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Cite this: DOI: 10.1039/c0xx00000x

www.rsc.org/xxxxxx

ARTICLE TYPE

Mechanisms of the Ammonia Oxidation by Hydrogen Peroxide over the Perfect and Defective Ti species of TS-1 zeolite: A Theoretical Calculation Study

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Received (in XXX, XXX) Xth XXXXXXXXX 20XX, Accepted Xth XXXXXXXXX 20XX
DOI: 10.1039/b000000x

Supporting Information

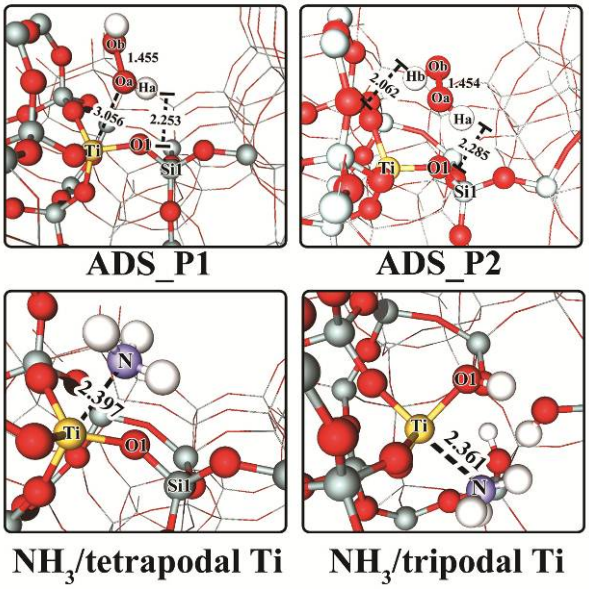


Figure S1. Illustration of the two modes of H_2O_2 adsorption on the perfect Ti active center (ADS_P1 and ADS_P2) and the adsorption complex of ammonia on both active sites of TS-1 zeolite: defective and perfect tetrahedral Ti centers. All distances are given in Å unit.

Reaction of NH_3 with ≡TiOOSi≡ species

The optimized structures and energetic profiles of this state are illustrated in Fig. S2. The following elementary reaction steps are proposed to be involved in the catalytic oxidation of NH_3 over the ≡TiOOSi≡ species:

≡Ti-O-O-Si≡ + NH_3 → ≡Ti-O-O-Si≡/NH_3 (I)
≡Ti-O-O-Si≡/NH_3 → ≡Ti-O-Si≡/ONH_3 (II)
≡Ti-O-Si≡/ONH3 → ≡Ti-O-Si≡/NH_2OH (III)

The interaction of ammonia with the hydrated [≡TiOOSi≡] species was determined as the first step of reaction by substitution of the water molecule as the proximal ligand on the [≡TiOOSi≡] species. The adsorption energy of NH_3 on the [≡TiOOSi≡] species with respect to the isolated systems is calculated to be -17.4 kcal/mol. This value is equal to the energy of H_2O desorption on this site. The adsorbed ammonia was oxidized by the peroxo-oxygen coordinated to the Ti center via the S_N2-like mechanism, leading to the formation of ammonia oxide-grafted Ti complex. The transition state structure of this step shows that a lone-pair electron from the ammonia attacks the peroxo oxygen atom (O_a) to form a covalent bond, concurrently eliminates the O-O bond of the peroxo moiety. At the transition state, the N-O bond distance was 2.303 Å with the geometrical changes of the peroxo bond and the distance between Ti and peroxo oxygen atoms are 1.711, 1.941 and 1.939 Å, respectively. For this process, the activation energy of 6.7 kcal/mol has to be overcome, which is lower than the barrier for H_2O_2 decomposition with one imaginary frequency value at 108*i* cm^{-1}. This imaginary frequency is associated with the stretching movement of proximal peroxo oxygen (O_a) to the nitrogen atom of ammonia, leading to the N-O_a bond forming and O_a-O1 bond breaking subsequently. Owing to the strongly exothermic character of this step by -33.5 kcal/mol, a reverse process back to the molecular ammonia adsorption complex is rather unlikely.

Furthermore, the energy stays below the reference state of gas molecules (NH_3, H_2O_2) and the catalyst (TS-1), indicating the grafted-Ti species is favorable. With the high desorption energy of NH_3O molecule from the Ti center of TS-1 zeolite (44.6 kcal/mol), the transformation of NH_3O to NH_2OH would take place on this active site of TS-1 zeolite. The direct proton transfer from the nitrogen to the adjacent oxygen in the ammonia oxide moiety as shown in the transition state TS_2 has to overcome a high energy barrier of 39.6 kcal/mol. At the TS_2 transition state, the migrating proton is at the midway point between the N and O atoms of ammonia oxide moiety (N-H and O-H bond distances are 1.137 and 1.245 Å). Next, the water-assisted NH_2OH formation was explored in search of lower activation energy on the catalytic profile. With additional water adsorbing on the NH_3O-Ti≡ species, this resulted in an energy decrease of -17.6 kcal/mol for the co-adsorption complex of H_2O/NH_3O/TS-1. As the proton-shuttling center, the transition state involves the transfer of a hydrogen atom from the ammonia oxide moiety to the water molecule, concurrently, a hydrogen atom of water to the NH_3O-ended oxygen atom, leading to the formation of hydroxylamine and water molecules co-adsorbed over the TS-1 zeolite. The imaginary frequency from vibrational analysis, 1455*i* cm^{-1} for this step is associated with the double proton transfers as mentioned earlier. The calculated barrier for this step is 18.8 kcal/mol, which is significantly lower than that for unimolecular transformation by about 2 times.

An alternative pathway for producing the hydroxylamaine was also demonstrated in Figure S2 called Route B, in which a framework oxygen of zeolite would facilitate the proton transfer from the nitrogen to the oxygen atoms of ammonia oxide. The reaction proceeds via three consecutive steps:

≡Ti-O-Si≡/ONH_3 → ≡Ti-O-NH_2---HO-Si≡ (IV)
≡Ti-O-NH_2---HO-Si≡ → ≡Ti-O-Si≡/NH_2OH (V)
≡Ti-O-Si≡/NH_2OH → ≡Ti-O-Si≡ + NH_2OH (VI)

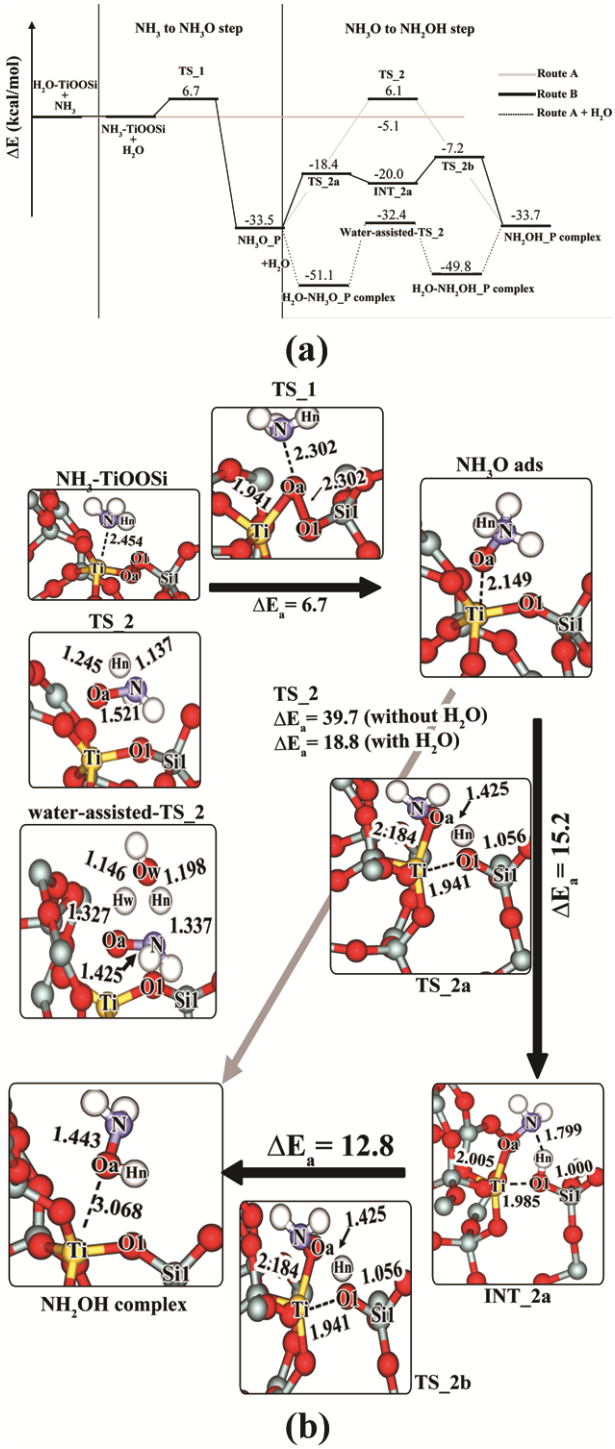


Figure S2. (a) The energetic profile along the pathway of ammonia oxidation over the hydrated [≡TiOOSi≡] active species. (b) Geometries of reaction intermediates and transition states for ammonia oxidation to hydroxylamine over the hydrated [≡TiOOSi≡] active site. All distances are given in Å unit.

Figure S2 shows that the reaction is an endothermic process by 13.5 kcal/mol, whereas a proton of ammonia oxide transfers to the framework oxygen atom via the **TS_2a** transition state structure. Activation energy of 15.1 kcal/mol has to be overcome for this step, which is lower than that for previous pathway with/without water assistance and the relative energy and stays below the reference state, indicating the favorable formation of NH_2O-grafted-Ti species. Then the oxyamine moiety abstracts the proton of the generated silanol moiety to produce the hydroxylamine. After this exothermic step with the activation energy of 12.8 kcal/mol, the active center of TS-1 zeolite is recovered. At the TS_2b transition state, the transferring proton (H1) is located between two terminal atoms, 1.056 and 1.425 Å for the H1-O1 and H1-O_a bond distances, respectively. The Ti-O1 bond distance was shortened to 1.941 and the elongation of the N-O_a and Ti-O_a bonds is observed to be 1.427 and 1.941 Å, respectively. The hydroxylamine product diffuses from the perfect tetrahedral Ti species by overcoming desorption energies of 16.4 kcal/mol. However, the H_2O_2 decomposition over the perfect Ti species is unlikely because the reaction involves a relatively high energy barrier of 24.7 and leads to the endothermic intermediate (H_2O/≡TiOOSi≡). So it can be concluded that the ≡TiOOSi≡ species is not the principal catalytic site for producing the hydroxylamine product.

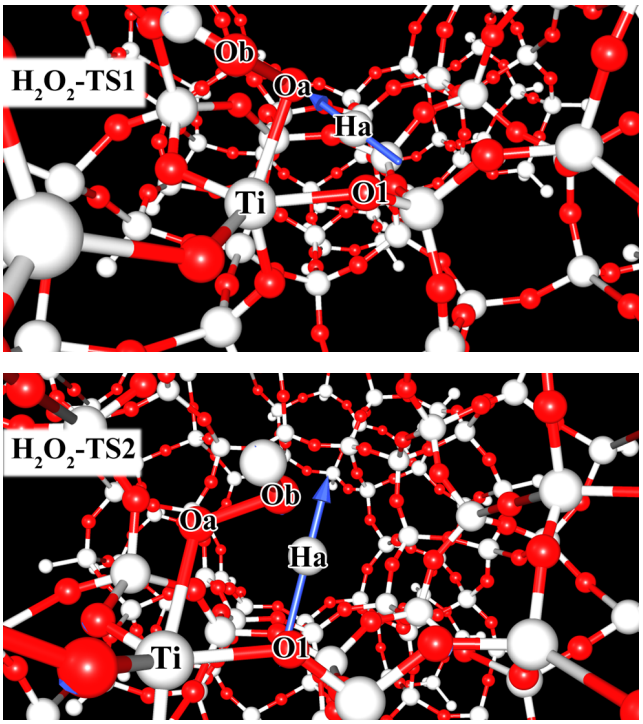


Figure S3 Shows the vibrational movements corresponding to the imaginary frequency at the transition states for H_2O_2 decomposition over perfect site of TS-1.

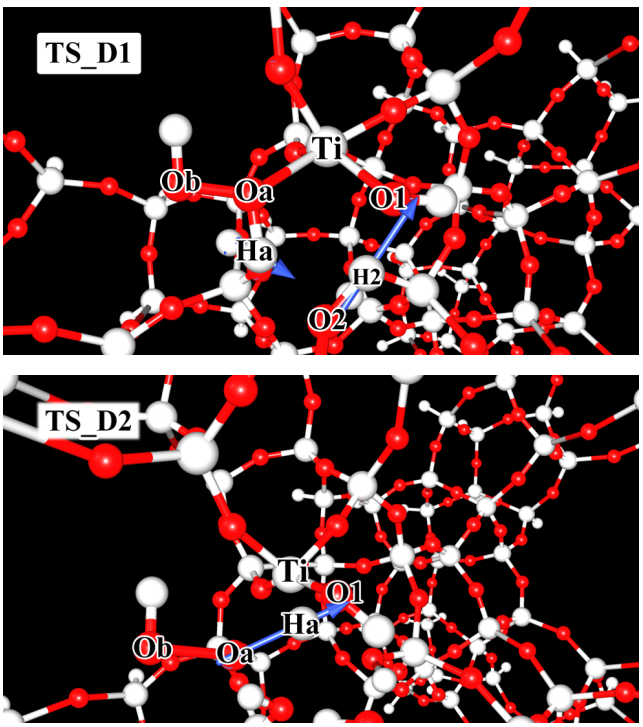
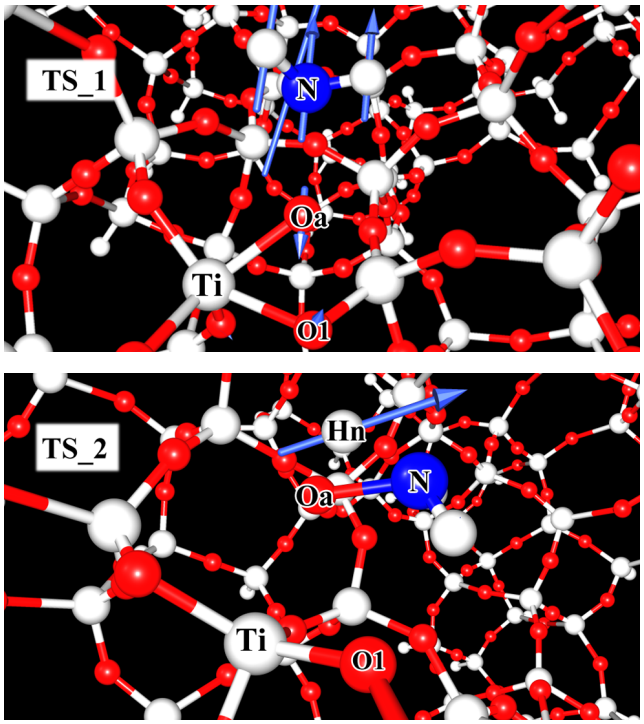


Figure S4 Shows the vibrational movements corresponding to the imaginary frequency at the transition states for H_2O_2 decomposition over defective site of TS-1.



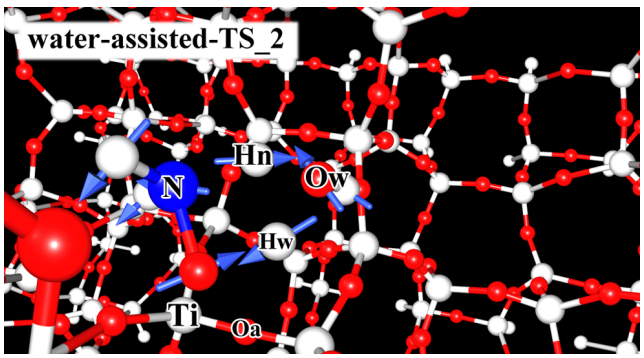


Figure S5 Shows the vibrational movements corresponding to the imaginary frequency at the transition states for NH_3 oxidation via route A over perfect site of TS-1.

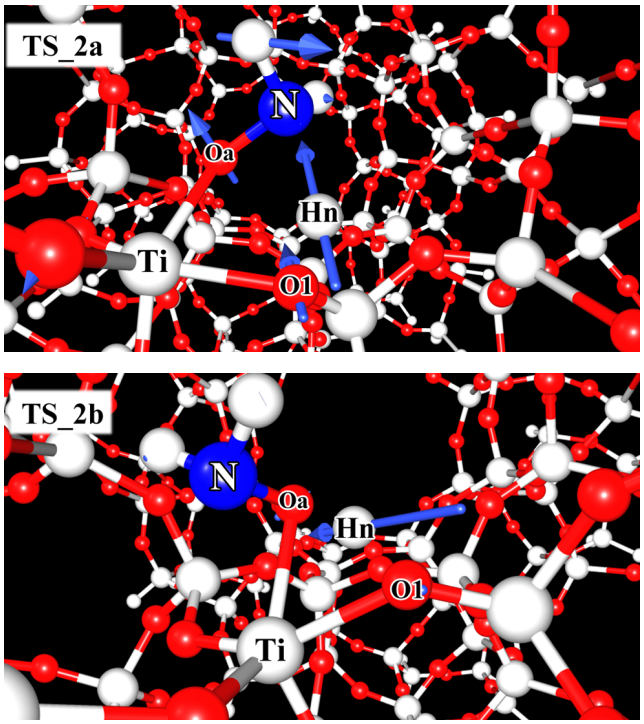
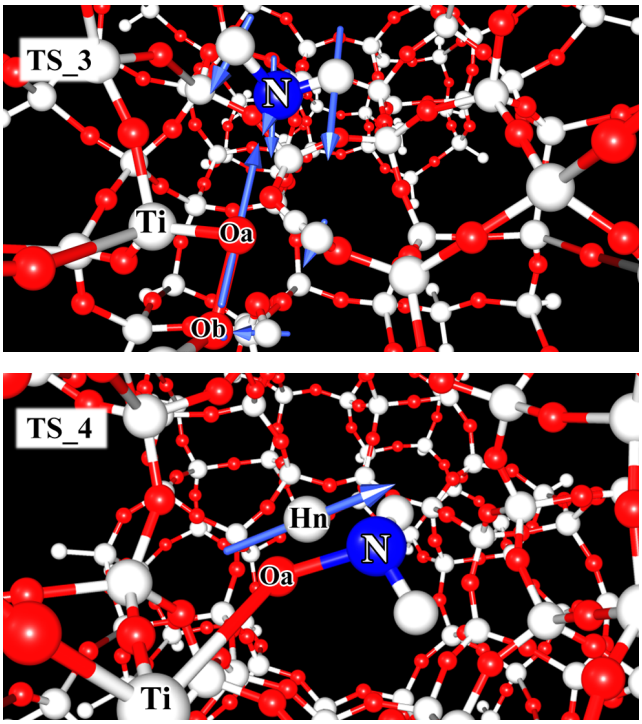


Figure S6 Shows the vibrational movements corresponding to the imaginary frequency at the transition states for NH_3 oxidation via route B over perfect site of TS-1.



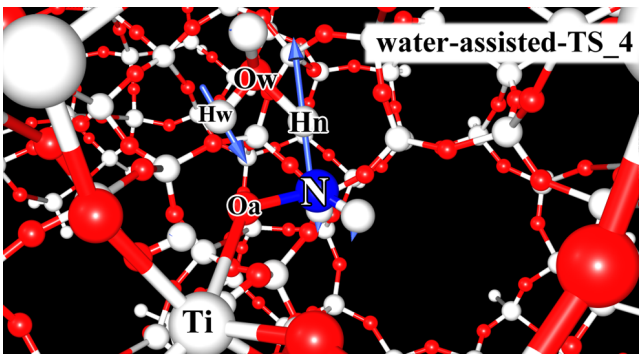


Figure S7 Shows the vibrational movements corresponding to the imaginary frequency at the transition states for NH_3 oxidation via route A over defective site of TS-1.

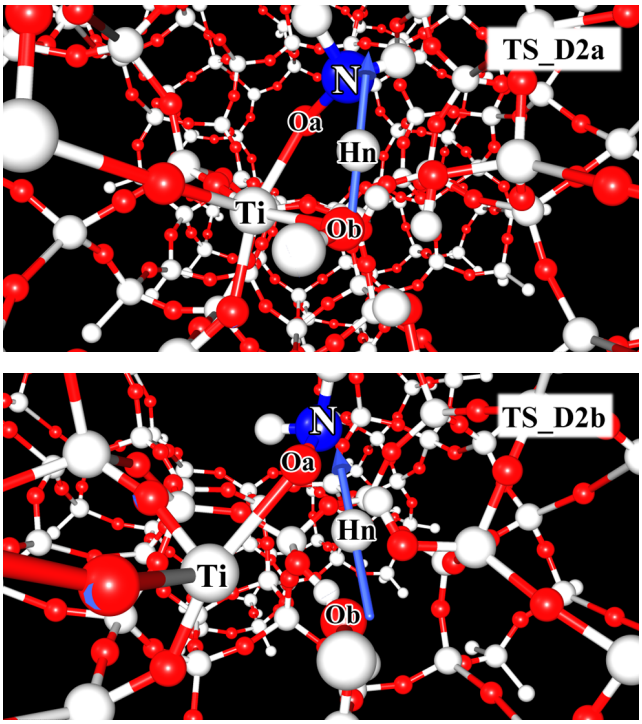


Figure S8 Shows the vibrational movements corresponding to the imaginary frequency at the transition states for NH_3 oxidation via hydrolysis of titano-oxyamine intermediate as shown in the Figure 5.

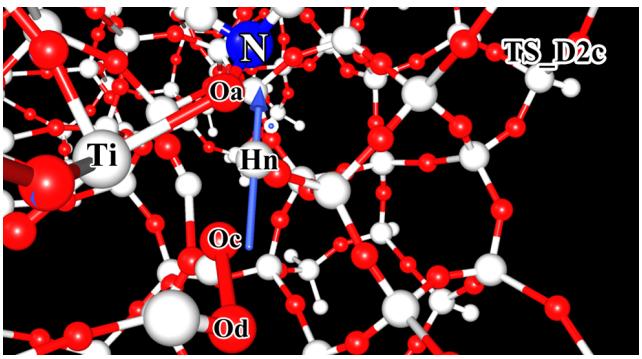


Figure S9 Shows the vibrational movements corresponding to the imaginary frequency at the transition states for NH_3 oxidation via the second H_2O_2 decomposition over the titano-oxyamine intermediate as shown in the Figure 6.

Table S1 Shows total energies of all stationary points along the H_2O_2 decomposition over the perfect site of TS-1 as shown in the Figure 2. All energies are obtained from the single point calculation energy from the ONIOM-optimized structures with the full DFT method (M06-L) for the whole 240T cluster model.

Steps	Energy (hartrees)
H_2O_2_P1	-101692.546082
H_2O_2_P2	-101692.544987
H_2O_2-TS1	-101692.505586
INT-TiOOH/HOSi	-101692.519564
H_2O_2-TS2	-101692.512175
Hydrated-TiOOSi	-101692.530612

Following is the optimized coordinates of atoms in the QM region of the ONIOM model for all catalytic steps in the Fig. 2.

H_2O_2_P1

Si	11.341930000	0.562537000	9.200349000
Ti	13.636763000	1.225060000	11.140759000
Si	14.571800000	3.446159000	12.885129000
Si	14.438869000	-1.220520000	13.055488000
Si	16.165748000	0.628242000	9.213550000
O	11.982463000	0.895171000	10.635137000
O	14.654202000	0.941669000	9.683175000
O	13.788049000	2.921207000	11.569163000
O	13.911975000	0.224789000	12.579783000
Si	8.434502000	1.139314000	8.877628000
Si	12.439292000	1.269065000	6.361500000
Si	11.406956000	-2.584309000	9.112300000
Si	13.755318000	-3.456989000	10.979618000
Si	17.629036000	-1.228222000	13.015122000
Si	13.870620000	-0.610814000	15.902754000
Si	17.692335000	3.430679000	12.933775000
Si	18.538812000	1.179861000	11.192127000
O	17.277196000	1.287357000	10.180417000
Si	16.192078000	-2.572314000	9.165075000
Si	15.652855000	1.233993000	6.309787000
Si	14.515269000	6.531232000	12.956987000
Si	13.872653000	2.581544000	15.828248000
O	11.874613000	1.325966000	7.894356000
O	9.860087000	0.992106000	9.573803000
O	11.482997000	-0.997237000	8.904355000
O	16.122970000	2.932412000	12.821655000
O	14.370508000	4.988351000	12.607390000
O	13.890929000	3.119487000	14.303573000
O	16.028411000	-1.097092000	12.926165000
O	13.909443000	-2.504781000	12.260871000
O	13.857691000	-1.446997000	14.520522000
O	16.419235000	1.221359000	7.744707000
O	16.274828000	-0.968688000	9.192441000
O	13.953677000	0.988005000	15.795494000
O	14.045854000	1.182752000	6.418845000
O	18.672141000	2.612406000	11.925839000
O	18.334306000	0.005222000	12.268403000
O	14.904349000	-3.185234000	9.897667000
O	11.302387000	1.308492000	14.407242000
H	10.904622000	2.029975000	14.919245000
O	11.418246000	1.956922000	13.110197000
H	10.893741000	1.360104000	12.552609000

H_2O_2_P2

Si	11.337414000	0.571686000	9.197079000
Ti	13.638099000	1.224940000	11.126440000
Si	14.578895000	3.452558000	12.895856000
Si	14.458898000	-1.235614000	13.048363000
Si	16.172727000	0.626193000	9.210631000
O	11.980948000	0.989037000	10.609714000
O	14.662713000	0.957675000	9.676537000
O	13.765611000	2.903833000	11.607901000
O	13.819101000	0.157609000	12.551106000
Si	8.430247000	1.138448000	8.877500000
Si	12.439566000	1.268919000	6.359248000
Si	11.407699000	-2.584589000	9.114383000
Si	13.756891000	-3.462797000	10.976667000
Si	17.641772000	-1.220595000	13.012579000
Si	13.870101000	-0.608521000	15.903723000
Si	17.694178000	3.430875000	12.933001000
Si	18.545597000	1.181387000	11.194776000
O	17.278625000	1.274684000	10.189333000
Si	16.189866000	-2.576277000	9.164892000
Si	15.654639000	1.233627000	6.310535000
Si	14.515710000	6.532038000	12.956175000
Si	13.864767000	2.591782000	15.832892000
O	11.865104000	1.323455000	7.885160000
O	9.854249000	0.981991000	9.574022000
O	11.510338000	-0.992219000	8.940944000
O	16.125518000	2.925568000	12.811963000
O	14.377602000	4.989160000	12.594984000
O	13.906347000	3.131852000	14.311253000
O	16.038699000	-1.040614000	12.907852000
O	13.956359000	-2.534349000	12.267433000
O	13.859604000	-1.441415000	14.512775000
O	16.429524000	1.217640000	7.742858000
O	16.260809000	-0.971492000	9.199309000
O	13.941488000	0.989476000	15.755856000
O	14.047258000	1.182599000	6.424650000
O	18.675131000	2.614645000	11.924775000
O	18.365650000	0.004549000	12.274544000
O	14.902264000	-3.195291000	9.890327000
O	11.208710000	0.489080000	13.867086000
H	12.028173000	0.058770000	13.567374000
O	11.408362000	1.805993000	13.284295000
H	10.880929000	1.725758000	12.472202000

H_2O_2-TS1

Si	11.336978000	0.612263000	9.155056000
Ti	13.691768000	1.092744000	11.244088000
Si	14.615305000	3.442054000	12.870570000
Si	14.474567000	-1.299039000	13.044740000
Si	16.090971000	0.644551000	9.224440000
O	11.960216000	1.395190000	10.441898000
O	14.532441000	0.866296000	9.639994000
O	13.983552000	2.808570000	11.531199000
O	14.782092000	0.099498000	12.287433000
Si	8.425490000	1.131497000	8.876385000
Si	12.439503000	1.269282000	6.338509000
Si	11.415381000	-2.582060000	9.126223000
Si	13.739897000	-3.445739000	11.003743000
Si	17.469428000	-1.339835000	13.081515000
Si	13.853401000	-0.553786000	15.936677000
Si	17.712802000	3.423506000	12.935981000
Si	18.443216000	1.119924000	11.194171000
O	17.230214000	1.366602000	10.126971000
Si	16.200252000	-2.551445000	9.168329000
Si	15.641517000	1.235312000	6.301816000
Si	14.512114000	6.524718000	12.954169000
Si	13.866828000	2.630970000	15.830508000
O	11.814490000	1.318928000	7.825928000
O	9.837754000	0.906958000	9.575292000
O	11.600790000	-0.964137000	9.079874000
O	16.155174000	2.955307000	12.870865000
O	14.343180000	4.975883000	12.591766000
O	13.910981000	3.105407000	14.288806000
O	15.954209000	-1.787673000	13.373031000
O	13.706486000	-2.493149000	12.305760000
O	13.695793000	-1.080665000	14.421597000
O	16.357295000	1.230493000	7.751904000
O	16.308988000	-0.948777000	9.185725000
O	13.887247000	1.039346000	15.866050000
O	14.035677000	1.181612000	6.393098000
O	18.669090000	2.547545000	11.945869000
O	17.875654000	-0.010700000	12.222806000
O	14.909993000	-3.116602000	9.954954000
O	12.373099000	1.271322000	13.200922000
H	12.814521000	0.825502000	13.946233000
O	12.102176000	0.137140000	12.333716000
H	11.584553000	0.871907000	11.336466000

INT-TiOOH/HOSi

Si	11.323158000	0.630985000	9.154772000
Ti	13.695671000	0.977478000	11.133878000
Si	14.586746000	3.398936000	12.927136000
Si	14.469675000	-1.304242000	13.024932000
Si	16.100783000	0.654381000	9.195205000
O	12.037862000	1.688338000	10.216458000
O	14.533971000	0.979079000	9.500701000
O	13.769130000	2.611056000	11.790956000
O	14.853137000	-0.134256000	11.955397000
Si	8.432749000	1.129822000	8.882050000
Si	12.428792000	1.265941000	6.341574000
Si	11.420050000	-2.576048000	9.130640000
Si	13.733645000	-3.441514000	11.037036000
Si	17.457784000	-1.344283000	13.088708000
Si	13.856806000	-0.521444000	15.955216000
Si	17.704998000	3.422586000	12.933213000
Si	18.437235000	1.111832000	11.196914000
O	17.225600000	1.361784000	10.127594000
Si	16.193624000	-2.550424000	9.173733000
Si	15.649281000	1.233833000	6.308686000
Si	14.510386000	6.508731000	12.952710000
Si	13.869465000	2.596413000	15.875696000
O	11.692878000	1.292543000	7.771320000
O	9.831043000	0.895842000	9.648953000
O	11.618104000	-0.941680000	9.105396000
O	16.138573000	2.951576000	12.838786000
O	14.332868000	4.938825000	12.599646000

O	13.901558000	3.026883000	14.330968000
O	15.945902000	-1.787646000	13.412135000
O	13.685810000	-2.561774000	12.391225000
O	13.746259000	-0.888720000	14.382864000
O	16.428681000	1.220520000	7.724603000
O	16.282113000	-0.943838000	9.187209000
O	13.891704000	1.045503000	16.100998000
O	14.033033000	1.178768000	6.438432000
O	18.658323000	2.546047000	11.942772000
O	17.866753000	-0.009312000	12.231925000
O	14.901452000	-3.100209000	9.978558000
O	11.240577000	0.773742000	12.492690000
H	10.487535000	0.169036000	12.417379000
O	12.319540000	-0.092975000	12.029970000
H	11.442359000	1.792900000	10.993247000

H_2O_2-TS2

Si	11.353155000	0.572142000	9.179434000
Ti	13.713893000	1.098387000	11.285169000
Si	14.572623000	3.449668000	12.906590000
Si	14.478125000	-1.332065000	13.078026000
Si	16.111294000	0.654152000	9.218831000
O	12.007304000	1.005446000	10.586261000
O	14.596662000	0.989511000	9.676601000
O	13.756536000	2.826964000	11.658095000
O	14.778597000	0.070247000	12.315998000
Si	8.436453000	1.137488000	8.878518000
Si	12.439836000	1.269619000	6.351587000
Si	11.410319000	-2.588438000	9.116813000
Si	13.742185000	-3.448994000	10.995369000
Si	17.470269000	-1.343616000	13.080520000
Si	13.855924000	-0.573852000	15.921171000
Si	17.692372000	3.423544000	12.937305000
Si	18.452194000	1.113308000	11.196338000
O	17.289877000	1.352340000	10.085087000
Si	16.195101000	-2.556888000	9.169296000
Si	15.644623000	1.233936000	6.301631000
Si	14.513412000	6.527796000	12.954010000
Si	13.868328000	2.600891000	15.840277000
O	11.855211000	1.328671000	7.870999000
O	9.865063000	0.982111000	9.579800000
O	11.509104000	-0.992780000	8.941285000
O	16.115736000	2.959840000	12.856720000
O	14.346451000	4.983684000	12.584143000
O	13.847957000	3.154311000	14.317505000
O	15.966214000	-1.814742000	13.360019000
O	13.693542000	-2.475881000	12.278942000
O	13.724934000	-1.237237000	14.466876000
O	16.380182000	1.217738000	7.738515000
O	16.260637000	-0.949828000	9.202814000
O	13.923926000	1.020256000	15.861437000
O	14.038001000	1.182417000	6.395120000
O	18.643445000	2.546011000	11.948209000
O	17.864972000	-0.010098000	12.219695000
O	14.911332000	-3.143032000	9.944432000
O	12.538414000	0.713706000	12.999211000
H	11.234975000	1.215642000	11.690322000
H	11.277883000	2.194461000	13.041842000
O	11.165745000	1.263283000	12.774291000

Hydrated-TiOOSi

Si	11.329405000	0.539905000	9.147873000
Ti	13.788176000	1.006875000	11.278921000
Si	14.537922000	3.436530000	12.890758000
Si	14.505750000	-1.317895000	13.086548000
Si	16.145892000	0.659264000	9.214054000
O	11.934173000	0.817558000	10.694069000
O	14.658274000	1.099393000	9.693645000
O	13.641851000	2.740822000	11.745737000
O	14.875775000	0.103601000	12.376630000
Si	8.435491000	1.143517000	8.879092000
Si	12.448843000	1.271138000	6.351206000
Si	11.408132000	-2.585495000	9.112775000
Si	13.742145000	-3.447285000	10.997766000
Si	17.464506000	-1.349987000	13.087092000
Si	13.853517000	-0.556577000	15.927130000
Si	17.678283000	3.425174000	12.938149000
Si	18.464448000	1.107073000	11.209957000
O	17.346955000	1.330407000	10.053615000
Si	16.188651000	-2.562811000	9.171334000
Si	15.649216000	1.233048000	6.299212000
Si	14.512265000	6.520338000	12.950032000
Si	13.870788000	2.610376000	15.841497000
O	11.917315000	1.342582000	7.905782000
O	9.882378000	1.032831000	9.560751000
O	11.432880000	-0.999690000	8.831073000
O	16.098254000	2.966167000	12.833830000
O	14.342968000	4.976127000	12.554804000
O	13.873012000	3.188476000	14.338553000
O	15.970987000	-1.846345000	13.400137000
O	13.739569000	-2.480423000	12.290035000
O	13.693220000	-1.165032000	14.439369000
O	16.393005000	1.207832000	7.728692000
O	16.214967000	-0.949166000	9.219476000
O	13.925306000	1.030368000	15.902079000
O	14.043732000	1.181054000	6.387592000
O	18.631606000	2.543723000	11.951105000
O	17.854754000	-0.016516000	12.220621000
O	14.908577000	-3.157159000	9.938457000
O	12.546322000	-0.473463000	11.166421000
H	11.785349000	1.869243000	13.167070000
O	12.258643000	1.056632000	13.381428000
H	11.656957000	0.339110000	13.146689000

Table S2 Shows total energies of all stationary points along the H_2O_2 decomposition over the defective active site of TS-1 as shown in the Figure 3. All energies are obtained from the single point calculation energy from the ONIOM-optimized structures with the full DFT method (M06-L) for the whole 239T cluster model.

Steps	Energy (hartrees)
Direct manner	
ADS-D2	-101405.294882
TS-D2	-101405.273987
H_2O/η^1-TiOOH	-101405.308285
Indirect manner	
ADS-D1	-101405.304763
TS-D1	-101405.291859
H_2O/η^1-TiOOH	-101405.308285

Following is the optimized coordinates of atoms in the QM region of the ONIOM model for all catalytic steps in the Fig. 3.

ADS-D2

Ti	13.266150000	1.219885000	10.878797000
Si	14.592669000	3.402129000	12.887042000
Si	14.436548000	-1.190795000	12.924947000
Si	16.021648000	0.634648000	9.235819000
O	11.531280000	1.633138000	11.278984000
O	14.478343000	1.067868000	9.496490000
O	13.924815000	2.700497000	11.604611000
O	13.716995000	-0.054688000	12.027298000
Si	8.453207000	1.134083000	8.879595000
Si	12.448933000	1.271494000	6.353558000
Si	11.413574000	-2.576698000	9.124038000
Si	13.755438000	-3.468864000	10.996968000
Si	17.638470000	-1.212067000	13.006263000
Si	13.869250000	-0.573834000	15.912202000
Si	17.703456000	3.430047000	12.933957000
Si	18.500337000	1.163126000	11.166981000
O	17.152537000	1.233475000	10.251237000
Si	16.168636000	-2.588648000	9.176035000
Si	15.660016000	1.230135000	6.316969000
Si	14.510666000	6.511145000	12.950753000
Si	13.865601000	2.600559000	15.840670000
O	11.900094000	1.373868000	7.921944000
O	9.954508000	0.959226000	9.484550000
O	11.580095000	-0.957015000	9.088980000
O	16.144501000	2.949263000	12.869252000
O	14.338332000	4.947907000	12.571395000
O	13.878436000	3.072860000	14.291372000
O	16.030242000	-0.973162000	12.868772000
O	14.023807000	-2.626578000	12.339509000
O	13.852369000	-1.191816000	14.416478000
O	16.414760000	1.188356000	7.762891000
O	16.122909000	-0.973364000	9.271703000
O	13.915500000	1.017028000	15.880964000
O	14.050961000	1.187556000	6.400170000
O	18.650466000	2.601058000	11.903604000
O	18.402230000	-0.005721000	12.273574000
O	14.893800000	-3.239799000	9.891183000
H	10.809860000	-0.456105000	9.399807000
H	10.698925000	1.292235000	10.910763000
H	12.229940000	2.212201000	8.308561000
H	10.663788000	1.197858000	8.827613000
O	12.640766000	3.576883000	9.352141000
H	13.382425000	3.855217000	9.917905000
O	11.491917000	4.076634000	10.083465000
H	11.348785000	3.315444000	10.700610000

TS-D2

Ti	13.180399000	1.212103000	10.791910000
Si	14.577958000	3.386122000	12.891044000
Si	14.417293000	-1.173356000	12.875837000
Si	16.026662000	0.642547000	9.236547000
O	11.340436000	1.254941000	11.661843000
O	14.492153000	1.102703000	9.519920000
O	13.852330000	2.522833000	11.746821000
O	13.685215000	-0.144051000	11.855794000
Si	8.471973000	1.132368000	8.887251000
Si	12.452542000	1.269026000	6.352025000
Si	11.412234000	-2.571251000	9.126383000
Si	13.750320000	-3.465223000	11.011441000
Si	17.631160000	-1.211748000	13.004713000
Si	13.868328000	-0.560788000	15.913592000
Si	17.699591000	3.430774000	12.933316000
Si	18.502069000	1.163019000	11.168799000
O	17.161065000	1.237840000	10.246987000
Si	16.167871000	-2.584491000	9.178017000
Si	15.659893000	1.229765000	6.315248000
Si	14.509515000	6.501691000	12.947943000
Si	13.866969000	2.605966000	15.848220000
O	11.911699000	1.367270000	7.910849000
O	9.967134000	0.962326000	9.503994000
O	11.577296000	-0.947323000	9.115044000
O	16.135965000	2.955951000	12.859971000
O	14.329146000	4.931231000	12.560094000
O	13.869545000	3.098362000	14.311880000
O	16.019091000	-0.961881000	12.850866000
O	14.020636000	-2.650743000	12.377597000
O	13.841936000	-1.088038000	14.377477000
O	16.413618000	1.189988000	7.761538000
O	16.122480000	-0.965659000	9.269440000
O	13.907018000	1.027572000	15.917245000
O	14.054396000	1.183235000	6.388554000
O	18.648040000	2.601295000	11.905941000
O	18.399476000	-0.006178000	12.274050000
O	14.893873000	-3.221807000	9.908671000
H	10.841103000	-0.458597000	9.533093000
H	11.373693000	1.349263000	12.620071000
H	11.805839000	2.312129000	8.171756000
H	10.641233000	1.091658000	8.801096000
O	11.125340000	3.528243000	9.129307000
H	11.478312000	4.428412000	9.110464000
O	11.814064000	3.034198000	10.318056000
H	11.176243000	2.277399000	11.034466000

H_2O/η^1-TiOOH

Ti	13.195889000	1.204929000	10.768270000
Si	14.577526000	3.378588000	12.891295000
Si	14.414817000	-1.173861000	12.884309000
Si	16.031461000	0.647249000	9.234282000
O	11.282538000	0.485288000	11.833774000

O	14.501908000	1.153722000	9.504946000
O	13.789548000	2.585705000	11.741382000
O	13.849463000	-0.100848000	11.824200000
Si	8.465307000	1.129457000	8.886407000
Si	12.450376000	1.264897000	6.346042000
Si	11.417563000	-2.573244000	9.129355000
Si	13.748879000	-3.462493000	11.015807000
Si	17.624877000	-1.218730000	13.011976000
Si	13.866232000	-0.559208000	15.913802000
Si	17.699953000	3.429075000	12.931721000
Si	18.501170000	1.162780000	11.170205000
O	17.166140000	1.245216000	10.239126000
Si	16.167268000	-2.582248000	9.177779000
Si	15.658672000	1.230019000	6.313515000
Si	14.510303000	6.502010000	12.947767000
Si	13.868351000	2.605653000	15.849460000
O	11.867271000	1.289709000	7.876071000
O	9.922845000	0.918482000	9.568557000
O	11.678736000	-0.955564000	9.204894000
O	16.135328000	2.943949000	12.846100000
O	14.331747000	4.931500000	12.550705000
O	13.879857000	3.109921000	14.318091000
O	16.018508000	-1.016624000	12.911633000
O	13.977617000	-2.641217000	12.383012000
O	13.823351000	-1.080091000	14.377753000
O	16.415170000	1.189463000	7.758257000
O	16.109154000	-0.961291000	9.261308000
O	13.908689000	1.029324000	15.923425000
O	14.054675000	1.182673000	6.387667000
O	18.652247000	2.602125000	11.905826000
O	18.371905000	-0.002841000	12.272581000
O	14.895676000	-3.216225000	9.916954000
H	11.098755000	-0.284530000	8.818252000
H	10.878146000	1.277290000	12.212520000
H	12.016376000	2.160064000	8.269748000
H	10.509863000	1.704798000	9.669043000
O	12.407860000	3.467592000	9.591170000
H	12.917273000	3.902153000	10.300042000
O	11.704216000	2.450651000	10.352419000
H	10.651210000	0.230076000	11.130377000

ADS-D1

Ti	13.131438000	1.176423000	10.917495000
Si	14.550508000	3.391398000	12.881554000
Si	14.460796000	-1.188807000	12.930186000
Si	15.964877000	0.628906000	9.265249000
O	11.381230000	0.832724000	11.583383000
O	14.430117000	1.058496000	9.598133000
O	13.676198000	2.699094000	11.713018000
O	13.823618000	0.014401000	12.061945000
Si	8.482457000	1.138900000	8.892416000
Si	12.441635000	1.259098000	6.341403000
Si	11.413752000	-2.569289000	9.125396000
Si	13.756748000	-3.472320000	10.982643000
Si	17.651166000	-1.211735000	13.006729000
Si	13.869232000	-0.577003000	15.907612000
Si	17.684371000	3.429141000	12.931209000
Si	18.490041000	1.156222000	11.158774000
O	17.134384000	1.206698000	10.256794000
Si	16.163374000	-2.596141000	9.176974000
Si	15.647274000	1.229222000	6.314542000
Si	14.510298000	6.508941000	12.948627000
Si	13.866258000	2.603573000	15.843054000
O	11.806131000	1.196846000	7.833566000
O	9.968111000	1.077852000	9.533313000
O	11.659532000	-0.962386000	9.214030000
O	16.108436000	2.946553000	12.834067000
O	14.326750000	4.945950000	12.550985000
O	13.874924000	3.122365000	14.316637000
O	16.048014000	-0.986246000	12.887112000
O	14.011508000	-2.596346000	12.310752000
O	13.844200000	-1.205529000	14.412606000
O	16.351120000	1.183906000	7.789161000
O	16.076047000	-0.982702000	9.290743000
O	13.916802000	1.016191000	15.853368000
O	14.043461000	1.179248000	6.385266000
O	18.623130000	2.596424000	11.898020000
O	18.417275000	-0.007610000	12.275664000
O	14.899044000	-3.275325000	9.881142000
H	11.432617000	-0.256560000	8.584011000
H	11.360862000	0.100599000	12.207812000
H	11.684836000	2.016390000	8.334093000
H	10.225092000	0.676833000	10.389569000
O	12.100049000	4.237054000	10.150506000
H	12.777384000	4.108413000	10.846703000
O	11.804554000	2.852266000	9.866458000
H	10.887252000	2.711704000	10.179256000

TS-D1

Ti	13.114420000	1.179353000	10.872070000
Si	14.541206000	3.388072000	12.868903000
Si	14.445899000	-1.177192000	12.919276000
Si	15.979279000	0.623857000	9.269704000
O	11.265739000	0.518754000	11.461517000
O	14.443452000	1.064511000	9.624754000
O	13.693676000	2.662593000	11.694728000
O	13.744653000	-0.014428000	12.038055000
Si	8.491101000	1.131552000	8.894802000
Si	12.456045000	1.265969000	6.337975000
Si	11.412386000	-2.565992000	9.117652000
Si	13.757817000	-3.473169000	10.984148000
Si	17.644788000	-1.210861000	13.005612000
Si	13.869711000	-0.575561000	15.907732000
Si	17.681153000	3.430447000	12.932095000
Si	18.495379000	1.157587000	11.164348000
O	17.143789000	1.209502000	10.253251000
Si	16.162239000	-2.599476000	9.177669000
Si	15.647127000	1.229855000	6.306677000
Si	14.509989000	6.506315000	12.947832000
Si	13.865694000	2.604345000	15.840579000
O	11.961947000	1.319277000	7.898582000
O	9.970117000	0.984565000	9.539530000
O	11.641733000	-0.957849000	9.112130000
O	16.105405000	2.952724000	12.830281000
O	14.328001000	4.943708000	12.543546000
O	13.875100000	3.113919000	14.308081000

O	16.038116000	-0.965088000	12.867240000
O	14.022092000	-2.601034000	12.311941000
O	13.852201000	-1.199191000	14.410068000
O	16.331568000	1.186971000	7.792483000
O	16.073454000	-0.984206000	9.296940000
O	13.918107000	1.017299000	15.855573000
O	14.054436000	1.185550000	6.333510000
O	18.622272000	2.598081000	11.899280000
O	18.416781000	-0.009248000	12.275327000
O	14.897811000	-3.277460000	9.879359000
H	10.974007000	-0.261675000	8.948127000
H	11.303071000	-0.399790000	11.749480000
H	12.203090000	2.198552000	8.225586000
H	10.465251000	0.643536000	10.633479000
O	12.218867000	3.637727000	9.445426000
H	12.841853000	3.997409000	10.104033000
O	11.594417000	2.629297000	10.285095000
H	10.840771000	2.166213000	9.726403000

Table S3 Shows total energies of all stationary points along the ammonia oxidation over the hydrated η^1-TiOOH active species as shown in the Figure 4. All energies are obtained from the single point calculation energy from the ONIOM-optimized structures with the full DFT method (M06-L) for the whole 239T cluster model.

Steps	Energy (hartrees)
NH_3-η^1TiOOH	-101385.455125
TS-3	-101385.429761
NH_3O-D	-101385.468388
Route A	
TS_4	-101385.412422
NH_2OH_D complex	-101385.489170
Route A + H_2O	
H_2O-NH_3O_D complex	-101461.908476
Water-assisted-TS_4	-101461.877552
H_2O-NH_2OH_D complex	-101461.920933

Following is the optimized coordinates of atoms in the QM region of the ONIOM model for all catalytic steps in the Fig. 4.

NH_3-η^1TiOOH

Ti	13.164382000	1.239328000	10.761174000
Si	14.579019000	3.380778000	12.893895000
Si	14.416778000	-1.164450000	12.870616000
Si	16.021427000	0.647600000	9.236180000
O	14.494878000	1.139913000	9.513142000
O	13.786539000	2.582819000	11.755931000
O	13.805510000	-0.108006000	11.828583000
Si	8.467677000	1.129185000	8.885035000
Si	12.447864000	1.265065000	6.350311000
Si	11.415564000	-2.569428000	9.124871000
Si	13.749998000	-3.462083000	11.015724000
Si	17.626728000	-1.217569000	13.010580000
Si	13.866373000	-0.557681000	15.913710000
Si	17.700636000	3.428912000	12.931549000
Si	18.498917000	1.162733000	11.166577000
O	17.164311000	1.243236000	10.238328000
Si	16.168742000	-2.580510000	9.177745000
Si	15.656917000	1.229931000	6.313878000
Si	14.510341000	6.502683000	12.948070000
Si	13.868297000	2.607332000	15.850382000
O	11.868585000	1.305754000	7.882464000
O	9.923726000	0.911190000	9.562757000
O	11.655687000	-0.955922000	9.172594000
O	16.135658000	2.945172000	12.849066000
O	14.330826000	4.932484000	12.553007000
O	13.880001000	3.106528000	14.320046000
O	16.018618000	-1.015266000	12.904477000
O	13.963374000	-2.637757000	12.387564000
O	13.816194000	-1.064064000	14.369691000
O	16.411488000	1.188826000	7.760337000
O	16.115662000	-0.962070000	9.263343000
O	13.902877000	1.030010000	15.928953000
O	14.053731000	1.182963000	6.387649000
O	18.651484000	2.601381000	11.905411000
O	18.373561000	-0.001382000	12.273537000
O	14.897557000	-3.214808000	9.920520000
H	10.962528000	-0.284097000	9.030801000
H	11.985828000	2.198357000	8.232869000
H	10.521183000	1.686588000	9.667695000
O	12.447315000	3.446240000	9.581732000
H	12.882257000	3.949889000	10.292898000
O	11.685260000	2.484941000	10.359168000
H	10.402933000	0.891780000	11.718556000
N	11.307729000	0.461681000	11.881004000
H	11.527881000	0.500539000	12.871638000
H	11.225226000	-0.518567000	11.625629000

TS-3

Ti	13.185476000	1.255777000	10.792359000
Si	14.596753000	3.393392000	12.897707000
Si	14.398196000	-1.148851000	12.869838000
Si	16.017964000	0.640558000	9.235179000
O	14.480878000	1.075917000	9.514345000
O	13.948121000	2.568825000	11.697467000
O	13.582292000	-0.097250000	11.946058000
Si	8.475180000	1.124777000	8.885731000
Si	12.437027000	1.262795000	6.359242000
Si	11.410752000	-2.560904000	9.119465000
Si	13.762311000	-3.470119000	10.992846000
Si	17.624309000	-1.211277000	13.004233000
Si	13.868041000	-0.571703000	15.905271000
Si	17.707306000	3.431043000	12.935376000
Si	18.497876000	1.163484000	11.164002000
O	17.154316000	1.237789000	10.248314000
Si	16.171007000	-2.584749000	9.175696000
Si	15.651799000	1.229117000	6.314328000
Si	14.509665000	6.504683000	12.948561000
Si	13.866691000	2.605977000	15.842241000
O	11.826585000	1.261181000	7.866155000
O	9.931492000	0.871326000	9.519808000
O	11.667074000	-0.959155000	9.187629000
O	16.149532000	2.961793000	12.891529000
O	14.323454000	4.936450000	12.558986000
O	13.864474000	3.107728000	14.308112000
O	16.003264000	-0.958302000	12.848457000
O	13.998382000	-2.627679000	12.349918000
O	13.828799000	-1.158775000	14.387459000

O	16.411585000	1.183204000	7.762661000
O	16.117787000	-0.971210000	9.284314000
O	13.907746000	1.020293000	15.872500000
O	14.049293000	1.180313000	6.396810000
O	18.651405000	2.599228000	11.906226000
O	18.387923000	-0.005275000	12.272381000
O	14.901713000	-3.244121000	9.896610000
H	10.975466000	-0.275481000	9.062499000
H	11.696314000	2.124413000	8.277396000
H	10.352122000	1.427158000	10.218315000
O	12.114019000	2.939045000	9.858778000
H	12.402584000	3.703484000	10.379864000
O	11.442816000	2.025386000	11.110992000
H	9.764254000	1.022193000	12.708742000
N	10.750445000	0.792724000	12.717266000
H	11.183506000	1.226727000	13.523080000
H	10.878679000	-0.225042000	12.749137000
H	11.404342000	-2.400138000	12.044688000
O	11.066631000	-2.115791000	12.905430000
H	11.809364000	-2.282368000	13.497337000

NH_3O-D

Ti	13.108631000	1.282843000	10.798660000
Si	14.569059000	3.412129000	12.926356000
Si	14.411754000	-1.178168000	12.833987000
Si	16.022461000	0.641683000	9.259668000
O	14.533283000	1.145496000	9.653645000
O	13.731476000	2.414697000	12.022595000
O	13.550258000	-0.229199000	11.876779000
Si	8.474244000	1.133301000	8.888851000
Si	12.438187000	1.265660000	6.346688000
Si	11.411585000	-2.571859000	9.127138000
Si	13.756445000	-3.468987000	11.011868000
Si	17.629332000	-1.209336000	13.004910000
Si	13.869137000	-0.569861000	15.896187000
Si	17.692946000	3.432368000	12.936510000
Si	18.510385000	1.158886000	11.173630000
O	17.194787000	1.223096000	10.232304000
Si	16.164173000	-2.587813000	9.178262000
Si	15.650098000	1.229825000	6.315824000
Si	14.509893000	6.503696000	12.943491000
Si	13.870143000	2.625889000	15.845638000
O	11.820718000	1.293752000	7.845442000
O	9.964028000	0.986484000	9.534135000
O	11.563489000	-0.950653000	9.122238000
O	16.121283000	2.971377000	12.883434000
O	14.331932000	4.938796000	12.523831000
O	13.839130000	3.266098000	14.376051000
O	16.015009000	-0.938193000	12.852462000
O	14.089993000	-2.693155000	12.386031000
O	13.821398000	-1.110936000	14.363904000
O	16.380346000	1.185344000	7.775586000
O	16.107262000	-0.969357000	9.277964000
O	13.894047000	1.034576000	15.811974000
O	14.045492000	1.185956000	6.405063000
O	18.635385000	2.599519000	11.910837000
O	18.409524000	-0.007201000	12.282588000
O	14.890407000	-3.238330000	9.896184000
H	10.835404000	-0.466373000	9.551854000
H	12.067621000	2.061845000	8.425680000
H	10.630738000	1.080815000	8.808686000
O	12.146628000	2.628174000	9.888627000
H	11.271417000	2.791473000	10.262679000
O	11.329186000	1.183105000	11.892095000
H	10.794522000	1.032056000	13.789385000
N	11.649748000	1.042308000	13.229405000
H	12.254102000	1.824139000	13.536828000
H	12.189119000	0.172443000	13.375514000

TS_4

Ti	13.169852000	1.201827000	10.817906000
Si	14.567266000	3.379689000	12.883923000
Si	14.420457000	-1.191059000	12.896792000
Si	16.011842000	0.647589000	9.243861000
O	11.621842000	0.629955000	12.260078000
O	14.485449000	1.135620000	9.542080000
O	13.740088000	2.612046000	11.741061000
O	13.876267000	-0.108284000	11.839976000
Si	8.473461000	1.133738000	8.887389000
Si	12.430724000	1.259491000	6.351059000
Si	11.418552000	-2.568081000	9.129033000
Si	13.746855000	-3.462960000	11.015733000
Si	17.625953000	-1.220050000	13.013219000
Si	13.866373000	-0.561637000	15.914406000
Si	17.694665000	3.428075000	12.930950000
Si	18.496353000	1.161461000	11.166280000
O	17.160726000	1.243507000	10.238622000
Si	16.167571000	-2.581075000	9.177847000
Si	15.650283000	1.230092000	6.316549000
Si	14.510725000	6.503296000	12.949366000
Si	13.868851000	2.602427000	15.848576000
O	11.738133000	1.213617000	7.815501000
O	9.900355000	0.972293000	9.652509000
O	11.696521000	-0.956912000	9.220087000
O	16.125651000	2.941600000	12.839212000
O	14.332334000	4.935120000	12.569141000
O	13.873251000	3.094033000	14.313466000
O	16.021075000	-1.031332000	12.926979000
O	13.973696000	-2.651382000	12.389871000
O	13.823517000	-1.096466000	14.387084000
O	16.395845000	1.193554000	7.766552000
O	16.115247000	-0.961088000	9.256442000
O	13.906172000	1.026699000	15.929261000
O	14.040573000	1.181081000	6.416940000
O	18.646131000	2.600804000	11.904783000
O	18.367304000	-0.001803000	12.272472000
O	14.897184000	-3.214059000	9.920474000
H	11.376981000	-0.275685000	8.608308000
H	11.927784000	1.935314000	8.454705000
H	10.530431000	1.728395000	9.656377000
O	11.886384000	2.461571000	9.995302000
H	12.060481000	3.366857000	10.266181000
N	10.188311000	1.208996000	12.352002000
H	9.709355000	0.556850000	12.962680000
H	9.829704000	1.192738000	11.383543000
H	11.178379000	1.675545000	12.718790000

NH_2OH_D complex

Ti	13.172354000	1.224402000	10.807553000
Si	14.562245000	3.389885000	12.891542000
Si	14.425873000	-1.178853000	12.897471000
Si	16.023186000	0.645557000	9.244955000
O	14.502342000	1.133078000	9.562992000
O	13.701034000	2.601100000	11.786120000
O	13.818178000	-0.082117000	11.898296000
Si	8.467845000	1.135462000	8.891138000
Si	12.435563000	1.259145000	6.347340000
Si	11.414430000	-2.570308000	9.124218000
Si	13.753122000	-3.466414000	11.006936000
Si	17.629986000	-1.218641000	13.011959000
Si	13.866356000	-0.562654000	15.913153000
Si	17.690975000	3.429190000	12.931349000
Si	18.502779000	1.164024000	11.169192000
O	17.176219000	1.238283000	10.231235000
Si	16.169217000	-2.582522000	9.176723000
Si	15.651254000	1.230000000	6.314800000
Si	14.510850000	6.504775000	12.947982000
Si	13.867766000	2.609589000	15.847230000
O	11.768529000	1.204621000	7.822315000
O	9.921637000	0.996521000	9.612051000
O	11.695449000	-0.963036000	9.225464000
O	16.120325000	2.940401000	12.830973000
O	14.336978000	4.939178000	12.553391000
O	13.884633000	3.135823000	14.328931000
O	16.022378000	-1.025771000	12.916143000
O	13.953974000	-2.630318000	12.371534000
O	13.812600000	-1.121054000	14.388038000
O	16.395056000	1.189869000	7.766499000
O	16.109275000	-0.964804000	9.265465000
O	13.910821000	1.026700000	15.892897000
O	14.044293000	1.180422000	6.409190000
O	18.644509000	2.602026000	11.906338000
O	18.371533000	-0.001954000	12.273167000
O	14.900146000	-3.225472000	9.914152000
H	11.412314000	-0.265380000	8.608532000
H	11.920706000	1.950851000	8.444019000
H	10.483114000	1.803585000	9.656260000
O	11.913989000	2.491499000	9.967750000
H	12.038250000	3.377577000	10.318595000
O	11.318251000	0.511156000	11.693284000
H	10.562148000	0.603845000	11.058850000
N	11.086185000	-0.789956000	12.273770000
H	11.520497000	-0.702760000	13.191203000
H	11.700761000	-1.415276000	11.747859000

H_2O-NH_3O_D complex

Ti	13.136017000	1.288116000	10.792242000
Si	14.569106000	3.413519000	12.932488000
Si	14.415297000	-1.175595000	12.835048000
Si	16.034193000	0.639873000	9.253789000
O	14.542893000	1.145443000	9.632281000
O	13.731950000	2.416014000	12.024279000
O	13.577086000	-0.225175000	11.861144000
Si	8.474543000	1.134562000	8.885452000
Si	12.435574000	1.265552000	6.350138000
Si	11.412028000	-2.572109000	9.127156000
Si	13.757110000	-3.467917000	11.013927000
Si	17.631107000	-1.209339000	13.005116000
Si	13.869058000	-0.568890000	15.895612000
Si	17.692832000	3.432388000	12.936292000
Si	18.512791000	1.159075000	11.176397000
O	17.195344000	1.221695000	10.236978000
Si	16.164687000	-2.588144000	9.178083000
Si	15.651853000	1.229607000	6.317589000
Si	14.509867000	6.503322000	12.943393000
Si	13.869041000	2.625862000	15.846359000
O	11.803237000	1.297713000	7.844847000
O	9.952724000	0.995810000	9.554703000
O	11.558856000	-0.949443000	9.115870000
O	16.121625000	2.970102000	12.878987000
O	14.333148000	4.938724000	12.521749000
O	13.842794000	3.269329000	14.378684000
O	16.018950000	-0.940693000	12.851185000
O	14.087290000	-2.691869000	12.388269000
O	13.821718000	-1.111578000	14.362377000
O	16.395085000	1.184558000	7.770812000
O	16.109404000	-0.970385000	9.275514000
O	13.898279000	1.034483000	15.811132000
O	14.044700000	1.184887000	6.414983000
O	18.637568000	2.600654000	11.910913000
O	18.413520000	-0.006973000	12.284819000
O	14.889781000	-3.236359000	9.896663000
H	10.846078000	-0.472099000	9.573852000
H	12.070415000	2.062629000	8.422531000
H	10.636634000	1.093547000	8.844155000
O	12.191413000	2.646809000	9.866723000
H	11.337700000	2.881075000	10.247524000
O	11.347167000	1.127258000	11.826290000
H	10.643299000	1.035172000	13.637065000
N	11.574233000	0.967332000	13.187002000
H	12.192609000	1.719298000	13.530048000
H	12.053920000	0.072786000	13.362942000
H	9.538356000	1.786613000	12.152254000
O	9.066930000	1.874593000	12.997689000
H	8.154123000	1.651311000	12.785675000

Water-assisted-TS_4

Ti	13.240912000	1.252452000	10.814873000
Si	14.551345000	3.409114000	12.946959000
Si	14.411955000	-1.214195000	12.832532000
Si	16.047432000	0.677169000	9.230980000
O	14.582961000	1.296515000	9.567058000
O	13.664026000	2.337556000	12.159078000
O	13.997859000	-0.279050000	11.619758000
Si	8.466861000	1.135592000	8.882308000
Si	12.436954000	1.265744000	6.354204000
Si	11.410990000	-2.576382000	9.122575000
Si	13.738101000	-3.459245000	11.038864000
Si	17.601050000	-1.236213000	13.026217000
Si	13.862516000	-0.542066000	15.902705000
Si	17.686669000	3.431605000	12.935703000
Si	18.502322000	1.165420000	11.171651000

O	17.218762000	1.264475000	10.193304000
Si	16.170476000	-2.564311000	9.180020000
Si	15.655409000	1.230323000	6.314064000
Si	14.509196000	6.496739000	12.939365000
Si	13.872020000	2.648264000	15.837581000
O	11.807078000	1.291239000	7.854715000
O	9.929629000	0.998652000	9.575069000
O	11.553701000	-0.956656000	9.084307000
O	16.110963000	2.965421000	12.862783000
O	14.331693000	4.930288000	12.490638000
O	13.874273000	3.369862000	14.415341000
O	15.993100000	-1.156405000	13.039531000
O	13.855176000	-2.690474000	12.462802000
O	13.731885000	-1.032615000	14.332329000
O	16.428241000	1.187334000	7.744341000
O	16.116843000	-0.939890000	9.246973000
O	13.900033000	1.053364000	15.840220000
O	14.047364000	1.183083000	6.416534000
O	18.641973000	2.599161000	11.917240000
O	18.277264000	0.005569000	12.266645000
O	14.901651000	-3.170229000	9.964420000
H	11.238976000	-0.549445000	9.912248000
H	12.094877000	2.017023000	8.455465000
H	10.628353000	0.871213000	8.889571000
O	12.070888000	2.517643000	10.058930000
H	11.109407000	2.430909000	10.119294000
O	11.101347000	-1.183629000	13.414119000
H	11.906851000	-1.210395000	13.981342000
O	11.577230000	0.268257000	11.559474000
H	11.498486000	-0.995808000	12.474526000
N	10.627975000	0.975126000	12.355520000
H	9.824507000	1.162428000	11.750394000
H	11.045172000	1.873160000	12.608040000
H	10.683088000	-0.178333000	13.363885000

H_2O-NH_2OH_D complex

Ti	13.190404000	1.244947000	10.794038000
Si	14.567679000	3.391317000	12.891088000
Si	14.433110000	-1.165623000	12.894199000
Si	16.031911000	0.645853000	9.239921000
O	11.920264000	2.496033000	9.966609000
O	14.511054000	1.140786000	9.548254000
O	13.711977000	2.625610000	11.764856000
O	13.847272000	-0.042894000	11.911348000
Si	8.462768000	1.133993000	8.895812000
Si	12.435463000	1.258941000	6.347967000
Si	11.413282000	-2.570810000	9.122595000
Si	13.755360000	-3.466512000	11.001937000
Si	17.633511000	-1.218606000	13.012442000
Si	13.866017000	-0.562121000	15.913505000
Si	17.693293000	3.429248000	12.930919000
Si	18.505390000	1.165076000	11.170498000
O	17.179146000	1.236798000	10.231882000
Si	16.169875000	-2.582922000	9.175887000
Si	15.652432000	1.229722000	6.314698000
Si	14.511118000	6.506376000	12.949043000
Si	13.867048000	2.608156000	15.848528000
O	11.769459000	1.203020000	7.823828000
O	9.923329000	0.989229000	9.618926000
O	11.697852000	-0.964991000	9.229089000
O	16.124102000	2.938053000	12.827553000
O	14.339454000	4.940475000	12.561269000
O	13.888109000	3.114971000	14.322632000
O	16.027435000	-1.031230000	12.923726000
O	13.943537000	-2.609674000	12.357132000
O	13.808776000	-1.116350000	14.383277000
O	16.405635000	1.186581000	7.762294000
O	16.104154000	-0.965533000	9.268128000
O	13.910125000	1.025468000	15.900950000
O	14.045542000	1.179875000	6.410798000
O	18.648394000	2.602884000	11.906553000
O	18.372788000	-0.000828000	12.274346000
O	14.901576000	-3.230711000	9.910434000
H	11.401085000	-0.262592000	8.622989000
H	11.910228000	1.954541000	8.440706000
H	10.473219000	1.801231000	9.664291000
H	12.033732000	3.383153000	10.318884000
O	11.345984000	0.492989000	11.677498000
H	10.569826000	0.575070000	11.056669000
N	11.210371000	-0.821995000	12.238300000
H	11.683900000	-0.739327000	13.136194000
H	11.799670000	-1.423428000	11.660636000
H	9.364052000	-0.921023000	12.397640000
O	8.431164000	-0.679457000	12.538329000
H	8.119161000	-1.340201000	13.158306000

Table S4 Shows total energies of all stationary points along the hydroxylamine formation via the hydrolysis of titano-oxyamine intermediate as shown in the Figure 5. All energies are obtained from the single point calculation energy from the ONIOM-optimized structures with the full DFT method (M06-L) for the whole 239T cluster model.

Steps	Energy (hartrees)
TS_D2a	-101385.473480
NH_2O-Ti/H_2O	-101385.486780
TS_D2b	-101385.460910

Following is the optimized coordinates of atoms in the QM region of the ONIOM model for all catalytic steps in the Fig. 5.

TS_D2a

Ti	13.173078000	1.218050000	10.838202000
Si	14.574053000	3.397294000	12.907344000
Si	14.427509000	-1.190115000	12.884979000
Si	16.001847000	0.646897000	9.240392000
O	11.450556000	1.031413000	11.757081000
O	14.480357000	1.129873000	9.518730000
O	13.787825000	2.598702000	11.770550000
O	13.771168000	-0.147360000	11.844747000
Si	8.470394000	1.132041000	8.881026000
Si	12.441910000	1.267370000	6.353850000
Si	11.412504000	-2.573956000	9.127400000
Si	13.752253000	-3.466317000	11.012146000
Si	17.634011000	-1.213174000	13.007340000
Si	13.868697000	-0.566418000	15.906846000
Si	17.695308000	3.429456000	12.934077000
Si	18.495192000	1.158347000	11.163647000
O	17.153325000	1.230019000	10.247584000

Si	16.166328000	-2.582947000	9.177688000
Si	15.656442000	1.229711000	6.317904000
Si	14.510831000	6.505688000	12.948012000
Si	13.868620000	2.607102000	15.845921000
O	11.840459000	1.322365000	7.875393000
O	9.952038000	0.978681000	9.527144000
O	11.565738000	-0.950601000	9.114287000
O	16.127129000	2.955655000	12.870666000
O	14.329679000	4.942918000	12.550401000
O	13.855960000	3.162293000	14.332941000
O	16.026771000	-0.981112000	12.880184000
O	14.017980000	-2.662687000	12.382615000
O	13.841315000	-1.119274000	14.383532000
O	16.409805000	1.187671000	7.763905000
O	16.108213000	-0.964906000	9.266973000
O	13.915085000	1.027277000	15.881383000
O	14.047959000	1.186273000	6.402794000
O	18.637341000	2.598458000	11.904011000
O	18.399487000	-0.005891000	12.275558000
O	14.893811000	-3.227046000	9.907480000
H	10.866198000	-0.478018000	9.596504000
H	12.059600000	2.132688000	8.396090000
H	10.646182000	1.084223000	8.827398000
O	12.059491000	2.834133000	9.889240000
H	12.616453000	3.602591000	10.057393000
H	10.734010000	2.625571000	12.663346000
N	10.650216000	2.182251000	11.747727000
H	9.685459000	1.892720000	11.588128000
H	11.161189000	2.768306000	10.800338000

NH_2O-Ti/H_2O

Ti	13.149952000	1.172805000	10.858941000
Si	14.552682000	3.378118000	12.869533000
Si	14.423472000	-1.202104000	12.906603000
Si	15.983854000	0.654389000	9.242657000
O	11.513443000	0.823018000	11.687506000
O	14.451022000	1.109084000	9.518525000
O	13.685833000	2.647271000	11.728177000
O	13.926458000	-0.132425000	11.820706000
Si	8.476638000	1.135885000	8.892723000
Si	12.442392000	1.260488000	6.343738000
Si	11.415685000	-2.568288000	9.125552000
Si	13.747555000	-3.461150000	11.021065000
Si	17.622691000	-1.224962000	13.016092000
Si	13.864138000	-0.552281000	15.921726000
Si	17.688812000	3.428421000	12.929943000
Si	18.483679000	1.163383000	11.156063000
O	17.145060000	1.250939000	10.232345000
Si	16.171773000	-2.572964000	9.178130000
Si	15.653309000	1.230956000	6.315567000
Si	14.510443000	6.504599000	12.950309000
Si	13.869043000	2.607002000	15.848499000
O	11.785835000	1.209771000	7.832139000
O	9.943388000	1.029794000	9.600174000
O	11.665794000	-0.956165000	9.209706000
O	16.116507000	2.943723000	12.824217000
O	14.328363000	4.939070000	12.569687000
O	13.893095000	3.081404000	14.312012000
O	16.016965000	-1.085524000	12.959552000
O	13.905486000	-2.646421000	12.407148000
O	13.801248000	-1.065748000	14.382810000
O	16.390494000	1.195401000	7.766055000
O	16.126410000	-0.957221000	9.253314000
O	13.902665000	1.031213000	15.952648000
O	14.044482000	1.180936000	6.393387000
O	18.639688000	2.598583000	11.903186000
O	18.336857000	0.000600000	12.264347000
O	14.900380000	-3.197538000	9.937070000
H	11.471062000	-0.253687000	8.564274000
H	11.791148000	2.022645000	8.357765000
H	10.034473000	0.346239000	10.296800000
O	11.809124000	2.828129000	9.896164000
H	11.997078000	3.579749000	10.469997000
H	10.451398000	-0.318125000	12.829331000
N	10.782693000	-0.367697000	11.866178000
H	11.463144000	-1.133681000	11.832961000
H	10.935989000	2.438581000	10.129197000

TS_D2b

Ti	13.210032000	1.237911000	10.808458000
Si	14.588081000	3.391243000	12.891704000
Si	14.413424000	-1.172755000	12.886564000
Si	16.040298000	0.636543000	9.235609000
O	11.377046000	1.285126000	11.773276000
O	14.503885000	1.076106000	9.543897000
O	13.873336000	2.614720000	11.682055000
O	13.645563000	-0.121553000	11.924680000
Si	8.480118000	1.128978000	8.888230000
Si	12.424244000	1.260510000	6.362009000
Si	11.416542000	-2.566565000	9.126911000
Si	13.751556000	-3.465823000	11.006450000
Si	17.629079000	-1.212349000	13.005059000
Si	13.868813000	-0.565225000	15.913163000
Si	17.703903000	3.430369000	12.932788000
Si	18.505756000	1.164448000	11.170934000
O	17.168624000	1.241148000	10.245091000
Si	16.169606000	-2.586010000	9.177696000
Si	15.648997000	1.229970000	6.316530000
Si	14.510188000	6.505886000	12.949835000
Si	13.866967000	2.602668000	15.846142000
O	11.734766000	1.199348000	7.828205000
O	9.933682000	0.948143000	9.574920000
O	11.688611000	-0.957149000	9.228838000
O	16.142298000	2.951697000	12.858174000
O	14.329092000	4.937972000	12.569582000
O	13.881056000	3.081200000	14.304263000
O	16.015345000	-0.965191000	12.850674000
O	14.006546000	-2.642634000	12.369209000
O	13.842016000	-1.127360000	14.392111000
O	16.410054000	1.190997000	7.762682000
O	16.132996000	-0.969584000	9.271557000
O	13.909864000	1.023096000	15.913150000
O	14.039839000	1.180797000	6.429651000
O	18.655613000	2.602398000	11.907483000
O	18.394423000	-0.004880000	12.274766000
O	14.897190000	-3.225510000	9.908056000

H	11.413563000	-0.255947000	8.607788000
H	11.658361000	1.946300000	8.455641000
H	9.930569000	0.361317000	10.361650000
H	10.101603000	0.341646000	12.898161000
N	10.565748000	0.130580000	12.015356000
H	11.247185000	-0.602546000	12.226050000
O	11.855591000	2.643245000	10.004040000
H	11.167196000	2.047357000	10.864154000
H	12.142449000	3.524048000	10.268655000

Table S5 Shows total energies of all stationary points along the hydroxylamine formation via the second H_2O_2 decomposition on the titano-oxyamine intermediate as shown in the Figure 6. All energies are obtained from the single point calculation energy from the ONIOM-optimized structures with the full DFT method (M06-L) for the whole 239T cluster model.

Steps	Energy (hartrees)
NH_2O-Ti/H_2O_2	-101460.600150
TS_D2c	-101460.575170
NH_2OH-η^1-TiOOH	-101460.596991

Atomic Coordinates in QM region of the ONIOM model for all steps of catalytic reaction in the Figure 6

NH_2O-Ti/H_2O_2

Ti	13.152009000	1.180610000	10.861133000
Si	14.558035000	3.378158000	12.872747000
Si	14.428260000	-1.195949000	12.912812000
Si	15.986971000	0.651090000	9.242671000
O	11.507410000	0.845913000	11.666248000
O	14.453354000	1.102839000	9.530611000
O	13.683465000	2.686508000	11.706227000
O	13.920892000	-0.082910000	11.873439000
Si	8.477188000	1.136185000	8.891494000
Si	12.440247000	1.259665000	6.344940000
Si	11.415251000	-2.568644000	9.124761000
Si	13.748959000	-3.463291000	11.011718000
Si	17.626380000	-1.223904000	13.015000000
Si	13.864834000	-0.558507000	15.918896000
Si	17.691069000	3.427679000	12.928814000
Si	18.486238000	1.162494000	11.156052000
O	17.147154000	1.246545000	10.233184000
Si	16.171337000	-2.576486000	9.176924000
Si	15.651834000	1.230335000	6.314713000
Si	14.510182000	6.506286000	12.949540000
Si	13.867955000	2.604716000	15.848073000
O	11.782747000	1.200332000	7.832727000
O	9.947163000	1.034791000	9.589716000
O	11.668123000	-0.957270000	9.212491000
O	16.118045000	2.938822000	12.820463000
O	14.326425000	4.938543000	12.564495000
O	13.892060000	3.078508000	14.308530000
O	16.020802000	-1.075071000	12.954750000
O	13.912027000	-2.627954000	12.383918000
O	13.804986000	-1.098395000	14.390214000
O	16.388445000	1.193213000	7.767255000
O	16.118351000	-0.960710000	9.258982000
O	13.907682000	1.026873000	15.930090000
O	14.043526000	1.179560000	6.399584000
O	18.641054000	2.598279000	11.902257000
O	18.344706000	0.000340000	12.265683000
O	14.901545000	-3.209911000	9.927881000
H	11.471201000	-0.253381000	8.567489000
H	11.680668000	2.019157000	8.341942000
H	10.037424000	0.353337000	10.286076000
H	10.433289000	-0.264214000	12.825660000
N	10.775163000	-0.339008000	11.867911000
H	11.453739000	-1.107181000	11.857762000
O	11.994369000	4.223738000	10.222878000
H	12.710718000	4.102322000	10.880504000
O	11.777978000	2.839475000	9.873698000
H	10.894592000	2.600882000	10.232237000

TS_D2c

Ti	13.201309000	1.231083000	10.799359000
Si	14.588264000	3.383338000	12.887099000
Si	14.414340000	-1.168443000	12.889430000
Si	16.040653000	0.637097000	9.235525000
O	11.384768000	1.328568000	11.782158000
O	14.503626000	1.080610000	9.547269000
O	13.854609000	2.649406000	11.655005000
O	13.654413000	-0.095211000	11.940876000
Si	8.480523000	1.130237000	8.888411000
Si	12.426383000	1.260991000	6.360231000
Si	11.416387000	-2.567078000	9.127431000
Si	13.751289000	-3.465839000	11.004008000
Si	17.629822000	-1.212479000	13.005121000
Si	13.868555000	-0.564865000	15.915143000
Si	17.704811000	3.429834000	12.931670000
Si	18.506209000	1.164643000	11.170673000
O	17.167065000	1.240298000	10.247181000
Si	16.169339000	-2.586560000	9.177733000
Si	15.649195000	1.229983000	6.315897000
Si	14.509860000	6.506338000	12.949892000
Si	13.866482000	2.600714000	15.847536000
O	11.747172000	1.198165000	7.834188000
O	9.938560000	0.953717000	9.574999000
O	11.690531000	-0.956682000	9.235026000
O	16.142332000	2.945249000	12.849125000
O	14.328629000	4.934160000	12.570349000
O	13.884945000	3.058768000	14.297378000
O	16.015688000	-0.967635000	12.851527000
O	13.998565000	-2.631178000	12.361899000
O	13.840605000	-1.124975000	14.393112000
O	16.409861000	1.189037000	7.763109000
O	16.126267000	-0.969697000	9.275986000
O	13.908225000	1.022199000	15.922820000
O	14.040889000	1.179166000	6.429049000
O	18.657487000	2.602481000	11.907226000
O	18.393763000	-0.004329000	12.274944000
O	14.897684000	-3.228227000	9.907118000
H	11.407149000	-0.256463000	8.617003000
H	11.624949000	1.960936000	8.430611000
H	9.929738000	0.390527000	10.376997000
H	10.051562000	0.482092000	12.919601000
N	10.534540000	0.212559000	12.062967000
H	11.191636000	-0.524570000	12.328870000

O	12.172397000	4.062208000	10.074742000
H	12.907358000	4.046580000	10.717730000
O	11.823069000	2.662754000	10.023724000
H	11.145446000	2.158908000	10.934308000

NH_2OH-η^1-TiOOH

Ti	13.179879000	1.303984000	10.705111000
Si	14.565385000	3.394553000	12.923003000
Si	14.384352000	-1.139115000	12.824886000
Si	16.083136000	0.638313000	9.232314000
O	11.304044000	1.068805000	12.207346000
O	14.571528000	1.107982000	9.587212000
O	13.706052000	2.480216000	11.929443000
O	13.571483000	-0.184879000	11.803516000
Si	8.488568000	1.131077000	8.895014000
Si	12.415221000	1.258428000	6.364808000
Si	11.416950000	-2.565942000	9.125872000
Si	13.750033000	-3.460575000	11.019166000
Si	17.617719000	-1.213412000	13.004706000
Si	13.867592000	-0.555043000	15.906713000
Si	17.694549000	3.431408000	12.934063000
Si	18.518594000	1.165043000	11.181092000
O	17.208358000	1.252088000	10.229072000
Si	16.172774000	-2.580987000	9.177275000
Si	15.647241000	1.230531000	6.318206000
Si	14.509408000	6.501096000	12.943861000
Si	13.868729000	2.619125000	15.852977000
O	11.677823000	1.167996000	7.801006000
O	9.940672000	0.967763000	9.616860000
O	11.687064000	-0.955935000	9.222042000
O	16.121703000	2.957120000	12.850789000
O	14.326272000	4.930939000	12.514989000
O	13.870052000	3.210896000	14.362872000
O	15.999646000	-0.957910000	12.834940000
O	13.994188000	-2.651780000	12.396884000
O	13.824984000	-1.038836000	14.351481000
O	16.423153000	1.193650000	7.756260000
O	16.166510000	-0.964967000	9.250497000
O	13.895150000	1.037983000	15.905019000
O	14.035601000	1.178730000	6.455140000
O	18.650555000	2.604522000	11.915489000
O	18.387318000	-0.004747000	12.278681000
O	14.896641000	-3.201262000	9.921811000
H	11.394509000	-0.268785000	8.591333000
H	11.573602000	1.871698000	8.473848000
H	9.941645000	0.417748000	10.422768000
H	10.153539000	-0.358647000	12.948595000
N	10.647793000	-0.205414000	12.072192000
H	11.398559000	-0.897426000	11.996384000
O	13.001866000	3.360431000	9.548291000
H	13.056384000	3.986151000	10.292608000
O	11.871253000	2.536092000	9.960259000
H	11.902998000	1.006006000	12.973075000

Table S6 Shows total energies of all stationary points along the ammonia oxidation over the hydrated [≡TiOOSi≡] active species as shown in the Figure S2. All energies are obtained from the single point calculation energy from the ONIOM-optimized structures with the full DFT method (M06-L) for the whole 240T cluster model.

Steps	Energy (hartrees)
NH_3-TiOOSi	-101672.668195
TS_1	-101672.657473
NH_3O_P	-101672.721651
Route A	
TS_2	-101672.658424
NH_2OH_P complex	-101672.721909
Route A + H_2O	
H_2O-NH_3O_P complex	-101749.160673
Water-assisted-TS_2	-101749.130771
H2O-NH2OH_P complex	-101749.158594
Route B	
TS_2a	-101672.697507
INT_2a	-101672.700008
TS_2b	-101672.679623

Following is the optimized coordinates of atoms in the QM region of the ONIOM model for all catalytic steps in the Fig. S2.

NH_3-TiOOSi

Si	11.327284000	0.530573000	9.122386000
Ti	13.742216000	1.007982000	11.339401000
Si	14.531110000	3.438901000	12.868822000
Si	14.505787000	-1.317856000	13.086399000
Si	16.122990000	0.658733000	9.234188000
O	11.933853000	0.738509000	10.663800000
O	14.670180000	1.120089000	9.770623000
O	13.635447000	2.775631000	11.715026000
O	14.856518000	0.136245000	12.447305000
Si	8.437788000	1.144838000	8.878982000
Si	12.452010000	1.271383000	6.343763000
Si	11.405144000	-2.581177000	9.108659000
Si	13.744115000	-3.451159000	10.991182000
Si	17.464474000	-1.348904000	13.087052000
Si	13.852895000	-0.569075000	15.922677000
Si	17.674706000	3.425171000	12.938157000
Si	18.463324000	1.103934000	11.203862000
O	17.370784000	1.309504000	10.026918000
Si	16.184794000	-2.567456000	9.172622000
Si	15.643350000	1.232365000	6.295449000
Si	14.512568000	6.523837000	12.951370000
Si	13.869956000	2.622906000	15.835171000
O	11.941324000	1.343122000	7.902435000
O	9.890532000	1.048064000	9.548574000
O	11.386827000	-1.005447000	8.779137000
O	16.092842000	2.971966000	12.840119000
O	14.342714000	4.982678000	12.566256000
O	13.869032000	3.166683000	14.324936000
O	15.970744000	-1.842465000	13.405939000
O	13.758842000	-2.483637000	12.283216000
O	13.681284000	-1.189746000	14.444962000
O	16.350608000	1.200717000	7.741019000
O	16.183114000	-0.954187000	9.238965000
O	13.898555000	1.028626000	15.842697000
O	14.041412000	1.181646000	6.352536000
O	18.621740000	2.541314000	11.948278000

O	17.848785000	-0.014596000	12.220987000
O	14.910969000	-3.182213000	9.931363000
O	12.614572000	-0.539803000	11.052743000
H	12.438815000	1.062574000	14.154301000
N	12.132624000	1.009824000	13.191735000
H	11.549835000	0.183853000	13.099396000
H	11.547792000	1.820703000	13.017328000

TS_1

Si	11.334396000	0.629263000	9.259500000
Ti	13.572263000	1.197456000	11.090966000
Si	14.608686000	3.439944000	12.909854000
Si	14.396888000	-1.228868000	13.055471000
Si	16.167891000	0.627789000	9.209048000
O	12.071306000	1.914747000	10.094505000
O	14.633716000	0.776274000	9.702010000
O	13.862546000	2.836951000	11.622791000
O	13.981478000	0.235237000	12.553451000
Si	8.433958000	1.132626000	8.877279000
Si	12.405462000	1.261021000	6.366981000
Si	11.413848000	-2.562151000	9.114809000
Si	13.752958000	-3.449210000	10.983175000
Si	17.588110000	-1.248570000	13.027563000
Si	13.863919000	-0.608715000	15.905307000
Si	17.710058000	3.429442000	12.934216000
Si	18.516787000	1.181877000	11.180929000
O	17.258847000	1.346969000	10.162583000
Si	16.211783000	-2.546716000	9.158202000
Si	15.632321000	1.237259000	6.306231000
Si	14.514735000	6.526268000	12.955882000
Si	13.866535000	2.590262000	15.835333000
O	11.688678000	1.255015000	7.803205000
O	9.816640000	0.913604000	9.628498000
O	11.577368000	-0.957896000	9.009824000
O	16.150207000	2.935644000	12.850043000
O	14.369731000	4.975511000	12.606314000
O	13.881016000	3.111488000	14.306268000
O	15.987844000	-1.238229000	13.041475000
O	13.812795000	-2.510465000	12.286476000
O	13.788281000	-1.427634000	14.518744000
O	16.378262000	1.252520000	7.751797000
O	16.395109000	-0.954798000	9.130620000
O	13.921245000	0.990832000	15.782506000
O	14.023778000	1.180322000	6.450892000
O	18.691464000	2.605147000	11.931146000
O	18.202522000	0.014750000	12.242576000
O	14.915362000	-3.112591000	9.930614000
O	11.730094000	0.585179000	11.115912000
N	10.984182000	-1.212452000	12.346618000
H	11.350856000	-2.154308000	12.299004000
H	10.037669000	-1.166846000	11.992115000
H	11.011011000	-0.864575000	13.295165000

NH_3O_P

Si	11.367066000	0.541652000	9.184844000
Ti	13.678992000	1.093816000	11.298688000
Si	14.547337000	3.451146000	12.892436000
Si	14.477186000	-1.343565000	13.068249000
Si	16.116902000	0.669061000	9.228045000
O	12.063434000	0.724968000	10.611613000
O	14.654175000	1.121655000	9.734184000
O	13.636249000	2.846429000	11.702302000
O	14.771788000	0.009291000	12.237668000
Si	8.450782000	1.139998000	8.881627000
Si	12.439626000	1.269823000	6.356763000
Si	11.404723000	-2.583638000	9.107949000
Si	13.739600000	-3.451121000	11.001702000
Si	17.464097000	-1.346069000	13.083784000
Si	13.855756000	-0.568147000	15.919959000
Si	17.680412000	3.422832000	12.937265000
Si	18.459536000	1.105537000	11.198677000
O	17.353761000	1.328142000	10.039413000
Si	16.188676000	-2.557360000	9.172301000
Si	15.643189000	1.232671000	6.300094000
Si	14.514278000	6.528989000	12.952880000
Si	13.872399000	2.607707000	15.836057000
O	11.878546000	1.334742000	7.891541000
O	9.888934000	1.019839000	9.588336000
O	11.421138000	-1.007775000	8.825977000
O	16.093949000	2.959135000	12.844948000
O	14.350315000	4.989790000	12.572670000
O	13.846284000	3.197691000	14.331030000
O	15.963027000	-1.820759000	13.381967000
O	13.685916000	-2.509196000	12.307249000
O	13.719532000	-1.207537000	14.455670000
O	16.374541000	1.206294000	7.735472000
O	16.208004000	-0.944636000	9.222392000
O	13.914547000	1.027471000	15.875089000
O	14.037551000	1.181366000	6.384856000
O	18.627778000	2.542509000	11.949710000
O	17.852143000	-0.009381000	12.221797000
O	14.909024000	-3.150813000	9.948809000
O	12.527338000	0.873141000	13.099307000
H	11.687117000	2.656320000	12.884624000
N	11.408329000	1.665949000	12.965867000
H	10.795289000	1.559772000	13.778025000
H	10.904327000	1.409827000	12.098276000

TS_2

Si	11.355587000	0.509219000	9.168962000
Ti	13.670678000	1.125544000	11.204999000
Si	14.560492000	3.441720000	12.879363000
Si	14.472963000	-1.312748000	13.042142000
Si	16.126742000	0.679556000	9.216185000
O	12.118475000	0.478536000	10.584564000
O	14.653551000	1.172578000	9.665233000
O	13.680989000	2.835330000	11.668343000
O	14.715399000	0.015973000	12.162873000
Si	8.455238000	1.140780000	8.885632000
Si	12.442667000	1.269752000	6.359812000
Si	11.397725000	-2.578692000	9.097373000
Si	13.737550000	-3.448061000	11.008499000
Si	17.476704000	-1.334597000	13.078982000
Si	13.854854000	-0.551848000	15.928726000
Si	17.688938000	3.423305000	12.933481000
Si	18.467449000	1.119620000	11.199748000

O	17.336526000	1.338728000	10.062558000
Si	16.189211000	-2.553266000	9.174197000
Si	15.650095000	1.231964000	6.302304000
Si	14.513868000	6.526581000	12.953701000
Si	13.870450000	2.613217000	15.838309000
O	11.898140000	1.333492000	7.906341000
O	9.901414000	1.021653000	9.593827000
O	11.343449000	-1.023478000	8.733406000
O	16.112388000	2.947085000	12.812945000
O	14.356827000	4.982666000	12.583750000
O	13.907058000	3.128507000	14.316672000
O	15.958177000	-1.765972000	13.365484000
O	13.671544000	-2.510880000	12.329376000
O	13.693689000	-1.136620000	14.425987000
O	16.412742000	1.198152000	7.723918000
O	16.198060000	-0.937147000	9.234183000
O	13.906338000	1.031239000	15.921917000
O	14.043746000	1.180434000	6.399804000
O	18.652756000	2.550860000	11.950155000
O	17.876780000	-0.004083000	12.223672000
O	14.912881000	-3.140785000	9.965215000
O	12.379487000	1.044619000	13.154640000
N	11.267429000	0.006419000	13.135923000
H	11.559772000	-0.755236000	13.745716000
H	11.135787000	-0.252957000	12.157554000
H	11.165683000	1.101439000	13.424376000

NH_2OH_P complex

Si	11.350097000	0.537791000	9.192191000
Ti	13.750788000	1.201576000	11.020027000
Si	14.550282000	3.438509000	12.887944000
Si	14.416917000	-1.276371000	13.027288000
Si	16.206624000	0.678152000	9.161866000
O	12.106116000	0.709054000	10.605344000
O	14.726574000	1.241578000	9.510251000
O	13.642935000	2.827094000	11.699917000
O	14.508215000	0.092952000	12.178310000
Si	8.446698000	1.140309000	8.884442000
Si	12.445638000	1.269033000	6.363444000
Si	11.403334000	-2.584681000	9.107566000
Si	13.734896000	-3.449933000	11.008505000
Si	17.505769000	-1.309144000	13.062308000
Si	13.854424000	-0.556971000	15.928977000
Si	17.685953000	3.426611000	12.934010000
Si	18.495957000	1.141564000	11.201051000
O	17.353269000	1.345671000	10.072742000
Si	16.188361000	-2.555976000	9.174229000
Si	15.667455000	1.230400000	6.306453000
Si	14.513906000	6.525780000	12.953582000
Si	13.870325000	2.613172000	15.841076000
O	11.882744000	1.329596000	7.900853000
O	9.885771000	1.013811000	9.592653000
O	11.427777000	-1.009728000	8.830423000
O	16.106166000	2.946462000	12.807504000
O	14.359831000	4.979527000	12.583468000
O	13.895782000	3.128749000	14.321859000
O	15.953283000	-1.613503000	13.255913000
O	13.700345000	-2.524260000	12.327963000
O	13.707455000	-1.149031000	14.440749000
O	16.524593000	1.183810000	7.678496000
O	16.203048000	-0.933181000	9.234132000
O	13.899069000	1.030787000	15.904708000
O	14.056906000	1.179214000	6.435510000
O	18.659612000	2.571635000	11.947137000
O	17.959853000	0.006938000	12.223944000
O	14.909238000	-3.135663000	9.959224000
H	11.034749000	-0.278381000	14.687903000
O	11.688227000	0.877749000	13.268326000
H	11.075163000	1.070720000	12.547891000
N	10.807185000	0.669934000	14.392110000
H	11.189691000	1.280038000	15.114979000

H_2O-NH_3O_P complex

Si	11.367595000	0.608368000	9.211390000
Ti	13.743562000	1.097107000	11.139485000
Si	14.571580000	3.435751000	12.905139000
Si	14.418808000	-1.146076000	12.984579000
Si	16.145536000	0.661885000	9.196954000
O	12.013139000	1.140709000	10.555503000
O	14.618784000	1.089121000	9.545469000
O	13.712490000	2.761142000	11.722396000
O	14.949593000	0.221855000	12.200029000
Si	8.437216000	1.134809000	8.871136000
Si	12.436177000	1.267303000	6.355129000
Si	11.410247000	-2.583232000	9.114865000
Si	13.767378000	-3.452709000	10.993072000
Si	17.469040000	-1.326661000	13.072614000
Si	13.862274000	-0.583228000	15.913863000
Si	17.693742000	3.425133000	12.934843000
Si	18.469740000	1.121616000	11.202295000
O	17.305014000	1.344143000	10.087007000
Si	16.190270000	-2.561681000	9.166970000
Si	15.654732000	1.231021000	6.308096000
Si	14.511781000	6.520379000	12.951838000
Si	13.867476000	2.602398000	15.840700000
O	11.797434000	1.310752000	7.846353000
O	9.846063000	0.948321000	9.588379000
O	11.532231000	-0.982383000	9.023719000
O	16.120588000	2.967348000	12.845493000
O	14.345430000	4.972644000	12.574969000
O	13.872881000	3.146295000	14.326357000
O	15.926484000	-1.683077000	13.297564000
O	13.773965000	-2.483983000	12.265162000
O	13.752441000	-1.263637000	14.466817000
O	16.452859000	1.196853000	7.712110000
O	16.219194000	-0.950401000	9.216781000
O	13.912101000	1.013799000	15.841417000
O	14.041493000	1.177713000	6.428144000
O	18.652125000	2.560557000	11.941659000
O	17.938579000	-0.009767000	12.224948000
O	14.901518000	-3.182052000	9.903309000
O	9.873783000	1.165113000	12.429744000
H	9.078763000	1.168396000	11.880690000
O	12.765109000	-0.198463000	12.525330000
H	10.520107000	1.625484000	11.866229000
N	11.571959000	-0.909615000	12.568786000

H	11.609129000	-1.675109000	11.881146000
H	10.769823000	-0.226603000	12.429734000
H	11.533514000	-1.331058000	13.503895000

Water-assisted-TS_2

Si	11.359467000	0.534339000	9.180514000
Ti	13.674596000	1.110943000	11.256375000
Si	14.544213000	3.447383000	12.888929000
Si	14.479648000	-1.336888000	13.057376000
Si	16.125503000	0.670441000	9.221136000
O	12.077367000	0.680136000	10.602563000
O	14.659874000	1.135881000	9.711813000
O	13.652245000	2.839877000	11.689874000
O	14.736428000	0.019338000	12.227702000
Si	8.450641000	1.140656000	8.882889000
Si	12.439955000	1.269734000	6.357940000
Si	11.402355000	-2.582042000	9.105843000
Si	13.736429000	-3.450802000	11.003153000
Si	17.469368000	-1.341809000	13.082430000
Si	13.856508000	-0.561707000	15.922612000
Si	17.679513000	3.423584000	12.937633000
Si	18.462577000	1.110160000	11.199129000
O	17.353613000	1.329243000	10.042860000
Si	16.188617000	-2.557113000	9.173274000
Si	15.645018000	1.232496000	6.300210000
Si	14.513865000	6.528078000	12.953176000
Si	13.871397000	2.610480000	15.837412000
O	11.884321000	1.333631000	7.894179000
O	9.891834000	1.026663000	9.583535000
O	11.408427000	-1.011087000	8.805156000
O	16.095164000	2.958932000	12.844207000
O	14.350154000	4.987293000	12.577953000
O	13.857327000	3.176713000	14.328855000
O	15.962810000	-1.800935000	13.381757000
O	13.684538000	-2.511642000	12.316247000
O	13.705757000	-1.179104000	14.443436000
O	16.389316000	1.203621000	7.730158000
O	16.205859000	-0.943459000	9.226896000
O	13.908055000	1.028035000	15.893282000
O	14.039998000	1.181478000	6.391488000
O	18.630479000	2.544708000	11.950511000
O	17.857043000	-0.007184000	12.222197000
O	14.911789000	-3.147700000	9.957061000
O	10.684969000	-0.606174000	13.614320000
H	10.641970000	-0.894496000	14.531304000
O	12.429892000	0.882170000	13.129190000
H	11.745290000	-0.218568000	13.414381000
N	11.216740000	1.627131000	13.067237000
H	11.029280000	1.857999000	12.087674000
H	11.356719000	2.485346000	13.598790000
H	10.513585000	0.573702000	13.496042000

H_2O-NH_2OH_P complex

Si	11.343934000	0.513221000	9.161622000
Ti	13.720299000	1.142386000	11.145800000
Si	14.541714000	3.441794000	12.876383000
Si	14.459146000	-1.310741000	13.038354000
Si	16.180050000	0.677893000	9.193236000
O	12.160575000	0.570909000	10.546025000
O	14.731654000	1.233729000	9.652135000
O	13.610031000	2.827432000	11.706679000
O	14.675031000	0.068665000	12.225999000
Si	8.453917000	1.141495000	8.886981000
Si	12.442221000	1.269995000	6.360060000
Si	11.393952000	-2.574675000	9.100723000
Si	13.734762000	-3.450819000	10.997743000
Si	17.479056000	-1.332610000	13.075507000
Si	13.854270000	-0.567102000	15.925362000
Si	17.680811000	3.424825000	12.935017000
Si	18.482327000	1.118387000	11.205018000
O	17.396309000	1.325232000	10.028304000
Si	16.188558000	-2.556540000	9.173817000
Si	15.653933000	1.231342000	6.300909000
Si	14.513475000	6.527581000	12.953670000
Si	13.863506000	2.620243000	15.841548000
O	11.891652000	1.338122000	7.898128000
O	9.904008000	1.044491000	9.588373000
O	11.371317000	-1.016685000	8.738269000
O	16.096147000	2.952719000	12.813287000
O	14.352352000	4.982570000	12.583341000
O	13.879172000	3.115083000	14.311580000
O	15.955218000	-1.750830000	13.333372000
O	13.668029000	-2.495224000	12.306130000
O	13.709170000	-1.154189000	14.433969000
O	16.451478000	1.191521000	7.703287000
O	16.187009000	-0.936888000	9.238990000
O	13.893601000	1.027641000	15.834402000
O	14.048363000	1.180982000	6.414696000
O	18.640925000	2.552986000	11.951076000
O	17.875877000	0.000593000	12.222151000
O	14.916654000	-3.146824000	9.961915000
O	10.407474000	-1.268955000	11.777863000
H	10.454573000	-2.103976000	12.253182000
O	12.206649000	0.802154000	13.062104000
H	11.294626000	-0.899146000	11.881912000
N	10.961554000	1.552092000	13.048406000
H	10.323648000	0.880693000	12.615762000
H	11.126790000	2.255297000	12.326860000
H	12.564759000	0.981900000	13.941815000

TS_2a

Si	11.335257000	0.621900000	9.157830000
Ti	13.681370000	1.027982000	11.184836000
Si	14.594679000	3.421248000	12.916098000
Si	14.471547000	-1.332450000	13.031681000
Si	16.072987000	0.652551000	9.205512000
O	12.003131000	1.558220000	10.323887000
O	14.509436000	0.945361000	9.525980000
O	13.835630000	2.705916000	11.701161000
O	14.809291000	-0.116258000	12.015043000
Si	8.431262000	1.129628000	8.878590000
Si	12.434394000	1.266917000	6.340280000
Si	11.419148000	-2.580199000	9.130218000
Si	13.735025000	-3.444913000	11.027287000
Si	17.461759000	-1.344380000	13.085888000
Si	13.857334000	-0.546242000	15.938396000

Si	17.705421000	3.422384000	12.935647000
Si	18.430091000	1.111981000	11.189471000
O	17.208376000	1.361451000	10.133307000
Si	16.195567000	-2.548788000	9.172674000
Si	15.648326000	1.233999000	6.307965000
Si	14.511616000	6.517211000	12.953968000
Si	13.869047000	2.601639000	15.857144000
O	11.737108000	1.300341000	7.790959000
O	9.833251000	0.893665000	9.614114000
O	11.621080000	-0.953039000	9.116708000
O	16.139190000	2.956115000	12.869775000
O	14.337536000	4.957892000	12.602063000
O	13.870150000	3.062881000	14.312708000
O	15.953727000	-1.800280000	13.399055000
O	13.666421000	-2.557373000	12.371828000
O	13.740177000	-1.037266000	14.413771000
O	16.407876000	1.221646000	7.734264000
O	16.287674000	-0.944524000	9.187943000
O	13.895697000	1.035667000	15.989176000
O	14.034964000	1.180048000	6.419520000
O	18.652446000	2.544179000	11.941909000
O	17.869117000	-0.010678000	12.229618000
O	14.904770000	-3.103818000	9.975599000
H	10.416252000	0.338723000	12.726167000
O	12.362447000	0.305298000	12.443950000
H	11.356931000	1.586311000	11.158411000
N	11.149559000	1.023292000	12.550331000
H	11.228354000	1.606915000	13.383747000

INT_2a

Si	11.339003000	0.600086000	9.163127000
Ti	13.881887000	1.038460000	11.054082000
Si	14.591436000	3.387160000	12.924043000
Si	14.409972000	-1.160760000	12.931199000
Si	16.177207000	0.662603000	9.157099000
O	11.995331000	1.312923000	10.501678000
O	14.613874000	1.085143000	9.401372000
O	13.804126000	2.678900000	11.713491000
O	15.076767000	0.010830000	11.900200000
Si	8.428588000	1.133903000	8.877944000
Si	12.452926000	1.269440000	6.344338000
Si	11.417928000	-2.588340000	9.125855000
Si	13.746081000	-3.440822000	11.049232000
Si	17.452191000	-1.330418000	13.085098000
Si	13.860928000	-0.508821000	15.968282000
Si	17.710965000	3.423604000	12.932084000
Si	18.462321000	1.116734000	11.207508000
O	17.275169000	1.367065000	10.108547000
Si	16.191704000	-2.551177000	9.171966000
Si	15.670124000	1.233021000	6.308688000
Si	14.510180000	6.509869000	12.957642000
Si	13.871296000	2.579356000	15.887035000
O	11.842034000	1.325661000	7.852743000
O	9.847209000	0.932129000	9.589035000
O	11.574507000	-0.970221000	9.050690000
O	16.145899000	2.954676000	12.835953000
O	14.327104000	4.934744000	12.647691000
O	13.911835000	2.907817000	14.308042000
O	15.908589000	-1.670209000	13.372992000
O	13.807056000	-2.601880000	12.414708000
O	13.757162000	-0.798556000	14.379920000
O	16.514390000	1.212159000	7.686439000
O	16.274727000	-0.938863000	9.175239000
O	13.873055000	1.047053000	16.207637000
O	14.054936000	1.180364000	6.422187000
O	18.671003000	2.558459000	11.941674000
O	17.915883000	-0.003240000	12.235982000
O	14.891390000	-3.097639000	9.959436000
H	11.152790000	-1.201991000	12.412537000
O	12.864899000	-0.332496000	12.106108000
H	11.435162000	1.036486000	11.283123000
N	11.517607000	-0.255158000	12.532241000
H	11.583556000	-0.108633000	13.541471000

TS_2b

Si	11.340235000	0.590538000	9.138850000
Ti	13.699875000	1.038056000	11.338762000
Si	14.591767000	3.436623000	12.869736000
Si	14.474560000	-1.294807000	13.062062000
Si	16.072179000	0.639559000	9.241946000
O	11.936453000	1.174846000	10.539775000
O	14.529725000	0.848458000	9.705122000
O	13.933783000	2.789815000	11.553179000
O	14.848682000	0.146998000	12.395915000
Si	8.424935000	1.134740000	8.873652000
Si	12.445741000	1.271240000	6.336906000
Si	11.414145000	-2.589131000	9.122529000
Si	13.747898000	-3.450242000	10.993438000
Si	17.466295000	-1.343010000	13.082703000
Si	13.856033000	-0.567358000	15.932502000
Si	17.702082000	3.424453000	12.938349000
Si	18.439672000	1.115721000	11.193467000
O	17.233238000	1.359602000	10.119342000
Si	16.198424000	-2.556015000	9.166590000
Si	15.639334000	1.235162000	6.300356000
Si	14.511503000	6.523030000	12.953642000
Si	13.868710000	2.620947000	15.829824000
O	11.866926000	1.337276000	7.852617000
O	9.849270000	0.940461000	9.550178000
O	11.557034000	-0.980556000	9.009707000
O	16.138390000	2.970980000	12.885803000
O	14.332744000	4.975591000	12.589863000
O	13.875223000	3.113319000	14.291446000
O	15.957539000	-1.801433000	13.374901000
O	13.760237000	-2.493960000	12.280155000
O	13.706934000	-1.166352000	14.453784000
O	16.321119000	1.229573000	7.764529000
O	16.298352000	-0.953562000	9.187166000
O	13.891400000	1.029479000	15.862178000
O	14.035630000	1.182726000	6.367349000
O	18.651840000	2.546106000	11.944882000
O	17.874693000	-0.014401000	12.221070000
O	14.907614000	-3.141096000	9.930972000
H	11.410890000	1.444197000	13.166652000
O	12.235596000	-0.207170000	12.374604000
H	11.639896000	0.476395000	11.274759000

N	12.331583000	1.010882000	13.111408000
H	12.635186000	0.772633000	14.050842000

Following is the fixed coordinates of atoms in the QM and MM regions of the ONIOM model.

Si	6.150000000	0.552000000	10.850000000
Si	1.427000000	0.542000000	10.900000000
Si	3.732000000	1.173000000	8.991000000
O	7.460000000	1.063000000	10.115000000
O	6.175000000	1.168000000	12.327000000
O	1.940000000	1.216000000	12.237000000
O	2.301000000	1.077000000	9.685000000
O	4.875000000	1.100000000	10.091000000
O	8.331000000	2.539000000	8.169000000
O	3.776000000	2.583000000	8.249000000
O	3.884000000	0.014000000	7.920000000
Si	3.849000000	2.590000000	4.209000000
Si	4.494000000	3.438000000	7.108000000
Si	7.597000000	3.445000000	7.090000000
Si	8.601000000	2.594000000	4.256000000
Si	6.266000000	3.448000000	2.418000000
O	3.834000000	3.088000000	5.717000000
O	6.047000000	3.092000000	7.077000000
O	8.189000000	3.212000000	5.652000000
O	7.670000000	3.140000000	3.086000000
O	5.110000000	3.172000000	3.450000000
O	3.910000000	1.015000000	4.194000000
O	8.473000000	1.033000000	4.324000000
O	10.091000000	3.041000000	3.911000000
Si	11.565000000	11.074000000	4.496000000
Si	13.872000000	10.501000000	2.533000000
Si	14.434000000	11.169000000	12.965000000
Si	17.576000000	11.203000000	13.026000000
Si	16.290000000	11.123000000	4.392000000
Si	11.560000000	6.517000000	4.379000000
Si	13.860000000	7.359000000	2.482000000
Si	17.608000000	6.505000000	12.984000000
Si	16.277000000	6.502000000	4.274000000
O	12.562000000	11.012000000	3.268000000
O	16.004000000	11.128000000	12.996000000
O	15.147000000	11.050000000	3.292000000
O	12.530000000	6.843000000	3.174000000
O	16.058000000	6.857000000	12.998000000
O	15.121000000	6.778000000	3.241000000
O	13.921000000	8.935000000	2.497000000
O	11.691000000	12.489000000	5.214000000
O	11.841000000	9.916000000	5.535000000
O	11.973000000	7.335000000	5.673000000
O	16.246000000	12.532000000	5.134000000
O	16.138000000	9.963000000	5.463000000
O	16.116000000	7.380000000	5.607000000
Si	18.468000000	8.825000000	11.188000000
Si	16.161000000	9.398000000	9.225000000
Si	15.599000000	8.730000000	6.274000000
Si	12.457000000	8.696000000	6.334000000
Si	11.438000000	9.408000000	9.174000000
Si	13.743000000	8.776000000	11.084000000
Si	18.473000000	13.382000000	11.070000000
Si	16.173000000	12.540000000	9.174000000
Si	15.528000000	13.388000000	6.275000000
Si	12.425000000	13.394000000	6.293000000
Si	11.421000000	12.544000000	9.127000000
Si	13.756000000	13.397000000	10.965000000
O	17.471000000	8.887000000	9.960000000
O	16.186000000	8.781000000	7.747000000
O	14.029000000	8.771000000	6.305000000
O	11.951000000	8.734000000	7.837000000
O	12.312000000	8.873000000	10.389000000
O	14.886000000	8.849000000	9.984000000
O	17.503000000	13.056000000	9.866000000
O	16.188000000	13.038000000	7.666000000
O	13.975000000	13.042000000	6.306000000
O	11.833000000	13.161000000	7.731000000
O	12.352000000	13.090000000	10.297000000
O	14.912000000	13.121000000	9.933000000
O	16.112000000	10.964000000	9.189000000
O	11.549000000	10.982000000	9.059000000
O	18.342000000	7.410000000	11.906000000
O	18.192000000	9.983000000	12.227000000
O	18.060000000	12.564000000	12.365000000
O	13.787000000	7.367000000	11.825000000
O	13.895000000	9.936000000	12.154000000
O	13.917000000	12.519000000	12.299000000
O	9.931000000	9.104000000	9.473000000
O	9.931000000	12.990000000	9.473000000
Si	11.560000000	3.433000000	4.379000000
Si	13.860000000	2.590000000	2.482000000
Si	16.277000000	3.448000000	4.274000000
O	12.530000000	3.106000000	3.174000000
O	15.121000000	3.172000000	3.241000000
O	13.921000000	1.015000000	2.497000000
O	11.841000000	0.034000000	5.535000000
O	11.973000000	2.615000000	5.673000000
O	16.116000000	2.569000000	5.607000000
Si	8.457000000	8.825000000	8.887000000
Si	6.150000000	9.398000000	10.850000000
Si	1.427000000	9.408000000	10.900000000
Si	3.732000000	8.776000000	8.991000000
Si	8.462000000	13.382000000	9.004000000
Si	6.162000000	12.540000000	10.901000000
Si	1.410000000	12.544000000	10.947000000
Si	3.745000000	13.397000000	9.109000000
O	7.460000000	8.887000000	10.115000000
O	6.175000000	8.781000000	12.327000000
O	1.940000000	8.734000000	12.237000000
O	2.301000000	8.873000000	9.685000000
O	4.875000000	8.849000000	10.091000000
O	7.492000000	13.056000000	10.209000000
O	6.177000000	13.038000000	12.409000000
O	1.822000000	13.161000000	12.343000000
O	2.341000000	13.090000000	9.778000000
O	4.901000000	13.121000000	10.142000000
O	6.101000000	10.964000000	10.886000000
O	1.538000000	10.982000000	11.016000000
O	8.331000000	7.410000000	8.169000000

O	8.181000000	9.983000000	7.848000000
O	8.049000000	12.564000000	7.710000000
O	3.776000000	7.367000000	8.249000000
O	3.884000000	9.936000000	7.920000000
O	3.906000000	12.519000000	7.776000000
Si	3.861000000	10.501000000	4.158000000
Si	4.423000000	11.169000000	7.109000000
Si	7.565000000	11.203000000	7.049000000
Si	8.584000000	10.491000000	4.209000000
Si	6.279000000	11.123000000	2.299000000
Si	3.849000000	7.359000000	4.209000000
Si	4.494000000	6.511000000	7.108000000
Si	7.597000000	6.505000000	7.090000000
Si	8.601000000	7.355000000	4.256000000
Si	6.266000000	6.502000000	2.418000000
O	3.836000000	11.118000000	5.636000000
O	5.993000000	11.128000000	7.078000000
O	8.071000000	11.165000000	5.546000000
O	7.710000000	11.026000000	2.994000000
O	5.136000000	11.050000000	3.399000000
O	3.834000000	6.861000000	5.717000000
O	6.047000000	6.857000000	7.077000000
O	8.189000000	6.738000000	5.652000000
O	7.670000000	6.809000000	3.086000000
O	5.110000000	6.778000000	3.450000000
O	3.910000000	8.935000000	4.194000000
O	8.473000000	8.917000000	4.324000000
O	10.091000000	10.795000000	3.911000000
O	10.091000000	6.909000000	3.911000000
O	6.239000000	4.975000000	1.957000000
O	4.239000000	4.975000000	7.466000000
O	7.839000000	4.975000000	7.509000000
O	11.629000000	4.975000000	4.738000000
O	16.250000000	4.975000000	4.735000000
O	17.850000000	4.975000000	12.565000000
Si	8.457000000	1.124000000	22.270000000
Si	6.150000000	0.552000000	24.233000000
Si	5.588000000	1.219000000	13.801000000
Si	2.446000000	1.253000000	13.740000000
Si	3.732000000	1.173000000	22.374000000
O	7.460000000	1.063000000	23.498000000
O	4.018000000	1.178000000	13.770000000
O	4.875000000	1.100000000	23.474000000
O	8.331000000	2.539000000	21.552000000
O	3.776000000	2.583000000	21.632000000
O	3.884000000	0.014000000	21.303000000
Si	1.549000000	3.433000000	15.696000000
Si	3.849000000	2.590000000	17.592000000
Si	4.494000000	3.438000000	20.491000000
Si	7.597000000	3.445000000	20.473000000
Si	8.601000000	2.594000000	17.639000000
Si	6.266000000	3.448000000	15.801000000
O	2.519000000	3.106000000	16.900000000
O	3.834000000	3.088000000	19.100000000
O	6.047000000	3.092000000	20.460000000
O	8.189000000	3.212000000	19.035000000
O	7.670000000	3.140000000	16.469000000
O	5.110000000	3.172000000	16.833000000
O	3.910000000	1.015000000	17.577000000
O	8.473000000	1.033000000	17.707000000
O	1.830000000	0.034000000	14.539000000
O	1.962000000	2.615000000	14.401000000
O	6.105000000	2.569000000	14.467000000
O	10.091000000	3.041000000	17.294000000
Si	11.565000000	11.074000000	17.879000000
Si	13.872000000	10.501000000	15.916000000
Si	18.595000000	10.491000000	15.866000000
Si	16.290000000	11.123000000	17.775000000
Si	11.560000000	6.517000000	17.762000000
Si	13.860000000	7.359000000	15.865000000
Si	18.612000000	7.355000000	15.819000000
Si	16.277000000	6.502000000	17.657000000
O	12.562000000	11.012000000	16.651000000
O	13.847000000	11.118000000	14.439000000
O	18.082000000	11.165000000	14.529000000
O	17.721000000	11.026000000	17.081000000
O	15.147000000	11.050000000	16.675000000
O	12.530000000	6.843000000	16.557000000
O	13.845000000	6.861000000	14.357000000
O	18.200000000	6.738000000	14.423000000
O	17.681000000	6.809000000	16.988000000
O	15.121000000	6.778000000	16.624000000
O	13.921000000	8.935000000	15.880000000
O	18.484000000	8.917000000	15.750000000
O	11.691000000	12.489000000	18.597000000
O	11.841000000	9.916000000	18.918000000
O	11.973000000	7.335000000	19.056000000
O	16.246000000	12.532000000	18.517000000
O	16.138000000	9.963000000	18.846000000
O	16.116000000	7.380000000	18.990000000
Si	16.161000000	9.398000000	22.608000000
Si	15.599000000	8.730000000	19.657000000
Si	12.457000000	8.696000000	19.717000000
Si	11.438000000	9.408000000	22.557000000
Si	13.743000000	8.776000000	24.467000000
Si	16.173000000	12.540000000	22.557000000
Si	15.528000000	13.388000000	19.658000000
Si	12.425000000	13.394000000	19.676000000
Si	11.421000000	12.544000000	22.510000000
Si	13.756000000	13.397000000	24.348000000
O	16.186000000	8.781000000	21.130000000
O	14.029000000	8.771000000	19.688000000
O	11.951000000	8.734000000	21.220000000
O	12.312000000	8.873000000	23.772000000
O	14.886000000	8.849000000	23.367000000
O	16.188000000	13.038000000	21.049000000
O	13.975000000	13.042000000	19.689000000
O	11.833000000	13.161000000	21.114000000
O	12.352000000	13.090000000	23.680000000
O	14.912000000	13.121000000	23.316000000
O	16.112000000	10.964000000	22.572000000
O	11.549000000	10.982000000	22.442000000
O	9.931000000	9.104000000	22.856000000
O	9.931000000	12.990000000	22.856000000
Si	11.560000000	3.433000000	17.762000000
Si	18.612000000	2.594000000	15.819000000

	Si	16.277000000	3.448000000	17.657000000
	O	12.530000000	3.106000000	16.557000000
	O	18.200000000	3.212000000	14.423000000
	O	17.681000000	3.140000000	16.988000000
5	O	15.121000000	3.172000000	16.624000000
	O	18.484000000	1.033000000	15.750000000
	O	11.841000000	0.034000000	18.918000000
	O	11.973000000	2.615000000	19.056000000
	O	16.116000000	2.569000000	18.990000000
10	Si	16.161000000	0.552000000	22.608000000
	Si	15.599000000	1.219000000	19.657000000
	Si	12.457000000	1.253000000	19.717000000
	Si	11.438000000	0.542000000	22.557000000
	Si	13.743000000	1.173000000	24.467000000
15	O	16.186000000	1.168000000	21.130000000
	O	14.029000000	1.178000000	19.688000000
	O	11.951000000	1.216000000	21.220000000
	O	12.312000000	1.077000000	23.772000000
	O	14.886000000	1.100000000	23.367000000
20	O	9.931000000	0.846000000	22.856000000
	Si	8.457000000	8.825000000	22.270000000
	Si	6.150000000	9.398000000	24.233000000
	Si	5.588000000	8.730000000	13.801000000
	Si	2.446000000	8.696000000	13.740000000
25	Si	3.732000000	8.776000000	22.374000000
	Si	8.462000000	13.382000000	22.387000000
	Si	6.162000000	12.540000000	24.284000000
	Si	5.517000000	13.388000000	13.799000000
	Si	2.414000000	13.394000000	13.782000000
30	Si	3.745000000	13.397000000	22.492000000
	O	7.460000000	8.887000000	23.498000000
	O	4.018000000	8.771000000	13.770000000
	O	4.875000000	8.849000000	23.474000000
	O	7.492000000	13.056000000	23.592000000
35	O	3.964000000	13.042000000	13.768000000
	O	4.901000000	13.121000000	23.525000000
	O	6.101000000	10.964000000	24.269000000
	O	8.331000000	7.410000000	21.552000000
	O	8.181000000	9.983000000	21.231000000
40	O	8.049000000	12.564000000	21.093000000
	O	3.776000000	7.367000000	21.632000000
	O	3.884000000	9.936000000	21.303000000
	O	3.906000000	12.519000000	21.159000000
	Si	1.554000000	11.074000000	15.578000000
45	Si	3.861000000	10.501000000	17.541000000
	Si	4.423000000	11.169000000	20.492000000
	Si	7.565000000	11.203000000	20.432000000
	Si	8.584000000	10.491000000	17.592000000
	Si	6.279000000	11.123000000	15.682000000
50	Si	1.549000000	6.517000000	15.696000000
	Si	3.849000000	7.359000000	17.592000000
	Si	4.494000000	6.511000000	20.491000000
	Si	7.597000000	6.505000000	20.473000000
	Si	8.601000000	7.355000000	17.639000000
55	Si	6.266000000	6.502000000	15.801000000
	O	2.551000000	11.012000000	16.806000000
	O	3.836000000	11.118000000	19.019000000
	O	5.993000000	11.128000000	20.461000000
	O	8.071000000	11.165000000	18.929000000
60	O	7.710000000	11.026000000	16.377000000
	O	5.136000000	11.050000000	16.782000000
	O	2.519000000	6.843000000	16.900000000
	O	3.834000000	6.861000000	19.100000000
	O	6.047000000	6.857000000	20.460000000
65	O	8.189000000	6.738000000	19.035000000
	O	7.670000000	6.809000000	16.469000000
	O	5.110000000	6.778000000	16.833000000
	O	3.910000000	8.935000000	17.577000000
	O	8.473000000	8.917000000	17.707000000
70	O	1.680000000	12.489000000	14.860000000
	O	1.830000000	9.916000000	14.539000000
	O	1.962000000	7.335000000	14.401000000
	O	6.235000000	12.532000000	14.941000000
	O	6.127000000	9.963000000	14.612000000
75	O	6.105000000	7.380000000	14.467000000
	O	10.091000000	10.795000000	17.294000000
	O	10.091000000	6.909000000	17.294000000
	O	1.618000000	4.975000000	15.337000000
	O	6.239000000	4.975000000	15.340000000
80	O	4.239000000	4.975000000	20.849000000
	O	7.839000000	4.975000000	20.892000000
	O	11.629000000	4.975000000	18.121000000
	O	16.250000000	4.975000000	18.118000000
	Si	8.462000000	-3.433000000	9.004000000
85	Si	6.162000000	-2.590000000	10.901000000
	Si	1.410000000	-2.594000000	10.947000000
	Si	3.745000000	-3.448000000	9.109000000
	O	7.492000000	-3.106000000	10.209000000
	O	6.177000000	-3.088000000	12.409000000
90	O	1.822000000	-3.212000000	12.343000000
	O	2.341000000	-3.140000000	9.778000000
	O	4.901000000	-3.172000000	10.142000000
	O	6.101000000	-1.015000000	10.886000000
	O	1.538000000	-1.033000000	11.016000000
95	O	8.181000000	-0.034000000	7.848000000
	O	8.049000000	-2.615000000	7.710000000
	O	3.906000000	-2.569000000	7.776000000
	Si	3.861000000	-0.552000000	4.158000000
	Si	4.423000000	-1.219000000	7.109000000
100	Si	7.565000000	-1.253000000	7.049000000
	Si	8.584000000	-0.542000000	4.209000000
	Si	6.279000000	-1.173000000	2.299000000
	O	3.836000000	-1.168000000	5.636000000
	O	5.993000000	-1.178000000	7.078000000
105	O	8.071000000	-1.216000000	5.546000000
	O	7.710000000	-1.077000000	2.994000000
	O	5.136000000	-1.100000000	3.399000000
	O	10.091000000	-0.846000000	3.911000000
	Si	11.565000000	-8.825000000	4.496000000
110	Si	13.872000000	-9.398000000	2.533000000
	Si	14.434000000	-8.730000000	12.965000000
	Si	17.576000000	-8.696000000	13.026000000
	Si	16.290000000	-8.776000000	4.392000000
	Si	11.560000000	-13.382000000	4.379000000
115	Si	13.860000000	-12.540000000	2.482000000
	Si	14.505000000	-13.388000000	12.967000000

Si	17.608000000	-13.394000000	12.984000000
Si	16.277000000	-13.397000000	4.274000000
O	12.562000000	-8.887000000	3.268000000
O	16.004000000	-8.771000000	12.996000000
O	15.147000000	-8.849000000	3.292000000
O	12.530000000	-13.056000000	3.174000000
O	16.058000000	-13.042000000	12.998000000
O	15.121000000	-13.121000000	3.241000000
O	13.921000000	-10.964000000	2.497000000
O	11.691000000	-7.410000000	5.214000000
O	11.841000000	-9.983000000	5.535000000
O	11.973000000	-12.564000000	5.673000000
O	16.246000000	-7.367000000	5.134000000
O	16.138000000	-9.936000000	5.463000000
O	16.116000000	-12.519000000	5.607000000
Si	18.468000000	-11.074000000	11.188000000
Si	16.161000000	-10.501000000	9.225000000
Si	15.599000000	-11.169000000	6.274000000
Si	12.457000000	-11.203000000	6.334000000
Si	11.438000000	-10.491000000	9.174000000
Si	13.743000000	-11.123000000	11.084000000
Si	18.473000000	-6.517000000	11.070000000
Si	16.173000000	-7.359000000	9.174000000
Si	15.528000000	-6.511000000	6.275000000
Si	12.425000000	-6.505000000	6.293000000
Si	11.421000000	-7.355000000	9.127000000
Si	13.756000000	-6.502000000	10.965000000
O	17.471000000	-11.012000000	9.960000000
O	16.186000000	-11.118000000	7.747000000
O	14.029000000	-11.128000000	6.305000000
O	11.951000000	-11.165000000	7.837000000
O	12.312000000	-11.026000000	10.389000000
O	14.886000000	-11.050000000	9.984000000
O	17.503000000	-6.843000000	9.866000000
O	16.188000000	-6.861000000	7.666000000
O	13.975000000	-6.857000000	6.306000000
O	11.833000000	-6.738000000	7.731000000
O	12.352000000	-6.809000000	10.297000000
O	14.912000000	-6.778000000	9.933000000
O	16.112000000	-8.935000000	9.189000000
O	11.549000000	-8.917000000	9.059000000
O	18.342000000	-12.489000000	11.906000000
O	18.192000000	-9.916000000	12.227000000
O	18.060000000	-7.335000000	12.365000000
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O	9.931000000	-6.909000000	9.473000000
Si	11.565000000	-1.124000000	4.496000000
Si	13.872000000	-0.552000000	2.533000000
Si	16.290000000	-1.173000000	4.392000000
O	12.562000000	-1.063000000	3.268000000
O	15.147000000	-1.100000000	3.292000000
O	11.691000000	-2.539000000	5.214000000
O	16.246000000	-2.583000000	5.134000000
O	16.138000000	-0.014000000	5.463000000
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Si	15.528000000	-3.438000000	6.275000000
Si	12.425000000	-3.445000000	6.293000000
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O	12.352000000	-3.140000000	10.297000000
O	18.060000000	-2.615000000	12.365000000
O	9.931000000	-3.041000000	9.473000000
Si	8.457000000	-11.074000000	8.887000000
Si	6.150000000	-10.501000000	10.850000000
Si	1.427000000	-10.491000000	10.900000000
Si	3.732000000	-11.123000000	8.991000000
Si	8.462000000	-6.517000000	9.004000000
Si	6.162000000	-7.359000000	10.901000000
Si	1.410000000	-7.355000000	10.947000000
Si	3.745000000	-6.502000000	9.109000000
O	7.460000000	-11.012000000	10.115000000
O	6.175000000	-11.118000000	12.327000000
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O	4.901000000	-6.778000000	10.142000000
O	6.101000000	-8.935000000	10.886000000
O	1.538000000	-8.917000000	11.016000000
O	8.331000000	-12.489000000	8.169000000
O	8.181000000	-9.916000000	7.848000000
O	8.049000000	-7.335000000	7.710000000
O	3.776000000	-12.532000000	8.249000000
O	3.884000000	-9.963000000	7.920000000
O	3.906000000	-7.381000000	7.776000000
Si	3.861000000	-9.398000000	4.158000000
Si	4.423000000	-8.730000000	7.109000000
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Si	3.849000000	-12.540000000	4.209000000
Si	4.494000000	-13.388000000	7.108000000
Si	7.597000000	-13.394000000	7.090000000
Si	8.601000000	-12.544000000	4.256000000
Si	6.266000000	-13.397000000	2.418000000
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Si	8.462000000	-3.433000000	22.387000000
Si	6.162000000	-2.590000000	24.284000000
Si	5.517000000	-3.438000000	13.799000000
Si	2.414000000	-3.445000000	13.782000000
Si	3.745000000	-3.448000000	22.492000000
O	7.492000000	-3.106000000	23.592000000
O	3.964000000	-3.092000000	13.768000000
O	4.901000000	-3.172000000	23.525000000
O	6.101000000	-1.015000000	24.269000000
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O	14.912000000	-6.778000000	23.316000000
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Si	6.150000000	-10.501000000	24.233000000
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Si	3.732000000	-11.123000000	22.374000000
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20	Si	8.584000000	-9.408000000	17.592000000
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