SUPPORTING INFORMATION

Quantum Chemical Characterization of the Mechanism of an Iron-based Water Oxidation Catalyst

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CONTENTS

Energetics of Pentacoordinated and Hexacoordinated {TAML–Fe} Complexes

As an alternative path to our proposed mechanism involving pentacoordinated {TAML–Fe} complexes, we have also investigated the possible formation of hexacoordinated {TAML–Fe} complexes. We found that approach of a water molecule to the sixth iron coordination site was in most cases repulsive at all distances. In those instances where binding was achieved, the free energy of the resulting complex was positive relative to the five-coordinate species, and no follow on reactions (deprotonation, oxidation, PCET) occurred at lower energy to generate reactive iron-oxo species. Calculated free energy changes and redox potentials for some of these species are listed in Table S1 and Table S2, respectively.

Table S1. Addition reactions to pentacoordinated {TAML–Fe} complexes to form hexacoordinated ones. The changes in free energies (ΔG, kcal/mol) are calculated at the M06-L level of theory with the SDD basis set on Fe and 6-31+G(d) basis set on all other atoms.

Possible Insertion Reactions	ΔG (kcal/mol)
$\{TAML–Fe^{III}–OH_2\}^- + H_2O \longrightarrow \{TAML–Fe^{III}–(OH_2)_2\}^-$	3.0
$\{TAML–Fe^{IV}–OH\}^- + H_2O \longrightarrow \{TAML–Fe^{IV}–(OH)_2\}^{2-} + H^+$	14.5
$\{TAML–Fe^{IV}–O\}^{2-} + H_2O \longrightarrow \{TAML–Fe^{IV}–(OH)_2\}^{2-}$	2.3
$\{TAML–Fe^{V}–OH\} + H_2O \longrightarrow \{TAML–Fe^{V}–(OH)_2\}^- + H^+$	6.2
$\{TAML–Fe^{V}–OH\} + H_2O \longrightarrow \{TAML–Fe^{V}–(OH)\ (O)\}^{2-} + 2\ H^+$	27.1
$\{TAML–Fe^{V}–O\}^- + H_2O \longrightarrow \{TAML–Fe^{V}–(OH)_2\}^-$	3.4
$\{TAML–Fe^{V}–O\}^- + H_2O \longrightarrow \{TAML–Fe^{V}–(OH)\ (O)\}^{2-} + H^+$	24.3
$\{TAML^{+\bullet}–Fe^{V}–O\} + H_2O \longrightarrow \{TAML^{+\bullet}–Fe^{V}–(OH)\ (O)\}^- + H^+$	13.8

Table S2. Redox reactions of hexacoordinated {TAML–Fe} complexes to form pentacoordinated ones. The oxidation potentials (in units of volts) are calculated at the M06-L level of theory with the SDD basis set on Fe and 6-31+G(d) basis set on all other atoms.

Possible Redox Reactions	E (Volts)
$\{TAML–Fe^{IV}–(OH)_2\}^{2-} + 2\ H^+ + e^- \longrightarrow \{TAML–Fe^{III}–OH_2\}^- + H_2O$	1.67
$\{TAML–Fe^{V}–(OH)_2\}^- + H^+ + e^- \longrightarrow \{TAML–Fe^{IV}–OH\}^- + H_2O$	1.37
$\{TAML–Fe^{V}–(OH)\ (O)\}^{2-} + 2\ H^+ + e^- \longrightarrow \{TAML–Fe^{IV}–OH\}^- + H_2O$	2.28
$\{TAML^{+\bullet}–Fe^{V}–(OH)\ (O)\}^- + 2\ H^+ + e^- \longrightarrow \{TAML–Fe^{V}–OH\} + H_2O$	2.07
$\{TAML^{+\bullet}–Fe^{V}–(OH)\ (O)\}^- + H^+ + e^- \longrightarrow \{TAML–Fe^{V}–O\}^- + H_2O$	1.95

Protonated {TAML–Fe} Complexes

We also examined possible protonation of the ligand in the pH = 0.7 aqueous solution, however protonation of the ligand at its most basic sites, the carbonyl group oxygens, was predicted to be unfavorable at the experimental pH, and no TS structures were located with sufficiently low energy to validate this pathway. As an example, the free energy of activation for the water nucleophilic attack TS for $\{H_2\text{-TAML–Fe}^{V}–O\}^+$ was found to be 23.0 kcal/mol. However, coupled with the protonation step (ΔG=31.0 kcal/mol), the overall free energy of activation corresponds to 54.0 kcal/mol with respect to the initial $\{TAML–Fe^{V}–O\}^-$ species. The free energy changes associated with the protonated {TAML–Fe-O} complexes are summarized in Table S3.

Table S3. Possible protonation reactions of pentacoordinated {TAML–Fe^{V}-O}. The changes in free energies (ΔG, kcal/mol) are calculated at the M06-L level of theory with the SDD basis set on Fe and 6-31+G(d) basis set on all other atoms.

Protonation Reactions	ΔG (kcal/mol)
$\{TAML–Fe^{V}–O\}^{-} + H^{+} \longrightarrow \{H\text{-}TAML–Fe^{V}–O\}$	12.7
$\{TAML–Fe^{V}–O\}^{-} + 2\,H^{+} \longrightarrow \{H_2\text{-}TAML–Fe^{V}–O\}^{+}$	31.0
$\{TAML^{+\bullet}–Fe^{V}–O\} + H^{+} \longrightarrow \{H\text{-}TAML^{+\bullet}–Fe^{V}–O\}$	21.9

Cartesian Coordinates and Electronic Energies

I – Pentacoordinated {TAML-Fe} Structures ($R^1 = R^2 = Cl$, $R^3 = R^4 = F$)

$\{TAML–Fe^{III}–OH_2\}^{-}$ (Quartet)

Energy: -2496.72415618 a.u.

C	-1.88044200	0.71214700	0.02887900
C	-1.88044800	-0.71200600	0.02890100
C	-3.08825700	-1.40813700	0.02033400
C	-4.29049400	-0.69820000	0.01761200
C	-4.29049900	0.69826500	0.01766800
C	-3.08829600	1.40824100	0.02041300
H	-3.08718200	-2.49273500	0.01106300
H	-3.08722100	2.49284000	0.01126800
N	-0.59268600	-1.26196900	0.01365300
N	-0.59281000	1.26213100	0.01353900
C	-0.25193400	-2.57076400	-0.17797100
C	-0.25193500	2.57105300	-0.17714000
C	1.27325800	-2.76954800	-0.35047200
C	1.27326900	2.76982200	-0.34981400
N	1.94844600	1.46935600	-0.11396000
N	1.94837600	-1.46924700	-0.11376900
C	3.28530700	-1.37066500	-0.26921600
C	3.28521300	1.37045500	-0.27071300
O	4.07274300	-2.23927700	-0.64404100
O	-1.02949300	-3.52297900	-0.25209800
O	-1.02945700	3.52332200	-0.25056100
O	4.07244600	2.23853400	-0.64712000
C	1.74279200	3.81658500	0.65927600

H	1.59316000	3.46270600	1.68879000
H	2.80558800	4.03475000	0.51444300
H	1.15943400	4.73577700	0.53265300
C	1.48465100	3.27075400	-1.78242600
H	2.53680300	3.51470900	-1.95102700
H	1.18305000	2.50447400	-2.50790100
H	0.86741100	4.16134200	-1.94853100
C	1.48506300	-3.26967600	-1.78328600
H	1.18371600	-2.50294200	-2.50837600
H	2.53728000	-3.51353100	-1.95165600
H	0.86789000	-4.16016900	-1.95016600
C	1.74229300	-3.81721000	0.65795800
H	2.80516900	-4.03519000	0.51357600
H	1.59218800	-3.46447000	1.68784700
H	1.15894500	-4.73627000	0.53034000
C	3.86575000	0.00017800	0.19565000
Fe	0.77784100	0.00031600	0.19106400
Cl	-5.78529800	1.59668900	0.01701600
Cl	-5.78526300	-1.59668200	0.01686100
F	3.73242900	0.00118400	1.61245400
F	5.18909300	0.00005400	-0.03503100
O	1.06835700	-0.00023100	2.43717300
H	1.66326100	-0.76876900	2.46895700
H	1.69468300	0.74338900	2.46136000

{TAML–Fe^{IV}–OH}$^{-}$ (Broken Symmetry Singlet)

Energy: -2496.08306724 a.u.

C	1.86416300	-0.71093500	0.01772400
C	1.86415700	0.71094500	0.01773000
C	3.07225800	1.41222700	0.01334600
C	4.26970000	0.70068600	0.01294200
C	4.26970600	-0.70066000	0.01292400
C	3.07226800	-1.41220900	0.01331600
H	3.07224900	2.49636900	0.00598600
H	3.07226800	-2.49635100	0.00592300
N	0.57822100	1.23562400	-0.00602200
N	0.57823200	-1.23562500	-0.00602400
C	0.23536400	2.54726500	-0.19931600
C	0.23538500	-2.54723900	-0.19953700
C	-1.28332800	2.74409700	-0.32415400
C	-1.28330900	-2.74409600	-0.32426800
N	-1.93855600	-1.42629900	-0.16066300
N	-1.93855900	1.42631000	-0.16049900

C	-3.28182500	1.35089200	-0.26987000
C	-3.28184200	-1.35089900	-0.26985100
O	-4.05533800	2.24489200	-0.61467700
O	1.02084500	3.48690000	-0.30787600
O	1.02086900	-3.48688200	-0.30799600
O	-4.05539900	-2.24487900	-0.61461500
C	-1.73122700	-3.71056300	0.77384500
H	-1.56486700	-3.27203100	1.76566900
H	-2.79529700	-3.94084800	0.66285600
H	-1.14972700	-4.63707100	0.70313400
C	-1.53146700	-3.33976900	-1.71452500
H	-2.58388500	-3.60735100	-1.83305800
H	-1.26270700	-2.61957100	-2.49744700
H	-0.90356200	-4.22991800	-1.83619100
C	-1.53144000	3.33966500	-1.71446900
H	-1.26259500	2.61943000	-2.49732800
H	-2.58386500	3.60718600	-1.83309400
H	-0.90357600	4.22984000	-1.83615000
C	-1.73136600	3.71061200	0.77385600
H	-2.79544500	3.94082600	0.66278900
H	-1.56503700	3.27216200	1.76572200
H	-1.14991600	4.63714800	0.70311600
C	-3.87795100	0.00000600	0.19389700
Fe	-0.79012800	-0.00001800	0.33581600
Cl	5.76563000	-1.59332300	0.01498400
Cl	5.76561800	1.59336000	0.01502400
F	-3.76091000	0.00001600	1.60526200
F	-5.19755900	0.00001000	-0.05888800
O	-0.89225800	-0.00012100	2.10063400
H	-1.84630200	0.00029000	2.30648600

{TAML–Fe^{IV}–OH}$^{-}$ (Triplet)

Energy: -2496.10235218 a.u.

C	1.86386300	-0.71196200	0.00253400
C	1.86385800	0.71184400	0.00220500
C	3.07305700	1.41286200	0.00660700
C	4.26939200	0.70132200	0.01296400
C	4.26939800	-0.70142300	0.01328400
C	3.07306200	-1.41297000	0.00726300
H	3.07319900	2.49699700	-0.00008800
H	3.07321400	-2.49710400	0.00104000
N	0.57998200	1.23568300	-0.03108900
N	0.57997800	-1.23583100	-0.03037600

C	0.23582900	2.55117100	-0.20820300
C	0.23577500	-2.55122700	-0.20811900
C	-1.28353000	2.75022300	-0.32279400
C	-1.28360300	-2.75021700	-0.32278900
N	-1.93850400	-1.43163700	-0.17072300
N	-1.93849600	1.43157100	-0.17109400
C	-3.28197300	1.35556800	-0.26500000
C	-3.28187000	-1.35551900	-0.26535500
O	-4.05955800	2.25117800	-0.59646000
O	1.02273000	3.48950200	-0.31116400
O	1.02267100	-3.48951700	-0.31155600
O	-4.05928100	-2.25101900	-0.59752000
C	-1.72480800	-3.70902600	0.78455400
H	-1.55203000	-3.26377000	1.77222900
H	-2.78977100	-3.93883300	0.68175300
H	-1.14507500	-4.63691600	0.71685500
C	-1.53865500	-3.35713100	-1.70718700
H	-2.59252600	-3.62277100	-1.81763300
H	-1.27245700	-2.64385100	-2.49722800
H	-0.91347700	-4.24988900	-1.82434000
C	-1.53831300	3.35743600	-1.70712600
H	-1.27176000	2.64437800	-2.49724800
H	-2.59218800	3.62295000	-1.81772500
H	-0.91325500	4.25032700	-1.82397100
C	-1.72446800	3.70891100	0.78475600
H	-2.78929200	3.93926700	0.68189700
H	-1.55202100	3.26328000	1.77232800
H	-1.14424900	4.63652300	0.71742300
C	-3.87575100	-0.00004300	0.19335700
Fe	-0.79135900	0.00000600	0.33079900
Cl	5.76561500	-1.59251800	0.02442400
Cl	5.76560500	1.59243300	0.02370300
F	-3.76191100	-0.00008400	1.60531700
F	-5.19493000	-0.00005400	-0.06179700
O	-0.89003000	0.00024100	2.10736600
H	-1.84270800	0.00142600	2.31601400

{TAML–Fe^{IV}–O}$^{2-}$ (Broken Symmetry Singlet)

Energy: -2495.46036336 a.u.

C	-1.87535800	0.71506300	0.02779500
C	-1.87538800	-0.71508000	0.02813600
C	-3.08951300	-1.40792300	-0.00518200
C	-4.29057600	-0.69737200	-0.03244500

C	-4.29055900	0.69733800	-0.03275100
C	-3.08949300	1.40789100	-0.00582800
H	-3.08358600	-2.49281900	-0.01806400
H	-3.08355500	2.49278300	-0.01916300
N	-0.60052900	-1.25888300	0.03073900
N	-0.60048400	1.25880500	0.02998800
C	-0.26183400	-2.55718200	-0.14538500
C	-0.26181100	2.55716300	-0.14560400
C	1.27033000	-2.76806100	-0.18531000
C	1.27035000	2.76805900	-0.18527100
N	1.93960700	1.44815300	-0.17482600
N	1.93958200	-1.44814600	-0.17447400
C	3.27421800	-1.39734600	-0.24735700
C	3.27428600	1.39734900	-0.24701100
O	4.05987100	-2.34534600	-0.41338400
O	-1.03921700	-3.51537300	-0.27739700
O	-1.03919100	3.51539000	-0.27738600
O	4.06011400	2.34531500	-0.41244200
C	1.65284900	3.56725800	1.06520000
H	1.43895300	2.97688300	1.96493300
H	2.72290500	3.80138100	1.04255000
H	1.07185600	4.49851600	1.10344800
C	1.58031100	3.56571800	-1.45524300
H	2.63446500	3.85454200	-1.47594200
H	1.36741600	2.96148600	-2.34737100
H	0.93925800	4.45567100	-1.48347100
C	1.58020800	-3.56515800	-1.45565100
H	1.36701200	-2.96062300	-2.34750000
H	2.63441800	-3.85376900	-1.47667900
H	0.93931900	-4.45521800	-1.48410400
C	1.65315400	-3.56772300	1.06474400
H	2.72325000	-3.80166200	1.04180900
H	1.43932600	-2.97780400	1.96479000
H	1.07232900	-4.49909800	1.10268400
C	3.93400100	-0.00004300	-0.04149300
Fe	0.79883400	-0.00004200	0.36550200
Cl	-5.79765200	1.60173000	-0.06578900
Cl	-5.79767800	-1.60175600	-0.06510800
F	4.37993300	-0.00022800	1.28051800
F	5.07233600	0.00002900	-0.80681700
O	0.91078000	0.00049300	1.99347200

{TAML–Fe^{IV}–O}$^{2-}$ (Triplet)

Energy: -2495.47937780 a.u.

C	-1.87617300	0.71504500	0.02363200
C	-1.87616500	-0.71504300	0.02321600
C	-3.09026800	-1.40794000	-0.00801700
C	-4.29139500	-0.69734900	-0.03302200
C	-4.29140600	0.69733400	-0.03265200
C	-3.09029300	1.40793100	-0.00725000
H	-3.08439800	-2.49282800	-0.02126400
H	-3.08445200	2.49282600	-0.01994800
N	-0.60099200	-1.25868300	0.02387700
N	-0.60102400	1.25872800	0.02474400
C	-0.26207200	-2.55774800	-0.14798700
C	-0.26217100	2.55777700	-0.14724000
C	1.27026000	-2.76939200	-0.18481100
C	1.27015500	2.76950300	-0.18384200
N	1.93944700	1.44970400	-0.17826200
N	1.93952600	-1.44957500	-0.17879300
C	3.27445600	-1.39869100	-0.24495600
C	3.27439300	1.39888500	-0.24435700
O	4.06141000	-2.34683300	-0.40297400
O	-1.03962400	-3.51596400	-0.27771100
O	-1.03978900	3.51592600	-0.27709800
O	4.06135900	2.34711000	-0.40183600
C	1.64993700	3.56457600	1.07016200
H	1.43442800	2.97107200	1.96742700
H	2.71997300	3.79898700	1.05044000
H	1.06867900	4.49557500	1.11043200
C	1.58275800	3.57168100	-1.45021700
H	2.63735300	3.85931200	-1.46794300
H	1.37065800	2.97113900	-2.34501000
H	0.94294000	4.46260100	-1.47608800
C	1.58275600	-3.57100300	-1.45157800
H	1.37026500	-2.97017500	-2.34608500
H	2.63743100	-3.85833500	-1.46965500
H	0.94319500	-4.46210400	-1.47764200
C	1.65024700	-3.56495800	1.06880100
H	2.72026700	-3.79940900	1.04880700
H	1.43491700	-2.97178000	1.96632500
H	1.06894000	-4.49593600	1.10881400
C	3.93395600	0.00007100	-0.04438700
Fe	0.79905500	-0.00013200	0.36545800
Cl	-5.79848900	1.60168000	-0.06323900
Cl	-5.79846200	-1.60170300	-0.06406600
F	4.38955000	-0.00018500	1.27406400
F	5.06684000	0.00027600	-0.81861500

O	0.91320000	-0.00064500	1.99220900

{TAML–Fe^{V}–OH} (Doublet)

Energy: -2495.94185902 a.u.

C	1.84315500	-0.72458800	0.06910000
C	1.84315300	0.72460500	0.06905400
C	3.05992200	1.42722900	0.01139600
C	4.24326700	0.71635400	-0.02977900
C	4.24326800	-0.71634300	-0.02972900
C	3.05992200	-1.42721600	0.01149800
H	3.06256400	2.51108000	0.01227400
H	3.06256400	-2.51106700	0.01246000
N	0.58635800	1.24035700	0.06363900
N	0.58636100	-1.24034700	0.06374200
C	0.23213000	2.58075500	-0.07991800
C	0.23214100	-2.58075900	-0.07971300
C	-1.27379500	2.76704900	-0.27892200
C	-1.27375300	-2.76705000	-0.27893100
N	-1.91226500	-1.42755600	-0.18547900
N	-1.91229900	1.42755600	-0.18541600
C	-3.26468600	1.34209500	-0.34837000
C	-3.26466400	-1.34212600	-0.34838500
O	-4.00680900	2.22762700	-0.74546400
O	1.02375200	3.50757000	-0.07823500
O	1.02382000	-3.50752400	-0.07840200
O	-4.00679300	-2.22772200	-0.74532000
C	-1.79697200	-3.69727600	0.81667300
H	-1.68032900	-3.24211700	1.80751800
H	-2.85481600	-3.91870800	0.65034000
H	-1.23090500	-4.63458000	0.79864200
C	-1.45028200	-3.39101300	-1.66976800
H	-2.49570500	-3.65510300	-1.83837500
H	-1.13302800	-2.69611200	-2.45655000
H	-0.83157200	-4.29244700	-1.73470000
C	-1.45049700	3.39101600	-1.66973200
H	-1.13331200	2.69613000	-2.45655400
H	-2.49595100	3.65507000	-1.83821100
H	-0.83182600	4.29247100	-1.73472700
C	-1.79688000	3.69727200	0.81675100
H	-2.85474300	3.91871100	0.65055700
H	-1.68011100	3.24210700	1.80757900
H	-1.23081100	4.63457500	0.79866100
C	-3.86938100	-0.00002300	0.12172600

Fe	-0.82202000	0.00000400	0.33024200
Cl	5.72951000	-1.57587400	-0.07217700
Cl	5.72950900	1.57588200	-0.07229100
F	-3.72252100	-0.00001900	1.52413800
F	-5.18035300	-0.00003400	-0.12671400
O	-0.84855300	0.00002900	2.09225500
H	-1.79368300	0.00043000	2.34215700

{TAML–Fe^{V}–OH} (Quartet)

Energy: -2495.94250800 a.u.

C	1.85646000	-0.71902100	0.04599800
C	1.85646400	0.71902400	0.04599700
C	3.06777900	1.42461500	0.02701900
C	4.25541200	0.71244700	0.01185600
C	4.25540900	-0.71245500	0.01185700
C	3.06777200	-1.42461800	0.02702100
H	3.07321800	2.50809300	0.02600500
H	3.07320600	-2.50809600	0.02600800
N	0.58521000	1.22522900	0.02365700
N	0.58520400	-1.22522100	0.02366300
C	0.23087900	2.56149100	-0.17381900
C	0.23086600	-2.56148000	-0.17383900
C	-1.27503100	2.76021400	-0.36679600
C	-1.27504500	-2.76020200	-0.36680200
N	-1.93035700	-1.44951600	-0.15335700
N	-1.93035100	1.44954400	-0.15327300
C	-3.28431900	1.34355000	-0.25875000
C	-3.28432800	-1.34353700	-0.25876300
O	-4.03703100	2.22301000	-0.65298400
O	1.03694700	3.47020400	-0.25350100
O	1.03694000	-3.47018100	-0.25360200
O	-4.03705900	-2.22301800	-0.65291400
C	-1.76519900	-3.78850300	0.65301000
H	-1.64283500	-3.41451500	1.67619600
H	-2.82080100	-4.01474600	0.48163600
H	-1.18108400	-4.70880700	0.54779900
C	-1.46652400	-3.25809000	-1.80402400
H	-2.51883100	-3.48943700	-1.98265300
H	-1.14313600	-2.50295300	-2.53006700
H	-0.86515000	-4.16144500	-1.95232600
C	-1.46648900	3.25800700	-1.80405500
H	-1.14308400	2.50282400	-2.53004400
H	-2.51879500	3.48933600	-1.98271800

H	-0.86511900	4.16135600	-1.95240800
C	-1.76519400	3.78858700	0.65293700
H	-2.82079200	4.01482700	0.48153500
H	-1.64284500	3.41467400	1.67615200
H	-1.18106900	4.70887900	0.54766900
C	-3.87313400	0.00000800	0.23593600
Fe	-0.84053100	0.00000100	0.37454900
Cl	5.74064800	-1.57851400	0.00062200
Cl	5.74065600	1.57849800	0.00061900
F	-3.68715400	0.00000000	1.62759100
F	-5.18920800	0.00001400	0.01797700
O	-0.85443300	-0.00007700	2.20643600
H	-1.76952000	0.00013300	2.53673300

{TAML–Fe^{V}–O}$^{-}$ (Doublet)

Energy: -2495.46279257 a.u.

C	1.86956200	-0.72216200	0.12345900
C	1.83491100	0.68879800	0.00495900
C	3.02529600	1.41336200	-0.08186900
C	4.23911000	0.72842600	-0.04770000
C	4.27169800	-0.66685000	0.06078500
C	3.08985300	-1.39944400	0.14370100
H	3.00605500	2.49224400	-0.17627300
H	3.10965200	-2.48101200	0.21600900
N	0.52895700	1.18485600	-0.04444500
N	0.59756200	-1.26738700	0.15264900
C	0.17933500	2.50012400	-0.25587800
C	0.27421900	-2.55675700	-0.13218600
C	-1.32807800	2.72696900	-0.27356200
C	-1.23181100	-2.72813600	-0.35332000
N	-1.86496000	-1.38836300	-0.23334200
N	-1.97547000	1.41445900	-0.11735300
C	-3.31684600	1.35574800	-0.15665400
C	-3.21914000	-1.31568200	-0.36240400
O	-4.09913100	2.28187600	-0.38302500
O	0.98732100	3.40966200	-0.41753100
O	1.06502200	-3.49084300	-0.25903900
O	-3.93295400	-2.23013800	-0.76521400
C	-1.76402500	-3.67783400	0.72147000
H	-1.66987200	-3.22603800	1.71694200
H	-2.81608800	-3.91588800	0.54015400
H	-1.17481500	-4.60212300	0.70252800

C	-1.39931500	-3.31797200	-1.75642600
H	-2.44119000	-3.58683800	-1.94122800
H	-1.08060100	-2.59736000	-2.51953300
H	-0.76272600	-4.20642000	-1.83837900
C	-1.66285700	3.38647000	-1.61596300
H	-1.47343000	2.69356500	-2.44512500
H	-2.71359700	3.68277300	-1.64231700
H	-1.02309600	4.26658700	-1.74901600
C	-1.67386700	3.65471600	0.89607500
H	-2.74127100	3.89369700	0.87355300
H	-1.44164900	3.17097400	1.85272500
H	-1.09025800	4.57967100	0.81931800
C	-3.89972100	-0.03434300	0.16438900
Fe	-0.80130500	-0.00915300	0.45878800
Cl	5.78604800	-1.52485500	0.10252600
Cl	5.71193300	1.65308500	-0.14076800
F	-3.91154200	-0.16353900	1.54949700
F	-5.19087500	-0.05895500	-0.23113000
O	-0.91146400	0.03933600	2.03370000

{TAML–Fe^{V}–O}$^{-}$ (Quartet)

Energy: -2495.45300391 a.u.

C	-1.85077300	0.71227000	-0.02319600
C	-1.85068300	-0.71185200	-0.02460300
C	-3.05805800	-1.41262100	0.00878800
C	-4.25483800	-0.70137000	0.03899000
C	-4.25492100	0.70135300	0.04022300
C	-3.05821300	1.41280300	0.01139300
H	-3.05744800	-2.49689400	-0.00005900
H	-3.05786200	2.49708600	0.00452000
N	-0.57178000	-1.24364400	-0.09570800
N	-0.57184800	1.24421000	-0.09266100
C	-0.21841900	-2.54665800	-0.30180000
C	-0.21855900	2.54713500	-0.30032400
C	1.30357900	-2.75531800	-0.34477300
C	1.30335000	2.75562200	-0.34407000
N	1.95628600	1.43954000	-0.15501500
N	1.95609900	-1.43858500	-0.15779600
C	3.30532000	-1.35332900	-0.17758500
C	3.30528000	1.35389100	-0.17684700
O	4.08769000	-2.25306100	-0.48071300
O	-1.00868500	-3.47473100	-0.46435200
O	-1.00887000	3.47494900	-0.46364100

O	4.08758500	2.25326700	-0.48142100
C	1.68403000	3.71029900	0.78862600
H	1.45981400	3.25946500	1.76297300
H	2.75321200	3.93898500	0.74286400
H	1.10985800	4.63909100	0.69220000
C	1.62927900	3.35973400	-1.71316100
H	2.68548900	3.63258100	-1.76806600
H	1.40935700	2.64404700	-2.51484700
H	1.00596200	4.24853700	-1.86430000
C	1.63010000	-3.36156600	-1.71265200
H	1.41078500	-2.64710200	-2.51558500
H	2.68624200	-3.63486000	-1.76667500
H	1.00663800	-4.25046000	-1.86276200
C	1.68373100	-3.70798700	0.78974800
H	2.75285400	-3.93706900	0.74468500
H	1.45935500	-3.25542600	1.76324500
H	1.10936900	-4.63682000	0.69478800
C	3.88317000	0.00016800	0.31124800
Fe	0.80551600	0.00002500	0.34213500
Cl	-5.74918400	1.59242000	0.08316000
Cl	-5.74901500	-1.59263700	0.08040400
F	3.72638100	-0.00041100	1.69412400
F	5.21014600	0.00022500	0.07266400
O	0.61753400	-0.00324000	1.96488300

{TAML–Fe^{V}–O}•H$_2$O‡ (Quartet)

Energy: -2801.09178009 a.u.

C	-1.56899100	0.95165700	-0.39606200
C	-1.61733300	-0.45712600	-0.63128600
C	-2.84465100	-1.08280100	-0.85594900
C	-4.01756700	-0.32298200	-0.86997000
C	-3.97000100	1.05900100	-0.67124700
C	-2.75044100	1.70022500	-0.42547900
H	-2.88464100	-2.15138800	-1.04127400
H	-2.70847500	2.77501700	-0.27924900
N	-0.35538100	-1.04162700	-0.66092800
N	-0.27848100	1.42860300	-0.19939400
C	-0.04230100	-2.34531100	-0.77840200
C	0.11435900	2.73785600	-0.18925700
C	1.47530400	-2.60414100	-0.85065600
C	1.64874300	2.89652400	-0.19366300
N	2.26574000	1.54839000	-0.17726700
N	2.17772600	-1.33269000	-0.55918300

C	3.52599000	-1.29280200	-0.59870100
C	3.60712100	1.43916200	-0.23378300
O	4.27939400	-2.20052800	-0.95532500
O	-0.85329300	-3.29360400	-0.82740700
O	-0.63638200	3.71509700	-0.19755800
O	4.42398100	2.35530000	-0.35444100
C	2.04481000	3.68801500	1.05416300
H	1.79365900	3.12386700	1.96175800
H	3.12149000	3.88351200	1.04889100
H	1.49920300	4.63893000	1.07583300
C	2.00078200	3.67515700	-1.46561400
H	3.06762800	3.91059500	-1.48397600
H	1.75819100	3.08513300	-2.35865600
H	1.41409500	4.60082500	-1.49536500
C	1.76500400	-3.11587000	-2.26697200
H	1.54781500	-2.33801100	-3.00965200
H	2.81568000	-3.40164800	-2.35922100
H	1.12602000	-3.98213600	-2.47718300
C	1.83255100	-3.65912300	0.19725400
H	2.88995900	-3.92777500	0.11323300
H	1.65312300	-3.26083800	1.20489600
H	1.21678500	-4.55467400	0.04671100
C	4.16926600	0.00166400	-0.01807000
Fe	1.05201000	0.09590600	-0.02658400
Cl	-5.42954400	2.01406800	-0.66002400
Cl	-5.54045600	-1.14424500	-1.10174800
F	4.18235600	-0.18802500	1.36704200
F	5.46629700	0.01155900	-0.40370500
O	1.03077300	-0.59108800	1.78615100
O	0.27200600	0.31435700	2.91032700
H	0.89151600	0.14533800	3.64022000
H	-0.59045800	-0.33235500	3.05781500
H	-2.51057300	-0.67105900	2.92619600
H	-1.63985400	-1.96356200	2.66816700
O	-1.70168000	-1.14847400	3.23457700
O	-3.91631300	0.27320800	2.41821600
H	-3.57458900	0.91800800	1.77399600
H	-4.51046500	-0.27365700	1.88228800
O	-1.70506700	-3.46637500	1.79827700
H	-1.55535200	-3.38715900	0.82646000
H	-0.97133300	-4.02582000	2.08642200

{H-TAML–Fe^{V}–O} (Doublet)

Energy: -2495.45300391 a.u.

C	1.82883000	-0.67266500	-0.04334900
C	1.89431500	0.73043200	0.10814200
C	3.11092200	1.39683800	0.18857700
C	4.29162000	0.66034500	0.11902700
C	4.23792700	-0.73280200	-0.04210200
C	3.01749700	-1.40233000	-0.12855200
H	3.15422700	2.47354700	0.31155500
H	2.99525800	-2.47789300	-0.25303300
N	0.61469500	1.29629600	0.12310800
N	0.52164300	-1.17225300	-0.11110200
C	0.21639500	2.46616600	-0.22781000
C	0.18107800	-2.50167600	-0.31952500
C	-1.26784800	2.68847000	-0.38423700
C	-1.32051600	-2.73986000	-0.30338900
N	-1.96600800	-1.42733400	-0.09141500
N	-1.89072600	1.34451100	-0.25735600
C	-3.25918900	1.29638400	-0.30349900
C	-3.31931800	-1.35948200	-0.11386300
C	-1.63647700	-3.69827500	0.84853100
H	-1.38012600	-3.24888000	1.81533700
H	-2.70256800	-3.94137600	0.84496900
H	-1.05605000	-4.61925200	0.72698000
C	-1.68649400	-3.35637700	-1.65855500
H	-2.72898700	-3.67868900	-1.66498900
H	-1.53623500	-2.63554900	-2.47110700
H	-1.03486000	-4.21844900	-1.83789500
C	-1.50955900	3.29201400	-1.77769600
H	-1.10147500	2.65001300	-2.56585700
H	-2.58118500	3.41517100	-1.93840700
H	-1.05345600	4.28859900	-1.86846700
C	-1.74822000	3.62762500	0.73214000
H	-2.80729300	3.85756000	0.59352500
H	-1.61076100	3.16004800	1.71348900
H	-1.18887900	4.57202000	0.71870800
C	-3.90564100	0.01556400	0.25653800
Fe	-0.82152600	-0.03437700	0.44160600
Cl	5.68973100	-1.66231100	-0.13212600
Cl	5.80039900	1.49315400	0.23381500
F	-3.81760400	0.14163300	1.63503900
F	-5.20870300	0.03109200	-0.06304400
O	-0.83247700	-0.01672000	2.01398000
O	1.08426100	3.44251400	-0.49231600
H	0.61556900	4.21931500	-0.84562200
O	1.00151800	-3.38719700	-0.50106300

O	-3.97333000	2.22537200	-0.65353600
O	-4.08348700	-2.28297000	-0.36488300

{H-TAML–Fe^{V}–O} (Quartet)

Energy: -2495.90257310 a.u.

C	1.84773100	-0.70287400	-0.03229900
C	1.87480900	0.71715900	-0.03162700
C	3.08065000	1.40934100	0.01022200
C	4.27555000	0.69387000	0.04835100
C	4.25619100	-0.71202600	0.04322900
C	3.05222200	-1.41057500	0.00539700
H	3.10699700	2.49320000	0.01668800
H	3.04790300	-2.49461400	0.00184900
N	0.58840300	1.27081400	-0.08522800
N	0.56883700	-1.23799400	-0.10509200
C	0.16638900	2.46796100	-0.30647400
C	0.22911500	-2.55574900	-0.31125400
C	-1.32745900	2.72274400	-0.33940100
C	-1.28732100	-2.78414200	-0.34647000
N	-1.93993800	-1.46141700	-0.15070900
N	-1.97185900	1.40128600	-0.20522600
C	-3.32802100	1.33526000	-0.17868800
C	-3.30318900	-1.36176200	-0.17670800
C	-1.66344400	-3.73734000	0.78647100
H	-1.43406700	-3.29506800	1.76296500
H	-2.73190500	-3.96796200	0.74394500
H	-1.09427900	-4.66726500	0.68207200
C	-1.61795000	-3.37607800	-1.71932600
H	-2.66844900	-3.66843000	-1.76845100
H	-1.41493600	-2.65418000	-2.51896000
H	-0.98542700	-4.25562900	-1.88032100
C	-1.67481300	3.38764200	-1.68063800
H	-1.37713700	2.75624500	-2.52469700
H	-2.75162600	3.55899400	-1.72850200
H	-1.18084000	4.36417500	-1.78681300
C	-1.69677300	3.62570000	0.84732200
H	-2.76963400	3.83406200	0.81859600
H	-1.45439600	3.13285800	1.79504000
H	-1.16471800	4.58540800	0.80584200
C	-3.88827700	-0.01856800	0.32564600
Fe	-0.83912600	-0.05026400	0.33295800
Cl	5.72892900	-1.60939200	0.09482000
Cl	5.76424400	1.56684400	0.10474200

F	-3.67629300	-0.00939500	1.69719300
F	-5.21164500	-0.03369100	0.11952200
O	-0.63451000	0.05066600	1.94210100
O	1.02162100	3.47088900	-0.50853600
H	0.53344400	4.28650300	-0.71880300
O	1.03587400	-3.46038900	-0.47120300
O	-4.10253600	2.24717200	-0.44207600
O	-4.06128800	-2.25865800	-0.51266900

{H_2-TAML–Fe^V–O} (Doublet)

Energy: -2496.25573028 a.u.

C	-1.86574300	0.68998300	-0.04873700
C	-1.88307100	-0.71805300	0.02638400
C	-3.08830000	-1.40643900	0.10235200
C	-4.28576600	-0.68999500	0.09844000
C	-4.27008100	0.71458700	0.01443100
C	-3.05941200	1.40505700	-0.06188600
H	-3.11678400	-2.48792900	0.17198200
H	-3.07516700	2.48677600	-0.11639100
N	-0.59341100	-1.27561000	0.00805900
N	-0.55887200	1.22416800	-0.09887000
C	-0.19536500	-2.46576600	-0.29812600
C	-0.15388400	2.43520800	-0.33938300
C	1.29304600	-2.70995800	-0.38113400
C	1.32844400	2.70734300	-0.33264500
N	1.96887900	1.38781100	-0.14630200
N	1.92205100	-1.36998100	-0.20780800
C	3.30028000	-1.30795300	-0.23461400
C	3.33550600	1.34338000	-0.12402100
C	1.64531500	3.63425300	0.85423100
H	1.38221300	3.16120700	1.80650800
H	2.71568600	3.85671500	0.85248500
H	1.10429800	4.58513400	0.77622500
C	1.70936300	3.35328700	-1.67432400
H	2.77722900	3.57524000	-1.68622500
H	1.47274200	2.69545800	-2.51705800
H	1.18160700	4.30545300	-1.82010400
C	1.60067700	-3.31457700	-1.75981400
H	1.27617300	-2.65401100	-2.57066800
H	2.67181100	-3.49481900	-1.85602000
H	1.10330700	-4.28571400	-1.88504100
C	1.70827800	-3.64753900	0.76306500
H	2.77268000	-3.88020500	0.67800900

H	1.52092300	-3.18563600	1.73858400
H	1.15353700	-4.59244800	0.71712700
C	3.91882600	-0.01126800	0.32733400
Fe	0.83116800	-0.00412100	0.39251500
Cl	-5.73041100	1.61344000	0.01294500
Cl	-5.76430900	-1.55111000	0.20061900
F	3.73810400	-0.07827900	1.69419000
F	5.22874900	-0.02330400	0.07801400
O	0.72991700	-0.00815100	1.96189500
O	-1.06510700	-3.42649600	-0.56060000
H	-0.61420900	-4.23697400	-0.86115000
O	4.01923600	-2.23043700	-0.56609300
O	4.08318200	2.27457000	-0.36496000
O	-1.02443300	3.39671200	-0.58073500
H	-0.56942300	4.22994100	-0.80499700

{H_2-TAML–Fe^V–O} (Quartet)

Energy: -2496.24676399 a.u.

C	-1.87121400	0.70940800	-0.04948800
C	-1.87119500	-0.70936000	-0.04943100
C	-3.07296700	-1.40839100	0.00413100
C	-4.27645600	-0.70512900	0.05763600
C	-4.27649200	0.70510400	0.05738400
C	-3.07301800	1.40839900	0.00381300
H	-3.09438700	-2.49191500	0.01258400
H	-3.09450400	2.49192300	0.01202200
N	-0.58365400	-1.26504700	-0.10243000
N	-0.58366700	1.26508900	-0.10244100
C	-0.17850000	-2.47524000	-0.32835900
C	-0.17849600	2.47539300	-0.32777200
C	1.31087800	-2.74547100	-0.35257000
C	1.31090800	2.74551200	-0.35240000
N	1.96192200	1.41869100	-0.18952200
N	1.96188000	-1.41858400	-0.18983400
C	3.33334000	-1.34033100	-0.16551200
C	3.33335200	1.34028600	-0.16576700
C	1.67499000	3.66586500	0.82118700
H	1.42613200	3.19883700	1.78005200
H	2.74696500	3.87798000	0.79539100
H	1.14696300	4.62509700	0.75393300
C	1.66371500	3.37970200	-1.70706900
H	2.73398600	3.58672100	-1.74824900
H	1.39570600	2.72155000	-2.53998500

H	1.14288700	4.33700600	-1.84137300
C	1.66426000	-3.38007100	-1.70683300
H	1.39670000	-2.72217600	-2.54010000
H	2.73453100	-3.58718600	-1.74746400
H	1.14343900	-4.33738500	-1.84112200
C	1.67444500	-3.66550000	0.82147800
H	2.74641800	-3.87771300	0.79611600
H	1.42528700	-3.19814800	1.78009600
H	1.14638200	-4.62471000	0.75423200
C	3.89778500	0.00003600	0.36176300
Fe	0.87567400	0.00000100	0.33210900
Cl	-5.74431000	1.58401700	0.12843000
Cl	-5.74423900	-1.58408500	0.12918800
F	3.61198800	0.00012900	1.71725000
F	5.21905500	-0.00000700	0.20499200
O	0.62607000	-0.00038400	1.93123600
O	-1.04754600	-3.44947100	-0.53952300
H	-0.59417000	-4.28843000	-0.74212400
O	4.08215100	-2.24997800	-0.47015700
O	4.08217600	2.24972700	-0.47103500
O	-1.04749700	3.44978200	-0.53823700
H	-0.59410500	4.28884100	-0.74035500

{H_2-TAML–Fe^V–O}•$H_2O^‡$ (Quartet)

Energy: -2801.91791593 a.u.

C	-1.51112500	0.87742000	-0.57591700
C	-1.53246900	-0.53532600	-0.69012300
C	-2.74736400	-1.20644900	-0.78859800
C	-3.93479000	-0.47594400	-0.78490400
C	-3.91557400	0.92456400	-0.70048200
C	-2.69934600	1.60000400	-0.59298300
H	-2.78409700	-2.28829200	-0.85467300
H	-2.69975900	2.68125500	-0.51051400
N	-0.25356100	-1.11766700	-0.66866200
N	-0.21240700	1.40123200	-0.42419000
C	0.14921200	-2.31171200	-0.96530200
C	0.25096500	2.60052000	-0.58008400
C	1.64113600	-2.58269800	-0.93098700
C	1.74518900	2.81540900	-0.44661500
N	2.31545700	1.49233900	-0.10389900
N	2.25456000	-1.35925700	-0.36762900
C	3.61453500	-1.28109100	-0.27190300
C	3.66888200	1.36770300	0.02739400

O	4.41295700	-2.11744300	-0.66347500
O	4.49687700	2.24393400	-0.16369400
C	2.01420000	3.82717700	0.67624400
H	1.61185200	3.47184900	1.63121500
H	3.09279900	3.97148500	0.77707500
H	1.56994000	4.80661800	0.45492100
C	2.26679300	3.33210900	-1.79819900
H	3.34504300	3.48955500	-1.73192900
H	2.06142100	2.61692500	-2.60199400
H	1.80686400	4.29256300	-2.06629000
C	2.08476700	-2.81235900	-2.38850500
H	1.86263800	-1.93883400	-3.01083200
H	3.16018800	-2.99985900	-2.41217400
H	1.57986300	-3.68319100	-2.82588700
C	1.95131900	-3.81015100	-0.06834600
H	3.02694100	-4.00164500	-0.09104100
H	1.63862000	-3.65357700	0.96830000
H	1.45122600	-4.71206900	-0.44707700
C	4.09987800	-0.03654100	0.51772000
Fe	1.11523400	0.06893100	0.08633700
Cl	-5.37274300	1.83626500	-0.70265000
Cl	-5.43220800	-1.33559000	-0.85474000
F	3.57283500	-0.17003300	1.79920400
F	5.42949400	-0.07569800	0.61293900
O	0.59890700	-0.31324200	1.85087000
O	-0.38189200	0.76056300	2.71303300
H	0.11646600	0.73019900	3.55117600
H	-1.26776700	0.12806400	2.84043000
H	-3.20582900	-0.51296200	2.70471100
H	-2.03964700	-1.60811700	2.57616400
O	-2.30355900	-0.76621600	3.01883100
O	-4.84001500	0.01507300	2.32687700
H	-5.36985000	0.30214400	3.08398300
H	-5.44850300	-0.50149600	1.77686100
O	-0.78853500	-2.72930800	1.89778800
H	-0.54007500	-3.39658800	2.55309800
H	-0.12106700	-2.01038900	1.98153400
O	-0.70130600	-3.24085300	-1.37146800
H	-0.23732300	-4.07831100	-1.55160900
O	-0.55582200	3.60955500	-0.87841900
H	-0.04931700	4.43371900	-0.99638200

{TAML$^{+\bullet}$–Fe^{V}–OH}$^{+}$ (Broken Symmetry Singlet)

Energy: -2495.64351052 a.u.

C	1.83875000	-0.72537200	0.09525900
C	1.83871800	0.72534100	0.09533300
C	3.04785000	1.43413200	0.02122900
C	4.23386500	0.72244000	-0.02159100
C	4.23390200	-0.72240400	-0.02171500
C	3.04791700	-1.43411800	0.02095800
H	3.05383800	2.51794400	0.01647600
H	3.05389300	-2.51793100	0.01598700
N	0.57770600	1.22607300	0.09799400
N	0.57777000	-1.22613500	0.09778600
C	0.22122800	2.56466900	-0.12141700
C	0.22125600	-2.56476600	-0.12100300
C	-1.28106300	2.73947000	-0.32948600
C	-1.28107100	-2.73944100	-0.32955300
N	-1.90440500	-1.40129900	-0.17819700
N	-1.90444900	1.40124000	-0.17829900
C	-3.27207000	1.31004000	-0.35218100
C	-3.27198600	-1.30985100	-0.35252400
O	-3.99796800	2.17721600	-0.79029100
O	1.01543800	3.47948000	-0.16443800
O	1.01525900	-3.47977900	-0.16340200
O	-3.99779700	-2.17686200	-0.79110400
C	-1.80214900	-3.68340100	0.76564000
H	-1.68324700	-3.24710000	1.76417600
H	-2.85830200	-3.90937500	0.59457600
H	-1.22809300	-4.61442700	0.72451400
C	-1.48280100	-3.33538300	-1.72741700
H	-2.52002000	-3.63725000	-1.88029500
H	-1.20336600	-2.62227900	-2.51104600
H	-0.84152700	-4.21806000	-1.81890800
C	-1.48316700	3.33564700	-1.72724200
H	-1.20433100	2.62250600	-2.51104600
H	-2.52034000	3.63790100	-1.87962700
H	-0.84156500	4.21807100	-1.81887900
C	-1.80179600	3.68331000	0.76594600
H	-2.85805300	3.90916100	0.59539100
H	-1.68235400	3.24702600	1.76443000
H	-1.22794800	4.61445500	0.72460800
C	-3.87512900	0.00001200	0.20126600
Fe	-0.81661300	-0.00002000	0.38433300
Cl	5.70675800	-1.56933700	-0.07111600
Cl	5.70666900	1.56946300	-0.07078800
F	-3.62309000	-0.00020000	1.57271400
F	-5.18770400	-0.00003400	0.02800300

O	-0.72399500	-0.00028900	2.12513400
H	-1.64514600	0.00061000	2.46171300

{TAML$^{+\bullet}$–Fe^{V}–OH}$^{+}$ (Triplet)

Energy: -2495.65209195 a.u.

C	1.83844000	-0.73127200	0.07126300
C	1.83843100	0.73134600	0.07120000
C	3.05228300	1.43893600	0.00427600
C	4.23253400	0.72733400	-0.04738800
C	4.23253900	-0.72726900	-0.04731200
C	3.05229100	-1.43886700	0.00442400
H	3.06047000	2.52291800	0.00884800
H	3.06047900	-2.52285100	0.00912700
N	0.58639700	1.22466300	0.10708900
N	0.58642000	-1.22460600	0.10724900
C	0.22990500	2.59439500	0.02166600
C	0.22996300	-2.59436100	0.02209400
C	-1.25832000	2.79297700	-0.26346400
C	-1.25816900	-2.79299000	-0.26344400
N	-1.88827100	-1.44684200	-0.18406500
N	-1.88834900	1.44680200	-0.18405300
C	-3.25371400	1.33321200	-0.37614500
C	-3.25364800	-1.33332100	-0.37614500
O	-3.95736500	2.20658900	-0.83929200
O	1.02980600	3.49604500	0.11274200
O	1.03004800	-3.49592400	0.11239300
O	-3.95729200	-2.20679100	-0.83912900
C	-1.84666700	-3.73990300	0.78142000
H	-1.79389100	-3.30790200	1.78719000
H	-2.88898200	-3.96645800	0.54326400
H	-1.27952400	-4.67591400	0.77842400
C	-1.35245500	-3.37658400	-1.68055600
H	-2.38892100	-3.62421900	-1.91687400
H	-0.97685400	-2.67237500	-2.43150600
H	-0.74946700	-4.28930000	-1.72573100
C	-1.35299300	3.37663500	-1.68051300
H	-0.97743700	2.67253000	-2.43158500
H	-2.38955900	3.62410000	-1.91658200
H	-0.75017200	4.28945700	-1.72576500
C	-1.84662300	3.73981200	0.78158900
H	-2.88899600	3.96636100	0.54368600
H	-1.79361100	3.30775700	1.78732300
H	-1.27950400	4.67583800	0.77852400

C	-3.86812100	-0.00007100	0.10282100
Fe	-0.86897700	0.00001400	0.32398300
Cl	5.70677200	-1.56587300	-0.11226900
Cl	5.70676300	1.56593600	-0.11244200
F	-3.69673800	-0.00006300	1.49466900
F	-5.16795200	-0.00010400	-0.14988000
O	-0.90143900	0.00004600	2.09590500
H	-1.83598000	0.00023000	2.38586000

{TAML$^{+\bullet}$–Fe^{V}–OH}$^{+}$ (Quintet)

Energy: -2495.64757109 a.u.

C	1.83791200	-0.73314300	-0.01084400
C	1.84501700	0.73797200	-0.00147600
C	3.06418700	1.43911800	0.03232800
C	4.24202000	0.72229100	0.04297900
C	4.23470700	-0.73590800	0.02860200
C	3.05001700	-1.44385400	0.00414900
H	3.07412600	2.52336600	0.04285100
H	3.05264700	-2.52804500	-0.00378800
N	0.59962600	1.23960000	-0.06245800
N	0.58580500	-1.22547100	-0.06476700
C	0.23185500	2.59603900	-0.21316700
C	0.20932800	-2.57504900	-0.26778700
C	-1.27496700	2.76369300	-0.41180300
C	-1.30197200	-2.75221300	-0.40442900
N	-1.92962400	-1.41771800	-0.21314800
N	-1.91899700	1.46858900	-0.06303500
C	-3.28909300	1.33901800	-0.17966000
C	-3.30222200	-1.31091000	-0.21121000
O	-4.02161700	2.19261600	-0.63872800
O	1.03531000	3.49931300	-0.26681800
O	1.01647000	-3.47029100	-0.37376500
O	-4.06002100	-2.18185400	-0.59210300
C	-1.76856000	-3.73832800	0.66922100
H	-1.61304600	-3.33328300	1.67560400
H	-2.82911300	-3.96503400	0.53602700
H	-1.19808900	-4.66782900	0.57515600
C	-1.55840300	-3.28523800	-1.82087600
H	-2.61881900	-3.51345600	-1.94534200
H	-1.26007000	-2.55814100	-2.58418000
H	-0.97417200	-4.20041400	-1.96306800
C	-1.46604300	3.10261300	-1.89890700
H	-1.12896600	2.28399100	-2.54512100

H	-2.52058500	3.30178600	-2.10168100
H	-0.88244800	3.99767200	-2.13771600
C	-1.77911800	3.88695800	0.49337000
H	-2.82945500	4.10188300	0.28476400
H	-1.67113700	3.62748400	1.55228100
H	-1.18960400	4.78875900	0.29945100
C	-3.85407800	0.01293600	0.36784900
Fe	-0.84433500	0.00244700	0.34967400
Cl	5.70464800	-1.57889400	0.04933500
Cl	5.72111500	1.55036900	0.07873300
F	-3.52297100	-0.00721900	1.72188000
F	-5.17607500	0.02086400	0.26058500
O	-0.72619500	-0.10647800	2.13510100
H	-1.43788900	0.36233300	2.60821600

{TAML$^{+\bullet}$–Fe^{V}–O} (Triplet)

Energy: -2495.29667208 a.u.

C	1.86000500	-0.72733000	0.15422300
C	1.81505700	0.71249700	0.02093200
C	3.00984400	1.43629400	-0.09837900
C	4.21403800	0.75063000	-0.08709900
C	4.25721000	-0.67688100	0.03367800
C	3.09324800	-1.40691900	0.15058500
H	2.99153300	2.51487000	-0.19584900
H	3.11575100	-2.48713300	0.24234600
N	0.53548900	1.19906800	-0.00468600
N	0.62360400	-1.26386500	0.21528600
C	0.17487100	2.54038300	-0.17256900
C	0.28125700	-2.59266200	0.02288000
C	-1.33053600	2.75024800	-0.20995300
C	-1.20163200	-2.73940800	-0.31809300
N	-1.82380600	-1.38248400	-0.26242900
N	-1.96180200	1.41697000	-0.10040900
C	-3.31330700	1.34209900	-0.17953900
C	-3.18070500	-1.30096000	-0.48283300
O	-4.07806200	2.26926100	-0.41548400
O	0.98857800	3.44058600	-0.28051500
O	1.06370500	-3.52720500	0.04085000
O	-3.84106200	-2.19206100	-0.98953600
C	-1.84389600	-3.66532000	0.71684400
H	-1.83839000	-3.20640700	1.71290100
H	-2.87632300	-3.89166300	0.43816100
H	-1.27448700	-4.59992300	0.76100300
C	-1.25140100	-3.33866100	-1.72871200

H	-2.27803500	-3.58642900	-2.00219800
H	-0.85062700	-2.63646600	-2.46925300
H	-0.63852500	-4.24629200	-1.74606600
C	-1.64558800	3.43793400	-1.54439000
H	-1.44619200	2.76759200	-2.38882900
H	-2.69315100	3.74070600	-1.57882700
H	-1.00642300	4.32167300	-1.64564300
C	-1.71151700	3.63923900	0.97881100
H	-2.78003500	3.86691000	0.93986900
H	-1.49279200	3.13880600	1.92954100
H	-1.14388500	4.57502000	0.93592100
C	-3.89322400	-0.05924000	0.08779800
Fe	-0.83005500	-0.00438100	0.45748700
Cl	5.76565100	-1.49515700	0.03895900
Cl	5.67078100	1.64399300	-0.22384400
F	-3.89640400	-0.24221600	1.46217300
F	-5.16982000	-0.08331900	-0.32242800
O	-0.96404000	-0.01023600	2.02695300

{TAML$^{+\bullet}$–Fe^{V}–O} (Quintet)

Energy: -2495.28997685 a.u.

C	1.84578800	-0.72469600	0.01959100
C	1.84578600	0.72480500	0.01955900
C	3.06264100	1.42727000	0.01468700
C	4.24769500	0.71632800	0.00841400
C	4.24770400	-0.71636100	0.00851500
C	3.06264400	-1.42723900	0.01483500
H	3.06586600	2.51111700	0.01371100
H	3.06571600	-2.51108800	0.01400800
N	0.59016600	1.24216000	-0.00595600
N	0.59023400	-1.24212600	-0.00594800
C	0.23289200	2.57833200	-0.16469500
C	0.23283100	-2.57824100	-0.16435100
C	-1.28074600	2.78245500	-0.29690400
C	-1.28081000	-2.78230400	-0.29712400
N	-1.92788200	-1.44926700	-0.19027400
N	-1.92802700	1.44966400	-0.18899000
C	-3.28970600	1.34971400	-0.25171400
C	-3.28960700	-1.34928700	-0.25313000
O	-4.04094000	2.24638700	-0.60374800
O	1.03436900	3.49359400	-0.23834700
O	1.03423500	-3.49365200	-0.23744700
O	-4.04074500	-2.24574900	-0.60581300

C	-1.74326900	-3.69945500	0.83586100
H	-1.58782000	-3.22594100	1.81221300
H	-2.80561700	-3.93074300	0.72048800
H	-1.17207600	-4.63332100	0.80437400
C	-1.52250500	-3.41577700	-1.67104700
H	-2.57652700	-3.67558300	-1.78606800
H	-1.23926000	-2.72987700	-2.47790500
H	-0.91227800	-4.32134900	-1.75551300
C	-1.52296900	3.41518800	-1.67112700
H	-1.23993300	2.72885500	-2.47769200
H	-2.57707400	3.67480200	-1.78584500
H	-0.91287300	4.32077400	-1.75630200
C	-1.74250100	3.70042800	0.83573400
H	-2.80482300	3.93194400	0.72068900
H	-1.58677200	3.22741400	1.81229000
H	-1.17099400	4.63407100	0.80346500
C	-3.88150600	-0.00004400	0.22715100
Fe	-0.86406600	0.00005400	0.32038100
Cl	5.73312400	-1.57598200	0.00604000
Cl	5.73310700	1.57595700	0.00574400
F	-3.72471500	-0.00083000	1.60496200
F	-5.19425000	0.00004600	-0.03440600
O	-0.78100400	-0.00117200	1.95104000

{TAML$^{+\bullet}$–Fe^{V}–O}•H_2O‡ (Broken Symmetry Singlet)

Energy: -2800.94641745 a.u.

C	-1.57377800	0.82128100	-0.44028300
C	-1.59377800	-0.59903300	-0.58026100
C	-2.80367400	-1.26444300	-0.79705800
C	-3.98771600	-0.53327300	-0.85905200
C	-3.96841400	0.86887300	-0.74150300
C	-2.76958700	1.54971400	-0.53314700
H	-2.82632300	-2.34279700	-0.91492600
H	-2.75286700	2.63230600	-0.45496300
N	-0.31882800	-1.14237800	-0.56641400
N	-0.29740700	1.31492900	-0.29103900
C	0.01999800	-2.46231400	-0.55366600
C	0.07319400	2.64536200	-0.29269700
C	1.52165900	-2.68950000	-0.71105400
C	1.58843800	2.81730600	-0.40221100
N	2.20048000	1.47216500	-0.25799000
N	2.17814400	-1.38145400	-0.48902700
C	3.53319900	-1.31413000	-0.55026800

C	3.55441000	1.36255700	-0.35639500
O	4.28852700	-2.19803900	-0.93830100
O	-0.78580400	-3.39118100	-0.39848700
O	-0.70865200	3.58611600	-0.26402100
O	4.32854200	2.26463200	-0.65105000
C	2.06779400	3.77663700	0.68560100
H	1.91305700	3.34879600	1.68257100
H	3.12983100	3.99988300	0.55540400
H	1.49305700	4.70694400	0.62053600
C	1.83875400	3.40539100	-1.79926200
H	2.90081900	3.62087900	-1.93346800
H	1.51937900	2.70657100	-2.58195800
H	1.26260200	4.33101900	-1.90700000
C	1.74150300	-3.22349900	-2.13283400
H	1.44208400	-2.47914700	-2.87993000
H	2.79621700	-3.46456600	-2.28268500
H	1.13924900	-4.12725100	-2.28140900
C	1.97311000	-3.70219600	0.34195100
H	3.03008700	-3.94429800	0.20526900
H	1.83627700	-3.29561000	1.35290900
H	1.37783200	-4.61695400	0.24870200
C	4.12499700	-0.01651000	0.04697200
Fe	1.03568200	0.03320600	0.02099600
Cl	-5.44250800	1.77978300	-0.78870000
Cl	-5.48149000	-1.38516900	-1.05540900
F	3.93627300	-0.11534000	1.42731300
F	5.44870000	-0.01091700	-0.16661000
O	0.92198500	-0.22883700	1.69742200
O	0.43726500	1.03799800	2.56822900
H	1.21480300	1.07824600	3.15455000
H	-0.74647000	0.11792500	3.04882100
H	-2.39928900	-0.04217200	2.97187400
H	-1.46850500	-1.37993300	2.76950000
O	-1.53794000	-0.49357300	3.27684600
O	-3.73081000	0.68228700	2.49339600
H	-3.57984600	1.15376600	1.65346800
H	-4.48375800	0.09903000	2.31255000
O	-1.71555700	-2.81654500	2.15497100
H	-1.49947600	-3.03378400	1.21640400
H	-1.34111100	-3.54338200	2.67166800

{TAML$^{+\bullet}$–Fe^{V}–O}•H$_2$O‡ (Triplet)

Energy: -2800.95319974 a.u.

C	-1.39411200	0.96357600	-0.55887800
C	-1.47595700	-0.45088000	-0.73489000
C	-2.71963000	-1.06044500	-0.91965100
C	-3.86885000	-0.27754000	-0.88231600
C	-3.78933600	1.11124700	-0.67559100
C	-2.55913100	1.73832300	-0.52375000
H	-2.79567200	-2.12816200	-1.09164400
H	-2.49463000	2.81028000	-0.37219000
N	-0.22847600	-1.05035800	-0.72170900
N	-0.09485300	1.40442900	-0.43252300
C	0.06164000	-2.37468200	-0.78161900
C	0.33980200	2.71326900	-0.42279900
C	1.56408300	-2.65445300	-0.75910100
C	1.85921800	2.82137700	-0.30206000
N	2.39590400	1.44911400	-0.12496400
N	2.24224400	-1.37662800	-0.43891800
C	3.60455300	-1.36331100	-0.36177500
C	3.74267200	1.28634200	-0.01529700
O	4.35463700	-2.26279700	-0.71509300
O	-0.77448200	-3.28846800	-0.84944200
O	-0.39673800	3.68558400	-0.52070200
O	4.59080300	2.15742400	-0.15633800
C	2.18031200	3.68996700	0.91564600
H	1.83301800	3.20818300	1.83812900
H	3.25788800	3.85832400	0.98893700
H	1.66943400	4.65384900	0.81658500
C	2.35760700	3.47111500	-1.59868000
H	3.42896300	3.67201300	-1.53618700
H	2.17153000	2.81837900	-2.45988500
H	1.81744200	4.41125200	-1.75531300
C	1.93629700	-3.18173100	-2.15092100
H	1.78547900	-2.40870800	-2.91343000
H	2.98193400	-3.49490700	-2.17255400
H	1.29562300	-4.03714900	-2.39297800
C	1.84610300	-3.69430000	0.32627300
H	2.90419300	-3.96999300	0.32044000
H	1.59250800	-3.30013800	1.31907300
H	1.24319900	-4.58943000	0.13784800
C	4.18039600	-0.13871500	0.38609500
Fe	1.12905400	0.07018000	0.02676200
Cl	-5.23483500	2.06609700	-0.53299800
Cl	-5.41057300	-1.06581100	-1.02049100
F	3.79058300	-0.30266900	1.71459800
F	5.51843600	-0.20569200	0.35380500
O	0.71708400	-0.19816800	1.64295900

O	-0.53112400	0.82831800	2.33279700
H	-0.01102400	0.98020400	3.14105000
H	-1.47232800	-0.14347100	2.56182600
H	-3.16129300	-0.53826200	2.53002600
H	-2.11566200	-1.74489300	2.23149100
O	-2.25081400	-0.89251500	2.76190800
O	-4.74459200	-0.07034700	2.25225900
H	-4.87501800	0.82065300	1.89032300
H	-5.21351900	-0.65155800	1.63123500
O	-2.18884000	-3.18940400	1.51146200
H	-1.74801200	-3.29793300	0.63523100
H	-1.86387600	-3.92070000	2.05405900

{TAML$^{+\bullet}$–Fe^{V}–O}•$H_2O^{‡}$•NO_3^- (Triplet)

Energy: -2928.52464320 a.u.

C	-0.81459800	1.67714400	-0.34240900
C	-1.23251000	0.35952900	-0.78640400
C	-2.58384600	0.11315500	-1.08169800
C	-3.50223200	1.13210400	-0.92082200
C	-3.08633900	2.43134600	-0.49128700
C	-1.76279700	2.70585800	-0.21472400
H	-2.90687900	-0.87170200	-1.39856700
H	-1.45064000	3.69051100	0.11361300
N	-0.20042700	-0.51910900	-0.85554400
N	0.51991200	1.75157300	-0.11054800
C	-0.21231700	-1.80128600	-1.37698100
C	1.26957200	2.87210200	0.17721400
C	1.15507900	-2.48495400	-1.26616000
C	2.76089700	2.54867100	0.32568400
N	2.94271200	1.08619000	0.14969900
N	2.11594900	-1.51247400	-0.68327800
C	3.40599000	-1.89550000	-0.53269700
C	4.19601300	0.58114400	0.22546100
O	3.91924500	-2.92619400	-0.96223400
O	-1.18080000	-2.32793300	-1.90458600
O	0.82656900	4.01131100	0.26746800
O	5.24248700	1.22425100	0.27897000
C	3.19895300	2.98354600	1.72609400
H	2.68452500	2.39165300	2.49291200
H	4.27797800	2.84468500	1.83972500
H	2.95189700	4.04080900	1.87653100
C	3.48896600	3.35579200	-0.75594600

H	4.57015900	3.26248500	-0.63591200
H	3.21648500	2.99819500	-1.75668400
H	3.19564500	4.40866600	-0.67370900
C	1.54699900	-2.91228600	-2.68447200
H	1.73721800	-2.03612400	-3.31698600
H	2.44795400	-3.52786600	-2.66322000
H	0.71863400	-3.48001800	-3.12297700
C	0.99533100	-3.69656400	-0.34398400
H	1.93066500	-4.26353500	-0.31167900
H	0.73293700	-3.37346400	0.66943500
H	0.19196600	-4.34130900	-0.71880900
C	4.26841700	-0.96002900	0.35067800
Fe	1.36063400	0.04738900	0.07685600
Cl	-4.25165000	3.69331600	-0.30639500
Cl	-5.16088300	0.81593000	-1.24025100
F	3.90910700	-1.24754100	1.66647700
F	5.55812500	-1.32983000	0.21648100
O	0.91916700	-0.30648400	1.58547300
O	-1.13041700	0.14298200	2.05301400
H	-0.71524000	0.20915200	2.92589400
H	-1.47314100	-1.15436900	1.79446900
H	-2.85291900	-2.10509600	0.98196500
H	-2.01512700	-2.65958000	2.28943600
O	-1.78518000	-2.16962300	1.48253700
N	-4.81889000	-2.58444100	1.41411300
O	-4.30309200	-3.06430800	2.44176200
O	-4.01966200	-2.04729600	0.51469700
O	-6.02268000	-2.57881300	1.18243300

{H-TAML$^{+\bullet}$–Fe^{V}–O} (Triplet)

Energy: -2495.62591126 a.u.

C	1.82471800	-0.67547400	-0.07166500
C	1.88635600	0.74928300	0.11473000
C	3.09844600	1.40785400	0.22109300
C	4.28098300	0.66579800	0.13439200
C	4.23281900	-0.74901000	-0.06878900
C	3.01894000	-1.40913700	-0.17433400
H	3.14927600	2.48059500	0.37211800
H	2.99415900	-2.48244900	-0.31870100
N	0.61299900	1.30623000	0.12958800
N	0.54221000	-1.16279100	-0.14177300
C	0.21761000	2.49165200	-0.21217000
C	0.18910100	-2.51210900	-0.35302000

C	-1.26493000	2.70603800	-0.37805900
C	-1.30863400	-2.75744900	-0.26885400
N	-1.94607600	-1.42352200	-0.14525900
N	-1.87990300	1.34980900	-0.26496200
C	-3.25302600	1.28411200	-0.34015100
C	-3.30684200	-1.36547300	-0.11819200
C	-1.57410300	-3.61273600	0.97650900
H	-1.28841600	-3.08699100	1.89488500
H	-2.63751300	-3.86206300	1.02983800
H	-0.99926500	-4.54201800	0.91067500
C	-1.72843400	-3.48383700	-1.55074100
H	-2.76343300	-3.82133300	-1.48243700
H	-1.62585900	-2.83640200	-2.42864000
H	-1.07976800	-4.35518200	-1.68569300
C	-1.49857300	3.32631100	-1.76611400
H	-1.10387800	2.68985500	-2.56494000
H	-2.56635100	3.47510100	-1.92801600
H	-1.02780900	4.31610600	-1.84185700
C	-1.76147200	3.62325100	0.75113400
H	-2.82203800	3.84203500	0.60417900
H	-1.62744900	3.14994800	1.72997800
H	-1.21875000	4.57619800	0.74981800
C	-3.90804400	0.01103300	0.23713800
Fe	-0.82534800	-0.01660100	0.41533900
Cl	5.67788700	-1.64736900	-0.16694600
Cl	5.76949200	1.47194900	0.27618300
F	-3.80839500	0.14882400	1.60531500
F	-5.20036500	0.01484500	-0.08930100
O	-0.86408900	-0.03923900	1.98239600
O	1.09112800	3.44987000	-0.45383800
H	0.65211300	4.24773200	-0.80525700
O	1.01233900	-3.37576700	-0.56865100
O	-3.95854700	2.20312800	-0.71068100
O	-4.06541600	-2.30538100	-0.29629100

{TAML–Fe^{IV}–OOH} (Broken Symmetry Singlet)

Energy: -2571.21095459 a.u.

C	1.83564700	-0.71080300	-0.08220200
C	1.83074700	0.71202400	-0.09662000
C	3.03823900	1.41404000	-0.10607700
C	4.23755600	0.70545500	-0.09965700
C	4.24181600	-0.69566900	-0.08671200
C	3.04498300	-1.40953700	-0.07843100

H	3.03549700	2.49811300	-0.12359500
H	3.04663700	-2.49407000	-0.08278700
N	0.54692400	1.23877400	-0.11564800
N	0.55097800	-1.24412500	-0.08283000
C	0.20224600	2.54805200	-0.31436400
C	0.20415700	-2.54927800	-0.29796800
C	-1.31923900	2.74569600	-0.39396200
C	-1.31612100	-2.73564600	-0.42286400
N	-1.96471400	-1.41886700	-0.22626400
N	-1.96845000	1.42766600	-0.20580600
C	-3.31698200	1.35107700	-0.28863700
C	-3.31198300	-1.34148900	-0.32377500
O	-4.09241800	2.25065000	-0.61020100
O	0.98746900	3.48402900	-0.45560500
O	0.98746000	-3.49141800	-0.41738100
O	-4.08278800	-2.23307800	-0.67809100
C	-1.76458600	-3.72161900	0.65826500
H	-1.61232000	-3.29351000	1.65761300
H	-2.82644100	-3.95678400	0.53899000
H	-1.17549400	-4.64275700	0.57898200
C	-1.56902700	-3.30318500	-1.82400000
H	-2.62453100	-3.55538700	-1.94837500
H	-1.29049400	-2.57174700	-2.59292100
H	-0.95248500	-4.19883400	-1.96250900
C	-1.60968200	3.34589400	-1.77369400
H	-1.37070400	2.62618300	-2.56677700
H	-2.66324700	3.62091500	-1.85840600
H	-0.98023400	4.23223300	-1.91361800
C	-1.72993800	3.70770100	0.72323600
H	-2.79626200	3.94130500	0.64657400
H	-1.53604800	3.26102500	1.70634500
H	-1.14764900	4.63272800	0.63957000
C	-3.90309400	-0.00273500	0.18017700
Fe	-0.81314700	0.00621300	0.26070100
Cl	5.73906000	-1.58532800	-0.08137200
Cl	5.73099000	1.60107400	-0.10774200
F	-3.76007300	-0.02167800	1.56807400
F	-5.22937500	-0.00201100	-0.06657800
O	-0.79073100	-0.01835700	2.04245400
O	0.52030700	0.03359000	2.59778700
H	0.79379800	-0.90278000	2.55000800

{TAML–Fe^{IV}–OOH} (Triplet)

Energy: -2571.22862303 a.u.

C	1.83167700	-0.71073200	-0.11623000
C	1.82801400	0.71408100	-0.12608800
C	3.03694600	1.41505700	-0.11650300
C	4.23453500	0.70576800	-0.09573800
C	4.23762100	-0.69670900	-0.08554700
C	3.04149000	-1.40996200	-0.09553500
H	3.03511100	2.49920500	-0.12972600
H	3.04283100	-2.49449800	-0.10113800
N	0.54603600	1.23993600	-0.15791100
N	0.54838900	-1.24142200	-0.13893500
C	0.20002700	2.55504000	-0.33247100
C	0.19907300	-2.55373000	-0.31764300
C	-1.32210200	2.75646000	-0.39264500
C	-1.32253500	-2.74469700	-0.42234800
N	-1.96965500	-1.42738300	-0.23279600
N	-1.96991700	1.43744800	-0.21588700
C	-3.31814800	1.35796200	-0.27678800
C	-3.31651400	-1.34577500	-0.30807300
O	-4.10154000	2.25592300	-0.58413600
O	0.98728100	3.48951500	-0.46470700
O	0.98406100	-3.49547700	-0.42049300
O	-4.09700400	-2.23547500	-0.64682800
C	-1.75715900	-3.72513200	0.66884100
H	-1.59307500	-3.29199000	1.66404900
H	-2.82057300	-3.95987600	0.56354100
H	-1.17029300	-4.64755400	0.58774900
C	-1.59040200	-3.32251700	-1.81704400
H	-2.64862600	-3.57030300	-1.92769300
H	-1.31714200	-2.59806500	-2.59439300
H	-0.97989500	-4.22254100	-1.95501600
C	-1.62691300	3.37205600	-1.76273800
H	-1.39574900	2.66146800	-2.56624500
H	-2.68213400	3.64533000	-1.83220600
H	-1.00086900	4.26142900	-1.89944100
C	-1.71963500	3.70771100	0.73804500
H	-2.78783400	3.93778700	0.67747400
H	-1.51172600	3.25258600	1.71443000
H	-1.14237800	4.63607100	0.65580100
C	-3.89501600	-0.00011400	0.19795900
Fe	-0.81384100	0.00563100	0.23305500
Cl	5.73453200	-1.58597200	-0.06024600
Cl	5.72897700	1.59902900	-0.08043900
F	-3.72553700	-0.01678500	1.58466900
F	-5.22527700	0.00159400	-0.02355400

O	-0.76673100	-0.04481800	2.05663900
O	0.55085700	0.03675000	2.56408800
H	0.82475700	-0.90070400	2.57047100

{TAML–Fe^{IV}–OO} (Triplet)

Energy: -2570.62265190 a.u.

C	1.88605400	-0.69306600	-0.01183700
C	1.89317600	0.73587900	0.01504200
C	3.10835800	1.42411900	-0.00966000
C	4.30753400	0.70926100	-0.05146600
C	4.30100800	-0.68414100	-0.07580300
C	3.09616700	-1.39007400	-0.05988800
H	3.10744300	2.50897100	-0.00502800
H	3.08582800	-2.47436600	-0.09225700
N	0.61651600	1.28952200	0.02824600
N	0.60607000	-1.23504300	-0.02496200
C	0.28896500	2.58663600	-0.18581300
C	0.26685900	-2.52187500	-0.28989900
C	-1.23852300	2.80144800	-0.31512100
C	-1.25856200	-2.71362800	-0.46352700
N	-1.93305500	-1.41017300	-0.26869800
N	-1.92147600	1.49431800	-0.19748500
C	-3.25090500	1.43137500	-0.35166600
C	-3.25796900	-1.32080200	-0.44469200
O	-4.02569200	2.35399200	-0.64922100
O	1.07365500	3.54005100	-0.30060000
O	1.04629200	-3.47431800	-0.43402800
O	-4.03632800	-2.20757300	-0.82837900
C	-1.73552900	-3.72696000	0.57936500
H	-1.60143100	-3.31349200	1.58656500
H	-2.79662900	-3.95040800	0.42213800
H	-1.14763900	-4.65013400	0.49026000
C	-1.46303200	-3.25865700	-1.88227600
H	-2.51613200	-3.50394600	-2.04505000
H	-1.15916900	-2.51145200	-2.62793000
H	-0.84037200	-4.15202700	-2.01758100
C	-1.47209800	3.45552000	-1.68135000
H	-1.20343500	2.76033400	-2.48795000
H	-2.52410100	3.73035300	-1.79637200
H	-0.83491900	4.34457300	-1.76789300
C	-1.67865900	3.73885000	0.81264000
H	-2.74308100	3.97541500	0.70707700
H	-1.52023800	3.25902600	1.78710000

H	-1.08894000	4.66424000	0.77696800
C	-3.88103800	0.04428200	-0.01806200
Fe	-0.78956600	0.02006800	0.31054900
Cl	5.80245900	-1.59464500	-0.12302200
Cl	5.81667400	1.60827800	-0.06866300
F	-3.98201200	-0.00108100	1.37546100
F	-5.16463700	0.06424900	-0.47184900
O	-0.89461200	0.06133700	2.30871900
O	-0.90595400	-1.10955500	2.89927800

{TAML–Fe^{IV}–OO} (Quintet)

Energy: -2570.62453601 a.u.

C	1.88518400	-0.69644100	-0.02463200
C	1.89208900	0.73400900	0.00365000
C	3.10753200	1.42181800	-0.01352900
C	4.30728200	0.70758800	-0.05049200
C	4.30112900	-0.68588600	-0.07653500
C	3.09654400	-1.39215100	-0.06713000
H	3.10622900	2.50679000	-0.00632700
H	3.08668100	-2.47658600	-0.09965200
N	0.61567100	1.28976200	0.01261400
N	0.60655300	-1.24119100	-0.04115100
C	0.28538300	2.58955000	-0.18563000
C	0.26587000	-2.53126600	-0.28671000
C	-1.24422400	2.80261900	-0.32161800
C	-1.26288100	-2.72464900	-0.45264700
N	-1.94034400	-1.42179700	-0.26334500
N	-1.92916600	1.49638300	-0.19925700
C	-3.25842500	1.42807200	-0.35470400
C	-3.26543100	-1.33186200	-0.43306100
O	-4.03790800	2.34349500	-0.66052800
O	1.06639100	3.54733300	-0.28547700
O	1.04179200	-3.48868600	-0.41759400
O	-4.05066500	-2.21746100	-0.80587300
C	-1.73493200	-3.73212000	0.59781900
H	-1.59972400	-3.31446700	1.60300800
H	-2.79639000	-3.95748200	0.44563100
H	-1.14641400	-4.65527400	0.51371100
C	-1.47385500	-3.27923000	-1.86661400
H	-2.52880900	-3.52111400	-2.02356000
H	-1.17019500	-2.53803500	-2.61834400
H	-0.85556200	-4.17615600	-1.99884300
C	-1.47273000	3.44819800	-1.69285000

H	-1.19507300	2.75039000	-2.49419000
H	-2.52605500	3.71542400	-1.81526900
H	-0.84153200	4.34142900	-1.78103600
C	-1.69029800	3.74691200	0.79752000
H	-2.75428800	3.98251600	0.68492000
H	-1.53715100	3.27337200	1.77584700
H	-1.10070000	4.67221900	0.75932600
C	-3.87930500	0.03881800	-0.00326600
Fe	-0.78773300	0.02174400	0.24461000
Cl	5.80334000	-1.59582600	-0.11848900
Cl	5.81641100	1.60705500	-0.06005700
F	-3.94692600	0.00108300	1.39347200
F	-5.17305200	0.05563100	-0.42664600
O	-0.85755100	0.12130100	2.37390500
O	-0.87937200	-1.05544000	2.92673300

{TAML–Fe^{V}–OO} (Doublet)

Energy: -2570.62152600 a.u.

C	-1.82112100	0.71292200	-0.12448900
C	-1.82106900	-0.71282800	-0.12494500
C	-3.02994900	-1.41262800	-0.09353100
C	-4.22611300	-0.70152700	-0.06061700
C	-4.22615200	0.70150800	-0.06021300
C	-3.03001200	1.41266900	-0.09267700
H	-3.02943200	-2.49698000	-0.10427200
H	-3.02950500	2.49702800	-0.10275500
N	-0.53930000	-1.24573500	-0.17248500
N	-0.53939300	1.24596600	-0.17151400
C	-0.19070500	-2.55638200	-0.36821800
C	-0.19080300	2.55649400	-0.36780500
C	1.33417900	-2.75063700	-0.44326100
C	1.33406700	2.75062800	-0.44351900
N	1.97967700	1.44313100	-0.18894900
N	1.97976900	-1.44318500	-0.18844700
C	3.32728400	-1.34998900	-0.23545200
C	3.32721600	1.34997200	-0.23594400
O	4.12656100	-2.22332200	-0.57050600
O	-0.97435500	-3.49315500	-0.50836300
O	-0.97443900	3.49329800	-0.50792100
O	4.12641800	2.22323400	-0.57134400
C	1.73818100	3.77078500	0.62208200
H	1.53231300	3.38247300	1.62779100
H	2.80679100	3.99360600	0.54487100

H	1.16195500	4.69284000	0.48315300
C	1.63968100	3.27924100	-1.84913200
H	2.69999700	3.52764700	-1.93938900
H	1.39075000	2.52709400	-2.60826100
H	1.03175600	4.17195900	-2.03689600
C	1.64039900	-3.27952600	-1.84862100
H	1.39231500	-2.52733100	-2.60798200
H	2.70063700	-3.52847200	-1.93826100
H	1.03213000	-4.17195500	-2.03664400
C	1.73773900	-3.77065300	0.62270800
H	2.80647300	-3.99317100	0.54626200
H	1.53102200	-3.38236500	1.62824900
H	1.16189300	-4.69289200	0.48341600
C	3.87000400	0.00011000	0.30376000
Fe	0.81273300	0.00003500	0.19812400
Cl	-5.72117100	1.59220400	-0.01938800
Cl	-5.72109100	-1.59232200	-0.02030500
F	3.59081600	0.00037000	1.67653100
F	5.21206200	0.00012600	0.18866900
O	0.57820700	-0.00061700	2.13952500
O	-0.59112100	-0.00006800	2.59942100

{TAML–Fe^{V}–OO} (Quartet)

Energy: -2570.60797080 a.u.

C	-1.82695300	0.71480000	-0.16085400
C	-1.82695000	-0.71477800	-0.16088700
C	-3.03670300	-1.41402300	-0.10816500
C	-4.23043600	-0.70278600	-0.05506800
C	-4.23043900	0.70278500	-0.05503000
C	-3.03671100	1.41403300	-0.10808900
H	-3.03618000	-2.49847800	-0.11548700
H	-3.03619400	2.49848900	-0.11533400
N	-0.55046900	-1.24653700	-0.22590600
N	-0.55047100	1.24657100	-0.22580300
C	-0.19941000	-2.56518600	-0.36605900
C	-0.19942500	2.56524000	-0.36578700
C	1.32768600	-2.75915800	-0.41886000
C	1.32766200	2.75919200	-0.41880800
N	1.97262600	1.44547300	-0.18839500
N	1.97263800	-1.44543100	-0.18848300
C	3.32209900	-1.35648300	-0.22435100
C	3.32209000	1.35653300	-0.22426300
O	4.11916500	-2.24057600	-0.53466500

O	-0.97959100	-3.50752400	-0.48122600
O	-0.97961200	3.50751300	-0.48143800
O	4.11915800	2.24062300	-0.53458100
C	1.72048400	3.75455500	0.67387800
H	1.50563000	3.34238400	1.66787800
H	2.78935000	3.98042700	0.61170100
H	1.14452300	4.67891300	0.55051000
C	1.64754400	3.31947300	-1.80950900
H	2.70822200	3.57146300	-1.88299700
H	1.40742100	2.58449800	-2.58809900
H	1.04002100	4.21543100	-1.98272900
C	1.64773300	-3.31951500	-1.80948500
H	1.40765900	-2.58460300	-2.58815000
H	2.70843400	-3.57145500	-1.88283200
H	1.04027200	-4.21551300	-1.98270900
C	1.72037700	-3.75446700	0.67392900
H	2.78924000	-3.98038600	0.61187400
H	1.50544300	-3.34222600	1.66788200
H	1.14439700	-4.67881500	0.55056500
C	3.87451800	0.00001000	0.29291000
Fe	0.79964100	0.00000500	0.13760500
Cl	-5.72489100	1.59062500	0.01052000
Cl	-5.72488300	-1.59063900	0.01042700
F	3.64270600	-0.00003300	1.67110400
F	5.21315100	0.00002200	0.13180300
O	0.65503000	-0.00024800	2.10621800
O	-0.53598900	-0.00001200	2.54882200

{TAML–Fe^{V}–OO} (Sextet)

Energy: -2570.61392817 a.u.

C	1.83107200	-0.70991700	-0.05800200
C	1.83107300	0.70991600	-0.05800100
C	3.03611500	1.40898300	-0.05764500
C	4.23783800	0.69844600	-0.05129000
C	4.23783700	-0.69845100	-0.05129100
C	3.03611300	-1.40898600	-0.05764700
H	3.03647800	2.49316400	-0.06887700
H	3.03647400	-2.49316700	-0.06888300
N	0.54238000	1.25619900	-0.08074100
N	0.54237800	-1.25619700	-0.08074600
C	0.20502600	2.55297300	-0.35964800
C	0.20502300	-2.55296900	-0.35966600
C	-1.31737100	2.75440500	-0.50581400

C	-1.31737500	-2.75440000	-0.50582100
N	-1.97402600	-1.46817000	-0.18516900
N	-1.97402500	1.46817500	-0.18516300
C	-3.32301000	1.34993400	-0.23836500
C	-3.32300900	-1.34992500	-0.23838200
O	-4.12563300	2.19661600	-0.62174100
O	0.99444000	3.48133100	-0.51976300
O	0.99443300	-3.48133800	-0.51973600
O	-4.12563200	-2.19662600	-0.62171800
C	-1.75864900	-3.84398300	0.47057700
H	-1.59995600	-3.52204700	1.50715900
H	-2.81951500	-4.07286200	0.33168400
H	-1.16450800	-4.74786200	0.29455300
C	-1.57600900	-3.17773300	-1.95405300
H	-2.63663000	-3.39952700	-2.10066200
H	-1.28387500	-2.38143100	-2.65009100
H	-0.97893300	-4.06839400	-2.18124600
C	-1.57599800	3.17774000	-1.95404700
H	-1.28386400	2.38143700	-2.65008500
H	-2.63661700	3.39953800	-2.10066100
H	-0.97891800	4.06839900	-2.18123700
C	-1.75864300	3.84398800	0.47058400
H	-2.81950800	4.07287100	0.33168700
H	-1.59995500	3.52205000	1.50716500
H	-1.16449800	4.74786500	0.29456300
C	-3.84751900	0.00000000	0.33016600
Fe	-0.84522400	0.00000100	0.15585100
Cl	5.73095900	-1.59585200	-0.04235600
Cl	5.73096100	1.59584500	-0.04235200
F	-3.50869100	-0.00000500	1.68353700
F	-5.19128400	0.00000000	0.26287900
O	-0.74364100	0.00000700	2.44779300
O	0.43412800	0.00000000	2.88489900

{TAML–Fe^{V}–OO}•H$_2$O‡ (Doublet)

Energy: -2799.88596625 a.u.

C	1.76286500	-0.74456600	-0.29698500
C	1.79071500	0.67157800	-0.41868300
C	3.00655100	1.32705000	-0.61573200
C	4.19041800	0.58821800	-0.65407300
C	4.16413900	-0.80190900	-0.51189900
C	2.95207400	-1.47221400	-0.34083700
H	3.03101700	2.40363100	-0.75208400

H	2.93703500	-2.55355700	-0.25368000
N	0.51982500	1.24401300	-0.38484300
N	0.46463200	-1.24791700	-0.22253700
C	0.21650000	2.56334100	-0.30510300
C	0.07759400	-2.54928100	-0.21496100
C	-1.29659800	2.83565400	-0.30262100
C	-1.41001100	-2.71905300	-0.56232600
N	-2.04755300	-1.38115500	-0.47490200
N	-1.99343900	1.52565200	-0.36081700
C	-3.33907100	1.50204100	-0.47570200
C	-3.35555800	-1.26035700	-0.78851100
O	-4.08367900	2.47970600	-0.54385200
O	1.03702500	3.48864900	-0.19932000
O	0.81658700	-3.51882100	0.01107700
O	-4.08627500	-2.15206300	-1.22105200
C	-2.04857400	-3.71209000	0.40678600
H	-2.05197700	-3.31604600	1.42969000
H	-3.08155300	-3.91667000	0.11164300
H	-1.47337600	-4.64508300	0.39962800
C	-1.43552400	-3.27014000	-1.99579300
H	-2.46468400	-3.47510100	-2.30085100
H	-0.99826700	-2.54772600	-2.69616100
H	-0.84791000	-4.19508500	-2.04100400
C	-1.60162000	3.72495500	-1.51015500
H	-1.43925400	3.17661700	-2.44659700
H	-2.63833500	4.06774800	-1.48436800
H	-0.92632000	4.58835600	-1.49452400
C	-1.62665500	3.55067200	1.01110400
H	-2.69712000	3.77393600	1.05447500
H	-1.35961400	2.92142200	1.87102500
H	-1.05546600	4.48381500	1.07830900
C	-4.02860900	0.10553300	-0.46506800
Fe	-0.88950000	0.04284800	0.00545600
Cl	5.63275000	-1.73419600	-0.55146600
Cl	5.69255500	1.44199800	-0.87546500
F	-4.52537400	-0.04824100	0.82824000
F	-5.11248600	0.20989800	-1.27520800
O	-1.93179100	-0.03941400	2.04201200
O	-1.84141900	-1.05690700	2.72323000
O	0.67692000	0.34045600	2.45136200
H	1.19442300	-0.48793900	2.48681900
H	1.32685400	1.07261100	2.43447100
O	1.49976700	-2.42051400	2.64496900
H	1.48063100	-2.88494100	1.78490900
H	0.64362600	-2.63804500	3.03914800

O	2.39474400	2.65202000	2.21379300
H	3.21048600	2.28275000	1.84617200
H	1.97625400	3.08206400	1.43895100

II – Solvent Optimized Pentacoordinated {TAML-Fe} Structures ($R^1 = R^2 = Cl$, $R^3 = R^4 = F$)

{$TAML^{+\bullet}$–Fe^{V}–O} (Triplet)

Energy: -2495.31934263 a.u.

C	1.85934000	-0.73329200	0.13260500
C	1.82062100	0.71287500	0.01004400
C	3.01614400	1.43435200	-0.10122400
C	4.21369500	0.74517200	-0.07349200
C	4.25190500	-0.68526900	0.05403300
C	3.08996700	-1.41509700	0.15046900
H	3.00926600	2.51263100	-0.19166200
H	3.11789100	-2.49328100	0.25148200
N	0.54775300	1.20713700	-0.01297200
N	0.62288300	-1.27019400	0.16709200
C	0.17864400	2.53670700	-0.21812200
C	0.27263700	-2.59092300	-0.05113900
C	-1.32505300	2.75159400	-0.24770300
C	-1.21486500	-2.75146100	-0.35219600
N	-1.86636100	-1.41804600	-0.19228900
N	-1.96533600	1.42213000	-0.12376800
C	-3.30161700	1.34200600	-0.16886400
C	-3.20767400	-1.32726100	-0.37347100
O	-4.09889500	2.25981800	-0.39736000
O	0.98905200	3.44143800	-0.34934900
O	1.06126800	-3.52524100	-0.07737100
O	-3.92431900	-2.22006200	-0.82227500
C	-1.79065200	-3.76429600	0.63593800
H	-1.73919400	-3.38771100	1.66388600
H	-2.82941600	-3.99858400	0.39205300
H	-1.20442600	-4.68760600	0.57635800
C	-1.30004000	-3.24849900	-1.79885500
H	-2.33394600	-3.47179500	-2.06835400
H	-0.90192500	-2.50400600	-2.49713100
H	-0.70783000	-4.16466700	-1.89444300
C	-1.65154700	3.43673200	-1.57727400
H	-1.46328600	2.76812300	-2.42437500
H	-2.69474900	3.75570100	-1.60195000

H	-1.01432700	4.32094500	-1.68513700
C	-1.68109100	3.64136100	0.94660100
H	-2.75198600	3.86247400	0.94273100
H	-1.42227900	3.15096300	1.89222700
H	-1.12952500	4.58525300	0.88074400
C	-3.88336500	-0.04716600	0.15220700
Fe	-0.81219000	-0.00282800	0.42997600
Cl	5.76074100	-1.49874300	0.09880200
Cl	5.67495800	1.63152200	-0.18610200
F	-3.91230200	-0.16519800	1.53642700
F	-5.17555400	-0.06958000	-0.24989400
O	-0.88815500	0.02759900	2.00956900

{TAML$^{+\bullet}$–Fe^{V}–O}•H$_2$O‡ (Triplet)

Energy: -2801.01276271 a.u.

C	-1.40507000	1.10068500	-0.42642200
C	-1.53154300	-0.32517900	-0.61687000
C	-2.79556900	-0.89230400	-0.83216100
C	-3.90772200	-0.06994100	-0.85054600
C	-3.78642200	1.33040500	-0.62685000
C	-2.55038500	1.91101200	-0.41867200
H	-2.90520000	-1.95769400	-0.99677700
H	-2.46798700	2.97782600	-0.25006200
N	-0.32141700	-0.96508500	-0.59828600
N	-0.10830500	1.50527300	-0.28494500
C	-0.04448800	-2.25222200	-0.97153600
C	0.37646000	2.79379500	-0.28598800
C	1.44274400	-2.60358500	-0.90673800
C	1.89546400	2.86844300	-0.11354000
N	2.42533400	1.47955400	-0.13324000
N	2.18731500	-1.37304900	-0.53331500
C	3.52263600	-1.41522100	-0.43911000
C	3.74456700	1.27825200	-0.03183700
O	4.27040200	-2.35486900	-0.74585300
O	-0.89227400	-3.07772600	-1.32847800
O	-0.32053200	3.79924200	-0.41379200
O	4.64238100	2.13398300	-0.04450300
C	2.15606200	3.51901300	1.24798600
H	1.72040900	2.92156300	2.05816500
H	3.23151900	3.61862400	1.42248200
H	1.70770400	4.51843300	1.27441300
C	2.44248100	3.72578900	-1.25538700

H	3.50077500	3.94661500	-1.10594900
H	2.31914800	3.22429800	-2.22211200
H	1.89154400	4.67180200	-1.28757800
C	1.84474600	-3.13425400	-2.28413300
H	1.79331600	-2.34515000	-3.04281900
H	2.85967200	-3.53560200	-2.26316400
H	1.15965200	-3.93765600	-2.57488900
C	1.60057600	-3.67677500	0.17442000
H	2.64374300	-3.99856700	0.24364300
H	1.28265800	-3.29929600	1.15426400
H	0.98693600	-4.54925700	-0.07723300
C	4.17842400	-0.18472200	0.23472800
Fe	1.11860800	0.10428000	0.02736400
Cl	-5.19152700	2.33044800	-0.60407400
Cl	-5.45666400	-0.76860000	-1.14435900
F	4.01483400	-0.37842600	1.60972200
F	5.51607700	-0.26360600	0.01671600
O	0.91437900	-0.07068500	1.65784100
O	-0.71005800	0.40668100	2.41561200
H	-0.26238100	0.55388700	3.26831200
H	-1.47719000	-0.88865500	2.61225100
H	-3.06574000	-1.27483800	2.72954700
H	-2.04328800	-2.41396800	2.15476400
O	-2.13436900	-1.66816500	2.83911800
O	-4.52060900	-0.56892800	2.67006800
H	-4.42198300	0.22100800	2.11408000
H	-5.10034800	-1.15043300	2.15236100
O	-2.05542200	-3.76082900	1.24750100
H	-1.80783500	-3.56018800	0.32417900
H	-1.31732800	-4.30278500	1.57040400

III – Hexacoordinated {TAML-Fe} Structures ($R^1 = R^2 = Cl$, $R^3 = R^4 = F$)

{TAML–Fe^{III}–$(OH_2)_2$}$^-$ (Quartet)

Energy: -2573.14449985 a.u.

C	1.92513900	0.71279400	-0.03122900
C	1.92430800	-0.71316100	-0.02375300
C	3.13268300	-1.40824100	-0.03067900
C	4.33519800	-0.69927800	-0.04583800
C	4.33585900	0.69712700	-0.05256200
C	3.13379900	1.40702800	-0.04477000
H	3.13069100	-2.49302500	-0.02381800
H	3.13263800	2.49183800	-0.04835200

N	0.64008500	-1.26972700	0.00044600
N	0.64093600	1.27076200	-0.01311100
C	0.29324100	-2.58793600	0.04963400
C	0.29535300	2.58938400	0.03972000
C	-1.24020700	-2.80051500	0.17176600
C	-1.23680000	2.80145000	0.17785300
N	-1.91361300	1.49022200	0.00744300
N	-1.91602400	-1.48690300	0.01407800
C	-3.25651500	-1.38459000	0.11821500
C	-3.25347900	1.38754600	0.11731400
O	-4.06460300	-2.25226300	0.45256300
O	1.06220400	-3.55059900	0.04174900
O	1.06483100	3.55166500	0.02702800
O	-4.05929300	2.25406500	0.46072200
C	-1.69646000	3.78633900	-0.89517800
H	-1.55142000	3.36806700	-1.90050000
H	-2.75773300	4.02257400	-0.76634000
H	-1.10471100	4.70607600	-0.82726200
C	-1.46312300	3.39968300	1.57136800
H	-2.52948400	3.56925600	1.74687000
H	-1.06395700	2.74223600	2.35554500
H	-0.92331500	4.35061300	1.64882300
C	-1.48144600	-3.42204700	1.55208800
H	-1.09857400	-2.77444700	2.35276900
H	-2.54860000	-3.60176500	1.71102700
H	-0.93470600	-4.36959000	1.62185500
C	-1.68938400	-3.76473400	-0.92447200
H	-2.75378600	-3.99708900	-0.81426500
H	-1.52606400	-3.32855000	-1.91917900
H	-1.10436800	-4.68930100	-0.86383600
C	-3.81297400	0.00200400	-0.35263200
Fe	-0.72362200	0.00027900	-0.07267000
Cl	5.83095500	1.59506700	-0.07269800
Cl	5.82965300	-1.59842400	-0.05743900
F	-3.63822500	-0.00078400	-1.76022200
F	-5.14346900	0.00367000	-0.15567900
O	-1.11055400	0.00109900	2.52535600
H	-1.68991200	-0.77225400	2.43406600
H	-1.71802100	0.75332600	2.44141900
O	-0.88981800	-0.01798000	-2.42513100
H	-1.58868300	-0.69387400	-2.42521100
H	-1.40386700	0.80425100	-2.48011000

{TAML–Fe^{IV}–$(OH)_2$}$^{2-}$ (Triplet)

Energy: -2571.90673091 a.u.

C	-1.89220100	-0.72006100	-0.02470900
C	-1.89511200	0.71575900	0.01581100
C	-3.11122500	1.40518700	-0.00925900
C	-4.31223400	0.69630800	-0.06503500
C	-4.31066100	-0.69837300	-0.09345100
C	-3.10986100	-1.40827700	-0.07326500
H	-3.10440500	2.49038800	0.01455400
H	-3.10222400	-2.49344600	-0.09500000
N	-0.63259400	1.28240800	0.09306100
N	-0.63306200	-1.28670000	-0.00208800
C	-0.26723900	2.58289300	0.08952800
C	-0.26628200	-2.58277200	0.09029700
C	1.27433100	2.78280200	0.18181500
C	1.27294700	-2.78131700	0.21039800
N	1.96472100	-1.48725300	0.04080400
N	1.96402300	1.49595800	-0.04600600
C	3.28877200	1.39451200	0.06303800
C	3.29226900	-1.39419700	0.07815300
O	4.10546300	2.28587100	0.34851000
O	-1.02838800	3.56312600	0.06552500
O	-1.02910700	-3.56119500	0.11913400
O	4.11651100	-2.29515700	0.30807600
C	1.70064400	-3.76539800	-0.88064900
H	1.53735900	-3.32358500	-1.87201500
H	2.76360500	-4.00527300	-0.77220600
H	1.10063300	-4.68083800	-0.80169100
C	1.53474900	-3.36013100	1.60584200
H	2.59799000	-3.60115700	1.71123000
H	1.26087400	-2.61947300	2.36637500
H	0.93146000	-4.26685600	1.74798600
C	1.55941300	3.33052200	1.58733500
H	1.34445100	2.56006000	2.33820700
H	2.61501400	3.60787700	1.67206700
H	0.92603400	4.20784200	1.77612100
C	1.68381400	3.80073000	-0.88340000
H	2.75526500	4.01287400	-0.79993400
H	1.47806300	3.40563000	-1.88674900
H	1.10760000	4.72517300	-0.75232900
C	3.85457200	-0.00060300	-0.36335400
Fe	0.76293900	-0.00809100	-0.00570000
Cl	-5.81649100	-1.60193500	-0.15701400
Cl	-5.81844700	1.60090300	-0.09366600
F	3.75504200	-0.00688500	-1.77588900

F	5.18642700	0.00292700	-0.10689100
O	0.66514900	-0.01721800	-1.86510200
H	1.53259800	0.32229500	-2.13958200
O	0.82944600	-0.04434200	1.88773700
H	0.04562400	0.45696100	2.16173900

{TAML–Fe^{V}–$(OH)_2$}$^{-}$ (Doublet)

Energy: -2571.87404721 a.u.

C	-1.87426800	-0.73122200	-0.04316200
C	-1.87896500	0.72763800	-0.04819400
C	-3.11090900	1.41620800	-0.06343600
C	-4.29040800	0.70231700	-0.07509400
C	-4.28582500	-0.72239600	-0.06830200
C	-3.10155300	-1.42815400	-0.05000700
H	-3.11194100	2.50092400	-0.06719700
H	-3.09563700	-2.51283600	-0.04138900
N	-0.64896100	1.28100300	-0.02366800
N	-0.64050300	-1.27520200	-0.01472400
C	-0.26895500	2.60795900	0.02746800
C	-0.25013400	-2.59332100	0.09708900
C	1.25717900	2.79498100	0.19008700
C	1.28321300	-2.77743000	0.20609900
N	1.95695500	-1.45799000	0.15557700
N	1.94056600	1.50375700	-0.05957000
C	3.26961900	1.39476800	0.09653800
C	3.29582000	-1.37474700	0.11972700
O	4.06043200	2.27636300	0.44299100
O	-1.04546700	3.55703800	-0.01132600
O	-1.01885800	-3.54944300	0.12851200
O	4.10644400	-2.28627200	0.30923300
C	1.71531200	-3.64635900	-0.98006300
H	1.54622500	-3.11227300	-1.92250400
H	2.77943800	-3.88466500	-0.89581600
H	1.13296100	-4.57512300	-0.98885900
C	1.55460100	-3.49488900	1.53298200
H	2.62701800	-3.68639700	1.63045600
H	1.22366000	-2.88428200	2.38299900
H	1.00588700	-4.44371600	1.56157500
C	1.46884500	3.28242600	1.63155600
H	1.16318500	2.50281000	2.33799900
H	2.52626200	3.51346800	1.78748100
H	0.86904300	4.18448400	1.80581700
C	1.72000100	3.84818200	-0.81644900

H	2.78332600	4.05680900	-0.66661600
H	1.57168600	3.49495800	-1.84455700
H	1.14303900	4.76998100	-0.68020000
C	3.84755300	0.01213400	-0.34048600
Fe	0.76357900	0.01097400	-0.01960400
Cl	-5.78291500	-1.59733400	-0.08396500
Cl	-5.79327100	1.56704300	-0.09851800
F	3.70886900	-0.01145600	-1.74378400
F	5.17419200	0.02683600	-0.10331100
O	0.71174900	-0.11548400	-1.86263000
H	1.56126500	0.24800000	-2.16378100
O	0.62984000	0.10550400	1.85742600
H	1.35288200	-0.45212900	2.18530500

{TAML–Fe^{V}–$(OH)_2$}$^{-}$ (Quartet)

Energy: -2571.87239115 a.u.

C	-1.87225800	-0.72728700	0.00365200
C	-1.87727100	0.72676400	-0.03459600
C	-3.10591200	1.41234200	-0.10095700
C	-4.28821800	0.69766300	-0.11224500
C	-4.28348100	-0.72148000	-0.05853200
C	-3.09576300	-1.42459500	0.00355500
H	-3.10694400	2.49661900	-0.13495900
H	-3.08898000	-2.50872000	0.04123000
N	-0.64624200	1.28816300	0.03120200
N	-0.63420700	-1.27640000	0.05805400
C	-0.27487300	2.61138000	0.07571800
C	-0.24785100	-2.58939900	0.18616000
C	1.25370000	2.79841300	0.22232100
C	1.28964500	-2.78048500	0.20239100
N	1.96709800	-1.46140000	0.16457700
N	1.93379600	1.51217300	-0.06201800
C	3.26585900	1.39347100	0.08360400
C	3.30317900	-1.37734300	0.06369500
O	4.05876500	2.26727000	0.44082400
O	-1.05149900	3.56310500	0.04740400
O	-1.01626800	-3.54588100	0.25621900
O	4.11883200	-2.29423700	0.18960000
C	1.64200300	-3.58550900	-1.05441600
H	1.40955900	-3.00246200	-1.95328800
H	2.71038600	-3.82136600	-1.05302700
H	1.06241100	-4.51596500	-1.07255800
C	1.64432100	-3.56647300	1.46757800

H	2.71679000	-3.77890600	1.48075000
H	1.38806600	-2.99928500	2.37256200
H	1.07873600	-4.50538900	1.48843900
C	1.48058600	3.25020100	1.67310300
H	1.18057600	2.45704500	2.36682400
H	2.54056000	3.47313800	1.82483200
H	0.88468600	4.14947100	1.87306500
C	1.70787600	3.87374200	-0.76272300
H	2.77118800	4.08490800	-0.61623900
H	1.55381600	3.54434300	-1.79802200
H	1.12658600	4.78891200	-0.60279900
C	3.83694400	0.01955900	-0.38934200
Fe	0.77690000	0.00991200	0.00357900
Cl	-5.77796200	-1.60260700	-0.07991100
Cl	-5.78903900	1.56381000	-0.19503800
F	3.66390500	0.01567100	-1.78566000
F	5.16920000	0.03698500	-0.18149100
O	0.65134400	-0.10715700	-1.82985500
H	1.39580900	0.42352900	-2.16018100
O	0.67768800	0.09299800	1.88138400
H	1.19351900	-0.67023600	2.18770300

{TAML–Fe^{V}–(OH)(O)}$^{2-}$ (Doublet)

Energy: -2571.24440972 a.u.

C	-1.89384400	-0.71793900	-0.01062700
C	-1.89969500	0.71683100	0.01241300
C	-3.11721000	1.40320800	-0.01269200
C	-4.31702500	0.69112500	-0.05078700
C	-4.31246700	-0.70338400	-0.06337900
C	-3.10950300	-1.40984300	-0.04367200
H	-3.11286000	2.48845000	-0.00133200
H	-3.09921500	-2.49508600	-0.05338800
N	-0.64010800	1.29169100	0.07056900
N	-0.63298500	-1.28241600	0.00784400
C	-0.28207200	2.59414900	0.05049800
C	-0.26605500	-2.57695600	0.09640400
C	1.25432800	2.80101500	0.17952100
C	1.27520400	-2.78569700	0.19895600
N	1.97358100	-1.49264600	0.08154400
N	1.95214300	1.52830900	-0.09940400
C	3.26968600	1.41416800	0.07820200
C	3.30163900	-1.39017000	0.10122900
O	4.07568100	2.29867700	0.40921100

O	-1.05061800	3.56692700	-0.00334500
O	-1.02682300	-3.55753600	0.12674500
O	4.12916500	-2.29765400	0.28628200
C	1.68978000	-3.71244700	-0.94734300
H	1.51951200	-3.21527400	-1.91024500
H	2.75247600	-3.96303600	-0.86103900
H	1.08565800	-4.62781200	-0.91013900
C	1.54916600	-3.43867900	1.55727800
H	2.61453500	-3.67675200	1.64587600
H	1.27219400	-2.74837800	2.36380200
H	0.95164300	-4.35479600	1.65245300
C	1.49408800	3.26688200	1.62349200
H	1.23371800	2.46146900	2.32120000
H	2.54946400	3.52212000	1.76339400
H	0.86750000	4.14367300	1.83618000
C	1.68602300	3.87817600	-0.81369900
H	2.75206100	4.09445300	-0.68497400
H	1.51625200	3.53870900	-1.84389500
H	1.09582900	4.78864200	-0.65129000
C	3.85828000	0.01513700	-0.31925400
Fe	0.75634700	0.01148700	0.01230700
Cl	-5.81620300	-1.61165500	-0.10749200
Cl	-5.82529800	1.59219300	-0.07857000
F	3.81931200	-0.00386100	-1.73030200
F	5.17888100	0.03148000	-0.00369500
O	0.70049800	-0.09011200	-1.85831800
H	1.49593700	0.38807800	-2.14283700
O	0.93605800	-0.06390800	1.74969800

{TAML–Fe^{V}–(OH)(O)}$^{2-}$ (Quartet)

Energy: -2571.24702171 a.u.

C	-1.89380400	-0.72138200	-0.04458500
C	-1.89450100	0.71201600	0.02114200
C	-3.10949800	1.40470300	0.03315500
C	-4.31135100	0.69891900	-0.01898400
C	-4.31184200	-0.69581000	-0.07606700
C	-3.11310400	-1.40779700	-0.08780900
H	-3.10090500	2.48882700	0.07867500
H	-3.10836400	-2.49231600	-0.12691000
N	-0.63137200	1.27153400	0.08665000
N	-0.63526400	-1.28447300	-0.03520300
C	-0.26698200	2.57731400	0.09409300
C	-0.28223100	-2.58028100	0.08419400

C	1.27063800	2.79254900	0.16535000
C	1.25334500	-2.78929300	0.22359500
N	1.94285200	-1.49177900	0.09889900
N	1.97071600	1.53059600	-0.15281300
C	3.28276200	1.41228400	0.04223200
C	3.27458400	-1.38749200	0.16421700
O	4.09662000	2.29645200	0.35913600
O	-1.04117700	3.54549900	0.07261400
O	-1.04766400	-3.55681400	0.12049800
O	4.08548800	-2.29705500	0.39783600
C	1.69946300	-3.73667300	-0.89290300
H	1.56016500	-3.25855900	-1.87046100
H	2.75756900	-3.99152600	-0.77115400
H	1.09007800	-4.64860400	-0.85626200
C	1.49370400	-3.41315800	1.60221000
H	2.55504200	-3.65355100	1.72280100
H	1.19984200	-2.70487900	2.38673100
H	0.88987500	-4.32447400	1.70148400
C	1.56059800	3.26108500	1.59966400
H	1.34587200	2.44657100	2.30173200
H	2.61408900	3.54152000	1.69663800
H	0.92295800	4.12305400	1.83863800
C	1.65435300	3.87665300	-0.84145600
H	2.72723100	4.08417800	-0.76103900
H	1.43387300	3.54505500	-1.86457400
H	1.08003400	4.79068500	-0.64499400
C	3.85969100	-0.00612000	-0.29790700
Fe	0.76745800	0.00788500	-0.05955200
Cl	-5.81995900	-1.59479500	-0.13962600
Cl	-5.81650800	1.60499500	-0.01253100
F	3.85195600	-0.08429000	-1.70488200
F	5.17331900	0.00037100	0.04846400
O	0.69399800	-0.05149100	-1.93510500
H	1.47032800	0.46103300	-2.21073000
O	0.92241100	0.03885800	1.71234700

{TAML$^{+\bullet}$–Fe^{V}–(OH)(O)}$^{-}$ (Broken Symmetry Singlet)

Energy: -2571.21019612 a.u.

C	-1.87742000	-0.72525300	-0.06363100
C	-1.88237900	0.72563400	-0.07394700
C	-3.10915600	1.41293600	-0.07606500
C	-4.29281700	0.69709600	-0.05903000
C	-4.28893200	-0.72119100	-0.02780900

C	-3.10028200	-1.42447000	-0.02151000
H	-3.11268700	2.49739900	-0.09159600
H	-3.09187500	-2.50886700	-0.00101700
N	-0.64118800	1.28394100	-0.02995100
N	-0.63557500	-1.26761700	-0.06428600
C	-0.27565300	2.61204700	0.01901800
C	-0.24308200	-2.58060800	0.10195000
C	1.24103600	2.79797500	0.24618400
C	1.28905900	-2.77158600	0.21830500
N	1.97079700	-1.47253500	0.05490700
N	1.93517500	1.53245100	-0.08505200
C	3.25376600	1.40126200	0.14798500
C	3.30743400	-1.35529700	0.13491600
O	4.02542300	2.25604800	0.58690900
O	-1.05631800	3.55707300	-0.03830700
O	-1.01391900	-3.53342500	0.15738400
O	4.11761300	-2.24397300	0.40351600
C	1.71897500	-3.72471100	-0.90242400
H	1.54120800	-3.26938900	-1.88384600
H	2.78551900	-3.94893700	-0.80441900
H	1.14344200	-4.65510600	-0.83458300
C	1.55704900	-3.38716200	1.59543200
H	2.62008700	-3.62349200	1.69343100
H	1.27729900	-2.67802000	2.38297600
H	0.96502400	-4.30306500	1.70958100
C	1.38370200	3.14068000	1.73798900
H	1.05376400	2.29593100	2.35537700
H	2.43153500	3.35059400	1.96965400
H	0.77272500	4.02001200	1.97696600
C	1.74027800	3.94172800	-0.63175400
H	2.79160000	4.14697800	-0.41032500
H	1.64756600	3.68395600	-1.69369300
H	1.14272000	4.84067100	-0.44221800
C	3.84641700	0.03626100	-0.32413500
Fe	0.76651100	0.03096400	-0.13151000
Cl	-5.78464300	-1.60182400	-0.00976300
Cl	-5.79332100	1.56730000	-0.07726300
F	3.69917600	0.02932000	-1.72638200
F	5.17290500	0.05965700	-0.09454500
O	0.72932400	-0.09790800	-1.95990900
H	1.60763900	0.19047600	-2.26088200
O	0.88030200	-0.19329500	1.64584200

{TAML$^{+\bullet}$–Fe^{V}–(OH)(O)}$^{-}$ (Triplet)

Energy: -2571.21204835 a.u.

C	-1.87390500	-0.73127400	-0.06001900
C	-1.87172500	0.72344400	0.00281500
C	-3.09903000	1.41699300	0.02551000
C	-4.28287900	0.70839500	-0.01119500
C	-4.28515700	-0.71414300	-0.06289000
C	-3.10330700	-1.42416700	-0.08455000
H	-3.09718000	2.50077000	0.06334700
H	-3.10111900	-2.50813500	-0.12415000
N	-0.63331900	1.26903700	0.05712300
N	-0.63980100	-1.27555700	-0.06092000
C	-0.26178200	2.60315800	0.04945600
C	-0.25946300	-2.59613800	0.04542700
C	1.26166100	2.79958700	0.19008000
C	1.26621700	-2.78012600	0.23406200
N	1.93759600	-1.47315800	0.09379900
N	1.94716000	1.53846100	-0.17226300
C	3.26180800	1.40831100	0.05808800
C	3.28052600	-1.34881600	0.19882400
O	4.05184300	2.27125400	0.45141500
O	-1.04989100	3.54043100	-0.01825300
O	-1.02807400	-3.55250500	0.04494000
O	4.07385500	-2.23491900	0.51169800
C	1.76237800	-3.73741100	-0.85381000
H	1.65305800	-3.28222300	-1.84527200
H	2.81714800	-3.97490600	-0.68754400
H	1.17098600	-4.65960200	-0.82107000
C	1.46848900	-3.37401800	1.63247900
H	2.52766100	-3.59609700	1.78870900
H	1.14233900	-2.65779100	2.39561400
H	0.88173200	-4.29530600	1.72848500
C	1.48419100	3.17347500	1.66613700
H	1.21763600	2.33016100	2.31443400
H	2.53702400	3.41826200	1.82980100
H	0.86359500	4.04021100	1.92666600
C	1.69947700	3.93561000	-0.73099100
H	2.76579600	4.13126900	-0.58422600
H	1.53112800	3.66951500	-1.78161700
H	1.12547700	4.84243100	-0.50873200
C	3.83694800	0.00996000	-0.33429900
Fe	0.76970500	0.01376000	-0.09058200
Cl	-5.78586800	-1.58203400	-0.10533500
Cl	-5.78085000	1.58134000	0.00574200
F	3.69849600	-0.08631300	-1.72780700

F	5.16344300	0.02335100	-0.09241700
O	0.64995600	-0.06929500	-1.94518400
H	1.44062200	0.39469000	-2.26521700
O	0.97736000	-0.07759900	1.67864700

{TAML$^{+\bullet}$–Fe^{V}–(OH)(O)}$^{-}$ (Quintet)

Energy: -2571.21777434 a.u.

C	-1.89085200	0.71443900	-0.00259600
C	-1.89085900	-0.71444700	-0.00245600
C	-3.10359200	-1.41121900	0.00256800
C	-4.30019400	-0.70170800	0.01458300
C	-4.30018900	0.70167000	0.01448000
C	-3.10359500	1.41119600	0.00234400
H	-3.10208600	-2.49534600	0.00320000
H	-3.10209600	2.49532300	0.00282600
N	-0.62222900	-1.26204200	-0.03842600
N	-0.62223500	1.26204500	-0.03877800
C	-0.27804700	-2.58192800	-0.10271200
C	-0.27808100	2.58195700	-0.10241100
C	1.24672200	-2.82441200	-0.17399000
C	1.24667100	2.82443000	-0.17395500
N	1.93195800	1.53760500	0.01811800
N	1.93201500	-1.53758300	0.01811200
C	3.26236600	-1.39534300	-0.17453700
C	3.26222400	1.39530300	-0.17503100
O	4.05800400	-2.27993100	-0.48168800
O	-1.06946500	-3.52385900	-0.12057000
O	-1.06950100	3.52390200	-0.11973500
O	4.05778600	2.27973700	-0.48281600
C	1.63743600	3.78405700	0.95222900
H	1.43826600	3.33340900	1.93163800
H	2.70316400	4.02519700	0.88069600
H	1.04752600	4.70345200	0.86429000
C	1.53173600	3.44030500	-1.54831900
H	2.57846300	3.74402100	-1.62407800
H	1.31932900	2.71332400	-2.34156200
H	0.88398300	4.31346300	-1.68736500
C	1.53212700	-3.44041400	-1.54820900
H	1.31975300	-2.71356400	-2.34157800
H	2.57891600	-3.74399200	-1.62370700
H	0.88454000	-4.31369200	-1.68727300
C	1.63718800	-3.78391000	0.95242300
H	2.70286900	-4.02528800	0.88107500

H	1.43799200	-3.33301600	1.93171400
H	1.04707800	-4.70318400	0.86456700
C	3.83037900	0.00006900	0.24835800
Fe	0.77048200	0.00000000	0.13648900
Cl	-5.79465100	1.59264700	0.03846300
Cl	-5.79465100	-1.59268600	0.03870100
F	3.73104100	0.00031300	1.65453900
F	5.14572700	0.00006900	-0.03233500
O	0.68009600	0.00009000	1.96771300
H	1.59690600	0.00149000	2.29014000
O	1.23994300	-0.00054100	-1.58974400

{TAML$^{+\bullet}$–Fe^{V}–(OH)(O)}•H$_2$O‡ (Triplet)

Energy: -2876.89125285 a.u.

C	-1.62908100	0.90578000	-0.40884000
C	-1.67910700	-0.50930800	-0.62022200
C	-2.91358000	-1.14591700	-0.76360500
C	-4.09208600	-0.39686200	-0.72423000
C	-4.04450800	0.98931300	-0.55220500
C	-2.81969700	1.64259300	-0.38150200
H	-2.95286800	-2.21899600	-0.92092200
H	-2.77865900	2.71913600	-0.24701600
N	-0.42736400	-1.10650300	-0.67712300
N	-0.34822700	1.40569300	-0.25960200
C	-0.10947400	-2.41035900	-0.65027500
C	0.03980800	2.69822100	-0.09291000
C	1.41155100	-2.68268000	-0.68746400
C	1.57848100	2.87664700	-0.12179300
N	2.21257700	1.53692900	-0.14568900
N	2.11783100	-1.41985400	-0.38053400
C	3.45774200	-1.38468500	-0.26212100
C	3.54437500	1.40695700	-0.02593100
O	4.22928800	-2.32833900	-0.44600500
O	-0.92395200	-3.35663200	-0.59508900
O	-0.71381900	3.66578900	0.04026200
O	4.37479500	2.32001800	-0.00890100
C	1.98306300	3.67734800	1.11694800
H	1.82229000	3.08982800	2.02963900
H	3.03816500	3.95741400	1.06699400
H	1.36078600	4.57750700	1.17599000
C	1.91366300	3.66258500	-1.39491400
H	2.99487300	3.82547800	-1.45281600
H	1.58163800	3.11745400	-2.28756400

H	1.39874700	4.63075300	-1.37893900
C	1.75177700	-3.16395200	-2.10332100
H	1.53923400	-2.37301800	-2.83169300
H	2.81338800	-3.42510000	-2.15852300
H	1.14813600	-4.04644900	-2.35019600
C	1.72538100	-3.75640900	0.35447100
H	2.77324200	-4.05855300	0.28346800
H	1.54557600	-3.36454700	1.36429500
H	1.07815000	-4.62529500	0.18637100
C	4.08415100	-0.03875900	0.23044500
Fe	1.00634800	0.12310900	-0.49054800
Cl	-5.50815600	1.93472800	-0.48517400
Cl	-5.61789700	-1.23245700	-0.86185800
F	4.12714400	-0.14911100	1.62180300
F	5.37724400	-0.04702700	-0.18143900
O	1.09824300	-0.42495200	1.40621600
O	0.35299700	0.58042000	2.37936500
H	1.05632400	0.65029000	3.04811200
H	-0.44274400	-0.10690000	2.77726300
H	-2.28153800	-0.47774400	3.02711200
H	-1.41757000	-1.76803000	2.74325900
O	-1.40507700	-0.89580400	3.22717900
O	-3.75633600	0.33778100	2.55696200
H	-3.48516800	0.96982800	1.86718900
H	-4.33102000	-0.27544600	2.07381800
O	-1.67741400	-3.31282900	2.04875200
H	-1.55293200	-3.32930800	1.06895800
H	-1.00783600	-3.93254500	2.36790200
O	1.10885300	0.31060000	-2.29969100
H	1.93904900	0.78469000	-2.46915700

IV – Pentacoordinated {TAML-Fe} Structures ($R^1 = R^2 = H$, $R^3 = R^4 = CH_3$)

{$TAML^{+\bullet}$–Fe^{V}–O} (Triplet)

Energy: -1456.31025437 a.u.

C	2.71988500	-0.61544900	0.08632400
C	2.61681300	0.81967500	-0.08194600
C	3.78570300	1.58460100	-0.25811500
C	5.00508300	0.93273300	-0.26127800
C	5.10476600	-0.47204800	-0.10449500
C	3.98241000	-1.25130600	0.06597800
H	3.71440300	2.65830100	-0.38159400
H	4.03626900	-2.32791800	0.18781300

N	1.31785200	1.25684000	-0.06957800
N	1.50386700	-1.19125300	0.19553200
C	0.89538400	2.57852200	-0.23135900
C	1.19476600	-2.53385600	0.07489400
C	-0.61915200	2.72896300	-0.18278900
C	-0.28578200	-2.73131500	-0.26343800
N	-0.95350900	-1.39335100	-0.23570800
N	-1.19211300	1.36570600	-0.10703700
C	-2.55090100	1.23516500	-0.13230600
C	-2.32118500	-1.35142700	-0.47975300
O	-3.31151400	2.19885800	-0.24031500
O	1.66115700	3.51514400	-0.38258700
O	1.99418800	-3.45295700	0.14092000
O	-2.88698000	-2.32296800	-0.97181000
C	-0.89676300	-3.65624500	0.79082800
H	-0.90306000	-3.17594200	1.77743100
H	-1.92148300	-3.92137600	0.51787200
H	-0.29644600	-4.57013000	0.85648700
C	-0.30076200	-3.36849400	-1.65934700
H	-1.31115800	-3.67736900	-1.92912400
H	0.06330600	-2.66248300	-2.41534600
H	0.36200400	-4.24088400	-1.65412500
C	-1.03076200	3.47366200	-1.45806000
H	-0.87866700	2.84578300	-2.34412100
H	-2.08144900	3.76217600	-1.41068000
H	-0.40796900	4.36921400	-1.55894200
C	-0.95533400	3.54579800	1.07150100
H	-2.03049400	3.73898600	1.10484700
H	-0.66476800	3.00553100	1.98077500
H	-0.41795100	4.50030100	1.04505900
C	-3.14945600	-0.16881900	0.01820100
Fe	0.00365600	0.01391000	0.43940200
O	-0.10723800	0.01658900	2.01917200
C	-3.35793700	-0.41031300	1.53282400
H	-3.84403300	-1.38121900	1.68919900
H	-2.41763000	-0.39219500	2.09431800
H	-4.01534600	0.37130700	1.93070300
C	-4.51255700	-0.19636000	-0.67331700
H	-5.13663300	0.61114200	-0.28442000
H	-4.41681600	-0.05796100	-1.75577100
H	-5.00360600	-1.15724600	-0.50010100
H	6.08699100	-0.94041700	-0.11677700
H	5.91459500	1.51691800	-0.38953000

{TAML$^{+\bullet}$–Fe^{V}–O}•H$_2$O‡ (Triplet)

Energy: -1761.96077658 a.u.

C	-1.95907000	1.24123500	-0.81986200
C	-2.18089700	-0.15970500	-0.97269100
C	-3.44508200	-0.63449500	-1.34197800
C	-4.47311700	0.28130200	-1.57488200
C	-4.25369400	1.65708500	-1.43149800
C	-3.00731400	2.14680400	-1.04306000
H	-3.60195300	-1.69893000	-1.48610500
H	-2.82086900	3.21089800	-0.94040200
N	-1.00920000	-0.88927100	-0.80638300
N	-0.63882100	1.53500700	-0.52323900
C	-0.84089100	-2.22784400	-0.87255500
C	-0.06629200	2.78296800	-0.46541800
C	0.62244400	-2.65749500	-0.75085200
C	1.44608000	2.72917100	-0.23830900
N	1.83266800	1.30325900	-0.07156900
N	1.41707300	-1.44414900	-0.44028900
C	2.78053900	-1.57143400	-0.30633200
C	3.16348100	1.00158900	0.08829900
O	3.37254200	-2.60802600	-0.60675100
O	-1.75063800	-3.06421800	-1.01401400
O	-0.67581900	3.83844800	-0.59665900
O	4.04228700	1.86251300	0.04724300
C	1.76420000	3.53000200	1.02649700
H	1.32702700	3.04717800	1.91038600
H	2.84525500	3.60899100	1.16511600
H	1.33351800	4.53341700	0.93574100
C	2.08471700	3.36764100	-1.47830900
H	3.16106000	3.48274300	-1.34087600
H	1.90625100	2.75180200	-2.36807200
H	1.62701900	4.34934600	-1.64290900
C	0.99857700	-3.29099500	-2.09658200
H	1.00557900	-2.53533100	-2.89079600
H	1.98621700	-3.75131500	-2.04457100
H	0.25146600	-4.05161100	-2.35003600
C	0.72631000	-3.66849200	0.39345800
H	1.74542400	-4.05929600	0.46192100
H	0.46316500	-3.19791100	1.35075200
H	0.03677700	-4.50055700	0.20911000
C	3.54743200	-0.44953400	0.41301400
Fe	0.43031600	0.08293700	0.00198900
O	-0.04757400	-0.20905400	1.60261500
O	-1.19747300	0.92528800	2.32005400

H	-0.61673600	1.10735600	3.07808600
H	-2.14565800	-0.14942900	2.59133400
H	-3.74213500	-0.21263500	2.32954000
H	-2.92510500	-1.62076600	2.15056200
O	-2.99244100	-0.77476300	2.71626300
O	-4.68055700	0.93355600	1.66093100
H	-4.14753700	1.74225800	1.59573400
H	-4.84335900	0.70516900	0.72626400
O	-3.11232000	-2.97487600	1.34584400
H	-2.71353400	-3.03483400	0.44204400
H	-2.80505800	-3.76492000	1.81043500
C	3.26126200	-0.64908800	1.91873400
H	2.19829200	-0.52558900	2.15996400
H	3.57227200	-1.65558900	2.22586100
H	3.83625900	0.08145800	2.50112300
C	5.04233300	-0.63279900	0.16431800
H	5.29068800	-0.50489400	-0.89441700
H	5.60844900	0.10985500	0.73158400
H	5.35026600	-1.63798800	0.46284100
H	-5.06402400	2.35818000	-1.62692100
H	-5.44944500	-0.08377900	-1.89077700