Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supplementary Information

How TiO_2 facets determine arsenic adsorption and photooxidation: Spectroscopic and DFT study

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Table S1. Summary of Characterization of three TiO_2 NPs.

Sample	HM	JR05	TG01
Crystalline phase	anatase	anatase	anatase
Particle size (nm)			
XRD	4.6	7.5	18.4
BET	4.3	8.6	20.1
TEM	5	7	20
S_{BET} (m^2/g)	336	167	71
Pore volume[a] (cm^3/g)	0.373	0.293	0.383
Mean pore diameter[b] (nm)	4.4	7.0	21.6
Acid concentration (mmol/g)	0.078	0.036	0.043
Exposed {001} facet (%)	4	17	7
pHzpc	5.3	6.5	6.1
As(III) adsorption capacity (mg/g)	136	138	71
As(V) adsorption capacity (mg/g)	140	144	106
As(III) surface coverage (molecules/nm^2)	3.2	6.6	8.0
As(V) surface coverage (molecules/nm^2)	3.3	6.9	12.0
As(III) loading (mol/mol acid)	23.2	51.1	22.0
As(V) loading (mol/mol acid)	23.9	53.3	32.9
As(III) photooxidation rate $k\times10000$ (min^{-1})	60.0	213	225

[a] Single point adsorption total pore volume.

[b] Adsorption average pore diameter (4V/A by BET).

Table S2. Langmuir modeling for As(III) and As(V) adsorbed on three TiO_2.

TiO_2 Samples	As(III)			As(V)		
	q_m (mg/g TiO_2)	K_L (L/mg)	R^2	q_m (mg/g TiO_2)	K_L (L/mg)	R^2
HM	136	0.019	0.967	140	0.005	0.950
JR05	138	0.018	0.969	144	0.012	0.917
TG01	71	0.004	0.979	106	0.003	0.976

1. X-ray diffraction.

The XRD patterns shown in Fig. S1 suggested that all TiO_2 NPs were in pure anatase phase. The XRD patterns of HM (JCPDS No. 21-1272), JR05 (JCPDS No. 21-1272), and TG01 (JCPDS No. 65-5714) indicated the 2θ diffraction positions match the standard anatase pattern. The particle sizes of the three TiO_2 NPs calculated using the Sherrer formula from peak widths in the X-ray diffractograms are reported in Table 1 in the main text.

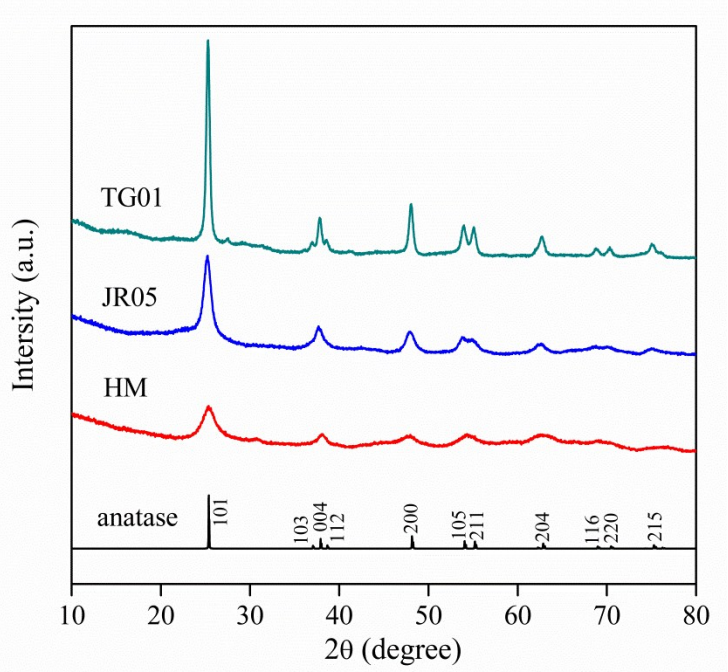

Fig. S1. The XRD patterns of three TiO_2 NPs and calculated diffraction patterns of bulk anatase (black).

2. BET surface area and BJH pore size distributions.

The N_2 adsorption-desorption isotherms and BJH pore size distributions of the three TiO_2 materials are presented in Fig. S2. The corresponding specific surface areas (S_{BET}) determined by N_2 adsorption are listed in Table 1, and total pore volumes and particle sizes derived from BET are summarized in Table S1. The average particle

size derived from BET is given by equation: $D=6000 / (S_{BET} \times \rho)$, where ρ is true density (4.2 g/mL for titania).[1] The particle sizes obtained from BET show no significant difference from those derived from XRD. All TiO_2 materials exhibited N_2 adsorption-desorption isotherms of type IV according to IUPAC classification (Fig. S2a).[2] Hysteresis loops at $P/P_0>0.5$ were observed for all TiO_2 samples, which indicate a high density of mesopores in these three materials. Fig. S2b shows that HM and JR05 have a narrow pore size distribution ranging from 3 to 8 nm with the peak located at *ca.*4 nm, and TG01 has a broad pore size distribution ranging from 5 to 35 nm with the peak resolved at *ca.*18 nm. Both the specific surface area and total pore volume of HM were larger than those of JR05, which can be attributable to the smaller particle size of HM (4.6 nm) than JR05 (7.5 nm).

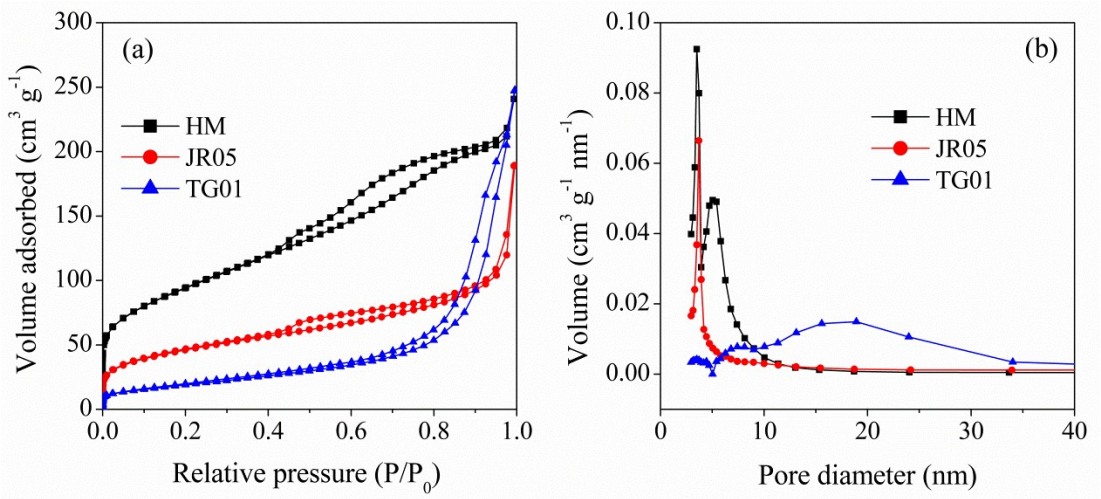

Fig. S2. (a) N_2 adsorption-desorption isotherms and (b) BJH pore size distribution curves of three TiO_2 NPs.

3. SEM and TEM analysis.

The SEM and TEM images of the three TiO_2 NPs are presented in Fig. S3. The SEM and TEM images demonstrate that the particle size of HM is about 5 nm (Fig.

S3a-c), and the measured lattice spacing of 3.5 Å indicates the presence of {101} facets.[3] JR05 exhibited a particle size of about 7 nm with two sets of lattice spacing of 3.5 and 1.9 Å, corresponding to {101} and {001} facets,[4, 5] respectively (Fig. S3d-f). The SEM (Fig. S3g) and TEM (Fig. S3h-i) images of TG01 suggest that the material exposed {101} facets and the average particle size is about 20 nm.

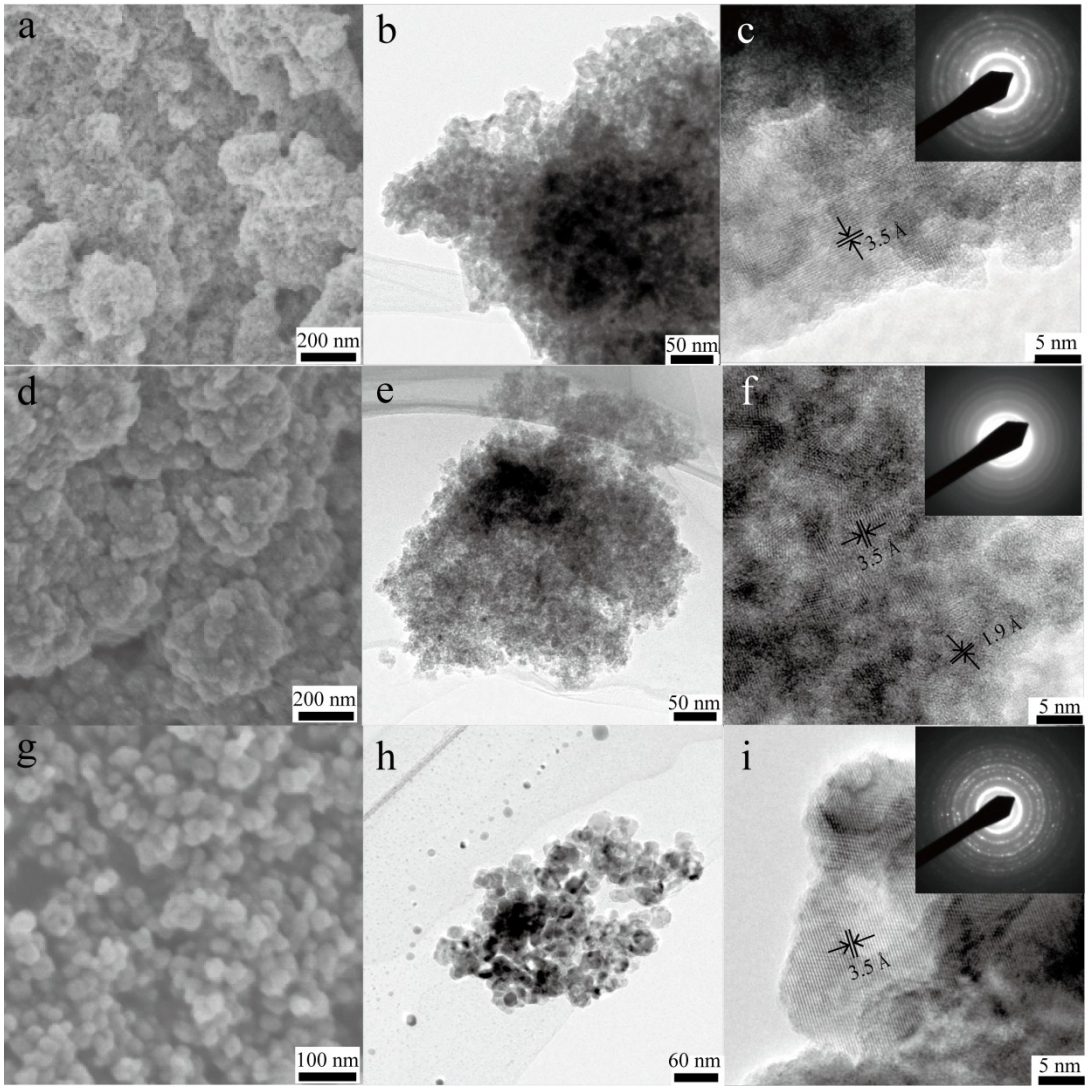

Fig. S3. FE-SEM and TEM images of three TiO_2.

4. X-ray photoelectron spectroscopy (XPS).

XPS was used to inspect the surface composition and chemical states of TiO_2. The XPS spectra of three TiO_2 NPs exhibited prominent peaks of C, Ti, and O (Fig. S4). The XPS spectra of the Ti 2p core level region of all samples are shown in Fig. S4b. The two peaks at about 458.9 and 464.5 eV could be assigned to the Ti $2p_{3/2}$ and $Ti2p_{1/2}$ spin orbital splitting photoelectrons in the Ti^{4+} chemical state, respectively. The primary peak at 530.0 eV in O 1s spectra (Fig. S4c) of the samples was assigned to Ti-O-Ti (lattice O).[6]

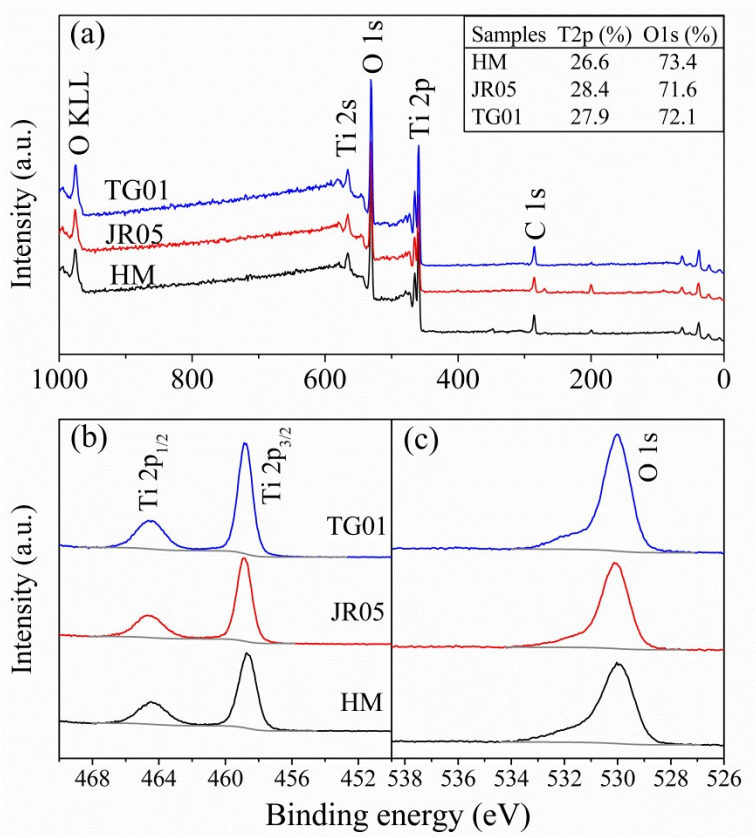

Fig. S4. XPS spectra of the three TiO_2 samples (a) with the inset showing their surface components, and of the core levels of Ti 2p (b), O 1s (1c).

5. Surface acid site determination.

FTIR spectroscopy of chemisorbed pyridine was performed to characterize the nature of the surface acid sites (Brønsted and Lewis).[7] Pyridine adsorbed on Brønsted acid sites exhibits characteristic IR bands around 1540 and 1635 cm^{-1}, whereas the band at 1445 cm^{-1} is assigned to pyridine coordinated with Lewis acid sites, which suggests that unsaturated Ti^{4+} sites are present on the TiO_2 surface. FTIR spectra of pyridine adsorption on the three TiO_2 NPs shown in Fig. S5a indicated that only Lewis acid sites existed on the TiO_2 surface.

The total amount of acid sites and the acid strength were determined with the NH_3-TPD technique.[8] The NH_3-TPD profiles were acquired by Quantachrome TPRWinV3.51 (ChemBET Pulsar TPR/TPD, Quantachrome Instruments, U.S.). About 50 mg of sample was heated at 550 °C with a He gas flow (60 mL/min) for 1 h to remove water vapor and impurities. After being cooled to ambient temperature, the sample was exposed to a flow of NH_3 gas at 60 mL/min for 1 h. After the saturation of NH_3 adsorption, the sample was heated to 100°C in a flow of He (60 mL/min) and maintained at 100 °C for 1 h in order to desorb all physi-sorbed species. Then, the temperature was increased to 800 °C at a ramp rate of 10 °C/min.

The integrated area under the desorption peak of the NH_3-TPD profile gives the acid site concentration (mmol/g), which corresponds to the amount of NH_3 bound to the acid sites on TiO_2 surfaces. Moreover, the desorption temperature indicates the acid strength of the sites on the samples. The higher the temperature of desorption, the stronger the acidity, which leads to a higher affinity toward the reacting molecules.[9]

The NH_3-TPD profiles of the three TiO_2 NPs are shown in Fig. 2, and the acid concentration is given in Table 1 in the main text. A broad TPD profile was observed for HM and TG01 with a NH_3 desorption peak at about 340 °C, which indicated a homogenous distribution of acid sites on the surface. In contrast, JR05 exhibited two distinct desorption peaks at 290 °C and 410 °C, which indicated that acid sites with different strength are heterogeneously distributed on the JR05 surface.

6. Model Building.

Anatase {001} and {101} facets were cleaved from the optimized bulk structure, six layers of atoms were extracted, and then a 4× 2 supercell was built. A vacuum slab of 15 Å was added to separate each slab in the direction along the surface normal.[10] All atoms were relaxed during the optimization. After NH_3, H_3AsO_3, and $H_2AsO_4^-$ molecules were individually geometry optimized in a periodic box of 10 Å side-lengths, they were added to the optimized anatase {001} and {101} facets to build the initial interfacial structure. Previous study indicates that TiO_2 is a heterogeneous catalyst with water-tolerant Lewis acid sites,[11] which implies that TiO_2 maintain their Lewis acidity even in water environment because water does not deactivate the Lewis acid sites. Therefore, DFT calculations of NH_3 and As adsorption on Ti_{5c} Lewis acid sites from different facets were performed without addition of water molecules to compromise the computational consumption.

The adsorption energy, E_{ads} in eV, for each NH_3/As-TiO_2 surface complex was calculated according to the following equation:[12]

$$E_{ads} = E_{NH3/As+surf} - (E_{surf} + E_{NH3/As})$$

where $E_{NH3/As+surf}$ is the total energy of the surface complexes, and E_{surf} and $E_{NH3/As}$ represent the energy of anatase facets and NH_3 or As, respectively.

To investigate the surface distortion effect on electron transfer from subsurface Ti_{6c} sites to surface Ti_{5c} sites, the energy obtained from surface distortion upon adsorption was calculated by subtracting the original surface energy from the energy of distorted surface.

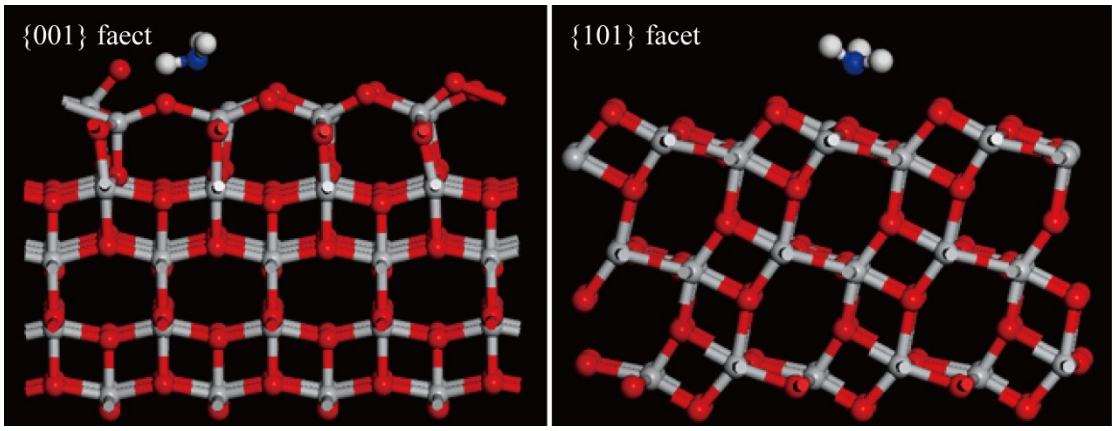

Fig. S5. Final NH_3 adsorption configurations on TiO_2 {001} and {101} facets. Ti: grey, O: red, N: blue, H: white.

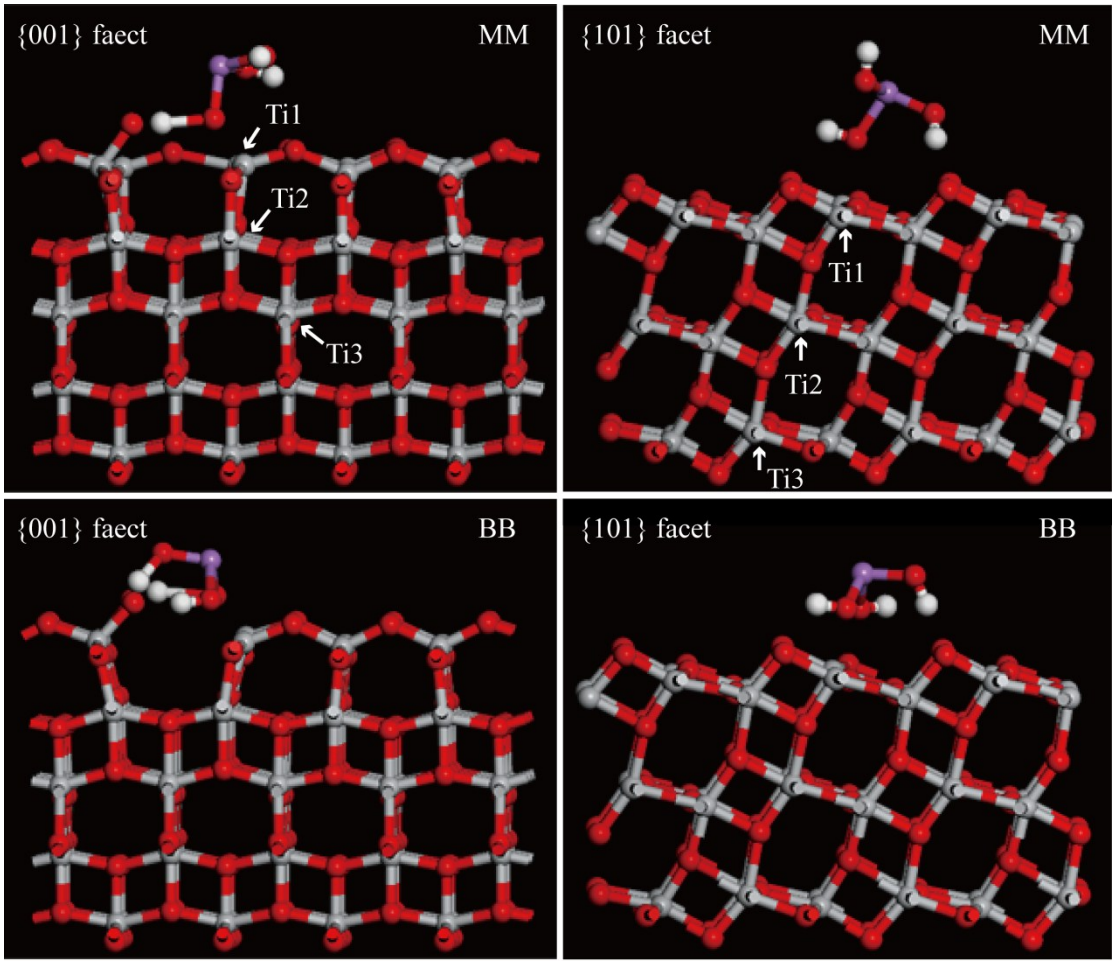

Fig. S6. Final As(III) adsorption configurations on TiO_2 {001} and {101} facets. Ti: grey, O: red, As: purple, H: white. The Ti1, Ti2, and Ti3 represented Ti atoms in the different atomic layers from surface to bulk region

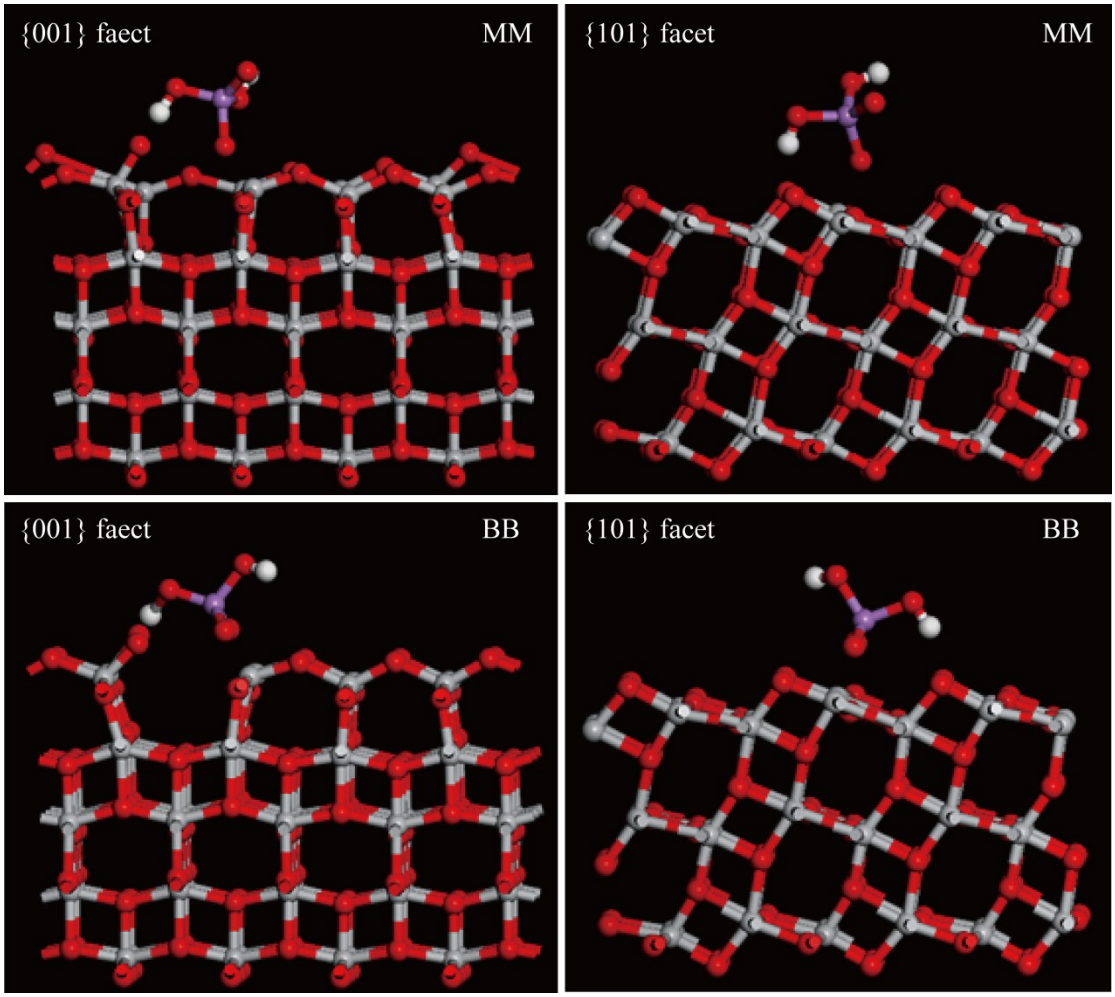

Fig. S7. Final As(V) adsorption configurations on TiO_2 {001} and {101} facets. Ti: grey, O: red, As: purple, H: white.

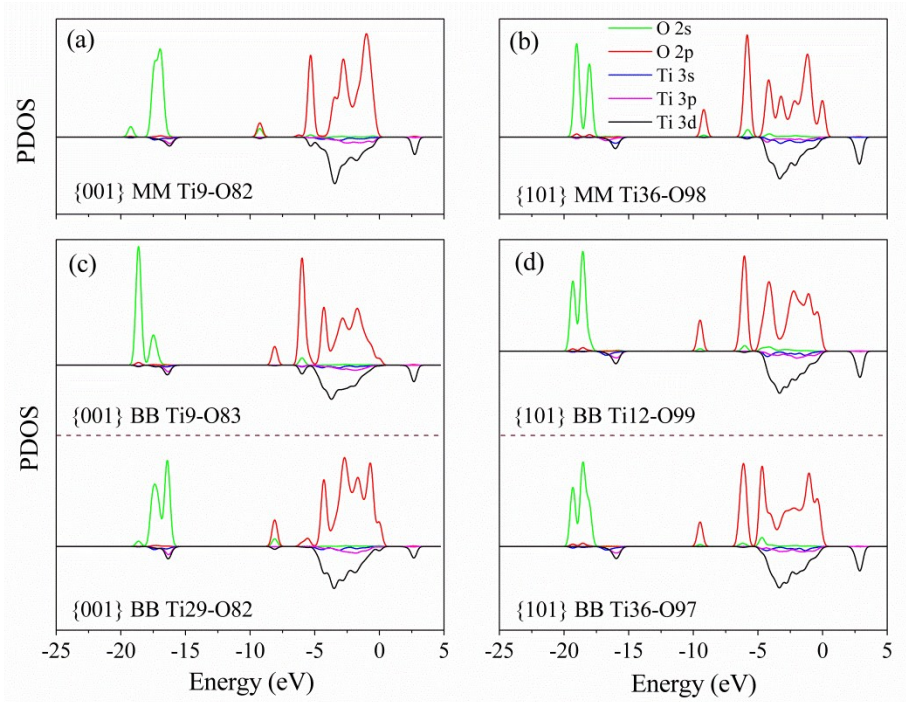

Fig. S8. PDOS analysis for As(III) adsorption configurations on TiO_2. (a) MM complex on {001} facet, (b) MM complex on {101} facet, (c) BB complex on {001} facet, (d) BB complex on {101} facet.

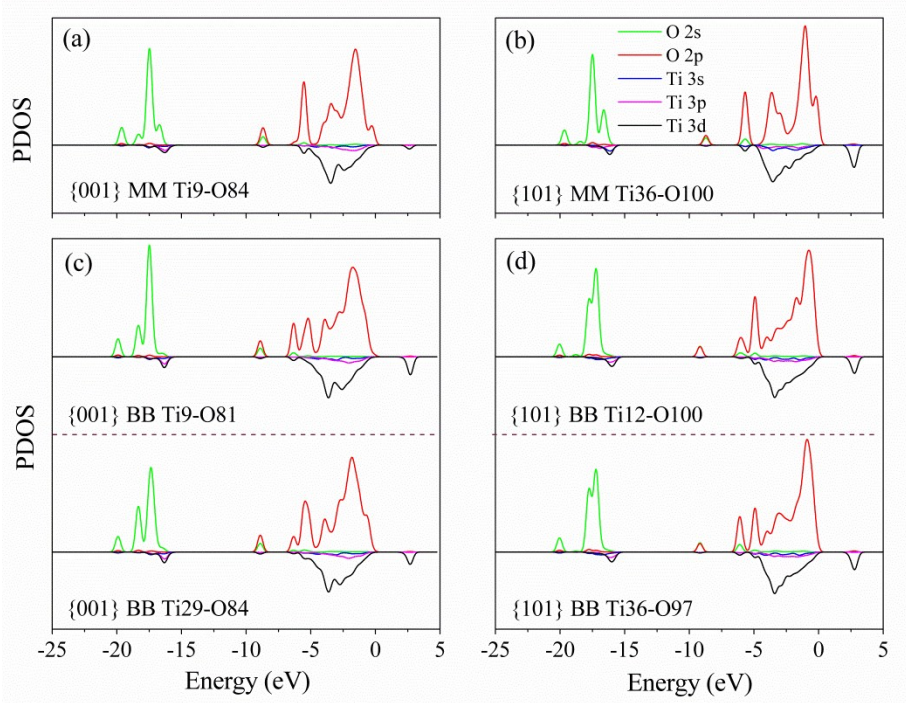

Fig. S9. PDOS analysis for As(V) adsorption configurations on TiO_2. (a) MM complex on {001} facet, (b) MM complex on {101} facet, (c) BB complex on {001} facet, (d) BB complex on {101} facet.

7. Raman analysis.

Raman measurements were performed on a Horiba JY HR800 Raman spectrometer (LabRAM HR Evolution, France) with exciting wavelength at 633 nm. Raman spectra of the three TiO_2 NPs are shown in Fig. 4a in the main text. All samples showed the characteristic peaks of TiO_2 at 144 (E_g), 397 (B_{1g}), 516 (A_{1g}), 639 cm^{-1} (E_g).[13, 14] The percentage of exposed anatase TiO_2 facets has a relationship with the intensity variations of the Raman vibrational mode E_g peak and A_{1g} peak according to a previous study.[15] Therefore, the percentage of exposed {001} facets in anatase TiO_2 can be quantitatively obtained by measuring the peak intensity ratio of the E_g and A_{1g} peaks at 144 and 514 cm^{-1}, respectively. Raman spectra measured at three different spots on each sample were averaged to quantify the peak intensity in this study. The percentage of exposed {001} facets is 4%, 17%, and 7% for HM, JR05, and TG01, respectively, as calculated in Table S3.

Table S3. Peak intensity and the ratio of the Raman vibrational modes between E_g and A_{1g}.

TiO_2 Samples	Peak intensity of E_g (144 cm^{-1})	Peak intensity of A_{1g} (514 cm^{-1})	Percentage of {001}
HM	14678.7	550.7	4%
JR05	7923.5	1358.5	17%
TG01	38333.0	2663.0	7%

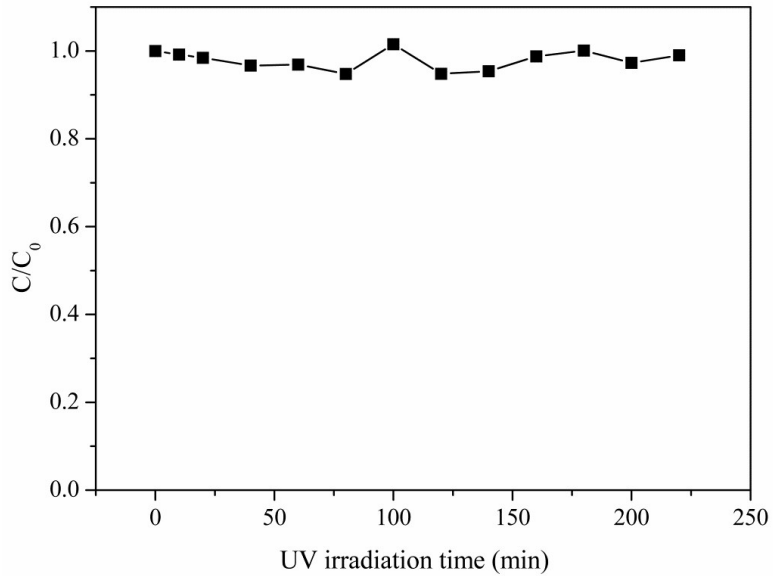

Fig. S10. As(III) oxidation kinetics in the absence of TiO_2. Initial As(III) concentration was 14 mg/L; pH=7.

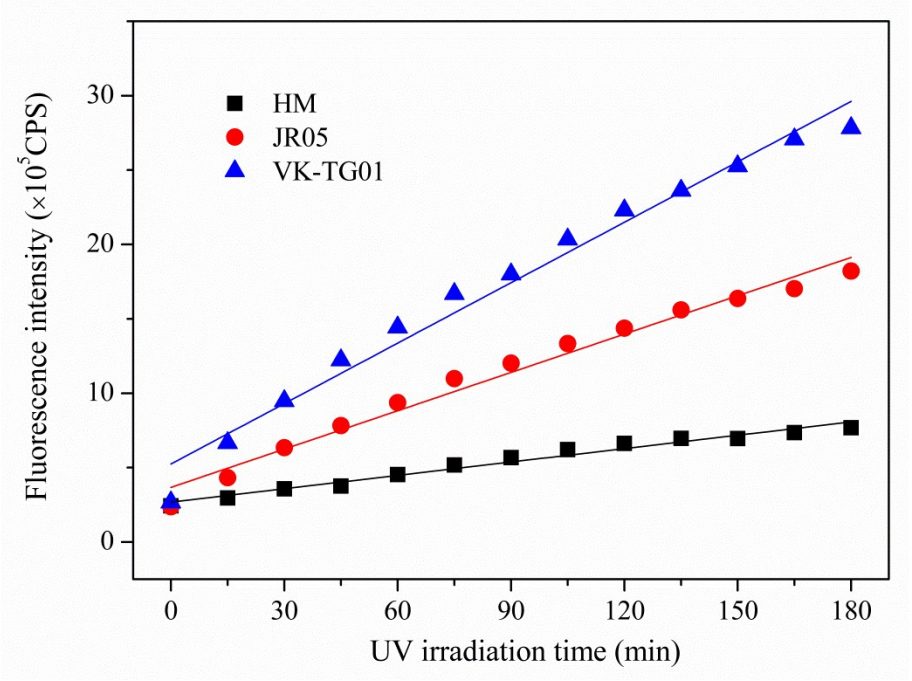

Fig. S11. Time dependence of the fluorescence intensity at 426 nm for three TiO_2 NPs.

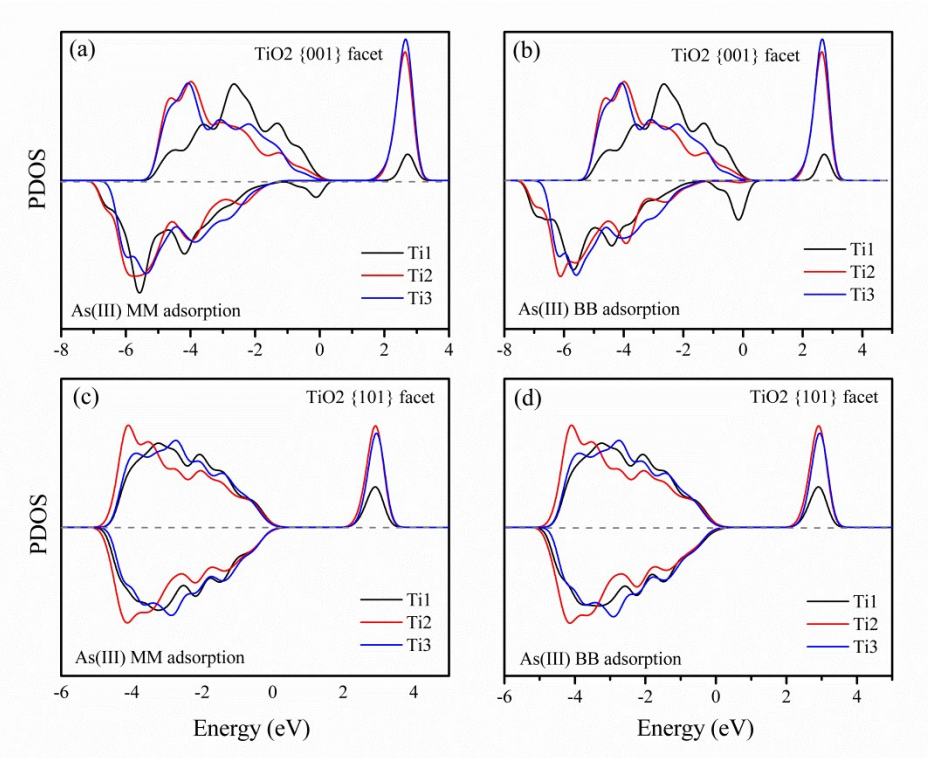

Fig. S12. PDOS for Ti atoms on {001} facets (a, b) and {101} facets (c, d) on the virgin surface (top half in each panel) and on the distorted surface upon As(III) adsorption (bottom half) in the first (Ti1), second (Ti2), and third (Ti3) atomic layers from surface to bulk (Fig. S6). Both MM (a, c) and BB (b, d) surface configurations are present.

References

1 K. J. A. Raj and B. Viswanathan, *Indian J. Chem. A*, 2009, **48**, 1378-1382.

2 S. Brunauer, L. S. Deming, W. E. Deming and E. Teller, *J. Am. Chem. Soc.*, 1940, **62**, 1723-1732.

3 N. Roy, Y. Sohn and D. Pradhan, *ACS Nano*, 2013, **7**, 2532-2540.

4 H. G. Yang, C. H. Sun, S. Z. Qiao, J. Zou, G. Liu, S. C. Smith, H. M. Cheng and G. Q. Lu, *Nature*, 2008, **453**, 638-641.

5 J. Pan, G. Liu, G. Q. M. Lu and H. M. Cheng, *Angew. Chem. Int. Ed.*, 2011, **50**, 2133-2137.

6 C. Hua, F. Chen, T. Lu, C. Lian, S. Zheng, Q. Hu, S. Duo and R. Zhang, *Appl. Surf. Sci.*, 2014, **317**, 648-656.

7 Y. Ma, Q. Xu, X. Zong, D. Wang, G. Wu, X. Wang and C. Li, *Energy Environ. Sci.*, 2012, **5**, 6345-6351.

8 A. Bordoloi and S. B. Halligudi, *Appl. Catal., A: General*, 2010, **379**, 141-147.

9 S. M. Kemdeo, V. S. Sapkal and G. N. Chaudhari, *J. Mol. Catal. A: Chem.*, 2010, **323**, 70-77.

10 L. Yan, S. Hu, J. Duan and C. Jing, *J. Phys. Chem. A*, 2014, **118**, 4759-4765.

11 K. Nakajima, R. Noma, M. Kitano and M. Hara, *J. Phys. Chem. C*, 2013, **117**, 16028-16033.

12 Y.N. Guo, X. Lu, H.P. Zhang, J. Weng, F. Watari and Y. Leng, *J. Phys. Chem. C*, 2011, **115**, 18572-18581.

13 T. Ohsaka, F. Izumi and Y. Fujiki, *J. Raman Spectrosc.*, 1978, **7**, 321-324.

14 Z. Xu and X. Meng, *J. Hazard. Mater.*, 2009, **168**, 747-752.

15 F. Tian, Y. Zhang, J. Zhang and C. Pan, *J. Phys. Chem. C*, 2012, **116**, 7515-7519.

Detail of DFT calculations.

Table S4. DFT calculated adsorption energies.

Molecule	Structure	$E_{mole+surf}^{*}$ (eV)	E_{surf}^{*} (eV)	E_{mole}^{*} (eV)	E_{ads} (eV)
NH_3	NH_3-{001}	-99567.89	-99246.10	-319.35	-2.43
	NH_3-{101}	-119422.78	-119102.29	-319.35	-1.14
H_3AsO_3	H_3AsO_3-{001}MM	-100778.89	-99246.10	-1530.30	-2.48
	H_3AsO_3-{001}BB	-100780.65	-99246.10	-1530.30	-4.24
	H_3AsO_3-{101}MM	-120633.21	-119102.29	-1530.30	-0.61
	H_3AsO_3-{101}BB	-120633.47	-119102.29	-1530.30	-0.88
H_2AsO_4	H_2AsO_4-{001}MM	-101196.01	-99246.10	-1947.41	-2.50
	H_2AsO_4-{001}BB	-101197.69	-99246.10	-1947.41	-4.18
	H_2AsO_4-{101}MM	-121050.33	-119102.29	-1947.41	-0.64
	H_2AsO_4-{101}BB	-121050.98	-119102.29	-1947.41	-1.29
O_2	O_2-{001}	-100113.78	-99246.10	-865.20	-2.48
	O_2-{101}	-119969.28	-119102.29	-865.20	-1.79

*: The absolute energies obtained directly from the computational output files.

Table S5. DFT calculated energy for surface distortion.

Structure	Surface	Original surface energy* (eV)	Distorted surface energy* (eV)	Energy for surface distortion (eV)
O2 adsorption	{001}	-99246.10	-99245.18	0.92
	{101}	-119102.29	-119101.49	0.80
As(III) adsorption	{001}	-99246.10	-99244.84	1.27
MM	{101}	-119102.29	-119102.10	0.19
As(III) adsorption	{001}	-99246.10	-99242.68	3.42
BB	{101}	-119102.29	-119101.86	0.43

*: The absolute energies obtained directly from the computational output files.

The structural parameters for optimized adsorption structures:

NH_3-{001}:

Atom	Number	v	w	x
H	1	-0.7150	-0.2246	-0.5398
H	2	-0.6286	-0.3303	-0.5122
H	3	-0.6301	-0.1124	-0.5132
N	1	-0.6448	-0.2231	-0.5349
O	1	0.1514	-0.0030	-0.0018
O	2	0.1298	0.0454	0.3828
O	3	0.0288	0.2772	0.1912
O	4	0.1511	0.2912	0.0969
O	5	0.0266	0.0319	0.2874
O	6	0.0261	0.0282	0.1303
O	7	0.1745	0.2770	0.3176
O	8	0.0268	0.2484	0.0359
O	9	-0.0630	0.2772	0.4472
O	10	0.1514	0.0257	0.2273
O	11	0.3997	-0.0022	-0.0021
O	12	0.4019	0.0194	0.3806
O	13	0.2739	0.2770	0.1922
O	14	0.4006	0.2905	0.0963
O	15	0.2777	0.0083	0.2880
O	16	0.2757	0.0282	0.1307
O	17	0.4047	0.2769	0.3182
O	18	0.2757	0.2481	0.0364
O	19	0.2846	0.2774	0.4146
O	20	0.3997	0.0292	0.2241
O	21	0.6510	-0.0017	-0.0027
O	22	0.6402	0.0256	0.3750
O	23	0.5249	0.2770	0.1893
O	24	0.6512	0.2906	0.0950
O	25	0.5274	0.0289	0.2830
O	26	0.5262	0.0280	0.1279
O	27	0.6531	0.2769	0.3160
O	28	0.5255	0.2508	0.0345
O	29	0.5180	0.2772	0.4186
O	30	0.6513	0.0266	0.2205
O	31	0.9025	-0.0025	-0.0023
O	32	0.8720	0.0253	0.3770
O	33	0.7782	0.2772	0.1889
O	34	0.9016	0.2910	0.0958
O	35	0.7759	0.0322	0.2824

O	36	0.7764	0.0282	0.1275
O	37	0.9037	0.2768	0.3187
O	38	0.7766	0.2510	0.0341
O	39	0.7399	0.2769	0.4254
O	40	0.9028	0.0266	0.2231
O	41	0.1514	0.4966	-0.0018
O	42	0.1298	0.5086	0.3829
O	43	0.0288	0.7772	0.1914
O	44	0.1512	0.7910	0.0967
O	45	0.0266	0.5214	0.2874
O	46	0.0260	0.5282	0.1303
O	47	0.1485	0.7769	0.3250
O	48	0.0268	0.7486	0.0359
O	49	-0.0101	0.7769	0.4227
O	50	0.1514	0.5292	0.2273
O	51	0.3997	0.4972	-0.0020
O	52	0.4020	0.5344	0.3805
O	53	0.2749	0.7770	0.1910
O	54	0.4006	0.7909	0.0960
O	55	0.2777	0.5452	0.2880
O	56	0.2758	0.5278	0.1307
O	57	0.4168	0.7770	0.3174
O	58	0.2757	0.7481	0.0360
O	59	0.1796	0.7770	0.4529
O	60	0.3997	0.5255	0.2241
O	61	0.6510	0.4986	-0.0027
O	62	0.6403	0.5284	0.3750
O	63	0.5239	0.7771	0.1895
O	64	0.6511	0.7906	0.0952
O	65	0.5274	0.5246	0.2830
O	66	0.5262	0.5281	0.1279
O	67	0.6599	0.7769	0.3148
O	68	0.5255	0.7508	0.0345
O	69	0.5377	0.7770	0.4198
O	70	0.6513	0.5283	0.2205
O	71	0.9025	0.4977	-0.0023
O	72	0.8717	0.5284	0.3769
O	73	0.7780	0.7772	0.1892
O	74	0.9017	0.7909	0.0959
O	75	0.7759	0.5212	0.2824
O	76	0.7763	0.5283	0.1276
O	77	0.9038	0.7768	0.3184
O	78	0.7766	0.7511	0.0343
O	79	0.7618	0.7772	0.4197

O	80	0.9028	0.5285	0.2231
Ti	1	0.1477	0.0189	0.3047
Ti	2	0.0262	0.2724	0.1128
Ti	3	0.1512	0.2804	0.0212
Ti	4	0.1746	0.2771	0.3894
Ti	5	0.0256	0.0272	0.2082
Ti	6	0.3999	0.0210	0.3005
Ti	7	0.2760	0.2723	0.1131
Ti	8	0.4003	0.2808	0.0207
Ti	9	0.4074	0.2769	0.3915
Ti	10	0.2748	0.0261	0.2084
Ti	11	0.6507	0.0290	0.2992
Ti	12	0.5261	0.2722	0.1112
Ti	13	0.6512	0.2817	0.0198
Ti	14	0.6379	0.2770	0.3925
Ti	15	0.5275	0.0273	0.2060
Ti	16	0.8982	0.0337	0.3040
Ti	17	0.7762	0.2724	0.1110
Ti	18	0.9020	0.2812	0.0203
Ti	19	0.8627	0.2768	0.4010
Ti	20	0.7787	0.0270	0.2057
Ti	21	0.1477	0.5348	0.3046
Ti	22	0.0262	0.7724	0.1128
Ti	23	0.1512	0.7807	0.0211
Ti	24	0.1095	0.7770	0.4031
Ti	25	0.0256	0.5268	0.2082
Ti	26	0.3999	0.5329	0.3005
Ti	27	0.2760	0.7723	0.1128
Ti	28	0.4003	0.7812	0.0206
Ti	29	0.4311	0.7768	0.3945
Ti	30	0.2748	0.5275	0.2083
Ti	31	0.6507	0.5249	0.2992
Ti	32	0.5261	0.7722	0.1112
Ti	33	0.6511	0.7817	0.0199
Ti	34	0.6561	0.7770	0.3901
Ti	35	0.5275	0.5268	0.2059
Ti	36	0.8981	0.5197	0.3040
Ti	37	0.7762	0.7724	0.1110
Ti	38	0.9021	0.7811	0.0204
Ti	39	0.8822	0.7768	0.3928
Ti	40	0.7787	0.5273	0.2057

NH_3-{101}:

Atom	Number	v	w	x
H	1	0.4297	0.8721	0.4571
H	2	0.3882	0.6458	0.4652
H	3	0.4644	0.7132	0.4454
N	1	0.4224	0.7403	0.4416
O	1	0.0107	0.3357	0.0566
O	2	0.0840	0.4089	0.2011
O	3	0.1587	0.4837	0.3555
O	4	0.1540	0.4789	0.0990
O	5	0.2300	0.0551	0.2422
O	6	0.0578	0.1322	0.3838
O	7	0.0814	0.1565	0.0296
O	8	0.1567	0.2320	0.1830
O	9	0.2298	0.3046	0.3284
O	10	0.1826	0.0075	0.0007
O	11	0.0103	0.0847	0.1428
O	12	0.0870	0.1625	0.2856
O	13	0.2606	0.3356	0.0566
O	14	0.3347	0.4100	0.2028
O	15	0.4095	0.4818	0.3548
O	16	0.4034	0.4788	0.0987
O	17	0.4805	0.0562	0.2412
O	18	0.3083	0.1337	0.3839
O	19	0.3310	0.1559	0.0291
O	20	0.4062	0.2312	0.1822
O	21	0.4802	0.3052	0.3267
O	22	0.4323	0.0075	0.0004
O	23	0.2608	0.0855	0.1428
O	24	0.3366	0.1609	0.2854
O	25	0.5105	0.3354	0.0558
O	26	0.5843	0.4091	0.2010
O	27	0.6586	0.4838	0.3557
O	28	0.6536	0.4785	0.0988
O	29	0.7301	0.0551	0.2423
O	30	0.5567	0.1297	0.3832
O	31	0.5812	0.1561	0.0292
O	32	0.6568	0.2316	0.1827
O	33	0.7293	0.3044	0.3285
O	34	0.6828	0.0077	0.0006
O	35	0.5106	0.0854	0.1419
O	36	0.5873	0.1620	0.2851
O	37	0.7605	0.3355	0.0564

O	38	0.8341	0.4091	0.2020
O	39	0.9093	0.4844	0.3561
O	40	0.9034	0.4785	0.0992
O	41	0.9802	0.0554	0.2422
O	42	0.8076	0.1327	0.3843
O	43	0.8312	0.1562	0.0295
O	44	0.9064	0.2314	0.1831
O	45	0.9796	0.3046	0.3282
O	46	0.9327	0.0077	0.0010
O	47	0.7605	0.0855	0.1429
O	48	0.8369	0.1619	0.2862
O	49	0.0107	0.8357	0.0563
O	50	0.0846	0.9095	0.2016
O	51	0.1594	0.9844	0.3556
O	52	0.1537	0.9788	0.0990
O	53	0.2299	0.5549	0.2427
O	54	0.0578	0.6335	0.3838
O	55	0.0814	0.6562	0.0296
O	56	0.1567	0.7314	0.1830
O	57	0.2298	0.8051	0.3284
O	58	0.1828	0.5078	0.0010
O	59	0.0103	0.5858	0.1428
O	60	0.0870	0.6612	0.2856
O	61	0.2606	0.8354	0.0566
O	62	0.3347	0.9093	0.2027
O	63	0.4097	0.9875	0.3554
O	64	0.4034	0.9779	0.0987
O	65	0.4806	0.5551	0.2412
O	66	0.3053	0.6306	0.3862
O	67	0.3310	0.6559	0.0290
O	68	0.4067	0.7316	0.1831
O	69	0.4788	0.8040	0.3267
O	70	0.4323	0.5067	0.0004
O	71	0.2610	0.5859	0.1439
O	72	0.3367	0.6621	0.2887
O	73	0.5104	0.8353	0.0556
O	74	0.5842	0.9091	0.2010
O	75	0.6588	0.9839	0.3558
O	76	0.6536	0.9785	0.0988
O	77	0.7299	0.5550	0.2424
O	78	0.5564	0.6346	0.3832
O	79	0.5812	0.6561	0.0291
O	80	0.6567	0.7318	0.1827
O	81	0.7293	0.8043	0.3285

O	82	0.6827	0.5076	0.0006
O	83	0.5106	0.5854	0.1419
O	84	0.5873	0.6621	0.2850
O	85	0.7605	0.8355	0.0564
O	86	0.8341	0.9092	0.2020
O	87	0.9093	0.9843	0.3561
O	88	0.9034	0.9784	0.0992
O	89	0.9802	0.5550	0.2422
O	90	0.8075	0.6326	0.3843
O	91	0.8312	0.6562	0.0294
O	92	0.9063	0.7314	0.1832
O	93	0.9795	0.8045	0.3279
O	94	0.9327	0.5076	0.0010
O	95	0.7605	0.5855	0.1429
O	96	0.8367	0.6618	0.2862
Ti	1	0.1070	0.4319	0.0383
Ti	2	0.1767	0.0018	0.1807
Ti	3	0.2492	0.0741	0.3273
Ti	4	-0.0090	0.0662	0.0576
Ti	5	0.0643	0.1402	0.2041
Ti	6	0.1340	0.2099	0.3464
Ti	7	0.3565	0.4316	0.0379
Ti	8	0.4265	0.0012	0.1800
Ti	9	0.4990	0.0736	0.3256
Ti	10	0.2409	0.0659	0.0573
Ti	11	0.3139	0.1386	0.2041
Ti	12	0.3837	0.2087	0.3458
Ti	13	0.6068	0.4317	0.0380
Ti	14	0.6772	0.0023	0.1806
Ti	15	0.7493	0.0742	0.3277
Ti	16	0.4909	0.0658	0.0569
Ti	17	0.5640	0.1389	0.2031
Ti	18	0.6332	0.2081	0.3463
Ti	19	0.8568	0.4318	0.0383
Ti	20	0.9270	0.0021	0.1809
Ti	21	0.9995	0.0743	0.3273
Ti	22	0.7410	0.0660	0.0574
Ti	23	0.8140	0.1389	0.2044
Ti	24	0.8838	0.2088	0.3470
Ti	25	0.1068	0.9317	0.0382
Ti	26	0.1783	0.5034	0.1806
Ti	27	0.2507	0.5757	0.3279
Ti	28	-0.0090	0.5660	0.0576
Ti	29	0.0643	0.6382	0.2041

Ti	30	0.1340	0.7079	0.3464
Ti	31	0.3565	0.9312	0.0379
Ti	32	0.4264	0.5019	0.1799
Ti	33	0.4988	0.5737	0.3252
Ti	34	0.2410	0.5659	0.0579
Ti	35	0.3144	0.6393	0.2074
Ti	36	0.3850	0.7104	0.3529
Ti	37	0.6069	0.9318	0.0379
Ti	38	0.6771	0.5021	0.1806
Ti	39	0.7492	0.5743	0.3277
Ti	40	0.4910	0.5659	0.0568
Ti	41	0.5640	0.6389	0.2030
Ti	42	0.6330	0.7082	0.3464
Ti	43	0.8568	0.9317	0.0383
Ti	44	0.9270	0.5022	0.1809
Ti	45	0.9995	0.5746	0.3273
Ti	46	0.7410	0.5660	0.0574
Ti	47	0.8139	0.6389	0.2044
Ti	48	0.8836	0.7087	0.3470

H_3AsO_3-{001} MM:

Atom	Number	v	w	x
H	1	0.4666	0.0903	0.5467
H	2	0.2464	0.2736	0.4588
H	3	0.4905	0.5271	0.5177
O	1	0.1514	-0.0031	-0.0005
O	2	0.1323	0.0268	0.3827
O	3	0.0280	0.2773	0.1921
O	4	0.1509	0.2914	0.0981
O	5	0.0248	0.0268	0.2868
O	6	0.0258	0.0283	0.1308
O	7	0.1445	0.2775	0.3236
O	8	0.0261	0.2494	0.0368
O	9	-0.0038	0.2777	0.4212
O	10	0.1515	0.0278	0.2276
O	11	0.3996	-0.0033	-0.0004
O	12	0.4021	0.0316	0.3848
O	13	0.2758	0.2775	0.1932
O	14	0.4000	0.2917	0.0981
O	15	0.2758	0.0365	0.2905
O	16	0.2754	0.0285	0.1327
O	17	0.4097	0.2771	0.3232

O	18	0.2755	0.2478	0.0377
O	19	0.1806	0.2772	0.4575
O	20	0.3992	0.0272	0.2281
O	21	0.6494	-0.0023	-0.0008
O	22	0.6475	0.0285	0.3785
O	23	0.5222	0.2775	0.1924
O	24	0.6499	0.2907	0.0974
O	25	0.5262	0.0273	0.2872
O	26	0.5249	0.0285	0.1311
O	27	0.6577	0.2777	0.3177
O	28	0.5246	0.2491	0.0370
O	29	0.5415	0.2800	0.4221
O	30	0.6491	0.0276	0.2235
O	31	0.9013	-0.0023	-0.0009
O	32	0.8839	0.0280	0.3776
O	33	0.7751	0.2772	0.1908
O	34	0.9008	0.2908	0.0972
O	35	0.7753	0.0243	0.2838
O	36	0.7755	0.0283	0.1290
O	37	0.8985	0.2774	0.3174
O	38	0.7753	0.2507	0.0360
O	39	0.7689	0.2777	0.4199
O	40	0.9011	0.0273	0.2233
O	41	0.1514	0.4970	-0.0005
O	42	0.1322	0.5284	0.3827
O	43	0.0281	0.7772	0.1921
O	44	0.1508	0.7913	0.0982
O	45	0.0248	0.5279	0.2868
O	46	0.0258	0.5283	0.1308
O	47	0.1580	0.7775	0.3214
O	48	0.0261	0.7494	0.0369
O	49	0.0019	0.7777	0.4191
O	50	0.1515	0.5275	0.2276
O	51	0.3996	0.4970	-0.0004
O	52	0.4020	0.5227	0.3845
O	53	0.2756	0.7775	0.1937
O	54	0.4000	0.7914	0.0982
O	55	0.2758	0.5180	0.2905
O	56	0.2754	0.5286	0.1327
O	57	0.4061	0.7772	0.3232
O	58	0.2755	0.7479	0.0379
O	59	0.2656	0.7778	0.4151
O	60	0.3992	0.5281	0.2280
O	61	0.6494	0.4974	-0.0008

O	62	0.6481	0.5273	0.3785
O	63	0.5226	0.7775	0.1923
O	64	0.6499	0.7910	0.0973
O	65	0.5263	0.5277	0.2872
O	66	0.5250	0.5285	0.1311
O	67	0.6560	0.7779	0.3182
O	68	0.5247	0.7492	0.0370
O	69	0.5235	0.7769	0.4181
O	70	0.6492	0.5276	0.2235
O	71	0.9013	0.4976	-0.0009
O	72	0.8839	0.5269	0.3776
O	73	0.7750	0.7771	0.1905
O	74	0.9008	0.7908	0.0972
O	75	0.7754	0.5306	0.2838
O	76	0.7754	0.5281	0.1290
O	77	0.9041	0.7774	0.3177
O	78	0.7753	0.7508	0.0359
O	79	0.7628	0.7779	0.4197
O	80	0.9011	0.5275	0.2232
O	81	0.4754	0.2181	0.5464
O	82	0.3620	0.2786	0.4644
O	83	0.4289	0.5433	0.5284
Ti	1	0.1483	0.0319	0.3062
Ti	2	0.0257	0.2724	0.1137
Ti	3	0.1511	0.2809	0.0224
Ti	4	0.1115	0.2776	0.4013
Ti	5	0.0268	0.0270	0.2089
Ti	6	0.3989	0.0334	0.3064
Ti	7	0.2754	0.2727	0.1149
Ti	8	0.3998	0.2808	0.0225
Ti	9	0.4294	0.2766	0.4035
Ti	10	0.2752	0.0276	0.2105
Ti	11	0.6496	0.0261	0.3014
Ti	12	0.5250	0.2726	0.1140
Ti	13	0.6495	0.2810	0.0219
Ti	14	0.6583	0.2777	0.3926
Ti	15	0.5236	0.0272	0.2092
Ti	16	0.8987	0.0246	0.3016
Ti	17	0.7754	0.2725	0.1124
Ti	18	0.9011	0.2811	0.0218
Ti	19	0.8846	0.2774	0.3921
Ti	20	0.7755	0.0269	0.2070
Ti	21	0.1483	0.5231	0.3062
Ti	22	0.0257	0.7724	0.1137

Ti	23	0.1511	0.7807	0.0225
Ti	24	0.1554	0.7776	0.3958
Ti	25	0.0268	0.5272	0.2089
Ti	26	0.3989	0.5211	0.3063
Ti	27	0.2754	0.7727	0.1150
Ti	28	0.3998	0.7807	0.0225
Ti	29	0.4118	0.7760	0.3969
Ti	30	0.2752	0.5271	0.2106
Ti	31	0.6497	0.5296	0.3014
Ti	32	0.5251	0.7726	0.1139
Ti	33	0.6496	0.7811	0.0219
Ti	34	0.6551	0.7780	0.3943
Ti	35	0.5237	0.5275	0.2092
Ti	36	0.8987	0.5302	0.3016
Ti	37	0.7754	0.7725	0.1124
Ti	38	0.9011	0.7811	0.0218
Ti	39	0.8964	0.7774	0.3947
Ti	40	0.7755	0.5270	0.2070
As	1	0.3750	0.3348	0.5328

H_3AsO_3-{001} BB:

Atom	Number	v	w	x
H	1	0.2021	0.3908	0.4806
H	2	0.2382	0.7527	0.4648
H	3	0.3001	0.2841	0.4520
O	1	0.1520	-0.0003	-0.0008
O	2	0.1178	0.0367	0.3813
O	3	0.0294	0.2803	0.1912
O	4	0.1511	0.2940	0.0978
O	5	0.0238	0.0311	0.2853
O	6	0.0257	0.0312	0.1298
O	7	0.1488	0.2843	0.3243
O	8	0.0265	0.2525	0.0362
O	9	-0.0045	0.2844	0.4238
O	10	0.1520	0.0312	0.2278
O	11	0.3991	-0.0011	-0.0007
O	12	0.4195	0.0240	0.3871
O	13	0.2765	0.2795	0.1938
O	14	0.3999	0.2930	0.0980
O	15	0.2753	0.0306	0.2920
O	16	0.2756	0.0306	0.1332
O	17	0.4063	0.2729	0.3249

O	18	0.2755	0.2497	0.0379
O	19	0.1916	0.2965	0.4522
O	20	0.3990	0.0267	0.2294
O	21	0.6490	-0.0002	-0.0016
O	22	0.6628	0.0272	0.3765
O	23	0.5214	0.2779	0.1919
O	24	0.6499	0.2915	0.0965
O	25	0.5267	0.0240	0.2873
O	26	0.5247	0.0294	0.1308
O	27	0.6544	0.2773	0.3166
O	28	0.5244	0.2506	0.0366
O	29	0.5539	0.2719	0.4230
O	30	0.6488	0.0289	0.2223
O	31	0.9017	0.0005	-0.0016
O	32	0.8857	0.0311	0.3760
O	33	0.7755	0.2787	0.1894
O	34	0.9008	0.2934	0.0963
O	35	0.7757	0.0289	0.2820
O	36	0.7755	0.0299	0.1277
O	37	0.8991	0.2804	0.3166
O	38	0.7754	0.2535	0.0348
O	39	0.7750	0.2791	0.4222
O	40	0.9014	0.0298	0.2215
O	41	0.1519	0.4996	-0.0008
O	42	0.1176	0.5346	0.3814
O	43	0.0294	0.7801	0.1912
O	44	0.1511	0.7941	0.0978
O	45	0.0241	0.5322	0.2854
O	46	0.0259	0.5312	0.1299
O	47	0.1484	0.7842	0.3243
O	48	0.0265	0.7527	0.0361
O	49	-0.0075	0.7835	0.4238
O	50	0.1524	0.5309	0.2281
O	51	0.3993	0.4985	-0.0007
O	52	0.4364	0.5234	0.3804
O	53	0.2760	0.7794	0.1937
O	54	0.3999	0.7932	0.0980
O	55	0.2765	0.5285	0.2922
O	56	0.2755	0.5305	0.1331
O	57	0.4023	0.7760	0.3260
O	58	0.2755	0.7495	0.0378
O	59	0.1795	0.7931	0.4535
O	60	0.3997	0.5293	0.2284
O	61	0.6489	0.4997	-0.0014

O	62	0.6617	0.5268	0.3767
O	63	0.5221	0.7782	0.1916
O	64	0.6498	0.7929	0.0964
O	65	0.5280	0.5292	0.2855
O	66	0.5254	0.5293	0.1301
O	67	0.6553	0.7769	0.3169
O	68	0.5244	0.7515	0.0364
O	69	0.5537	0.7780	0.4239
O	70	0.6499	0.5278	0.2218
O	71	0.9016	0.5006	-0.0016
O	72	0.8858	0.5303	0.3760
O	73	0.7752	0.7790	0.1894
O	74	0.9008	0.7930	0.0962
O	75	0.7759	0.5287	0.2821
O	76	0.7754	0.5300	0.1277
O	77	0.8984	0.7805	0.3166
O	78	0.7753	0.7538	0.0348
O	79	0.7737	0.7786	0.4229
O	80	0.9018	0.5296	0.2215
O	81	0.2546	0.5188	0.5178
O	82	0.3709	0.7134	0.4594
O	83	0.3656	0.3132	0.4564
Ti	1	0.1486	0.0335	0.3070
Ti	2	0.0258	0.2754	0.1129
Ti	3	0.1515	0.2833	0.0221
Ti	4	0.1098	0.2854	0.4008
Ti	5	0.0279	0.0300	0.2080
Ti	6	0.3989	0.0234	0.3073
Ti	7	0.2755	0.2749	0.1150
Ti	8	0.3995	0.2826	0.0222
Ti	9	0.4430	0.2724	0.3991
Ti	10	0.2751	0.0294	0.2109
Ti	11	0.6504	0.0263	0.2997
Ti	12	0.5251	0.2733	0.1133
Ti	13	0.6493	0.2828	0.0211
Ti	14	0.6657	0.2768	0.3920
Ti	15	0.5233	0.0279	0.2088
Ti	16	0.8994	0.0302	0.2997
Ti	17	0.7754	0.2743	0.1112
Ti	18	0.9014	0.2840	0.0209
Ti	19	0.8869	0.2808	0.3924
Ti	20	0.7762	0.0289	0.2056
Ti	21	0.1499	0.5333	0.3069
Ti	22	0.0257	0.7751	0.1129

Ti	23	0.1515	0.7836	0.0221
Ti	24	0.1072	0.7856	0.4002
Ti	25	0.0280	0.5301	0.2081
Ti	26	0.4019	0.5287	0.3065
Ti	27	0.2755	0.7745	0.1151
Ti	28	0.3994	0.7826	0.0222
Ti	29	0.4398	0.7698	0.4034
Ti	30	0.2758	0.5292	0.2111
Ti	31	0.6517	0.5276	0.2997
Ti	32	0.5251	0.7737	0.1132
Ti	33	0.6493	0.7834	0.0210
Ti	34	0.6642	0.7771	0.3927
Ti	35	0.5242	0.5281	0.2082
Ti	36	0.9001	0.5306	0.2997
Ti	37	0.7754	0.7746	0.1112
Ti	38	0.9014	0.7838	0.0209
Ti	39	0.8852	0.7805	0.3924
Ti	40	0.7761	0.5287	0.2054
As	1	0.3623	0.5307	0.5081

H_3AsO_3-{101} MM:

Atom	Number	v	w	x
H	1	0.4301	0.5203	0.5647
H	2	0.3627	0.6651	0.4558
H	3	0.5333	0.7198	0.4447
O	1	0.0086	0.3345	0.0563
O	2	0.0821	0.4082	0.2018
O	3	0.1567	0.4830	0.3562
O	4	0.1519	0.4780	0.0998
O	5	0.2278	0.0539	0.2428
O	6	0.0555	0.1316	0.3841
O	7	0.0794	0.1555	0.0298
O	8	0.1547	0.2313	0.1837
O	9	0.2275	0.3035	0.3290
O	10	0.1809	0.0068	0.0014
O	11	0.0085	0.0844	0.1427
O	12	0.0850	0.1611	0.2860
O	13	0.2586	0.3347	0.0577
O	14	0.3326	0.4094	0.2036
O	15	0.4076	0.4822	0.3537
O	16	0.4013	0.4782	0.0999
O	17	0.4788	0.0558	0.2421

O	18	0.3062	0.1334	0.3844
O	19	0.3290	0.1551	0.0299
O	20	0.4043	0.2308	0.1835
O	21	0.4787	0.3060	0.3276
O	22	0.4303	0.0064	0.0014
O	23	0.2586	0.0850	0.1435
O	24	0.3344	0.1605	0.2861
O	25	0.5085	0.3345	0.0567
O	26	0.5825	0.4084	0.2016
O	27	0.6574	0.4840	0.3561
O	28	0.6516	0.4776	0.0990
O	29	0.7284	0.0545	0.2422
O	30	0.5556	0.1341	0.3836
O	31	0.5790	0.1550	0.0296
O	32	0.6548	0.2309	0.1829
O	33	0.7280	0.3045	0.3282
O	34	0.6804	0.0062	0.0008
O	35	0.5085	0.0843	0.1428
O	36	0.5857	0.1611	0.2856
O	37	0.7584	0.3342	0.0562
O	38	0.8323	0.4082	0.2019
O	39	0.9074	0.4837	0.3562
O	40	0.9015	0.4773	0.0989
O	41	0.9781	0.0544	0.2421
O	42	0.8058	0.1320	0.3842
O	43	0.8292	0.1549	0.0294
O	44	0.9045	0.2305	0.1829
O	45	0.9777	0.3040	0.3281
O	46	0.9306	0.0063	0.0007
O	47	0.7586	0.0845	0.1428
O	48	0.8353	0.1614	0.2860
O	49	0.0086	0.8345	0.0562
O	50	0.0822	0.9084	0.2018
O	51	0.1571	0.9836	0.3563
O	52	0.1515	0.9776	0.0995
O	53	0.2282	0.5546	0.2435
O	54	0.0555	0.6323	0.3842
O	55	0.0795	0.6551	0.0298
O	56	0.1547	0.7306	0.1837
O	57	0.2277	0.8044	0.3294
O	58	0.1811	0.5068	0.0018
O	59	0.0085	0.5846	0.1427
O	60	0.0850	0.6616	0.2860
O	61	0.2586	0.8346	0.0576

O	62	0.3325	0.9086	0.2033
O	63	0.4075	0.9876	0.3544
O	64	0.4013	0.9770	0.0998
O	65	0.4789	0.5556	0.2423
O	66	0.3029	0.6277	0.3869
O	67	0.3291	0.6551	0.0300
O	68	0.4048	0.7311	0.1844
O	69	0.4774	0.8046	0.3288
O	70	0.4303	0.5060	0.0015
O	71	0.2591	0.5851	0.1446
O	72	0.3354	0.6632	0.2899
O	73	0.5085	0.8344	0.0567
O	74	0.5825	0.9085	0.2016
O	75	0.6574	0.9838	0.3559
O	76	0.6516	0.9777	0.0990
O	77	0.7284	0.5546	0.2422
O	78	0.5552	0.6341	0.3841
O	79	0.5790	0.6550	0.0296
O	80	0.6548	0.7308	0.1828
O	81	0.7275	0.8039	0.3281
O	82	0.6804	0.5061	0.0008
O	83	0.5085	0.5844	0.1429
O	84	0.5859	0.6613	0.2857
O	85	0.7584	0.8342	0.0562
O	86	0.8323	0.9082	0.2019
O	87	0.9074	0.9837	0.3562
O	88	0.9015	0.9773	0.0989
O	89	0.9782	0.5542	0.2421
O	90	0.8057	0.6324	0.3842
O	91	0.8291	0.6548	0.0294
O	92	0.9045	0.7305	0.1829
O	93	0.9776	0.8039	0.3280
O	94	0.9306	0.5064	0.0007
O	95	0.7586	0.5844	0.1428
O	96	0.8353	0.6615	0.2860
O	97	0.4247	0.5344	0.5253
O	98	0.4069	0.7319	0.4443
O	99	0.5309	0.8007	0.4764
Ti	1	0.1051	0.4309	0.0388
Ti	2	0.1748	0.0011	0.1813
Ti	3	0.2473	0.0735	0.3281
Ti	4	-0.0111	0.0648	0.0574
Ti	5	0.0620	0.1387	0.2043
Ti	6	0.1318	0.2086	0.3469

Ti	7	0.3545	0.4307	0.0390
Ti	8	0.4247	0.0009	0.1811
Ti	9	0.4975	0.0751	0.3267
Ti	10	0.2390	0.0649	0.0582
Ti	11	0.3118	0.1379	0.2050
Ti	12	0.3817	0.2086	0.3466
Ti	13	0.6047	0.4305	0.0383
Ti	14	0.6753	0.0016	0.1807
Ti	15	0.7475	0.0742	0.3276
Ti	16	0.4890	0.0648	0.0579
Ti	17	0.5622	0.1382	0.2040
Ti	18	0.6317	0.2079	0.3469
Ti	19	0.8547	0.4304	0.0381
Ti	20	0.9251	0.0011	0.1806
Ti	21	0.9975	0.0737	0.3276
Ti	22	0.7389	0.0646	0.0574
Ti	23	0.8122	0.1380	0.2043
Ti	24	0.8819	0.2081	0.3470
Ti	25	0.1048	0.9307	0.0386
Ti	26	0.1759	0.5022	0.1814
Ti	27	0.2481	0.5741	0.3288
Ti	28	-0.0111	0.5646	0.0574
Ti	29	0.0620	0.6375	0.2044
Ti	30	0.1318	0.7078	0.3470
Ti	31	0.3546	0.9305	0.0389
Ti	32	0.4245	0.5015	0.1810
Ti	33	0.4963	0.5731	0.3257
Ti	34	0.2391	0.5650	0.0588
Ti	35	0.3122	0.6386	0.2077
Ti	36	0.3831	0.7119	0.3530
Ti	37	0.6047	0.9307	0.0383
Ti	38	0.6753	0.5013	0.1807
Ti	39	0.7475	0.5737	0.3276
Ti	40	0.4891	0.5649	0.0579
Ti	41	0.5625	0.6384	0.2039
Ti	42	0.6319	0.7081	0.3466
Ti	43	0.8547	0.9304	0.0381
Ti	44	0.9251	0.5012	0.1807
Ti	45	0.9975	0.5738	0.3276
Ti	46	0.7389	0.5645	0.0574
Ti	47	0.8122	0.6380	0.2043
Ti	48	0.8819	0.7082	0.3470
As	1	0.4580	0.7791	0.5062

H_3AsO_3-{101} BB:

Atom	Number	v	w	x
H	1	0.4691	0.8080	0.4392
H	2	0.5316	0.5851	0.4450
H	3	0.3580	0.2471	0.4508
O	1	0.0108	0.3359	0.0563
O	2	0.0837	0.4084	0.2020
O	3	0.1578	0.4812	0.3566
O	4	0.1536	0.4783	0.1003
O	5	0.2295	0.0534	0.2439
O	6	0.0566	0.1307	0.3842
O	7	0.0817	0.1569	0.0300
O	8	0.1565	0.2312	0.1844
O	9	0.2288	0.3026	0.3294
O	10	0.1833	0.0084	0.0023
O	11	0.0104	0.0852	0.1427
O	12	0.0862	0.1607	0.2861
O	13	0.2606	0.3361	0.0587
O	14	0.3348	0.4102	0.2053
O	15	0.4071	0.4833	0.3439
O	16	0.4028	0.4784	0.0996
O	17	0.4804	0.0570	0.2415
O	18	0.3052	0.1299	0.3863
O	19	0.3306	0.1560	0.0298
O	20	0.4059	0.2317	0.1836
O	21	0.4794	0.3047	0.3280
O	22	0.4318	0.0074	0.0010
O	23	0.2607	0.0873	0.1450
O	24	0.3361	0.1526	0.2888
O	25	0.5105	0.3358	0.0557
O	26	0.5844	0.4096	0.2001
O	27	0.6585	0.4834	0.3549
O	28	0.6537	0.4788	0.0979
O	29	0.7299	0.0551	0.2413
O	30	0.5570	0.1284	0.3833
O	31	0.5810	0.1566	0.0287
O	32	0.6567	0.2322	0.1820
O	33	0.7291	0.3039	0.3275
O	34	0.6825	0.0079	-0.0003
O	35	0.5100	0.0853	0.1422
O	36	0.5871	0.1639	0.2848
O	37	0.7605	0.3360	0.0552
O	38	0.8340	0.4091	0.2013

O	39	0.9084	0.4830	0.3556
O	40	0.9036	0.4789	0.0986
O	41	0.9796	0.0546	0.2420
O	42	0.8068	0.1312	0.3834
O	43	0.8314	0.1568	0.0289
O	44	0.9064	0.2315	0.1825
O	45	0.9789	0.3035	0.3280
O	46	0.9330	0.0083	0.0004
O	47	0.7606	0.0862	0.1419
O	48	0.8366	0.1613	0.2853
O	49	0.0107	0.8359	0.0562
O	50	0.0838	0.9085	0.2021
O	51	0.1580	0.9820	0.3565
O	52	0.1536	0.9786	0.1002
O	53	0.2293	0.5535	0.2442
O	54	0.0564	0.6308	0.3844
O	55	0.0817	0.6568	0.0301
O	56	0.1566	0.7312	0.1843
O	57	0.2286	0.8019	0.3309
O	58	0.1834	0.5092	0.0023
O	59	0.0104	0.5854	0.1428
O	60	0.0864	0.6604	0.2863
O	61	0.2608	0.8362	0.0591
O	62	0.3343	0.9096	0.2031
O	63	0.4100	0.9855	0.3571
O	64	0.4032	0.9785	0.0994
O	65	0.4814	0.5557	0.2404
O	66	0.3057	0.6232	0.3869
O	67	0.3306	0.6560	0.0299
O	68	0.4061	0.7312	0.1841
O	69	0.4803	0.8064	0.3266
O	70	0.4318	0.5072	0.0011
O	71	0.2607	0.5850	0.1453
O	72	0.3357	0.6711	0.2894
O	73	0.5105	0.8362	0.0556
O	74	0.5843	0.9102	0.2004
O	75	0.6585	0.9830	0.3545
O	76	0.6537	0.9798	0.0979
O	77	0.7299	0.5552	0.2413
O	78	0.5563	0.6310	0.3821
O	79	0.5809	0.6564	0.0287
O	80	0.6568	0.7323	0.1814
O	81	0.7289	0.8035	0.3273
O	82	0.6825	0.5081	-0.0003

O	83	0.5102	0.5860	0.1413
O	84	0.5876	0.6625	0.2837
O	85	0.7605	0.8360	0.0553
O	86	0.8340	0.9091	0.2012
O	87	0.9084	0.9830	0.3556
O	88	0.9036	0.9789	0.0986
O	89	0.9797	0.5546	0.2421
O	90	0.8068	0.6318	0.3834
O	91	0.8314	0.6568	0.0289
O	92	0.9064	0.7315	0.1826
O	93	0.9789	0.8034	0.3279
O	94	0.9330	0.5082	0.0005
O	95	0.7606	0.5856	0.1419
O	96	0.8366	0.6613	0.2853
O	97	0.4278	0.7057	0.4379
O	98	0.5138	0.5676	0.4837
O	99	0.4038	0.3129	0.4442
Ti	1	0.1072	0.4322	0.0391
Ti	2	0.1770	0.0018	0.1819
Ti	3	0.2486	0.0714	0.3289
Ti	4	-0.0089	0.0664	0.0573
Ti	5	0.0638	0.1387	0.2045
Ti	6	0.1329	0.2072	0.3471
Ti	7	0.3561	0.4316	0.0386
Ti	8	0.4262	0.0018	0.1806
Ti	9	0.4986	0.0735	0.3261
Ti	10	0.2411	0.0665	0.0593
Ti	11	0.3137	0.1383	0.2074
Ti	12	0.3843	0.2109	0.3504
Ti	13	0.6067	0.4319	0.0371
Ti	14	0.6773	0.0035	0.1796
Ti	15	0.7488	0.0735	0.3266
Ti	16	0.4908	0.0664	0.0571
Ti	17	0.5640	0.1395	0.2032
Ti	18	0.6331	0.2080	0.3459
Ti	19	0.8570	0.4324	0.0376
Ti	20	0.9270	0.0021	0.1804
Ti	21	0.9988	0.0733	0.3275
Ti	22	0.7410	0.0665	0.0564
Ti	23	0.8140	0.1391	0.2036
Ti	24	0.8830	0.2077	0.3464
Ti	25	0.1071	0.9321	0.0391
Ti	26	0.1774	0.5020	0.1820
Ti	27	0.2493	0.5726	0.3290

Ti	28	-0.0089	0.5663	0.0574
Ti	29	0.0638	0.6382	0.2046
Ti	30	0.1328	0.7062	0.3475
Ti	31	0.3562	0.9315	0.0387
Ti	32	0.4253	0.5009	0.1798
Ti	33	0.4971	0.5735	0.3216
Ti	34	0.2411	0.5665	0.0595
Ti	35	0.3139	0.6400	0.2083
Ti	36	0.3835	0.7092	0.3525
Ti	37	0.6067	0.9326	0.0371
Ti	38	0.6773	0.5023	0.1796
Ti	39	0.7488	0.5735	0.3268
Ti	40	0.4912	0.5668	0.0571
Ti	41	0.5648	0.6401	0.2017
Ti	42	0.6329	0.7076	0.3450
Ti	43	0.8570	0.9324	0.0376
Ti	44	0.9270	0.5022	0.1804
Ti	45	0.9987	0.5732	0.3275
Ti	46	0.7410	0.5665	0.0563
Ti	47	0.8140	0.6390	0.2036
Ti	48	0.8831	0.7078	0.3464
As	1	0.4325	0.5221	0.4880

H_2AsO_4-{001} MM:

Atom	Number	v	w	x
H	1	-0.7908	0.3063	0.5063
H	2	-0.5793	0.5724	0.5569
O	1	0.1520	-0.0018	-0.0006
O	2	0.1316	0.0114	0.3841
O	3	0.0290	0.2766	0.1917
O	4	0.1519	0.2893	0.0973
O	5	0.0267	0.0215	0.2878
O	6	0.0269	0.0275	0.1307
O	7	0.1486	0.2757	0.3250
O	8	0.0275	0.2503	0.0360
O	9	-0.0122	0.2763	0.4211
O	10	0.1517	0.0288	0.2279
O	11	0.4002	-0.0012	-0.0010
O	12	0.4078	0.0291	0.3801
O	13	0.2753	0.2762	0.1916
O	14	0.4012	0.2887	0.0965
O	15	0.2780	0.0407	0.2884

O	16	0.2764	0.0271	0.1312
O	17	0.4130	0.2749	0.3193
O	18	0.2763	0.2495	0.0361
O	19	0.1628	0.2781	0.4605
O	20	0.4002	0.0246	0.2243
O	21	0.6515	-0.0001	-0.0016
O	22	0.6433	0.0265	0.3750
O	23	0.5238	0.2758	0.1895
O	24	0.6517	0.2879	0.0954
O	25	0.5275	0.0257	0.2831
O	26	0.5267	0.0268	0.1279
O	27	0.6594	0.2755	0.3150
O	28	0.5261	0.2518	0.0343
O	29	0.5411	0.2760	0.4209
O	30	0.6513	0.0269	0.2204
O	31	0.9034	-0.0004	-0.0011
O	32	0.8719	0.0270	0.3765
O	33	0.7782	0.2762	0.1893
O	34	0.9023	0.2887	0.0963
O	35	0.7758	0.0194	0.2822
O	36	0.7769	0.0273	0.1274
O	37	0.9013	0.2762	0.3175
O	38	0.7773	0.2524	0.0340
O	39	0.7624	0.2759	0.4205
O	40	0.9030	0.0271	0.2232
O	41	0.1521	0.4985	-0.0006
O	42	0.1316	0.5408	0.3838
O	43	0.0295	0.7766	0.1916
O	44	0.1518	0.7893	0.0974
O	45	0.0267	0.5303	0.2878
O	46	0.0268	0.5277	0.1307
O	47	0.1722	0.7762	0.3189
O	48	0.0275	0.7501	0.0360
O	49	-0.0584	0.7769	0.4448
O	50	0.1517	0.5249	0.2278
O	51	0.4002	0.4992	-0.0010
O	52	0.4073	0.5199	0.3803
O	53	0.2741	0.7762	0.1926
O	54	0.4013	0.7888	0.0967
O	55	0.2778	0.5099	0.2884
O	56	0.2765	0.5274	0.1312
O	57	0.4058	0.7744	0.3193
O	58	0.2763	0.7496	0.0365
O	59	0.2850	0.7762	0.4129

O	60	0.4001	0.5276	0.2244
O	61	0.6515	0.4997	-0.0016
O	62	0.6434	0.5247	0.3750
O	63	0.5247	0.7757	0.1895
O	64	0.6518	0.7880	0.0953
O	65	0.5275	0.5243	0.2832
O	66	0.5267	0.5268	0.1279
O	67	0.6517	0.7755	0.3158
O	68	0.5261	0.7519	0.0343
O	69	0.5226	0.7754	0.4186
O	70	0.6513	0.5256	0.2204
O	71	0.9033	0.4992	-0.0011
O	72	0.8717	0.5256	0.3765
O	73	0.7781	0.7761	0.1889
O	74	0.9022	0.7890	0.0962
O	75	0.7758	0.5318	0.2822
O	76	0.7769	0.5271	0.1274
O	77	0.9028	0.7762	0.3182
O	78	0.7773	0.7525	0.0338
O	79	0.7435	0.7761	0.4250
O	80	0.9030	0.5267	0.2232
O	81	-0.5844	0.1971	0.5645
O	82	-0.7515	0.3309	0.5403
O	83	-0.6025	0.5392	0.5225
O	84	-0.6373	0.2703	0.4595
Ti	1	0.1493	0.0342	0.3055
Ti	2	0.0270	0.2718	0.1138
Ti	3	0.1520	0.2806	0.0218
Ti	4	0.1069	0.2754	0.4047
Ti	5	0.0266	0.0263	0.2090
Ti	6	0.4014	0.0323	0.3031
Ti	7	0.2767	0.2712	0.1140
Ti	8	0.4006	0.2809	0.0212
Ti	9	0.4307	0.2738	0.4001
Ti	10	0.2761	0.0267	0.2097
Ti	11	0.6510	0.0240	0.2994
Ti	12	0.5265	0.2708	0.1119
Ti	13	0.6516	0.2807	0.0204
Ti	14	0.6557	0.2756	0.3907
Ti	15	0.5260	0.0255	0.2065
Ti	16	0.8991	0.0197	0.3032
Ti	17	0.7769	0.2712	0.1116
Ti	18	0.9029	0.2807	0.0211
Ti	19	0.8794	0.2765	0.3920

Ti	20	0.7776	0.0260	0.2061
Ti	21	0.1491	0.5173	0.3058
Ti	22	0.0271	0.7717	0.1137
Ti	23	0.1520	0.7804	0.0218
Ti	24	0.1746	0.7763	0.3909
Ti	25	0.0268	0.5269	0.2091
Ti	26	0.4012	0.5174	0.3029
Ti	27	0.2766	0.7713	0.1143
Ti	28	0.4006	0.7808	0.0213
Ti	29	0.4102	0.7735	0.3929
Ti	30	0.2759	0.5255	0.2097
Ti	31	0.6510	0.5269	0.2994
Ti	32	0.5266	0.7707	0.1119
Ti	33	0.6516	0.7809	0.0203
Ti	34	0.6396	0.7756	0.3926
Ti	35	0.5261	0.5258	0.2066
Ti	36	0.8990	0.5328	0.3032
Ti	37	0.7769	0.7711	0.1116
Ti	38	0.9029	0.7809	0.0210
Ti	39	0.8633	0.7764	0.3995
Ti	40	0.7778	0.5262	0.2061
As	1	-0.6425	0.3214	0.5249

H_2AsO_4-{001} BB:

Atom	Number	v	w	x
H	1	-0.7976	0.6830	0.4808
H	2	-0.5282	0.4542	0.5426
O	1	0.1538	-0.0013	-0.0013
O	2	0.1115	0.0243	0.3793
O	3	0.0315	0.2757	0.1894
O	4	0.1526	0.2886	0.0964
O	5	0.0252	0.0244	0.2834
O	6	0.0272	0.0268	0.1279
O	7	0.1521	0.2764	0.3219
O	8	0.0282	0.2511	0.0339
O	9	-0.0152	0.2755	0.4255
O	10	0.1535	0.0254	0.2265
O	11	0.4002	-0.0019	-0.0015
O	12	0.4160	0.0287	0.3873
O	13	0.2774	0.2764	0.1924
O	14	0.4014	0.2891	0.0965
O	15	0.2771	0.0265	0.2905

O	16	0.2769	0.0274	0.1319
O	17	0.4066	0.2759	0.3245
O	18	0.2770	0.2483	0.0362
O	19	0.1815	0.2743	0.4462
O	20	0.4004	0.0276	0.2280
O	21	0.6504	-0.0006	-0.0027
O	22	0.6613	0.0264	0.3735
O	23	0.5229	0.2757	0.1897
O	24	0.6514	0.2877	0.0944
O	25	0.5282	0.0270	0.2852
O	26	0.5263	0.0270	0.1285
O	27	0.6579	0.2764	0.3136
O	28	0.5257	0.2501	0.0343
O	29	0.5515	0.2730	0.4204
O	30	0.6500	0.0256	0.2197
O	31	0.9035	-0.0003	-0.0025
O	32	0.8810	0.0256	0.3733
O	33	0.7766	0.2751	0.1869
O	34	0.9024	0.2875	0.0944
O	35	0.7774	0.0274	0.2793
O	36	0.7770	0.0263	0.1251
O	37	0.9033	0.2757	0.3148
O	38	0.7769	0.2528	0.0322
O	39	0.7699	0.2766	0.4215
O	40	0.9032	0.0261	0.2190
O	41	0.1537	0.4985	-0.0013
O	42	0.1105	0.5278	0.3790
O	43	0.0312	0.7756	0.1892
O	44	0.1526	0.7887	0.0964
O	45	0.0254	0.5271	0.2834
O	46	0.0272	0.5268	0.1279
O	47	0.1525	0.7760	0.3230
O	48	0.0282	0.7512	0.0338
O	49	-0.0123	0.7755	0.4231
O	50	0.1538	0.5265	0.2267
O	51	0.4004	0.4981	-0.0015
O	52	0.4327	0.5283	0.3795
O	53	0.2777	0.7765	0.1924
O	54	0.4014	0.7890	0.0964
O	55	0.2786	0.5273	0.2905
O	56	0.2768	0.5274	0.1317
O	57	0.4071	0.7801	0.3241
O	58	0.2770	0.7482	0.0361
O	59	0.1743	0.7655	0.4529

O	60	0.4012	0.5262	0.2266
O	61	0.6503	0.4994	-0.0026
O	62	0.6591	0.5261	0.3738
O	63	0.5225	0.7763	0.1897
O	64	0.6514	0.7883	0.0944
O	65	0.5292	0.5268	0.2837
O	66	0.5269	0.5270	0.1281
O	67	0.6587	0.7759	0.3133
O	68	0.5257	0.7508	0.0342
O	69	0.5536	0.7829	0.4199
O	70	0.6510	0.5258	0.2192
O	71	0.9035	0.4996	-0.0025
O	72	0.8812	0.5259	0.3733
O	73	0.7770	0.7755	0.1870
O	74	0.9024	0.7874	0.0943
O	75	0.7775	0.5242	0.2793
O	76	0.7770	0.5264	0.1251
O	77	0.9007	0.7757	0.3143
O	78	0.7769	0.7528	0.0322
O	79	0.7714	0.7756	0.4209
O	80	0.9034	0.5252	0.2192
O	81	-0.6213	0.3472	0.4626
O	82	-0.7516	0.5569	0.5164
O	83	-0.5796	0.5272	0.5509
O	84	-0.6187	0.7178	0.4613
Ti	1	0.1494	0.0246	0.3066
Ti	2	0.0273	0.2707	0.1119
Ti	3	0.1533	0.2801	0.0210
Ti	4	0.1040	0.2763	0.3994
Ti	5	0.0297	0.0255	0.2068
Ti	6	0.4000	0.0281	0.3063
Ti	7	0.2770	0.2715	0.1144
Ti	8	0.4008	0.2803	0.0209
Ti	9	0.4386	0.2806	0.4015
Ti	10	0.2762	0.0264	0.2104
Ti	11	0.6518	0.0266	0.2972
Ti	12	0.5266	0.2705	0.1118
Ti	13	0.6507	0.2807	0.0194
Ti	14	0.6639	0.2757	0.3897
Ti	15	0.5245	0.0258	0.2072
Ti	16	0.9004	0.0267	0.2984
Ti	17	0.7768	0.2703	0.1094
Ti	18	0.9031	0.2805	0.0195
Ti	19	0.8838	0.2758	0.3916

Ti	20	0.7784	0.0252	0.2036
Ti	21	0.1504	0.5240	0.3062
Ti	22	0.0273	0.7706	0.1118
Ti	23	0.1533	0.7802	0.0210
Ti	24	0.1038	0.7756	0.3999
Ti	25	0.0295	0.5258	0.2069
Ti	26	0.4030	0.5278	0.3053
Ti	27	0.2771	0.7712	0.1144
Ti	28	0.4007	0.7802	0.0209
Ti	29	0.4409	0.7781	0.4007
Ti	30	0.2769	0.5265	0.2104
Ti	31	0.6530	0.5256	0.2971
Ti	32	0.5266	0.7711	0.1118
Ti	33	0.6507	0.7808	0.0193
Ti	34	0.6647	0.7763	0.3891
Ti	35	0.5251	0.5258	0.2065
Ti	36	0.9010	0.5247	0.2984
Ti	37	0.7768	0.7707	0.1094
Ti	38	0.9031	0.7805	0.0194
Ti	39	0.8833	0.7757	0.3902
Ti	40	0.7781	0.5251	0.2034
As	1	-0.6492	0.5345	0.4969

H_2AsO_4-{101} MM:

Atom	Number	v	w	x
H	1	0.3077	0.5724	0.4567
H	2	0.4583	0.8958	0.5536
O	1	0.0115	0.3353	0.0565
O	2	0.0844	0.4076	0.2024
O	3	0.1596	0.4818	0.3568
O	4	0.1543	0.4777	0.1009
O	5	0.2307	0.0533	0.2439
O	6	0.0584	0.1308	0.3846
O	7	0.0827	0.1566	0.0305
O	8	0.1578	0.2314	0.1848
O	9	0.2308	0.3024	0.3306
O	10	0.1841	0.0079	0.0026
O	11	0.0116	0.0849	0.1429
O	12	0.0880	0.1610	0.2865
O	13	0.2615	0.3357	0.0595
O	14	0.3355	0.4098	0.2044
O	15	0.4110	0.4821	0.3530

O	16	0.4040	0.4796	0.0998
O	17	0.4821	0.0589	0.2412
O	18	0.3102	0.1337	0.3850
O	19	0.3315	0.1556	0.0303
O	20	0.4068	0.2307	0.1830
O	21	0.4824	0.3059	0.3273
O	22	0.4325	0.0068	0.0014
O	23	0.2615	0.0853	0.1446
O	24	0.3376	0.1616	0.2866
O	25	0.5111	0.3352	0.0561
O	26	0.5855	0.4094	0.2003
O	27	0.6607	0.4843	0.3542
O	28	0.6546	0.4785	0.0980
O	29	0.7314	0.0553	0.2412
O	30	0.5596	0.1319	0.3823
O	31	0.5816	0.1558	0.0288
O	32	0.6580	0.2319	0.1818
O	33	0.7317	0.3053	0.3273
O	34	0.6832	0.0072	-0.0002
O	35	0.5113	0.0845	0.1419
O	36	0.5890	0.1624	0.2842
O	37	0.7613	0.3353	0.0552
O	38	0.8352	0.4088	0.2010
O	39	0.9104	0.4837	0.3554
O	40	0.9046	0.4787	0.0988
O	41	0.9810	0.0546	0.2423
O	42	0.8092	0.1327	0.3833
O	43	0.8323	0.1563	0.0291
O	44	0.9078	0.2315	0.1827
O	45	0.9811	0.3044	0.3283
O	46	0.9338	0.0079	0.0006
O	47	0.7617	0.0854	0.1418
O	48	0.8385	0.1619	0.2851
O	49	0.0115	0.8353	0.0563
O	50	0.0851	0.9083	0.2025
O	51	0.1602	0.9825	0.3567
O	52	0.1543	0.9780	0.1006
O	53	0.2301	0.5530	0.2454
O	54	0.0586	0.6319	0.3846
O	55	0.0827	0.6563	0.0305
O	56	0.1577	0.7306	0.1847
O	57	0.2313	0.8040	0.3312
O	58	0.1846	0.5091	0.0033
O	59	0.0116	0.5852	0.1429

O	60	0.0882	0.6608	0.2865
O	61	0.2616	0.8356	0.0596
O	62	0.3356	0.9090	0.2045
O	63	0.4107	0.9869	0.3525
O	64	0.4039	0.9768	0.0998
O	65	0.4819	0.5530	0.2414
O	66	0.3063	0.6234	0.3887
O	67	0.3315	0.6556	0.0306
O	68	0.4077	0.7316	0.1854
O	69	0.4812	0.8050	0.3252
O	70	0.4326	0.5065	0.0014
O	71	0.2616	0.5856	0.1465
O	72	0.3369	0.6612	0.2910
O	73	0.5112	0.8353	0.0559
O	74	0.5854	0.9092	0.2004
O	75	0.6609	0.9845	0.3542
O	76	0.6545	0.9787	0.0981
O	77	0.7314	0.5551	0.2412
O	78	0.5595	0.6345	0.3824
O	79	0.5817	0.6557	0.0289
O	80	0.6580	0.7319	0.1819
O	81	0.7317	0.8052	0.3273
O	82	0.6831	0.5072	-0.0002
O	83	0.5112	0.5856	0.1421
O	84	0.5891	0.6628	0.2843
O	85	0.7613	0.8353	0.0552
O	86	0.8352	0.9089	0.2010
O	87	0.9103	0.9836	0.3554
O	88	0.9046	0.9785	0.0988
O	89	0.9811	0.5547	0.2423
O	90	0.8091	0.6323	0.3834
O	91	0.8323	0.6563	0.0290
O	92	0.9078	0.7315	0.1827
O	93	0.9810	0.8042	0.3281
O	94	0.9338	0.5074	0.0006
O	95	0.7617	0.5856	0.1418
O	96	0.8385	0.6618	0.2852
O	97	0.4457	0.5296	0.5135
O	98	0.3224	0.5622	0.4953
O	99	0.4140	0.8476	0.5407
O	100	0.4263	0.7580	0.4318
Ti	1	0.1084	0.4320	0.0396
Ti	2	0.1774	0.0005	0.1825
Ti	3	0.2505	0.0723	0.3292

Ti	4	-0.0080	0.0662	0.0575
Ti	5	0.0650	0.1398	0.2048
Ti	6	0.1348	0.2080	0.3477
Ti	7	0.3569	0.4314	0.0391
Ti	8	0.4273	0.0007	0.1808
Ti	9	0.5013	0.0744	0.3255
Ti	10	0.2419	0.0662	0.0594
Ti	11	0.3146	0.1386	0.2059
Ti	12	0.3854	0.2099	0.3470
Ti	13	0.6075	0.4315	0.0373
Ti	14	0.6785	0.0024	0.1797
Ti	15	0.7512	0.0745	0.3266
Ti	16	0.4917	0.0659	0.0573
Ti	17	0.5655	0.1396	0.2027
Ti	18	0.6354	0.2090	0.3453
Ti	19	0.8579	0.4319	0.0378
Ti	20	0.9284	0.0021	0.1806
Ti	21	1.0008	0.0737	0.3278
Ti	22	0.7418	0.0659	0.0564
Ti	23	0.8153	0.1391	0.2034
Ti	24	0.8852	0.2086	0.3462
Ti	25	0.1079	0.9315	0.0395
Ti	26	0.1797	0.5029	0.1825
Ti	27	0.2519	0.5731	0.3296
Ti	28	-0.0080	0.5657	0.0575
Ti	29	0.0651	0.6370	0.2048
Ti	30	0.1349	0.7065	0.3477
Ti	31	0.3569	0.9305	0.0391
Ti	32	0.4273	0.5013	0.1808
Ti	33	0.5011	0.5751	0.3257
Ti	34	0.2420	0.5662	0.0609
Ti	35	0.3159	0.6400	0.2115
Ti	36	0.3886	0.7130	0.3569
Ti	37	0.6075	0.9315	0.0373
Ti	38	0.6786	0.5025	0.1796
Ti	39	0.7511	0.5744	0.3266
Ti	40	0.4917	0.5660	0.0574
Ti	41	0.5655	0.6394	0.2029
Ti	42	0.6354	0.7092	0.3454
Ti	43	0.8580	0.9319	0.0378
Ti	44	0.9285	0.5022	0.1806
Ti	45	1.0009	0.5740	0.3278
Ti	46	0.7418	0.5659	0.0563
Ti	47	0.8153	0.6391	0.2035

Ti	48	0.8852	0.7085	0.3462
As	1	0.4042	0.6628	0.4949

H_2AsO_4-{101} BB:

Atom	Number	v	w	x
H	1	0.5360	0.6036	0.4550
H	2	0.3561	0.5247	0.5250
O	1	0.0115	0.3371	0.0557
O	2	0.0833	0.4089	0.2010
O	3	0.1559	0.4814	0.3557
O	4	0.1539	0.4794	0.1003
O	5	0.2280	0.0535	0.2451
O	6	0.0554	0.1310	0.3832
O	7	0.0828	0.1583	0.0297
O	8	0.1568	0.2325	0.1841
O	9	0.2281	0.3038	0.3307
O	10	0.1852	0.0109	0.0030
O	11	0.0104	0.0858	0.1419
O	12	0.0857	0.1603	0.2851
O	13	0.2616	0.3376	0.0603
O	14	0.3347	0.4108	0.2068
O	15	0.4055	0.4822	0.3422
O	16	0.4025	0.4784	0.0994
O	17	0.4797	0.0558	0.2409
O	18	0.3027	0.1271	0.3880
O	19	0.3309	0.1569	0.0297
O	20	0.4055	0.2318	0.1839
O	21	0.4793	0.3054	0.3250
O	22	0.4324	0.0083	0.0011
O	23	0.2609	0.0875	0.1466
O	24	0.3346	0.1554	0.2910
O	25	0.5108	0.3367	0.0555
O	26	0.5838	0.4093	0.1995
O	27	0.6575	0.4834	0.3538
O	28	0.6536	0.4794	0.0976
O	29	0.7294	0.0549	0.2409
O	30	0.5564	0.1325	0.3822
O	31	0.5813	0.1573	0.0284
O	32	0.6565	0.2324	0.1817
O	33	0.7286	0.3039	0.3271
O	34	0.6831	0.0089	-0.0005
O	35	0.5097	0.0855	0.1418

O	36	0.5867	0.1619	0.2837
O	37	0.7611	0.3366	0.0552
O	38	0.8338	0.4090	0.2008
O	39	0.9076	0.4826	0.3550
O	40	0.9037	0.4793	0.0980
O	41	0.9792	0.0548	0.2412
O	42	0.8060	0.1305	0.3830
O	43	0.8318	0.1573	0.0283
O	44	0.9061	0.2314	0.1819
O	45	0.9780	0.3030	0.3269
O	46	0.9337	0.0092	0.0000
O	47	0.7604	0.0860	0.1416
O	48	0.8360	0.1607	0.2848
O	49	0.0115	0.8371	0.0558
O	50	0.0832	0.9087	0.2009
O	51	0.1560	0.9819	0.3560
O	52	0.1538	0.9799	0.1004
O	53	0.2280	0.5541	0.2449
O	54	0.0551	0.6302	0.3834
O	55	0.0828	0.6584	0.0299
O	56	0.1568	0.7324	0.1840
O	57	0.2274	0.8031	0.3310
O	58	0.1852	0.5111	0.0029
O	59	0.0103	0.5855	0.1420
O	60	0.0857	0.6614	0.2852
O	61	0.2616	0.8376	0.0605
O	62	0.3343	0.9104	0.2056
O	63	0.4092	0.9863	0.3580
O	64	0.4029	0.9795	0.0994
O	65	0.4808	0.5576	0.2393
O	66	0.3028	0.6301	0.3878
O	67	0.3310	0.6568	0.0297
O	68	0.4053	0.7312	0.1836
O	69	0.4793	0.8066	0.3253
O	70	0.4323	0.5084	0.0009
O	71	0.2610	0.5865	0.1464
O	72	0.3345	0.6666	0.2908
O	73	0.5108	0.8371	0.0556
O	74	0.5838	0.9099	0.1993
O	75	0.6574	0.9825	0.3539
O	76	0.6537	0.9802	0.0976
O	77	0.7294	0.5554	0.2409
O	78	0.5549	0.6296	0.3812
O	79	0.5812	0.6573	0.0282

O	80	0.6565	0.7324	0.1810
O	81	0.7282	0.8036	0.3269
O	82	0.6831	0.5088	-0.0005
O	83	0.5100	0.5856	0.1406
O	84	0.5868	0.6626	0.2827
O	85	0.7610	0.8366	0.0553
O	86	0.8338	0.9090	0.2007
O	87	0.9077	0.9828	0.3550
O	88	0.9037	0.9793	0.0980
O	89	0.9792	0.5546	0.2412
O	90	0.8060	0.6317	0.3829
O	91	0.8318	0.6573	0.0283
O	92	0.9061	0.7314	0.1820
O	93	0.9780	0.8031	0.3269
O	94	0.9338	0.5093	0.0000
O	95	0.7604	0.5854	0.1416
O	96	0.8360	0.6610	0.2848
O	97	0.4172	0.6849	0.4334
O	98	0.5098	0.5832	0.4893
O	99	0.3904	0.4717	0.5280
O	100	0.4171	0.3063	0.4335
Ti	1	0.1085	0.4340	0.0387
Ti	2	0.1788	0.0043	0.1819
Ti	3	0.2488	0.0739	0.3296
Ti	4	-0.0080	0.0677	0.0570
Ti	5	0.0646	0.1404	0.2038
Ti	6	0.1324	0.2079	0.3465
Ti	7	0.3563	0.4321	0.0382
Ti	8	0.4254	0.0010	0.1803
Ti	9	0.4971	0.0720	0.3260
Ti	10	0.2421	0.0682	0.0613
Ti	11	0.3147	0.1403	0.2130
Ti	12	0.3842	0.2124	0.3596
Ti	13	0.6072	0.4328	0.0366
Ti	14	0.6772	0.0034	0.1792
Ti	15	0.7479	0.0725	0.3263
Ti	16	0.4912	0.0676	0.0572
Ti	17	0.5638	0.1400	0.2029
Ti	18	0.6322	0.2077	0.3449
Ti	19	0.8577	0.4331	0.0369
Ti	20	0.9271	0.0022	0.1797
Ti	21	0.9982	0.0729	0.3264
Ti	22	0.7415	0.0674	0.0562
Ti	23	0.8140	0.1395	0.2033

Ti	24	0.8823	0.2073	0.3460
Ti	25	0.1085	0.9341	0.0388
Ti	26	0.1786	0.5040	0.1819
Ti	27	0.2488	0.5750	0.3295
Ti	28	-0.0080	0.5678	0.0570
Ti	29	0.0645	0.6407	0.2038
Ti	30	0.1321	0.7079	0.3466
Ti	31	0.3564	0.9324	0.0385
Ti	32	0.4244	0.4998	0.1792
Ti	33	0.4954	0.5698	0.3206
Ti	34	0.2421	0.5682	0.0610
Ti	35	0.3145	0.6413	0.2124
Ti	36	0.3842	0.7099	0.3587
Ti	37	0.6072	0.9336	0.0366
Ti	38	0.6772	0.5022	0.1792
Ti	39	0.7479	0.5731	0.3262
Ti	40	0.4917	0.5680	0.0568
Ti	41	0.5645	0.6408	0.2011
Ti	42	0.6313	0.7069	0.3443
Ti	43	0.8576	0.9331	0.0369
Ti	44	0.9271	0.5021	0.1797
Ti	45	0.9980	0.5728	0.3265
Ti	46	0.7415	0.5673	0.0562
Ti	47	0.8140	0.6396	0.2033
Ti	48	0.8823	0.7075	0.3460
As	1	0.4323	0.5109	0.4668

O_2-{001}:

Atom	Number	v	w	x
O	1	0.1499	-0.0039	-0.0021
O	2	0.1284	0.0103	0.3823
O	3	0.0271	0.2777	0.1912
O	4	0.1499	0.2918	0.0967
O	5	0.0250	0.0231	0.2871
O	6	0.0249	0.0288	0.1301
O	7	0.1480	0.2785	0.3241
O	8	0.0254	0.2480	0.0358
O	9	-0.0151	0.2785	0.4233
O	10	0.1501	0.0294	0.2270
O	11	0.3980	-0.0035	-0.0029
O	12	0.4030	0.0308	0.3788
O	13	0.2734	0.2780	0.1907

O	14	0.3993	0.2918	0.0956
O	15	0.2766	0.0464	0.2874
O	16	0.2746	0.0288	0.1303
O	17	0.4127	0.2784	0.3204
O	18	0.2742	0.2476	0.0356
O	19	0.1722	0.2791	0.4548
O	20	0.3987	0.0276	0.2232
O	21	0.6496	-0.0024	-0.0036
O	22	0.6396	0.0297	0.3742
O	23	0.5227	0.2776	0.1887
O	24	0.6496	0.2911	0.0946
O	25	0.5256	0.0301	0.2825
O	26	0.5249	0.0287	0.1272
O	27	0.6588	0.2783	0.3141
O	28	0.5241	0.2501	0.0337
O	29	0.5376	0.2795	0.4197
O	30	0.6496	0.0278	0.2199
O	31	0.9015	-0.0025	-0.0027
O	32	0.8686	0.0296	0.3763
O	33	0.7765	0.2775	0.1887
O	34	0.9002	0.2912	0.0958
O	35	0.7743	0.0226	0.2818
O	36	0.7747	0.0287	0.1270
O	37	0.9025	0.2783	0.3180
O	38	0.7753	0.2507	0.0337
O	39	0.7592	0.2786	0.4203
O	40	0.9012	0.0283	0.2228
O	41	0.1498	0.4965	-0.0021
O	42	0.1282	0.5468	0.3822
O	43	0.0274	0.7777	0.1910
O	44	0.1498	0.7920	0.0968
O	45	0.0250	0.5333	0.2870
O	46	0.0248	0.5288	0.1301
O	47	0.1735	0.7785	0.3173
O	48	0.0254	0.7480	0.0358
O	49	-0.0671	0.7787	0.4473
O	50	0.1500	0.5270	0.2270
O	51	0.3980	0.4970	-0.0029
O	52	0.4031	0.5262	0.3789
O	53	0.2729	0.7780	0.1919
O	54	0.3993	0.7918	0.0959
O	55	0.2766	0.5102	0.2874
O	56	0.2746	0.5292	0.1304
O	57	0.4041	0.7785	0.3176

O	58	0.2742	0.7477	0.0360
O	59	0.2833	0.7786	0.4133
O	60	0.3987	0.5286	0.2232
O	61	0.6496	0.4977	-0.0036
O	62	0.6399	0.5273	0.3742
O	63	0.5230	0.7776	0.1887
O	64	0.6497	0.7911	0.0946
O	65	0.5257	0.5265	0.2825
O	66	0.5249	0.5287	0.1272
O	67	0.6501	0.7784	0.3149
O	68	0.5240	0.7502	0.0338
O	69	0.5188	0.7786	0.4186
O	70	0.6497	0.5278	0.2198
O	71	0.9015	0.4972	-0.0027
O	72	0.8686	0.5271	0.3763
O	73	0.7767	0.7775	0.1883
O	74	0.9002	0.7916	0.0957
O	75	0.7743	0.5338	0.2818
O	76	0.7748	0.5285	0.1269
O	77	0.9018	0.7784	0.3182
O	78	0.7753	0.7507	0.0336
O	79	0.7377	0.7787	0.4256
O	80	0.9012	0.5277	0.2228
O	81	-0.6265	0.1891	-0.5312
O	82	-0.6291	0.3651	-0.5317
Ti	1	0.1474	0.0372	0.3048
Ti	2	0.0250	0.2725	0.1133
Ti	3	0.1498	0.2803	0.0213
Ti	4	0.1069	0.2787	0.4041
Ti	5	0.0247	0.0272	0.2087
Ti	6	0.3997	0.0370	0.3027
Ti	7	0.2746	0.2725	0.1132
Ti	8	0.3986	0.2808	0.0205
Ti	9	0.4265	0.2783	0.4019
Ti	10	0.2746	0.0285	0.2090
Ti	11	0.6492	0.0268	0.2986
Ti	12	0.5246	0.2722	0.1111
Ti	13	0.6496	0.2811	0.0196
Ti	14	0.6540	0.2784	0.3896
Ti	15	0.5241	0.0274	0.2059
Ti	16	0.8969	0.0218	0.3037
Ti	17	0.7747	0.2722	0.1109
Ti	18	0.9009	0.2809	0.0207
Ti	19	0.8793	0.2784	0.3926

Ti	20	0.7765	0.0273	0.2057
Ti	21	0.1474	0.5198	0.3048
Ti	22	0.0250	0.7725	0.1131
Ti	23	0.1499	0.7802	0.0214
Ti	24	0.1737	0.7786	0.3892
Ti	25	0.0246	0.5279	0.2087
Ti	26	0.3997	0.5198	0.3028
Ti	27	0.2746	0.7725	0.1136
Ti	28	0.3986	0.7805	0.0206
Ti	29	0.4070	0.7784	0.3914
Ti	30	0.2746	0.5271	0.2091
Ti	31	0.6493	0.5300	0.2986
Ti	32	0.5246	0.7722	0.1111
Ti	33	0.6496	0.7811	0.0197
Ti	34	0.6359	0.7785	0.3919
Ti	35	0.5241	0.5277	0.2059
Ti	36	0.8970	0.5351	0.3037
Ti	37	0.7748	0.7722	0.1109
Ti	38	0.9008	0.7811	0.0206
Ti	39	0.8594	0.7784	0.4005
Ti	40	0.7765	0.5274	0.2056

O_2-{101}:

Atom	Number	v	w	x
O	1	0.0103	0.3353	0.0559
O	2	0.0828	0.4078	0.2013
O	3	0.1580	0.4828	0.3563
O	4	0.1524	0.4775	0.0994
O	5	0.2287	0.0534	0.2424
O	6	0.0576	0.1319	0.3839
O	7	0.0812	0.1560	0.0291
O	8	0.1566	0.2324	0.1829
O	9	0.2294	0.3040	0.3296
O	10	0.1828	0.0080	0.0008
O	11	0.0102	0.0847	0.1425
O	12	0.0869	0.1626	0.2856
O	13	0.2606	0.3357	0.0571
O	14	0.3344	0.4107	0.2039
O	15	0.4090	0.4785	0.3508
O	16	0.4032	0.4796	0.1000
O	17	0.4809	0.0556	0.2417
O	18	0.3087	0.1340	0.3840
O	19	0.3311	0.1565	0.0299

O	20	0.4059	0.2315	0.1834
O	21	0.4817	0.3076	0.3265
O	22	0.4322	0.0074	0.0016
O	23	0.2605	0.0861	0.1431
O	24	0.3343	0.1603	0.2853
O	25	0.5106	0.3360	0.0563
O	26	0.5844	0.4099	0.2012
O	27	0.6594	0.4849	0.3552
O	28	0.6536	0.4790	0.0990
O	29	0.7302	0.0557	0.2423
O	30	0.5578	0.1351	0.3832
O	31	0.5811	0.1564	0.0294
O	32	0.6570	0.2325	0.1826
O	33	0.7303	0.3057	0.3283
O	34	0.6825	0.0077	0.0007
O	35	0.5102	0.0861	0.1424
O	36	0.5878	0.1606	0.2847
O	37	0.7604	0.3355	0.0562
O	38	0.8342	0.4093	0.2018
O	39	0.9095	0.4846	0.3564
O	40	0.9033	0.4782	0.0989
O	41	0.9800	0.0548	0.2422
O	42	0.8081	0.1334	0.3844
O	43	0.8311	0.1562	0.0292
O	44	0.9065	0.2316	0.1829
O	45	0.9797	0.3047	0.3281
O	46	0.9326	0.0072	0.0006
O	47	0.7606	0.0858	0.1427
O	48	0.8373	0.1624	0.2859
O	49	0.0106	0.8356	0.0561
O	50	0.0845	0.9094	0.2015
O	51	0.1588	0.9837	0.3561
O	52	0.1534	0.9784	0.0989
O	53	0.2290	0.5540	0.2443
O	54	0.0576	0.6332	0.3839
O	55	0.0812	0.6563	0.0291
O	56	0.1566	0.7307	0.1829
O	57	0.2296	0.8046	0.3299
O	58	0.1835	0.5087	0.0019
O	59	0.0102	0.5855	0.1426
O	60	0.0870	0.6610	0.2856
O	61	0.2606	0.8362	0.0571
O	62	0.3344	0.9092	0.2038
O	63	0.4091	0.9919	0.3507

O	64	0.4032	0.9778	0.0999
O	65	0.4808	0.5577	0.2418
O	66	0.3036	0.6268	0.3890
O	67	0.3312	0.6565	0.0305
O	68	0.4069	0.7325	0.1853
O	69	0.4794	0.8056	0.3310
O	70	0.4322	0.5077	0.0016
O	71	0.2597	0.5850	0.1442
O	72	0.3356	0.6620	0.2912
O	73	0.5107	0.8360	0.0564
O	74	0.5843	0.9098	0.2004
O	75	0.6596	0.9852	0.3562
O	76	0.6537	0.9792	0.0989
O	77	0.7303	0.5558	0.2423
O	78	0.5578	0.6322	0.3832
O	79	0.5811	0.6564	0.0294
O	80	0.6570	0.7324	0.1827
O	81	0.7303	0.8059	0.3283
O	82	0.6825	0.5076	0.0007
O	83	0.5102	0.5852	0.1425
O	84	0.5877	0.6661	0.2847
O	85	0.7604	0.8356	0.0562
O	86	0.8342	0.9094	0.2018
O	87	0.9095	0.9845	0.3564
O	88	0.9033	0.9786	0.0989
O	89	0.9800	0.5553	0.2422
O	90	0.8079	0.6334	0.3842
O	91	0.8310	0.6561	0.0292
O	92	0.9064	0.7315	0.1827
O	93	0.9796	0.8046	0.3280
O	94	0.9326	0.5078	0.0006
O	95	0.7606	0.5857	0.1427
O	96	0.8373	0.6624	0.2858
O	97	0.4130	0.8300	0.4420
O	98	0.4177	0.6600	0.4409
Ti	1	0.1076	0.4325	0.0379
Ti	2	0.1766	0.0016	0.1812
Ti	3	0.2496	0.0743	0.3283
Ti	4	-0.0089	0.0665	0.0577
Ti	5	0.0651	0.1425	0.2041
Ti	6	0.1342	0.2104	0.3465
Ti	7	0.3564	0.4322	0.0392
Ti	8	0.4260	0.0009	0.1812
Ti	9	0.4984	0.0735	0.3258

Ti	10	0.2408	0.0662	0.0581
Ti	11	0.3136	0.1392	0.2051
Ti	12	0.3841	0.2108	0.3451
Ti	13	0.6068	0.4321	0.0384
Ti	14	0.6774	0.0030	0.1809
Ti	15	0.7493	0.0746	0.3279
Ti	16	0.4910	0.0664	0.0582
Ti	17	0.5642	0.1394	0.2037
Ti	18	0.6330	0.2083	0.3463
Ti	19	0.8569	0.4319	0.0382
Ti	20	0.9277	0.0028	0.1810
Ti	21	0.9997	0.0744	0.3274
Ti	22	0.7410	0.0662	0.0576
Ti	23	0.8145	0.1395	0.2044
Ti	24	0.8839	0.2090	0.3468
Ti	25	0.1068	0.9317	0.0382
Ti	26	0.1808	0.5058	0.1804
Ti	27	0.2518	0.5763	0.3290
Ti	28	-0.0089	0.5658	0.0577
Ti	29	0.0651	0.6372	0.2041
Ti	30	0.1342	0.7076	0.3465
Ti	31	0.3564	0.9314	0.0392
Ti	32	0.4260	0.5029	0.1812
Ti	33	0.4981	0.5746	0.3260
Ti	34	0.2412	0.5666	0.0607
Ti	35	0.3166	0.6422	0.2156
Ti	36	0.3875	0.7150	0.3665
Ti	37	0.6068	0.9321	0.0383
Ti	38	0.6773	0.5030	0.1810
Ti	39	0.7491	0.5746	0.3276
Ti	40	0.4910	0.5664	0.0582
Ti	41	0.5642	0.6397	0.2038
Ti	42	0.6329	0.7088	0.3463
Ti	43	0.8569	0.9319	0.0382
Ti	44	0.9277	0.5030	0.1810
Ti	45	0.9997	0.5748	0.3274
Ti	46	0.7410	0.5662	0.0577
Ti	47	0.8145	0.6395	0.2043
Ti	48	0.8838	0.7088	0.3468