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Supporting Information

Titanium Defective Sites in TS-1: Structural Insights by Combining Spectroscopy and Simulation

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S1. Experimental details

S1.1. Characterization

A multi-technique approach has been applied to the characterization of the two TS-1 catalysts, employing diffuse reflectance UV-vis spectroscopy, X-ray absorption near edge structure (XANES) spectroscopy at Ti K-edge and near edge X-ray absorption fine structure (NEXAFS) spectroscopy at the and $L_{2,3}$- edges of Ti.

UV-vis spectra were measured with a Varian Cary5000 spectrophotometer, equipped with a diffuse reflectance sphere. The samples were measured in pure form (i.e. without dilution in a non-absorbing matrix) in a home-made bulb quartz cell, allowing thermal treatments to be performed. All the materials were measured after heating up to 500 °C with a ramp of 5 °C/min under dynamic vacuum (< 10^{-3} mbar); after 1 hour of outgassing at 500 °C, 50 mbar of pure O_2 were dosed in the cell and left in contact for 1 further hour in order to oxidize the residuals of organic pollutants. The same sample treatment has been adopted for all the measurements described hereafter.

Ti K-edge XANES spectra were collected at the XAFS beamline of Elettra Sincrotrone Trieste. The samples were prepared in the form of self-supporting pellets, then activated (by

following the same protocol described for UV-vis) and measured in a home-made quartz cell equipped with x-ray transparent Kapton windows. Spectra were collected in transmission mode using three ionization chambers. A Ti metal foil was positioned after the second ionization chamber for on-line energy calibration. The white beam emitted from the bending magnet source was monochromatized by a double Si(111) monochromator, detuned to 50% to minimize the third harmonic contamination. The energy resolution was $\Delta E/E < 10^{-4}$ (i.e. < 0.5 eV at 5000 eV). XANES spectra were collected with a step of 5.0 eV in the pre-edge region (4750-4940 eV), that progressively reduces to 0.25 eV in the edge region (4965-5000 eV), and progressively increases in the post edge region in order to guarantee an excellent evaluation of the edge jump. The data were normalized using VIPER software,[1,2] because it provides a procedure for taking in account the μ displacement, due to the energy dependence in (i) source/optics properties, (ii) efficiency of ionization chambers, (iii) transmittance of windows, air paths etc. by interpolating the pre-edge region with a modified Victoreen polynomial ($aE^{-3}+b$, a and b coefficients are found by the standard least-squares method). The construction of the post-edge is done by a smoothing spline, while the EXAFS normalization procedure is shown in Figure S1 (the inset shows the equation adopted).

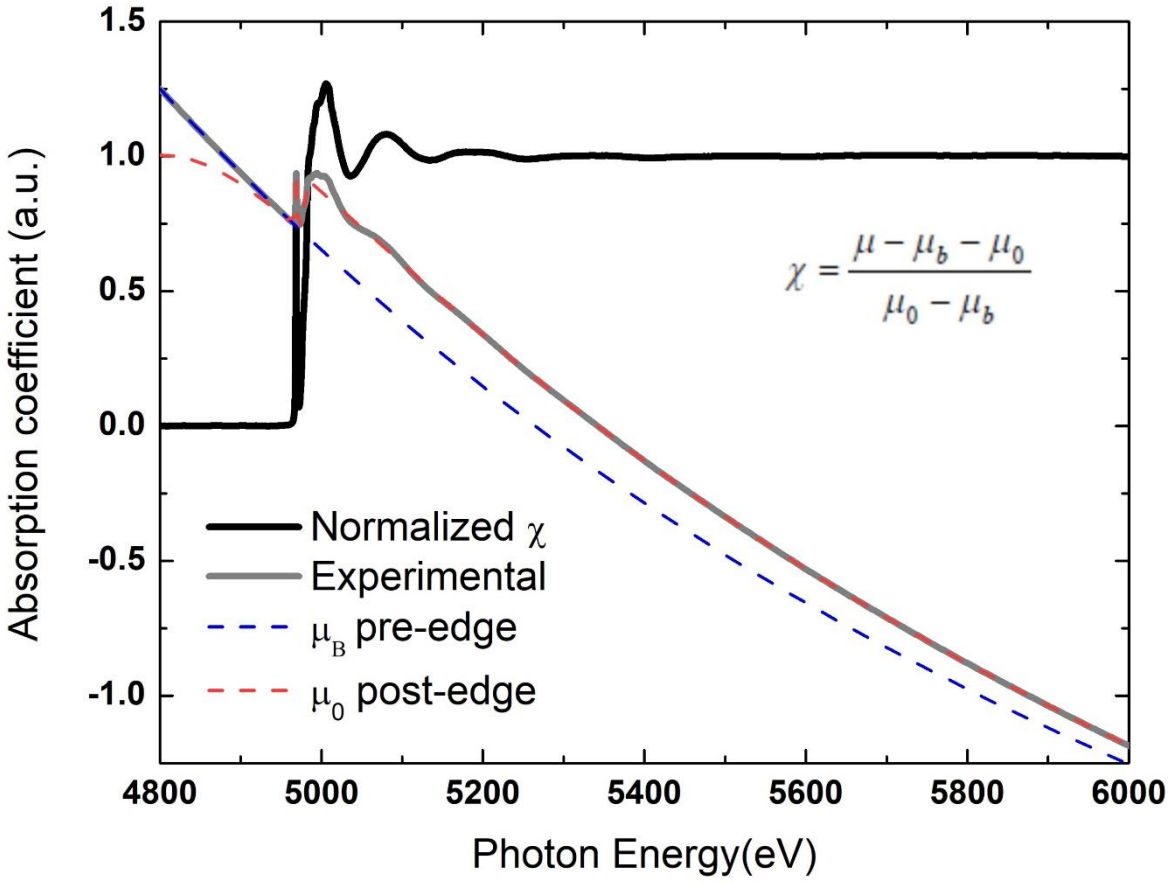

Figure S1. Graphical representation of the Ti K-edge XAS data extraction procedure.

Ti $L_{2,3}$-edges NEXAFS spectra were collected at the APE-HE beamline of the Elettra Sincrotrone Trieste facility in total electron yield (TEY) mode. A newly developed environmental NEXAFS cell[3] was used to pre-activate the samples *in situ* at 400 °C under 5 ml/min of He at 1 bar, thus recording the spectra after cooling at RT still under He flow. A liquid nitrogen trap has been employed to remove water contaminations. The spectra were collected with 0.1 eV energy step and 0.18 s of integration time in the 400-480 eV range by adopting the fast scan mode, therefore the grating monochromator is scanned continuously through the wanted energy range and the picoammeter signal is recorded in the streaming mode. The signal collected from the sample, I_s, is divided by the signal, I_m, of the beam measured on a metal mesh located in the X-ray tube before the sample. The data extraction has been performed with a custom Python script, as it follows: first, the spectra have been energy calibrated by exploiting the $1s \rightarrow \pi^*$ transition (peaked at 399.8 eV) of a small

nitrogen contamination on the optics,[4] as present in traces in the beamline. The soft X-rays interact easily with all the medium and all these interactions yield electronic signal that produce anomalous backgrounds, therefore these phenomena must be considered. The background subtraction has been performed normalizing the I_s/I_m with the simulation of the mean free path of the transmission spectrum in the soft X-ray range in a medium of Si_3N_4 membrane with a thickness of 100 nm (corresponding to the thickness of two membranes employed in APE-HE setup)[3] at 1 bar and thorough a medium of He gas with a thickness of 500 μm (distance between sample and Si_3N_4 membrane) at 1 bar (taken from CXRO database[5]). Finally, a 6-knots cubic spline was subtracted to flatten the spectra and the spectra have been normalized to the intensity of the most intense feature of the Ti L_3-edge.

S1.2. Computational details

The defective models (as well as the reference one for perfect tetrahedral Ti) were constructed starting from the structures reported in a previous contribution.[6] According to the relative stabilities there reported, we chose as starting model the perfect tetrahedral Ti substituting Si in the T10 crystallographic position of monoclinic MFI framework, we found to be the most stable among the 24 possible. Such periodic model was modified to generate different defective Ti structures (vide infra for their description). These periodic models have been geometry relaxed (main structural details are given in Table S1), thus cluster models of comparable size and identical topology have been cut from the periodic structures for the following simulations. The dangling bonds, intentionally left on Si atoms, were saturated by H atoms positioned along the direction of the pristine Si-O bonds at a fixed length of 1.45 Å. Cluster models have been applied in the calculation of optical spectra (through the TD-DFT formalism), K-edge XANES spectra (by finite difference method) and $L_{2,3}$-edges NEXAFS (via DFT/ROCIS) spectra.

The periodic calculations have been carried out with the CRYSTAL17 code, using a computational method giving a good performance-accuracy balance in the case of Ti-zeolites.[6,7] The B3LYP hybrid functional[8,9] was adopted in combination with the D3 empirical scheme by Grimme[10] to include dispersive forces (hereafter referred as B3LYP-D3). The basis set includes the 88-31G(d1) and 8-411G(d1) basis proposed by Nada et al. for Si and O respectively,[11] the 86-411G(d31) by D'Arco for Ti,[12] the 8-511G from Dovesi for Na[13] and the 3-11G basis of Gatti to describe H.[14] The five integral truncation cutoffs (TOLINTEG keyword) were set to 7 7 7 7 14. The reciprocal space was sampled by a net of 8 real k points, defined by setting the SHRINK keyword to 2 2. The maximum order of shell multipoles in the long-range zone for the electron-electron Coulomb interaction (POLEORDR keyword) was set to 6. All the remaining parameters default to the standard values reported in the CRYSTAL17 manual.[15]

The as-cut clusters were directly exploited in the spectroscopic simulations. The cluster calculations simulating optical spectra were performed with the Gaussian16 (Rev. C01) code,[16] at the same level of theory exploited in periodic calculation. *Optical transitions* were simulated by TD-DFT, including 350 states in the calculation.

Ti K-edge XANES spectra were computed with the FDMNES code in its parallelized version.[17,18] The calculations are based on the finite difference method to solve the Schrodinger equation. The Fermi energy is determined over the occupied state where the initial potential is calculated every time at the beginning of each computational cycle (Self-consistent calculation, SCF). The cluster radius from the Ti absorber atom adopted for the SCF calculation was 5 Å. The quadrupole calculation has been also inserted in the Fermi golden rule. The output spectra calculated were convoluted using a Lorentzian to eliminate the occupied states, while to simulate the experimental resolution we convoluted with a Gaussian function of width equal 1.3 eV after the Lorentzian.

Ti $L_{2,3}$-edge NEXAFS simulations were performed with the ORCA (v 4.1.2) code,[19] by adopting the DFT/ROCIS method[20] as proposed in the ORCA manual,[21] where the B3LYP functional and the def2-TZVP[22] basis set are used. This method yielded excellent agreement with experimental results in the study of Ti metallorganic compounds and TiO_2 large clusters.[23–25] Since the L-edge transitions involve core electrons, relativistic corrections have been included through the ZORA formalism.[26] The orbitals part of the excitation space have been manually selected, including the only the Ti 2p as donor orbitals and the 100 lower energy unoccupied orbitals as acceptor ones: 100 transitions were calculated per spin state. The spin-orbit coupling correction was included in the calculations. The same formalism was adopted in the simulation of the K-edge pre-edge transitions, as shown in Figure S8.

All the spectra have been energy scaled by a multiplicative factor, derived from the comparison of the experimental spectrum of perfect TS-1 and the simulated one for a perfect tetrahedral Ti. In detail, we calculated this corrective factor as the ratio of the energy of a given fingerprint in the experimental spectrum on the corresponding one for the simulated one. In the case multiple features can be adopted for the same technique (e.g. in NEXAFS spectra), the procedure was repeated for each fingerprint and the final corrective factor was derived by averaging all the obtained coefficients.

S2. Geometrical parameters of periodic structures

Table S1. Main geometrical parameters for the periodic structures: cell parameters (*a, b, c*), cell angles (α, β, γ) and cell volume (V). All the lengths are given in Å, the angles in °, the volume in Å^3.

Ti model	Label[a]	*a*	*b*	*c*	α	β	γ	V
Perfect tetracoordinated	A	19.652	19.882	13.281	89.7	91.3	89.9	5188
Bipodal tetracoordinated	B	19.600	19.839	13.288	89.6	91.2	89.6	5166
H-terminated pentacoordinated	C	19.548	19.571	13.240	89.1	89.5	89.5	5064
Na-terminated pentacoordinated	D	19.556	19.554	13.243	89.1	89.5	89.6	5063
H-terminated hexacoordinated	E	19.533	19.583	13.266	90.0	89.9	89.4	5074
Na-terminated hexacoordinated	F	19.580	19.558	13.261	89.7	89.7	89.7	5078
Dimeric tetracoordinated	G	19.680	19.899	13.294	89.8	91.3	89.8	5205

[a] labels referred to Figure 1.

The cartesian coordinates of atoms for each model follow:

Model A (perfect tetracoordinated)

O	0.083653	0.376684	0.769689
O	0.080049	0.315799	0.942621
O	0.040903	0.204056	0.036287
O	0.083789	0.112208	0.904029
O	0.050840	0.123644	0.708163
O	0.052838	0.246059	0.778269
O	0.854798	0.357525	0.718732
O	0.839176	0.317523	0.905414
O	0.855190	0.202033	0.002073
O	0.838997	0.069334	0.914131
O	0.853839	0.109667	0.722339
O	0.889355	0.234503	0.766675
O	0.963669	0.335085	0.840108
O	0.960509	0.083343	0.841401
O	0.128611	0.429743	0.599558
O	0.000867	0.384028	0.615841
O	0.878550	0.419304	0.547944
O	0.145979	0.208985	0.647814
O	0.020086	0.225240	0.584668
O	0.888423	0.193913	0.576319
O	0.064182	0.004854	0.788543
O	0.880577	0.984776	0.773445
O	0.759317	0.433835	0.628986
O	0.772333	0.208542	0.667451
O	0.750272	0.280084	0.040551
O	0.745118	0.115246	0.074502
O	0.447166	0.374502	0.723347

O	0.469794	0.318771	0.902674
O	0.428005	0.200668	0.973667
O	0.455951	0.074758	0.926845
O	0.437980	0.111976	0.732818
O	0.450726	0.243153	0.743747
O	0.685664	0.369926	0.763531
O	0.639765	0.319221	0.935704
O	0.644483	0.196463	0.013342
O	0.677310	0.085581	0.911283
O	0.679052	0.115656	0.717034
O	0.674644	0.237680	0.792834
O	0.564722	0.314764	0.764198
O	0.561547	0.095747	0.809677
O	0.381528	0.441417	0.576500
O	0.513990	0.421547	0.562855
O	0.642600	0.382501	0.572623
O	0.388412	0.187981	0.585300
O	0.522313	0.174606	0.611442
O	0.648724	0.220608	0.597337
O	0.480713	0.989873	0.783253
O	0.645158	0.992977	0.775239
O	0.931649	0.621646	0.211812
O	0.935205	0.680567	0.036337
O	0.972755	0.795501	0.949734
O	0.932323	0.892901	0.076171
O	0.966908	0.872452	0.271548
O	0.961176	0.751771	0.198965
O	0.160557	0.639049	0.260026
O	0.176475	0.684456	0.076807
O	0.165690	0.801683	0.985815
O	0.176765	0.926207	0.052116
O	0.169225	0.886954	0.246328
O	0.124398	0.762590	0.218593
O	0.051571	0.662826	0.139768
O	0.058647	0.904640	0.134108
O	0.888202	0.567600	0.382805
O	0.014866	0.615943	0.365952
O	0.136928	0.577656	0.431208
O	0.870298	0.789128	0.332621
O	0.996448	0.770158	0.393191
O	0.125679	0.812280	0.401497
O	0.968433	0.992283	0.202902
O	0.133081	0.009422	0.192855
O	0.257092	0.565764	0.352226
O	0.243205	0.787872	0.316084
O	0.264606	0.717326	0.938541
O	0.261438	0.882984	0.912687
O	0.568314	0.624558	0.259227
O	0.547820	0.679385	0.079119
O	0.584653	0.799311	0.009666
O	0.557570	0.925601	0.056586

O	0.576241	0.887420	0.249278
O	0.565037	0.755924	0.237611
O	0.330648	0.628953	0.216415
O	0.375976	0.681146	0.044455
O	0.366449	0.804073	0.966813
O	0.335591	0.914361	0.070392
O	0.334687	0.882956	0.264670
O	0.340594	0.761335	0.188378
O	0.451239	0.684709	0.215589
O	0.451858	0.902229	0.172188
O	0.634548	0.557581	0.405565
O	0.502017	0.576943	0.419657
O	0.373721	0.616854	0.407555
O	0.628718	0.811049	0.394422
O	0.494267	0.824030	0.371744
O	0.367577	0.778027	0.383404
O	0.530854	0.009053	0.201445
O	0.369583	0.006016	0.205585
O	0.438263	0.871784	0.721774
O	0.433286	0.814780	0.546772
O	0.472387	0.704437	0.451740
O	0.436764	0.609928	0.584084
O	0.476978	0.620464	0.779192
O	0.463359	0.741388	0.708028
O	0.667263	0.865283	0.730394
O	0.675812	0.784280	0.578016
O	0.653963	0.684332	0.449599
O	0.691316	0.590765	0.583871
O	0.660718	0.609738	0.774661
O	0.624159	0.738393	0.747450
O	0.553768	0.826391	0.637429
O	0.563708	0.587834	0.636548
O	0.390680	0.923434	0.890542
O	0.519895	0.878194	0.877993
O	0.649967	0.899970	0.920806
O	0.377902	0.698667	0.846318
O	0.503136	0.723707	0.900706
O	0.632037	0.686061	0.929865
O	0.467548	0.503220	0.699610
O	0.646087	0.488778	0.695928
O	0.761804	0.934588	0.826747
O	0.744594	0.707883	0.832084
O	0.755209	0.768432	0.421838
O	0.761374	0.603016	0.419875
O	0.032663	0.883856	0.728520
O	0.053402	0.814136	0.563775
O	0.087049	0.695698	0.487340
O	0.034423	0.580002	0.554668
O	0.080110	0.623922	0.733079
O	0.074850	0.757652	0.743481
O	0.842663	0.867193	0.704148

O	0.862628	0.811293	0.529036
O	0.862406	0.687236	0.460859
O	0.848378	0.576999	0.570787
O	0.825698	0.613324	0.761671
O	0.826090	0.735061	0.681758
O	0.949384	0.784644	0.681954
O	0.950302	0.595333	0.702959
O	0.132966	0.902224	0.863212
O	0.003818	0.922245	0.914854
O	0.874577	0.880126	0.898199
O	0.140416	0.688021	0.883283
O	0.005731	0.680001	0.870876
O	0.875296	0.718738	0.867458
O	0.041158	0.496491	0.709159
O	0.866803	0.490205	0.717478
O	0.575365	0.127454	0.258698
O	0.581609	0.183642	0.434839
O	0.543781	0.294227	0.530153
O	0.578295	0.388763	0.397310
O	0.538090	0.378632	0.201959
O	0.553465	0.258123	0.274002
O	0.347764	0.133637	0.251041
O	0.339217	0.215190	0.402753
O	0.363007	0.314704	0.530955
O	0.324231	0.409126	0.398525
O	0.353000	0.389297	0.207616
O	0.389867	0.260665	0.232022
O	0.461132	0.174290	0.343765
O	0.451456	0.410909	0.344309
O	0.614544	0.075942	0.084564
O	0.487608	0.120800	0.109477
O	0.360208	0.099271	0.058998
O	0.637755	0.301810	0.134160
O	0.512608	0.274133	0.081724
O	0.385271	0.316110	0.051354
O	0.548257	0.495694	0.282435
O	0.369869	0.510284	0.284863
O	0.252014	0.063291	0.159584
O	0.270851	0.291486	0.142246
O	0.261785	0.230670	0.561151
O	0.255175	0.394594	0.562936
O	0.991921	0.117363	0.251146
O	0.960567	0.184817	0.413676
O	0.934830	0.305121	0.486783
O	0.983396	0.423721	0.428120
O	0.937107	0.375230	0.252358
O	0.942075	0.241585	0.233305
O	0.163923	0.124941	0.279512
O	0.156012	0.186089	0.451865
O	0.154420	0.310540	0.518493
O	0.168318	0.421945	0.412194

O	0.191757	0.381969	0.224253
O	0.194351	0.256278	0.293359
O	0.067380	0.219808	0.304459
O	0.066792	0.403017	0.279319
O	0.887912	0.085647	0.128035
O	0.014550	0.075670	0.064162
O	0.142143	0.121225	0.082774
O	0.872429	0.316828	0.101970
O	0.007777	0.322030	0.106588
O	0.138368	0.281713	0.113933
O	0.976978	0.503253	0.270754
O	0.151834	0.506443	0.262462
Si	0.063925	0.422603	0.672096
Si	0.044512	0.318421	0.831719
Si	0.067243	0.281148	0.051021
Si	0.070286	0.128392	0.021245
Si	0.039683	0.080689	0.810571
Si	0.067102	0.201235	0.679917
Si	0.839555	0.425257	0.654283
Si	0.887224	0.311490	0.808156
Si	0.829644	0.279604	0.012831
Si	0.883119	0.061887	0.812625
Si	0.851203	0.186904	0.683352
Si	0.452778	0.433946	0.640424
Si	0.483213	0.312816	0.783463
Si	0.448989	0.277464	0.002412
Si	0.432821	0.124190	0.016088
Si	0.483624	0.068425	0.813007
Si	0.449889	0.180090	0.667524
Si	0.682878	0.418912	0.665072
Si	0.640912	0.310925	0.814483
Si	0.668769	0.274072	0.030264
Si	0.669673	0.118664	0.021696
Si	0.640583	0.072183	0.802871
Si	0.693752	0.194550	0.693287
Si	0.952539	0.576302	0.309614
Si	0.970523	0.678933	0.147471
Si	0.946650	0.718785	0.930064
Si	0.946105	0.872593	0.960065
Si	0.981264	0.915513	0.170603
Si	0.949019	0.795359	0.299151
Si	0.176876	0.572188	0.325625
Si	0.127645	0.686788	0.173346
Si	0.186360	0.723194	0.970370
Si	0.184036	0.878611	0.953608
Si	0.135124	0.931828	0.156065
Si	0.165411	0.812317	0.295697
Si	0.563156	0.564888	0.341844
Si	0.532934	0.686087	0.197889
Si	0.566937	0.721973	0.979683
Si	0.578135	0.875582	0.966704

Si	0.529474	0.930681	0.170221
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Si	0.333353	0.580348	0.315329
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Si	0.345819	0.725556	0.949892
Si	0.338629	0.881023	0.959749
Si	0.372978	0.926568	0.178675
Si	0.321381	0.803752	0.288551
Si	0.456836	0.916178	0.820300
Si	0.472912	0.813874	0.654689
Si	0.441851	0.780254	0.437860
Si	0.446160	0.627335	0.465517
Si	0.485889	0.580560	0.674252
Si	0.455869	0.696386	0.808707
Si	0.680813	0.923117	0.813295
Si	0.629946	0.803671	0.673385
Si	0.678159	0.762266	0.460808
Si	0.685422	0.608897	0.464322
Si	0.640689	0.568789	0.673201
Si	0.665755	0.685163	0.819877
Si	0.058466	0.927522	0.824646
Si	0.027972	0.809992	0.678625
Si	0.065989	0.773235	0.460833
Si	0.068509	0.618076	0.460740
Si	0.027367	0.573772	0.675711
Si	0.074943	0.688017	0.807952
Si	0.839503	0.916398	0.800442
Si	0.870609	0.800507	0.649709
Si	0.836852	0.763721	0.436544
Si	0.840153	0.608555	0.459023
Si	0.872615	0.569337	0.687439
Si	0.818698	0.692886	0.786614
Si	0.552551	0.082890	0.162201
Si	0.542118	0.185723	0.326811
Si	0.574071	0.218308	0.543908
Si	0.569713	0.371411	0.516031
Si	0.529363	0.418375	0.307134
Si	0.559959	0.302852	0.172792
Si	0.332908	0.075696	0.168726
Si	0.384792	0.195839	0.307024
Si	0.338366	0.236863	0.520174
Si	0.330942	0.389985	0.517587
Si	0.374431	0.430321	0.308305
Si	0.349255	0.314644	0.159611
Si	0.965842	0.068405	0.161497
Si	0.989726	0.191256	0.300920
Si	0.950874	0.227068	0.516248
Si	0.949084	0.382443	0.518901
Si	0.990324	0.426341	0.306646
Si	0.940139	0.313211	0.173353
Si	0.173242	0.080110	0.179280

Si	0.145151	0.195871	0.331398
Si	0.180207	0.234275	0.544385
Si	0.176588	0.389247	0.523085
Si	0.144812	0.427937	0.295170
Si	0.197708	0.303498	0.192809
Ti	0.831563	0.116250	0.029758

Model B (bipodal tetracoordinated)

H	0.502253	0.319100	0.546150
H	0.546539	0.550896	0.506079
H	0.455078	0.463385	0.798566
H	0.450309	0.452407	0.371679
O	0.752271	0.763039	0.238237
O	0.749209	0.700961	0.410371
O	0.710914	0.589985	0.507709
O	0.750686	0.499067	0.370928
O	0.710718	0.509571	0.178633
O	0.722808	0.632448	0.245040
O	0.523226	0.743083	0.187111
O	0.507094	0.700231	0.372390
O	0.544922	0.589736	0.460663
O	0.499555	0.454293	0.380416
O	0.525275	0.494532	0.189110
O	0.561322	0.620458	0.229975
O	0.632286	0.721061	0.308464
O	0.625539	0.466188	0.320120
O	0.797421	0.815308	0.067279
O	0.669886	0.769354	0.083176
O	0.547355	0.806057	0.016708
O	0.812801	0.587629	0.115159
O	0.687764	0.610942	0.051965
O	0.555589	0.578953	0.041033
O	0.729979	0.390851	0.258091
O	0.548757	0.369999	0.242380
O	0.428195	0.821019	0.097733
O	0.441776	0.592987	0.138435
O	0.425036	0.650247	0.508357
O	0.406300	0.492418	0.560787
O	0.115933	0.757647	0.192314
O	0.139181	0.703932	0.372996
O	0.097506	0.585841	0.444355
O	0.124553	0.458916	0.400864
O	0.110377	0.495713	0.206375
O	0.127205	0.626354	0.215219
O	0.358747	0.754117	0.233713
O	0.316045	0.702078	0.407190
O	0.314112	0.576845	0.477735
O	0.353437	0.464981	0.382636
O	0.350068	0.498300	0.189967

O	0.341678	0.621190	0.260025
O	0.236306	0.704841	0.238248
O	0.233236	0.480036	0.288869
O	0.050832	0.825463	0.046202
O	0.183290	0.803768	0.031523
O	0.312591	0.764794	0.044384
O	0.057868	0.572120	0.061570
O	0.192344	0.555363	0.078225
O	0.319204	0.600000	0.064066
O	0.152973	0.373754	0.259115
O	0.313219	0.375825	0.245886
O	0.598404	0.009493	0.684670
O	0.603382	0.066184	0.507673
O	0.642185	0.180147	0.420786
O	0.597263	0.278417	0.543956
O	0.629484	0.261337	0.739981
O	0.629469	0.139606	0.668373
O	0.830853	0.023957	0.729333
O	0.843350	0.070322	0.546415
O	0.833057	0.188312	0.455951
O	0.839780	0.314349	0.516947
O	0.836859	0.272334	0.709836
O	0.791693	0.147626	0.689896
O	0.719271	0.047798	0.612641
O	0.722923	0.293287	0.605626
O	0.558470	0.951788	0.855060
O	0.684387	0.002326	0.834620
O	0.806816	0.964802	0.902282
O	0.536350	0.174660	0.801047
O	0.663049	0.159654	0.862735
O	0.791935	0.202162	0.869013
O	0.626797	0.381309	0.664805
O	0.799389	0.396025	0.662599
O	0.926461	0.947873	0.821565
O	0.910352	0.174540	0.787008
O	0.932875	0.103373	0.410719
O	0.929132	0.269293	0.382955
O	0.237093	0.007355	0.731386
O	0.216452	0.061788	0.551531
O	0.254017	0.181138	0.481314
O	0.227463	0.308148	0.527045
O	0.244113	0.270651	0.720248
O	0.233911	0.138984	0.709674
O	0.999749	0.012053	0.686802
O	0.044719	0.066372	0.516209
O	0.034666	0.189550	0.437820
O	0.002244	0.299461	0.541427
O	0.003597	0.267893	0.735760
O	0.008415	0.145359	0.661329
O	0.119744	0.068743	0.687822
O	0.120037	0.285318	0.639609

O	0.303572	0.939505	0.877210
O	0.170645	0.960249	0.891560
O	0.041959	0.001328	0.878336
O	0.294260	0.194644	0.868575
O	0.160262	0.208117	0.840689
O	0.034089	0.162816	0.856869
O	0.198474	0.392106	0.670892
O	0.039489	0.390856	0.674540
O	0.107109	0.257559	0.192791
O	0.101981	0.199318	0.018511
O	0.140385	0.088590	0.922770
O	0.104775	0.994122	0.055115
O	0.144309	0.003977	0.250023
O	0.132081	0.126238	0.180577
O	0.337740	0.248389	0.198878
O	0.343923	0.164731	0.049714
O	0.321427	0.066836	0.918756
O	0.360342	0.974070	0.054229
O	0.330856	0.993324	0.244778
O	0.292068	0.122501	0.221233
O	0.222630	0.210809	0.109241
O	0.232487	0.973560	0.108004
O	0.059065	0.308910	0.361898
O	0.187668	0.259453	0.350398
O	0.318602	0.281075	0.389584
O	0.045994	0.083604	0.317996
O	0.171564	0.106020	0.373057
O	0.300562	0.067087	0.401704
O	0.137763	0.886591	0.168628
O	0.313380	0.872269	0.165816
O	0.430305	0.319513	0.296961
O	0.412981	0.092567	0.304685
O	0.421588	0.151962	0.890483
O	0.430323	0.986399	0.889810
O	0.697420	0.269390	0.198648
O	0.721582	0.201263	0.033395
O	0.755749	0.083935	0.953141
O	0.702917	0.968925	0.024004
O	0.749435	0.009421	0.203092
O	0.742067	0.143324	0.212885
O	0.510457	0.252586	0.172316
O	0.528278	0.195986	0.997731
O	0.530526	0.072089	0.928969
O	0.516776	0.963238	0.042169
O	0.494586	0.998441	0.233698
O	0.493353	0.120188	0.152687
O	0.616814	0.168884	0.148598
O	0.619045	0.981968	0.173257
O	0.801089	0.286903	0.327726
O	0.673115	0.307045	0.386393
O	0.543560	0.264216	0.365944

O	0.809426	0.074639	0.352270
O	0.674756	0.064511	0.341927
O	0.544149	0.104571	0.337768
O	0.709441	0.882489	0.175686
O	0.536443	0.875601	0.187506
O	0.246666	0.510041	0.723913
O	0.251914	0.565272	0.901621
O	0.214583	0.676026	0.000154
O	0.249581	0.770671	0.867710
O	0.214333	0.761723	0.670776
O	0.224100	0.640718	0.741880
O	0.015234	0.518177	0.722076
O	0.010826	0.597341	0.876621
O	0.031945	0.697908	0.003360
O	0.995228	0.792061	0.868780
O	0.021357	0.774255	0.677524
O	0.058266	0.645071	0.704514
O	0.131487	0.556260	0.810454
O	0.122593	0.790694	0.810261
O	0.275694	0.457666	0.543389
O	0.152207	0.505455	0.584437
O	0.026209	0.485668	0.528992
O	0.312070	0.679943	0.603226
O	0.185206	0.658330	0.549673
O	0.056904	0.701244	0.523924
O	0.217434	0.878360	0.754044
O	0.042022	0.893999	0.757931
O	0.920267	0.445967	0.631599
O	0.940439	0.676538	0.610165
O	0.930659	0.612956	0.032793
O	0.924206	0.778866	0.032168
O	0.662053	0.504211	0.718050
O	0.628669	0.570605	0.880469
O	0.602661	0.691274	0.954097
O	0.651742	0.809756	0.895578
O	0.604875	0.762585	0.719158
O	0.610821	0.628744	0.701234
O	0.831888	0.512144	0.745254
O	0.826045	0.570995	0.919180
O	0.823155	0.693894	0.993538
O	0.837250	0.803254	0.880636
O	0.861054	0.768448	0.691117
O	0.863669	0.643051	0.762051
O	0.736179	0.607425	0.774162
O	0.735321	0.787513	0.747472
O	0.556072	0.483301	0.592683
O	0.684455	0.461347	0.532728
O	0.812639	0.505294	0.547553
O	0.539998	0.703249	0.569523
O	0.676353	0.709090	0.574148
O	0.807563	0.668135	0.582240

O	0.646748	0.889959	0.738625
O	0.818935	0.891673	0.734803
O	0.471143	0.355286	0.562664
O	0.464391	0.431865	0.745808
Si	0.732506	0.808209	0.139769
Si	0.713331	0.704257	0.299764
Si	0.736154	0.667497	0.519541
Si	0.739610	0.514397	0.488906
Si	0.703537	0.466330	0.281988
Si	0.733306	0.585363	0.148132
Si	0.508607	0.811321	0.123441
Si	0.556189	0.696270	0.275956
Si	0.504398	0.659297	0.479451
Si	0.548716	0.447268	0.284142
Si	0.521436	0.571962	0.150645
Si	0.122351	0.817363	0.109671
Si	0.154699	0.698051	0.254535
Si	0.119982	0.662283	0.473112
Si	0.099848	0.509446	0.488002
Si	0.154871	0.452496	0.288669
Si	0.121790	0.563336	0.139425
Si	0.352593	0.803138	0.135214
Si	0.313102	0.696147	0.285651
Si	0.343219	0.652546	0.498549
Si	0.337657	0.498793	0.492359
Si	0.311547	0.454822	0.275701
Si	0.363330	0.577394	0.162881
Si	0.621664	0.962426	0.779958
Si	0.638208	0.065615	0.619185
Si	0.615391	0.103563	0.400900
Si	0.614871	0.257251	0.428677
Si	0.644844	0.304053	0.639109
Si	0.615083	0.183236	0.768106
Si	0.846055	0.957092	0.796246
Si	0.795674	0.071872	0.644318
Si	0.854110	0.109534	0.440672
Si	0.850849	0.265039	0.421134
Si	0.800531	0.318948	0.623210
Si	0.832619	0.199079	0.763956
Si	0.231950	0.947412	0.813737
Si	0.201660	0.069212	0.670145
Si	0.235593	0.103878	0.451665
Si	0.247086	0.257361	0.437551
Si	0.197847	0.313597	0.639730
Si	0.233190	0.202287	0.785470
Si	0.002999	0.963613	0.786143
Si	0.043396	0.072638	0.637646
Si	0.014249	0.110889	0.421676
Si	0.006344	0.266661	0.430535
Si	0.041333	0.311033	0.648571
Si	0.989163	0.188831	0.760541

Si	0.125978	0.300282	0.292812
Si	0.141542	0.198662	0.126457
Si	0.109145	0.164584	0.909485
Si	0.114458	0.011312	0.936544
Si	0.154434	0.964656	0.144882
Si	0.124159	0.080293	0.280411
Si	0.349592	0.305575	0.283056
Si	0.298725	0.186603	0.144788
Si	0.345023	0.144816	0.931646
Si	0.354140	0.991591	0.934579
Si	0.309523	0.952723	0.143726
Si	0.334551	0.068353	0.291860
Si	0.725656	0.313138	0.293052
Si	0.694981	0.195670	0.147532
Si	0.733363	0.161752	0.928992
Si	0.737701	0.005713	0.929599
Si	0.696213	0.960419	0.144687
Si	0.743561	0.073601	0.277724
Si	0.508199	0.301550	0.268730
Si	0.537580	0.185224	0.118122
Si	0.503463	0.148422	0.904995
Si	0.509042	0.993121	0.929420
Si	0.541612	0.955013	0.158364
Si	0.487160	0.078160	0.258003
Si	0.218988	0.465802	0.629566
Si	0.212599	0.567846	0.793391
Si	0.244298	0.599324	0.011152
Si	0.240141	0.753529	0.986349
Si	0.201250	0.799996	0.776211
Si	0.233811	0.685073	0.640683
Si	0.000942	0.460425	0.639298
Si	0.054297	0.579185	0.778001
Si	0.007889	0.619827	0.993448
Si	0.000443	0.773607	0.988033
Si	0.045327	0.813368	0.778456
Si	0.018759	0.699243	0.630402
Si	0.632619	0.458794	0.626326
Si	0.658814	0.578190	0.768408
Si	0.618691	0.612823	0.983052
Si	0.617686	0.768445	0.986653
Si	0.658805	0.812371	0.774110
Si	0.608060	0.700337	0.640212
Si	0.841331	0.465581	0.647136
Si	0.814216	0.582650	0.799427
Si	0.848809	0.616621	0.015044
Si	0.845467	0.772687	0.992939
Si	0.813303	0.812388	0.764312
Si	0.867084	0.689652	0.660540
Ti	0.474442	0.438362	0.611997

Model C (H-terminated pentacoordinated)

H	0.500495	0.735806	0.802680
H	0.626465	0.388098	0.326471
O	0.742175	0.779078	0.407278
O	0.722957	0.739028	0.598273
O	0.720713	0.616446	0.680538
O	0.712483	0.493443	0.601377
O	0.743333	0.518062	0.409482
O	0.744572	0.648577	0.455092
O	0.505124	0.771451	0.473704
O	0.542717	0.659805	0.592916
O	0.509544	0.523501	0.335451
O	0.518391	0.648999	0.400393
O	0.627209	0.719033	0.459416
O	0.612482	0.506472	0.465364
O	0.799251	0.847866	0.255183
O	0.664137	0.845430	0.269482
O	0.539857	0.793269	0.280256
O	0.801604	0.604314	0.284064
O	0.665917	0.606353	0.308720
O	0.550321	0.623998	0.209716
O	0.690730	0.398939	0.465317
O	0.507448	0.423971	0.469659
O	0.422143	0.839500	0.346629
O	0.422088	0.615834	0.270931
O	0.430483	0.686675	0.721739
O	0.444002	0.555315	0.684037
O	0.153299	0.788854	0.399068
O	0.102571	0.725765	0.562426
O	0.123189	0.632033	0.709031
O	0.124646	0.547184	0.551804
O	0.139690	0.532585	0.354151
O	0.109515	0.662691	0.389656
O	0.308910	0.772619	0.396652
O	0.339354	0.732343	0.580299
O	0.322041	0.614951	0.667377
O	0.357220	0.500094	0.566301
O	0.349426	0.518078	0.365650
O	0.343336	0.643585	0.429057
O	0.223681	0.689547	0.489670
O	0.238627	0.498599	0.478615
O	0.048175	0.827395	0.281237
O	0.176099	0.847851	0.220268
O	0.312245	0.846130	0.231802
O	0.037345	0.593933	0.259791
O	0.160299	0.628177	0.210500
O	0.289874	0.610576	0.248193
O	0.126491	0.422582	0.467010
O	0.327069	0.397643	0.450994
O	0.654158	0.053513	0.946511

O	0.618340	0.103245	0.769328
O	0.579610	0.215531	0.667709
O	0.638821	0.315324	0.770747
O	0.592546	0.315571	0.957703
O	0.604199	0.180973	0.928518
O	0.828968	0.061042	0.920041
O	0.825228	0.109024	0.735030
O	0.815829	0.234945	0.667219
O	0.802038	0.348769	0.765870
O	0.819840	0.313052	0.959551
O	0.855898	0.192228	0.883806
O	0.729320	0.149572	0.866012
O	0.707819	0.379460	0.906715
O	0.545978	0.018901	0.059792
O	0.671995	0.991329	0.123158
O	0.803851	0.026598	0.111215
O	0.550195	0.227445	0.097316
O	0.682101	0.242337	0.061993
O	0.808700	0.197606	0.070878
O	0.585775	0.431376	0.849757
O	0.828126	0.441794	0.897452
O	0.916587	0.983746	0.027293
O	0.928483	0.248014	0.028622
O	0.924290	0.159605	0.616520
O	0.914818	0.326898	0.650897
O	0.232949	0.076619	0.981009
O	0.246840	0.120332	0.792741
O	0.208221	0.221243	0.669411
O	0.251880	0.327622	0.778036
O	0.232879	0.328173	0.978285
O	0.197791	0.203673	0.932770
O	0.997269	0.077819	0.949692
O	0.007285	0.128318	0.769280
O	0.023970	0.242953	0.667473
O	0.003126	0.345788	0.791532
O	0.031267	0.332173	0.985861
O	0.039166	0.204991	0.928072
O	0.121080	0.103243	0.872042
O	0.130880	0.352581	0.850424
O	0.292738	0.989635	0.110057
O	0.158299	0.001955	0.112786
O	0.025841	0.028808	0.129337
O	0.303621	0.223062	0.052017
O	0.178547	0.248562	0.120545
O	0.042423	0.236688	0.126321
O	0.229960	0.443647	0.879176
O	0.043299	0.452169	0.896217
O	0.108667	0.288004	0.465073
O	0.114890	0.221803	0.291973
O	0.120494	0.128619	0.142402
O	0.102717	0.038389	0.289287

O	0.118477	0.027347	0.484984
O	0.152260	0.157429	0.456760
O	0.362306	0.271136	0.429256
O	0.322634	0.234446	0.248618
O	0.316996	0.112774	0.171866
O	0.350932	0.007776	0.291622
O	0.328119	0.028352	0.488289
O	0.314381	0.148768	0.408127
O	0.229839	0.256614	0.389772
O	0.224695	0.007287	0.360857
O	0.039245	0.365972	0.595219
O	0.171888	0.347661	0.619631
O	0.300435	0.306067	0.598377
O	0.048967	0.124254	0.578042
O	0.177396	0.094170	0.629600
O	0.307056	0.134255	0.611225
O	0.123485	0.916984	0.375082
O	0.311405	0.906376	0.411386
O	0.426011	0.341170	0.568087
O	0.425285	0.123051	0.519486
O	0.422564	0.192924	0.124562
O	0.421760	0.029886	0.127186
O	0.745935	0.281708	0.415741
O	0.743296	0.229013	0.239399
O	0.706768	0.119478	0.142282
O	0.741769	0.025478	0.285075
O	0.726266	0.031942	0.485023
O	0.709623	0.151899	0.400799
O	0.525872	0.290346	0.453405
O	0.496465	0.231338	0.280490
O	0.519133	0.111532	0.198751
O	0.517994	0.980409	0.250823
O	0.501446	0.028048	0.438132
O	0.545349	0.157234	0.432355
O	0.625072	0.247633	0.336145
O	0.623833	0.996516	0.370633
O	0.796385	0.351279	0.568193
O	0.675053	0.289374	0.582929
O	0.554767	0.347834	0.624453
O	0.805613	0.133335	0.538829
O	0.676058	0.133573	0.595416
O	0.545531	0.091608	0.603849
O	0.732774	0.913391	0.400660
O	0.534685	0.897731	0.409128
O	0.245714	0.576791	0.879782
O	0.246619	0.632541	0.058696
O	0.245220	0.732044	0.195270
O	0.252622	0.829788	0.056015
O	0.236754	0.830719	0.856724
O	0.203761	0.704883	0.900728
O	0.012561	0.582881	0.870341

O	0.005482	0.607510	0.065412
O	0.028774	0.718174	0.170941
O	0.015033	0.842769	0.087798
O	0.011233	0.833313	0.886178
O	0.032912	0.705929	0.933741
O	0.126397	0.606439	0.971402
O	0.129271	0.843929	0.979371
O	0.325985	0.498960	0.762533
O	0.194928	0.516543	0.717348
O	0.059464	0.512349	0.716578
O	0.310208	0.729832	0.777821
O	0.184592	0.752074	0.713956
O	0.050532	0.745426	0.742172
O	0.220095	0.944307	0.957343
O	0.041800	0.949386	0.969703
O	0.935265	0.488230	0.786979
O	0.926636	0.743064	0.813527
O	0.919754	0.643569	0.213500
O	0.923730	0.798687	0.221099
O	0.618685	0.539370	0.955619
O	0.668790	0.604446	0.112595
O	0.644798	0.721118	0.205053
O	0.594706	0.826632	0.101900
O	0.601401	0.803051	0.904446
O	0.621502	0.675216	0.958516
O	0.862892	0.570023	0.900540
O	0.824709	0.602866	0.089081
O	0.812530	0.722859	0.185263
O	0.844273	0.829507	0.067787
O	0.817819	0.819028	0.872008
O	0.836410	0.697105	0.947904
O	0.736306	0.606152	0.938094
O	0.715484	0.828815	0.006260
O	0.564313	0.565698	0.777022
O	0.686551	0.507265	0.791449
O	0.812559	0.519850	0.728780
O	0.539749	0.705000	0.805291
O	0.672794	0.722133	0.782673
O	0.805489	0.710303	0.752124
O	0.620975	0.925344	0.967958
O	0.796232	0.935643	0.964894
O	0.592626	0.421771	0.307075
Si	0.734798	0.845143	0.333276
Si	0.708571	0.721468	0.480882
Si	0.731145	0.696450	0.703768
Si	0.733493	0.535489	0.699931
Si	0.690327	0.480631	0.486886
Si	0.739471	0.594958	0.362962
Si	0.500503	0.825523	0.378288
Si	0.548154	0.699191	0.483967
Si	0.556504	0.468117	0.393935

Si	0.500729	0.603058	0.304415
Si	0.124916	0.844664	0.318166
Si	0.147467	0.716917	0.459788
Si	0.115035	0.713273	0.681958
Si	0.126061	0.552865	0.673638
Si	0.157142	0.499284	0.463703
Si	0.112945	0.603945	0.305231
Si	0.339830	0.841464	0.347463
Si	0.303958	0.709558	0.475601
Si	0.351339	0.691679	0.687524
Si	0.362825	0.541409	0.669854
Si	0.318307	0.479136	0.464738
Si	0.350541	0.597432	0.327884
Si	0.622658	0.997875	0.024563
Si	0.651151	0.122099	0.877127
Si	0.604521	0.136006	0.658046
Si	0.611413	0.292074	0.662275
Si	0.630596	0.361726	0.871000
Si	0.606917	0.241668	0.011033
Si	0.836924	0.001943	0.005253
Si	0.809364	0.127049	0.852145
Si	0.843191	0.159027	0.639308
Si	0.833717	0.315603	0.665059
Si	0.788704	0.369949	0.882168
Si	0.852705	0.238790	0.985156
Si	0.225919	0.003946	0.040264
Si	0.199555	0.125376	0.894240
Si	0.236208	0.142481	0.675145
Si	0.232521	0.300533	0.666864
Si	0.211594	0.363499	0.871389
Si	0.228195	0.250542	0.021675
Si	0.995033	0.009340	0.019429
Si	0.041858	0.129256	0.879602
Si	0.001363	0.163802	0.658498
Si	0.995289	0.320854	0.676216
Si	0.052770	0.370375	0.881231
Si	0.010122	0.254533	0.016778
Si	0.111778	0.355175	0.535962
Si	0.150879	0.231480	0.400545
Si	0.114236	0.208906	0.171872
Si	0.101457	0.049661	0.168504
Si	0.142995	0.996719	0.377523
Si	0.123461	0.101293	0.537541
Si	0.353673	0.330510	0.512547
Si	0.306816	0.227520	0.368027
Si	0.341591	0.190601	0.149484
Si	0.345309	0.034463	0.175264
Si	0.303164	0.987800	0.388821
Si	0.344083	0.108686	0.507833
Si	0.727674	0.330453	0.509648
Si	0.705548	0.226975	0.348326

Si	0.735293	0.197055	0.128293
Si	0.731182	0.041030	0.166320
Si	0.705707	0.991165	0.384390
Si	0.728866	0.113151	0.506170
Si	0.503650	0.351290	0.528336
Si	0.547574	0.231565	0.376331
Si	0.497614	0.190930	0.174272
Si	0.501183	0.034919	0.160294
Si	0.544433	0.975573	0.367095
Si	0.503876	0.099782	0.497974
Si	0.249247	0.509651	0.809662
Si	0.205333	0.629350	0.952833
Si	0.236388	0.651282	0.176763
Si	0.246474	0.813777	0.175893
Si	0.209294	0.862256	0.962433
Si	0.234253	0.754101	0.811531
Si	0.012292	0.509068	0.817704
Si	0.045635	0.625591	0.960818
Si	0.998100	0.640812	0.176539
Si	0.004183	0.796822	0.189266
Si	0.049623	0.866954	0.981613
Si	0.005421	0.756253	0.843494
Si	0.610190	0.511037	0.840732
Si	0.661156	0.604893	0.991587
Si	0.631696	0.639547	0.208578
Si	0.610181	0.796344	0.214430
Si	0.634006	0.845972	0.996810
Si	0.611339	0.726433	0.863315
Si	0.858525	0.504028	0.828247
Si	0.815363	0.618188	0.970029
Si	0.839139	0.643839	0.192111
Si	0.845269	0.799360	0.182636
Si	0.793095	0.853273	0.977874
Si	0.846859	0.743103	0.845190
Ti	0.504024	0.623811	0.707296

Model D (Na-terminated pentacoordinated)

H	0.627939	0.388467	0.331624
O	0.742394	0.782523	0.410982
O	0.720388	0.739223	0.600134
O	0.722285	0.615417	0.677681
O	0.707361	0.489931	0.609684
O	0.743043	0.520434	0.419152
O	0.747865	0.652030	0.453886
O	0.507022	0.771384	0.474758
O	0.549733	0.665140	0.601493
O	0.509568	0.522834	0.338313
O	0.517983	0.644625	0.413996
O	0.628441	0.718136	0.455681
O	0.610473	0.504260	0.472783

O	0.798695	0.846335	0.253646
O	0.663638	0.844692	0.269471
O	0.540538	0.790608	0.280505
O	0.801319	0.600485	0.284269
O	0.666281	0.604703	0.313176
O	0.550308	0.626186	0.218961
O	0.691290	0.399763	0.465283
O	0.506814	0.424803	0.476238
O	0.420619	0.831056	0.345854
O	0.423051	0.617716	0.277743
O	0.430689	0.693236	0.704319
O	0.445144	0.559107	0.699950
O	0.148364	0.789390	0.403466
O	0.100678	0.726751	0.567953
O	0.123260	0.632945	0.713542
O	0.125507	0.550290	0.553433
O	0.147628	0.538165	0.357374
O	0.100120	0.663541	0.395435
O	0.300433	0.776740	0.396176
O	0.329923	0.737150	0.579825
O	0.321984	0.617875	0.667432
O	0.364294	0.503022	0.573469
O	0.351043	0.521235	0.373949
O	0.340690	0.648690	0.429089
O	0.218539	0.687752	0.485135
O	0.241857	0.501298	0.490524
O	0.046719	0.828219	0.281815
O	0.175136	0.841249	0.220751
O	0.310692	0.852569	0.233847
O	0.042658	0.590679	0.255613
O	0.163256	0.640268	0.221846
O	0.291642	0.608590	0.248204
O	0.129609	0.426316	0.467183
O	0.329726	0.401171	0.459057
O	0.653441	0.051082	0.942563
O	0.617685	0.104145	0.767681
O	0.579533	0.216440	0.665447
O	0.641556	0.316829	0.766285
O	0.593572	0.315334	0.952248
O	0.605555	0.179984	0.928549
O	0.829385	0.059750	0.918130
O	0.825571	0.108472	0.733153
O	0.817400	0.234752	0.664624
O	0.804257	0.348239	0.764380
O	0.823016	0.312780	0.957773
O	0.856309	0.191371	0.881568
O	0.729695	0.148020	0.864548
O	0.710385	0.377815	0.905841
O	0.545197	0.018572	0.056363
O	0.670691	0.991343	0.120829
O	0.802394	0.027930	0.109801

O	0.550172	0.229744	0.094041
O	0.682483	0.244540	0.060773
O	0.808338	0.196991	0.067586
O	0.589684	0.432033	0.845069
O	0.829885	0.441707	0.896157
O	0.916341	0.985157	0.029403
O	0.929386	0.245052	0.028225
O	0.925402	0.158713	0.615123
O	0.916236	0.327451	0.646960
O	0.233480	0.078393	0.980979
O	0.247928	0.121090	0.792032
O	0.207907	0.222125	0.670768
O	0.252294	0.329742	0.777285
O	0.233594	0.329211	0.977557
O	0.198275	0.204800	0.931231
O	0.998101	0.077938	0.948847
O	0.007990	0.129792	0.768747
O	0.024876	0.243521	0.663242
O	0.004091	0.345952	0.788539
O	0.029586	0.332494	0.983553
O	0.040994	0.205128	0.927947
O	0.121991	0.103545	0.870407
O	0.131071	0.352177	0.850408
O	0.292411	0.991181	0.110169
O	0.158245	0.002727	0.111443
O	0.026034	0.030260	0.129962
O	0.304344	0.224146	0.050057
O	0.179740	0.249416	0.119798
O	0.043566	0.238491	0.125542
O	0.229158	0.444871	0.880179
O	0.044120	0.452299	0.895161
O	0.110110	0.291381	0.461392
O	0.115609	0.222184	0.290880
O	0.120860	0.129794	0.140176
O	0.105445	0.040332	0.288327
O	0.120955	0.028298	0.482801
O	0.152927	0.160038	0.457337
O	0.362539	0.275085	0.426189
O	0.324138	0.236586	0.246440
O	0.316902	0.114443	0.171516
O	0.352927	0.010420	0.290899
O	0.329276	0.031626	0.487911
O	0.315375	0.151831	0.407405
O	0.230571	0.258727	0.386961
O	0.227294	0.006687	0.359881
O	0.040961	0.367512	0.592949
O	0.173408	0.348745	0.617711
O	0.301304	0.304706	0.599016
O	0.050441	0.123492	0.578070
O	0.179465	0.094825	0.627723
O	0.308419	0.137615	0.610632

O	0.125359	0.917763	0.370611
O	0.318025	0.909112	0.414253
O	0.427558	0.338034	0.569413
O	0.426608	0.126339	0.517356
O	0.422986	0.193735	0.121941
O	0.421343	0.032201	0.124280
O	0.746853	0.283883	0.411308
O	0.744891	0.228198	0.236836
O	0.704673	0.120408	0.137178
O	0.738503	0.029091	0.282791
O	0.724048	0.033048	0.482923
O	0.710158	0.153713	0.400698
O	0.528044	0.290597	0.448872
O	0.497372	0.231403	0.277510
O	0.520485	0.112469	0.193976
O	0.516661	0.981583	0.247967
O	0.500165	0.028826	0.435603
O	0.546953	0.157346	0.429448
O	0.626460	0.248025	0.331803
O	0.621930	0.995225	0.369574
O	0.796889	0.351279	0.567057
O	0.674990	0.288961	0.577976
O	0.555906	0.349087	0.622300
O	0.806229	0.132806	0.537378
O	0.676819	0.135077	0.595027
O	0.546190	0.092268	0.600940
O	0.733538	0.915774	0.395910
O	0.530165	0.897740	0.405114
O	0.243001	0.578227	0.881827
O	0.244497	0.630699	0.062588
O	0.257920	0.733332	0.191090
O	0.252326	0.833534	0.056800
O	0.237911	0.832093	0.857602
O	0.205145	0.706718	0.905253
O	0.012901	0.583236	0.871267
O	0.002698	0.607307	0.066374
O	0.028365	0.716918	0.173979
O	0.016018	0.841433	0.088415
O	0.009393	0.834125	0.887793
O	0.030104	0.706777	0.937286
O	0.124719	0.609222	0.975398
O	0.129204	0.845217	0.977330
O	0.325406	0.502110	0.766089
O	0.194650	0.517275	0.718524
O	0.059566	0.513289	0.716288
O	0.310894	0.730661	0.779188
O	0.184350	0.752706	0.717978
O	0.049838	0.745748	0.746695
O	0.219940	0.946380	0.955680
O	0.041264	0.949665	0.971767
O	0.936261	0.488441	0.786400

O	0.924943	0.742543	0.815441
O	0.921660	0.639799	0.222029
O	0.923411	0.797986	0.220406
O	0.613033	0.545882	0.949824
O	0.665223	0.598460	0.117721
O	0.647448	0.719501	0.206840
O	0.594418	0.823638	0.101657
O	0.600038	0.800660	0.902349
O	0.629848	0.680429	0.970348
O	0.862886	0.570627	0.898528
O	0.830045	0.601374	0.090353
O	0.814362	0.719845	0.188288
O	0.843199	0.826575	0.067236
O	0.816401	0.818452	0.871926
O	0.833367	0.696252	0.948288
O	0.736830	0.600206	0.946818
O	0.714261	0.828550	0.006518
O	0.568709	0.556285	0.755993
O	0.692509	0.509336	0.800533
O	0.814569	0.518791	0.725620
O	0.541633	0.688481	0.820457
O	0.672030	0.718569	0.786085
O	0.804372	0.709709	0.751591
O	0.619078	0.922845	0.967688
O	0.796750	0.934556	0.966748
O	0.591675	0.419376	0.311985
Na	0.525609	0.481422	0.642235
Si	0.734586	0.845865	0.332255
Si	0.709035	0.723215	0.481735
Si	0.729219	0.695781	0.705020
Si	0.734804	0.535326	0.702725
Si	0.689865	0.480685	0.492495
Si	0.740445	0.595805	0.366138
Si	0.499854	0.823038	0.377114
Si	0.550312	0.699895	0.489580
Si	0.556015	0.467518	0.396041
Si	0.500918	0.603925	0.312540
Si	0.123897	0.843752	0.318269
Si	0.141897	0.717090	0.462754
Si	0.114506	0.714208	0.686879
Si	0.126335	0.554477	0.675416
Si	0.161074	0.503103	0.467281
Si	0.114549	0.607318	0.309029
Si	0.339073	0.842449	0.348485
Si	0.297658	0.712737	0.474259
Si	0.349972	0.695966	0.683749
Si	0.365267	0.546402	0.677635
Si	0.321573	0.482758	0.474393
Si	0.350485	0.599711	0.331744
Si	0.621551	0.995922	0.021751
Si	0.651381	0.120764	0.875833

Si	0.604786	0.136526	0.656301
Si	0.613041	0.292149	0.659670
Si	0.633445	0.362119	0.868141
Si	0.607798	0.242234	0.008453
Si	0.836664	0.001722	0.005416
Si	0.809778	0.125810	0.850517
Si	0.844291	0.158412	0.637683
Si	0.835391	0.315501	0.662998
Si	0.791339	0.369481	0.880779
Si	0.853863	0.237671	0.983145
Si	0.226126	0.005359	0.039441
Si	0.200275	0.126276	0.893197
Si	0.237306	0.143744	0.674671
Si	0.232750	0.301306	0.667003
Si	0.211592	0.364642	0.871197
Si	0.228843	0.251443	0.020375
Si	0.994963	0.010146	0.020341
Si	0.042864	0.129481	0.878890
Si	0.002497	0.163929	0.657050
Si	0.996719	0.321581	0.672858
Si	0.052804	0.370486	0.879502
Si	0.010713	0.254436	0.015877
Si	0.113680	0.357880	0.533775
Si	0.151652	0.233386	0.398965
Si	0.115062	0.209926	0.170644
Si	0.102116	0.050826	0.167586
Si	0.145375	0.997313	0.375458
Si	0.125062	0.102076	0.536317
Si	0.353995	0.331145	0.514101
Si	0.307544	0.230088	0.365575
Si	0.342118	0.191922	0.147647
Si	0.345495	0.036147	0.174343
Si	0.306087	0.989623	0.388802
Si	0.345157	0.111902	0.507084
Si	0.728813	0.330820	0.507117
Si	0.706947	0.227679	0.345391
Si	0.735163	0.197434	0.125175
Si	0.729177	0.042116	0.163243
Si	0.703957	0.992530	0.381614
Si	0.728997	0.113894	0.505237
Si	0.503964	0.348112	0.525915
Si	0.549359	0.230911	0.371815
Si	0.498233	0.191637	0.170437
Si	0.500961	0.035690	0.156666
Si	0.542248	0.975449	0.364424
Si	0.504290	0.100440	0.495364
Si	0.248349	0.511466	0.811516
Si	0.204030	0.630768	0.956140
Si	0.239816	0.653490	0.179464
Si	0.248523	0.815036	0.175871
Si	0.209311	0.864162	0.961997

Si	0.235388	0.754952	0.814132
Si	0.012928	0.509703	0.817739
Si	0.043850	0.626471	0.962953
Si	0.998904	0.638894	0.179031
Si	0.003918	0.795928	0.189930
Si	0.049393	0.867160	0.982286
Si	0.003265	0.756731	0.846276
Si	0.612644	0.513365	0.836934
Si	0.660674	0.605301	0.996079
Si	0.632158	0.638213	0.212818
Si	0.610768	0.794210	0.214031
Si	0.632282	0.842856	0.994872
Si	0.609069	0.721794	0.867014
Si	0.859534	0.504371	0.826730
Si	0.815819	0.616574	0.972217
Si	0.841559	0.641055	0.195311
Si	0.844966	0.797372	0.182413
Si	0.791877	0.851981	0.978302
Si	0.844773	0.742232	0.845624
Ti	0.506812	0.636776	0.718369

Model E (H-terminated hexacoordinated)

H	0.504960	0.528433	0.775715
H	0.499467	0.733178	0.779958
O	0.756049	0.780586	0.417013
O	0.729692	0.737435	0.604462
O	0.710636	0.616452	0.695424
O	0.745867	0.508866	0.580217
O	0.719644	0.522601	0.387890
O	0.739896	0.648016	0.459271
O	0.510195	0.784156	0.473018
O	0.555083	0.680758	0.595583
O	0.493642	0.565126	0.561892
O	0.526726	0.531370	0.372811
O	0.531572	0.663870	0.396340
O	0.635028	0.737444	0.458884
O	0.617081	0.518213	0.522096
O	0.803832	0.851595	0.263536
O	0.672700	0.824561	0.267056
O	0.539989	0.801898	0.277051
O	0.807291	0.604665	0.296933
O	0.674546	0.632222	0.290535
O	0.551932	0.609822	0.214631
O	0.687227	0.406333	0.477694
O	0.510539	0.434783	0.502662
O	0.419170	0.835510	0.345627
O	0.429619	0.610287	0.288962
O	0.427233	0.686467	0.670047
O	0.432321	0.560019	0.737733
O	0.140857	0.789744	0.410051

O	0.107021	0.721565	0.571712
O	0.116861	0.628274	0.718518
O	0.121919	0.549018	0.554712
O	0.143622	0.537029	0.359226
O	0.092829	0.662933	0.395044
O	0.300481	0.779549	0.400332
O	0.314101	0.732773	0.584317
O	0.314506	0.611248	0.673481
O	0.360539	0.497738	0.589343
O	0.355978	0.520744	0.390490
O	0.345112	0.652098	0.430485
O	0.216737	0.683717	0.463903
O	0.240953	0.506127	0.491947
O	0.046642	0.833462	0.279589
O	0.174542	0.826666	0.222434
O	0.308481	0.850519	0.234200
O	0.046082	0.591556	0.244375
O	0.169499	0.641438	0.234820
O	0.298126	0.602673	0.253699
O	0.131616	0.425370	0.468195
O	0.323907	0.400780	0.466578
O	0.657203	0.049311	0.938421
O	0.616306	0.099442	0.765074
O	0.580391	0.210139	0.661711
O	0.646378	0.304373	0.766092
O	0.595277	0.308927	0.951538
O	0.602960	0.174173	0.929993
O	0.825733	0.057154	0.913066
O	0.825705	0.108330	0.730766
O	0.817845	0.234874	0.666944
O	0.813055	0.349152	0.768224
O	0.823291	0.310065	0.961399
O	0.855064	0.188437	0.884439
O	0.728042	0.147891	0.859909
O	0.711114	0.373301	0.902172
O	0.546573	0.020309	0.048652
O	0.671819	0.987793	0.112923
O	0.803632	0.026294	0.105966
O	0.549737	0.229978	0.095823
O	0.682237	0.238490	0.061451
O	0.808056	0.194297	0.070874
O	0.588838	0.419421	0.841426
O	0.825652	0.441086	0.906608
O	0.915847	0.983169	0.020181
O	0.928978	0.240478	0.032376
O	0.925384	0.158279	0.614788
O	0.916210	0.325803	0.636376
O	0.235058	0.074054	0.977512
O	0.246280	0.119834	0.791157
O	0.207032	0.221712	0.671362
O	0.251282	0.328354	0.779777

O	0.231625	0.325482	0.979623
O	0.197217	0.200795	0.934712
O	0.995520	0.075354	0.938802
O	0.012036	0.130055	0.762639
O	0.026136	0.242829	0.656028
O	0.000886	0.343383	0.783862
O	0.023390	0.330551	0.979595
O	0.039685	0.202445	0.927495
O	0.121555	0.099704	0.872174
O	0.127656	0.341134	0.851198
O	0.293701	0.989771	0.109170
O	0.158625	0.001104	0.107251
O	0.025546	0.031372	0.121332
O	0.305238	0.222116	0.050488
O	0.182037	0.246650	0.123680
O	0.045989	0.239704	0.123073
O	0.217352	0.440196	0.886364
O	0.046749	0.447969	0.890008
O	0.110468	0.290901	0.460560
O	0.114931	0.220011	0.290777
O	0.120871	0.128420	0.138377
O	0.103862	0.037022	0.282442
O	0.123052	0.027866	0.476230
O	0.154043	0.159721	0.456632
O	0.362424	0.276774	0.426975
O	0.324790	0.235845	0.247350
O	0.317693	0.113506	0.171422
O	0.356127	0.009439	0.287811
O	0.331283	0.033236	0.484709
O	0.316851	0.153028	0.408309
O	0.230516	0.258114	0.386137
O	0.229424	0.013337	0.352163
O	0.042343	0.367453	0.592348
O	0.175346	0.348246	0.617337
O	0.303221	0.301782	0.602370
O	0.049101	0.121942	0.570144
O	0.177063	0.094634	0.626796
O	0.306272	0.136643	0.611133
O	0.135977	0.917025	0.363426
O	0.314548	0.912083	0.411390
O	0.427791	0.341270	0.569852
O	0.425904	0.128701	0.525261
O	0.423479	0.192278	0.122839
O	0.422485	0.032838	0.119673
O	0.743494	0.290364	0.409182
O	0.743433	0.226856	0.239427
O	0.705643	0.116545	0.141130
O	0.739947	0.019673	0.277749
O	0.728719	0.033328	0.475370
O	0.708773	0.157255	0.403441
O	0.527439	0.306858	0.441285

O	0.495680	0.232463	0.279360
O	0.522641	0.113077	0.191413
O	0.520155	0.982778	0.238561
O	0.497668	0.042149	0.417565
O	0.542595	0.171028	0.442189
O	0.624031	0.249090	0.331280
O	0.621131	0.002256	0.367322
O	0.792191	0.351649	0.572929
O	0.672111	0.287009	0.572155
O	0.554731	0.342014	0.631402
O	0.807359	0.134039	0.535144
O	0.679716	0.129110	0.596692
O	0.548916	0.087175	0.592549
O	0.722307	0.911292	0.397756
O	0.526327	0.908796	0.403055
O	0.233717	0.572854	0.886382
O	0.244469	0.620407	0.071283
O	0.267361	0.727170	0.189158
O	0.250093	0.828206	0.058633
O	0.242426	0.826023	0.860240
O	0.214305	0.702677	0.917198
O	0.015568	0.579026	0.872655
O	0.996516	0.612078	0.062526
O	0.030658	0.719440	0.173080
O	0.018710	0.842484	0.085141
O	0.006449	0.833121	0.885815
O	0.029377	0.706118	0.931013
O	0.122434	0.614183	0.986450
O	0.129215	0.842683	0.969029
O	0.314846	0.494755	0.775618
O	0.185232	0.510684	0.722742
O	0.050454	0.510652	0.711351
O	0.317616	0.724814	0.783244
O	0.188822	0.740501	0.727576
O	0.052781	0.747548	0.744519
O	0.222160	0.941312	0.955978
O	0.042183	0.948607	0.966445
O	0.932334	0.484433	0.796530
O	0.925427	0.740284	0.806986
O	0.923291	0.644812	0.223629
O	0.925280	0.801049	0.214891
O	0.633115	0.530474	0.930017
O	0.661359	0.597710	0.099286
O	0.621362	0.720244	0.164672
O	0.595870	0.842005	0.104178
O	0.590039	0.794815	0.913679
O	0.618272	0.663545	0.938740
O	0.868954	0.565981	0.921948
O	0.822600	0.607002	0.100747
O	0.813776	0.724439	0.198896
O	0.836081	0.828567	0.072688

O	0.819457	0.815942	0.875540
O	0.844881	0.696265	0.955052
O	0.742188	0.608482	0.939135
O	0.710674	0.825988	0.995401
O	0.553675	0.542867	0.765488
O	0.680383	0.492162	0.749470
O	0.810509	0.528567	0.749934
O	0.532264	0.697920	0.798819
O	0.666621	0.730571	0.779428
O	0.800790	0.703771	0.765382
O	0.618066	0.923361	0.953764
O	0.793665	0.933088	0.963331
Si	0.738150	0.841171	0.337056
Si	0.714957	0.725659	0.485510
Si	0.727147	0.696929	0.710793
Si	0.738103	0.537890	0.693676
Si	0.692307	0.488418	0.491900
Si	0.735979	0.601127	0.358172
Si	0.499303	0.832908	0.374595
Si	0.557062	0.714901	0.484473
Si	0.536387	0.512148	0.491223
Si	0.509513	0.604152	0.319405
Si	0.124817	0.841528	0.318417
Si	0.139090	0.714880	0.460356
Si	0.116608	0.709205	0.690764
Si	0.119131	0.550421	0.676500
Si	0.159923	0.503176	0.468467
Si	0.114150	0.607010	0.309598
Si	0.337325	0.844267	0.348935
Si	0.294474	0.712432	0.469827
Si	0.343894	0.688900	0.678809
Si	0.357797	0.540024	0.694748
Si	0.320333	0.482381	0.485402
Si	0.356037	0.596423	0.340519
Si	0.622370	0.995270	0.013956
Si	0.650810	0.118277	0.872422
Si	0.606216	0.130939	0.653006
Si	0.613167	0.285726	0.658141
Si	0.635278	0.351479	0.865589
Si	0.607204	0.237023	0.009825
Si	0.835443	0.000165	0.999819
Si	0.808173	0.124451	0.847962
Si	0.844474	0.158673	0.637334
Si	0.835989	0.315369	0.662381
Si	0.793066	0.366663	0.883828
Si	0.853003	0.234471	0.986948
Si	0.227342	0.002476	0.037505
Si	0.200024	0.122944	0.893199
Si	0.235458	0.143104	0.674636
Si	0.233785	0.300071	0.667815
Si	0.207239	0.358925	0.873779

Si	0.228954	0.248366	0.022758
Si	0.994210	0.009274	0.012108
Si	0.042732	0.127467	0.875335
Si	0.003669	0.163350	0.651839
Si	0.996376	0.320355	0.666652
Si	0.050170	0.365475	0.876323
Si	0.009529	0.252498	0.015206
Si	0.115149	0.357448	0.533680
Si	0.152005	0.232424	0.398360
Si	0.115888	0.208555	0.170348
Si	0.101780	0.049559	0.162306
Si	0.148428	0.997996	0.368397
Si	0.124964	0.101429	0.532018
Si	0.353949	0.331662	0.517621
Si	0.308193	0.230624	0.366120
Si	0.342836	0.190739	0.148560
Si	0.347370	0.035658	0.172145
Si	0.307245	0.992532	0.384209
Si	0.345188	0.113367	0.508371
Si	0.724239	0.334755	0.508376
Si	0.704638	0.230673	0.347037
Si	0.735087	0.193725	0.128715
Si	0.730174	0.037684	0.160045
Si	0.702810	0.990742	0.378443
Si	0.730366	0.113894	0.502653
Si	0.505519	0.355931	0.534778
Si	0.546864	0.240199	0.375130
Si	0.498743	0.192173	0.172432
Si	0.502821	0.037233	0.149668
Si	0.541153	0.983910	0.357120
Si	0.503287	0.106987	0.493388
Si	0.237596	0.505127	0.817761
Si	0.203182	0.627385	0.965636
Si	0.245165	0.647713	0.186767
Si	0.249501	0.807723	0.176250
Si	0.210273	0.859608	0.961811
Si	0.241327	0.747387	0.821761
Si	0.010839	0.505559	0.818430
Si	0.041924	0.627139	0.962704
Si	0.999270	0.642345	0.176315
Si	0.005818	0.798787	0.186698
Si	0.049817	0.866388	0.977784
Si	0.003357	0.756169	0.841108
Si	0.614271	0.496833	0.822062
Si	0.664011	0.599632	0.977822
Si	0.627143	0.639988	0.191925
Si	0.607287	0.797051	0.205999
Si	0.629257	0.845563	0.992098
Si	0.603591	0.722587	0.857225
Si	0.858121	0.503883	0.843155
Si	0.819920	0.619306	0.980757

Si	0.841888	0.645787	0.204832
Si	0.845016	0.801261	0.187004
Si	0.789243	0.851142	0.977632
Si	0.847945	0.739787	0.849824
Ti	0.497782	0.623123	0.669572

Model F (Na-terminated hexacoordinated)

O	0.747950	0.778366	0.410499
O	0.720998	0.735064	0.600360
O	0.725174	0.612966	0.684689
O	0.733906	0.495001	0.595518
O	0.737985	0.514364	0.401087
O	0.738330	0.644433	0.460186
O	0.513103	0.788774	0.478067
O	0.554526	0.682863	0.602853
O	0.506988	0.562889	0.573981
O	0.516413	0.535891	0.376361
O	0.511113	0.666600	0.410233
O	0.630002	0.724283	0.450040
O	0.619364	0.511398	0.498582
O	0.800567	0.849901	0.260523
O	0.666289	0.839362	0.268820
O	0.538794	0.799310	0.278430
O	0.803980	0.604979	0.293483
O	0.667145	0.607919	0.304740
O	0.547934	0.621225	0.222618
O	0.688734	0.396972	0.472940
O	0.507348	0.433376	0.497731
O	0.416584	0.826047	0.349224
O	0.423376	0.612359	0.284058
O	0.427059	0.683488	0.668558
O	0.432954	0.562262	0.748259
O	0.137980	0.790635	0.411719
O	0.099228	0.721449	0.571999
O	0.118882	0.630250	0.719696
O	0.120641	0.551380	0.555070
O	0.145213	0.539100	0.360676
O	0.090753	0.663837	0.393246
O	0.293003	0.781402	0.401242
O	0.318510	0.728414	0.578474
O	0.312534	0.616812	0.692549
O	0.364351	0.520715	0.582613
O	0.351549	0.521589	0.386152
O	0.335027	0.651844	0.418560
O	0.211164	0.684566	0.471430
O	0.240610	0.509864	0.497204
O	0.045280	0.833130	0.280107
O	0.173930	0.827840	0.224166
O	0.308025	0.850822	0.234921
O	0.043480	0.589990	0.248376

O	0.165559	0.641290	0.229667
O	0.292173	0.598347	0.242198
O	0.133371	0.426932	0.470617
O	0.326993	0.407150	0.488492
O	0.656360	0.046145	0.937052
O	0.616247	0.098385	0.765936
O	0.581357	0.210915	0.666740
O	0.648908	0.310533	0.761339
O	0.594378	0.310156	0.943394
O	0.603806	0.173494	0.930039
O	0.826581	0.056837	0.914875
O	0.824657	0.107108	0.730820
O	0.821585	0.235055	0.672376
O	0.810908	0.352241	0.766145
O	0.823751	0.309769	0.957629
O	0.855656	0.187697	0.882679
O	0.728136	0.146125	0.861336
O	0.710751	0.373108	0.904944
O	0.545618	0.018978	0.046140
O	0.669687	0.986895	0.114032
O	0.801257	0.026652	0.108373
O	0.548285	0.233869	0.090164
O	0.681034	0.240566	0.059229
O	0.806439	0.193924	0.066896
O	0.591623	0.426090	0.836379
O	0.825273	0.441394	0.908172
O	0.914700	0.984389	0.026169
O	0.928260	0.241300	0.031075
O	0.925463	0.155879	0.614983
O	0.917816	0.328779	0.640507
O	0.233626	0.074917	0.980539
O	0.245594	0.118869	0.793323
O	0.206759	0.220477	0.672951
O	0.253240	0.327192	0.778841
O	0.234031	0.325553	0.979378
O	0.196924	0.201322	0.935389
O	0.995051	0.076284	0.943127
O	0.011000	0.130267	0.765319
O	0.024789	0.242634	0.656363
O	0.003689	0.342671	0.786746
O	0.025355	0.331239	0.981945
O	0.039721	0.203252	0.928960
O	0.120659	0.100199	0.873999
O	0.130099	0.338282	0.852176
O	0.293832	0.990873	0.110832
O	0.158537	0.001591	0.112074
O	0.025458	0.031482	0.125496
O	0.304013	0.221290	0.051929
O	0.180180	0.248511	0.123216
O	0.044099	0.239239	0.125121
O	0.218710	0.439199	0.883183

O	0.054373	0.447727	0.889438
O	0.110241	0.292277	0.460733
O	0.114257	0.220410	0.291793
O	0.120483	0.129367	0.138841
O	0.104631	0.039550	0.285695
O	0.123908	0.028170	0.478184
O	0.154000	0.160935	0.458564
O	0.360033	0.286167	0.421700
O	0.324537	0.237480	0.247452
O	0.318552	0.114164	0.174471
O	0.356900	0.009661	0.288476
O	0.330791	0.035479	0.483854
O	0.317533	0.158417	0.412776
O	0.229420	0.260309	0.385109
O	0.229953	0.011314	0.353335
O	0.045084	0.367985	0.596059
O	0.178237	0.347240	0.615886
O	0.304909	0.297255	0.602356
O	0.049890	0.121538	0.573383
O	0.177812	0.093756	0.627728
O	0.306994	0.135915	0.614193
O	0.133463	0.917859	0.363731
O	0.317937	0.912244	0.412580
O	0.430729	0.336431	0.571694
O	0.426146	0.130179	0.525015
O	0.423067	0.194085	0.122475
O	0.423056	0.033680	0.120648
O	0.748128	0.283830	0.407749
O	0.743265	0.224447	0.235904
O	0.702721	0.116539	0.136339
O	0.735163	0.021869	0.278857
O	0.729827	0.033357	0.478101
O	0.707345	0.154095	0.401531
O	0.527692	0.306977	0.436171
O	0.497736	0.232390	0.276472
O	0.524217	0.115287	0.184564
O	0.523521	0.986263	0.237980
O	0.498077	0.043619	0.417624
O	0.543423	0.171766	0.441678
O	0.625999	0.249143	0.330235
O	0.620514	0.997065	0.377109
O	0.795387	0.347947	0.569490
O	0.676039	0.280321	0.572151
O	0.559723	0.342370	0.623398
O	0.805824	0.137566	0.536174
O	0.678425	0.129081	0.596753
O	0.547624	0.088845	0.594235
O	0.727989	0.912587	0.401669
O	0.518047	0.909754	0.398418
O	0.235656	0.571248	0.884970
O	0.242832	0.627100	0.063777

O	0.265347	0.727297	0.193864
O	0.248840	0.826336	0.058921
O	0.235468	0.829686	0.859365
O	0.211732	0.702702	0.904133
O	0.015108	0.578554	0.875065
O	0.998432	0.609949	0.065291
O	0.028352	0.718578	0.175946
O	0.014074	0.841803	0.087237
O	0.006288	0.833760	0.888020
O	0.027512	0.706169	0.935307
O	0.122767	0.614042	0.981444
O	0.126832	0.843409	0.977605
O	0.313835	0.492594	0.766539
O	0.183865	0.511151	0.721939
O	0.049701	0.513295	0.712175
O	0.316819	0.737701	0.777874
O	0.187835	0.745835	0.718123
O	0.052955	0.747881	0.749339
O	0.220631	0.941895	0.960745
O	0.040273	0.949196	0.970426
O	0.936849	0.478684	0.807847
O	0.925123	0.740192	0.810946
O	0.921309	0.642815	0.223195
O	0.922900	0.799791	0.219215
O	0.619601	0.537049	0.939010
O	0.659374	0.596741	0.109549
O	0.638808	0.718550	0.197845
O	0.594179	0.825929	0.099178
O	0.592600	0.793933	0.900939
O	0.622227	0.672625	0.958402
O	0.866372	0.568048	0.915757
O	0.823168	0.605338	0.097779
O	0.812642	0.723093	0.195455
O	0.837213	0.827742	0.071421
O	0.820009	0.818128	0.874909
O	0.836666	0.695954	0.950773
O	0.737501	0.602409	0.943859
O	0.711006	0.824536	0.995718
O	0.576209	0.556754	0.748123
O	0.694761	0.498593	0.783671
O	0.822655	0.522622	0.739600
O	0.533674	0.682377	0.807452
O	0.665930	0.715999	0.780242
O	0.802115	0.710393	0.756727
O	0.616241	0.918980	0.959388
O	0.793186	0.933301	0.966579
Na	0.629046	0.599018	0.599808
Na	0.423610	0.628553	0.517316
Si	0.735237	0.843637	0.335602
Si	0.710024	0.722150	0.480686
Si	0.728627	0.695148	0.708129

Si	0.745429	0.532455	0.702384
Si	0.695333	0.477766	0.491236
Si	0.737848	0.593175	0.362945
Si	0.497245	0.831498	0.374744
Si	0.551873	0.715495	0.492206
Si	0.534803	0.510731	0.491395
Si	0.502038	0.608952	0.322292
Si	0.122997	0.842250	0.319068
Si	0.133995	0.715767	0.462121
Si	0.115155	0.711161	0.690355
Si	0.118766	0.552498	0.677065
Si	0.160128	0.505418	0.470784
Si	0.112484	0.607196	0.309448
Si	0.336021	0.843231	0.350079
Si	0.288514	0.712974	0.468415
Si	0.346119	0.693365	0.683387
Si	0.359082	0.546579	0.701041
Si	0.320357	0.488960	0.490316
Si	0.348531	0.595263	0.329078
Si	0.621292	0.992320	0.014049
Si	0.650705	0.116520	0.873359
Si	0.605625	0.131322	0.654860
Si	0.615917	0.285773	0.656750
Si	0.635280	0.356854	0.861430
Si	0.606936	0.239293	0.004802
Si	0.834612	0.000468	0.003282
Si	0.808144	0.123453	0.848473
Si	0.844669	0.158608	0.638610
Si	0.837599	0.316041	0.664023
Si	0.791903	0.367488	0.883357
Si	0.852878	0.234348	0.984302
Si	0.226792	0.003278	0.041219
Si	0.199051	0.123194	0.895168
Si	0.235718	0.142051	0.676576
Si	0.235172	0.298309	0.667771
Si	0.209354	0.357700	0.872926
Si	0.228664	0.248569	0.023515
Si	0.993103	0.010071	0.016778
Si	0.042106	0.128038	0.877696
Si	0.003111	0.162704	0.653550
Si	0.997721	0.320818	0.669409
Si	0.053622	0.364801	0.877869
Si	0.009063	0.253018	0.016493
Si	0.116897	0.357936	0.535029
Si	0.151452	0.233447	0.398866
Si	0.114674	0.209419	0.171162
Si	0.101552	0.050548	0.165179
Si	0.148554	0.998490	0.370052
Si	0.125451	0.101703	0.533981
Si	0.355751	0.332913	0.522145
Si	0.307696	0.234958	0.366487

Si	0.342846	0.191667	0.149762
Si	0.348054	0.036401	0.173062
Si	0.308076	0.992675	0.385095
Si	0.345408	0.115279	0.509777
Si	0.728149	0.327361	0.506765
Si	0.705660	0.227496	0.344317
Si	0.733227	0.193679	0.124193
Si	0.727013	0.038034	0.160154
Si	0.702776	0.990667	0.382211
Si	0.729839	0.114187	0.503702
Si	0.506914	0.354375	0.531409
Si	0.548374	0.240081	0.372158
Si	0.499211	0.194202	0.168045
Si	0.503694	0.038673	0.147476
Si	0.540375	0.984424	0.357736
Si	0.503416	0.108073	0.493924
Si	0.237917	0.504506	0.814128
Si	0.202702	0.628587	0.957291
Si	0.240863	0.648906	0.180752
Si	0.248567	0.808149	0.177806
Si	0.207470	0.860302	0.965082
Si	0.238773	0.752922	0.814389
Si	0.014086	0.504645	0.822033
Si	0.041922	0.626891	0.964053
Si	0.997915	0.640824	0.178512
Si	0.003169	0.797854	0.189410
Si	0.047524	0.866910	0.981712
Si	0.002604	0.756502	0.844930
Si	0.615644	0.506228	0.824463
Si	0.659136	0.601330	0.987281
Si	0.628514	0.636871	0.205989
Si	0.608553	0.795498	0.211082
Si	0.628600	0.839126	0.988339
Si	0.600353	0.715861	0.857839
Si	0.861463	0.501787	0.843636
Si	0.815439	0.617708	0.978034
Si	0.840509	0.644697	0.201426
Si	0.843672	0.800199	0.186006
Si	0.788896	0.850991	0.978164
Si	0.846355	0.741566	0.848258
Ti	0.503511	0.622816	0.706345

Model G (dimeric tetracoordinated)

O	0.752777	0.763221	0.238363
O	0.745393	0.707625	0.414495
O	0.710532	0.594324	0.506288
O	0.746437	0.498013	0.378456
O	0.714528	0.509755	0.182808
O	0.730113	0.631578	0.253796
O	0.527876	0.738088	0.173889

O	0.508338	0.700650	0.361174
O	0.533210	0.578646	0.478909
O	0.495521	0.464341	0.352675
O	0.533662	0.493642	0.164638
O	0.559597	0.615781	0.227707
O	0.633247	0.717433	0.301662
O	0.624193	0.464112	0.311731
O	0.798924	0.813269	0.068479
O	0.668433	0.775755	0.086629
O	0.546697	0.806294	0.010741
O	0.810418	0.588998	0.110423
O	0.682089	0.614936	0.067200
O	0.551409	0.591241	0.030592
O	0.732236	0.390998	0.261634
O	0.544227	0.369893	0.231199
O	0.427379	0.812895	0.099312
O	0.440366	0.589472	0.134691
O	0.411216	0.655230	0.509140
O	0.412863	0.498135	0.530106
O	0.116421	0.755961	0.195286
O	0.135258	0.697250	0.371931
O	0.095462	0.579555	0.443595
O	0.136699	0.457804	0.392467
O	0.102641	0.493351	0.201424
O	0.112366	0.624834	0.209407
O	0.350509	0.748146	0.232194
O	0.302765	0.697372	0.404101
O	0.304573	0.574087	0.481946
O	0.334837	0.461623	0.379882
O	0.353713	0.494016	0.188193
O	0.343652	0.616363	0.263673
O	0.230434	0.688980	0.232821
O	0.229935	0.475274	0.255060
O	0.050080	0.817500	0.044924
O	0.183409	0.802908	0.035521
O	0.311471	0.762913	0.040625
O	0.048765	0.565608	0.054596
O	0.183644	0.556943	0.076189
O	0.313375	0.597629	0.071574
O	0.145828	0.370607	0.247586
O	0.313638	0.371081	0.238267
O	0.601372	0.012744	0.685918
O	0.603338	0.074280	0.513675
O	0.637450	0.185784	0.417227
O	0.603966	0.279450	0.554895
O	0.634784	0.262237	0.751414
O	0.634877	0.141751	0.679379
O	0.827832	0.025801	0.733756
O	0.847848	0.073022	0.553477
O	0.833941	0.187634	0.456905
O	0.843802	0.312022	0.522216

O	0.843356	0.273578	0.717112
O	0.793899	0.150294	0.694931
O	0.721221	0.052639	0.610883
O	0.729203	0.290658	0.616117
O	0.559955	0.954535	0.855318
O	0.682555	0.012556	0.841982
O	0.802569	0.964558	0.903368
O	0.540672	0.175503	0.809948
O	0.666449	0.162369	0.875442
O	0.795466	0.204191	0.875021
O	0.640192	0.381016	0.679828
O	0.805870	0.396502	0.663263
O	0.925567	0.957729	0.831620
O	0.912538	0.172736	0.792326
O	0.932098	0.102083	0.408228
O	0.930321	0.267849	0.384907
O	0.236419	0.006765	0.726228
O	0.215685	0.062742	0.547442
O	0.253866	0.181645	0.476356
O	0.226011	0.307032	0.529279
O	0.244726	0.269529	0.721274
O	0.232666	0.138308	0.707121
O	0.998866	0.011790	0.687386
O	0.042466	0.064671	0.515344
O	0.034758	0.187129	0.436369
O	0.003338	0.294956	0.544873
O	0.005202	0.265123	0.740066
O	0.008270	0.144059	0.661656
O	0.119310	0.067343	0.684313
O	0.120362	0.283926	0.643866
O	0.306258	0.940757	0.870107
O	0.174508	0.960187	0.890392
O	0.046396	0.000045	0.875999
O	0.297280	0.191908	0.864012
O	0.163089	0.206434	0.843232
O	0.037310	0.158951	0.856167
O	0.198092	0.390825	0.673870
O	0.036830	0.387527	0.678735
O	0.104143	0.250381	0.197605
O	0.102916	0.197667	0.018703
O	0.143540	0.087330	0.924169
O	0.106638	0.991690	0.053314
O	0.144042	0.001260	0.249660
O	0.130841	0.121283	0.176858
O	0.337085	0.241746	0.207593
O	0.342867	0.167623	0.048274
O	0.324269	0.066221	0.922049
O	0.358747	0.969628	0.052918
O	0.330443	0.989017	0.244579
O	0.291479	0.115894	0.213577
O	0.221558	0.208889	0.113915

O	0.231846	0.966553	0.109308
O	0.059958	0.307254	0.365625
O	0.188859	0.262867	0.348913
O	0.318315	0.284751	0.393070
O	0.045807	0.080623	0.317456
O	0.171288	0.106082	0.368977
O	0.299647	0.067086	0.397890
O	0.132180	0.884509	0.168267
O	0.314960	0.868140	0.166672
O	0.429883	0.316811	0.297739
O	0.412017	0.089484	0.300277
O	0.424048	0.152278	0.893922
O	0.432279	0.986115	0.893107
O	0.696215	0.269448	0.208020
O	0.728713	0.203171	0.043458
O	0.760870	0.086413	0.960205
O	0.702138	0.973282	0.028576
O	0.747297	0.012783	0.208226
O	0.745087	0.145873	0.223363
O	0.515086	0.245110	0.188047
O	0.528866	0.196119	0.005924
O	0.531353	0.072553	0.934999
O	0.518858	0.962007	0.044003
O	0.495443	0.994898	0.236957
O	0.498241	0.114979	0.154411
O	0.621400	0.165983	0.149384
O	0.619243	0.976442	0.179498
O	0.802531	0.287975	0.332824
O	0.676514	0.311027	0.395462
O	0.544798	0.278811	0.377939
O	0.806336	0.072052	0.362701
O	0.671894	0.068545	0.345614
O	0.541158	0.103428	0.343149
O	0.716719	0.885075	0.178263
O	0.534131	0.871815	0.185498
O	0.244580	0.508800	0.730624
O	0.249047	0.565071	0.905722
O	0.212169	0.675701	0.000547
O	0.244968	0.770654	0.867519
O	0.202704	0.759821	0.673998
O	0.218698	0.639144	0.745573
O	0.019502	0.518415	0.704193
O	0.005223	0.589968	0.867193
O	0.029463	0.690838	0.994441
O	0.991609	0.787881	0.867357
O	0.024022	0.772141	0.676155
O	0.061431	0.645112	0.707056
O	0.128862	0.552966	0.813152
O	0.118763	0.797987	0.816874
O	0.286953	0.453888	0.561888
O	0.160422	0.502587	0.577295

O	0.036450	0.470593	0.520003
O	0.300582	0.681385	0.603209
O	0.176253	0.655624	0.553404
O	0.049326	0.694023	0.521148
O	0.218033	0.877770	0.751877
O	0.031647	0.892452	0.756923
O	0.923606	0.446803	0.613444
O	0.940277	0.671368	0.625151
O	0.923718	0.610147	0.017253
O	0.924029	0.770919	0.033622
O	0.622286	0.509126	0.713262
O	0.639327	0.572681	0.886828
O	0.612877	0.696482	0.947735
O	0.656131	0.818868	0.901288
O	0.609211	0.773911	0.724003
O	0.613474	0.640524	0.719623
O	0.847452	0.510783	0.745273
O	0.812246	0.570116	0.914326
O	0.818140	0.693596	0.986539
O	0.841691	0.805955	0.883779
O	0.863067	0.768567	0.694177
O	0.850784	0.644962	0.764929
O	0.733471	0.580970	0.747111
O	0.739256	0.792320	0.753422
O	0.552586	0.447105	0.565490
O	0.683623	0.467491	0.545666
O	0.811348	0.508861	0.552418
O	0.546116	0.709211	0.579366
O	0.681289	0.711890	0.585607
O	0.810739	0.670970	0.577598
O	0.656294	0.898620	0.745278
O	0.826587	0.893153	0.736757
Si	0.734399	0.809890	0.141561
Si	0.714864	0.704825	0.300985
Si	0.737016	0.671071	0.522243
Si	0.737921	0.517625	0.495663
Si	0.704197	0.465786	0.284240
Si	0.733851	0.586206	0.153355
Si	0.508420	0.807973	0.118186
Si	0.557926	0.693606	0.266193
Si	0.549103	0.448189	0.264185
Si	0.520872	0.572545	0.139281
Si	0.120660	0.814055	0.110670
Si	0.148949	0.691599	0.252630
Si	0.114064	0.656878	0.472077
Si	0.107093	0.503025	0.482254
Si	0.153054	0.449430	0.273999
Si	0.112039	0.560970	0.134284
Si	0.350914	0.798007	0.134935
Si	0.306658	0.688516	0.283140
Si	0.329462	0.651606	0.499205

Si	0.334579	0.497641	0.488589
Si	0.308361	0.450332	0.265425
Si	0.362848	0.573486	0.163636
Si	0.624153	0.968803	0.783873
Si	0.640772	0.070208	0.622930
Si	0.612976	0.108152	0.404163
Si	0.615831	0.263542	0.436903
Si	0.651612	0.303356	0.649928
Si	0.619568	0.184705	0.779345
Si	0.845863	0.960282	0.800692
Si	0.797121	0.075010	0.647836
Si	0.854918	0.108991	0.444598
Si	0.852624	0.264203	0.424353
Si	0.806075	0.318225	0.629281
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Si	0.200829	0.068675	0.666248
Si	0.235192	0.104361	0.447591
Si	0.246819	0.258748	0.437504
Si	0.197754	0.312443	0.642482
Si	0.234463	0.200675	0.784758
Si	0.001141	0.965072	0.787979
Si	0.042488	0.071493	0.636764
Si	0.013427	0.108810	0.420164
Si	0.007182	0.264223	0.432511
Si	0.041636	0.308055	0.652202
Si	0.990734	0.186217	0.762943
Si	0.124213	0.298206	0.291950
Si	0.140654	0.194926	0.127848
Si	0.111576	0.162536	0.910149
Si	0.117868	0.010000	0.935775
Si	0.153547	0.961159	0.144769
Si	0.123399	0.077519	0.278544
Si	0.349471	0.303495	0.284196
Si	0.297678	0.183740	0.145562
Si	0.346950	0.144577	0.931820
Si	0.355489	0.990602	0.934477
Si	0.309181	0.947973	0.143537
Si	0.333846	0.064962	0.288297
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Si	0.698197	0.196243	0.155222
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Si	0.737613	0.009843	0.934785
Si	0.697067	0.961576	0.148850
Si	0.742221	0.075491	0.285328
Si	0.508456	0.302185	0.273134
Si	0.541480	0.181588	0.124867
Si	0.505475	0.148906	0.911593
Si	0.510673	0.993598	0.932518
Si	0.541766	0.951577	0.160642
Si	0.487514	0.074770	0.259858

Si	0.222822	0.463516	0.634534
Si	0.209657	0.566437	0.797953
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Si	0.237945	0.752594	0.986011
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Si	0.004474	0.455923	0.629827
Si	0.053968	0.576239	0.772702
Si	0.001964	0.613917	0.983566
Si	0.999021	0.766951	0.985586
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Si	0.621450	0.618544	0.983229
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Si	0.664706	0.821136	0.780258
Si	0.613138	0.708319	0.652016
Si	0.847006	0.465806	0.643362
Si	0.810762	0.576088	0.792745
Si	0.842049	0.615965	0.006463
Si	0.845533	0.770653	0.992943
Si	0.818022	0.814780	0.767587
Si	0.865455	0.689481	0.664853
Ti	0.499729	0.663029	0.483915
Ti	0.498055	0.494730	0.481420

S3. Local detail of Ti structures

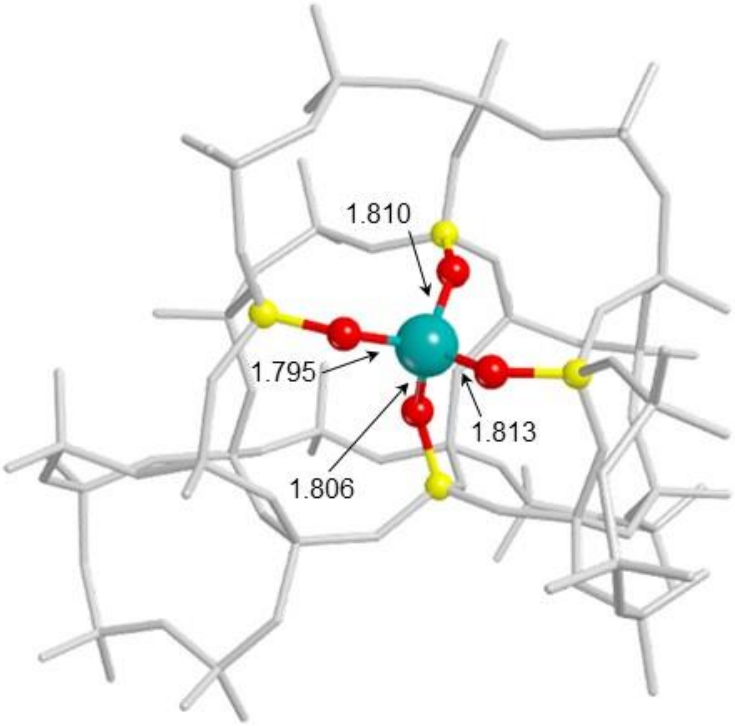

Figure S2. Structural detail of the perfect tetracoordinated Ti model (A in Figure 1). Distances are given in Å.

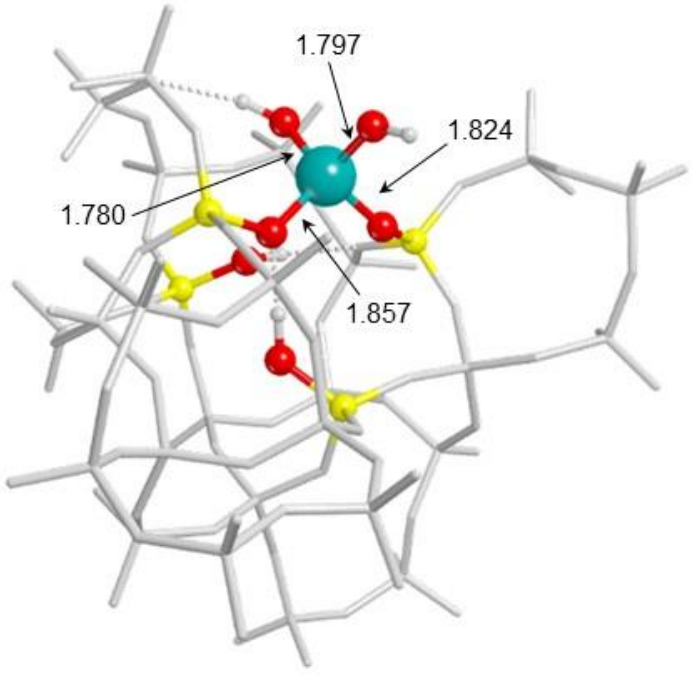

Figure S3. Structural detail of the bipodal tetracoordinated Ti model (B in Figure 1). Distances are given in Å.

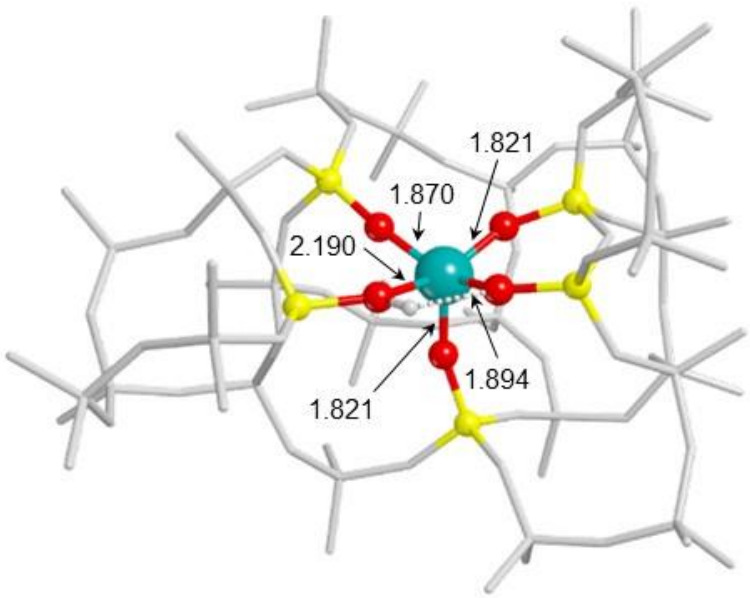

Figure S4. Structural detail of the H-terminated pentacoordinated Ti model (C in Figure 1). Distances are given in Å.

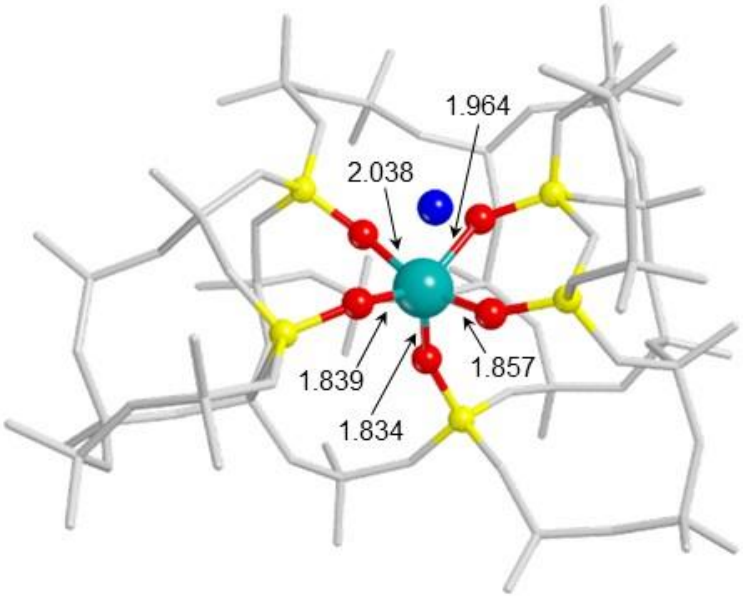

Figure S5. Structural detail of the Na-terminated pentacoordinated Ti model (D in Figure 1). Distances are given in Å.

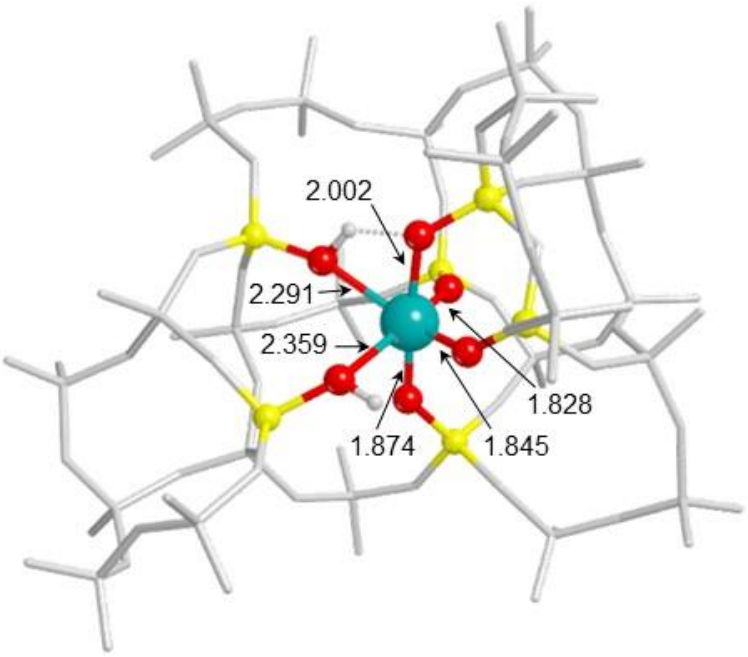

Figure S6. Structural detail of the H-terminated hexacoordinated Ti model (E in Figure 1). Distances are given in Å.

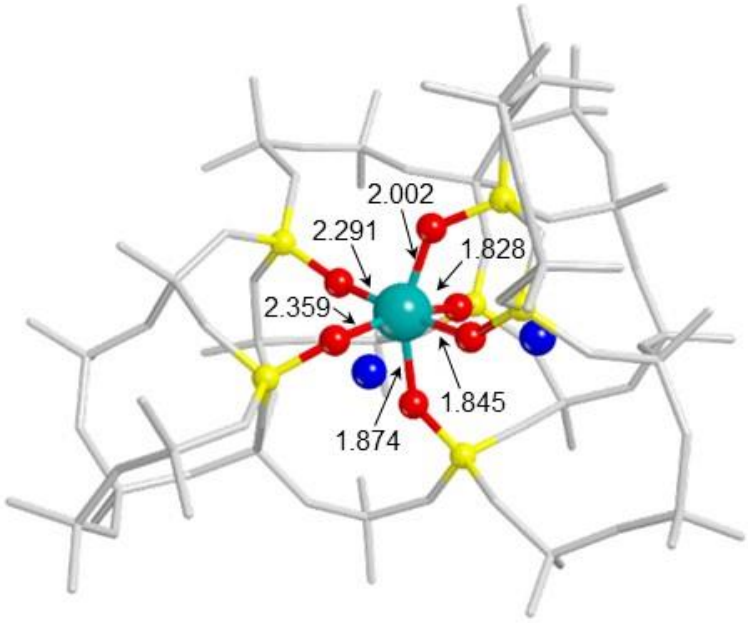

Figure S7. Structural detail of the Na-terminated hexacoordinated Ti model (F in Figure 1). Distances are given in Å.

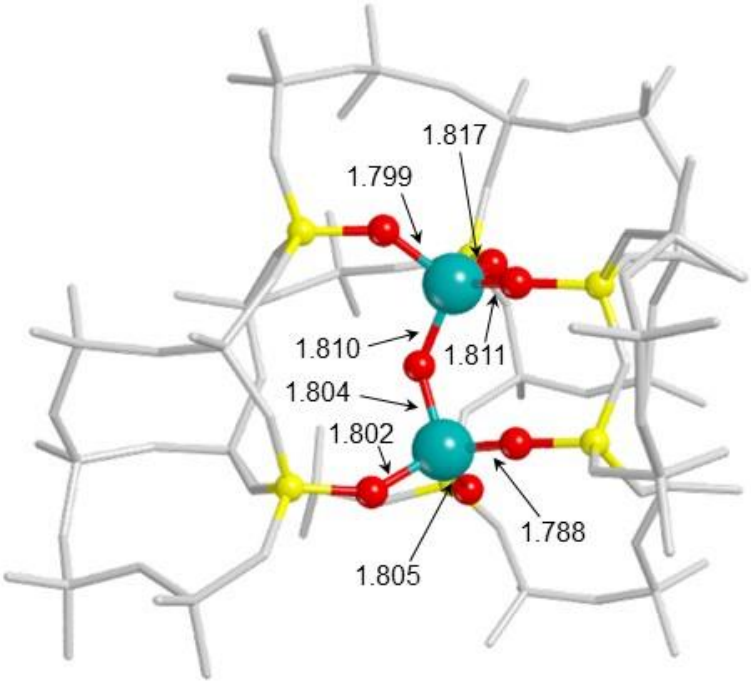

Figure S8. Structural detail of the dimeric tetracoordinated Ti model (G in Figure 1). Distances are given in Å.

S4. Ti K-edge XANES: pre-edge region

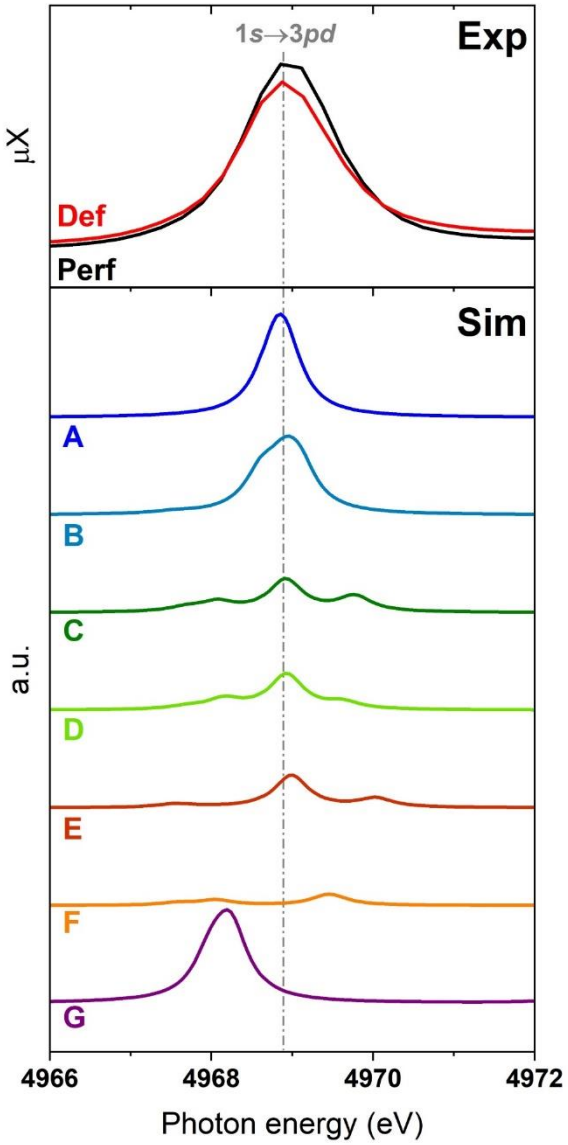

Figure S9. In the top panel (Exp), experimental Ti K-edges XANES spectra (in the pre-edge region) for the perfect TS-1A (Perf) and the defective TS-1B (Def) samples. In the bottom panel (Sim), the simulated Ti K-edges XANES spectra for the seven models reported in Figure 1: **A**, perfect tetracoordinated Ti; **B**, bipodal tetracoordinated Ti; **C**, H-terminated pentacoordinated Ti; **D**, Na-terminated pentacoordinated Ti; **E**, H-terminated hexacoordinated Ti; **F**, Na-terminated hexacoordinated Ti; and **G**, dimeric tetracoordinated Ti.

The principal feature in the pre-edge region of Ti K-edge XANES of TS-1 is the narrow peak at 4969 eV, associated to the Ti *1s* → *3pd* electronic transition occurring in tetrahedral Ti species. According to simulation, this assignment to the perfect tetracoordinated Ti is confirmed (model A in Figure 1). The presence of bipodal tetracoordinated Ti (model B in Figure 1) would only cause an asymmetric broadening of the pre-edge peak, which is not

observed but cannot be excluded a priori if the concentration of these species is low. The presence of dimeric tetracoordinated sites (model G in Figure 1) should instead be easily detected, since they cause a shift of the Ti *1s* $\rightarrow$ *3pd* transition of -0.8 eV, which is recognizable within the photon resolution (0.25 eV) adopted in the collection of this portion of spectrum. Thereby, the presence of a significant amount of dimeric species can be excluded in our samples. The higher coordination Ti species (models C-F in Figure 1), instead, produces pre-edge fingerprints having an intensity negligible compared to that of tetracoordinated sites, thus this portion of XANES spectrum cannot be effectively used in a complete assessment of the coordination environment of defective Ti sites. This observation is in line with the selection rules for the Ti *1s* $\rightarrow$ *3pd* transitions, which become Laporte forbidden in the case the *d* orbitals are (approximately) centrosymmetric. This is clearly the case of octahedral Ti sites (e.g. model F of Figure 1), but simulation demonstrate as also pentacoordinated Ti sites show the same intensity drop.

S5. Ti K-edge XANES: benchmark calculations

Figure S10 shows the benchmark calculation for the XANES spectra of TiO_2 (anatase) and ETS-10, compared to the corresponding experimental spectra (collected as described in section S1.1). The structural models adopted in the calculations where obtained by optimizing the experimental structures for anatase[27] and ETS-10[28] (in Na form) at the same level of theory proposed in section S1.2. These test simulations demonstrates the reliability of the FDMNES based method, since the agreement with experimental data obtained for the edge/post-edge feature for these well-defined systems is remarkable. Instead, the procedure is not suitable for an accurate description of pre-edge features, as already commented in the main text and in section S4.

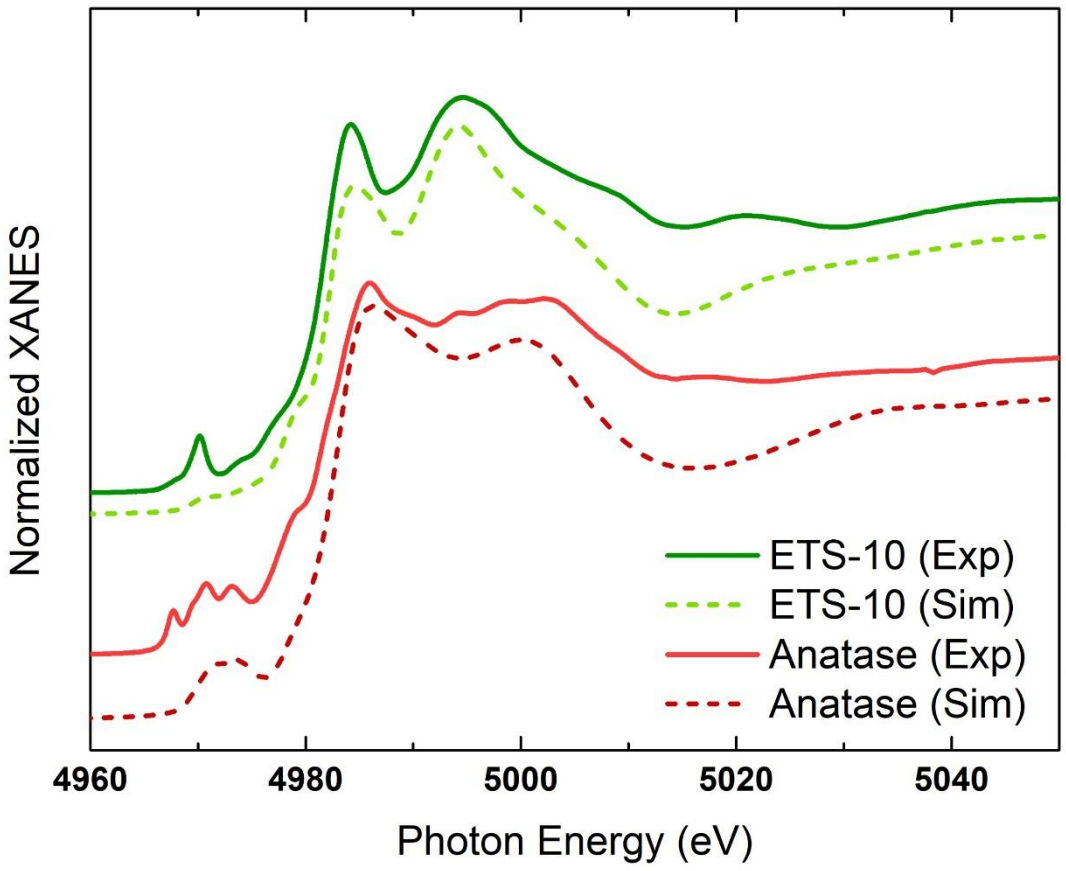

Figure S10. Benchmark calculation of Ti K-edge XANES simulation methodology on ETS-10 and TiO_2 (anatase), compared to the corresponding experimental results.

S6. Ti K-edge EXAFS

The k^2-weighted EXAFS spectra of TS-1A and TS-1B have been extracted in the 2.4-14.5 $Å^{-1}$ k-range. The magnitude and the imaginary part of the Fourier are shown in Figure S11.

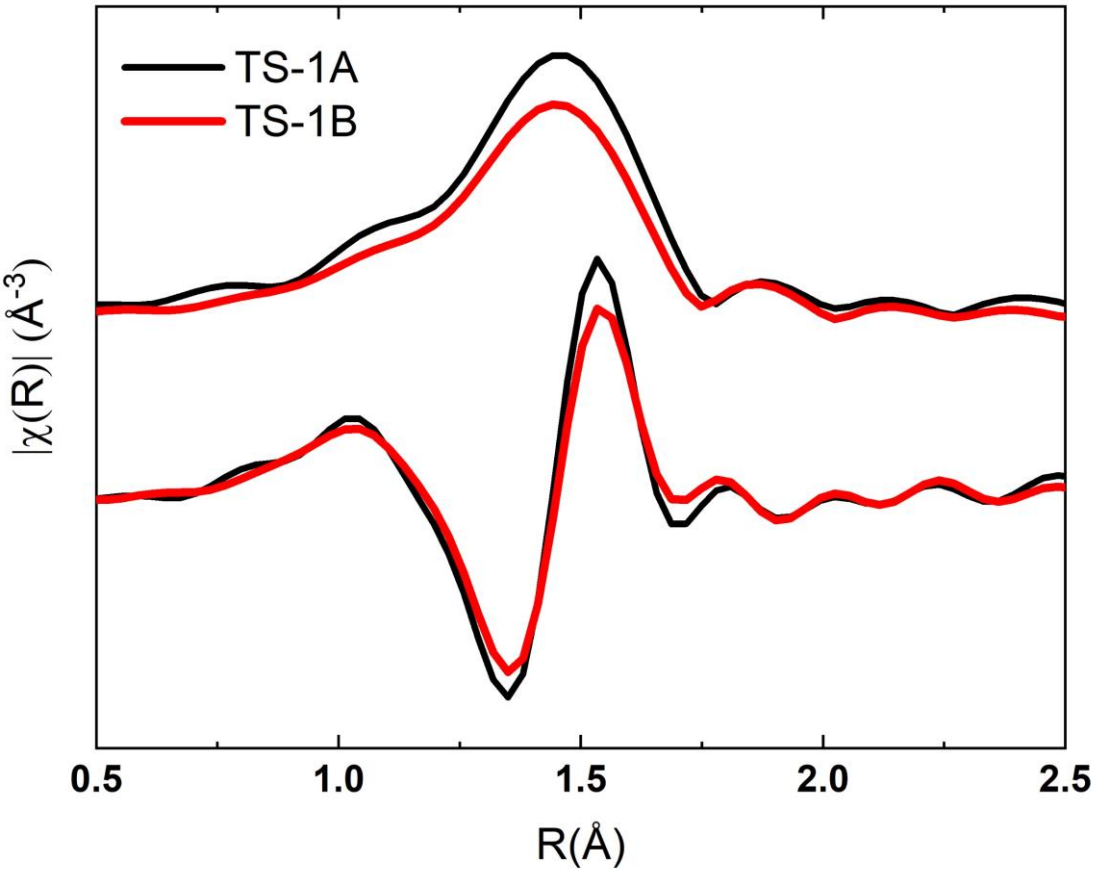

Figure S11. Magnitude and imaginary part of the Fourier transform of the EXAFS spectrum of TS-1A (black) and TS-1B (red).

In the 1st shell, TS-1A shows a more intense peak than TS-1B. The possible interpretations are: i) Ti sites in TS-1A have more scatterer neighbours in 1st shell (even though this is against our previous findings); ii) there are intense paths in antiphase that dump the signal of TS-1B. In order to clarify this point, a complete EXAFS analysis has been performed. Therefore, we calculated the scattering paths with FEFF6 code[29] by using the model A (perfect tetracoordinated Ti) to represent TS-1A, whereas the model F (Na-terminated hexacoordinated Ti) has been chosen to represent the fraction of defective sites in TS-1B.

First, we performed the EXAFS fit of TS-1A (R-range 1.0-2.8 Å), by fixing the coordination number and fitting the amplitude scattering factor (S_0^2), the Debye Waller factors for O in perfect Ti sites (σ_{Operf}^2), the energy shift (ΔE) and a single expansion coefficient α that multiplies all the Ti-O distances. The obtained EXAFS fit parameters are shown in Table 2. The quality of the fit can be appreciated graphically in the left panel of Figure S12. If the obtained value of the expansion coefficient approaches 1, it means that the model reliably describes the structureof the system. Since a value of 0.998±0.003 was obtained, we confirmed the reliability of the model A toward the description of the perfect tetrahedral Ti sites in TS-1A.

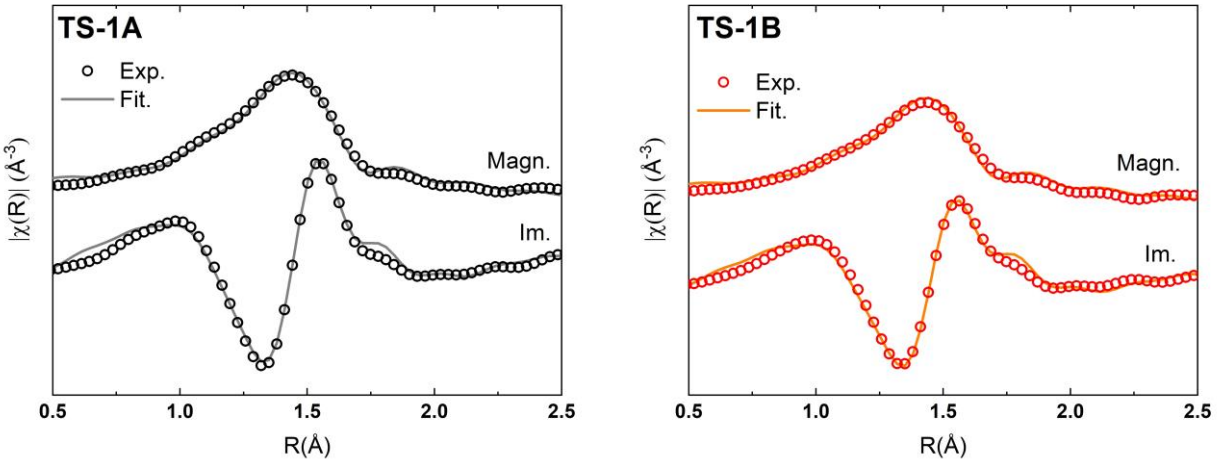

Figure S12. k^2-weighted, phase uncorrected, magnitude and imaginary part of the experimental (empty circles) and best fit (solid lines) FT EXAFS spectra for TS-1A (left panel) and TS-1B (right panel).

The EXAFS of TS-1B is more complicated because we assume the coexistence of at least two structural components, that increases significantly the number of variables to fit. Therefore, we performed a 2-phases fit, whereby the contribution of the perfect tetrahedral Ti phase (accounted by model A) was weighted by a free compositional variable x, while the contribution of the defective Ti sites (accounted by model F) was weighted by a factor $1-x$. We set α, S_0^2, ΔE and σ_{Operf}^2 to the values obtained from the TS-1A fit. For the second phase, we introduced a single expansion coefficient β that multiplies all the Ti-O distances, and the

Debye Waller factor (σ_{Odef}^2) for the O atom of the defective sites. The results of the fit are reported in Table 2. β resulted into a value of 0.98, thus confirming the validity of the structural hypothesis. σ_{Odef}^2 resulted into 0.01±0.01 Å^2, i.e. much higher than σ_{Operf}^2, refleting the greater static disorder of defective sites. The quality of the fit is reasonable and it can be appreciate in the right panel of Figure S12.

The decrease in the magnitude of the 1st-shell peak is thus ascribable to an antiphase effect, since the model adopted to represent the defective Ti sites (model F) is characterized by six first neighbors around the Ti absorber. The Ti-O single scattering paths computed for the models A and F, as shown in Figure S13, clearly confirms this scenario.

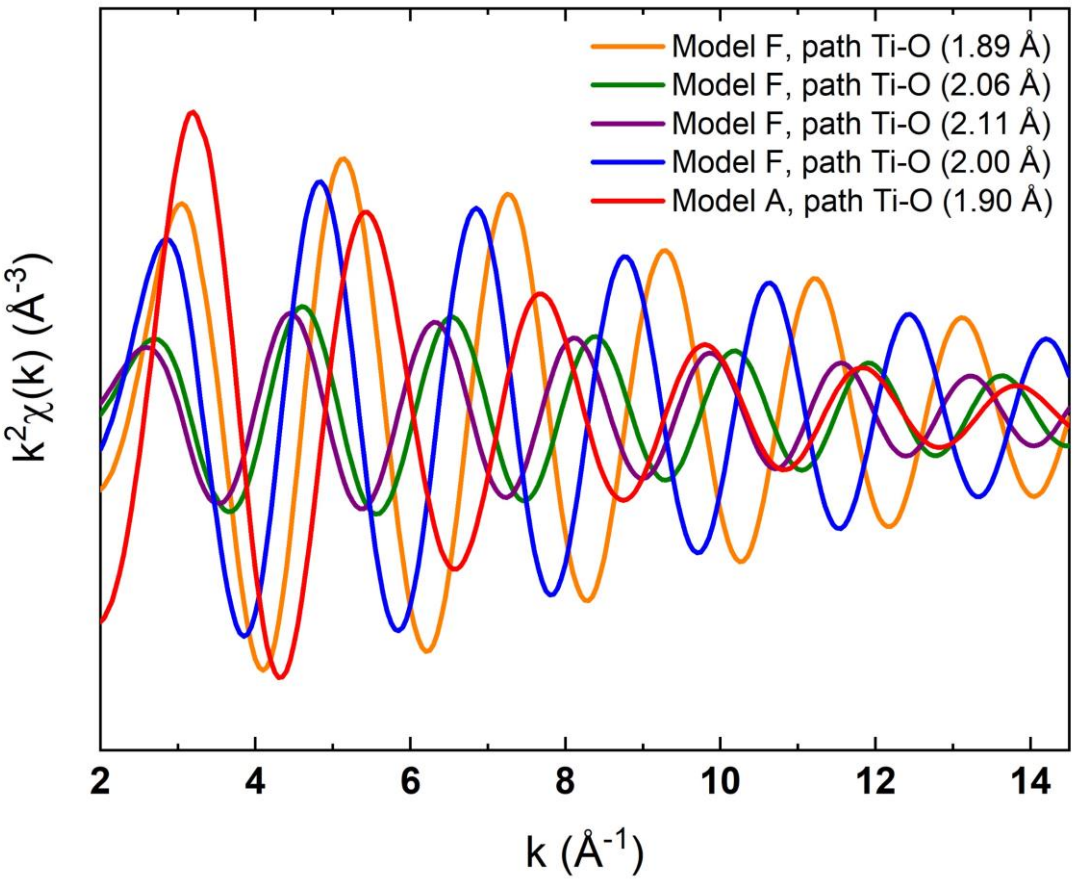

Figure S13. The k^2-weighted EXAFS spectra of Ti-O single scattering paths calculated for the structural models A and F.

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