS-HSM

-6 5			
W	-2.08813000	2.45493400	1.52946900
W	0.16623000	3.40868400	-0.84547500
W	-1.39618400	-2.34113900	-2.18919600
W	0.90657300	-1.08624800	3.31645400
W	-1.16398800	0.85159000	-3.18391900
W	3.43878100	-0.07680800	0.72600900
W	2.19168500	-2.35199500	-1.38135300
W	2.44433500	0.86116600	-2.33677700
W	-3.42647700	-0.02165300	-0.82808400
W	1.21353100	2.46907100	2.18817400
W	-0.31943800	-3.38307700	1.23784900
Si	-0.00939600	-0.03890800	0.07791500
O	1.84144600	-1.28520600	4.74893200
O	-3.14829200	-1.70620900	-1.77988300
O	-1.12291600	-0.30258700	-1.10644000
O	-0.77007600	-1.09758500	3.95484200
O	-5.13501300	0.10561800	-0.95948000
O	0.51308300	-2.35205100	-2.29986500
O	1.66472600	2.38322300	-1.52484500
O	-0.14656700	1.52602000	0.57167500
O	0.92014700	0.84853400	3.12171300
O	1.32469500	-3.05646800	0.07180100
O	-0.84079700	2.41181300	-2.13612300
O	0.72273900	0.61865100	-3.17118100
O	-2.29866400	1.01988800	2.53775800

O	-3.31324800	3.52252200	2.10712000
O	1.49722100	-0.28978300	-0.53987600
O	-1.20180000	-3.10988700	-0.48233600
O	-1.40933000	1.53464800	-4.73935600
O	-2.96596700	1.60371800	0.03107500
O	-3.30578500	-0.94384900	0.77006200
O	0.40100900	4.89286400	-1.67817100
O	2.64935200	1.56943300	1.30802400
O	-0.27794000	-1.05822600	1.33000000
O	-1.82721500	-3.12926300	2.14173400
O	-1.37022300	3.75941300	0.11891800
O	1.22707300	3.72669800	0.72286500
O	-2.94840000	0.82451300	-2.53266800
O	2.48292300	-0.91857200	2.05376800
O	-1.35727100	-1.00577400	-3.59553500
O	3.63215400	-1.71482700	-0.25831200
O	-1.79469500	-3.71678000	-3.13639000
O	3.77599700	0.82888900	-0.98378800
O	2.96096200	-3.72301500	-2.07971200
O	3.33271600	1.56761700	-3.62732700
O	5.01344700	0.04590800	1.40617600
O	-0.15798400	-5.09888600	1.26484500
O	-0.56065300	3.07168100	2.56598900
O	2.07231700	3.38754300	3.35788000
O	2.77662200	-0.98695000	-2.65882000
O	0.82822300	-2.91279500	2.71427100
N	-3.89547300	-1.32531900	3.64811800
O	-4.00659200	-1.43942600	4.87025400
H	-4.86401200	-1.45535900	2.79090500
Fe	-2.17234200	-1.05125900	2.48240300
O	-5.44829900	-1.56299300	1.76328400
H	-6.05476300	-0.81782300	1.65685900
H	-4.58529500	-1.33160800	1.18585200

SiW₁₁Fe^{II}-NHOH-TS-PCM

-6 6			
W	-1.61985100	2.76734800	1.56841400
W	-1.98384100	2.26327100	-1.77230400
W	-1.16638100	-3.21182300	0.78942900
W	3.19305500	1.03982800	1.36298000
W	-3.17958900	-1.17214400	-0.94798300
W	2.57715300	0.47439600	-2.27415700
W	1.66072000	-2.64908400	-1.50852300
W	-0.38022000	-0.69473000	-3.33223500
W	-2.65498800	-0.62526500	2.38206300
W	0.94196700	3.32283000	-0.55129200
W	2.10600000	-2.03836300	2.17285900
Si	0.02532500	0.00046600	0.12864300
O	4.76103000	1.73464600	1.41955800
O	-2.30135500	-2.51926500	2.18046300
O	-1.29037100	-0.92671500	0.47620400
O	2.61746800	1.44667800	3.09258400
O	-3.96789700	-0.66353700	3.49841900
O	0.01808500	-3.24049600	-0.70217200
O	-0.99514000	1.04831900	-2.89647000
O	-0.48615000	1.55001600	-0.08844000
O	2.08779900	2.52224000	0.71604200

O	2.31580100	-2.38206600	0.18159800
O	-2.99224500	0.67334700	-1.32241800
O	-1.81237100	-1.37521800	-2.35933900
O	-0.38937800	2.21157300	2.71579600
O	-2.50667200	3.94603200	2.46329200
O	0.71879200	-0.53346700	-1.26731200
O	0.37038900	-2.81868100	1.84509700
O	-4.58490500	-1.56420000	-1.85419200
O	-2.68820600	1.21359600	1.77653000
O	-1.26439000	-0.32734800	3.42704600
O	-3.02635200	2.98780800	-2.92880400
O	1.74972400	2.11278000	-1.83764700
O	1.10214700	-0.07979500	1.36884600
O	1.62308100	-1.29671900	3.71377000
O	-2.56843900	3.06727500	-0.20244000
O	-0.49945500	3.45300800	-1.85605400
O	-3.87601500	-0.90388600	0.72371700
O	3.23379000	0.51584900	-0.47870300
O	-2.62091700	-2.95171600	-0.42623000
O	2.93805000	-1.42533600	-2.25567700
O	-1.35162600	-4.89095300	1.09602800
O	1.35499800	0.16446200	-3.68412100
O	2.37296600	-4.14625700	-1.96579500
O	-0.92373600	-0.86505900	-4.95397100
O	3.94881900	1.01092100	-3.15854800
O	3.01711900	-3.40600600	2.69025600
O	-0.26136900	3.96612200	0.73574100
O	1.78930800	4.76793100	-0.92745700
O	0.60098900	-2.30921400	-3.12396000
O	3.55024700	-0.75711300	1.88271900
Fe	0.64716200	0.58263800	3.32819600
N	0.79521800	1.38255700	5.04688500
O	1.77232600	2.27564900	5.12877100
H	0.02306600	1.69349600	5.64232400
H	2.38430900	1.94840200	4.14903400

SiW₁₁Fe^{II}-NHOH-TS-HSM

-6 6			
W	-0.91664600	2.73225400	2.11835100
W	-2.81724700	2.03424400	-0.62337300
W	-0.42634000	-3.25617700	1.23900100
W	3.29358500	1.32883200	-0.32067200
W	-3.17543500	-1.46109900	0.60128800
W	1.14508000	0.55664700	-3.25398000
W	0.90286200	-2.58216400	-2.13749600
W	-1.87801400	-0.81429100	-2.81073000
W	-1.22682400	-0.69882000	3.28849000
W	0.23312500	3.35197100	-0.99097200
W	3.00115000	-1.80029600	0.87314300
Si	0.05077300	0.01449400	0.07090900
O	4.67219300	2.12968900	-0.95713500
O	-0.84968700	-2.60090800	2.96848700
O	-0.87543500	-0.99743700	0.98184000
O	3.52386100	1.72548900	1.50739100
O	-1.80926300	-0.77668400	4.91011300
O	-0.08645200	-3.25225700	-0.64784200
O	-2.37663200	0.87290500	-2.10453100

O	-0.62141300	1.51631300	0.12785900
O	1.93099200	2.68973400	-0.41278300
O	2.26988800	-2.18283600	-0.97767100
O	-3.33433400	0.40574500	0.24976200
O	-2.63177700	-1.57240800	-1.26810300
O	0.72840200	2.30741500	2.60367100
O	-1.39669700	3.88051400	3.31222600
O	0.04524900	-0.51397400	-1.49112800
O	1.39694000	-2.70770500	1.42266200
O	-4.80735400	-1.97724400	0.46688900
O	-1.65755500	1.10594000	2.79164500
O	0.48673600	-0.32907900	3.48693100
O	-4.33767700	2.63722300	-1.14547200
O	0.46303700	2.15189400	-2.48373000
O	1.58781300	0.06296700	0.66001800
O	3.29841800	-1.04785700	2.46651600
O	-2.63054000	2.87955700	1.01117200
O	-1.64350200	3.33649700	-1.41793500
O	-3.02571300	-1.16916800	2.41512300
O	2.54469800	0.70872900	-1.98586500
O	-2.29725200	-3.16493400	0.81256500
O	1.57838800	-1.30724100	-3.42183600
O	-0.29619700	-4.93167300	1.58727500
O	-0.59177900	0.13354700	-3.92036100
O	1.43117000	-4.04170100	-2.87744300
O	-3.10768000	-1.08597800	-3.97948500
O	1.88728700	1.15806100	-4.68129800
O	4.15712100	-3.07576100	0.86176400
O	-0.21486000	3.96236200	0.73499500
O	0.68693500	4.83784400	-1.72005600
O	-0.81144200	-2.37037200	-3.06132600
O	4.02015200	-0.41368800	-0.04678600
Fe	2.04536900	0.72787800	2.62601400
N	2.61829100	1.23011000	4.37032900
O	3.75595600	1.79976000	4.69487800
H	1.87934100	1.60240200	4.97730500
O	5.18639900	0.85781700	2.97130500
H	4.82496000	-0.04977100	2.90023800
H	4.45799500	1.35892600	2.13724500
H	4.62014800	1.27967100	3.82372800