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Supporting Information

Mechanism by which Tungsten Oxide Promotes the Activity of Supported V_2O_5/TiO_2 Catalysts for NO_X Abatement: Structural Effects Revealed by ^{51}V MAS NMR Spectroscopy

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Supporting Information

Methods

Sample Preparation

V_2O_5-WO_3/TiO_2 catalyst samples were prepared by incipient wetness impregnation. An aqueous solution of ammonium metatungstate (0.06 M, Pfaltz & Bauer, 99.5%) or ammonium metavanadate (0.35 M, Aldrich) was added to P25 TiO2 (Degussa, ~55 m2/g) until inceptively wet and the sample was subsequently mixed for 30 minutes. The sample was then dried overnight and subsequent impregnation was repeated with the second metal precursor (if applicable) as previously described[1]. After the second drying step, all samples were dried with flowing air (0.1 L/min) at 120°C for 4 hours. The samples were calcined at 550°C for 4 hours under flowing air and a 1°C/min ramp rate.

Prior to magnetic resonance measurements, catalyst samples were dried in flowing dry air (~20 sccm/mg) at 400°C for 3 hours to dehydrate the surface. The samples were sealed under dry air at elevated temperature with isolation valves at each end of the reactor tube and transferred to a dry, N_2 purged glovebox through an antechamber for further processing. The samples were then loaded into 2.5 mm pencil-type Bruker NMR rotors and sealed prior to transfer and analysis in the Bruker 600WB spectrometer (1.6 mm for the 850 MHz measurements). Dehydration of the materials before and after the experiment were confirmed by ^{1}H NMR.

SCR Activity Tests

SCR reactivity of the supported V_2O_5(-WO_3)/TiO_2 catalysts was investigated in a fixed-bed reactor (Altamira AMI-200 temperature programmed system) equipped with an online quadrupole mass spectrometer (Dycor Dymaxion DME200MS) designated for effluent analysis. Typically, 30 mg of catalyst was loaded into a U-type quartz tubes (0.25" OD standard 6.5" AI-2210) and initially treated with 10% O_2/Ar at 400°C for 1 h to activate the catalyst. The reactor system was subsequently flushed with He for 10 min and the SCR reaction mixture was introduced (35 mL/min of NH_3/He (2000 ppm), 35 mL/min of NO/He (2000 ppm), 5 mL/min of 5% O_2/He). The steady-state SCR reaction was performed for 2 h at 200°C. The following m/z ratios were analyzed for the identification of the exiting gas composition: O_2 (m/z = 32), N_2 (m/z = 28), NH_3 (m/z = 17), NO (m/z = 30), NO_2 (m/z = 46) and N_2O (m/z = 44). Activity data was calculated based on NO conversion.

NMR Spectroscopy

^{51}V MAS NMR experiments were conducted with a 14.0921 T Bruker 600WB spectrometer utilizing a commercial 2.5 mm pencil-type MAS probe and a Varian-Inova 850 MHz spectrometer equipped with a commercial 1.6 mm pencil-type probe. The corresponding ^{51}V Larmor frequencies are 157.778 and 223.367 MHz. Single pulse NMR experiments were conducted with a $3\pi/16$ pulse width of 1.5 µs, a delay time of 0.2 s, a spectral width of 1 MHz, and an acquisition time of 4.096 ms (1.85 µs, 0.2 s, 5 MHz). Typically, 40,000 scans were collected per ^{51}V MAS NMR spectrum. Chemical shifts were externally referenced to the centerband of bulk V_2O_5 at -613.8 ppm relative to $VOCl_3$. Spinning rates of 32-35 kHz were used for all 600 MHz experiments, which proved a superior option in removing sideband overlap compared to 850 MHz experiments. Comparison of the current results to our previous work will show a chemical shift difference of a few ppm due to our direct utilization of $VOCl_3$ as the standard instead of the secondary reference V_2O_5, which has an isotropic chemical shift of -613.8 ppm relative to $VOCl_3$ and was previously reported as -610 ppm (see Figure S8 and S9).

^1H MAS NMR experiments were conducted to verify the dehydrated state of the material and collected with a π pulse width of 1.25 μs, a delay time of 2 s, a spectral width of 0.5 MHz, and an acquisition time of 8.192 ms. Typically, 1024 scans were collected per spectrum. Chemical shifts were externally referenced to adamantine at 1.82 ppm. To account for only the signal generated by the sample, rotor and probe background signals were subtracted from each spectra.

X-ray Diffraction

XRD patterns were collected using a PANalytical X'Pert MPD system with a vertical θ-θ goniometer with a 220 mm radius. The X-ray source is a long-fine-focus ceramic X-ray tube with a CuK- alpha anode (1.54056 Å). The operating power was 45 kV at 40 mA (1.8 kW). The scans were collected over the range of 10° to 80° (2θ) at a rate of 1.5 deg/min and a step size of 0.04°. Rietveld Refinement was conducted with the aid of the Materials Analysis Using Diffraction software.[2]

Raman Spectroscopy

Raman analysis of the catalysts were determined with a visible (532 nm) laser excitation on a single stage Horiba-Jobin Yvon Laboratory Ram-HR Raman spectrometer with a confocal microscope (Olympus BX-30) and a notch filter (Kaiser Super Notch). The visible excitation was generated by an Nd-YAG double diode pumped laser (Coherent Compass 315M-150, output power of 150 mW with power at the sample of 10 mW). The scattered photons were directed into a single monochromator and focused onto a UV-sensitive liquid N_2 cooled CCD detector (Horiba-Jobin Yvon CCD-3000V) with a spectral resolution of ~1 cm^{-1} for the given parameters. Powder samples were loaded into a Harrick Scientific cell (HVC-DRP4) connected to a gas control system. The temperature of the reaction chamber was controlled by the Harrick ATC Temperature Controller unit.

Electron Paramagnetic Resonance

Continuous Wave Electron Paramagnetic Resonance (CW-EPR) X-band (9.30 GHz) spectra were collected with a Bruker Elexsys 580 EPR spectrometer. The field was modulated at 100 kHz and a microwave power of 30 dB, with a receiver gain of 80 and 4 repetitions. The sample temperature was maintained at 125 K for all analyses. The weight percent of vanadium in the reduced state was calculated using a 0.5 mM solution of VO_2 dissolved with a small amount of HCl and converted the integral to equivalent mg of vanadium and dividing by the weight of the sample.

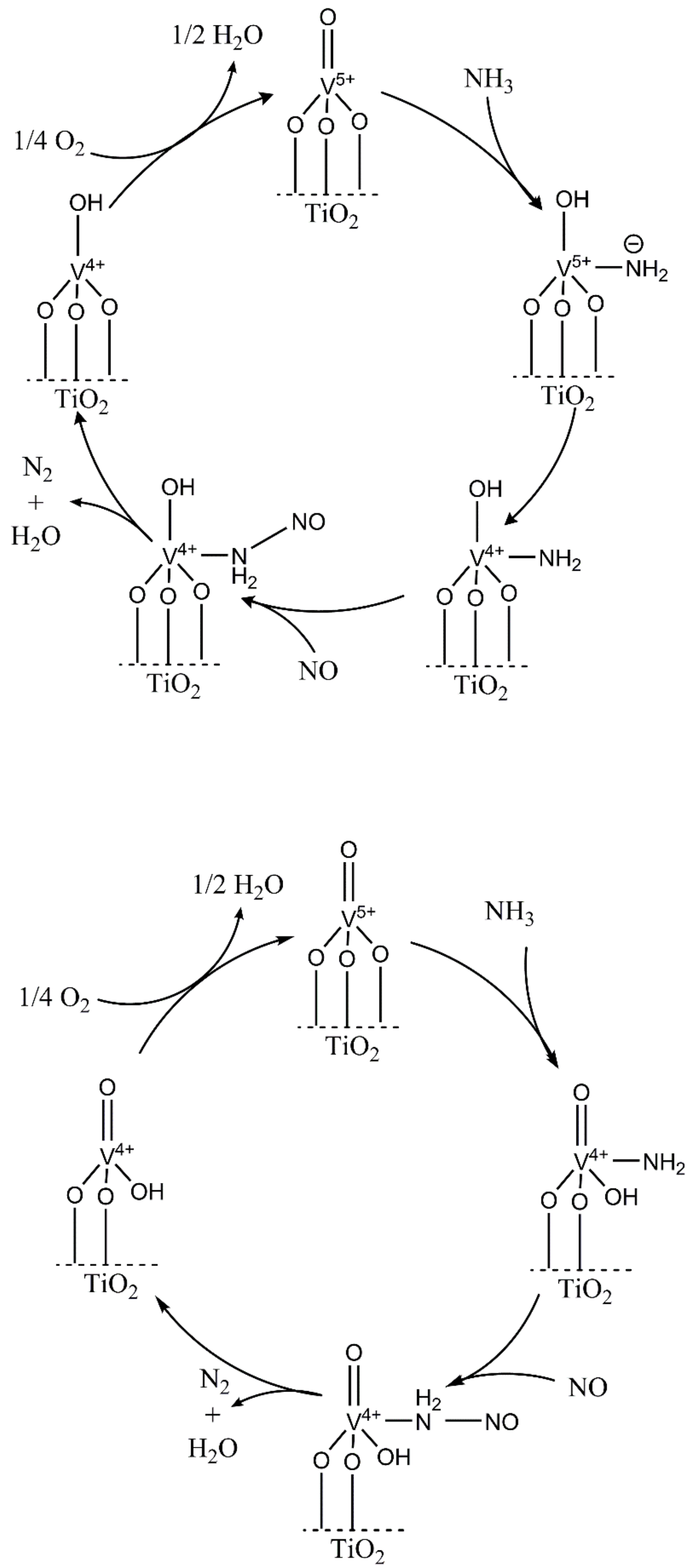
Scanning Transmission Electron Microscopy

STEM images were acquired using an FEI Titan 80-300 STEM equipped with a condenser lens spherical aberration corrector. Samples were exposed to ambient atmosphere prior to insertion into the column under ultra-high vacuum.

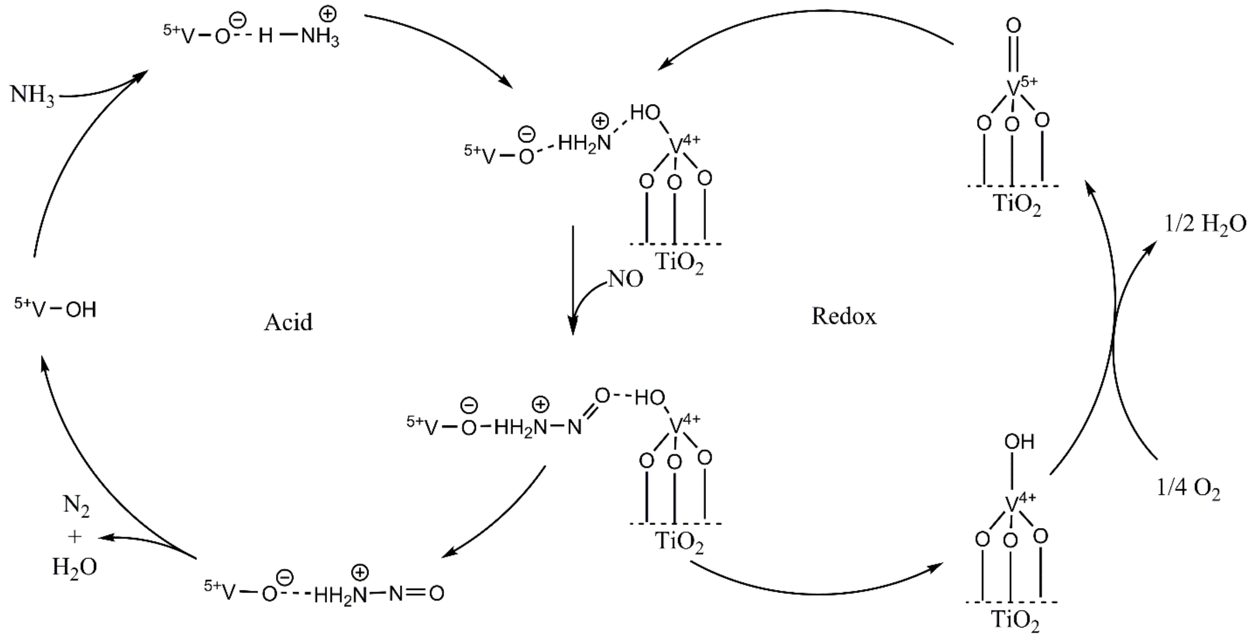
Density Functional Theory Calculations

The interpretation of the NMR spectra was aided by NMR chemical shift calculations using density functional theory as implemented in the Amsterdam Density Functional (ADF) software[3-5] and in Gaussian-16.[6] Large model cluster geometries were optimized using the generalized gradient approximation with Grimme's third generation dispersion-corrections applied to the Beck-Lee-Yang-Parr functional (GGA: BLYP-D3).[7-9] Scalar relativistic effects were accounted for using the zero-order regular approximation (ZORA).[10-11] A Slater-type, all-electron, triple- ζ, two-polarization function (TZ2P) was used as the basis set.[12]

Diffraction patterns of both the impregnated and co-precipitated samples demonstrate anatase as the primary polymorph (see Figure S3). As such, cluster models were constructed to mimic the (101) and (001) planes of anatase. Howard et al.'s structural determination of anatase was used as the base model whereby the crystal was cut along the aforementioned faces.[13] The models provided two layers of depth, where the bottom layer was frozen to preserve the crystal structure. Terminal oxygen atoms were charged balanced with protons at a length of 9.7 Å in the direction of the removed Ti atoms. The vanadium structure was placed atop this surface model and optimized as described above. The smaller model cluster calculations were performed with Gaussian 16.[6] The geometries were optimized at the B3LYP[7, 14] level with the aug-cc-pVDZ(-PP)[15-17] pseudopotentials on the V, Ti, and W. The NMR chemical shift calculations were done with ADF using the BLYP functional and the TZ2P basis set with ZORA as described above. To correlate the calculated nuclear shielding from DFT to the observed NMR chemical shifts, vanadium oxytrichloride ($VOCl_3$) was used as the computational standard at 0 ppm.[18-19] The calculated shielding relates to the chemical shift by $\delta(^{51}V) = \sigma_{calc, ref} - \sigma_{calc}$. Our model of V_2O_5 predicts peaks at -618 and -607 ppm for the average and center vanadium atoms, respectively, which correlates with the experimental value of -613.8 ppm, providing a validation of our computational approach.



Scheme S1. Representative mechanistic interpretation of the one-site SCR of NO by NH_3 with vanadia-based catalysts where the proton is transferred to the vanadyl bond (top) or a V-O-Ti bridging bond (bottom).



Scheme S2. Representative mechanistic interpretation of the two-site SCR of NO by NH_3 with vanadia-based catalysts involving both an acid site and redox site.

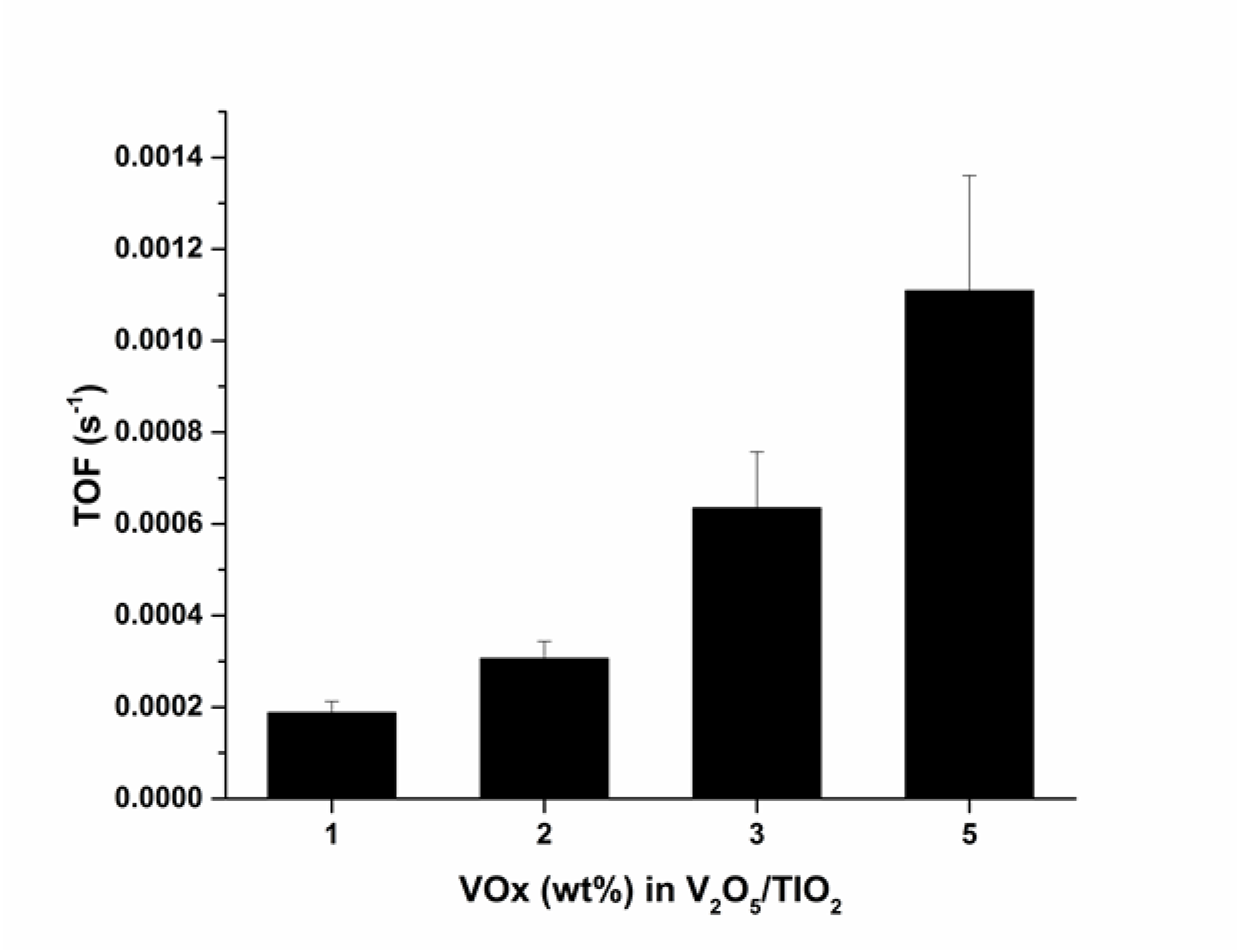


Figure S1. Turn-over-frequency plot (per vanadia per second) of the SCR reaction of NO_X by NH_3 as a function of surface vanadia loading. Reactions were conducted at 200°C.

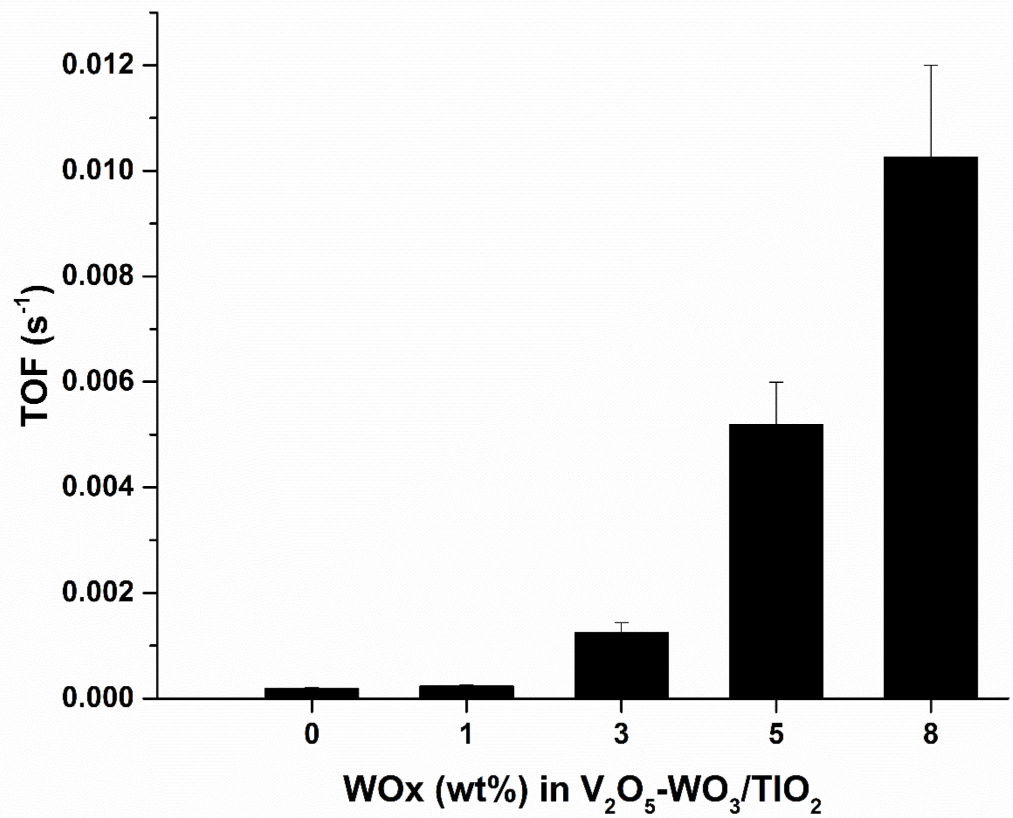


Figure S2. Turn-over-frequency plot (per vanadia per second) of the SCR reaction of NO_X by NH_3 as a function of surface tungsta loading at a constant 1% V_2O_5 coverage. Reactions were conducted at 200°C.

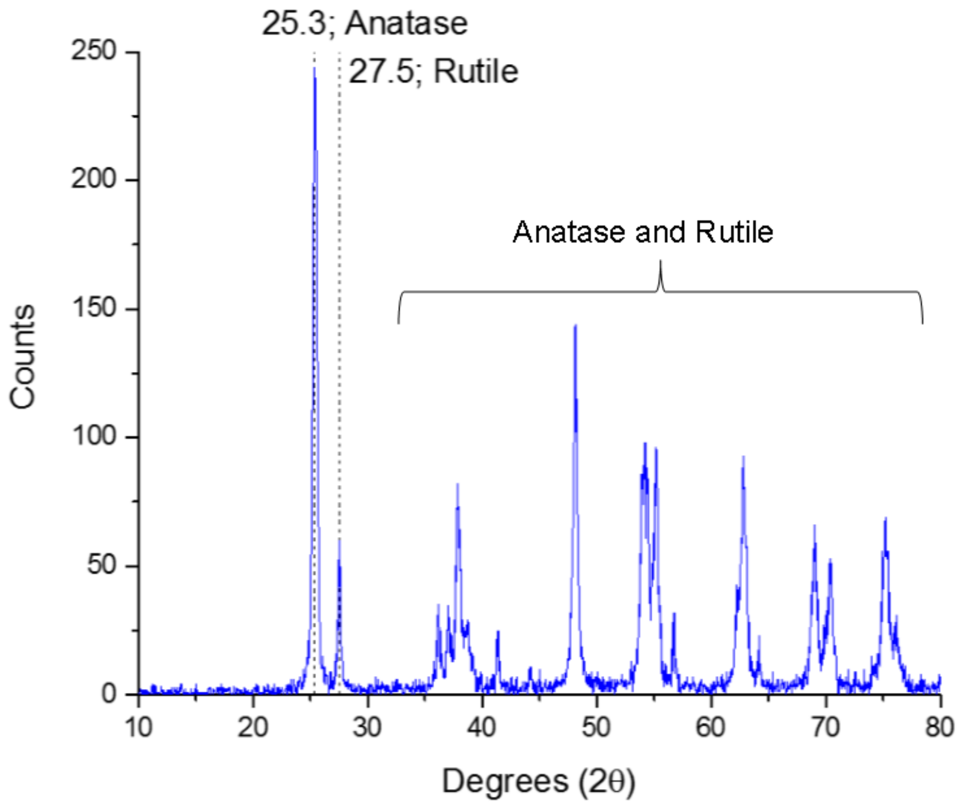


Figure S3. X-ray diffraction (XRD) patterns of 5% V_2O_5/TiO_2 prepared by incipient wetness impregnation demonstrating the observance of only the anatase and rutile phases of TiO_2 from the P25 support material. Signature features are marked at 25.3 and 27.5 where the remaining diffraction pattern also reflects these TiO_2 phases. Rietveld refinement of the XRD pattern reveals an approximate composition of 84% anatase and 16% rutile TiO_2.

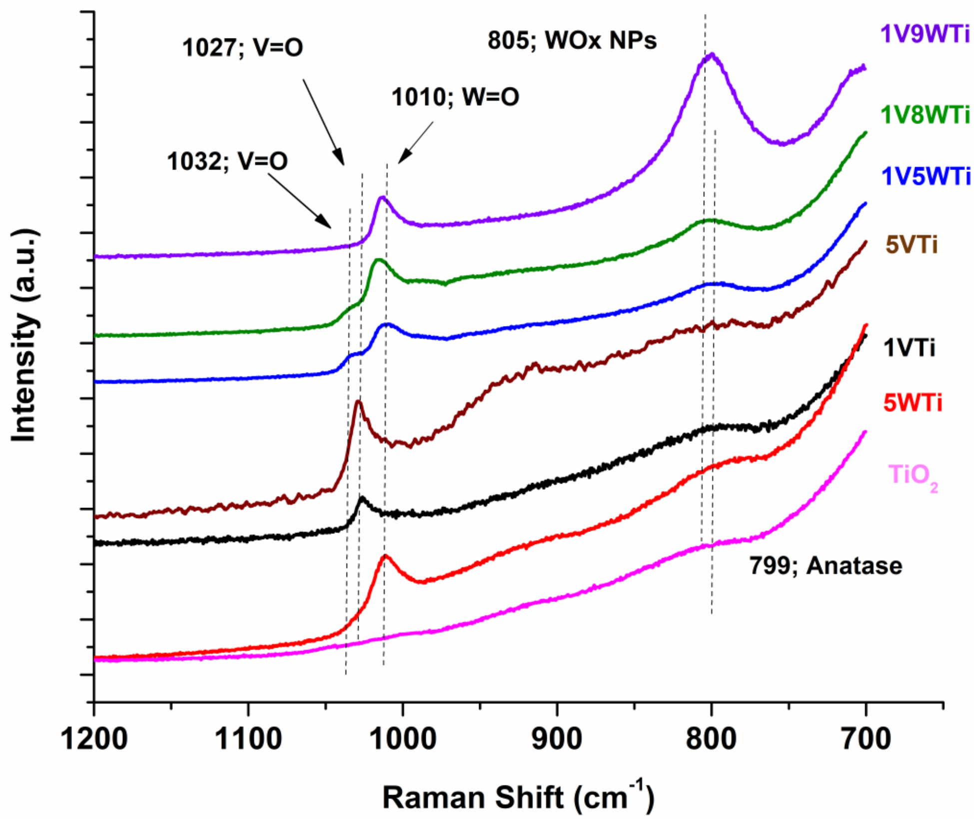


Figure S4. Raman spectra of dehydrated supported vanadium and tungsten oxides on titania. The formation of both vanadyl V=O (1032 cm^{-1}) and bridging V-O-Ti (950 cm^{-1}) vibrations are apparent upon introduction of vanadium oxide. The tungstanyl W=O vibration is also formed at 1010 cm^{-1} when tungsten oxide is introduced to the catalyst. No vibrations from bulk V_2O_5, WO_3, mixed V-W-O oxides phases are present. The weak and broad feature at 799 cm^{-1} is from the TiO_2 anatase overtone band.

The *in situ* Raman spectra (Figure S4) of the bare TiO_2, supported 1% V_2O_5/TiO_2, and supported 5% V_2O_5/TiO_2 exhibit the formation of a band around 1032 cm^{-1} for vanadia-containing catalysts that has been ascribed to vanadyl (V=O) vibrations of surface VO_4 sites.[20] The terminal V=O band slightly blue shifts with increasing surface vanadia coverage due to vibrational coupling of adjacent V=O bonds, which provides evidence for oligomerization of the surface vanadia sites with increasing surface vanadia coverage.[21-24] This effect has been extensively noted on different metal oxide supports (ZrO_2, TiO_2, Al_2O_3) and shown small shifts in the observed wavenumber with increasing polymeric vanadia content. In addition, weak and broad bands at ~930 cm^{-1} and

~799 cm^{-1} are present that that arise from bridging V-O-Ti vibrations of the surface VO_4 sites and TiO_2 anatase overtones, respectively.[20, 25-26] The 930 cm^{-1} band is a broad and weak feature not easily observed on these samples for low vanadia loadings (1%). This band becomes more apparent at high surface VOx coverage due to the presence of more vanadia on the surface (and thus more V-O-Ti linkages). The presence of additional VOx species at higher loadings directly form additional V-O-Ti bonds that can then be detected by Raman spectroscopy. Since the quantity of vanadia in 1% VOx-(x%) WOx/TiO_2 samples remains low, no additional V-O-Ti linkages are expected compared to 1VTi. In fact, fewer of these linkages will be present with tungsten addition due to oligomerization of surface vanadia and the increase in V-O-V bonds. For example, two VO_4 monomers will have 6 V-O-Ti linkages (3 each). Upon dimer formation, two of these become V-O-V linkages, lowering the abundance of V-O-Ti. Numerous experimental and theoretical studies have ascribed this peak to V-O-Ti linkages[20, 25-28], however it is noted that some debate remains where this peak is alternatively identified as V-O-V vibrations. Theoretical works predict this bridging V-O-V will arise at ~800 cm^{-1}. [25-28] The absence of a Raman band at 995 cm^{-1} from crystalline V_2O_5 nanoparticles reveals that the vanadia in these catalyst samples are 100% dispersed on the titania support. The peak at 799 cm^{-1} is ascribed to the overtone bands on anatase TiO_2, evidenced by its presence on the bare TiO_2 sample. Any overlapping V-O stretches in this region would be overshadowed by the relatively intense overtone at the same position.

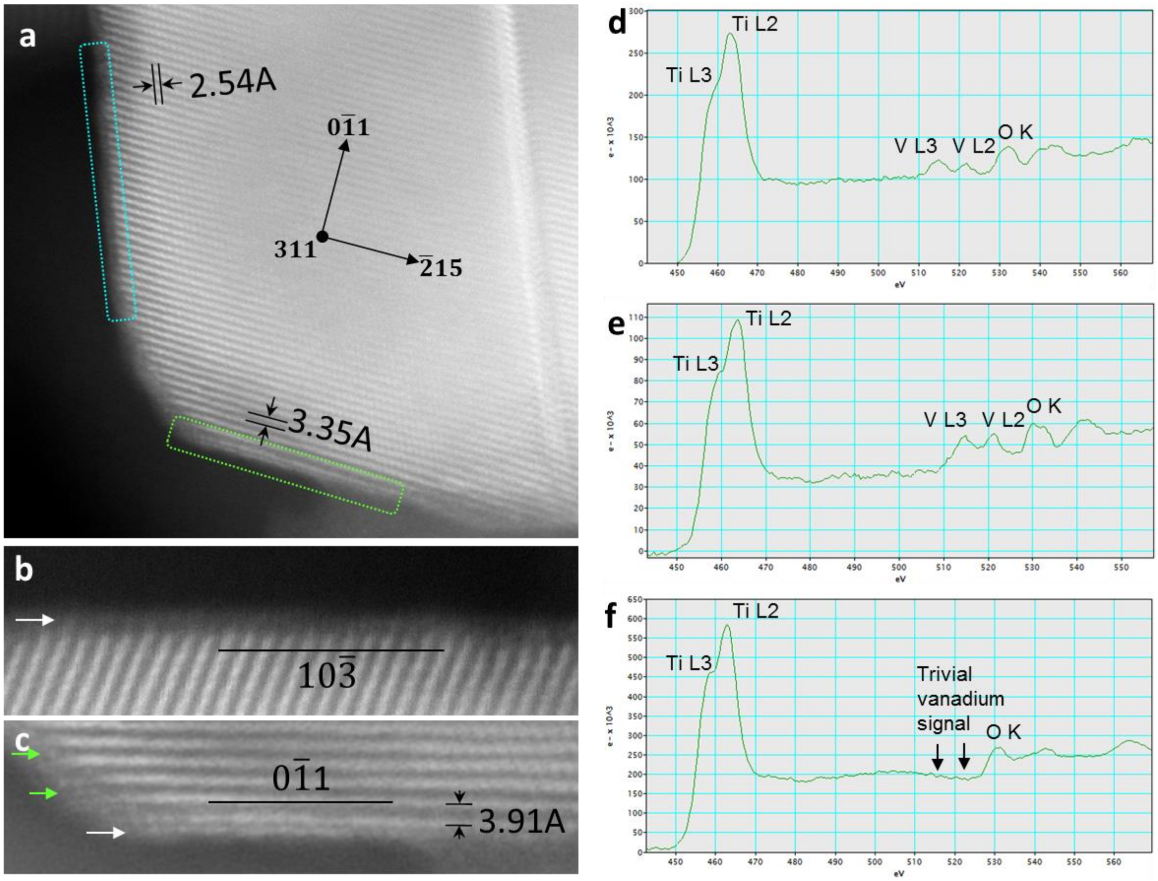


Figure S5. (a) Atomic resolution Z-contrast STEM image of a TiO_2 particle for the supported 5% V_2O_5/TiO_2 catalyst after ambient exposure, but under UHV showing the TiO_2 lattice. (b) Enlarged image of the cyan box region in panel (a) and corresponding EELS spectrum (d) of the thin surface layer (indicated by white arrow in (b)) showing presence of vanadium on the $(10\bar{3})$ surface of the particle. (c) Enlarged image of the green box region in panel (a) and corresponding EELS spectrum (e) of the thin surface layer (indicated by white arrow in (c)) showing presence of vanadium on the $(0\bar{1}1)$ surface of the TiO_2 particle. Vanadium atoms also seems to have widened the spacing of $(0\bar{1}1)$ planes near the edge (indicated by green arrows in (c)). The d-spacing of TiO2 $(0\bar{1}1)$ planes were expanded by the surface vanadia overlayer (as shown in (c)). (f) EELS spectrum collected from inside of the TiO_2 particle showing no discernable peaks from vanadium, which would likely be smeared by the signal form titanium as the electron travels through the thickness direction of the particle.

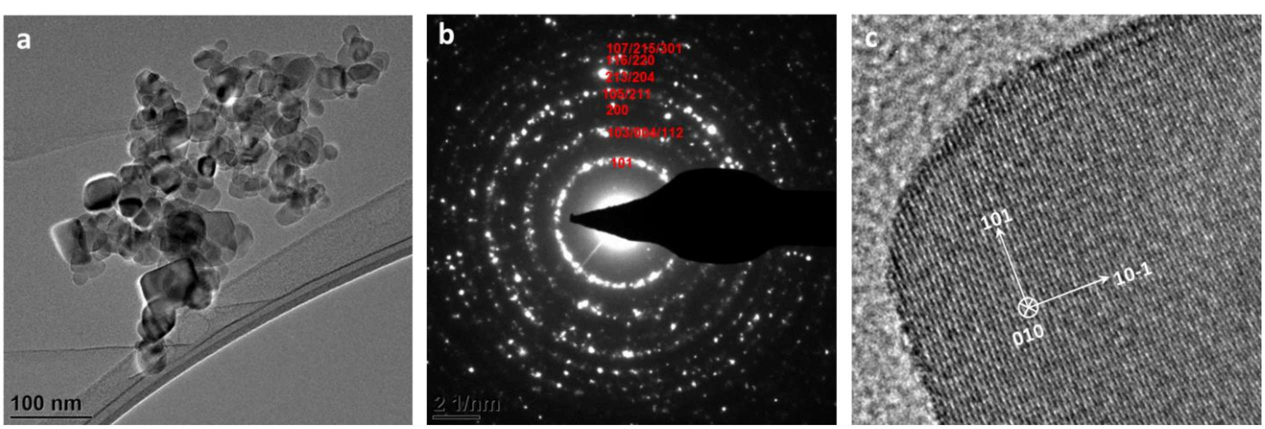


Figure S6. Microstructural characterization of the TiO_2 particles (for supported 5% V_2O_5/TiO_2-I), including (a) Low magnification TEM image of the particles, (b) electron diffraction pattern of the particles in panel (a) which shows a typical pattern of anatase TiO_2, an indication minor rutile presence at 3.26 A and no obvious signal from vanadium oxides, and (c) high resolution TEM image of the edge of a particle demonstrating that each particle is in fact a single crystal. The shape (or surface facet) of the particles are not uniform; but (101) surfaces appears to be the dominant facet.

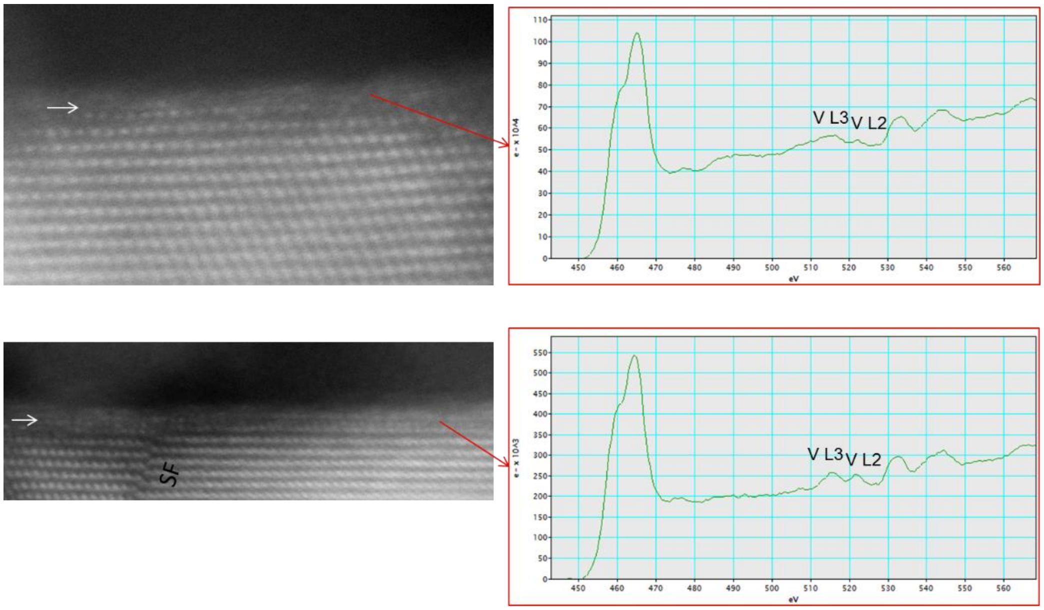


Figure S7. Atomic resolution Z-contrast STEM image of the supported, impregnated 5% V_2O_5/TiO_2 catalyst particle (left) and EEELS spectra (right) providing further evidence of surface vanadium inserted atop titania rows on the particle edges.

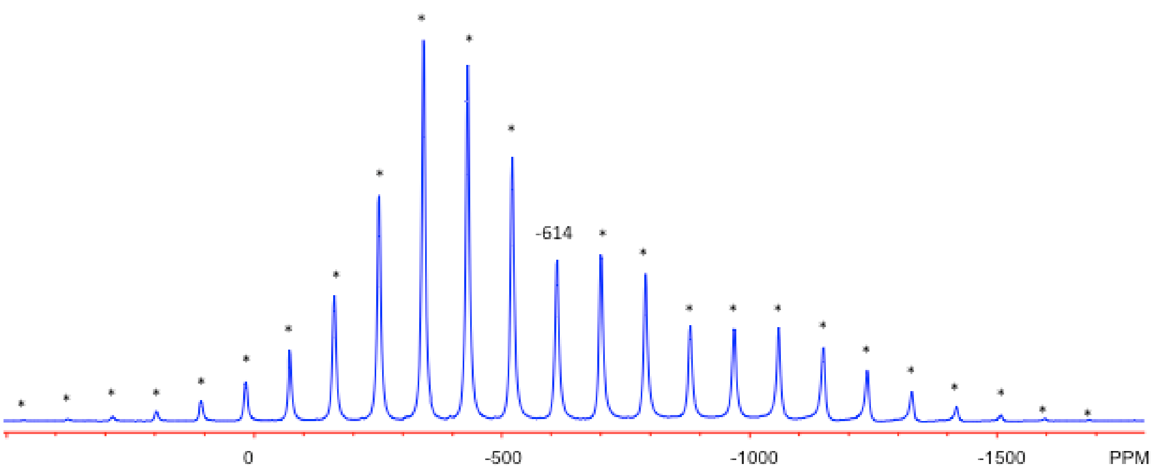


Figure S8. ^{51}V MAS NMR spectrum of bulk V_2O_5 at high field relative to $VOCl_3$ measured in this study at 0 ppm. The centerband of the bulk V_2O_5 secondary reference is -613.8 ppm. * denotes spinning side band.

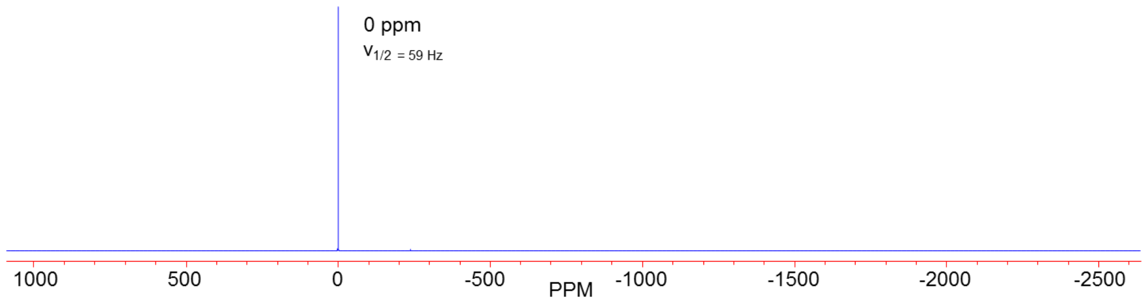


Figure S9. ^{51}V NMR spectrum of $VOCl_3$ referenced to 0 ppm.

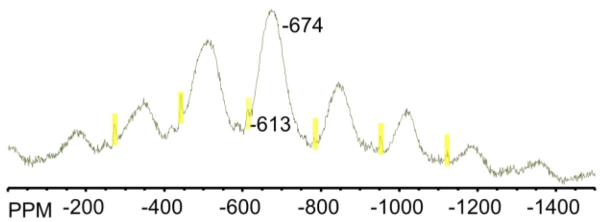


Figure S10. ^{51}V MAS NMR spectrum of 7% V_2O_5/SiO_2. The primary, broad centerband feature at -674 ppm is indicative of dispersed vanadia species on the silica support. The peak at -613 ppm exhibits the chemical shift sideband pattern of bulk V_2O_5, demonstrating a less complicated spectrum compared to titania-supported vanadia.

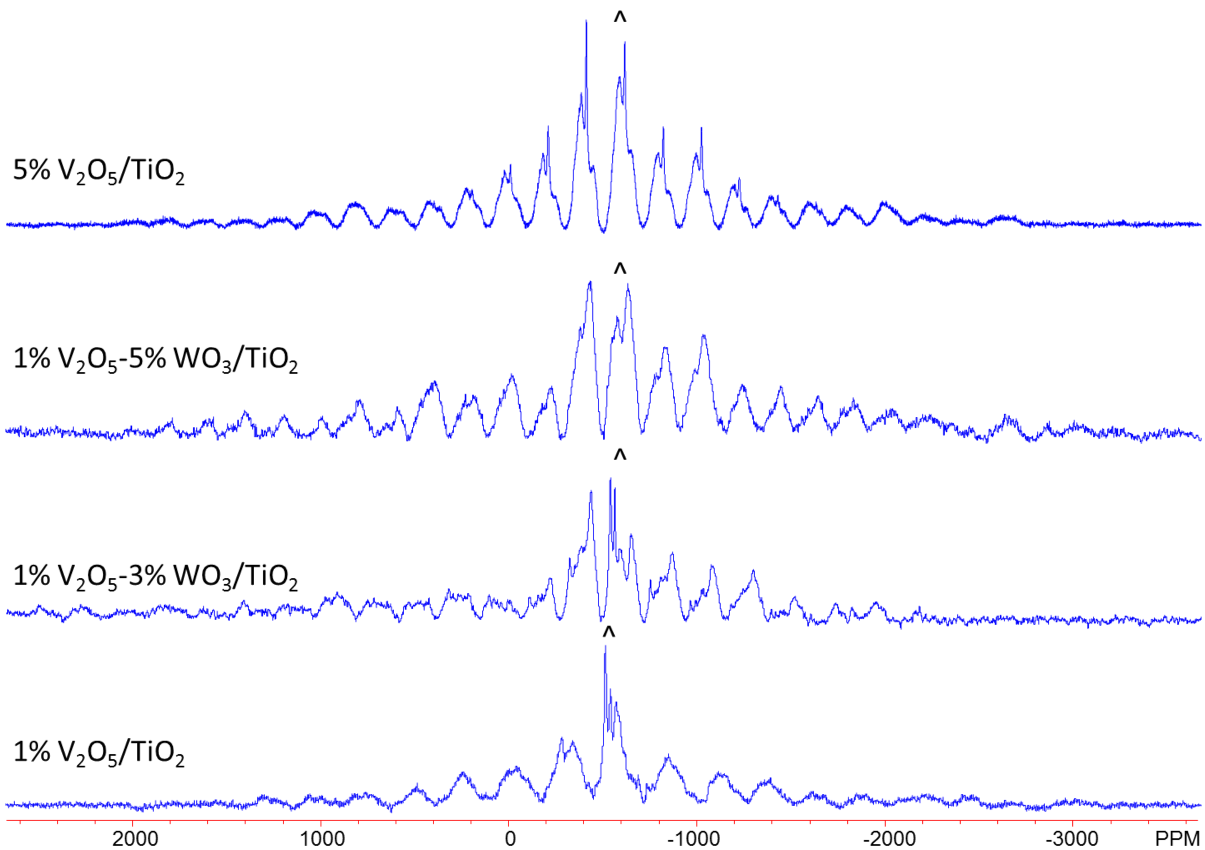


Figure S11. Spinning sideband patterns for the ^{51}V MAS NMR spectra of dehydrated, impregnated V_2O_5/TiO_2 catalysts at 14T and ~35 kHz spinning rate. ^ indicates center band.

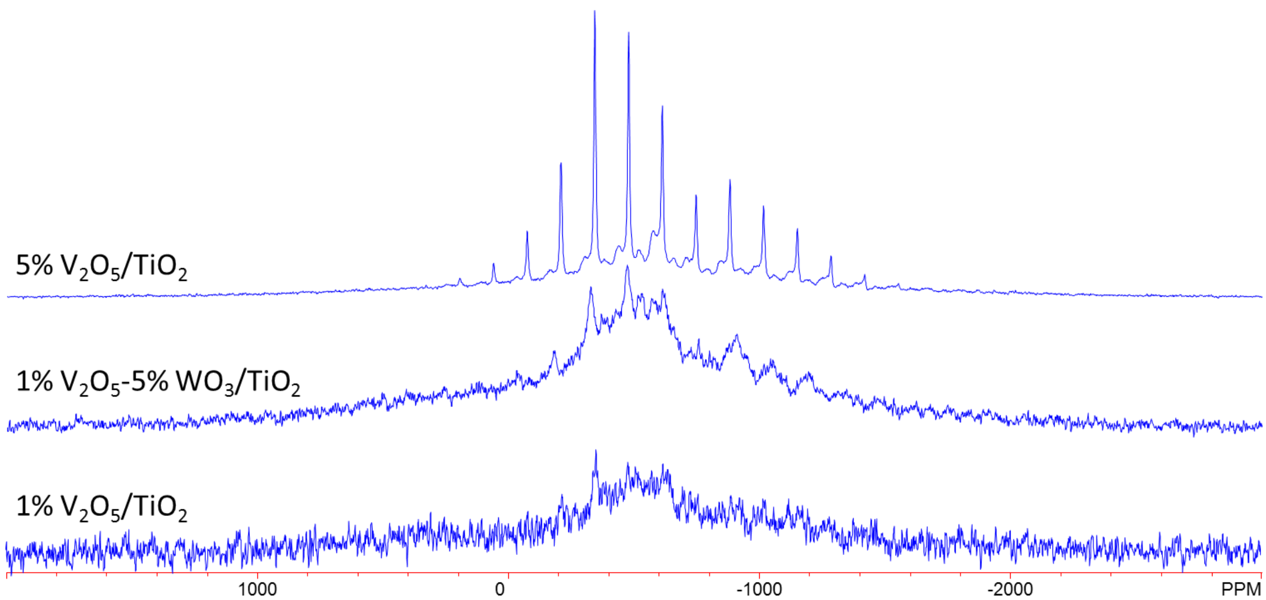


Figure S12. [51]V MAS NMR spectra at 21T of dehydrated, supported 1% V_2O_5/TiO_2, 1% V_2O_5-5% WO_3/TiO_2, and 5% V_2O_5/TiO_2 catalysts prepared by impregnation and collected with sample spinning rates of 30, 32.5, and 30 kHz and 38,000, 308,000, and 77,000 repetitions, respectively.

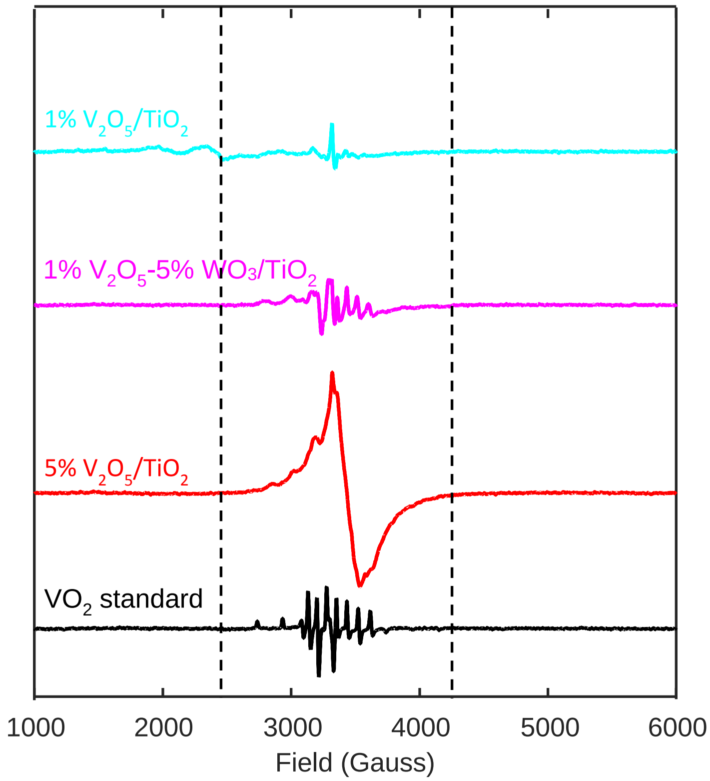


Figure S13. Electron paramagnetic resonance (EPR) spectra of the same dehydrated supported vanadium oxide catalysts probed above by NMR. Small quantities of V^{4+} are present on the samples. G-values are determined as 2.0014 (1% V_2O_5/TiO_2), 1.9829 (1% V_2O_5-5% WO_3/TiO_2), and 1.9376 (5% V_2O_5/TiO_2). The broader lines of the 5% V_2O_5/TiO_2 impregnated catalyst reflect V^{4+} in close proximity to each other.

Table S1. Content of reduced vanadium oxide species determined by EPR line integration, surface vanadium density, average V-V distance, surface tungsten density, and fractional surface coverage of V or W with respect to monolayer coverage.

Sample	**%V as V^{4+}**	**V/nm^2**	**Avg. V-V dist. Å**	**W/nm^2**	**Θ(V/W)**
1% V_2O_5/TiO_2	0.25%	1	8.9	-	0.2
5% V_2O_5/TiO_2	1.02%	7	5.2	-	0.6
1% V_2O_5-5% WO_3/TiO_2	0.62%	1	10.3	2.4	0.15/0.53

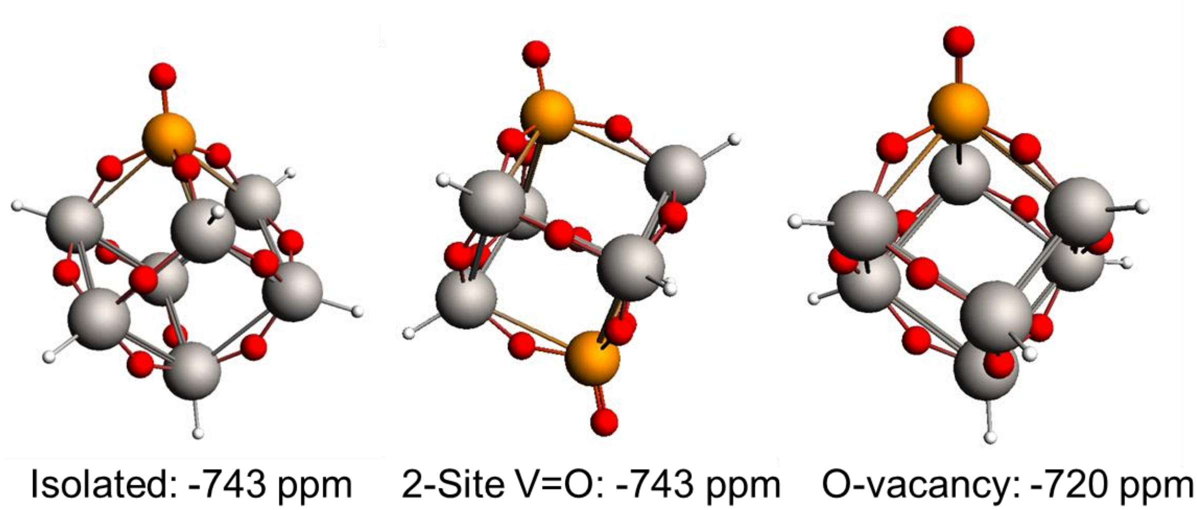


Figure S14. Optimized Goodrow DFT cluster models used to gain an understanding of the impact of oxygen vacancies on the ^{51}V NMR chemical shift. A nearby oxygen vacancy on TiO_2 is predicted to deshield ^{51}V nuclei by approximately 20 ppm.

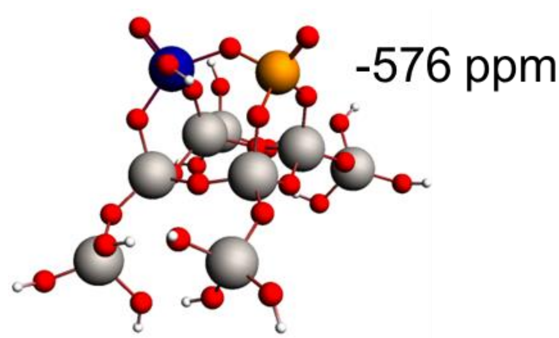


Figure S15. DFT-optimized small cluster model of a VO_X-WO_X dimeric structure. Atoms represented include vanadium (orange), titanium (grey), oxygen (red), tungsten (blue), and hydrogen (white).

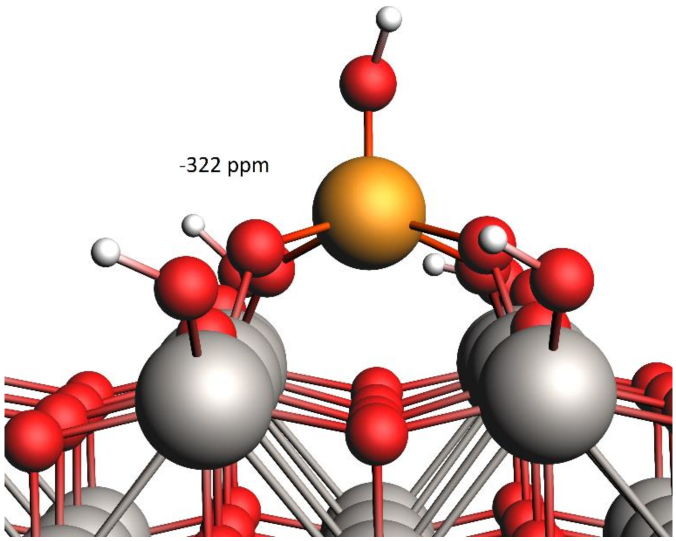


Figure S16. DFT-optimized structure of a vanadia monomer with a protonated vanadyl bond. The predicted chemical shift is far from any resonance observed experimentally.

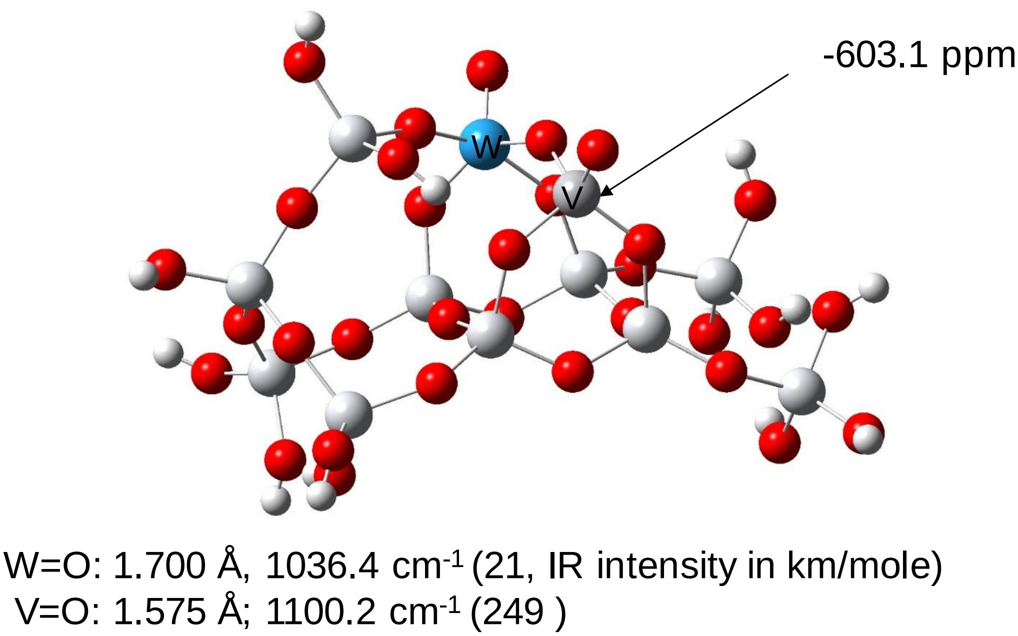


Figure S17. DFT-optimized structure of a VO_X-WO_X dimer on a TiO_2 cluster. The cluster was optimized in Gaussian-16 with B3LYP/aug-cc-pVDZ(H,O)/aug-cc-pVDZ-PP(V,Ti,W). ^{51}V NMR shielding calculations were conducted using ADF with ZORA and BLYP/TZ2P, referenced to $VOCl_3$.

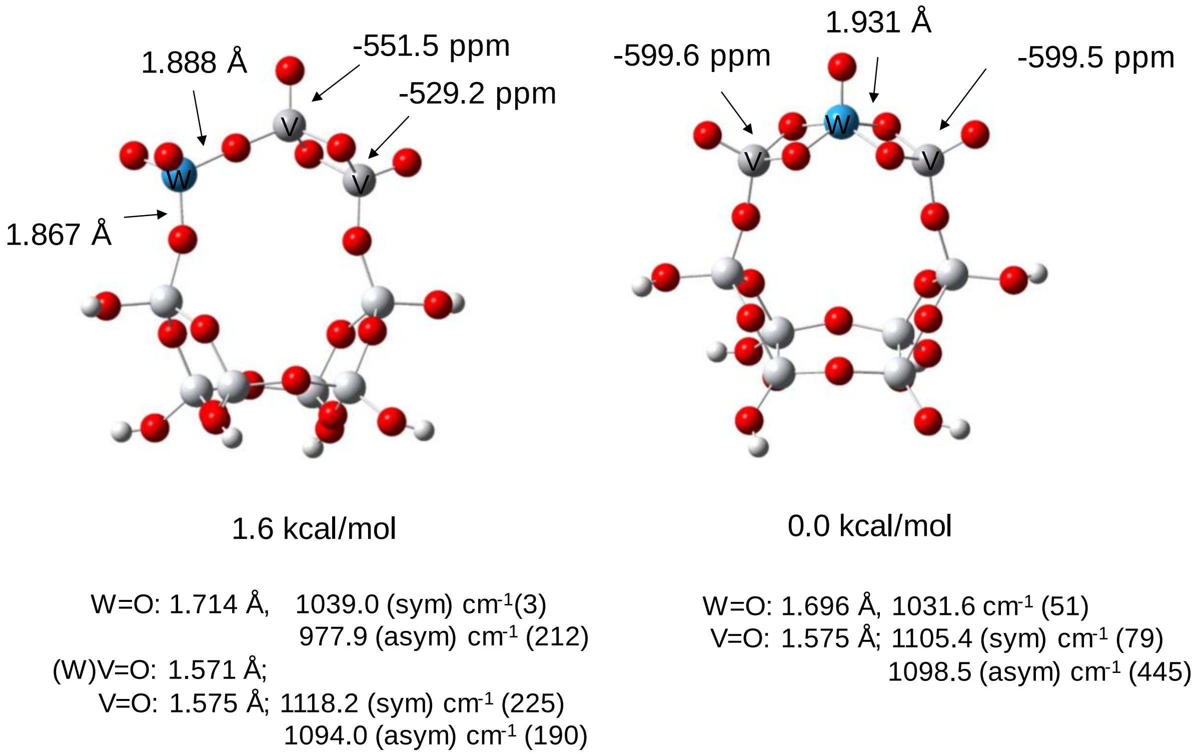


Figure S18. DFT-optimized structure of A) $2VO_X$-WO_X trimer (left) and B) VO_X-WO_X-VO_X trimer on TiO_2 cluster 1. The clusters were optimized in Gaussian-16 with B3LYP/aug-cc-pVDZ(H,O)/aug-cc-pVDZ-PP(V,Ti,W). ^{51}V NMR shielding calculations were conducted using ADF with ZORA and BLYP/TZ2P, referenced to $VOCl_3$.

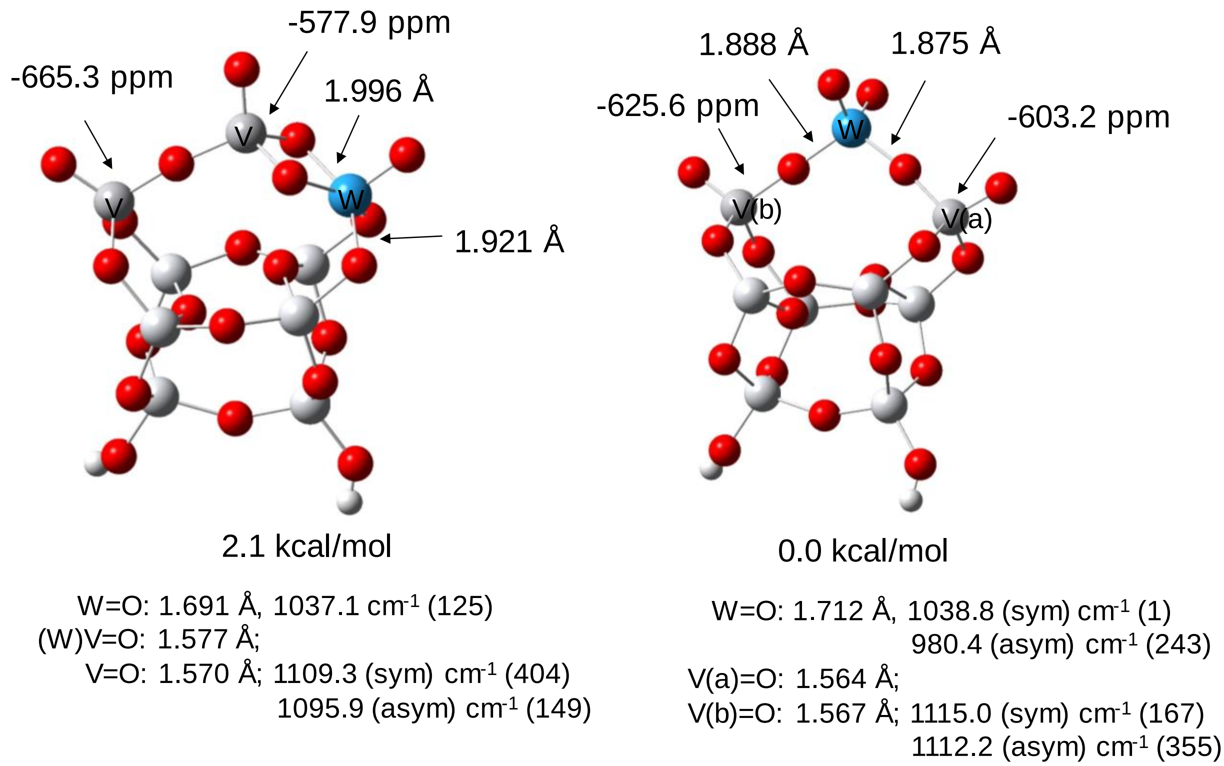


Figure S19. DFT-optimized structure of A) 2VO_X-WO_X trimer (left) and B) VO_X-WO_X-VO_X trimer on TiO_2 cluster 2. The clusters were optimized in Gaussian-16 with B3LYP/aug-cc-pVDZ(H,O)/aug-cc-pVDZ-PP(V,Ti,W). ^{51}V NMR shielding calculations were conducted using ADF with ZORA and BLYP/TZ2P, referenced to $VOCl_3$.

To explore the possibility of surface VO_x-WO_x dimers on TiO_2, we evaluated a number of W^{VI}-O_x-V^V on Ti(IV) cluster models (Figure S15-18). The smallest raw model (O=)(HO)W^{VI}-O-V^V(=O) had a predicted chemical shift of -576 ppm. A larger cluster, (O=)W^{VI}-O-V^V(=O) single O bridge dimer predicted a ^{51}V chemical shift of -603 ppm. These two models potentially represent a portion of the signals observed from the NMR spectra on the basis of chemical shift. Additional configurations were also considered with a slightly smaller cluster model. In these, structures with two V^V bonded to a single W^{VI} were examined. A structure with two O bridge atoms between with the W and each V (VWV) on cluster 1 (trimer B) leads to ^{51}V chemical shifts of -600 ppm, which slightly higher than observed, but similar to the larger cluster model. An asymmetric structure containing a W connected with two bridge bonds to a central V which is connected to an additional V by a single bridge O and provided ^{51}V chemical shifts of -578 ppm for the central V and -665 ppm for the terminal V. In this trimer, the central vanadium nucleus well-reflects the observed signal, but a rise in -665 ppm features was not observed for promoted catalysts refuting its presence. However, a second asymmetric structure with a VVW ($W(=O)_2$) motif (trimer A on cluster 1) was found to be 1.6 kcal/mol higher in energy, but more agreeable on the basis of chemical shift. The calculated ^{51}V chemical shift for the central V is -552 ppm and that for the V bonded only to a V and a Ti through O bridges is -529 ppm; signals that are both apparently present in the NMR spectrum and also result in vanadia in close proximity to each other, satisfying the two-site requirement. A second TiO_2 cluster (cluster 2) was used to generate two additional structures, one with a W connected with two bridge bonds to a central V which is connected to an additional V by a single bridge O (trimer A on cluster 2) and one with a WO_2 unit single bridge bonded to two V centers (trimer B on cluster 2). The former is 2.1 kcal/mol above the latter. Trimer A on cluster 2 has ^{51}V chemical shifts of -578 ppm for the central V and -665 ppm for the terminal V, again dissimilar to the observed spectral trend. The latter, lower energy structure (trimer B on cluster 2) has two asymmetric V sites with ^{51}V chemical shifts of -603 and -626 ppm, which may be possible, but are less likely due to the primary signal in that region being the -613 ppm feature of familiar position and lineshape present in unpromoted catalysts. Thus, the actual local structure of the TiO_2 can influence how the V and W centers will bind. We note that the structures prefer to have the W between the two V atoms by a small amount of energy independent of whether the W has one or two W=O bonds, however, the chemical shift agreement for these structures is mild.

References

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DFT Cluster Model Coordinates

Figure3**Fehler! Verweisquelle konnte nicht gefunden werden.**a

O	3.93753683	-40.85743801	-1.56398586
O	11.35350000	-35.35496000	-6.30138900
O	7.56900000	-31.67621400	-7.76468300
O	12.42120071	-25.65142880	-1.83066739
O	5.67675000	-27.32575400	-5.42226000
O	7.56900000	-35.35496000	-6.30138900
O	9.46125000	-30.23528300	-6.30138900
O	9.46848356	-24.87751533	-4.20085746
O	3.78852860	-33.90043239	-2.41885377
O	9.46125000	-27.32575400	-5.42226000
O	1.85102195	-36.05186271	-1.81176589
O	13.24575000	-33.88636100	-6.88555300
O	13.25249997	-35.33481901	-4.18902039
O	-1.02705771	-28.54125859	-1.51494231
O	5.71672443	-39.00185925	-2.66289623
O	11.35350000	-32.44543000	-5.42226000
O	15.13800000	-39.00603700	-6.88555300
O	3.78450000	-32.44543000	-5.42226000
O	9.55587558	-35.33895879	-4.18497292
O	5.67675000	-30.23528300	-6.30138900
O	13.24575000	-30.23528300	-6.30138900
O	1.92850094	-35.36577586	-4.22487320
O	13.35200954	-36.15157496	-1.83006758
O	1.89225000	-40.47463600	-6.30138900
O	15.13800000	-35.35496000	-6.30138900
O	1.89225000	-37.56510700	-5.42226000
O	-0.91208086	-39.63807633	-1.48059492
O	0.00000000	-42.68478300	-5.42226000
O	2.04144815	-39.03172321	-2.43321931
O	0.00000000	-31.67621400	-7.76468300
O	5.63392473	-35.34444692	-4.19856349
O	3.75746857	-30.26660948	-4.21874881
O	0.38646175	-27.21492148	-3.22455529
O	9.46600943	-39.03809741	-2.71569619
O	9.52661108	-36.07310170	-1.75923861
O	7.55497075	-40.57835564	-1.41779872
O	3.78450000	-28.76668500	-6.88555300
O	5.67675000	-33.88636100	-6.88555300
O	7.59799905	-37.48427448	-3.30064317
O	2.54771663	-25.79535761	-1.86416129
O	5.68194715	-36.07770193	-1.76775578
O	5.67675000	-36.79589000	-7.76468300
O	9.46125000	-40.47463600	-6.30138900
O	9.46125000	-37.56510700	-5.42226000
O	7.56900000	-42.68478300	-5.42226000
O	1.93753931	-32.52624930	-3.38342946
O	3.78450000	-42.68478300	-5.42226000
O	7.60485877	-30.25477060	-4.21866891
O	-1.87117001	-32.28218603	-3.44976121
O	7.55524023	-40.30858170	-4.46661113
O	7.56900000	-39.00603700	-6.88555300
O	7.56900000	-32.44543000	-5.42226000
O	13.27198250	-39.07880523	-2.68241612
O	14.63610011	-33.68935983	-1.64274591
O	11.40267645	-37.57006881	-3.29594335
O	0.98789571	-41.69033791	-2.30907056
O	-1.89225000	-33.88636100	-6.88555300
O	11.20403885	-30.21406509	-4.25976941
O	9.46125000	-36.79589000	-7.76468300
O	11.35350000	-28.76668500	-6.88555300
O	11.35350000	-31.67621400	-7.76468300
O	0.12881668	-30.99441372	-1.79875130
O	9.48869443	-32.44176165	-3.36142148
O	12.26471627	-25.02121382	-4.47747239
O	7.59246989	-34.02216591	-2.82707211
O	13.28717184	-32.48376807	-3.54032564
O	3.76256983	-40.29407427	-4.46878095
O	3.78450000	-39.00603700	-6.88555300
O	7.56900000	-28.76668500	-6.88555300
O	15.28897842	-37.38865905	-3.57440455
O	4.02455329	-31.02646101	-1.78804046
O	0.03548868	-37.70591477	-3.40902187
O	15.13800000	-28.76668500	-6.88555300
O	1.89225000	-30.23528300	-6.30138900
O	6.27113307	-25.11479405	-3.99492908
O	11.39479402	-33.84686287	-2.35580110
O	-1.89225000	-40.47463600	-6.30138900
O	0.01931313	-40.23313322	-4.46906730
O	0.00000000	-39.00603700	-6.88555300
O	0.00000000	-28.76668500	-6.88555300
O	9.46125000	-33.88636100	-6.88555300
O	11.35350000	-42.68478300	-5.42226000
O	12.92194595	-28.49823515	-2.41964454
O	13.24575000	-40.47463600	-6.30138900
O	1.89225000	-36.79589000	-7.76468300
O	1.89225000	-27.32575400	-5.42226000
O	-1.89225000	-30.23528300	-6.30138900
O	9.34217494	-29.07507241	-2.08577314
O	5.44153608	-26.13172499	-1.63660214
O	3.78450000	-35.35496000	-6.30138900
O	9.40306615	-26.00228548	-1.67481198
O	13.24575000	-37.56510700	-5.42226000
O	0.12696960	-33.84386553	-2.32927804
O	13.24575000	-27.32575400	-5.42226000
O	5.66305458	-32.51590280	-3.44200730
O	11.34913403	-40.33835501	-4.46766707
O	1.89225000	-33.88636100	-6.88555300
O	2.08909923	-24.84997871	-4.37943436
O	0.00000000	-32.44543000	-5.42226000
O	0.00000000	-35.35496000	-6.30138900
O	11.52720573	-30.92374385	-1.88996357
O	7.63247123	-27.46128382	-3.33374818
O	14.74132743	-26.37098955	-3.19468613
O	2.19079598	-28.94957538	-2.12580766
O	11.35350000	-39.00603700	-6.88555300
O	0.15408629	-30.17110233	-4.16530749
O	11.02232739	-27.41880783	-3.40927573
O	13.24575000	-36.79589000	-7.76468300

O	5.67675000	-40.47463600	-6.30138900
O	5.67675000	-37.56510700	-5.42226000
O	11.29826267	-40.55253550	-1.37116369
O	7.47811010	-31.18740245	-1.78844542
O	5.75252053	-28.84918590	-2.34730695
O	3.78450000	-31.67621400	-7.76468300
O	3.79950185	-37.53495982	-3.33921049
O	3.91199825	-27.41031668	-3.51583021
O	9.01884335	-33.43378235	-0.65826702
O	6.07163103	-33.39934752	-0.68903077
O	7.54273435	-31.71095230	1.00374492
Ti	12.90404821	-26.47610690	-3.38409029
Ti	9.49983867	-34.34981478	-2.26495060
Ti	1.93654820	-37.21971871	-3.22567298
Ti	1.89225000	-28.39591000	-7.03303600
Ti	13.47073891	-37.18405984	-3.38813404
Ti	3.82702903	-32.17459372	-3.42240551
Ti	11.37530188	-32.05753226	-3.28214900
Ti	5.67675000	-28.39591000	-7.03303600
Ti	9.37572624	-26.55024717	-3.48571123
Ti	1.89225000	-38.63526300	-7.03303600
Ti	11.35350000	-40.84541000	-6.15390700
Ti	-0.05034073	-32.00701797	-3.32471104
Ti	9.46125000	-38.63526300	-7.03303600
Ti	7.62168712	-39.43910146	-2.86095379
Ti	9.46125000	-28.39591000	-7.03303600
Ti	3.94256165	-39.52667536	-2.82510380
Ti	7.62060379	-32.27769203	-3.51718094
Ti	5.67675000	-38.63526300	-7.03303600
Ti	11.35350000	-30.60605700	-6.15390700
Ti	5.67675000	-35.72573400	-6.15390700
Ti	7.58560771	-29.32508725	-2.64592258
Ti	7.56900000	-33.51558700	-7.03303600
Ti	2.16591482	-26.47303410	-3.50067163
Ti	5.72192038	-37.04617473	-3.36734353
Ti	13.24575000	-38.63526300	-7.03303600
Ti	11.35350000	-33.51558700	-7.03303600
Ti	5.81534056	-26.77198015	-3.37840716
Ti	1.96784052	-34.41325166	-2.68422778
Ti	3.78450000	-30.60605700	-6.15390700
Ti	13.19768165	-34.48072998	-2.53834232
Ti	11.12627456	-29.24131442	-2.68665200
Ti	7.56900000	-30.60605700	-6.15390700
Ti	0.00000000	-40.84541000	-6.15390700
Ti	9.55177515	-37.04095385	-3.36796036
Ti	7.56900000	-40.84541000	-6.15390700
Ti	13.24575000	-35.72573400	-6.15390700
Ti	3.78450000	-40.84541000	-6.15390700
Ti	11.30659939	-39.46240077	-2.85172723
Ti	0.00000000	-33.51558700	-7.03303600
Ti	3.89815799	-29.17935279	-2.73230453
Ti	3.78450000	-33.51558700	-7.03303600
Ti	0.41849215	-39.98748037	-2.69070250
Ti	0.00000000	-30.60605700	-6.15390700
Ti	0.37467127	-29.30564243	-2.48539330
Ti	13.24575000	-28.39591000	-7.03303600
Ti	5.70190696	-34.35911027	-2.29966295
Ti	1.89225000	-35.72573400	-6.15390700
Ti	9.46125000	-35.72573400	-6.15390700
H	3.45262803	-25.85491300	-1.47399698
H	15.19654711	-34.26396741	-1.09167452
H	13.69226354	-28.94473922	-2.03147699
H	15.11964183	-26.02665378	-2.36636646
H	15.13800000	-34.45364600	-6.65990500
H	14.19634000	-33.70183500	-6.94237500
H	15.13800000	-39.90735100	-6.52703800
H	13.98094502	-39.61449660	-2.29049846
H	6.70476578	-40.86133826	-1.02974911
H	14.19364500	-30.42990000	-6.23415700
H	3.78450000	-43.21602500	-6.22187400
H	-1.87885700	-29.34208100	-6.67942400
H	13.92464946	-32.00620791	-2.97629132
H	3.12340336	-41.37376437	-1.39052002
H	-0.94912600	-35.54093500	-6.22741400
H	15.67410698	-37.54401798	-4.45881910
H	11.48010768	-25.54820660	-1.56305216
H	15.13800000	-29.66799800	-6.52703800
H	-0.93934200	-28.58262700	-6.95876600
H	0.00000000	-43.21602500	-6.22187400
H	9.30371457	-26.71108502	-1.01221877
H	11.35350000	-43.21602500	-6.22187400
H	-2.26346974	-32.49503110	-4.31823636
H	7.56900000	-43.21602500	-6.22187400
H	-1.89225000	-39.58261400	-6.65620900
H	-1.34242119	-38.76402439	-1.50577605
H	5.83388414	-25.26358843	-1.43221165
H	12.51092463	-25.18435341	-5.40550114
H	7.10002770	-24.67020012	-4.25460542
H	-0.22306187	-37.88590097	-4.33095853
H	-1.59495447	-29.14477776	-1.00383753
H	1.07284045	-42.35873137	-3.01862121
H	14.19301100	-40.66200500	-6.20925100
H	10.42575909	-24.65507503	-4.39477319
H	-0.25272380	-26.75444172	-2.64687617
H	1.82758120	-24.92425634	-5.31512147
H	-1.88980400	-34.79123900	-6.53613900
H	-0.61493048	-34.41690589	-2.07084077
H	10.47129937	-40.78714590	-0.90947817
H	-0.89789200	-38.83396100	-6.96424100
H	4.80790892	-31.29557877	-1.26713467
V	7.55985520	-32.44607497	-0.42215713

Figure 3**Fehler! Verweisquelle konnte nicht gefunden werden.**b

O	3.91979600	-40.88311000	-1.56271800
O	11.35350000	-35.35496000	-6.30138900
O	7.56900000	-31.67621400	-7.76468300
O	12.25127200	-25.09582100	-2.50296100
O	5.67675000	-27.32575400	-5.42226000
O	7.56900000	-35.35496000	-6.30138900
O	9.46125000	-30.23528300	-6.30138900
O	9.91014600	-24.98144700	-4.38392700

O	3.79709400	-33.87508600	-2.32889900
O	9.46125000	-27.32575400	-5.42226000
O	1.86214200	-36.05820800	-1.81378700
O	13.24575000	-33.88636100	-6.88555300
O	13.25859100	-35.33106100	-4.19103300
O	-1.06201500	-28.52671400	-1.52555600
O	5.70763500	-39.01414900	-2.63606700
O	11.35350000	-32.44543000	-5.42226000
O	15.13800000	-39.00603700	-6.88555300
O	3.78450000	-32.44543000	-5.42226000
O	9.51580900	-35.34518200	-4.17519900
O	5.67675000	-30.23528300	-6.30138900
O	13.24575000	-30.23528300	-6.30138900
O	1.94726500	-35.37532900	-4.21846700
O	13.34692800	-36.15630500	-1.83681700
O	1.89225000	-40.47463600	-6.30138900
O	15.13800000	-35.35496000	-6.30138900
O	1.89225000	-37.56510700	-5.42226000
O	-0.92177800	-39.63608700	-1.48333100
O	0.00000000	-42.68478300	-5.42226000
O	2.03438800	-39.04195600	-2.43210600
O	0.00000000	-31.67621400	-7.76468300
O	5.60963600	-35.33223200	-4.19513800
O	3.86086200	-30.19819200	-4.23094900
O	0.19913900	-27.25757000	-3.44284100
O	9.46602900	-39.05349100	-2.69681200
O	9.50142500	-36.08105500	-1.76235100
O	7.53166000	-40.62345600	-1.42696800
O	3.78450000	-28.76668500	-6.88555300
O	5.67675000	-33.88636100	-6.88555300
O	7.58711400	-37.51592400	-3.30339200
O	1.97634500	-25.75276500	-1.83943100
O	5.67972000	-36.06941300	-1.80561300
O	5.67675000	-36.79589000	-7.76468300
O	9.46125000	-40.47463600	-6.30138900
O	9.46125000	-37.56510700	-5.42226000
O	7.56900000	-42.68478300	-5.42226000
O	1.94877800	-32.54936200	-3.42346000
O	3.78450000	-42.68478300	-5.42226000
O	7.57442500	-30.27321500	-4.23054200
O	-1.82315500	-32.31435300	-3.37645800
O	7.55213900	-40.31218300	-4.46357400
O	7.56900000	-39.00603700	-6.88555300
O	7.56900000	-32.44543000	-5.42226000
O	13.28090600	-39.07763000	-2.70093000
O	14.57156600	-33.69337700	-1.55712400
O	11.39088800	-37.57131400	-3.29406700
O	0.97351300	-41.69930300	-2.30785000
O	-1.89225000	-33.88636100	-6.88555300
O	11.31009000	-30.21153600	-4.22614600
O	9.46125000	-36.79589000	-7.76468300
O	11.35350000	-28.76668500	-6.88555300
O	11.35350000	-31.67621400	-7.76468300
O	0.22620300	-30.92903900	-1.82149700
O	9.46433600	-32.49939700	-3.41682200
O	14.21273000	-25.07730000	-4.42504100

O	7.55450900	-33.98042500	-2.72204100
O	13.27223200	-32.49077100	-3.48742500
O	3.76414100	-40.30068900	-4.46528500
O	3.78450000	-39.00603700	-6.88555300
O	7.56900000	-28.76668500	-6.88555300
O	15.30424700	-37.36689600	-3.56879500
O	3.80898400	-30.93265600	-1.83875500
O	0.03173700	-37.69826600	-3.40302900
O	15.13800000	-28.76668500	-6.88555300
O	1.89225000	-30.23528300	-6.30138900
O	5.37506500	-24.98695400	-4.03986800
O	11.36974200	-33.89186800	-2.38243500
O	-1.89225000	-40.47463600	-6.30138900
O	0.01762100	-40.23061300	-4.46851400
O	0.00000000	-39.00603700	-6.88555300
O	0.00000000	-28.76668500	-6.88555300
O	9.46125000	-33.88636100	-6.88555300
O	11.35350000	-42.68478300	-5.42226000
O	12.24330200	-28.64640900	-1.11489000
O	13.24575000	-40.47463600	-6.30138900
O	1.89225000	-36.79589000	-7.76468300
O	1.89225000	-27.32575400	-5.42226000
O	-1.89225000	-30.23528300	-6.30138900
O	9.30857600	-29.00159300	-2.12337800
O	6.24320400	-26.05582900	-1.67563700
O	3.78450000	-35.35496000	-6.30138900
O	9.21125400	-25.97012300	-1.87259400
O	13.24575000	-37.56510700	-5.42226000
O	0.19516900	-33.80677600	-2.23769100
O	13.24575000	-27.32575400	-5.42226000
O	5.65694100	-32.49526300	-3.41392600
O	11.34591200	-40.33720300	-4.46737400
O	1.89225000	-33.88636100	-6.88555300
O	2.51984900	-25.05510400	-4.29726200
O	0.00000000	-32.44543000	-5.42226000
O	0.00000000	-35.35496000	-6.30138900
O	11.34461200	-31.02801800	-1.85885600
O	7.63268100	-27.44087200	-3.52307800
O	14.11987000	-27.40204900	-2.59437500
O	2.11468500	-28.67123500	-2.39880100
O	11.35350000	-39.00603700	-6.88555300
O	0.10447600	-30.18226000	-4.19247000
O	11.26294900	-27.46362900	-3.36144600
O	13.24575000	-36.79589000	-7.76468300
O	5.67675000	-40.47463600	-6.30138900
O	5.67675000	-37.56510700	-5.42226000
O	11.32577700	-40.54895900	-1.37119400
O	7.57984500	-31.18995500	-1.78873500
O	5.78386400	-28.90385000	-2.27808600
O	3.78450000	-31.67621400	-7.76468300
O	3.79907400	-37.56020900	-3.33809600
O	3.99775200	-27.31331600	-3.27282200
O	9.08100200	-33.40390300	-0.64990700
O	6.08469000	-33.39224300	-0.58889100
O	7.70516400	-31.62464500	0.97762800
Ti	13.09814200	-26.31783100	-3.60940800

Ti	9.50462400	-34.35957900	-2.30017600
Ti	1.92562100	-37.20828400	-3.22362300
Ti	1.89225000	-28.39591000	-7.03303600
Ti	13.48586400	-37.16563700	-3.38957000
Ti	3.81217300	-32.05526300	-3.29532200
Ti	11.34325700	-32.02423200	-3.32088300
Ti	5.67675000	-28.39591000	-7.03303600
Ti	9.57779100	-26.59745500	-3.56054300
Ti	1.89225000	-38.63526300	-7.03303600
Ti	11.35350000	-40.84541000	-6.15390700
Ti	-0.00437000	-31.99274400	-3.30764600
Ti	9.46125000	-38.63526300	-7.03303600
Ti	7.63653000	-39.46613600	-2.85060800
Ti	9.46125000	-28.39591000	-7.03303600
Ti	3.91779600	-39.54645400	-2.81749500
Ti	7.61444100	-32.22301000	-3.50202900
Ti	5.67675000	-38.63526300	-7.03303600
Ti	11.35350000	-30.60605700	-6.15390700
Ti	5.67675000	-35.72573400	-6.15390700
Ti	7.55056300	-29.15855900	-2.75424000
Ti	7.56900000	-33.51558700	-7.03303600
Ti	2.12717600	-26.70912400	-3.39405900
Ti	5.71160100	-37.12406100	-3.32782700
Ti	13.24575000	-38.63526300	-7.03303600
Ti	11.35350000	-33.51558700	-7.03303600
Ti	5.77706400	-26.64579000	-3.41606100
Ti	2.00494200	-34.39554200	-2.68366300
Ti	3.78450000	-30.60605700	-6.15390700
Ti	13.17605300	-34.46544300	-2.53448500
Ti	11.06850700	-29.22148600	-2.49502400
Ti	7.56900000	-30.60605700	-6.15390700
Ti	0.00000000	-40.84541000	-6.15390700
Ti	9.54631400	-37.05535800	-3.35940200
Ti	7.56900000	-40.84541000	-6.15390700
Ti	13.24575000	-35.72573400	-6.15390700
Ti	3.78450000	-40.84541000	-6.15390700
Ti	11.32398400	-39.45955100	-2.85280600
Ti	0.00000000	-33.51558700	-7.03303600
Ti	3.94113100	-29.26529800	-2.64814100
Ti	3.78450000	-33.51558700	-7.03303600
Ti	0.41099800	-39.99362100	-2.68913800
Ti	0.00000000	-30.60605700	-6.15390700
Ti	0.31476000	-29.23996900	-2.56625800
Ti	13.24575000	-28.39591000	-7.03303600
Ti	5.67694100	-34.39909800	-2.53753700
Ti	1.89225000	-35.72573400	-6.15390700
Ti	9.46125000	-35.72573400	-6.15390700
H	1.97018200	-24.78148800	-1.79432700
H	15.11489500	-34.28507500	-1.00703800
H	12.45294500	-29.33950900	-0.46289200
H	13.61897200	-27.84293400	-1.84961400
H	15.13800000	-34.45364600	-6.65990500
H	14.19634000	-33.70183500	-6.94237500
H	15.13800000	-39.90735100	-6.52703800
H	13.98005500	-39.59952500	-2.27417900
H	6.67913700	-40.90347300	-1.04219100
H	14.19364500	-30.42990000	-6.23415700
H	3.78450000	-43.21602500	-6.22187400
H	-1.87885700	-29.34208100	-6.67942400
H	13.89833200	-31.98937000	-2.93134800
H	3.11029800	-41.40945200	-1.39673600
H	-0.94912600	-35.54093500	-6.22741400
H	15.68479200	-37.51531700	-4.45651400
H	11.67717400	-25.34274300	-1.75360300
H	15.13800000	-29.66799800	-6.52703800
H	-0.93934200	-28.58262700	-6.95876600
H	0.00000000	-43.21602500	-6.22187400
H	8.29275800	-25.93180600	-1.51941000
H	11.35350000	-43.21602500	-6.22187400
H	-2.22872400	-32.50805500	-4.24321300
H	7.56900000	-43.21602500	-6.22187400
H	-1.89225000	-39.58261400	-6.65620900
H	-1.34784300	-38.76004200	-1.51570000
H	5.86750700	-25.20052200	-1.40268300
H	14.91140800	-25.38415300	-5.02857700
H	4.40979000	-24.81790100	-4.20872100
H	-0.21956400	-37.88163200	-4.32658700
H	-1.56640800	-29.14926100	-0.97226000
H	1.04978200	-42.36674900	-3.01946500
H	14.19301100	-40.66200500	-6.20925100
H	10.25823200	-24.28841000	-3.78919200
H	-0.39258800	-26.76074400	-2.84600000
H	2.40379800	-25.17071500	-5.25752900
H	-1.88980400	-34.79123900	-6.53613900
H	-0.54389700	-34.38155600	-1.97427600
H	10.51048900	-40.78346500	-0.89031300
H	-0.89789200	-38.83396100	-6.96424100
H	5.34187800	-33.21819000	0.01757400
V	7.67885300	-32.37759200	-0.43353500

Figure 3**Fehler! Verweisquelle konnte nicht gefunden werden.**c

O	3.92574607	-40.89528507	-1.58217120
O	11.35350000	-35.35496000	-6.30138900
O	7.56900000	-31.67621400	-7.76468300
O	12.47365811	-25.66799086	-1.83193499
O	5.67675000	-27.32575400	-5.42226000
O	7.56900000	-35.35496000	-6.30138900
O	9.46125000	-30.23528300	-6.30138900
O	9.74370581	-24.82949992	-4.34409004
O	3.79470341	-33.94054866	-2.51676900
O	9.46125000	-27.32575400	-5.42226000
O	1.85913361	-36.04393131	-1.81670696
O	13.24575000	-33.88636100	-6.88555300
O	13.22178449	-35.33506885	-4.17686715
O	-0.90327735	-28.53946733	-1.37849001
O	5.71572916	-39.02289899	-2.62897830
O	11.35350000	-32.44543000	-5.42226000
O	15.13800000	-39.00603700	-6.88555300
O	3.78450000	-32.44543000	-5.42226000
O	9.53163465	-35.32435826	-4.22289378
O	5.67675000	-30.23528300	-6.30138900

O	13.24575000	-30.23528300	-6.30138900	O	-1.89225000	-40.47463600	-6.30138900
O	1.92235545	-35.37686118	-4.23014815	O	0.01975546	-40.22744091	-4.46987434
O	13.27051520	-36.16147012	-1.82566696	O	0.00000000	-39.00603700	-6.88555300
O	1.89225000	-40.47463600	-6.30138900	O	0.00000000	-28.76668500	-6.88555300
O	15.13800000	-35.35496000	-6.30138900	O	9.46125000	-33.88636100	-6.88555300
O	1.89225000	-37.56510700	-5.42226000	O	11.35350000	-42.68478300	-5.42226000
O	-0.89979841	-39.65978567	-1.47564068	O	12.91539703	-28.50175717	-2.40123386
O	0.00000000	-42.68478300	-5.42226000	O	13.24575000	-40.47463600	-6.30138900
O	2.05107391	-39.03082493	-2.42891790	O	1.89225000	-36.79589000	-7.76468300
O	0.00000000	-31.67621400	-7.76468300	O	1.89225000	-27.32575400	-5.42226000
O	5.70459394	-35.35048553	-4.17985863	O	-1.89225000	-30.23528300	-6.30138900
O	3.76623298	-30.27015044	-4.21599430	O	9.32838436	-29.06722054	-2.08800333
O	0.41536785	-27.26220928	-3.17463594	O	5.34507477	-25.98143581	-1.65273113
O	9.45829304	-39.04077569	-2.65098991	O	3.78450000	-35.35496000	-6.30138900
O	9.50696768	-36.03182729	-1.83400796	O	9.51839436	-25.83504239	-1.76249877
O	7.54691399	-40.65723544	-1.42716304	O	13.24575000	-37.56510700	-5.42226000
O	3.78450000	-28.76668500	-6.88555300	O	0.10778088	-33.86266235	-2.40779159
O	5.67675000	-33.88636100	-6.88555300	O	13.24575000	-27.32575400	-5.42226000
O	7.59561099	-37.52925426	-3.30430901	O	5.71026513	-32.59500788	-3.49541081
O	2.52105500	-25.63315986	-1.96991381	O	11.34072998	-40.34032693	-4.46154105
O	5.70549127	-36.08349670	-1.76217534	O	1.89225000	-33.88636100	-6.88555300
O	5.67675000	-36.79589000	-7.76468300	O	1.86777918	-24.78890213	-4.49840973
O	9.46125000	-40.47463600	-6.30138900	O	0.00000000	-32.44543000	-5.42226000
O	9.46125000	-37.56510700	-5.42226000	O	0.00000000	-35.35496000	-6.30138900
O	7.56900000	-42.68478300	-5.42226000	O	11.51362573	-30.88028884	-1.87184581
O	1.95149260	-32.49094094	-3.34516848	O	7.66182598	-27.30792211	-3.29043877
O	3.78450000	-42.68478300	-5.42226000	O	14.82322582	-26.47064113	-3.15701568
O	7.62818507	-30.22967014	-4.21482120	O	2.21793293	-29.09555257	-2.00562768
O	-1.92928671	-32.25603597	-3.47758498	O	11.35350000	-39.00603700	-6.88555300
O	7.56333725	-40.31233281	-4.45948195	O	0.16520212	-30.18258577	-4.14377183
O	7.56900000	-39.00603700	-6.88555300	O	11.04794761	-27.38616039	-3.43764558
O	7.56900000	-32.44543000	-5.42226000	O	13.24575000	-36.79589000	-7.76468300
O	13.25737424	-39.08477330	-2.64898246	O	5.67675000	-40.47463600	-6.30138900
O	14.54041961	-33.71830327	-1.55673503	O	5.67675000	-37.56510700	-5.42226000
O	11.37808530	-37.61295788	-3.30887224	O	11.25552018	-40.67248079	-1.42430121
O	1.00855807	-41.69354894	-2.33223961	O	7.22277170	-31.04801809	-1.82018629
O	-1.89225000	-33.88636100	-6.88555300	O	5.73139122	-28.77036822	-2.35932820
O	11.19406815	-30.21037406	-4.24983382	O	3.78450000	-31.67621400	-7.76468300
O	9.46125000	-36.79589000	-7.76468300	O	3.81301293	-37.53739625	-3.33499586
O	11.35350000	-28.76668500	-6.88555300	O	3.78119686	-27.40595147	-3.50561425
O	11.35350000	-31.67621400	-7.76468300	O	5.70423230	-30.80681707	0.55705686
O	0.06320878	-31.03890888	-1.78758881	O	5.72175283	-33.27385925	-0.70710990
O	9.45848292	-32.42131517	-3.30871588	H	-0.89789200	-38.83396100	-6.96424100
O	12.47734923	-24.98987711	-4.45598764	H	3.42916145	-25.62600175	-1.56318141
O	7.64068598	-33.91765321	-2.52463952	H	15.08546700	-34.31011282	-1.00866691
O	13.25695143	-32.49377964	-3.48608655	H	13.64430990	-28.95635321	-1.94952583
O	3.76710859	-40.29034328	-4.46816853	H	15.20746426	-26.09197416	-2.34687981
O	3.78450000	-39.00603700	-6.88555300	H	15.13800000	-34.45364600	-6.65990500
O	7.56900000	-28.76668500	-6.88555300	H	14.19634000	-33.70183500	-6.94237500
O	15.26565194	-37.37011004	-3.52828741	H	15.13800000	-39.90735100	-6.52703800
O	4.20987439	-31.08056753	-1.82882606	H	13.97290313	-39.59913370	-2.24020039
O	0.04373893	-37.71188566	-3.39315606	H	6.71153076	-40.96018990	-1.02294145
O	15.13800000	-28.76668500	-6.88555300	H	14.19364500	-30.42990000	-6.23415700
O	1.89225000	-30.23528300	-6.30138900	H	3.78450000	-43.21602500	-6.22187400
O	5.91668227	-24.98430397	-4.12114194	H	-1.87885700	-29.34208100	-6.67942400
O	11.32981867	-33.83562934	-2.32718971	H	13.90147693	-32.01229236	-2.93396283

H	3.11149357	-41.42084521	-1.43565155
H	-0.94912600	-35.54093500	-6.22741400
H	15.67178633	-37.49853074	-4.40740578
H	11.52820985	-25.53516648	-1.58262425
H	15.13800000	-29.66799800	-6.52703800
H	-0.93934200	-28.58262700	-6.95876600
H	0.00000000	-43.21602500	-6.22187400
H	9.17137622	-26.39550028	-1.04593538
H	11.35350000	-43.21602500	-6.22187400
H	-2.30921797	-32.43347156	-4.35966689
H	7.56900000	-43.21602500	-6.22187400
H	-1.89225000	-39.58261400	-6.65620900
H	-1.34840234	-38.79489714	-1.48748548
H	10.46181318	-40.88221820	-0.89859749
H	12.77712163	-25.12335108	-5.37265533
H	6.14657470	-25.13427658	-5.05618096
H	-0.21832472	-37.88033649	-4.31631385
H	-1.46311469	-29.12683264	-0.84136007
H	1.07018885	-42.35960650	-3.04620479
H	14.19301100	-40.66200500	-6.20925100
H	10.73272866	-24.67901661	-4.45898119
H	-0.19994427	-26.83207627	-2.54815393
H	1.61273762	-24.90893571	-5.43029239
H	-1.88980400	-34.79123900	-6.53613900
H	-0.62701481	-34.44735025	-2.15652796
Ti	0.00000000	-33.51558700	-7.03303600
Ti	3.89174145	-29.10422492	-2.75042827
Ti	3.78450000	-33.51558700	-7.03303600
Ti	0.42561429	-39.98924289	-2.69399895
Ti	0.00000000	-30.60605700	-6.15390700
Ti	0.42314938	-29.33440875	-2.42724584
Ti	13.24575000	-28.39591000	-7.03303600
Ti	5.72215726	-34.36137569	-2.30970016
Ti	1.89225000	-35.72573400	-6.15390700
Ti	9.46125000	-35.72573400	-6.15390700
Ti	12.98623515	-26.49606916	-3.36397748
Ti	9.48848723	-34.39730477	-2.66037218
Ti	1.93786434	-37.20865483	-3.22364215
Ti	1.89225000	-28.39591000	-7.03303600
Ti	13.44495782	-37.16826412	-3.38535782
Ti	3.78957204	-32.13921678	-3.44064548
Ti	11.35864116	-31.98140625	-3.24552218
Ti	5.67675000	-28.39591000	-7.03303600
Ti	9.42067573	-26.41486698	-3.55228707
Ti	1.89225000	-38.63526300	-7.03303600
Ti	11.35350000	-40.84541000	-6.15390700
Ti	-0.11242495	-31.99265508	-3.33151265
Ti	9.46125000	-38.63526300	-7.03303600
Ti	7.58640828	-39.48237942	-2.83948759
Ti	9.46125000	-28.39591000	-7.03303600
Ti	3.93124650	-39.54234074	-2.81636416
Ti	7.55292962	-32.13668607	-3.44027223
Ti	5.67675000	-38.63526300	-7.03303600
Ti	11.35350000	-30.60605700	-6.15390700
Ti	5.67675000	-35.72573400	-6.15390700
Ti	7.57366535	-29.10081520	-2.72504347
Ti	7.56900000	-33.51558700	-7.03303600
Ti	2.10268101	-26.36609048	-3.55949478
Ti	5.70837735	-37.05077289	-3.35673693
Ti	13.24575000	-38.63526300	-7.03303600
Ti	11.35350000	-33.51558700	-7.03303600
Ti	5.69867522	-26.58579294	-3.16659394
Ti	1.97364032	-34.40298871	-2.70253910
Ti	3.78450000	-30.60605700	-6.15390700
Ti	13.12872001	-34.47189265	-2.51608688
Ti	11.09009954	-29.15668912	-2.70499896
Ti	7.56900000	-30.60605700	-6.15390700
Ti	0.00000000	-40.84541000	-6.15390700
Ti	9.52615472	-37.16294474	-3.31163522
Ti	7.56900000	-40.84541000	-6.15390700
Ti	13.24575000	-35.72573400	-6.15390700
Ti	3.78450000	-40.84541000	-6.15390700
Ti	11.32636498	-39.50873904	-2.83571492
V	5.71082443	-31.52800418	-0.87186297

Figure 3**Fehler! Verweisquelle konnte nicht gefunden werden.**d

H	23.17714917	-4.58311174	-5.10650442
H	0.94312400	-1.89225000	-6.93684300
H	21.76387600	-1.89225000	-6.93684300
H	18.92250000	4.73362600	-7.33460700
H	3.78450000	-12.30262600	-7.33460700
H	11.35350000	4.73362600	-7.33460700
H	21.76387600	-9.46125000	-6.93684300
H	0.94312400	1.89225000	-6.93684300
H	10.08481996	3.52626539	-3.01863397
H	23.34523030	-2.23662912	-4.36566113
H	6.74888658	2.95916925	-3.01038414
H	21.76048000	1.97279300	-6.93671200
H	21.76387600	-5.67675000	-6.93684300
H	7.53108900	-12.30189700	-7.33473800
H	23.13422327	-7.80187078	-4.97685522
H	10.50761915	-11.24601084	-3.50450470
H	18.04998168	2.86811919	-3.04048973
H	0.94312400	-9.46125000	-6.93684300
H	18.12267919	-10.40471755	-3.04474444
H	11.34876300	-12.30264200	-7.33473800
H	7.56900000	4.73362600	-7.33460700
H	6.26368154	-10.85639650	-3.06117278
H	15.10555800	-12.30209900	-7.33473800
H	0.94312400	-5.67675000	-6.93684300
H	2.97853203	-5.23071895	-4.84095529
H	2.87714784	-1.96566792	-4.86853691
H	21.59193701	-10.34135189	-2.85144834
H	2.98679961	-9.05492822	-4.76228177
H	2.98186078	1.59897548	-4.74436656
H	14.25023624	3.37270581	-3.09060468
H	18.97682800	-12.30109800	-7.33473800
H	21.65928607	2.75076403	-2.87475191
H	23.02192630	0.10156212	-5.13945984
H	15.13800000	4.73362600	-7.33460700
H	3.78450000	4.73362600	-7.33460700

H	13.79419381	-10.95999260	-2.91431197
H	8.36426346	-7.68512667	-3.40837162
V	11.39828533	-3.61628216	-2.74840245
Ti	17.02950458	-5.50426713	-4.80598147
Ti	11.35350000	-1.89225000	-7.13572500
Ti	3.78450000	-9.46125000	-7.13572500
Ti	5.75420157	-5.48994519	-4.79969853
Ti	11.35350000	1.89225000	-7.13572500
Ti	17.05400425	1.39636109	-4.75168142
Ti	18.92250000	1.89225000	-7.13572500
Ti	17.07268834	-8.96172331	-4.73970542
Ti	9.53278393	-5.91289024	-4.73205684
Ti	7.56900000	1.89225000	-7.13572500
Ti	9.51452834	-1.60806392	-4.66844921
Ti	15.13800000	1.89225000	-7.13572500
Ti	18.92250000	-5.67675000	-7.13572500
Ti	13.29535918	-9.29255593	-4.74686729
Ti	7.56900000	-9.46125000	-7.13572500
Ti	5.73667936	-8.97769830	-4.68088625
Ti	11.35350000	-9.46125000	-7.13572500
Ti	17.01288932	-2.05758750	-4.80461441
Ti	20.87077910	1.23623817	-4.69386115
Ti	3.78450000	-5.67675000	-7.13572500
Ti	18.92250000	-9.46125000	-7.13572500
Ti	15.13800000	-1.89225000	-7.13572500
Ti	3.78450000	-1.89225000	-7.13572500
Ti	13.26289463	1.80001675	-4.76203804
Ti	9.48292329	-9.45033459	-4.80676291
Ti	18.92250000	-1.89225000	-7.13572500
Ti	3.78450000	1.89225000	-7.13572500
Ti	20.87293845	-5.46217144	-4.70332038
Ti	9.46541681	1.79456763	-4.76178002
Ti	15.13800000	-9.46125000	-7.13572500
Ti	11.35350000	-5.67675000	-7.13572500
Ti	13.23567298	-1.60537979	-4.67897663
Ti	20.83625456	-2.09752217	-4.71226057
Ti	7.56900000	-5.67675000	-7.13572500
Ti	5.74795773	1.43239020	-4.68791850
Ti	7.56900000	-1.89225000	-7.13572500
Ti	13.23523297	-5.95269316	-4.71156888
Ti	5.75876937	-2.02971362	-4.80431229
Ti	20.87651001	-8.81784012	-4.69930236
Ti	15.13800000	-5.67675000	-7.13572500
O	17.04366708	-7.23941009	-4.11185265
O	5.67675000	-1.89225000	-6.73669500
O	15.11521213	-5.57094887	-5.17239380
O	22.69255663	-8.66325002	-5.11716847
O	11.36613863	-1.78679233	-5.23928590
O	18.94725980	-5.50478011	-5.24705748
O	9.33210701	3.10780279	-3.47296831
O	11.35350000	-11.35350000	-7.53475500
O	5.67675000	-5.67675000	-6.73669500
O	3.78450000	-11.35350000	-7.53475500
O	9.46125000	-1.89225000	-6.73669500
O	17.23212088	-10.13390184	-3.34345332
O	7.56900000	-11.35350000	-7.53475500
O	15.13800000	-7.56900000	-7.53475500
O	13.24575000	-5.67675000	-6.73669500
O	18.92250000	-11.35350000	-7.53475500
O	13.11371175	-10.69600598	-3.55917862
O	18.95052151	1.55796301	-5.22597429
O	20.81162831	-10.09941240	-3.38062759
O	13.24575000	-9.46125000	-6.73669500
O	17.03025000	-1.89225000	-6.73669500
O	11.34400465	-6.11718735	-5.27305288
O	5.74791258	-0.31222151	-4.10224696
O	17.03025000	1.89225000	-6.73669500
O	17.03025000	-9.46125000	-6.73669500
O	9.99436307	-4.87213491	-3.44499363
O	15.10438705	-2.01110520	-5.15703086
O	22.74497058	-5.45435983	-5.01798898
O	13.39872603	3.12343912	-3.49555449
O	18.95319825	-9.12683766	-5.23066061
O	22.74366607	-2.06290157	-5.11182909
O	20.69948161	-0.44968264	-3.92245230
O	11.35350000	3.78450000	-7.53475500
O	3.78450000	-7.56900000	-7.53475500
O	9.99953842	-2.43701096	-3.14842632
O	20.81475000	-5.67675000	-6.73669500
O	12.76155004	-2.42245148	-3.13967849
O	3.78450000	-3.78450000	-7.53475500
O	13.28614208	0.10926704	-4.11886757
O	11.35350000	0.00000000	-7.53475500
O	15.13800000	-3.78450000	-7.53475500
O	22.67445832	1.01951184	-5.11698122
O	17.03552992	-3.78460047	-4.07627602
O	9.46125000	-5.67675000	-6.73669500
O	18.92250000	-3.78450000	-7.53475500
O	17.17123597	2.59291535	-3.36626871
O	3.78450000	0.00000000	-7.53475500
O	20.81475000	1.89225000	-6.73669500
O	3.81335610	-2.00987321	-5.13620786
O	9.46125000	1.89225000	-6.73669500
O	1.89225000	-1.89225000	-6.73669500
O	7.56900000	3.78450000	-7.53475500
O	3.81967723	-5.63965024	-5.11584897
O	1.89225000	-5.67675000	-6.73669500
O	15.17968730	1.77702790	-5.18898295
O	9.23581935	-7.70853091	-3.86072281
O	7.63614657	-5.58754320	-5.15917333
O	20.86659057	2.53713775	-3.39793080
O	11.38458183	-3.82146813	-1.17062220
O	5.85458988	-9.97827223	-3.15562614
O	7.57214769	1.78014810	-5.19916756
O	9.46516889	0.10863743	-4.10849890
O	11.35350000	-3.78450000	-7.53475500
O	3.86148592	-9.29625872	-5.11973274
O	11.35350000	-7.56900000	-7.53475500
O	7.59342215	-9.40339257	-5.17407975
O	20.73275430	-7.13155455	-3.95580288
O	5.67675000	-9.46125000	-6.73669500
O	15.13800000	0.00000000	-7.53475500

O	3.78450000	3.78450000	-7.53475500
O	9.61327464	-10.92199914	-3.74138422
O	3.86694624	1.77200573	-5.11415942
O	7.56900000	-7.56900000	-7.53475500
O	1.89225000	1.89225000	-6.73669500
O	17.04038438	-0.33318229	-4.11261631
O	7.56900000	-3.78450000	-7.53475500
O	20.77632337	-3.76899369	-3.91567941
O	1.89225000	-9.46125000	-6.73669500
O	5.72917342	-3.79951022	-4.08619603
O	11.33022504	-9.27157698	-5.17171006
O	5.67675000	1.89225000	-6.73669500
O	11.36054526	1.94604319	-5.16458172
O	15.17338227	-9.36697558	-5.16803585
O	13.35735000	-7.65752513	-4.01024795
O	9.46125000	-9.46125000	-6.73669500
O	18.92250000	0.00000000	-7.53475500
O	5.83021173	-7.27367975	-4.08793801
O	18.92250000	-7.56900000	-7.53475500
O	20.81475000	-1.89225000	-6.73669500
O	13.24575000	-1.89225000	-6.73669500
O	15.13800000	3.78450000	-7.53475500
O	18.94410069	-2.05904681	-5.25022750
O	18.92250000	3.78450000	-7.53475500
O	13.24575000	1.89225000	-6.73669500
O	20.81475000	-9.46125000	-6.73669500
O	12.67607326	-4.89300188	-3.43036084
O	7.56900000	0.00000000	-7.53475500
O	15.13800000	-11.35350000	-7.53475500
O	7.63108964	-2.01579648	-5.14314522
O	5.90702928	2.51206014	-3.22834490
O	17.03025000	-5.67675000	-6.73669500

Figure 3**Fehler! Verweisquelle konnte nicht gefunden werden.**e

H	23.18312033	-4.59336796	-5.10906360
H	0.94312400	-1.89225000	-6.93684300
H	21.76387600	-1.89225000	-6.93684300
H	18.92250000	4.73362600	-7.33460700
H	3.78450000	-12.30262600	-7.33460700
H	11.35350000	4.73362600	-7.33460700
H	21.76387600	-9.46125000	-6.93684300
H	0.94312400	1.89225000	-6.93684300
H	10.17437924	3.56223970	-3.09408484
H	23.34793555	-2.25429080	-4.36891071
H	6.70024322	2.96015880	-2.99326229
H	21.76048000	1.97279300	-6.93671200
H	21.76387600	-5.67675000	-6.93684300
H	7.53108900	-12.30189700	-7.33473800
H	23.12856528	-7.79944146	-4.97823844
H	10.09863139	-11.05725518	-3.03475443
H	18.02609214	2.86306394	-3.02949057
H	0.94312400	-9.46125000	-6.93684300
H	18.07030154	-10.43344833	-3.04418668
H	11.34876300	-12.30264200	-7.33473800
H	7.56900000	4.73362600	-7.33460700
H	6.75805008	-10.50618582	-3.00649911
H	15.10555800	-12.30209900	-7.33473800
H	0.94312400	-5.67675000	-6.93684300
H	2.89000617	-5.67946881	-4.85366219
H	3.05303202	-2.60153108	-4.87628879
H	21.61173202	-10.34835187	-2.86761458
H	2.97988520	-9.18023157	-4.74195903
H	2.99499858	1.45925102	-4.76543527
H	14.22847427	3.31389233	-3.08097420
H	18.97682800	-12.30109800	-7.33473800
H	21.67038318	2.74567700	-2.88054797
H	23.02209492	0.08823888	-5.13774747
H	15.13800000	4.73362600	-7.33460700
H	3.78450000	4.73362600	-7.33460700
H	14.22034856	-10.99010364	-3.09652043
H	9.12644143	-2.99154762	-2.72653576
O	17.03025000	-5.67675000	-6.73669500
O	17.04116172	-7.24232714	-4.11661862
O	5.67675000	-1.89225000	-6.73669500
O	15.10693342	-5.56788177	-5.16233261
O	22.68700025	-8.66041768	-5.12029944
O	11.33089473	-1.77166635	-5.23339606
O	18.94671355	-5.50154938	-5.24602735
O	9.39670338	3.12215081	-3.48213037
O	11.35350000	-11.35350000	-7.53475500
O	5.67675000	-5.67675000	-6.73669500
O	3.78450000	-11.35350000	-7.53475500
O	9.46125000	-1.89225000	-6.73669500
O	17.18683227	-10.16443939	-3.36375838
O	7.56900000	-11.35350000	-7.53475500
O	15.13800000	-7.56900000	-7.53475500
O	13.24575000	-5.67675000	-6.73669500
O	18.92250000	-11.35350000	-7.53475500
O	13.37764655	-10.72372979	-3.50860024
O	18.94868571	1.55189699	-5.22438731
O	20.82261367	-10.10424498	-3.38265226
O	13.24575000	-9.46125000	-6.73669500
O	17.03025000	-1.89225000	-6.73669500
O	11.38281135	-5.81471457	-5.24652514
O	5.75985448	-0.33481553	-4.11405053
O	17.03025000	1.89225000	-6.73669500
O	17.03025000	-9.46125000	-6.73669500
O	10.04087980	-4.97136384	-3.24116315
O	15.10011894	-2.02374488	-5.15868733
O	22.74584663	-5.46082895	-5.01207443
O	13.37708053	3.05288527	-3.47939564
O	18.95038943	-9.13529510	-5.22824153
O	22.74546749	-2.06239429	-5.10983857
O	20.69688817	-0.45455788	-3.92166539
O	11.35350000	3.78450000	-7.53475500
O	3.78450000	-7.56900000	-7.53475500
O	20.81475000	-5.67675000	-6.73669500
O	5.88641949	2.46772016	-3.21332067
O	3.78450000	-3.78450000	-7.53475500
O	13.26819867	0.04476733	-4.09826579
O	11.35350000	0.00000000	-7.53475500

O	15.13800000	-3.78450000	-7.53475500
O	22.67392434	1.00634014	-5.12175161
O	17.03330078	-3.78825847	-4.07356280
O	9.46125000	-5.67675000	-6.73669500
O	18.92250000	-3.78450000	-7.53475500
O	17.15393307	2.58061613	-3.36609545
O	3.78450000	0.00000000	-7.53475500
O	20.81475000	1.89225000	-6.73669500
O	3.81093154	-2.03535897	-5.11232101
O	9.46125000	1.89225000	-6.73669500
O	1.89225000	-1.89225000	-6.73669500
O	7.56900000	3.78450000	-7.53475500
O	3.81187048	-5.53107920	-5.13294781
O	1.89225000	-5.67675000	-6.73669500
O	15.17190169	1.74347094	-5.18690220
O	9.47341228	-7.62629000	-4.09347917
O	7.63704013	-5.54759299	-5.14572188
O	20.87496202	2.52898262	-3.39828585
O	11.49330793	-3.90536734	-1.10115117
O	5.91210925	-10.07014061	-3.23069981
O	7.57468656	1.79706634	-5.19465915
O	9.44238522	0.10112276	-4.13552237
O	11.35350000	-3.78450000	-7.53475500
O	3.86773254	-9.33558642	-5.11291147
O	11.35350000	-7.56900000	-7.53475500
O	7.57635794	-9.31870409	-5.19737038
O	20.72740553	-7.13262249	-3.95578971
O	5.67675000	-9.46125000	-6.73669500
O	15.13800000	0.00000000	-7.53475500
O	3.78450000	3.78450000	-7.53475500
O	9.33938998	-10.61651662	-3.45635574
O	3.86354504	1.73584535	-5.11331992
O	7.56900000	-7.56900000	-7.53475500
O	1.89225000	1.89225000	-6.73669500
O	17.03981269	-0.34404787	-4.10981819
O	7.56900000	-3.78450000	-7.53475500
O	20.77766274	-3.77028290	-3.91470895
O	1.89225000	-9.46125000	-6.73669500
O	5.75418126	-3.78568794	-4.05298803
O	11.35827336	-9.49709458	-5.16450321
O	5.67675000	1.89225000	-6.73669500
O	11.36138243	1.91173556	-5.16900236
O	15.17945100	-9.36353360	-5.18686115
O	13.30202668	-7.69762038	-4.11990789
O	9.46125000	-9.46125000	-6.73669500
O	18.92250000	0.00000000	-7.53475500
O	5.74213557	-7.24597120	-4.09314469
O	18.92250000	-7.56900000	-7.53475500
O	20.81475000	-1.89225000	-6.73669500
O	13.24575000	-1.89225000	-6.73669500
O	15.13800000	3.78450000	-7.53475500
O	18.94307874	-2.06425722	-5.25049177
O	18.92250000	3.78450000	-7.53475500
O	13.24575000	1.89225000	-6.73669500
O	20.81475000	-9.46125000	-6.73669500
O	12.81615413	-5.16228081	-3.15016493
O	7.56900000	0.00000000	-7.53475500
O	15.13800000	-11.35350000	-7.53475500
O	9.87916822	-2.51686789	-3.13127721
O	12.69785432	-2.62360575	-3.26867079
O	7.65396489	-2.02863162	-5.14520497
Ti	3.78450000	-5.67675000	-7.13572500
Ti	18.92250000	-9.46125000	-7.13572500
Ti	15.13800000	-1.89225000	-7.13572500
Ti	3.78450000	-1.89225000	-7.13572500
Ti	13.26477102	1.73910092	-4.75656433
Ti	9.46446216	-9.31659916	-4.75661416
Ti	18.92250000	-1.89225000	-7.13572500
Ti	3.78450000	1.89225000	-7.13572500
Ti	20.87412208	-5.46802711	-4.70206838
Ti	9.45980603	1.81304827	-4.77202851
Ti	15.13800000	-9.46125000	-7.13572500
Ti	11.35350000	-5.67675000	-7.13572500
Ti	13.22691213	-1.66216312	-4.69476594
Ti	20.83947841	-2.10302833	-4.71156758
Ti	7.56900000	-5.67675000	-7.13572500
Ti	5.74047534	1.40400118	-4.68708422
Ti	7.56900000	-1.89225000	-7.13572500
Ti	13.25531234	-5.99894632	-4.70950254
Ti	5.74169866	-2.07731154	-4.79378208
Ti	20.87141928	-8.82350382	-4.70061746
Ti	15.13800000	-5.67675000	-7.13572500
Ti	17.03504139	-5.51543108	-4.80442436
Ti	11.35350000	-1.89225000	-7.13572500
Ti	3.78450000	-9.46125000	-7.13572500
Ti	5.75645554	-5.52600113	-4.79687889
Ti	11.35350000	1.89225000	-7.13572500
Ti	17.05747884	1.38306740	-4.75134552
Ti	18.92250000	1.89225000	-7.13572500
Ti	17.05586653	-8.97361471	-4.75094843
Ti	9.52378167	-5.91994227	-4.69112970
Ti	7.56900000	1.89225000	-7.13572500
Ti	9.49328604	-1.57090870	-4.76060424
Ti	15.13800000	1.89225000	-7.13572500
Ti	18.92250000	-5.67675000	-7.13572500
Ti	13.26417129	-9.39047358	-4.76600764
Ti	7.56900000	-9.46125000	-7.13572500
Ti	5.74657134	-8.98718412	-4.68652025
Ti	11.35350000	-9.46125000	-7.13572500
Ti	17.01831880	-2.06909133	-4.80449536
Ti	20.87359899	1.22904000	-4.69437956
V	11.53955677	-3.95930192	-2.69239424

Figure S14 Isolated

Ti	3.81346007	4.83796898	4.56558848
Ti	2.44636180	4.39915287	1.38359711
V	1.02369137	1.37029603	2.36471232
Ti	2.36200031	1.81802767	5.55223073
Ti	0.91976709	6.53765757	5.55858999
Ti	-0.43233893	6.11770275	2.35926610

Ti	-1.84116692	3.08456880	3.36810217
Ti	-0.51745645	3.50954308	6.57023214
O	3.57808163	4.75943586	2.76126201
O	1.87899614	2.66914097	1.47781462
O	1.82493334	1.13684321	3.94864617
O	3.52553158	3.19086205	5.28761097
O	2.64955834	6.03782988	5.28608922
O	1.01948566	5.52624853	1.43208175
O	-0.66551636	1.89030773	2.65013216
O	0.91940583	2.39252555	6.49959208
O	-1.57909900	4.73097296	2.64060415
O	-1.63163926	3.15597308	5.17351937
O	0.04315358	5.23930272	6.48697735
H	5.41121483	5.33100166	4.90488466
H	3.27643942	4.61484319	-0.08949212
O	1.05159160	0.01269020	1.52359583
H	3.14720271	0.58401323	6.42760850
H	0.89033377	7.98725566	6.45784577
H	-3.42476637	2.56415818	3.01178759
H	-1.35396249	3.26040071	8.03623149
O	0.09817959	6.81091715	3.95657068
H	-1.22352700	7.32921682	1.45525269

Figure S14 Dimer

Ti	-2.64888748	-1.11140704	-0.90053218
Ti	-1.45896651	2.09343006	-1.59670701
V	-0.45522719	2.47341878	1.71982480
Ti	-1.64448569	-0.73051466	2.41287137
V	0.45453281	-2.47324943	-1.72041896
Ti	1.64221361	0.73081548	-2.41428989
Ti	2.64943899	1.10855876	0.90294961
Ti	1.46213658	-2.09132877	1.59656975
O	-2.48796759	0.59535581	-1.51018550
O	-1.13369501	2.72470340	0.08188784
O	-1.25236572	1.04881759	2.45544543
O	-2.60606427	-1.12153399	0.91845692
O	-1.29762889	-2.14004936	-1.56217011
O	0.11115470	1.71378535	-2.43411243
O	1.29596341	2.13280211	1.56675328
O	-0.10910917	-1.70669926	2.42958589
O	2.60046753	1.11453732	-0.91590626
O	2.49804944	-0.59760997	1.51676481
O	1.13961184	-2.71790375	-0.08424731
H	-4.13291414	-1.75969062	-1.43082583
H	-2.28880541	3.29405581	-2.47630650
H	-2.56874848	-1.11466736	3.79199007
O	0.69343723	-3.76981229	-2.62137344
H	4.13231596	1.76473543	1.42671401
H	2.28349503	-3.29760634	2.47638137
O	1.24286276	-1.04677352	-2.46184414
H	2.57287144	1.11383348	-3.78941132
O	-0.69156234	3.76908427	2.62274473

Figure S14 Vacant

Ti	3.86058412	4.81337006	4.64693797
Ti	2.39516197	4.37010460	1.50970821
V	1.01930802	1.27136598	2.41432061
Ti	2.35362495	1.80366316	5.58358182
Ti	1.04580632	6.53006190	5.51341047
Ti	-0.08911016	5.91239955	2.25239814
Ti	-1.76303033	3.00792182	3.27565736
Ti	-0.53591225	3.57377131	6.49092753
O	3.51964390	4.83871050	2.85528080
O	1.73847493	2.67446861	1.55941282
O	1.85650084	1.07963985	3.98543986
O	3.55411917	3.14003017	5.29963455
O	2.79474807	6.02035049	5.49710828
O	-0.70902894	1.62637481	2.71469829
O	0.89244498	2.44414887	6.45823527
O	-1.26988249	4.54244999	2.42909473
O	-1.62929072	3.21958099	5.07720748
O	0.04003572	5.29790451	6.40086592
H	5.49646370	5.22850484	4.90272614
H	2.82925499	4.93667426	-0.05765665
O	1.17084837	-0.05980361	1.54398269
H	3.08204941	0.58602340	6.52975433
H	0.90607354	8.04059082	6.29645819
H	-3.38318905	2.65692887	2.87435343
H	-1.40117816	3.34609829	7.94432340
O	0.44004745	6.69569676	3.80206207
H	-0.42575602	7.00460655	0.96479515

Figure S15

Ti	-1.78288125	0.91950806	-0.70588723
W	-0.93300251	3.89222084	1.11823912
O	-1.92667644	2.48535628	0.22627863
O	-0.17448038	0.26294044	-0.09592954
Ti	1.20565395	1.28153014	0.54933855
O	0.33676141	2.53228265	1.59696087
Ti	-1.01668909	2.51515928	-3.73442093
V	-0.85984829	5.31247484	-1.99177885
O	-1.55525083	4.20909512	-3.22216658
O	0.82028252	2.56105845	-3.60762449
Ti	1.82962172	3.36210558	-2.30729772
O	0.88537691	4.88629264	-1.80134336
O	-1.55475514	4.99142512	-0.38304711
O	1.86334757	2.26846277	-0.84704577
O	3.53598061	3.70448718	-2.80715849
O	2.54130401	0.35861212	1.35907053
O	-1.60762702	1.34657777	-2.47814063
O	-3.18746011	-0.20724824	-0.47645908
O	-1.67387427	1.99991148	-5.35058150
O	-1.88710873	4.22964995	2.50310567
O	-1.06563574	6.84813041	-2.40748180
Ti	5.22655129	3.08743015	-2.37337754
Ti	4.37978288	0.20786264	1.24476601
Ti	-4.45206351	-1.20156545	-1.37468834
Ti	-2.87511491	0.74235039	-5.96177137
O	5.61908936	3.69679485	-0.64163768
O	6.44382960	3.72998745	-3.56768035
O	5.20750872	1.31202111	-2.30051011
O	4.76829044	-0.55662834	-0.42553122

O	4.99937335	-0.84063454	2.60144326
O	5.11358727	1.82827592	1.23158787
O	-4.19857406	-0.94770404	-3.17253025
O	-6.09514651	-0.62726407	-0.85334464
O	-4.19140677	-2.97830929	-1.03584953
O	-4.50306358	1.07530283	-5.12141075
O	-2.39694437	-0.91487512	-5.40002123
O	-2.98912309	0.77591948	-7.77932237
H	6.23150917	4.41163908	-0.40069182
H	7.09083671	3.28249668	-4.13810344
H	5.06042031	0.55019434	-1.66642599
H	4.98346079	-1.48427741	-0.61708488
H	5.66996193	-0.68141925	3.28649804
H	5.32724477	2.57695325	0.60274505
H	-4.51358358	-0.20251794	-3.74060167
H	-6.44443220	0.02317158	-0.22405568
H	-4.63587464	-3.59376244	-0.43025481
H	-5.36387521	1.29330580	-5.51503269
H	-2.80532723	-1.26530652	-4.57248953
H	-2.71858576	1.43240635	-8.44232742
O	0.46849459	5.19792385	1.28654707
H	1.05757678	5.44436074	0.54779955

Figure S16: Vanadyl bond protonation

H	23.1791	-4.57999	-5.10269
H	0.943124	-1.89225	-6.93684
H	21.76388	-1.89225	-6.93684
H	18.9225	4.733626	-7.33461
H	3.7845	-12.3026	-7.33461
H	11.3535	4.733626	-7.33461
H	21.76388	-9.46125	-6.93684
H	0.943124	1.89225	-6.93684
H	10.20431	3.519939	-3.12989
H	23.34543	-2.24973	-4.3665
H	6.71147	2.955999	-2.99317
H	21.76048	1.972793	-6.93671
H	21.76388	-5.67675	-6.93684
H	7.531089	-12.3019	-7.33474
H	23.12775	-7.78353	-4.98203
H	10.1537	-11.0845	-3.08061
H	18.04291	2.870881	-3.0415
H	0.943124	-9.46125	-6.93684
H	18.03517	-10.4364	-3.03769
H	11.34876	-12.3026	-7.33474
H	7.569	4.733626	-7.33461
H	6.731227	-10.5122	-2.99917
H	15.10556	-12.3021	-7.33474
H	0.943124	-5.67675	-6.93684
H	2.908039	-5.34588	-4.86829
H	2.89667	-2.1956	-4.87541
H	21.63883	-10.3371	-2.87882
H	2.989876	-9.05116	-4.76309
H	2.990435	1.493442	-4.76079
H	14.20965	3.370452	-3.10849
H	18.97683	-12.3011	-7.33474
H	21.66984	2.753195	-2.88494
H	23.02376	0.094008	-5.13539
H	15.138	4.733626	-7.33461
H	3.7845	4.733626	-7.33461
H	14.24542	-10.9181	-3.11747
O	17.03025	-5.67675	-6.7367
V	11.36719	-3.79692	-2.76011
Ti	17.02864	-5.50478	-4.80588
Ti	11.3535	-1.89225	-7.13573
Ti	3.7845	-9.46125	-7.13573
Ti	5.750566	-5.50992	-4.79731
Ti	11.3535	1.89225	-7.13573
Ti	17.05681	1.390943	-4.75064
Ti	18.9225	1.89225	-7.13573
Ti	17.05575	-8.96043	-4.75298
Ti	9.5045	-5.94823	-4.70858
Ti	7.569	1.89225	-7.13573
Ti	9.507385	-1.62649	-4.71418
Ti	15.138	1.89225	-7.13573
Ti	18.9225	-5.67675	-7.13573
Ti	13.26103	-9.32865	-4.7617
Ti	7.569	-9.46125	-7.13573
Ti	5.74267	-8.9773	-4.68545
Ti	11.3535	-9.46125	-7.13573
Ti	17.01813	-2.06132	-4.80402
Ti	20.87386	1.233107	-4.69557
Ti	3.7845	-5.67675	-7.13573
Ti	18.9225	-9.46125	-7.13573
Ti	15.138	-1.89225	-7.13573
Ti	3.7845	-1.89225	-7.13573
Ti	13.26383	1.759477	-4.75914
Ti	9.455888	-9.33112	-4.76006
Ti	18.9225	-1.89225	-7.13573
Ti	3.7845	1.89225	-7.13573
Ti	20.87196	-5.46189	-4.70369
Ti	9.45856	1.755948	-4.76219
Ti	15.138	-9.46125	-7.13573
Ti	11.3535	-5.67675	-7.13573
Ti	13.23049	-1.61901	-4.71247
Ti	20.83742	-2.09846	-4.71021
Ti	7.569	-5.67675	-7.13573
Ti	5.744373	1.406523	-4.68432
Ti	7.569	-1.89225	-7.13573
Ti	13.22995	-5.94338	-4.71262
Ti	5.746934	-2.06287	-4.79918
Ti	20.87356	-8.81559	-4.70217
Ti	15.138	-5.67675	-7.13573
O	17.0407	-7.23111	-4.11425
O	5.67675	-1.89225	-6.7367
O	15.10164	-5.54625	-5.15954
O	22.68663	-8.64354	-5.13142
O	11.35956	-1.68791	-5.26225
O	18.94539	-5.49938	-5.24713
O	9.413129	3.060486	-3.46524
O	11.3535	-11.3535	-7.53476
O	5.67675	-5.67675	-6.7367
O	3.7845	-11.3535	-7.53476

O	9.46125	-1.89225	-6.7367
O	17.15881	-10.1567	-3.36648
O	7.569	-11.3535	-7.53476
O	15.138	-7.569	-7.53476
O	13.24575	-5.67675	-6.7367
O	18.9225	-11.3535	-7.53476
O	13.38654	-10.6488	-3.49406
O	18.94937	1.555051	-5.22488
O	20.84253	-10.0957	-3.38397
O	13.24575	-9.46125	-6.7367
O	17.03025	-1.89225	-6.7367
O	11.36495	-5.87038	-5.25871
O	5.773239	-0.3262	-4.10053
O	17.03025	1.89225	-6.7367
O	17.03025	-9.46125	-6.7367
O	10.05064	-4.99977	-3.25308
O	15.10455	-2.01542	-5.16238
O	22.744	-5.44934	-5.01331
O	13.35994	3.092959	-3.49895
O	18.95001	-9.13272-	5.22476
O	22.74371	-2.06086-	5.10876
O	20.69761	-0.44945	-3.92041
O	11.3535	3.7845	-7.53476
O	3.7845	-7.569	-7.53476
O	10.09611	-2.57358	-3.24264
O	20.81475	-5.67675	-6.7367
O	12.67964	-2.58398	-3.28031
O	3.7845	-3.7845	-7.53476
O	13.30716	0.072172	-4.08032
O	11.3535	0	-7.53476
O	15.138	-3.7845	-7.53476
O	22.67541	1.011962	-5.12084
O	17.0352	-3.7806	-4.07024
O	9.46125	-5.67675	-6.7367
O	18.9225	-3.7845	-7.53476
O	17.16586	2.588476	-3.36552
O	3.7845	0	-7.53476
O	20.81475	1.89225	-6.7367
O	3.810866	-1.9745	-5.1313
O	9.46125	1.89225	-6.7367
O	1.89225	-1.89225	-6.7367
O	7.569	3.7845	-7.53476
O	3.813121	-5.59263	-5.13197
O	1.89225	-5.67675	-6.7367
O	15.17488	1.763548	-5.18654
O	9.435915	-7.64042	-4.09002
O	7.637307	-5.53668	-5.15151
O	20.87392	2.536189	-3.40181
O	11.37289	-3.78381	-0.98774
O	5.893627	-10.0641	-3.22801
O	7.578047	1.782527	-5.19302
O	9.423696	0.057136	-4.09102
O	11.3535	-3.7845	-7.53476
O	3.863403	-9.30748	-5.11272
O	11.3535	-7.569	-7.53476
O	7.576457	-9.34271	-5.19525
O	20.72835	-7.12597	-3.95457
O	5.67675	-9.46125	-6.7367
O	15.138	0	-7.53476
O	3.7845	3.7845	-7.53476
O	9.378584	-10.6413	-3.4697
O	3.865646	1.740449	-5.11296
O	7.569	-7.569	-7.53476
O	1.89225	1.89225	-6.7367
O	17.03767	-0.33638	-4.10893
O	7.569	-3.7845	-7.53476
O	20.773	-3.76532	-3.91332
O	1.89225	-9.46125	-6.7367
O	5.719676	-3.7838	-4.06506
O	11.36355	-9.46805	-5.16366
O	5.67675	1.89225	-6.7367
O	11.36119	1.883727	-5.16647
O	15.17496	-9.32703	-5.18913
O	13.31066	-7.6308	-4.09704
O	9.46125	-9.46125	-6.7367
O	18.9225	0	-7.53476
O	5.768761	-7.24392	-4.09807
O	18.9225	-7.569	-7.53476
O	20.81475	-1.89225	-6.7367
O	13.24575	-1.89225	-6.7367
O	15.138	3.7845	-7.53476
O	18.9431	-2.05763	-5.25013
O	18.9225	3.7845	-7.53476
O	13.24575	1.89225	-6.7367
O	20.81475	-9.46125	-6.7367
O	12.65294	-5.00761	-3.23586
O	7.569	0	-7.53476
O	15.138	-11.3535	-7.53476
O	7.640748	-2.04216	-5.14819
O	5.888402	2.480595	-3.21588
H	10.94413	-3.01668	-0.55802

Figure S17: V-W dimer on TiO_2 cluster (large)

TI	2.344860	-0.953508	1.188524
W	-0.163418	-2.569092	-0.844317
O	1.509331	-1.970792	-0.049723
O	0.969765	-0.594922	2.346007
TI	-0.762537	-0.612575	1.813270
O	-0.926137	-2.163727	0.856320
TI	2.530289	1.737843	-0.986229
V	0.650946	-0.020684	-3.045199
O	2.148717	0.726904	-2.480005
O	0.958149	2.597689	-0.619185
TI	-0.717442	1.911285	-0.773194
O	-0.691777	0.932968	-2.355993
O	0.477715	-1.671242	-2.420074
O	-0.966897	0.700282	0.561405
O	-2.034418	3.117104	-0.732810
O	-1.978864	-0.439372	3.139141
O	2.838794	0.595730	0.366817
O	3.798161	-1.722005	1.932752
O	3.982614	2.789558	-1.183815

O	0.115347	-4.237028	-0.969865
O	0.584087	-0.023253	-4.618633
TI	-3.676409	3.446515	0.054767
TI	-3.642797	0.184342	3.554428
TI	5.609476	-1.612306	2.174783
TI	5.737785	2.818944	-0.655004
O	-4.666497	1.922273	-0.146156
O	-4.490432	4.851514	-0.744901
O	-3.448333	3.737866	1.789669
O	-3.518045	1.998851	3.921513
O	-4.293967	-0.695105	4.984571
O	-4.673187	0.016027	2.107928
O	6.204209	-0.069805	1.419003
O	6.356115	-3.053519	1.390445
O	5.989847	-1.531988	3.943119
O	6.491350	1.212941	-1.146393
O	5.859429	2.869081	1.137563
O	6.587774	4.235523	-1.380933
H	-4.759982	5.704935	-0.388705
H	-3.467468	3.188479	2.606542
H	-3.485912	2.381358	4.806187
H	-5.073578	-1.236575	5.146659
H	6.421038	0.108149	0.484393
H	6.012160	-3.815119	0.912904
H	6.268911	-2.212330	4.564767
H	7.159758	1.045794	-1.819813
H	5.941477	2.040057	1.643847
H	6.347633	4.849357	-2.083083
O	-1.893795	-2.382853	-1.560340
TI	-5.181016	0.272302	0.353298
TI	-3.504910	-1.695066	-2.120697
O	-4.321404	-0.934994	-0.680442
O	-3.144421	-0.434094	-3.339680
H	-2.446903	0.240197	-3.305462
O	-4.558165	-2.974189	-2.840951
H	-4.706734	-3.218122	-3.761242
O	-6.971696	0.092431	0.209375
H	-7.656754	0.578405	-0.260655

Figure S18a: V_2W trimer A on TiO_2 cluster 1

TI	-3.595748	1.174615	1.627348
O	-2.215281	2.280027	-1.506030
TI	-1.564280	3.187262	-0.072136
TI	-3.574570	1.082418	-1.702734
O	-2.229078	2.387561	1.397756
O	-4.304174	0.979392	-0.043848
O	-2.939525	-0.426886	2.122843
TI	-2.635200	-2.184795	1.709062
O	-0.815210	-2.572465	-1.385919
TI	0.162420	-2.961228	0.072756
TI	-2.618769	-2.275177	-1.619850
O	-0.858276	-2.507759	1.512438
O	-3.321382	-2.473845	0.050082
O	-2.921159	-0.572419	-2.126086
O	-4.779975	1.608239	-2.935262
H	-5.271558	2.415558	-3.117372
O	-4.826379	1.802216	2.786175
H	-5.255701	1.451327	3.573258
O	-3.396416	-3.257107	2.941940
H	-3.253751	-4.159696	3.244930
O	-3.321971	-3.472291	-2.769681
H	-3.897283	-3.420278	-3.539794
O	1.732465	-1.985274	0.052759
O	0.283992	3.083211	-0.025037
V	1.931706	3.660471	0.043642
O	-2.109958	4.898752	-0.172593
H	-2.231809	5.616484	0.457932
O	0.513877	-4.723159	0.138052
H	0.655616	-5.408811	-0.523710
O	3.049652	2.948968	-1.180406
O	2.983302	2.833214	1.254136
O	4.212310	-2.290369	-1.464461
O	3.825137	0.270531	-0.052801
O	2.029539	5.229803	0.128596
O	4.355917	-2.291690	1.308736
O	5.503383	2.518116	0.086826
W	3.557112	-1.598444	-0.039348
V	4.007297	2.041620	0.023879

Figure S18b: V_2W trimer B on TiO_2 cluster 1

TI	-3.206779	1.775688	1.643048
O	-1.583662	2.543121	-1.476160
TI	-0.744499	3.262336	-0.025731
TI	-3.190255	1.720278	-1.682279
O	-1.580685	2.614266	1.430859
O	-3.938189	1.794685	-0.026719
O	-2.975653	0.048937	2.102185
TI	-3.191700	-1.719486	1.682119
O	-1.581744	-2.616398	-1.431475
TI	-0.745286	-3.262401	0.026045
TI	-3.206450	-1.775327	-1.643303
O	-1.584521	-2.541717	1.475280
O	-3.938601	-1.793435	0.026349
O	-2.973436	-0.048504	-2.100884
O	-4.226178	2.530730	-2.917022
H	-4.352347	3.439851	-3.207357
O	-4.242502	2.669272	2.818989
H	-4.783310	2.415932	3.574021
O	-4.227099	-2.531315	2.916396
H	-4.367811	-3.442802	3.192267
O	-4.242964	-2.666970	-2.820005
H	-4.789326	-2.411865	-3.570427
O	1.021726	-2.745631	-0.014177
O	1.022534	2.745977	0.014239
V	2.760368	2.529982	0.021759
V	2.759565	-2.530268	-0.021511
O	-0.899725	5.055401	-0.096525
H	-0.933935	5.760491	0.558405
O	-0.899903	-5.055510	0.098828
H	-0.935785	-5.760638	-0.555981
O	3.362322	1.379642	-1.213733

O	3.348417	1.350460	1.237910
O	3.348055	-1.350862	-1.237752
O	3.361884	-1.380029	1.213882
O	3.553505	3.891020	0.045621
O	3.552304	-3.891529	-0.045265
W	3.957322	-0.000353	-0.000007
O	5.653053	-0.000640	-0.000056

Figure S19a: V2W trimer A on TiO_2 cluster 2

TI	-3.898754	0.135987	0.013624
O	-1.727004	0.636429	0.008768
TI	-1.755526	1.235352	1.740348
TI	-1.765648	1.239394	-1.717838
O	-3.522998	0.896815	1.710251
O	-3.535600	0.910018	-1.687181
TI	-2.135498	-2.923253	0.010301
O	0.401494	-0.588545	0.001564
TI	0.210178	-1.338548	1.659417
TI	0.196726	-1.336174	-1.655512
O	-1.004745	-2.638769	1.446923
O	-1.017244	-2.636913	-1.435459
O	-1.192370	2.954298	-1.451899
O	-0.608241	0.059358	-2.538463
O	-1.184591	2.950726	1.469580
O	-0.589379	0.056242	2.548329
O	1.966056	-1.897087	-1.500543
O	1.978485	-1.899438	1.488458
V	-0.314504	3.523520	0.007519
O	1.280620	2.792168	0.001787
V	2.814676	1.826218	-0.006038
O	-0.220396	5.090851	0.009065
W	2.799135	-1.019142	-0.008541
O	2.870200	0.557958	1.212290
O	2.859042	0.560270	-1.227220
O	4.109630	2.725767	-0.011222
O	4.382453	-1.613365	-0.015923
O	-5.689040	0.138627	-0.040185
H	-6.360932	0.385340	-0.684306
O	-2.828553	-4.577834	0.012208
H	-3.713362	-4.957658	0.036846
O	-3.390091	-1.644564	0.016117

Figure S19b: V2W trimer A on TiO_2 cluster 2

TI	3.503732	1.955969	0.009616
O	0.317724	1.077139	-0.001042
TI	0.734774	1.638574	-1.659085
TI	0.721202	1.649255	1.656947
O	2.416632	2.252983	-1.455130
O	2.403868	2.262682	1.463123
TI	3.601829	-1.586341	0.016377
O	1.444512	-1.078560	0.009266
TI	1.215867	-1.585281	-1.729438
TI	1.206241	-1.574055	1.753027
O	2.934676	-2.098708	-1.702252
O	2.927908	-2.077215	1.729883
O	-0.616527	2.924486	1.544317
O	0.735047	0.019622	2.533432
O	-0.603634	2.914602	-1.566235
O	0.754818	0.004257	-2.526432
O	-0.112643	-2.834400	1.471284
O	-0.105691	-2.843610	-1.452174
V	-1.527191	2.907913	-0.014560
O	-2.606681	1.466657	-0.014473
O	-2.432135	4.183420	-0.022181
O	-2.278150	-1.614629	-0.002260
O	-4.497153	-0.277620	1.388021
O	-4.505984	-0.291075	-1.389492
O	-1.874153	-4.347280	0.010821
O	3.970364	0.216817	0.017496
O	5.181075	-2.428875	-0.038932
H	5.652416	-2.982232	-0.670360
V	-1.116823	-2.975559	0.007767
W	-3.505529	-0.178260	-0.004426
O	4.926803	3.047990	0.011643
H	5.883480	2.941205	0.040896