

Supporting Information

DFT Investigation of the Impact of Inner-Sphere Water Molecules on RE Nitrate Binding to Internal Pore and External Surface of MCM-22

Tamalika Ash*,^{1,2} Yong Han,^{1,3} James W. Evans^{1,3} and Theresa L. Windus*,^{1,4}

¹Ames National Laboratory, U.S. Department of Energy, Ames, Iowa 50011, USA

²Department of Aerospace Engineering, Iowa State University, Ames, Iowa 50011, USA

³Department of Physics & Astronomy, Iowa State University, Ames, Iowa 50011, USA

⁴Department of Chemistry, Iowa State University, Ames, Iowa 50011, USA

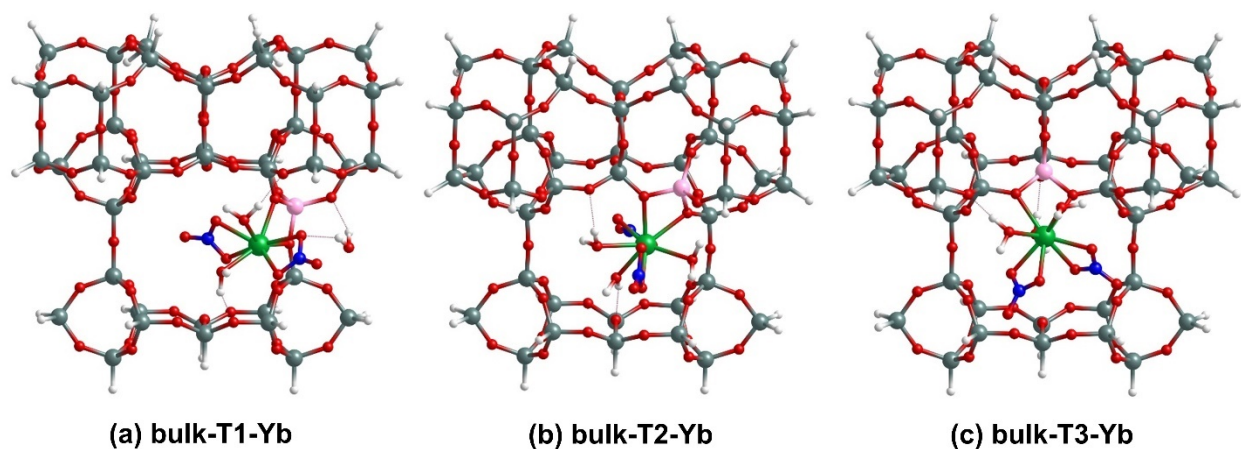


Figure S1. Lowest energy optimized geometries for $[\text{Yb}(\text{NO}_3)_3(\text{H}_2\text{O})_3]$ binding to T1, T2 and T3 BASs at internal pore using cluster models.

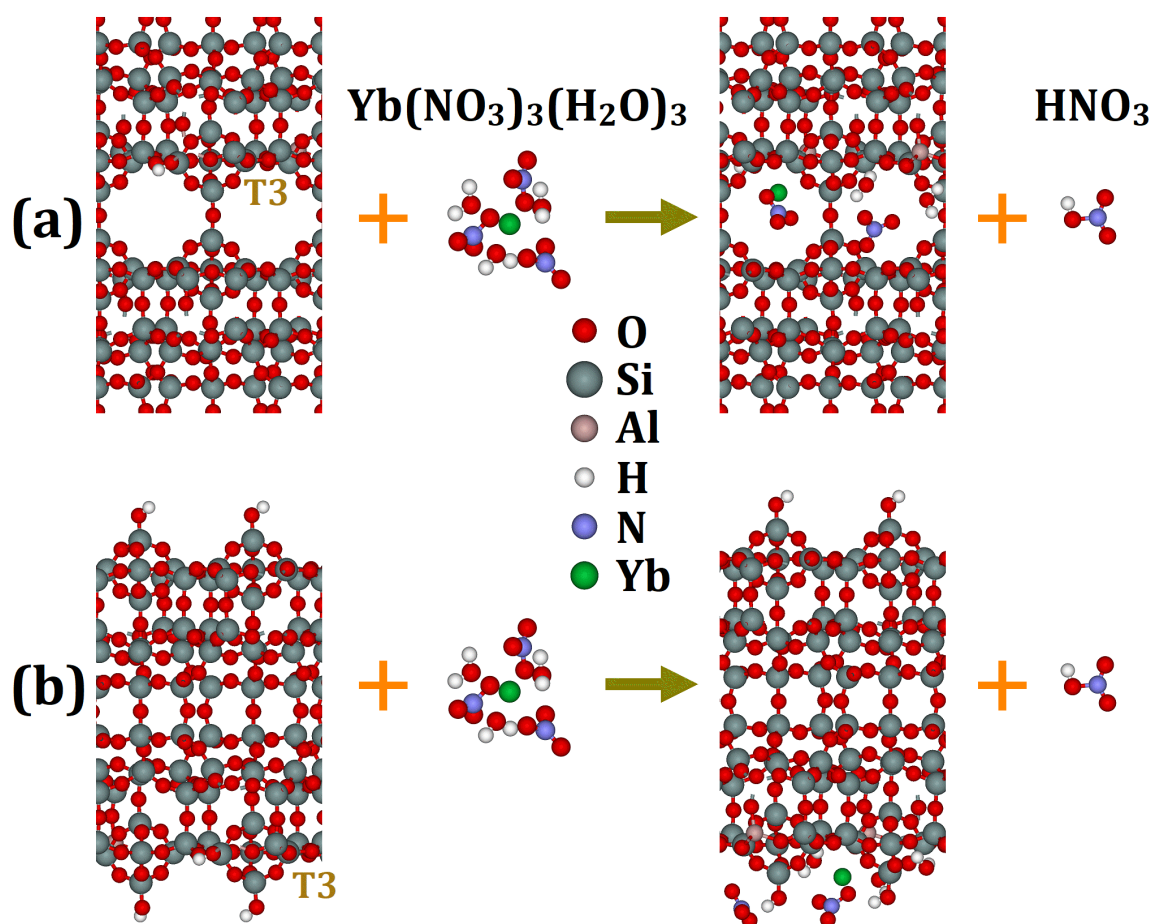


Figure S2. Binding of $\text{Yb}(\text{NO}_3)_3(\text{H}_2\text{O})_3$ complexes at BASs at (a) internal and (b) external surfaces of MCM-22. The overall reaction mechanism indicating all reactants and products is shown by using plus signs and arrows. All structures are optimized from our plane-wave DFT calculations. Yb nitrate binding reactions with an Al atom at the T3 site of the MCM-22 reactant.

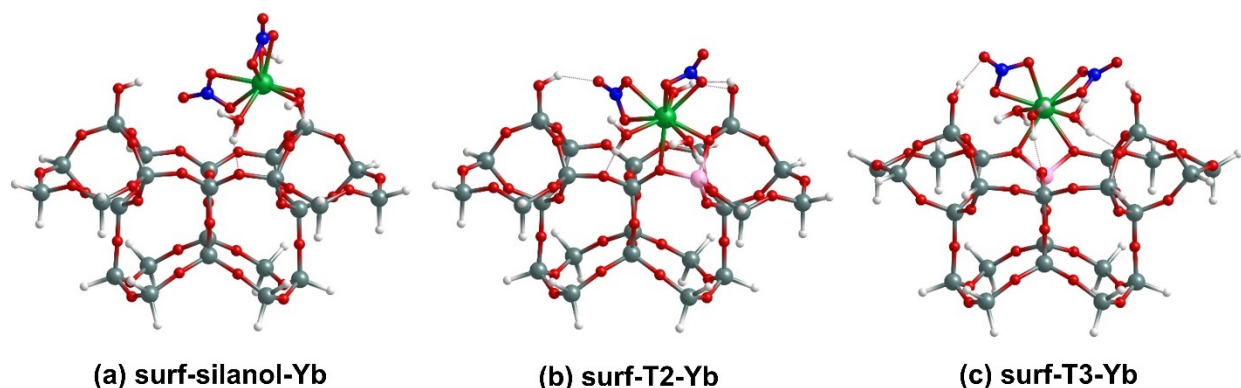


Figure S3. Lowest energy optimized geometries for $[\text{Yb}(\text{NO}_3)_3(\text{H}_2\text{O})_3]$ binding to silanol site and T2, and T3 BASs at external surface using cluster models.

Table S1. Geometrical parameters associated with the highest binding bulk and surface structures of Nd and Yb complexes. Bond lengths are given in Å.

X-bound MCM-22 clusters	X-Al	X-O	X-O
bulk-T1-Nd	3.34	2.45	2.61
surf-T3-Nd	3.32	2.53	2.55
bulk-T1-Yb	3.19	2.31	2.42
surf-T2-Yb	3.18	2.37	2.42

Table S2. Comparison of binding energies (in eV) for $\text{X}(\text{NO}_3)_3$ and $[\text{X}(\text{NO}_3)_3(\text{H}_2\text{O})_n]$ at bulk-T3 and surf-T3 BASs from periodic model calculations.

$\text{X}(\text{NO}_3)_3$ at bulk-T3	-1.80 (Nd)	-1.61 (Yb)
$[\text{X}(\text{NO}_3)_3(\text{H}_2\text{O})_4]$ at bulk-T3	-2.22 (Nd)	-1.76 (Yb)
$\text{X}(\text{NO}_3)_3$ at surf-T3	-1.41 (Nd)	-1.27 (Yb)
$[\text{X}(\text{NO}_3)_3(\text{H}_2\text{O})_4]$ at surf-T3	-2.01 (Nd)	-1.61 (Yb)

The Cartesian coordinates x , y , and z (in Å) of all optimized geometries from DFT calculations.

$[\text{Nd}(\text{NO}_3)_3(\text{H}_2\text{O})_4]$:

Nd	0.032947380	0.022288280	-0.184684480
O	1.266522240	1.982046890	-1.062836920
N	0.591782300	2.899626210	-0.508100440
O	-0.391507430	2.495511700	0.188157200
O	0.855406850	4.056100100	-0.634905710
O	2.161593850	-1.219269340	-0.253490920
O	0.802516170	-1.837506450	1.279179450
N	1.888679390	-2.055068240	0.665428910
O	-3.441756960	-0.737797120	1.952467500
O	-1.471819620	0.124310810	1.786566680
O	-2.344007430	-0.846786670	0.094319040
N	-2.462668640	-0.495570230	1.318062990
O	2.606448950	-2.970097820	0.926494510

O	-1.755118540	1.007668320	-1.763024450
O	-0.539988580	-2.052221030	-1.514994420
O	1.167285130	0.901157020	1.893584240
O	1.173613630	-0.267653890	-2.549106520
H	1.482708560	0.628330630	-2.745524730
H	1.956896090	-0.739717350	-2.222744340
H	1.065668300	0.182850180	2.534303670
H	0.585719160	1.607152540	2.209146910
H	-1.853469880	1.918706010	-1.449868850
H	-2.502010660	0.529500540	-1.364792230
H	-1.442890800	-2.339312650	-1.324521670
H	-0.462880780	-1.916233510	-2.467683240

[Yb(NO₃)₃(H₂O)₃]:

Yb	-0.099230290	0.032023160	-0.071238960
O	1.099119010	1.397941810	-1.500003900
N	0.790017820	2.506817570	-0.977367490
O	0.031947390	2.415263460	0.047664700
O	1.165933660	3.554139070	-1.400193390
O	1.897165790	-1.165164990	-0.353706150
O	0.519249940	-1.862893570	1.120630420
N	1.651247260	-2.011187980	0.559093770
O	-3.331034110	-1.183874470	1.878134160
O	-1.610683800	0.111853640	1.700362840
O	-2.107379110	-1.206765190	0.096729660
N	-2.395195810	-0.782879440	1.260897070
O	2.411141700	-2.876733600	0.863479030
O	-1.854432620	1.096786420	-1.289333960
O	-0.346619640	-1.386688620	-1.957311650
O	1.129579930	0.726783550	1.838260350
H	0.799466690	0.264130670	2.619969510
H	0.957657920	1.668479150	1.978436500
H	-2.054139940	1.973543410	-0.935800670
H	-2.675670120	0.589231500	-1.296609070
H	-0.900967470	-2.154181460	-1.761933790
H	0.516565280	-1.727470820	-2.229371400

Internal pore cluster model:

H	-2.822156840	-8.793391720	0.426277410
H	-5.061929110	-4.913936560	0.426276250
H	-2.821191410	-8.809408860	4.684232690
H	-5.075356400	-4.905101820	4.684244970
O	2.038483880	-3.416932390	-5.220439010
O	-0.633038290	-3.414958190	-5.226225240
O	0.704434400	-5.724294840	-5.198247740
O	3.035409810	-1.306006320	-6.539326900
H	-2.790885790	-3.537091400	-6.559402120
H	1.897767730	-7.515026880	-6.559402230
H	-0.494180280	-7.515026880	-6.559402230
O	-1.631561710	-1.306019430	-6.540608460
H	4.194373240	-3.537091400	-6.559402120

O	2.033392450	-3.371079950	-7.903326100
O	-0.630194140	-3.371442090	-7.904709570
O	0.702403990	-5.717331610	-7.900397200
H	0.701793720	-4.172572010	-9.893425710
Si	0.699612280	-4.175867780	-4.680297810
Si	2.856193720	-2.928692010	-6.554325710
Si	-1.452706280	-2.928692010	-6.554325710
Si	0.701793720	-6.660322010	-6.554325710
Si	0.701793720	-4.172572010	-8.423425710
O	0.674201290	-4.146666630	-3.079908030
O	2.016635110	-3.457713580	-0.934472790
O	-0.655610280	-3.432061930	-0.910490820
O	0.659670760	-5.755013820	-1.000023360
O	3.029809450	-1.305181820	0.311720660
O	-2.972656200	-3.542878900	0.410977620
H	1.897767730	-7.515026880	0.369850810
O	-0.586395330	-7.661689850	0.420769690
O	-1.637566120	-1.296782930	0.342949810
H	4.194373240	-3.537091400	0.369850710
O	2.016580410	-3.328529390	1.734180800
O	-0.658863740	-3.345433530	1.756222870
O	0.680840720	-5.655774170	1.675697170
O	0.697357100	-4.174139150	3.872387300
O	-2.179920600	-7.641386450	2.571744090
O	-3.731885400	-4.927220350	2.571922610
O	-2.828934940	-6.210826850	0.433679560
O	-2.869729690	-6.234470340	4.721526200
O	3.039866200	-1.323431820	4.679660370
O	-2.934275330	-3.557722380	4.687357100
H	1.892493360	-7.579591290	4.814913270
O	-0.583603670	-7.627974250	4.675172490
O	-1.585794050	-1.322728420	4.715885980
H	4.247676960	-3.500233910	4.814916200
O	1.999000360	-3.401843710	6.068726390
O	-0.626009920	-3.433977640	6.070138730
O	0.702171020	-5.683864200	6.072452060
H	4.006170520	-2.264706550	6.884849580
H	-2.602683070	-2.264706550	6.884849580
H	0.701793720	-7.988200490	6.884848860
Si	0.666803140	-4.193995880	-1.481579010
Si	2.856193720	-2.928692010	0.364774290
Si	-1.479832180	-2.910016500	0.396004810
Si	0.701793720	-6.660322010	0.364774290
Si	-2.132006280	-7.609422010	0.958074290
Si	-3.691506280	-4.908272010	0.958074290
Si	0.688131010	-4.128270300	2.262248720
Si	0.694868400	-4.171547740	5.504990440
Si	-2.131706280	-7.609892010	4.187574290
Si	-3.691806280	-4.907802010	4.187574290
Si	3.368793720	-2.632752010	5.612374290
Si	-1.965306280	-2.632752010	5.612374290

Si	0.701793720	-7.252192010	5.612374290
O	-0.633066760	3.414986820	-5.226215180
O	2.038510810	3.416962710	-5.220429220
O	0.704433170	5.724270590	-5.198256710
O	-1.631561760	1.306036530	-6.540621300
H	4.194390310	3.537069820	-6.559402190
H	-0.494197430	7.514988850	-6.559402300
H	1.897784880	7.514988850	-6.559402300
O	3.035409870	1.306023460	-6.539338810
H	-2.790902870	3.537069820	-6.559402190
O	-0.630207570	3.371506530	-7.904699730
O	2.033402150	3.371139320	-7.903315720
O	0.702403130	5.717369900	-7.900426390
H	0.701793720	4.172607990	-9.893425710
H	2.314873180	0.000007990	-8.616648930
H	-0.911285740	0.000007990	-8.616648930
O	0.702103490	0.000006740	-6.638892910
Si	0.699610650	4.175847280	-4.680291050
Si	-1.452706280	2.928707990	-6.554325710
Si	2.856193720	2.928707990	-6.554325710
Si	0.701793720	6.660307990	-6.554325710
Si	2.261293720	0.000007990	-7.147625710
Si	-0.857706280	0.000007990	-7.147625710
Si	0.701793720	4.172607990	-8.423425710
O	0.674194760	4.146661350	-3.079902900
O	-0.655620800	3.432077430	-0.910476320
O	2.016713080	3.457850840	-0.934475830
O	0.659634260	5.755016850	-1.000034950
O	-1.637589120	1.296791740	0.342966880
H	4.194390310	3.537069820	0.369850770
O	-0.586388810	7.661682870	0.420789650
H	-5.061929310	4.913918250	0.426276170
H	1.897784880	7.514988850	0.369850890
O	3.029811640	1.305198020	0.311705870
O	-2.972661740	3.542904260	0.410979240
H	-2.822167100	8.793368160	0.426269500
O	-0.658901390	3.345465800	1.756243200
O	2.016597340	3.328565150	1.734179050
O	0.680850740	5.655761730	1.675692990
O	0.697362100	4.174140050	3.872387040
O	-0.845249190	-0.000002200	2.545343220
O	-2.179935100	7.641370040	2.571743410
O	2.274327490	0.000009630	2.522327220
O	-3.731888170	4.927270220	2.571922340
O	0.697276600	0.000002160	0.391384510
O	-2.828927670	6.210831000	0.433644290
O	0.725190570	0.000007230	4.689802930
O	-2.869849650	6.234551150	4.721535740
O	-1.585879330	1.322627600	4.715942610
H	4.247657740	3.500225390	4.814933640
O	-0.583619800	7.628028230	4.675210880

H	-5.075356350	4.905080530	4.684244950
H	1.892504820	7.579546880	4.814905590
O	3.039908450	1.323366220	4.679688580
O	-2.934319440	3.557728370	4.687437630
H	-2.821194890	8.809421810	4.684235200
O	-0.625989380	3.433906900	6.070134710
O	1.999022540	3.401857320	6.068707080
O	0.702130810	5.683861880	6.072434980
H	-2.602689010	2.264713790	6.884861430
H	4.006176450	2.264713790	6.884861430
H	0.701793720	7.988195980	6.884860710
Si	0.666795790	4.193989260	-1.481574210
Si	-1.479842920	2.910025590	0.396017190
Si	2.856193720	2.928707990	0.364774290
Si	0.701793720	6.660307990	0.364774290
Si	-0.851393660	0.000007650	0.924373600
Si	-2.132006280	7.609407990	0.958074290
Si	2.253520120	0.000014140	0.900559310
Si	-3.691506280	4.908307990	0.958074290
Si	0.688120910	4.128259760	2.262252840
Si	0.694861570	4.171531290	5.504989680
Si	-0.827211050	-0.000013490	4.167963080
Si	-2.131706280	7.609907990	4.187574290
Si	2.270120840	-0.000014560	4.146221850
Si	-3.691806280	4.907807990	4.187574290
Si	-1.965306280	2.632707990	5.612374290
Si	3.368793720	2.632707990	5.612374290
Si	0.701793720	7.252207990	5.612374290

External surface cluster model:

O	-2.526831580	2.411661790	2.992989470
O	-5.207859580	2.381375780	2.888023200
O	-3.868689140	0.099616850	2.872070510
O	2.024150250	-3.307240940	2.871886900
O	4.669243370	-3.317114940	2.889551160
O	3.359580560	-0.984315540	2.993078030
O	-1.537597400	4.472213970	1.583743760
H	-7.383577460	2.241526570	1.550084960
O	-2.574031770	-1.848454950	1.572803370
H	1.039495460	-5.273485860	1.550084960
O	6.995356470	-3.180292270	1.552652030
O	2.014352150	0.890023760	1.647921320
H	-5.086922240	-1.736396950	1.550084960
O	-6.251098940	4.468112230	1.554218800
O	-0.233474280	2.191808230	1.644152830
O	4.641824180	0.906315820	1.584220010
H	5.632805890	-5.273485870	1.550084960
O	-0.312822350	-3.151191300	1.576519660
O	-2.535735130	2.354948940	0.307860330
O	-5.197670890	2.402058810	0.206677630
O	-3.874479090	0.050342780	0.194021190

O	1.978422160	-3.326516520	0.194127890
O	4.676637760	-3.301038030	0.207771960
O	3.308543210	-1.017139570	0.307450700
O	-3.792394600	1.620195360	-1.911356700
O	3.299067090	-2.473638990	-1.911296620
O	-1.046755460	-1.816188040	-0.616667840
O	0.521981400	0.900129070	-0.586416030
O	-0.276773080	-0.475700470	1.536720600
O	-0.266208130	-0.457881980	-2.752648930
H	-1.535729000	4.340777690	-2.894991580
O	-2.571761660	-1.812584850	-2.778334810
H	0.980939740	-5.301234120	-2.894991580
O	2.037667710	0.879970920	-2.755893220
H	-5.081675070	-1.800981830	-2.894991580
O	-0.256318250	2.206115380	-2.754517250
H	4.526886460	0.840525020	-2.894991580
O	-0.284137360	-3.132499610	-2.779630720
O	-2.581811420	2.356355910	-4.152371490
H	-5.086849990	2.296511730	-4.046900160
O	-3.922110510	0.097909230	-4.133818390
O	2.045852150	-3.347785990	-4.133657620
H	4.532061020	-3.256969060	-4.046900270
O	3.332960910	-1.057706250	-4.152565890
H	-0.586524160	3.513858200	-4.964882460
H	-3.890939770	-2.209557850	-4.964882310
H	0.031734870	-4.474315110	-4.964882310
H	3.336150760	1.249100780	-4.964882460
Si	-3.885159210	1.621857120	3.485128600
Si	3.345409790	-2.555514540	3.485602140
Si	-1.716261940	2.859497100	1.642884580
Si	-6.045400190	2.849931220	1.555122120
Si	-3.890939780	-0.881703680	1.555122120
Si	1.181690310	-3.810388030	1.555122120
Si	5.490611150	-3.810388030	1.555122120
Si	3.336085940	-0.057125080	1.643741720
Si	-1.049922300	-1.818313430	1.003487450
Si	0.505683400	0.875010370	1.036702890
Si	-3.858911440	1.608850200	-0.301928930
Si	3.321749420	-2.536238480	-0.301933170
Si	-3.890939780	1.606052430	-3.542951020
Si	3.336150960	-2.566509610	-3.542951020
Si	-1.042631130	-1.805314020	-2.239263350
Si	0.509090410	0.882458630	-2.214133430
Si	-1.223906890	3.145865570	-3.692394870
Si	-3.890939770	-1.473571630	-3.692394870
Si	0.669117630	-4.106322000	-3.692394870
Si	3.336151160	0.513114830	-3.692394870
O	3.328942330	-2.617026180	5.112837290
O	-3.946366490	1.601015970	5.112246550
H	-6.130747010	6.968250560	1.493657950
H	-1.651132620	6.968250600	1.493657970

H	-2.277873830	5.778615570	-0.507210300
H	-5.504005720	5.778615570	-0.507210300
O	-3.890851780	5.743778970	1.477641030
Si	-2.331434090	5.778615570	0.961813630
Si	-5.450445460	5.778615570	0.961813630
H	6.860046570	2.054319010	1.493657970
H	9.099853730	-1.825140870	1.493657950
H	6.143163010	0.916727680	-0.507210300
H	7.756228960	-1.877184490	-0.507210300
O	6.918332080	-0.498275040	1.478213160
Si	6.169943140	0.870343140	0.961813630
Si	7.729448830	-1.830799950	0.961813630
H	-3.148012200	1.883665940	5.566939070
H	3.360570630	-1.769448220	5.564954790

bulk-T1-Nd:

H	-2.545855100	-8.501420080	0.778409300
H	-4.785627370	-4.621964920	0.778408140
H	-2.544889670	-8.517437220	5.036364580
H	-4.799054660	-4.613130180	5.036376860
O	2.351037110	-3.150934300	-4.842244100
O	-0.290669100	-2.940842790	-4.895620660
O	0.955041680	-5.384817970	-4.869650080
O	3.311162850	-1.016084160	-6.186531010
H	-2.514584050	-3.245119760	-6.207270230
H	2.174069470	-7.223055240	-6.207270340
H	-0.217878540	-7.223055240	-6.207270340
O	-1.447783490	-1.009068050	-6.256165410
H	4.470674980	-3.245119760	-6.207270230
O	2.283571540	-3.058817870	-7.537438300
O	-0.376989680	-3.112008730	-7.545747920
O	0.991569620	-5.428067490	-7.554014890
H	0.978095460	-3.880600370	-9.541293820
Si	0.975199890	-3.848949980	-4.323930800
Si	3.132495460	-2.636720370	-6.202193820
Si	-1.176404540	-2.636720370	-6.202193820
Si	0.978095460	-6.368350370	-6.202193820
Si	0.978095460	-3.880600370	-8.071293820
O	0.604123090	-3.696281180	-2.772752370
O	2.275268400	-3.144602930	-0.535746760
O	-0.622909990	-3.055040650	-0.557932660
O	0.752352680	-5.586705120	-0.686441180
O	3.344559990	-1.007177730	0.697093390
O	-2.763788380	-3.147135750	0.976218260
H	2.174069470	-7.223055240	0.721982700
O	-0.285062480	-7.406465180	0.892342870
O	-1.444240930	-0.972249690	0.939351890
H	4.470674980	-3.245119760	0.721982600
O	2.345184620	-2.992242240	2.146340980
O	-0.324755840	-3.082155430	2.129227680
O	1.039800000	-5.336654310	1.999046040

O	0.996308090	-3.926189400	4.242330340
O	-1.990963330	-7.331934720	2.923407690
O	-3.480525620	-4.735557100	2.925316750
O	-2.479352890	-5.869356370	0.745773330
O	-2.574082730	-5.931016840	5.095764770
O	3.332584620	-1.032084350	5.027966090
O	-2.663601130	-3.248569240	5.014019040
H	2.168795100	-7.287619650	5.167045160
O	-0.296470440	-7.328805060	4.999890000
O	-1.276980680	-1.048231110	5.049780750
H	4.523978700	-3.208262270	5.167048090
O	2.266997490	-3.096080290	6.429083240
O	-0.362767320	-3.164156190	6.420800890
O	0.983439940	-5.399014240	6.452186650
H	4.282472260	-1.972734910	7.236981470
H	-2.326381330	-1.972734910	7.236981470
H	0.978095460	-7.696228850	7.236980750
Al	0.859624890	-3.906005620	-1.081428330
Si	3.132495460	-2.636720370	0.716906180
Si	-1.237098370	-2.578044360	0.883418700
Si	0.978095460	-6.368350370	0.716906180
Si	-1.855704540	-7.317450370	1.310206180
Si	-3.415204540	-4.616300370	1.310206180
Si	1.042179100	-3.836288260	2.635686970
Si	0.973674130	-3.890034850	5.873266030
Si	-1.855404540	-7.317920370	4.539706180
Si	-3.415504540	-4.615830370	4.539706180
Si	3.645095460	-2.340780370	5.964506180
Si	-1.689004540	-2.340780370	5.964506180
Si	0.978095460	-6.960220370	5.964506180
O	-0.364137430	3.712625920	-4.878877540
O	2.311096870	3.707395930	-4.872752720
O	0.980579130	6.008420970	-4.854787730
O	-1.366213060	1.585409130	-6.168600590
H	4.470692050	3.829041460	-6.207270300
H	-0.217895690	7.806960490	-6.207270410
H	2.174086620	7.806960490	-6.207270410
O	3.298880000	1.597233270	-6.186020020
H	-2.514601130	3.829041460	-6.207270300
O	-0.346412540	3.636903410	-7.555788460
O	2.313788300	3.668073410	-7.553723800
O	0.961143320	6.008080680	-7.550479810
H	0.978095460	4.464579630	-9.541293820
H	2.591174920	0.291979630	-8.264517040
H	-0.634984000	0.291979630	-8.264517040
O	0.970821040	0.244628440	-6.308242950
Si	0.973972120	4.461561580	-4.323451310
Si	-1.176404540	3.220679630	-6.202193820
Si	3.132495460	3.220679630	-6.202193820
Si	0.978095460	6.952279630	-6.202193820
Si	2.537595460	0.291979630	-6.795493820

Si	-0.581404540	0.291979630	-6.795493820
Si	0.978095460	4.464579630	-8.071293820
O	0.943804560	4.462275410	-2.727548160
O	-0.389497800	3.734583080	-0.553291320
O	2.295707260	3.734993390	-0.590817840
O	0.947008180	6.030473720	-0.633565180
O	-1.358358690	1.599328650	0.734504650
H	4.470692050	3.829041460	0.721982660
O	-0.313944890	7.952333060	0.761581340
H	-4.785627570	5.205889890	0.778408060
H	2.174086620	7.806960490	0.721982780
O	3.287106150	1.598236510	0.687134320
O	-2.703561280	3.830437050	0.765983170
H	-2.545865360	9.085339800	0.778401390
O	-0.387254550	3.666993890	2.113084820
O	2.290907030	3.647091620	2.077491750
O	0.953365350	5.973446140	2.047262590
O	0.981223020	4.472004110	4.227443000
O	-0.464764840	0.398628330	2.947227540
O	-1.901698850	7.934945820	2.923804440
O	2.517742310	0.302983630	2.891988730
O	-3.464492430	5.225662860	2.923938760
O	0.975865120	0.231652300	0.744126320
O	-2.553505490	6.502300270	0.786259010
O	1.027219000	0.291186410	5.118419210
O	-2.592817010	6.525619850	5.073763360
O	-1.316713270	1.588045810	5.116774360
H	4.523959480	3.792197030	5.167065530
O	-0.308699370	7.919146550	5.029665880
H	-4.799054610	5.197052170	5.036376840
H	2.168806560	7.871518520	5.167037480
O	3.333477670	1.615486580	5.030242160
O	-2.654481680	3.843636260	5.025647270
H	-2.544893150	9.101393450	5.036367090
O	-0.353420470	3.734139700	6.415788900
O	2.272260580	3.688336470	6.422768940
O	0.983648390	5.977345070	6.430141870
H	-2.326387270	2.556685430	7.236993320
H	4.282478190	2.556685430	7.236993320
H	0.978095460	8.280167620	7.236992600
Si	0.944274560	4.470383670	-1.128982290
Si	-1.201598790	3.213928410	0.756075880
Si	3.132495460	3.220679630	0.716906180
Si	0.978095460	6.952279630	0.716906180
Si	-0.543890300	0.326627040	1.329591700
Si	-1.855704540	7.901379630	1.310206180
Si	2.533828770	0.275444280	1.267185150
Si	-3.415204540	5.200279630	1.310206180
Si	0.966168300	4.440199690	2.617135960
Si	0.973425400	4.466142940	5.858567670
Si	-0.512695580	0.298164590	4.561965410

Si	-1.855404540	7.901879630	4.539706180
Si	2.553073840	0.292227060	4.513238920
Si	-3.415504540	5.199779630	4.539706180
Si	-1.689004540	2.924679630	5.964506180
Si	3.645095460	2.924679630	5.964506180
Si	0.978095460	7.544179630	5.964506180
O	-0.129485000	-0.663399910	-3.597241340
O	0.342648030	1.196331450	-2.605638010
O	-0.895102010	-0.293511360	-1.650692580
N	-0.200819140	0.130652300	-2.619994700
H	-2.505147410	-0.471621120	-4.836946500
O	-2.884423140	-0.713255990	-3.972575360
H	-3.811539310	-0.948378110	-4.107292520
O	-3.328648150	-1.336656790	-1.131326830
H	-2.911937660	-0.533655210	-0.781033080
H	-3.532510140	-1.877660900	-0.349597350
Nd	-1.676704010	-2.438737280	-2.680390640
O	-4.007140000	-3.093198140	-3.384387930
N	-4.268093330	-3.852919190	-2.406394530
O	-3.320282390	-4.015487900	-1.583840480
O	-5.329437760	-4.388418670	-2.272501270
O	-1.856392270	-4.769651970	-3.832184350
H	-2.716762040	-4.922292470	-4.236927060
H	-1.738537080	-5.499445340	-3.144803850
O	-1.566556280	-6.430549720	-1.913322430
H	-0.659175240	-6.320832290	-1.563634320
H	-2.119883260	-6.029862760	-1.221754570

bulk-T2-Nd:

H	-2.638198280	-8.659538610	0.752682720
H	-4.877970550	-4.780083450	0.752681560
H	-2.637232850	-8.675555750	5.010638000
H	-4.891397840	-4.771248710	5.010650280
O	2.262733400	-3.348578550	-4.904226830
O	-0.389288440	-3.177364710	-4.893834140
O	0.797965680	-5.575077780	-4.896478380
O	3.191761750	-1.168386860	-6.191161860
H	-2.606927230	-3.403238290	-6.232996810
H	2.081726290	-7.381173770	-6.232996920
H	-0.310221720	-7.381173770	-6.232996920
O	-1.450725640	-1.173932420	-6.254748530
H	4.378331800	-3.403238290	-6.232996810
O	2.188215020	-3.186515830	-7.577608290
O	-0.470833620	-3.279359500	-7.574030330
O	0.934177010	-5.583030260	-7.577969090
H	0.885752280	-4.038718900	-9.567020400
Si	0.899752640	-4.039951850	-4.352992580
Si	3.040152280	-2.794838900	-6.227920400
Si	-1.268747720	-2.794838900	-6.227920400
Si	0.885752280	-6.526468900	-6.227920400
Si	0.885752280	-4.038718900	-8.097020400

O	0.892943480	-4.141878330	-2.764382980
O	2.282941550	-3.568692250	-0.543220330
O	-0.367793210	-3.165727930	-0.692827370
O	0.678437350	-5.675037370	-0.709006080
O	2.929839910	-1.178640700	0.445151160
O	-2.805017940	-3.425519570	0.774374480
H	2.081726290	-7.381173770	0.696256120
O	-0.389135310	-7.547695290	0.795701630
O	-1.277859180	-1.033844620	0.390660810
H	4.378331800	-3.403238290	0.696256020
O	2.323848870	-3.175301110	2.127662240
O	-0.330158580	-3.097174590	2.233506330
O	0.915047700	-5.458910160	1.936156850
O	1.064998570	-4.182193240	4.231270030
O	-2.034060030	-7.489718260	2.895285760
O	-3.552571730	-4.903332170	2.900747800
O	-2.635009140	-6.086542660	0.695257360
O	-2.670751240	-6.092528360	5.071858520
O	3.128293650	-1.172198670	5.088884210
O	-2.763986890	-3.385479840	4.972194460
H	2.076451920	-7.445738180	5.141318580
O	-0.390693430	-7.489633400	4.979091680
O	-1.325160470	-1.125952930	5.205398260
H	4.431635520	-3.366380800	5.141321510
O	2.202677200	-3.288356940	6.445661320
O	-0.445087830	-3.347633470	6.317214370
O	0.885427200	-5.572363410	6.468234030
H	4.190129080	-2.130853440	7.211254890
H	-2.418724510	-2.130853440	7.211254890
H	0.885752280	-7.854347380	7.211254170
Si	0.875517330	-4.096890500	-1.156961330
Si	3.040152280	-2.794838900	0.691179600
Al	-1.233999530	-2.757594240	0.803694780
Si	0.885752280	-6.526468900	0.691179600
Si	-1.948047720	-7.475568900	1.284479600
Si	-3.507547720	-4.774418900	1.284479600
Si	0.967088820	-3.963214780	2.631712930
Si	0.919633950	-4.076522130	5.849859750
Si	-1.947747720	-7.476038900	4.513979600
Si	-3.507847720	-4.773948900	4.513979600
Si	3.552752280	-2.498898900	5.938779600
Si	-1.781347720	-2.498898900	5.938779600
Si	0.885752280	-7.118338900	5.938779600
O	-0.453353310	3.506493020	-4.880695830
O	2.208230550	3.530268850	-4.896216170
O	0.870719540	5.836001010	-4.884109130
O	-1.446380280	1.432466530	-6.181806590
H	4.378348870	3.670922930	-6.232996880
H	-0.310238870	7.648841960	-6.232996990
H	2.081743440	7.648841960	-6.232996990
O	3.213446750	1.441094510	-6.224251730

H	-2.606944310	3.670922930	-6.232996880
O	-0.434901060	3.480936260	-7.571918800
O	2.219111760	3.511441440	-7.576291650
O	0.870143870	5.849056020	-7.574312520
H	0.885752280	4.306461100	-9.567020400
H	2.498831740	0.133861100	-8.290243620
H	-0.727327180	0.133861100	-8.290243620
O	0.881399760	0.161403830	-6.276869290
Si	0.879193180	4.294876120	-4.348507680
Si	-1.268747720	3.062561100	-6.227920400
Si	3.040152280	3.062561100	-6.227920400
Si	0.885752280	6.794161100	-6.227920400
Si	2.445252280	0.133861100	-6.821220400
Si	-0.673747720	0.133861100	-6.821220400
Si	0.885752280	4.306461100	-8.097020400
O	0.847240370	4.266860380	-2.749876450
O	-0.462453490	3.535961370	-0.607106420
O	2.216594900	3.719462510	-0.562838060
O	0.744533210	5.920304770	-0.691636760
O	-1.437399780	1.499576310	0.685029280
H	4.378348870	3.670922930	0.696256080
O	-0.391739230	7.802674130	0.791722720
H	-4.877970750	5.047771360	0.752681480
H	2.081743440	7.648841960	0.696256200
O	3.141692900	1.445269790	0.528988730
O	-2.773368340	3.698427390	0.704521840
H	-2.638208540	8.927221270	0.752674810
O	-0.465730890	3.559958840	2.100513600
O	2.214463550	3.413368490	2.088417120
O	0.950326850	5.780991730	1.987831720
O	0.913675940	4.335689590	4.218545310
O	-1.296182510	0.005696230	2.864196570
O	-2.021455240	7.772156980	2.898298610
O	3.056967050	0.074822160	2.795444100
O	-3.536215350	5.046763720	2.895501050
O	0.861080150	0.318987760	1.399386230
O	-2.640859510	6.343765700	0.755692610
O	0.902202770	0.143176770	4.415744760
O	-2.684471420	6.365990280	5.047270890
O	-1.298929450	1.497018580	5.043632100
H	4.431616300	3.634078500	5.141338950
O	-0.395752420	7.753226720	4.988581480
H	-4.891397790	5.038933640	5.010650260
H	2.076463380	7.713399990	5.141310900
O	3.135458190	1.467955440	5.034879820
O	-2.765020970	3.680304790	5.013437300
H	-2.637236330	8.943274920	5.010640510
O	-0.459774470	3.605443770	6.402494390
O	2.194973460	3.556191400	6.419109320
O	0.889177760	5.827696590	6.420948170
H	-2.418730450	2.398566900	7.211266740

H	4.190135010	2.398566900	7.211266740
H	0.885752280	8.122049090	7.211266020
Si	0.848378670	4.358081740	-1.150436790
Si	-1.267534080	3.100865270	0.756153800
Si	3.040152280	3.062561100	0.691179600
Si	0.885752280	6.794161100	0.691179600
Si	-0.756578040	0.172320690	1.342590270
Si	-1.948047720	7.743261100	1.284479600
Si	2.475639870	0.155254010	1.272575020
Si	-3.507547720	5.042161100	1.284479600
Si	0.923398950	4.270754620	2.613521500
Si	0.884220220	4.314031440	5.856023490
Si	-0.728911870	0.126999100	4.388572560
Si	-1.947747720	7.743761100	4.513979600
Si	2.534088920	0.130361760	4.340688870
Si	-3.507847720	5.041661100	4.513979600
Si	-1.781347720	2.766561100	5.938779600
Si	3.552752280	2.766561100	5.938779600
Si	0.885752280	7.386061100	5.938779600
O	-3.085485790	-0.821517760	-3.657817970
O	-3.609280050	-0.697606310	-1.581930300
Nd	-1.216346170	-1.104696440	-2.057996910
O	-5.131446240	-0.443035890	-3.088966080
N	-3.992364860	-0.644748330	-2.786040630
H	-2.972362540	-3.200946380	-3.352393720
O	-2.304209550	-3.203977860	-2.659867740
H	-2.131635290	-4.153388000	-2.399552350
O	-0.409530340	0.341726670	-3.851837480
O	-1.942713760	1.337980540	-2.029377860
H	-2.605493250	1.427352360	-1.330785100
H	-1.237588860	1.964196070	-1.802200870
H	0.333963750	0.241627800	-4.465925050
H	-1.065459410	0.914007960	-4.273837570
H	-0.993202330	-5.981837870	-1.975380900
O	-1.921497800	-5.708833790	-2.020342000
H	-2.234751420	-5.837424860	-1.105282770
O	1.179709430	-1.362168670	-2.643798480
N	1.582186110	-0.262581300	-2.154517860
O	2.638854230	0.213847360	-2.447535480
O	0.775685270	0.301453990	-1.364769900

bulk-T3-Nd:

H	-2.458528330	-8.740437440	0.752824970
H	-4.698300600	-4.860982280	0.752823810
H	-2.457562900	-8.756454580	5.010780250
H	-4.711727890	-4.852147540	5.010792530
O	2.474407520	-3.407027690	-4.869872890
O	-0.151978760	-3.334007630	-4.983870000
O	1.081895120	-5.690009710	-4.856068060
O	3.375483320	-1.249015320	-6.188455000
H	-2.427257280	-3.484137120	-6.232854560

H	2.261396240	-7.462072600	-6.232854670
H	-0.130551770	-7.462072600	-6.232854670
O	-1.262034520	-1.244332620	-6.207681810
H	4.558001750	-3.484137120	-6.232854560
O	2.382117940	-3.295102450	-7.570537460
O	-0.285225910	-3.316727220	-7.606135120
O	1.080752840	-5.658829120	-7.567352460
H	1.065422230	-4.119617730	-9.566878150
Si	1.103509540	-4.136241090	-4.358499970
Si	3.219822230	-2.875737730	-6.227778150
Si	-1.089077770	-2.875737730	-6.227778150
Si	1.065422230	-6.607367730	-6.227778150
Si	1.065422230	-4.119617730	-8.096878150
O	1.067085070	-4.058834920	-2.756078820
O	2.239966530	-3.345642030	-0.535562580
O	-0.426196960	-3.624493770	-0.619301160
O	1.115549650	-5.773882340	-0.726042330
O	3.454959080	-1.260031980	0.634674750
O	-2.629631280	-3.418152090	0.898278760
H	2.261396240	-7.462072600	0.696398370
O	-0.221570570	-7.608296760	0.751432680
O	-1.251185460	-1.284418110	0.348715420
H	4.558001750	-3.484137120	0.696398270
O	2.463567920	-3.292337050	2.109004450
O	-0.194467090	-3.135487480	1.995483410
O	0.987099860	-5.532277300	1.940789740
O	0.993969890	-4.103294060	4.172787650
O	-1.823480320	-7.589415480	2.896942090
O	-3.415057520	-4.935458480	2.899572320
O	-2.432119030	-6.130659330	0.754876270
O	-2.496056780	-6.176751910	5.052857480
O	3.420194300	-1.265414660	5.003851690
O	-2.562114440	-3.494104860	4.978681150
H	2.256121870	-7.526637010	5.141460830
O	-0.218499680	-7.581375440	4.999258770
O	-1.198835920	-1.256567570	5.093462540
H	4.611305470	-3.447279630	5.141463760
O	2.346032730	-3.338032720	6.360642760
O	-0.284790860	-3.414887690	6.407969090
O	1.082329940	-5.627312700	6.373210450
H	4.369799030	-2.211752270	7.211397140
H	-2.239054560	-2.211752270	7.211397140
H	1.065422230	-7.935246210	7.211396420
Si	0.999237000	-4.209062320	-1.165391010
Si	3.219822230	-2.875737730	0.691321850
Si	-1.107889240	-2.871135350	0.655414390
Si	1.065422230	-6.607367730	0.691321850
Si	-1.768377770	-7.556467730	1.284621850
Si	-3.327877770	-4.855317730	1.284621850
Si	1.069625930	-4.017427570	2.564793020
Si	1.040654110	-4.113806660	5.809052540

Si	-1.768077770	-7.556937730	4.514121850
Si	-3.328177770	-4.854847730	4.514121850
Si	3.732422230	-2.579797730	5.938921850
Si	-1.601677770	-2.579797730	5.938921850
Si	1.065422230	-7.199237730	5.938921850
O	-0.243994960	3.418684780	-4.893569610
O	2.414727640	3.472720710	-4.889687400
O	1.045755660	5.767689480	-4.878819860
O	-1.287957670	1.351932490	-6.189155980
H	4.558018820	3.590024100	-6.232854630
H	-0.130568920	7.567943130	-6.232854740
H	2.261413390	7.567943130	-6.232854740
O	3.403438820	1.360470250	-6.217535430
H	-2.427274360	3.590024100	-6.232854630
O	-0.264378190	3.413622150	-7.574542890
O	2.393205320	3.426249530	-7.572497600
O	1.058333280	5.768508740	-7.572662110
H	1.065422230	4.225562270	-9.566878150
H	2.678501690	0.052962270	-8.290101370
H	-0.547657230	0.052962270	-8.290101370
O	1.062436420	0.103574610	-6.305399760
Si	1.073317520	4.224691540	-4.357708780
Si	-1.089077770	2.981662270	-6.227778150
Si	3.219822230	2.981662270	-6.227778150
Si	1.065422230	6.713262270	-6.227778150
Si	2.624922230	0.052962270	-6.821078150
Si	-0.494077770	0.052962270	-6.821078150
Si	1.065422230	4.225562270	-8.096878150
O	1.058473390	4.193466530	-2.761259220
O	-0.379683690	3.603070100	-0.658404180
O	2.300904800	3.442576940	-0.584608350
O	1.089161660	5.832486230	-0.696213510
O	-1.349963020	1.342822850	0.376360590
H	4.558018820	3.590024100	0.696398330
O	-0.227138210	7.711092060	0.731979550
H	-4.698300800	4.966872530	0.752823730
H	2.261413390	7.567943130	0.696398450
O	3.508455220	1.374550790	0.666032430
O	-2.648916120	3.570592030	0.721735810
H	-2.458538590	8.846322440	0.752817060
O	-0.283269990	3.284993770	1.982610660
O	2.388033970	3.386839310	2.067084080
O	0.970468990	5.659168200	1.961630670
O	0.956393130	4.184440850	4.163647550
O	-0.553419110	0.041018190	2.883748810
O	-1.814422210	7.688994380	2.895829510
O	2.651771210	0.045675310	2.825953080
O	-3.367074080	4.968760970	2.893078610
O	1.178853380	0.127876180	0.580373480
O	-2.458492840	6.252816220	0.757230220
O	1.103712740	0.059952210	4.997280480

O	-2.511998330	6.290640960	5.040855310
O	-1.193409340	1.383349320	5.066410580
H	4.611286250	3.553179670	5.141481200
O	-0.222496220	7.687751460	5.004228090
H	-4.711727840	4.958034810	5.010792510
H	2.256133330	7.632501160	5.141453150
O	3.423462990	1.375232020	4.996441650
O	-2.571831480	3.609819790	5.004175030
H	-2.457566380	8.862376090	5.010782760
O	-0.288902670	3.522619260	6.419610660
O	2.342877630	3.445248790	6.347033300
O	1.080729670	5.729919540	6.354647210
H	-2.239060500	2.317668070	7.211408990
H	4.369804960	2.317668070	7.211408990
H	1.065422230	8.041150260	7.211408270
Si	1.020389700	4.270509320	-1.163656270
Si	-1.134315970	2.930190780	0.622232510
Si	3.219822230	2.981662270	0.691321850
Si	1.065422230	6.713262270	0.691321850
Al	-0.453987570	0.046835060	1.193283380
Si	-1.768377770	7.662362270	1.284621850
Si	2.679633800	0.066743480	1.199131620
Si	-3.327877770	4.961262270	1.284621850
Si	1.013139490	4.127648450	2.553624460
Si	1.031501250	4.212493100	5.800802800
Si	-0.458153670	0.054120250	4.478609800
Si	-1.768077770	7.662862270	4.514121850
Si	2.644967910	0.053329820	4.453944630
Si	-3.328177770	4.960762270	4.514121850
Si	-1.601677770	2.685662270	5.938921850
Si	3.732422230	2.685662270	5.938921850
Si	1.065422230	7.305162270	5.938921850
H	-3.627473070	2.611061520	-0.416331130
H	-2.054133770	0.995327340	-4.282845700
H	-0.851330550	1.474799300	-3.438310420
O	-5.060023120	-0.152078360	-1.895132290
O	-3.850038220	-0.422623860	-3.633634380
N	-5.007322830	-0.401986160	-3.144210780
O	-5.992961070	-0.596409320	-3.790126750
O	-1.804877380	1.318680420	-3.402417130
O	-3.789243350	2.026483410	-1.178578000
H	-4.717250150	1.754039690	-1.191948330
Nd	-2.525419780	-0.084958570	-1.505303880
H	-4.808851440	-1.053686150	-0.100028180
H	-3.664349270	-1.723111580	0.692323670
O	-4.010977060	-0.856971560	0.415447400
O	0.092089530	0.109991740	-1.910536630
H	0.277332530	-0.744434270	-2.326448410
H	0.685778330	0.163999510	-1.129569940
O	-3.183396550	-2.443555820	-1.733787660
O	-1.507556410	-1.849932470	-2.908930270

N	-2.337725910	-2.758479650	-2.619115240
O	-2.330356880	-3.836728680	-3.135676660

surf-silanol-Nd:

O	-2.585370940	2.207023390	1.472913750
O	-5.210576890	2.153616550	1.689205800
O	-3.842148260	-0.146036830	1.636015360
O	2.373465080	-3.628877230	1.458164040
O	4.984811020	-3.552604960	1.715584350
O	3.633235110	-1.274925520	1.664598530
O	-1.367920220	4.244549300	0.252450510
H	-7.241218050	2.028592860	0.270763200
O	-2.412109030	-2.016179150	0.440787630
H	1.181854870	-5.486419570	0.270763200
O	7.144898550	-3.424609720	0.180685210
O	2.112557380	0.605193700	0.553917770
H	-4.944562830	-1.949330660	0.270763200
O	-6.116808250	4.254505380	0.257746080
O	-0.135770000	1.909999740	0.558400360
O	4.754258210	0.693845450	0.244856620
H	5.775165300	-5.486419580	0.270763200
O	-0.129905420	-3.301419410	0.484742220
O	-2.223718190	2.123641440	-1.153750560
O	-4.915397670	2.209405040	-0.978327120
O	-3.643020070	-0.152444200	-1.063509880
O	1.975616790	-3.501561010	-1.160928530
O	4.685357850	-3.476494030	-0.963464650
O	3.313699010	-1.187269850	-1.005480030
O	-3.708764400	1.379870150	-3.193109390
O	3.448540180	-2.694420770	-3.187692090
O	-1.152857260	-2.481078880	-1.828843700
O	0.898380180	1.131647890	-1.786597760
O	-0.155621190	-0.676678540	-0.169102960
O	-0.124505850	-0.669197840	-3.498593740
H	-1.393369590	4.127843980	-4.174313340
O	-2.398659280	-1.958093360	-4.085238920
H	1.123299150	-5.514167830	-4.174313340
O	2.148841870	0.622402060	-4.062922330
H	-4.939315660	-2.013915540	-4.174313340
O	-0.138866930	1.938424370	-4.072906780
H	4.669245870	0.627591310	-4.174313340
O	-0.119226310	-3.279278820	-4.115713000
O	-2.450453390	2.159628400	-5.423139490
H	-4.944490580	2.083578020	-5.326221920
O	-3.795638080	-0.113237880	-5.422550100
O	2.199883320	-3.579266080	-5.416494530
H	4.674420430	-3.469902770	-5.326222030
O	3.482148340	-1.271046320	-5.435048540
H	-0.444164750	3.300924490	-6.244204220
H	-3.748580360	-2.422491560	-6.244204070
H	0.174094280	-4.687248820	-6.244204070

H	3.478510170	1.036167070	-6.244204220
Si	-3.835767900	1.419278260	2.210099120
Si	3.597361240	-2.830829210	2.207844320
Si	-1.585225550	2.632886740	0.276990540
Si	-5.903040780	2.636997510	0.275800360
Si	-3.748580370	-1.094637390	0.275800360
Si	1.324049720	-4.023321740	0.275800360
Si	5.632970560	-4.023321740	0.275800360
Si	3.470219210	-0.299716030	0.378225270
Si	-0.938490070	-2.102684220	-0.259374950
Si	0.687196680	0.710274850	-0.228171090
Si	-3.631527250	1.397063910	-1.591073720
Si	3.362038530	-2.726689440	-1.574952410
Si	-3.748580370	1.393118720	-4.822272780
Si	3.478510370	-2.779443320	-4.822272780
Si	-0.936291670	-2.083481690	-3.392097590
Si	0.691780440	0.739432490	-3.363393610
Si	-1.081547480	2.932931860	-4.971716630
Si	-3.748580360	-1.686505340	-4.971716630
Si	0.811477040	-4.319255710	-4.971716630
Si	3.478510570	0.300181120	-4.971716630
O	3.475560050	-2.891080710	3.826260930
O	-3.598839270	1.459221710	3.788596440
H	-5.988387600	6.755316850	0.214336190
H	-1.508773210	6.755316890	0.214336210
H	-2.135514420	5.565681860	-1.786532060
H	-5.361646310	5.565681860	-1.786532060
O	-3.746643580	5.519926440	0.206940760
Si	-2.189074680	5.565681860	-0.317508130
Si	-5.308086050	5.565681860	-0.317508130
H	7.002405980	1.841385300	0.214336210
H	9.242213140	-2.038074580	0.214336190
H	6.285522420	0.703793970	-1.786532060
H	7.898588370	-2.090118200	-1.786532060
O	7.049419800	-0.717072660	0.205401350
Si	6.312302550	0.657409430	-0.317508130
Si	7.871808240	-2.043733660	-0.317508130
H	2.640117660	-2.509296860	4.131276290
H	-0.022769000	2.086983290	2.534466180
Nd	-1.658020710	0.791475450	4.844987080
H	-3.243446210	2.916280050	4.817215030
H	0.605448390	2.557018800	3.887293890
H	-3.240798620	0.489478710	7.291433250
H	-4.249511390	1.059834860	6.263372200
O	0.079860030	2.003299090	6.149048280
O	-1.083917670	0.571790510	7.235959110
N	-0.149964740	1.434949240	7.255345320
O	0.947181900	-1.718393110	2.901768990
O	0.255128200	-0.770242150	4.702031280
O	-0.738817080	-0.383685480	2.842286470
N	0.179855520	-0.983747100	3.465847590

O	0.456451650	1.692074650	8.249654470
O	-3.641892130	0.326031330	6.424380610
O	-0.228485890	2.330190530	3.456537830
O	-2.870589510	-1.374974040	4.282132710
O	-2.668156880	3.013105430	5.608173750
H	-3.090427660	-1.299999060	3.338243450
H	-3.715371950	-1.323396760	4.747854840
H	-2.129598180	3.802333430	5.483807300

surf-T2-Nd:

O	-2.524603690	1.956517760	2.112257120
O	-5.188667620	2.181530810	1.932093810
O	-4.047868390	-0.211357580	1.766550910
O	2.183226050	-3.690797060	1.758074180
O	4.832010950	-3.719362100	1.912351050
O	3.532847300	-1.410752060	1.964510440
O	-1.448995080	4.148316580	0.618457320
H	-7.322402810	1.864467160	0.511773030
O	-2.395842570	-2.016600770	0.811392470
H	1.100677190	-5.650552840	0.511773030
O	7.058989170	-3.574262890	0.456972580
O	2.126275630	0.502484320	0.763507290
H	-5.025742810	-2.113462840	0.511773030
O	-6.220524500	4.083242600	0.432793580
O	-0.174075820	1.595935650	0.971971020
O	4.698930030	0.526279510	0.533265090
H	5.693987190	-5.650552840	0.511773030
O	-0.254644400	-3.536045340	0.673566450
O	-2.416175540	1.860023630	-0.841042160
O	-5.084055600	1.902582140	-0.734719480
O	-3.754660050	-0.443853210	-0.906394300
O	1.934594000	-3.676843720	-0.898444730
O	4.646857540	-3.661169680	-0.764761930
O	3.285660940	-1.376705140	-0.736612490
O	-3.832421790	1.189370950	-2.960350420
O	3.363953620	-2.847349120	-2.947247310
O	-1.313907750	-2.587439710	-1.574367710
O	0.782552080	0.981543090	-1.514971970
O	-0.041099830	-0.948294210	0.109483890
O	-0.191621950	-0.835708990	-3.236994540
H	-1.474552810	3.963717160	-3.933296970
O	-2.458155700	-2.138970820	-3.881690660
H	1.042117190	-5.678292840	-3.933296970
O	2.082365760	0.456026690	-3.786697840
H	-5.020492810	-2.178042840	-3.933296970
O	-0.205230670	1.778296110	-3.832648310
H	4.588067190	0.463457160	-3.933296970
O	-0.175156980	-3.453025870	-3.822095700
O	-2.525744270	1.990632780	-5.175353300
H	-5.025672810	1.919447160	-5.085206970
O	-3.862222350	-0.279108260	-5.189609580

O	2.118063270	-3.741631790	-5.176046330
H	4.593237190	-3.634032840	-5.085206970
O	3.398305700	-1.434780270	-5.194401320
H	-0.525342810	3.136797160	-6.003186970
H	-3.829762810	-2.586622840	-6.003186970
H	0.092917190	-4.851382840	-6.003186970
H	3.397327190	0.872037160	-6.003186970
Si	-3.967533900	1.256161280	2.496041890
Si	3.482991650	-2.986152470	2.477553970
Al	-1.693149870	2.421197620	0.602380090
Si	-5.984222810	2.472867160	0.516813030
Si	-3.829762810	-1.258762840	0.516813030
Si	1.242867190	-4.187452840	0.516813030
Si	5.551787190	-4.187452840	0.516813030
Si	3.432713400	-0.487720410	0.633454390
Si	-0.996615600	-2.263306310	-0.015394110
Si	0.640866210	0.527851230	0.044340170
Si	-3.763475860	1.143620350	-1.353750090
Si	3.313320710	-2.907259650	-1.338132110
Si	-3.829762810	1.228987160	-4.581256970
Si	3.397327190	-2.943572840	-4.581256970
Si	-1.020959370	-2.242390560	-3.146692050
Si	0.611884360	0.582604390	-3.103794820
Si	-1.162722810	2.768797160	-4.730706970
Si	-3.829762810	-1.850632840	-4.730706970
Si	0.730297190	-4.483382840	-4.730706970
Si	3.397327190	0.136047160	-4.730706970
O	3.468643010	-3.098198490	4.086840910
O	-4.099171450	0.980376520	4.103633450
H	-6.069562810	6.591187160	0.455353030
H	-1.589952810	6.591187160	0.455353030
H	-2.216692810	5.401557160	-1.545516970
H	-5.442822810	5.401557160	-1.545516970
O	-3.830909920	5.342548010	0.457753760
Si	-2.270252810	5.401557160	-0.076496970
Si	-5.389262810	5.401557160	-0.076496970
H	6.921227190	1.677257160	0.455353030
H	9.161037190	-2.202202840	0.455353030
H	6.204347190	0.539667160	-1.545516970
H	7.817407190	-2.254252840	-1.545516970
O	6.969804320	-0.879636480	0.441869480
Si	6.231127190	0.493277160	-0.076496970
Si	7.790627190	-2.207862840	-0.076496970
H	-3.611329030	1.525104710	4.748502550
H	2.666880460	-2.736430450	4.505738480
Nd	-0.468760020	1.711499190	3.590372620
H	-2.425802000	4.100845300	3.030100890
H	2.622005310	1.600155780	3.736034660
O	-0.219962260	2.927121040	5.680836760
O	-1.916576720	1.634169240	5.553548350
N	-1.279507100	2.508363000	6.227771190

O	1.205954210	-1.808599580	4.840952930
O	0.713446330	0.258907270	5.152035810
O	0.738987830	-0.528902900	3.166884090
N	0.898831080	-0.727695970	4.395658890
O	-1.662624880	2.897759450	7.284958050
O	2.035211130	1.982147810	3.071794060
O	-1.793866870	-0.454753410	3.726405200
O	-2.038477930	3.884987660	3.888486580
H	-1.856188050	-1.085619690	2.995618560
H	-2.690935260	-0.362164370	4.095224060
H	-1.424782500	4.604004690	4.086682260
H	2.165356750	1.442705860	2.259183780
O	0.313252970	3.968698070	2.629414690
H	1.237015460	3.828168080	2.383329190
H	-0.175570600	4.239435690	1.818736310

surf-T3-Nd:

O	-2.960599970	2.078474700	1.989776980
O	-5.580952770	1.866573080	2.014830280
O	-4.083034550	-0.342683990	1.987917830
O	1.744824590	-3.642493840	1.943753520
O	4.390184020	-3.860505300	2.021171590
O	3.312017950	-1.463836110	2.098984800
O	-1.727417360	4.073917580	0.666251230
H	-7.653635640	1.819411690	0.650384730
O	-2.924003220	-2.375382440	0.618880960
H	0.769437280	-5.695600740	0.650384730
O	6.724172610	-3.593062670	0.665108750
O	1.757289010	0.429517770	1.038023530
H	-5.356980420	-2.158511830	0.650384730
O	-6.513250430	4.050634840	0.673268870
O	-0.480300840	1.811998670	0.960900240
O	4.343056910	0.545843600	0.663940560
H	5.362747710	-5.695600750	0.650384730
O	-0.608538580	-3.634279550	0.646651460
O	-2.672909520	1.934413040	-0.647594490
O	-5.361251170	2.047860170	-0.647037820
O	-4.101247330	-0.333154390	-0.678059080
O	1.710950330	-3.761821090	-0.714420220
O	4.407713480	-3.629333070	-0.655317490
O	2.948544310	-1.396784860	-0.570974450
O	-4.058205580	1.210387040	-2.806703830
O	3.038997590	-2.867237670	-2.804434310
O	-1.298805430	-2.223187000	-1.509611100
O	0.308129520	0.480403720	-1.529236290
O	-0.701345300	-0.963446920	0.770521940
O	-0.546238430	-0.886088950	-3.683525700
H	-1.805787180	3.918662810	-3.794691810
O	-2.847789800	-2.240076400	-3.668371790
H	0.710881560	-5.723349000	-3.794691810
O	1.752782170	0.467068260	-3.709283330

H	-5.351733250	-2.223096710	-3.794691810
O	-0.531597470	1.778575310	-3.673502830
H	4.256828280	0.418410140	-3.794691810
O	-0.555924620	-3.557662280	-3.676864830
O	-2.862906220	1.950487890	-5.055112760
H	-5.356908170	1.874396850	-4.946600390
O	-4.189194770	-0.323489860	-5.031060000
O	1.778098630	-3.771510860	-5.027837930
H	4.262002840	-3.679083940	-4.946600500
O	3.081731360	-1.481827240	-5.054382990
H	-0.856582340	3.091743320	-5.864582690
H	-4.160997950	-2.631672730	-5.864582540
H	-0.238323310	-4.896429990	-5.864582540
H	3.066092580	0.826985900	-5.864582690
Si	-4.201236180	1.184056930	2.595936840
Si	3.110719700	-3.024596070	2.622679990
Si	-1.976007360	2.440790440	0.759175590
Si	-6.315458370	2.427816340	0.655421890
Si	-4.160997960	-1.303818560	0.655421890
Si	0.911632130	-4.232502910	0.655421890
Si	5.220552970	-4.232502910	0.655421890
Si	3.075337760	-0.510860820	0.804558210
Si	-1.374191250	-2.293233390	0.114109600
Al	0.208414320	0.386914840	0.152975990
Si	-4.055833910	1.216249980	-1.194008820
Si	3.027676420	-2.925234100	-1.193336610
Si	-4.160997960	1.183937550	-4.442651250
Si	3.066092780	-2.988624490	-4.442651250
Si	-1.311894190	-2.223958950	-3.135057830
Si	0.235399960	0.451408700	-3.127709710
Si	-1.493965070	2.723750690	-4.592095100
Si	-4.160997950	-1.895686510	-4.592095100
Si	0.399059450	-4.528436880	-4.592095100
Si	3.066092980	0.090999950	-4.592095100
O	3.026515360	-3.086853680	4.233083490
O	-4.168517310	1.158659290	4.211771980
H	-6.400805190	6.546135680	0.593957720
H	-1.921190800	6.546135720	0.593957740
H	-2.547932010	5.356500690	-1.406910530
H	-5.774063900	5.356500690	-1.406910530
O	-4.152533950	5.300479260	0.578831220
Si	-2.601492270	5.356500690	0.062113400
Si	-5.720503640	5.356500690	0.062113400
H	6.589988390	1.632204130	0.593957740
H	8.829795550	-2.247255750	0.593957720
H	5.873104830	0.494612800	-1.406910530
H	7.486170780	-2.299299370	-1.406910530
O	6.625402550	-0.922984510	0.579553330
Si	5.899884960	0.448228260	0.062113400
Si	7.459390650	-2.252914830	0.062113400
H	-3.535149910	1.750761170	4.650755360

H	3.228384810	-2.256608710	4.703438750
H	-0.085783230	4.321785330	1.367168510
H	1.791695840	4.082489400	4.995392450
H	1.501189320	4.652798160	3.571196120
O	-0.910953010	3.208448520	3.638447160
O	0.031634670	2.114765170	5.209365030
N	-1.013635170	2.664203500	4.769795180
O	-2.046320370	2.663171500	5.390315150
O	2.046416770	4.018062630	4.066748520
O	0.811179630	4.259072550	1.757571140
H	1.439777070	4.233603260	1.024773560
Nd	1.090000110	1.923575380	2.964010320
H	3.712067590	3.144237520	2.452480340
O	1.767408610	-0.135062970	4.217348430
H	3.651828920	2.109244110	1.302131450
O	3.253625280	1.387126030	4.122685770
N	2.940517420	0.224218500	4.485014200
O	3.151452220	2.836472680	1.726521310
O	-0.689098980	0.162626240	3.223530670
H	-0.415382620	-0.484386580	3.887300820
H	-0.899314600	-0.358108050	2.413965660
O	3.723035750	-0.505129630	5.042482970

bulk-T1-Yb:

H	-2.531359740	-8.493215440	0.783684680
H	-4.771132010	-4.613760280	0.783683520
H	-2.530394310	-8.509232580	5.041639960
H	-4.784559300	-4.604925540	5.041652240
O	2.284454020	-3.065590030	-4.865003080
O	-0.417891170	-3.045017400	-4.806458870
O	1.020253440	-5.361148730	-4.873255810
O	3.333930640	-1.009946580	-6.206290750
H	-2.500088690	-3.236915120	-6.201994850
H	2.188564830	-7.214850600	-6.201994960
H	-0.203383180	-7.214850600	-6.201994960
O	-1.387569350	-0.990826730	-6.169239590
H	4.485170340	-3.236915120	-6.201994850
O	2.342795250	-3.108034070	-7.545274460
O	-0.290311840	-3.014323060	-7.511224790
O	0.943508600	-5.415089000	-7.547615710
H	0.992590820	-3.872395730	-9.536018440
Si	0.969226440	-3.842688420	-4.311037920
Si	3.146990820	-2.628515730	-6.196918440
Si	-1.161909180	-2.628515730	-6.196918440
Si	0.992590820	-6.360145730	-6.196918440
Si	0.992590820	-3.872395730	-8.066018440
O	0.650690290	-3.599620280	-2.758743950
O	2.363275100	-3.100777900	-0.590248970
O	-0.496236790	-2.893799720	-0.582136450
O	0.809350060	-5.520422340	-0.645282330
O	3.372152950	-0.998856500	0.743625390

O	-2.744074330	-3.179662260	0.808964950
H	2.188564830	-7.214850600	0.727258080
O	-0.276901200	-7.393323060	0.870891070
O	-1.463536720	-0.962745440	0.967246460
H	4.485170340	-3.236915120	0.727257980
O	2.290641240	-2.996326740	2.104375100
O	-0.377982830	-3.146613830	2.105418320
O	1.045091010	-5.375045690	2.050716510
O	0.980726460	-3.876708680	4.241436440
O	-1.959542870	-7.332682020	2.931999570
O	-3.450239490	-4.625462760	2.927566440
O	-2.492900790	-5.875499910	0.787051640
O	-2.570588750	-5.926022090	5.085466150
O	3.347438410	-1.025744300	5.030170020
O	-2.653966690	-3.247905670	5.041960970
H	2.183290460	-7.279415010	5.172320540
O	-0.288163170	-7.319219740	5.018099730
O	-1.267089450	-1.044788780	5.047033310
H	4.538474060	-3.200057630	5.172323470
O	2.281813480	-3.088860660	6.428802580
O	-0.347088710	-3.148284310	6.438296400
O	0.999736980	-5.385782730	6.440330120
H	4.296967620	-1.964530270	7.242256850
H	-2.311885970	-1.964530270	7.242256850
H	0.992590820	-7.688024210	7.242256130
Al	0.925186650	-3.864426080	-1.074986000
Si	3.146990820	-2.628515730	0.722181560
Si	-1.223797680	-2.566844770	0.846373170
Si	0.992590820	-6.360145730	0.722181560
Si	-1.841209180	-7.309245730	1.315481560
Si	-3.400709180	-4.608095730	1.315481560
Si	1.011821620	-3.855770200	2.631680180
Si	0.982617570	-3.873079640	5.873217630
Si	-1.840909180	-7.309715730	4.544981560
Si	-3.401009180	-4.607625730	4.544981560
Si	3.659590820	-2.332575730	5.969781560
Si	-1.674509180	-2.332575730	5.969781560
Si	0.992590820	-6.952015730	5.969781560
O	-0.344575840	3.702415550	-4.868646530
O	2.327827960	3.719959000	-4.867821080
O	0.984979100	6.013328240	-4.851770480
O	-1.355636610	1.593340030	-6.169551770
H	4.485187410	3.837246100	-6.201994920
H	-0.203400330	7.815165130	-6.201995030
H	2.188581980	7.815165130	-6.201995030
O	3.313362380	1.605234520	-6.178508440
H	-2.500105770	3.837246100	-6.201994920
O	-0.334078750	3.648617950	-7.549430270
O	2.325377350	3.672660730	-7.547932740
O	0.979125880	6.016290670	-7.545344240
H	0.992590820	4.472784270	-9.536018440

H	2.605670280	0.300184270	-8.259241660
H	-0.620488640	0.300184270	-8.259241660
O	0.985425710	0.267853520	-6.299757390
Si	0.988752070	4.468024280	-4.318118870
Si	-1.161909180	3.228884270	-6.196918440
Si	3.146990820	3.228884270	-6.196918440
Si	0.992590820	6.960484270	-6.196918440
Si	2.552090820	0.300184270	-6.790218440
Si	-0.566909180	0.300184270	-6.790218440
Si	0.992590820	4.472784270	-8.066018440
O	0.955934320	4.471962080	-2.722740600
O	-0.373258590	3.719625430	-0.560926700
O	2.314185460	3.751596390	-0.584621820
O	0.946346090	6.031659720	-0.623019470
O	-1.343552780	1.602700680	0.745619140
H	4.485187410	3.837246100	0.727258040
O	-0.299321990	7.961289970	0.767126140
H	-4.771132210	5.214094530	0.783683440
H	2.188581980	7.815165130	0.727258160
O	3.283785200	1.605210310	0.693712150
O	-2.686082310	3.840322030	0.765457400
H	-2.531370000	9.093544440	0.783676770
O	-0.367489320	3.681722370	2.106969020
O	2.310491780	3.663355330	2.083760500
O	0.971281310	5.988210030	2.057337670
O	0.990135880	4.478616370	4.231664860
O	-0.449021740	0.407677480	2.961498600
O	-1.887308290	7.941121880	2.929008780
O	2.516761060	0.328814790	2.910759900
O	-3.449275840	5.229520580	2.928715000
O	0.984818120	0.210430630	0.766375510
O	-2.541119420	6.511450900	0.791220220
O	1.038788150	0.294241590	5.139801060
O	-2.580002730	6.534374900	5.078580650
O	-1.302227830	1.594719610	5.126031590
H	4.538454840	3.800401670	5.172340910
O	-0.294602120	7.926651480	5.035156190
H	-4.784559250	5.205256810	5.041652220
H	2.183301920	7.879723160	5.172312860
O	3.348108990	1.620249650	5.043896520
O	-2.639952600	3.851362580	5.030257340
H	-2.530397790	9.109598090	5.041642470
O	-0.339727920	3.743213780	6.421646110
O	2.285877010	3.696219050	6.425506280
O	0.998201820	5.985403890	6.433797480
H	-2.311891910	2.564890070	7.242268700
H	4.296973550	2.564890070	7.242268700
H	0.992590820	8.288372260	7.242267980
Si	0.957415350	4.473448380	-1.123814460
Si	-1.185596690	3.218531240	0.757232360
Si	3.146990820	3.228884270	0.722181560

Si	0.992590820	6.960484270	0.722181560
Si	-0.535626450	0.327052960	1.346634780
Si	-1.841209180	7.909584270	1.315481560
Si	2.543545650	0.280710730	1.287997770
Si	-3.400709180	5.208484270	1.315481560
Si	0.983626860	4.452920340	2.621482690
Si	0.986982690	4.474213970	5.863026690
Si	-0.498159940	0.303896570	4.575675740
Si	-1.840909180	7.910084270	4.544981560
Si	2.563054750	0.300241230	4.529547190
Si	-3.401009180	5.207984270	4.544981560
Si	-1.674509180	2.932884270	5.969781560
Si	3.659590820	2.932884270	5.969781560
Si	0.992590820	7.552384270	5.969781560
O	0.345772050	-0.690614700	-3.427258670
O	0.815483460	1.196088040	-2.478616510
O	-0.608051970	-0.174355580	-1.601448880
N	0.216856980	0.165951930	-2.499723320
H	-2.207110900	-0.355266500	-4.696463710
O	-2.416201510	-0.406351980	-3.745088870
H	-3.362179650	-0.592369210	-3.687837520
O	-3.077218210	-1.393080690	-1.296661110
H	-2.809541110	-0.609922940	-0.788701010
H	-3.348126380	-2.043616040	-0.620745450
Yb	-1.275199950	-2.146229440	-2.628199800
O	-3.169914850	-2.969158060	-3.786090330
N	-3.400800780	-3.944606930	-3.013711130
O	-2.582064230	-4.038429350	-2.045452270
O	-4.305450470	-4.701903490	-3.169820260
O	-1.034729760	-6.280483690	-2.749991400
H	-1.703125880	-5.801809510	-2.241456440
H	-0.292588470	-6.312090300	-2.130660680

bulk-T2-Yb:

H	-2.644670610	-8.638905840	0.716541040
H	-4.884442880	-4.759450680	0.716539880
H	-2.643705180	-8.654922980	4.974496320
H	-4.897870170	-4.750615940	4.974508600
O	2.224960900	-3.298885240	-4.950130530
O	-0.433971430	-3.160957140	-4.902707840
O	0.792297610	-5.539547640	-4.950255670
O	3.196116750	-1.146760910	-6.238450390
H	-2.613399560	-3.382605520	-6.269138490
H	2.075253960	-7.360541000	-6.269138600
H	-0.316694050	-7.360541000	-6.269138600
O	-1.462161040	-1.149870170	-6.289554580
H	4.371859470	-3.382605520	-6.269138490
O	2.191960660	-3.176248520	-7.619393580
O	-0.464432660	-3.243072130	-7.603353130
O	0.914670450	-5.565646550	-7.620990820
H	0.879279950	-4.018086130	-9.603162080

Si	0.876747050	-4.013838590	-4.383723250
Si	3.033679950	-2.774206130	-6.264062080
Si	-1.275220050	-2.774206130	-6.264062080
Si	0.879279950	-6.505836130	-6.264062080
Si	0.879279950	-4.018086130	-8.133162080
O	0.909937930	-4.145338920	-2.801389930
O	2.318062500	-3.527927200	-0.615552320
O	-0.289484630	-3.037118730	-0.723296720
O	0.657079130	-5.594730650	-0.688617690
O	2.934534760	-1.154211580	0.418303580
O	-2.773409900	-3.476124410	0.561935330
H	2.075253960	-7.360541000	0.660114440
O	-0.392077200	-7.526693460	0.770807260
O	-1.301245460	-1.008878100	0.342584060
H	4.371859470	-3.382605520	0.660114340
O	2.269259100	-3.144132300	2.066554850
O	-0.387104890	-3.139171420	2.204918590
O	0.932743210	-5.476800380	1.943754620
O	1.066486340	-4.133463180	4.201545550
O	-2.030039320	-7.489264300	2.865723760
O	-3.534119570	-4.746219520	2.862038170
O	-2.687929460	-6.089229080	0.721154070
O	-2.690386970	-6.074712270	5.017080870
O	3.120008250	-1.154186600	5.046455430
O	-2.780316300	-3.370312440	4.965125150
H	2.069979590	-7.425105410	5.105176900
O	-0.403853480	-7.459735590	4.956733290
O	-1.337389920	-1.103257680	5.170829400
H	4.425163190	-3.345748030	5.105179830
O	2.199237510	-3.264228250	6.421303580
O	-0.448040840	-3.320639220	6.284199570
O	0.884425750	-5.549319140	6.429034820
H	4.183656750	-2.110220670	7.175113210
H	-2.425196840	-2.110220670	7.175113210
H	0.879279950	-7.833714610	7.175112490
Si	0.891802620	-4.057511180	-1.199378210
Si	3.033679950	-2.774206130	0.655037920
Al	-1.228944830	-2.738622480	0.759745750
Si	0.879279950	-6.505836130	0.655037920
Si	-1.954520050	-7.454936130	1.248337920
Si	-3.514020050	-4.753786130	1.248337920
Si	0.942990820	-3.968764640	2.597698400
Si	0.916816730	-4.050446750	5.819304060
Si	-1.954220050	-7.455406130	4.477837920
Si	-3.514320050	-4.753316130	4.477837920
Si	3.546279950	-2.478266130	5.902637920
Si	-1.787820050	-2.478266130	5.902637920
Si	0.879279950	-7.097706130	5.902637920
O	-0.465331320	3.550143190	-4.922241710
O	2.199679200	3.551812910	-4.932715210
O	0.876373340	5.864966330	-4.913801780

O	-1.449207610	1.448639660	-6.201809780
H	4.371876540	3.691555700	-6.269138560
H	-0.316711200	7.669474730	-6.269138670
H	2.075271110	7.669474730	-6.269138670
O	3.203194140	1.462419970	-6.257796730
H	-2.613416640	3.691555700	-6.269138560
O	-0.437692650	3.489894970	-7.610346900
O	2.215816200	3.537238680	-7.612755440
O	0.854061220	5.867533640	-7.607762030
H	0.879279950	4.327093870	-9.603162080
H	2.492359410	0.154493870	-8.326385300
H	-0.733799510	0.154493870	-8.326385300
O	0.872940460	0.164735050	-6.305074880
Si	0.872960210	4.321631350	-4.384392440
Si	-1.275220050	3.083193870	-6.264062080
Si	3.033679950	3.083193870	-6.264062080
Si	0.879279950	6.814793870	-6.264062080
Si	2.438779950	0.154493870	-6.857362080
Si	-0.680220050	0.154493870	-6.857362080
Si	0.879279950	4.327093870	-8.133162080
O	0.835888890	4.280458830	-2.784517730
O	-0.442710230	3.530719220	-0.625338650
O	2.226064140	3.745877410	-0.608044070
O	0.732666760	5.935049620	-0.724168360
O	-1.469606980	1.523570510	0.683164470
H	4.371876540	3.691555700	0.660114400
O	-0.398452910	7.822891970	0.753963150
H	-4.884443080	5.068404130	0.716539800
H	2.075271110	7.669474730	0.660114520
O	3.124630280	1.467234460	0.483889680
O	-2.772903450	3.727897850	0.660352020
H	-2.644680870	8.947854040	0.716533130
O	-0.477532840	3.584393280	2.079867220
O	2.201001960	3.433619580	2.046994930
O	0.942847400	5.803582200	1.953333640
O	0.917622860	4.361011230	4.185849770
O	-1.298145300	-0.003995520	2.827640320
O	-2.026435550	7.792301480	2.862104350
O	3.038251870	0.111161120	2.759968690
O	-3.539861720	5.061113390	2.859192050
O	0.846982330	0.343641390	1.347053910
O	-2.650723280	6.366787530	0.720543360
O	0.891200860	0.168231430	4.384106640
O	-2.692103390	6.387358790	5.009989590
O	-1.316242840	1.520663980	4.993732810
H	4.425143970	3.654711270	5.105197270
O	-0.402007980	7.773398300	4.951870770
H	-4.897870120	5.059566410	4.974508580
H	2.069991050	7.734032760	5.105169220
O	3.124618250	1.487837860	5.003932190
O	-2.771838250	3.704155320	4.982578460

H	-2.643708660	8.963907690	4.974498830
O	-0.460814200	3.617994650	6.363469060
O	2.192827430	3.581868510	6.387538410
O	0.876969880	5.848990490	6.388292180
H	-2.425202780	2.419199670	7.175125060
H	4.183662680	2.419199670	7.175125060
H	0.879279950	8.142681860	7.175124340
Si	0.847395510	4.374125100	-1.184472940
Si	-1.270721430	3.127268280	0.730482340
Si	3.033679950	3.083193870	0.655037920
Si	0.879279950	6.814793870	0.655037920
Si	-0.769003940	0.185650370	1.307123300
Si	-1.954520050	7.763893870	1.248337920
Si	2.465481680	0.176976080	1.234312270
Si	-3.514020050	5.062793870	1.248337920
Si	0.916638140	4.294871110	2.581556930
Si	0.880927950	4.335547360	5.823248270
Si	-0.739005530	0.146009360	4.354199470
Si	-1.954220050	7.764393870	4.477837920
Si	2.523088890	0.151857680	4.307518930
Si	-3.514320050	5.062293870	4.477837920
Si	-1.787820050	2.787193870	5.902637920
Si	3.546279950	2.787193870	5.902637920
Si	0.879279950	7.406693870	5.902637920
O	1.075632860	-1.449629900	-2.730038740
O	2.616962180	0.033600860	-2.437041590
O	-2.957120340	-0.989148270	-3.547811710
O	-3.455822320	-0.930312940	-1.472836090
O	0.726581760	0.174247630	-1.400456910
Yb	-1.158894400	-1.140797590	-2.015499310
N	1.531957850	-0.395417610	-2.193740150
O	-5.000891240	-0.619091170	-2.950455550
N	-3.860596520	-0.832166350	-2.665624690
H	-2.977601790	-3.295799950	-2.969487910
O	-2.217053060	-3.303173970	-2.377181000
H	-2.532975150	-3.626304160	-1.511634920
O	-0.537774040	0.193288420	-3.838226770
O	-1.901923570	1.109414500	-1.910964190
H	-2.367062150	1.239135400	-1.070290110
H	-1.166989070	1.740774740	-1.888001400
H	0.201855080	0.062663000	-4.450826010
H	-1.253237270	0.630244440	-4.323111440

bulk-T3-Yb:

H	-2.461220600	-8.741370290	0.717919320
H	-4.700992870	-4.861915130	0.717918160
H	-2.460255170	-8.757387430	4.975874600
H	-4.714420160	-4.853080390	4.975886880
O	2.461107860	-3.393587270	-4.906758510
O	-0.182481990	-3.336714970	-4.986918280
O	1.076556380	-5.685826680	-4.896992760

O	3.393007010	-1.252363910	-6.237812560
H	-2.429949550	-3.485069970	-6.267760210
H	2.258703970	-7.463005450	-6.267760320
H	-0.133244040	-7.463005450	-6.267760320
O	-1.274147710	-1.254282530	-6.265663080
H	4.555309480	-3.485069970	-6.267760210
O	2.383862000	-3.307124620	-7.604375380
O	-0.282388220	-3.332084120	-7.628415160
O	1.079536760	-5.664527830	-7.605616850
H	1.062729960	-4.120550580	-9.601783800
Si	1.097441690	-4.131615810	-4.401972770
Si	3.217129960	-2.876670580	-6.262683800
Si	-1.091770040	-2.876670580	-6.262683800
Si	1.062729960	-6.608300580	-6.262683800
Si	1.062729960	-4.120550580	-8.131783800
O	1.083583030	-4.082858130	-2.798608690
O	2.229076480	-3.344642010	-0.564092400
O	-0.449171880	-3.608132540	-0.717181310
O	1.095788270	-5.762077670	-0.749720210
O	3.445361040	-1.259738500	0.604292700
O	-2.644429820	-3.417373520	0.816770550
H	2.258703970	-7.463005450	0.661492720
O	-0.225497750	-7.609480160	0.716519920
O	-1.208105500	-1.269113880	0.296152310
H	4.555309480	-3.485069970	0.661492620
O	2.455755330	-3.295106420	2.073278170
O	-0.205112120	-3.160804200	1.908779010
O	0.992456280	-5.547586320	1.919754090
O	0.955883730	-4.080001150	4.125452280
O	-1.829887090	-7.586236460	2.862044900
O	-3.409367280	-4.915651360	2.862966540
O	-2.438241320	-6.132417190	0.720660390
O	-2.501589560	-6.177913870	5.015413650
O	3.430587660	-1.261311040	4.971786920
O	-2.568063920	-3.493110680	4.944914400
H	2.253429600	-7.527569860	5.106555180
O	-0.223110990	-7.584521520	4.966954050
O	-1.201016190	-1.254108170	5.068151000
H	4.608613200	-3.448212480	5.106558110
O	2.336370280	-3.333670710	6.308700460
O	-0.292215370	-3.419252970	6.377969740
O	1.081353690	-5.624245980	6.320304910
H	4.367106760	-2.212685120	7.176491490
H	-2.241746830	-2.212685120	7.176491490
H	1.062729960	-7.936179060	7.176490770
Si	0.993917670	-4.201511180	-1.210631440
Si	3.217129960	-2.876670580	0.656416200
Si	-1.118685660	-2.869860240	0.572222050
Si	1.062729960	-6.608300580	0.656416200
Si	-1.771070040	-7.557400580	1.249716200
Si	-3.330570040	-4.856250580	1.249716200

Si	1.057351730	-4.020705330	2.516046290
Si	1.029834940	-4.109468340	5.760904490
Si	-1.770770040	-7.557870580	4.479216200
Si	-3.330870040	-4.855780580	4.479216200
Si	3.729729960	-2.580730580	5.904016200
Si	-1.604370040	-2.580730580	5.904016200
Si	1.062729960	-7.200170580	5.904016200
O	-0.256503330	3.484991770	-4.948781590
O	2.412241440	3.468101380	-4.923134540
O	1.083116140	5.787013690	-4.901280750
O	-1.247849360	1.359113090	-6.241316030
H	4.555326550	3.589091250	-6.267760280
H	-0.133261190	7.567010280	-6.267760390
H	2.258721120	7.567010280	-6.267760390
O	3.396118410	1.358077680	-6.246225870
H	-2.429966630	3.589091250	-6.267760280
O	-0.264637010	3.419077890	-7.616880010
O	2.398425190	3.429513760	-7.610142510
O	1.061790500	5.769753330	-7.607279940
H	1.062729960	4.224629420	-9.601783800
H	2.675809420	0.052029420	-8.325007020
H	-0.550349500	0.052029420	-8.325007020
O	1.065912270	0.044855990	-6.337852760
Si	1.071231210	4.233519480	-4.399736540
Si	-1.091770040	2.980729420	-6.262683800
Si	3.217129960	2.980729420	-6.262683800
Si	1.062729960	6.712329420	-6.262683800
Si	2.622229960	0.052029420	-6.855983800
Si	-0.496770040	0.052029420	-6.855983800
Si	1.062729960	4.224629420	-8.131783800
O	1.071885550	4.210144950	-2.798179500
O	-0.381270390	3.606741830	-0.680665870
O	2.290972740	3.406558840	-0.623589080
O	1.103119490	5.811473070	-0.712888290
O	-1.359680730	1.340230930	0.383199240
H	4.555326550	3.589091250	0.661492680
O	-0.233637270	7.707094670	0.688714730
H	-4.700993070	4.965939680	0.717918080
H	2.258721120	7.567010280	0.661492800
O	3.530737320	1.376292590	0.662031330
O	-2.656633170	3.563551140	0.680439340
H	-2.461230860	8.845389590	0.717911410
O	-0.292548170	3.291436550	1.962691190
O	2.379851290	3.398539510	2.026537100
O	0.956017120	5.672924300	1.942124080
O	0.957854860	4.184552120	4.133641870
O	-0.527061050	0.022326150	2.869682680
O	-1.818005720	7.685590530	2.860881500
O	2.627477990	0.032950760	2.797503470
O	-3.371081660	4.958301670	2.857435340
O	1.187019320	0.171488980	0.540236730

O	-2.462383500	6.249565240	0.724102860
O	1.110598240	0.056930780	4.992040850
O	-2.515793490	6.289121010	5.004206580
O	-1.191439750	1.384212100	5.030555610
H	4.608593980	3.552246820	5.106575550
O	-0.226370640	7.684483490	4.970371720
H	-4.714420110	4.957101960	4.975886860
H	2.253441060	7.631568310	5.106547500
O	3.423564390	1.379127670	4.953254310
O	-2.578079070	3.606237260	4.969734610
H	-2.460258650	8.861443240	4.975877110
O	-0.294218680	3.524884750	6.385120240
O	2.338126090	3.439271610	6.316616960
O	1.080650350	5.729479310	6.323814410
H	-2.241752770	2.316735220	7.176503340
H	4.367112690	2.316735220	7.176503340
H	1.062729960	8.040217410	7.176502620
Si	1.023253220	4.256006660	-1.207449770
Si	-1.129747400	2.938737820	0.596054250
Si	3.217129960	2.980729420	0.656416200
Si	1.062729960	6.712329420	0.656416200
Al	-0.426640220	0.045160170	1.186445590
Si	-1.771070040	7.661429420	1.249716200
Si	2.683206760	0.073375390	1.170335160
Si	-3.330570040	4.960329420	1.249716200
Si	1.009657520	4.138968230	2.522995100
Si	1.030070930	4.212190440	5.770070100
Si	-0.446633870	0.051981680	4.464670120
Si	-1.770770040	7.661929420	4.479216200
Si	2.645545090	0.051836130	4.425312980
Si	-3.330870040	4.959829420	4.479216200
Si	-1.604370040	2.684729420	5.904016200
Si	3.729729960	2.684729420	5.904016200
Si	1.062729960	7.304229420	5.904016200
H	-3.641187640	2.409266630	-0.169882810
O	-3.998104730	0.265499690	-3.033085000
O	-2.279929440	1.531263890	-3.137627240
N	-3.380970070	1.183181680	-3.656832760
O	-3.821811720	1.696774080	-4.641887930
O	-3.964507020	1.677028430	-0.734686260
H	-4.489409710	2.066616150	-1.442161120
Yb	-2.349899440	0.017805520	-1.366531830
H	-4.750581340	-0.544983330	0.260651570
H	-3.700202470	-1.669658820	0.538228030
O	-3.810921100	-0.714015880	0.388620230
O	-0.070389870	0.401227330	-1.862382140
H	0.230886300	-0.075555710	-2.646165650
H	0.623700770	0.331238590	-1.172050770
O	-3.123152810	-2.127586600	-1.748447150
O	-1.658982940	-1.396339600	-3.098492630
N	-2.479303530	-2.317447990	-2.823033340

O -2.647646900 -3.278554820 -3.508052080

surf-silanol-Yb:

O -2.392735430 2.353853310 1.706879580
O -5.047115890 2.318959800 1.748153780
O -3.763224320 0.037603570 1.534287370
O 2.401803830 -3.528178390 1.543357470
O 5.031825760 -3.509844970 1.747091580
O 3.700897950 -1.207476330 1.727004250
O -1.273979680 4.288081410 0.308087360
H -7.148838840 2.071000840 0.319903970
O -2.318282320 -1.966213820 0.511747790
H 1.274234080 -5.444011590 0.319903970
O 7.235829490 -3.375613400 0.252298350
O 2.212668980 0.677149550 0.592106550
H -4.852183620 -1.906922680 0.319903970
O -6.039899550 4.291630180 0.257747890
O -0.026181670 1.965618840 0.585364640
O 4.848486160 0.741967360 0.297454500
H 5.867544510 -5.444011600 0.319903970
O -0.049247850 -3.279873880 0.508664000
O -2.202736870 2.100707570 -0.977245980
O -4.867982160 2.165809740 -0.929880610
O -3.557895990 -0.205554460 -1.099150080
O 2.096359490 -3.472321120 -1.100487960
O 4.803086670 -3.426032340 -0.930596220
O 3.407456090 -1.146103850 -0.946977740
O -3.576171490 1.457260910 -3.140254070
O 3.542084170 -2.643178790 -3.138388890
O -1.047582320 -2.376227480 -1.776320140
O 0.964577680 1.124359230 -1.749145880
O -0.046239390 -0.644270210 -0.034992410
O -0.030846830 -0.631341700 -3.517305080
H -1.300990380 4.170251960 -4.125172570
O -2.305513220 -1.932908850 -4.045471340
H 1.215678360 -5.471759850 -4.125172570
O 2.246162970 0.675900750 -4.012942290
H -4.846936450 -1.971507560 -4.125172570
O -0.043933020 1.992238280 -4.014524730
H 4.761625080 0.669999290 -4.125172570
O -0.026793670 -3.253843710 -4.045496780
O -2.354067640 2.196471620 -5.381309010
H -4.852111370 2.125986000 -5.277081150
O -3.704466560 -0.070592380 -5.365125090
O 2.289593350 -3.531921120 -5.365832330
H 4.766799640 -3.427494790 -5.277081260
O 3.572034950 -1.228281430 -5.385282350
H -0.351785540 3.343332470 -6.195063450
H -3.656201150 -2.380083580 -6.195063300
H 0.266473490 -4.644840840 -6.195063300
H 3.570889380 1.078575050 -6.195063450

Si	-3.726954410	1.494219260	2.285588210
Si	3.664314080	-2.766766770	2.264688900
Si	-1.497022890	2.675701300	0.380542610
Si	-5.810661570	2.679405490	0.324941130
Si	-3.656201160	-1.052229410	0.324941130
Si	1.416428930	-3.980913760	0.324941130
Si	5.725349770	-3.980913760	0.324941130
Si	3.562168850	-0.246056190	0.427603810
Si	-0.853883670	-2.056207580	-0.193024160
Si	0.780171770	0.740993590	-0.184646660
Si	-3.570946200	1.369922480	-1.534912270
Si	3.469137700	-2.683028920	-1.526354170
Si	-3.656201160	1.435526700	-4.773132010
Si	3.570889580	-2.737035340	-4.773132010
Si	-0.844313050	-2.039723710	-3.353226130
Si	0.778843060	0.772112420	-3.337085150
Si	-0.989168270	2.975339840	-4.922575860
Si	-3.656201150	-1.644097360	-4.922575860
Si	0.903856250	-4.276847730	-4.922575860
Si	3.570889780	0.342589100	-4.922575860
O	3.549562000	-2.806431430	3.883118090
O	-3.445922680	1.389597430	3.849705940
H	-5.896008390	6.797724830	0.263476960
H	-1.416394000	6.797724870	0.263476980
H	-2.043135210	5.608089840	-1.737391290
H	-5.269267100	5.608089840	-1.737391290
O	-3.652442010	5.544035420	0.264334090
Si	-2.096695470	5.608089840	-0.268367360
Si	-5.215706840	5.608089840	-0.268367360
H	7.094785190	1.883793280	0.263476980
H	9.334592350	-1.995666600	0.263476960
H	6.377901630	0.746201950	-1.737391290
H	7.990967580	-2.047710220	-1.737391290
O	7.138593250	-0.675799850	0.253534980
Si	6.404681760	0.699817410	-0.268367360
Si	7.964187450	-2.001325680	-0.268367360
H	2.740546710	-2.375500520	4.198704190
H	0.469127740	2.230881410	2.284823960
Yb	-1.398385250	1.556584180	4.543001440
H	-2.274354460	3.886347860	3.219912000
H	1.235318020	2.395150700	3.645674830
O	-0.016941860	2.926229870	5.874489570
O	-1.660432150	1.937289120	6.806292520
N	-0.659074780	2.711165410	6.946253830
O	0.903531570	-1.495652370	3.472489120
O	0.424888480	0.089817170	4.858688280
O	-0.761961910	-0.174643260	3.105164840
N	0.214978270	-0.566477230	3.804217930
O	-0.357576780	3.190501240	7.992268220
O	0.370203100	2.479199690	3.226445170
O	-2.427789610	-0.366445130	5.506570410

O	-1.943706870	3.825031220	4.129121960
H	-3.282589390	-0.169149660	5.081501050
H	-2.559781770	-0.251069860	6.456280760
H	-1.118101740	4.327222040	4.148777080

surf-T2-Yb:

O	-2.458263220	1.974888680	2.200467340
O	-5.128662050	2.264943880	1.898481800
O	-4.035150000	-0.146095990	1.777809510
O	2.216383890	-3.663253310	1.752112880
O	4.857912300	-3.589353050	1.901362410
O	3.455013040	-1.327564310	1.997248540
O	-1.454142380	4.210019170	0.611084360
H	-7.321411160	1.934941900	0.511358180
O	-2.381785280	-1.924530770	0.802090630
H	1.101661760	-5.580070530	0.511358180
O	7.062191080	-3.510573660	0.441284410
O	2.124160960	0.581867100	0.725941610
H	-5.024755940	-2.042981620	0.511358180
O	-6.221428690	4.152356220	0.434433140
O	-0.207307570	1.591717980	0.995168220
O	4.706772240	0.575785240	0.557816440
H	5.694972190	-5.580070540	0.511358180
O	-0.242402130	-3.447211530	0.687856360
O	-2.465118150	1.913808470	-0.763623220
O	-5.130893850	1.959465070	-0.765469590
O	-3.788422510	-0.381229670	-0.911453320
O	1.927313890	-3.602620670	-0.901403030
O	4.639011130	-3.623415880	-0.771989760
O	3.311381650	-1.325602650	-0.716266990
O	-3.796973750	1.267915730	-2.957463510
O	3.363620780	-2.772317440	-2.946747210
O	-1.343331650	-2.576547050	-1.580019270
O	0.776879660	1.117404950	-1.527269840
O	-0.023944230	-0.890512280	-0.028000500
O	-0.189975280	-0.771325560	-3.183343940
H	-1.473562700	4.034193020	-3.933718360
O	-2.450243630	-2.055182040	-3.889655890
H	1.043106040	-5.607818790	-3.933718360
O	2.081236470	0.511149620	-3.782648520
H	-5.019508770	-2.107566500	-3.933718360
O	-0.208123600	1.828634770	-3.856703890
H	4.589052760	0.533940350	-3.933718360
O	-0.170206010	-3.375110190	-3.829363250
O	-2.528616160	2.066047570	-5.181333710
H	-5.024683690	1.989927060	-5.085626940
O	-3.872055590	-0.208361050	-5.188110430
O	2.121397060	-3.674519190	-5.175954720
H	4.594227320	-3.563553730	-5.085627050
O	3.402985780	-1.364583300	-5.196300940
H	-0.524357860	3.207273530	-6.003609240

H	-3.828773470	-2.516142520	-6.003609090
H	0.093901170	-4.780899780	-6.003609090
H	3.398317060	0.942516110	-6.003609240
Si	-3.946641100	1.323593590	2.504632000
Si	3.484753010	-2.916805550	2.479048970
Al	-1.701935970	2.492275070	0.651639340
Si	-5.983233890	2.543346550	0.516395340
Si	-3.828773480	-1.188288350	0.516395340
Si	1.243856610	-4.116972700	0.516395340
Si	5.552777450	-4.116972700	0.516395340
Si	3.425518400	-0.420630070	0.644231200
Si	-0.993707650	-2.198795910	-0.036649080
Si	0.636275780	0.592353300	0.008377330
Si	-3.788338400	1.211121940	-1.347897690
Si	3.315039330	-2.847956300	-1.338165800
Si	-3.828773480	1.299467760	-4.581677800
Si	3.398317260	-2.873094280	-4.581677800
Si	-1.023708920	-2.179589570	-3.136885640
Si	0.610510650	0.653711620	-3.101459130
Si	-1.161740590	2.839280900	-4.731121650
Si	-3.828773470	-1.780156300	-4.731121650
Si	0.731283930	-4.412906670	-4.731121650
Si	3.398317460	0.206530160	-4.731121650
O	3.519183680	-3.056499850	4.091643060
O	-4.141263250	1.059806150	4.116042900
H	-6.068580710	6.661665890	0.454931170
H	-1.588966320	6.661665930	0.454931190
H	-2.215707530	5.472030900	-1.545937080
H	-5.441839420	5.472030900	-1.545937080
O	-3.832141390	5.419910860	0.443277180
Si	-2.269267790	5.472030900	-0.076913150
Si	-5.388279160	5.472030900	-0.076913150
H	6.922212870	1.747734340	0.454931190
H	9.162020030	-2.131725540	0.454931170
H	6.205329310	0.610143010	-1.545937080
H	7.818395260	-2.183769160	-1.545937080
O	6.975713240	-0.807414620	0.440664610
Si	6.232109440	0.563758470	-0.076913150
Si	7.791615130	-2.137384620	-0.076913150
H	-3.673786880	1.682667100	4.703595310
H	2.691840380	-2.807157940	4.530379710
Yb	-0.477260420	1.441347970	3.397109420
H	-0.754592770	4.189651160	2.172767720
H	2.375079960	1.624626690	3.734785040
O	0.153540820	2.574443210	5.349991180
O	-1.906493050	2.134144980	5.071091530
N	-1.014700820	2.701747980	5.797019980
O	0.991506840	-2.123187060	4.222282110
O	0.711215870	-0.059206660	4.785113320
O	0.405264800	-0.649882970	2.765041430
N	0.720604030	-0.984380340	3.941099620

O	-1.287205560	3.289613050	6.792961600
O	1.792622640	1.974105090	3.047986390
O	-1.924483360	-0.434447710	3.809436750
O	-0.384198930	3.769754430	2.987682730
H	-2.054838220	-1.086682460	3.105589420
H	-2.811200730	-0.216860980	4.161842950
H	0.540281230	4.041240180	3.048035290
H	2.076749850	1.565622290	2.200185460

surf-T3-Yb:

O	-2.975308000	2.080596410	1.963837060
O	-5.583548150	1.873634420	2.079292610
O	-4.073615800	-0.335973910	2.053246970
O	1.776322000	-3.609202630	1.993772580
O	4.419708050	-3.873721170	2.091821920
O	3.397073970	-1.460854130	2.076438630
O	-1.696474980	4.103394240	0.739198700
H	-7.628806310	1.841616420	0.703514350
O	-2.907935630	-2.366982320	0.672447030
H	0.794266610	-5.673396010	0.703514350
O	6.748908860	-3.571946230	0.716337340
O	1.753741530	0.438884190	1.101911260
H	-5.332151090	-2.136307100	0.703514350
O	-6.488803670	4.072047200	0.725483550
O	-0.453795090	1.817505710	1.029287350
O	4.348868890	0.585176480	0.683411730
H	5.387577040	-5.673396020	0.703514350
O	-0.586789390	-3.618582600	0.708614140
O	-2.602344900	1.971705190	-0.642848460
O	-5.304245460	2.077514860	-0.574332470
O	-4.039479180	-0.297924880	-0.612731900
O	1.726944570	-3.733823730	-0.663324730
O	4.418913070	-3.570720350	-0.576226320
O	2.926710870	-1.345716170	-0.559764320
O	-4.041339840	1.227485820	-2.753574930
O	3.067477350	-2.857338510	-2.752272060
O	-1.276908430	-2.218725620	-1.460177710
O	0.328331100	0.505377050	-1.487219970
O	-0.691171170	-0.952138110	0.804046400
O	-0.524470440	-0.870609850	-3.631919390
H	-1.780957850	3.940867540	-3.741562190
O	-2.826730370	-2.222852270	-3.612769700
H	0.735710890	-5.701144270	-3.741562190
O	1.776561890	0.483383770	-3.657471880
H	-5.326903920	-2.200891980	-3.741562190
O	-0.505071840	1.796183850	-3.629575880
H	4.281657610	0.440614870	-3.741562190
O	-0.534854700	-3.540981520	-3.624508930
O	-2.838715090	1.973848200	-5.000184450
H	-5.332078840	1.896601580	-4.893470770
O	-4.158587660	-0.301640110	-4.978291520

O	1.799865480	-3.744225100	-4.974529240
H	4.286832170	-3.656879210	-4.893470880
O	3.108716710	-1.459645460	-4.999098520
H	-0.831753010	3.113948050	-5.811453070
H	-4.136168620	-2.609468000	-5.811452920
H	-0.213493980	-4.874225260	-5.811452920
H	3.090921910	0.849190630	-5.811453070
Si	-4.188826500	1.203305450	2.637542390
Si	3.154554920	-2.991555640	2.655528650
Si	-1.943819670	2.473147400	0.787306730
Si	-6.290629040	2.450021070	0.708551510
Si	-4.136168630	-1.281613830	0.708551510
Si	0.936461460	-4.210298180	0.708551510
Si	5.245382300	-4.210298180	0.708551510
Si	3.087391050	-0.480226220	0.825517140
Si	-1.362571040	-2.290419610	0.160110770
Al	0.217195070	0.396996260	0.186103290
Si	-4.005209570	1.248926440	-1.141338940
Si	3.038484730	-2.889073890	-1.142702830
Si	-4.136168630	1.206142280	-4.389521630
Si	3.090922110	-2.966419760	-4.389521630
Si	-1.290762610	-2.208503460	-3.085396670
Si	0.257531000	0.469450790	-3.085552760
Si	-1.469135740	2.745955420	-4.538965480
Si	-4.136168620	-1.873481780	-4.538965480
Si	0.423888780	-4.506232150	-4.538965480
Si	3.090922310	0.113204680	-4.538965480
O	3.075869950	-2.969251620	4.270946340
O	-4.119512110	1.215056390	4.251137020
H	-6.375975860	6.568340410	0.647087340
H	-1.896361470	6.568340450	0.647087360
H	-2.523102680	5.378705420	-1.353780910
H	-5.749234570	5.378705420	-1.353780910
O	-4.128082430	5.320282820	0.630607340
Si	-2.576662940	5.378705420	0.115243020
Si	-5.695674310	5.378705420	0.115243020
H	6.614817720	1.654408860	0.647087360
H	8.854624880	-2.225051020	0.647087340
H	5.897934160	0.516817530	-1.353780910
H	7.511000110	-2.277094640	-1.353780910
O	6.641240920	-0.904185600	0.635973770
Si	5.924714290	0.470432990	0.115243020
Si	7.484219980	-2.230710100	0.115243020
H	-3.4211131120	1.728245310	4.691509680
H	3.232226860	-2.107978580	4.693229880
H	-0.007418150	4.316575890	1.886870820
O	0.865114210	4.066007780	2.243330020
H	1.527073900	4.280203050	1.573960050
Yb	0.982571130	1.809617900	2.926445500
H	3.540117290	2.096558400	1.347658070
O	1.877791990	-0.072039410	3.995119980

H	3.669032750	2.760605850	2.724596350
O	2.956155510	1.716438490	4.381059250
N	2.866798870	0.472568540	4.553572430
O	3.085760880	2.719733420	1.950923870
O	-0.597962280	0.088422260	3.212238570
H	-0.264476130	-0.564975670	3.841849420
H	-0.842757750	-0.417208980	2.397410460
O	3.668788120	-0.164855680	5.182406450
O	0.241614900	1.928131740	5.145503590
O	-0.971028380	2.878377660	3.687302410
N	-0.890017180	2.392787270	4.844546360
O	-1.829591570	2.352632760	5.594632210