Supplementary Material

Sorption of Arsenate on Cerium Oxide: A Simulated Infrared and Raman Spectroscopic Identification

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The adsorption energy is calculated using:

$$E_{\text{ads}} = \frac{E_{\text{surf+ars}} - (E_{\text{surf}} + n_{\text{ars}} \times E_{\text{ars}})}{n_{\text{ars}}} \qquad \text{Equation S1}$$

where $E_{\text{surf+ars}}$ is the energy of the surface with the adsorbed Arsenate, E_{surf} is the energy of the bare surface, and E_{ars} and n_{ars} are the energy and the number of arsenate species adsorbed to the surface. Table S1 lists the adsorption energies, while Table S2 reports the degree of dissociation of the H_3AsO_4 molecule when adsorbed to the three surfaces in different configurations.

***Table S1**: Adsorption energies of all stable configurations of arsenic acid adsorbed onto the stoichiometric {111}, {110}, and {100} surfaces of CeO_2. The labelling scheme for the configurations is described in the text.*

Surface	Configuration	Adsorption energy (eV)		
		This work (PBE+*U*)	Previous work – Phosphate (PBE+U)[1]	ΔE (As-P)
{111}	{111}-5OAs-1O_s	-1.90	-1.13	-0.77
	{111}-4OAs-2O_s	-1.31	-1.56	0.25
	{111}-4OAs-3O_s	-1.66	-1.76	0.1
{110}	{110}-5OAs-1O_s	-2.14	-1.34	-0.8
	{110}-4OAs-2O_s	-2.98	-2.93	-0.05
	{110}-4OAs-3O_s	-2.36	-2.46	0.1
{100}	{100}-5OAs-2O_s	-2.79	-1.92	-0.87
	{100}-4OAs-1O_s	-2.26	-2.33	0.07
	{100}-4OAs-2O_s	-3.47	-3.56	0.09
	{100}-4OAs-3O_s	-4.14	-4.53	0.39

***Table S2**: Degree of dissociation of arsenic acid when adsorbed onto the stoichiometric {111}, {110}, and {100} surfaces of CeO_2 in different configurations. The labelling scheme for the configurations is described in the text.*

Surface	Configuration	Dissociation of H_3AsO_4
{111}	{111}-5OAs-1O_s	$H_3AsO_4 \rightarrow H_2AsO_4^- + H^+$
	{111}-4OAs-2O_s	$H_3AsO_4 \rightarrow HAsO_4^{2-} + 2H^+$
	{111}-4OAs-3O_s	$H_3AsO_4 \rightarrow HAsO_4^{2-} + 2H^+$
{110}	{110}-5OAs-1O_s	No dissociation
	{110}-4OAs-2O_s	$H_3AsO_4 \rightarrow H_2AsO_4^- + H^+$
	{110}-4OAs-3O_s	$H_3AsO_4 \rightarrow HAsO_4^{2-} + 2H^+$
{100}	{100}-5OAs-2O_s	No dissociation
	{100}-4OAs-1O_s	$H_3AsO_4 \rightarrow H_2AsO_4^- + H^+$
	{100}-4OAs-2O_s	$H_3AsO_4 \rightarrow HAsO_4^{2-} + 2H^+$
	{100}-4OAs-3O_s	$H_3AsO_4 \rightarrow HAsO_4^{2-} + 2H^+$

Table S3 compares selected bond lengths from our models to experimental measurements and previous DFT calculations on cerium gasparite ($CeAsO_4$), and arsenic acid (H_3AsO_4). As described in the text, we use the notation O_p to denote phosphoryl oxygen atoms, O_{surf} for surface oxygen atoms, and $*O_{surf}$ for the surface O atoms bound directly to As atoms.

***Table S3**. Comparison of selected bond lengths in our models to experimental measurements and previous DFT arsenic acid (H_3AsO_4). O_{surf}, $*O_{surf}$, O_p, O_{As} denote, respectively, surface oxygen atoms, surface oxygen atom directly bound to phosphorus atoms, the phosphoryl oxygen atoms, and the arsenic oxygen atoms.*

	Bond	Bond length (Å)	
		This work (PBE+*U*)	**Literature (Experimental.)[2]**
$CeAsO_4$ (Cerium Gasparite)	As-O_{As}	-	1.68, 1.69, 1.70
	Ce-O_{As}	-	2.47, 2.46, 2.56
	As-O_{As}	-	
	Ce-O_{As}	-	
H_3AsO_4 (DFT)	As-O_{As}	1.77	
	As=O_{As}	1.64	
{111}-5OAs-1O_{surf}	As-$*O_{surf}$	2.01	
	As -O_{As}	1.72, 1.82, 1.84, 1.71	
	Ce-O_{As}	2.39, 2.65, 2.40	
	Ce-$*O_{surf}$	2.39, 2.31, 2.38	
{110}-5OAs-1O_{surf}	As-$*O_{surf}$	1.81	
	As -O_{As}	1.80, 1.89, 1.73, 1.86	
	Ce-O_{As}	2.33, 2.53	
	Ce-$*O_{surf}$	2.54, 2.64	
{100}-5OAs-2O_{surf}	As-$*O_{surf}$	1.80	
	As -O_{As}	1.76, 1.97, 1.77, 1.80	
	Ce-O_{As}	2.57, 2.66, 2.45, 2.43	
	Ce-$*O_{surf}$	2.41, 2.48	
{111}-4OAs-3O_{surf}	Ce-O_{As}	2.36, 2.42, 2.54	
{110}-4OAs-3O_{surf}	Ce-O_{As}	2.36, 2.61, 2.61	
{100}-4OAs-3O_{surf}	Ce-O_{As}	2.34, 2.38, 2.47, 2.63, 2.79	
{111}-4OAs-2O_{surf}	Ce-O_{As}	2.30, 2.30	
{110}-4OAs-2O_{surf}	Ce-O_{As}	2.34, 2.34	
{100}-4OAs-2O_{surf}	Ce-O_{As}	2.39, 2.48, 2.60, 2.51	
{100}-4OAs-1O_{surf}	Ce-O_{As}	2.39, 2.41	

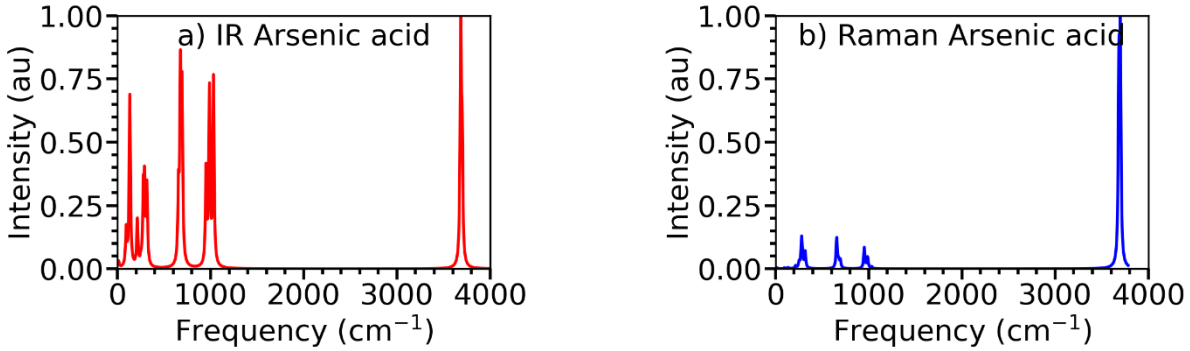

***Figure S1:** Simulated IR (a) and Raman spectra (b) of isolated H_3AsO_4.*

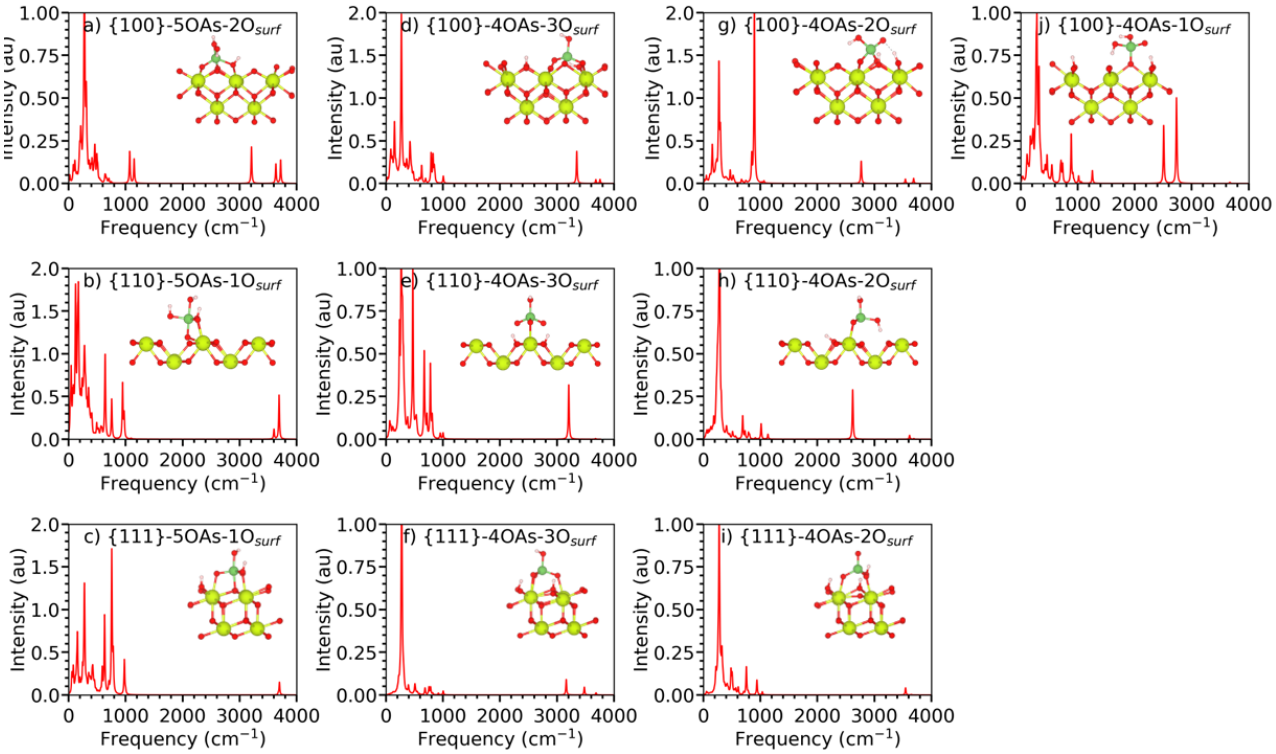

***Figure S2**: Simulated IR spectra of raw data of arsenate species adsorbed onto the {111}, {110}, and {100} stoichiometric surfaces of CeO_2.*

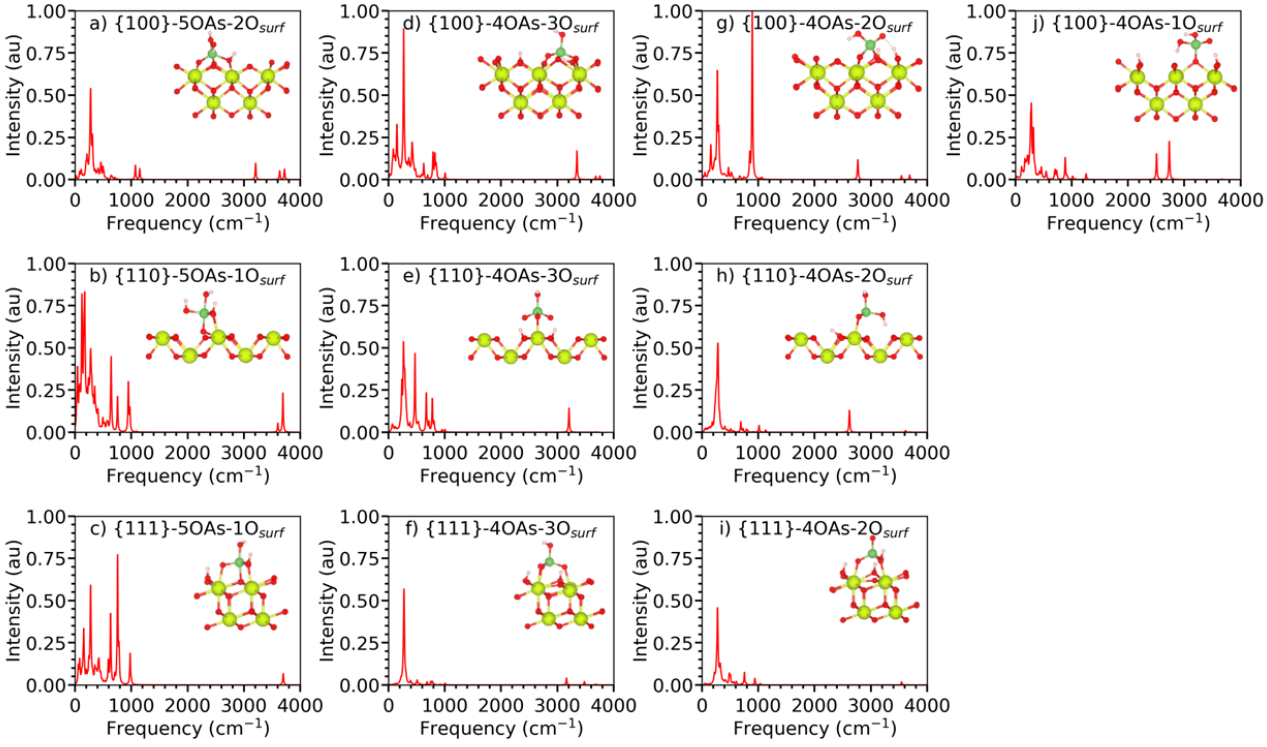

***Figure S3:** Simulated IR spectra of arsenate species adsorbed onto the {111}, {110}, and {100} stoichiometric surfaces of CeO_2. The spectra are normalised relative to each other such that the highest absolute intensity across all the spectra is set to unity.*

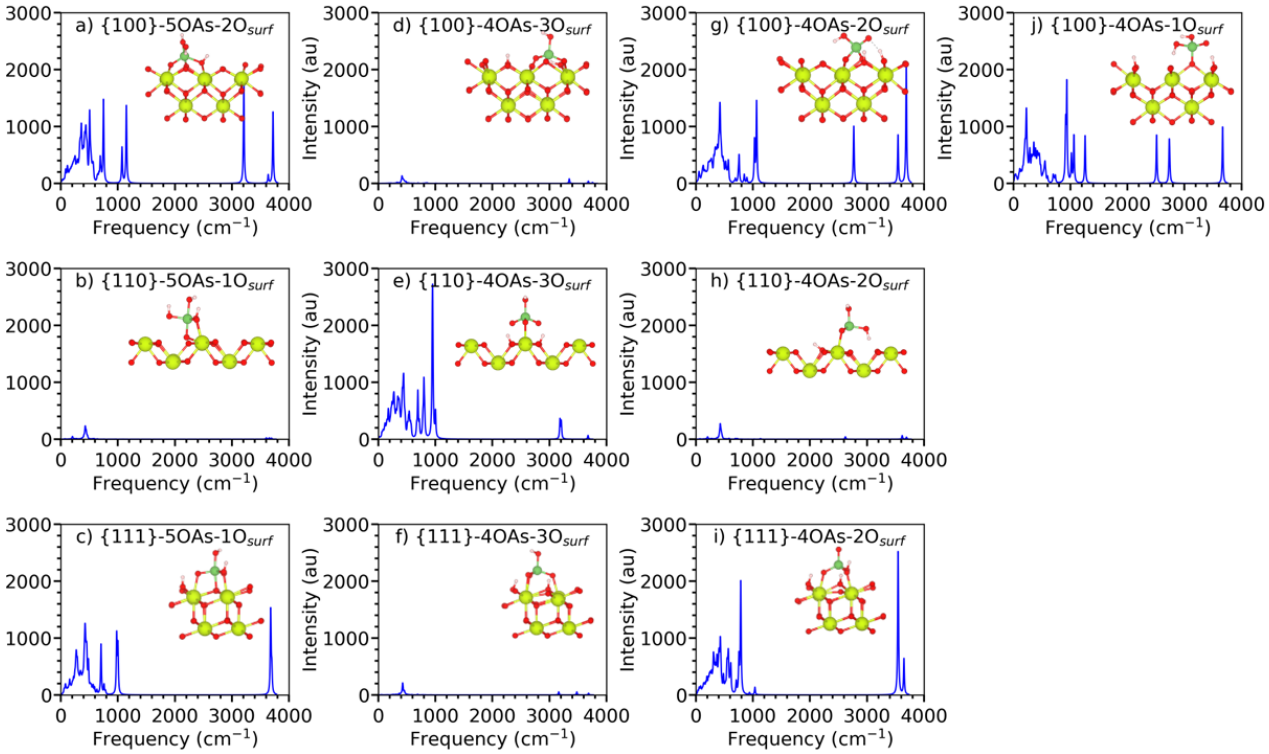

***Figure S4**: Simulated Raman spectra of raw data of arsenate species adsorbed onto the {111}, {110}, and {100} stoichiometric surfaces of CeO_2.*

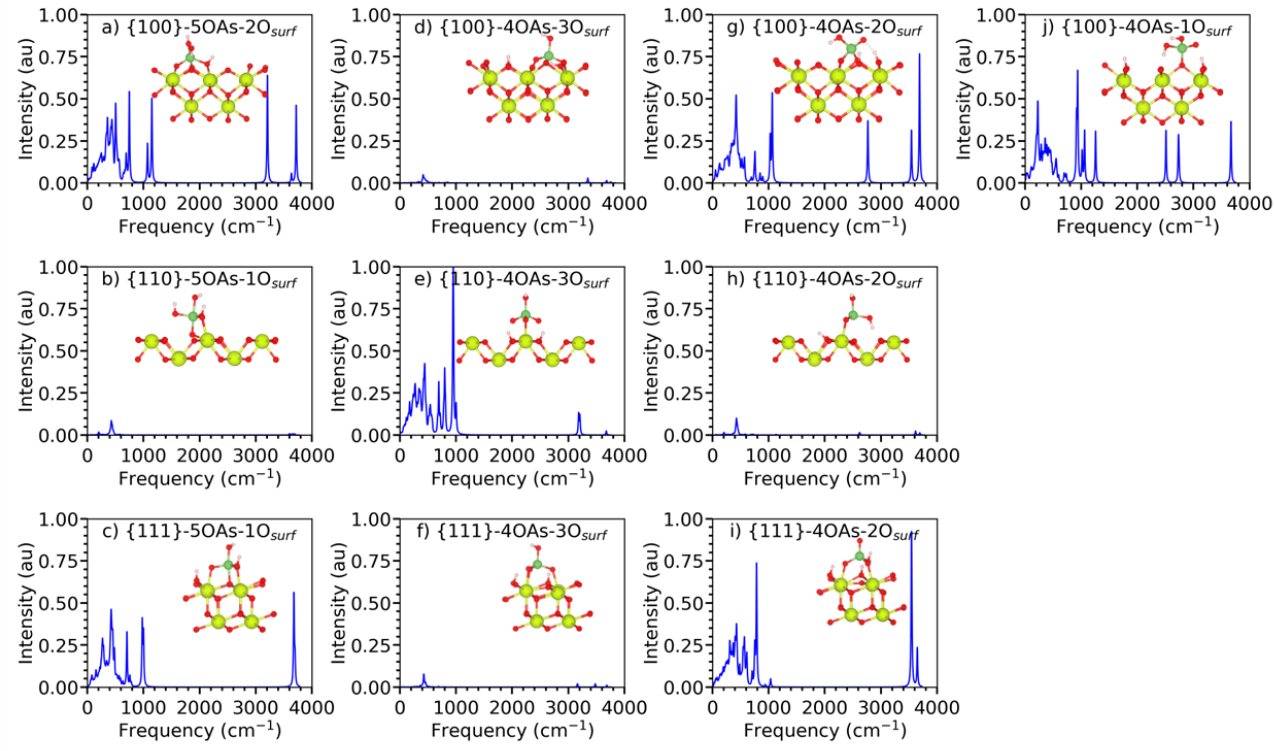

***Figure S5**: Simulated Raman spectra of arsenate species adsorbed onto the {111}, {110}, and {100} stoichiometric surfaces of CeO_2. The spectra are normalised relative to each other such that the highest absolute intensity across all the spectra is set to unity.*

***Table S4**: Assignment of the major features in the simulated IR spectra of arsenate species adsorbed onto the {111}, {110}, and {100} stoichiometric surfaces of CeO_2 with different binding modes. The mode labelling scheme is described in the text, and we additionally denote motion parallel or perpendicular to the surface where appropriate with the symbols || and ⊥ in parentheses. Vibrational frequencies from previous computational studies are also give for comparison.*

	Frequency (cm^{-1})	IR Relative intensity (AU)	Raman Relative intensity (AU)	Mode
	95.12	0.19		*Breathing modes
	133.85	0.69		scAs-OH_{As}, ρO_{As}-H_{As}
	214.76	0.25		scAs-OH_{As}, ρO_{As}-H_{As}
	278.25	0.16		δAs-OH_{As}
	280.38	0.19	0.13	δAs-OH_{As}, δAs-O_{As}, ρO_{As}-H_{As}
	291.95	0.39		δAs-OH_{As}, δAs-O_{As}
	317.36	0.42	0.08	scAs-OH_{As}, ρO_{As}-H_{As}
	656.29	0.35	0.15	v_sAs-OH_{As}
H_3AsO_4	676.99	0.87		v_{as}As-OH_{As}
	694.96	0.78		v_sAs-OH_{As}, vAs-OH_{As} (⊥)
	952.21	0.50	0.10	vAs=O_{As}, ρO_{As}-H_{As}
	986.12	0.39		ρO_{As}-H_{As}
	990.26	0.60		scAs-OH_{As}, vAs=O_{As}
	1031.67	0.77		vAs=O_{As}, δAs-OH_{As}
	3683.79	1.00	0.68	vO_{As}-H_{As}, ωAs-OH_{As}
	3686.38	0.29	0.22	vO_{As}-H_{As}
	3699.49	0.60	1.00	vO_{As}-H_{As}
	55.91	0.09		*Breathing mode of surface and Arsenate
	80.21	0.08		*Breathing mode of surface and Arsenate
	84.39	0.06		*Breathing mode of surface and Arsenate
	154.76	0.28	0.09	*Breathing mode of surface and Arsenate
	245.16	0.10		*Breathing mode of surface
	262.19		0.07	Complex v_sCe-O_{bulk}
	269.00		0.06	Complex v_sCe-O_{bulk}, v_sCe-O_{surf}
	270.80		0.12	Complex v_sCe-O_{bulk}
	272.15		0.05	Complex v_sCe-O_{bulk}
	274.16	0.21		Complex v_sCe-O_{bulk}, v_sCe-O_{surf}
	278.62	0.16		Complex vCe-O_{bulk}, vCe-O_{surf}
	279.20	0.18		v_sCe-O_{bulk} (L)
	289.88		0.10	Complex ωCe-O_{bulk}, δAs-O_{As}, ρO_{As}-H_{As}
	292.87		0.07	Complex v_sCe-O_{bulk}, ρO_{As}-H_{As}
	343.47		0.08	ρCe-O_{bulk} (L), v_sCe-O_{surf} (T), δAs-O_{As}
	349.65	0.06		v_sCe-O_{bulk} (L), v_sCe-O_{surf} (T), δAs-O_{As}, ρO_{As}-H_{As}
	363.73		0.07	v_sCe-O_{bulk} (T), v_sCe-O_{surf} (L)
	379.56		0.05	v_sCe-O_{bulk} (L), v_sCe-O_{surf} (L), ρAs-O_{As}
	410.60		0.05	v_sCe-O_{bulk} (L), v_sCe-O_{surf} (L), ρAs-O_{As}, ρO_{As}-H_{As}
	413.23	0.05		v_sCe-O_{bulk} (T), v_sCe-O_{surf} (T), δAs-O_{As}
	414.47		0.05	v_sCe-O_{bulk} (T), v_sCe-O_{surf} (T), δAs-O_{As}, ρO_{As}-H_{As}
	419.17		0.13	v_sCe-O_{bulk} (T), v_sCe-O_{surf} (T), ρAs-O_{As}, ρO_{As}-H_{As}
	422.50	0.07	0.13	ρO_{As}-H_{As}, v_sCe-O_{bulk} (T), v_sCe-O_{surf} (T)
	426.75		0.07	v_sCe-O_{bulk} (L), ρO_{As}-H_{As}
	427.42		0.08	v_sCe-O_{bulk} (L), v_sCe-O_{surf} (L)
{111}-5OAs-1O_{surf}	432.76		0.14	v_sCe-O_{bulk} (T), v_sCe-O_{surf} (L), ρO_{As}-H_{As}
	439.38		0.05	v_{as}Ce-O_{bulk} (T)
	449.51		0.10	v_{as}Ce-O_{bulk} (L), v_{as}Ce-O_{surf} (L)
	449.92		0.05	v_{as}Ce-O_{bulk} (L), v_{as}Ce-O_{surf} (L)
	456.08		0.08	v_{as}Ce-O_{surf} (L), ρAs-O_{As}, ρO_{As}-H_{As}
	456.31		0.17	v_{as}Ce-O_{surf} (L), ρAs-O_{As}, ρO_{As}-H_{As}
	480.44		0.07	v_{as}Ce-O_{surf} (T), ωAs-O_{As}
	484.23		0.09	ρO_{surf}-H_{surf}
	484.29		0.16	ρAs-O_{As}, ρO_{surf}-H_{surf}, v_sCe-O_{surf} (L), ρO_{As}-H_{As}
	590.81	0.13		v_sAs-OH_{As}
	631.36	0.42		vAs-OH_{As} (⊥)
	705.20		0.15	ρO_{surf}-H_{surf}
	705.24		0.41	ρO_{surf}-H_{surf}, v_sAs-O_{As}
	756.59	0.76		v_sAs-O_{As}
	758.11		0.10	v_sAs-O_{As}
	782.78	0.19		v_{as}As-O_{As}
	979.03	0.18	0.44	vAs-OH_{As} (⊥)
	980.74		0.20	ρO_{As}-H_{As}
	1000.59		0.37	ρO_{As}-H_{As}
	1003.55		0.16	vAs-OH_{As} (⊥), ρO_{As}-H_{As} (⊥)
	3679.98		0.35	vO_{As}-H_{As}, vO_{surf}-H_{surf}
	3680.35		0.42	vO_{As}-H_{As}, vO_{surf}-H_{surf}
	3684.70		0.08	vO_{As}-H_{As} (⊥), vO_{surf}-H_{surf}
	3685.01		0.11	vO_{As}-H_{As} (⊥), vO_{surf}-H_{surf}
	3700.34	0.07	0.05	vO_{As}-H_{As}
	3700.668		0.19	vO_{As}-H_{As}, vO_{surf}-H_{surf},
{110}-5OAs-1O_{surf}	29.35	0.12		*Breathing mode of surface and Arsenate

	44.29	0.32		*Breathing mode of surface and Arsenate
	71.07	0.07		*Breathing mode of surface and Arsenate
	72.32	0.08		*Breathing mode of surface and Arsenate
	84.16	0.14		*Breathing mode of surface and Arsenate
	95.30	0.05		*Breathing mode of surface and Arsenate
	117.39	0.13		*Breathing mode of surface and Arsenate
	121.79	0.26		*Breathing mode of surface and Arsenate
	124.86	0.22		*Breathing mode of surface and Arsenate
	126.05	0.08		*Breathing mode of surface and Arsenate
	127.57	0.07		*Breathing mode of surface and Arsenate
	151.66	0.20		*Breathing mode of surface and Arsenate
	160.39	0.34		*Breathing mode of surface and Arsenate
	168.99	0.06		*Breathing mode of surface and Arsenate
	172.69	0.45		*Breathing mode of surface and Arsenate
	173.60	0.11		*Breathing mode of surface and Arsenate
	195.53	0.07		*Breathing mode of surface and Arsenate
	218.13	0.06		*Breathing mode of surface and Arsenate
	237.07	0.13		$v_sCe\text{-}O_{surf}$ (L), $v_sCe\text{-}O_{bulk}$ (L)
	256.75	0.06		Complex $v_sCe\text{-}O_{surf}$, $v_sCe\text{-}O_{bulk}$
	266.96	0.09		$v_sCe\text{-}O_{bulk}$ (L), $\rho Ce\text{-}O_{surf}$
	274.81	0.12		$v_sCe\text{-}O_{bulk}$ (L)
	280.71	0.18		$\rho Ce\text{-}O_{bulk}$, $\rho Ce\text{-}O_{surf}$
	287.03	0.09		$v_sCe\text{-}O_{surf}$ (L), $v_sCe\text{-}O_{bulk}$ (L)
	294.74	0.06		$v_sCe\text{-}O_{surf}$ (L), $v_sCe\text{-}O_{bulk}$ (L)
	300.024	0.06		$\rho Ce\text{-}O_{bulk}$, $\rho Ce\text{-}O_{surf}$
	324.25	0.11		$v_sCe\text{-}O_{surf}$ (T), $v_sCe\text{-}O_{bulk}$ (T), $\delta As\text{-}OH_{As}$
	349.74	0.12		$v_sCe\text{-}O_{surf}$ (T), $v_sCe\text{-}O_{bulk}$ (T), $\delta As\text{-}OH_{As}$
	409.31	0.05		$v_{as}Ce\text{-}O_{surf}$ (T), $v_{as}Ce\text{-}O_{bulk}$ (T), $\rho O_{As}\text{-}H_{As}$ (⊥),$\delta As\text{-}OH_{As}$, $\delta As\text{-}{*}O_{surf}$
	426.87		0.06	$v_sCe\text{-}O_{bulk}$ (L), $v_{as}Ce\text{-}O_{surf}$ (T)
	493.21	0.07		$v_sOH_{As}\text{-}As\text{-}{*}O_{surf}$, $v_sAs\text{-}(OH_{As})_2$
	634.93	0.13		$v_{as}OH_{As}\text{-}As\text{-}{*}O_{surf}$ (⊥), $v_{as}As\text{-}(O_{As})_2$
	642.01	0.36		$v_s(OH_{As})_3\text{-}As\text{-}{*}O_{surf}$
	755.73	0.20		$vAs\text{-}O_{As}$, $vAs\text{-}{*}O_{surf}$
	947.82	0.29		$vAs\text{-}OH_{As}$ (⊥)
	975.11	0.12		$\delta As\text{-}OH_{As}$
	3604.20	0.05		$vO_{As}\text{-}H_{As}$ (||)
	3694.10	0.23		$vO_{As}\text{-}H_{As}$
	85.39		0.06	*Breathing mode of surface
	194.34	0.06		$v_sCe\text{-}O_{surf}$ (L)
	212.11	0.10		$v_sCe\text{-}O_{surf}$ (L), breathing modes of arsenate
	234.36		0.07	$v_sCe\text{-}O_{bulk}$ (L)
	270.33	0.20		$v_sCe\text{-}O_{bulk}$ (L)
	278.76	0.34		$v_sCe\text{-}O_{bulk}$ (L)
	291.67		0.05	$v_sCe\text{-}O_{bulk}$ (T), $scAs\text{-}OH_{as}$
	309.84	0.18		$v_sCe\text{-}O_{surf}$ (L), $v_sCe\text{-}O_{bulk}$ (T)
	329.19		0.05	$\rho Ce\text{-}O_{bulk}$
	330.05		0.08	$v_sCe\text{-}O$(T), $\delta As\text{-}O_{as}$, $scAs\text{-}OH_{as}$
	337.97		0.08	$\rho Ce\text{-}O_{bulk}$, $\rho O_{surf}\text{-}H_{surf}$
	339.66		0.05	$\rho Ce\text{-}O_{bulk}$, $scAs\text{-}OH_{As}$
	350.87		0.05	Complex ρCe-O
	358.03		0.07	$\rho Ce\text{-}O_{bulk}$
	360.42		0.15	$\rho Ce\text{-}O_{bulk}$, $\rho O_{surf}\text{-}H_{surf}$
	364.54		0.08	$v_sCe\text{-}O_{surf}$ (T), $v_sCe\text{-}O_{bulk}$ (L)
	367.38		0.05	$v_{as}Ce\text{-}O_{bulk}$ (L)
	386.75		0.10	$v_{as}Ce\text{-}O_{bulk}$ (T), $vAs\text{-}{*}O_{surf}$, $\rho O_{surf}\text{-}H_{surf}$, $\delta As\text{-}O_{As}$
	397.14		0.06	$v_sCe\text{-}O_{surf}$ (T), $v_sCe\text{-}O_{bulk}$ (T), $vAs\text{-}{*}O_{surf}$, $\delta As\text{-}O_{As}$, $scAs\text{-}OH_{As}$
	416.69		0.08	$v_{as}Ce\text{-}O_{bulk}$ (T), $\rho O_{surf}\text{-}H_{surf}$
{100}-5OAs-2O$_{surf}$	420.87		0.11	$v_{as}Ce\text{-}O_{bulk}$ (T), $scO_{As}\text{-}As\text{-}{*}O_{surf}$, $\rho O_{surf}\text{-}H_{surf}$
	431.30		0.14	$v_sCe\text{-}O_{surf}$ (T), $v_sCe\text{-}O_{bulk}$ (T), $\rho O_{surf}\text{-}H_{surf}$
	439.86		0.14	$v_{as}Ce\text{-}O_{bulk}$ (L)
	442.49		0.09	Complex vCe-O, $tO_{As}\text{-}As$
	451.68		0.06	$v_{as}Ce\text{-}O_{bulk}$ (L)
	458.62		0.08	$v_{as}Ce\text{-}O_{bulk}$ (L), $v_{as}Ce\text{-}O_{surf}$ (T), $vAs\text{-}{*}O_{surf}$
	462.11		0.07	$v_{as}Ce\text{-}O_{bulk}$ (L), $v_{as}Ce\text{-}O_{surf}$ (L), $\rho O_{surf}\text{-}H_{surf}$
	463.68	0.05		$v_{as}Ce\text{-}O_{surf}$ (T), $\delta As\text{-}{*}O_{surf}$, $\delta As\text{-}O_{As}$
	495.86	0.06		$v_{as}Ce\text{-}O_{surf}$ (T), $vAs\text{-}{*}O_{surf}$, $\omega As\text{-}O_{As}$, $\rho O_{As}\text{-}H_{As}$, $\rho O_{surf}\text{-}H_{surf}$
	504.34		0.11	$v_{as}Ce\text{-}O$ (T), $\rho O_{As}\text{-}H_{As}$
	504.84		0.44	$v_{as}As\text{-}O_{As}$, $\rho O_{As}\text{-}H_{As}$
	505.59		0.09	$v_{as}Ce\text{-}O_{bulk}$ (T), $\rho O_{As}\text{-}H_{As}$
	516.36		0.06	$tO_{As}\text{-}As$, $vAs\text{-}{*}O_{surf}$, $\rho O_{As}\text{-}H_{As}$
	567.42		0.06	$v_sCe\text{-}O_{bulk}$ (L), $\omega As\text{-}O_{As}$
	668.04		0.05	$v_sAs\text{-}O_{As}$, $v_sAs\text{-}OH_{As}$
	691.39		0.16	$v_{as}As\text{-}O_{As}$, $\rho O_{surf}\text{-}H_{surf}$, $\rho O_{As}\text{-}H_{As}$
	691.40		0.09	$v_{as}As\text{-}O_{As}$, $\rho O_{surf}\text{-}H_{surf}$, $\rho O_{As}\text{-}H_{As}$
	705.52		0.06	$v_{as}OH_{as}\text{-}As\text{-}O_{As}$, $v_sAs\text{-}O_{As}$
	748.099		0.43	$pO_{As}\text{-}H_{As}$, $\rho O_{surf}\text{-}H_{surf}$
	748.10		0.49	$pO_{As}\text{-}H_{As}$, $\rho O_{surf}\text{-}H_{surf}$
	1072.06	0.08	0.24	$\delta O_{As}\text{-}As\text{-}O_{As}$, $\rho O_{As}\text{-}H_{As}$

	1075.61		0.17	ρO_{As}-H_{As}
	1149.56	0.06	0.71	v_{as}As-O_{As}, δO_{As}-As-O_{As}, ρO_{As}-H_{As}
	3208.45	0.08	0.20	vO_{As}-H_{As}
	3209.6		0.89	vO_{As}-H_{As}
	3637.37	0.05	0.05	vO_{As}-H_{As}
	3637.92		0.04	vO_{As}-H_{As}
	3721.69	0.06	0.65	vO_{surf}-H_{surf}
	3722.22		0.14	vO_{surf}-H_{surf}
{100}-4OAs-1O$_{surf}$	38.32		0.05	*Breathing mode of surface
	166.99	0.08		*Breathing mode of surface and arsenate
	182.33		0.07	*Breathing mode of surface and arsenate
	192.53		0.07	*Breathing mode of surface and arsenate
	201.18		0.07	*Breathing mode of surface
	217.52		0.06	ρCe-O
	222.22		0.15	*Breathing mode of surface
	228.79		0.44	v_sCe-O_{bulk} (L), δAs-O_{As}, ρO_{As}-H_{As}
	253.52	0.05		v_sCe-O_{bulk} (L)
	271.85	0.11		v_sCe-O_{bulk} (L), v_sCe-O_{surf} (T)
	272.25	0.11		v_sCe-O_{bulk} (L), v_sCe-O_{surf} (T)
	277.93		0.09	ρCe-O, δAs-OH_{As}, ρO_{As}-H_{As}, tAs-O_{As}
	283.53	0.16		v_sCe-O_{surf} (T), ρO_{As}-H_{As}
	284.58	0.15		v_sCe-O_{surf} (T), ρO_{As}-H_{As}
	287.71		0.14	v_sCe-O_{surf} (T), ρO_{As}-H_{As}
	319.64	0.19		v_sCe-O_{surf} (T), δAs-O_{As}
	320.88	0.05		v_sCe-O_{bulk} (T), δAs-O_{As}
	353.17		0.06	ωAs-O_{As}, v_sCe-O_{surf} (T), ρCe-O_{bulk}
	358.78		0.06	ρCe-O_{bulk}
	360.74		0.08	v_{as}Ce-O_{bulk} (T), δAs-O_{As}
	389.38		0.08	ωCe-O_{bulk} (T), δAs-O_{As}
	415.54		0.06	Complex vCe-O
	419.80		0.11	v_sCe-O
	430.46		0.08	ρCe-O_{bulk}
	445.61		0.05	Complex vCe-O, δAs-O_{As}
	455.74		0.06	v_{as}Ce-O_{bulk} (L)
	480.94		0.05	v_{as}Ce-O_{surf} (L)
	554.49		0.10	v_sCe-O (T)
	734.76		0.06	vAs-OH_{As} (||), vAs-O_{As}
	885.39	0.12		vAs-O_{As} (||), ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	916.367		0.52	ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	916.371		0.08	ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	936.37		0.05	ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	936.73		0.67	ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	1016.3		0.14	$v_{as}O_{As}$-As-OH_{As}, δAs-O_{As}, ρO_{As}-H_{As}
	1016.8		0.17	$v_{as}O_{As}$-As-OH_{As}, δAs-O_{As}, ρO_{As}-H_{As}
	1060.33		0.29	pO_{surf}-H_{surf}
	1060.43		0.23	pO_{surf}-H_{surf}
	1256.54		0.07	ρO_{As}-H_{As} (||)
	1257.17		0.45	ρO_{As}-H_{As} (||)
	2507.26	0.12	0.02	vO_{surf}-H_{surf}
	2511.76		0.52	vO_{surf}-H_{surf}
	2732.62	0.21	0.39	vO_{As}-H_{As}
	2740.83		0.19	vO_{As}-H_{As}
	3669.80		0.08	vO_{As}-H_{As}
	3669.87		0.54	vO_{As}-H_{As}
{111}-4OAs-2O$_{surf}$	172.91		0.05	Complex breathing mode of surface
	238.51		0.05	Complex vCe-O_{bulk}, vCe-O_{surf}
	258.61	0.06		Complex vCe-O_{bulk}, vCe-O_{surf}
	265.27		0.06	v_{as}Ce-O_{bulk} (T), v_{as}Ce-O_{surf} (T)
	273.15	0.05		Complex v_{as}Ce-O_{bulk} (T), v_{as}Ce-O_{surf} (T)
	276.06	0.21		v_sCe-O_{bulk} (L), v_sCe-O_{surf} (L)
	276.46		0.06	v_sCe-O_{bulk} (L), v_sCe-O_{surf} (L)
	280.47	0.12		v_sCe-O_{bulk} (L)
	286.92	0.06		v_sCe-O_{bulk} (T), v_sCe-O_{surf} (T)
	306.20		0.08	v_{as}Ce-O_{bulk} (T), v_{as}Ce-O_{surf} (T), ωAs-O_{As}
	308.08		0.05	Complex vCe-O, ρO_{As}-H_{As}
	309.20		0.10	v_{as}Ce-O_{bulk} (T), v_{as}Ce-O_{surf} (T), ρO_{As}-H_{As}
	319.12		0.06	ωAs-O_{As}, v_{as}Ce-O_{bulk} (T), v_{as}Ce-O_{surf} (T), ρO_{surf}-H_{surf}
	319.69		0.06	Complex vCe-O
	339.58		0.05	v_{as}Ce-O_{bulk} (L), v_{as}Ce-O_{surf} (L), ρO_{surf}-H_{surf}, ρO_{As}-H_{As}
	340.11		0.07	Complex vCe-O, pO_{As}-H_{As}
	357.79		0.07	v_{as}Ce-O_{bulk} (T), v_{as}Ce-O_{surf} (T)
	367.24		0.16	v_{as}Ce-O_{surf} (T), pO_{surf}-H_{surf}, pO_{As}-H_{As}, scAs-O_{As}
	370.13		0.07	v_{as}Ce-O_{surf} (T), scOH_{As}-As-O_{As}, pO_{surf}-H_{surf}, pO_{As}-H_{As}
	396.92		0.06	v_{as}Ce-O_{surf} (T), pO_{As}-H_{As}
	401.76		0.07	V_sCe-O_{surf} (T), pO_{surf}-O_{surf}, V_sCe-O_{bulk} (T), scOH_{As}-As-O_{As}, pO_{As}-H_{As}
	404.53		0.06	V_sCe-O_{surf} (T), pO_{As}-H_{As}, V_sCe-O_{bulk} (T), scOH_{As}-As-O_{As}, pO_{As}-H_{As}, pO_{surf}-H_{surf}
	406.31		0.07	V_sCe-O_{surf} (T), pO_{As}-H_{As}, V_sCe-O_{bulk} (T), scOH_{As}-As-O_{As}, pO_{As}-H_{As} , pO_{surf}-H_{surf}
	409.09		0.07	V_sCe-O_{surf} (L), pO_{As}-H_{As}, V_sCe-O_{bulk} (L)

	425.08		0.05	$V_{as}Ce\text{-}O_{surf}$ (L), $V_{as}Ce\text{-}O_{bulk}$ (L), ωAs-O_{As}, ρO_{surf}-H_{surf}
	426.81		0.07	$V_{as}Ce\text{-}O_{surf}$ (L), $V_{as}Ce\text{-}O_{bulk}$ (L),
	427.58		0.24	$V_{s}Ce\text{-}O_{surf}$ (T), $V_{s}Ce\text{-}O_{bulk}$ (T), δAs-OH_{As}
	431.13		0.07	$V_{s}Ce\text{-}O_{surf}$ (T), $V_{s}Ce\text{-}O_{bulk}$ (T), δO_{As}-H_{As}
	479.01		0.06	$V_{as}Ce\text{-}O_{surf}$ (L), $V_{as}Ce\text{-}O_{bulk}$ (L)
	484.40	0.06	0.07	$v_{s}Ce\text{-}O_{surf}$ (T), $v_{s}Ce\text{-}O_{bulk}$ (T), vAs-OH_{As}, ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	486.17		0.05	$v_{s}Ce\text{-}O_{surf}$ (T), ρAs-OH_{As}, ρO_{surf}-H_{surf}
	542.82		0.17	$v_{as}Ce\text{-}O_{surf}$ (T), scAs-O_{As}, ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	550.7		0.14	ρCe-O_{bulk}, scAs-O_{As}, ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	560.78		0.10	$v_{s}Ce\text{-}O_{surf}$ (T), $v_{s}Ce\text{-}O_{bulk}$ (T), $v_{s}As\text{-}O_{As}$, ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	568.64		0.19	$v_{s}Ce\text{-}O_{surf}$ (T), $v_{s}Ce\text{-}O_{bulk}$ (T), ωAs-O_{As}, ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	571.64		0.15	$v_{s}Ce\text{-}O_{surf}$ (T), $v_{s}Ce\text{-}O_{bulk}$ (T), ωAs-O_{As}, ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	597.51		0.05	$v_{s}Ce\text{-}O_{surf}$ (T), ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	612.13		0.20	$v_{s}Ce\text{-}O_{surf}$ (T), ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	612.66		0.09	ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	706.95		0.10	$v_{s}As\text{-}O_{As}$, ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	753.24		0.14	$v_{s}As\text{-}O_{As}$, ρO_{surf}-H_{surf}, ρO_{As}-H_{As}
	754.28	0.06	0.17	$v_{s}As\text{-}O_{As}$, ρO_{surf}-H_{surf}, ρO_{As}-H_{As}
	758.13		0.06	$v_{s}As\text{-}O_{As}$, vAs-OH_{As} (‖), ρO_{surf}-H_{surf}, ρO_{As}-H_{As}
	785.91		0.70	$v_{s}As\text{-}O_{As}$, ρO_{surf}-H_{surf}, ρO_{As}-H_{As}
	786.45		0.53	$v_{s}As\text{-}O_{As}$, ρO_{surf}-H_{surf}, ρO_{As}-H_{As}
	1034.92		0.07	ρO_{As}-H_{As}, vAs-OH_{As} (⊥)
	3544.46		0.63	vO_{As}-H_{As}
	3545.00		0.38	vO_{surf}-H_{surf}, vO_{As}-H_{As}
	3548.50	0.02	0.18	vO_{As}-H_{As}, vO_{surf}-H_{surf}
	3549.39		0.50	vO_{surf}-H_{surf}, vO_{As}-H_{As}
	3549.49		0.19	vO_{surf}-H_{surf}
	3650.00		0.20	vO_{As}-H_{As}
{110}-4OAs-2O_{surf}	228.72	0.07		*Breathing mode of surface
	246.12	0.08		$v_{s}Ce\text{-}O_{surf}$ (L)
	258.76	0.08		$v_{s}Ce\text{-}O_{bulk}$ (L), $v_{as}Ce\text{-}O_{surf}$ (T)
	271.10	0.05		$v_{s}Ce\text{-}O_{bulk}$ (L), ρCe-O_{surf}
	271.52	0.07		$v_{s}Ce\text{-}O_{bulk}$ (L), ρCe-O_{surf}
	279.87	0.22		ρCe-O_{surf}
	287.42	0.20		$v_{s}Ce\text{-}O_{bulk}$ (L), ρCe-O_{surf}, tAs-O_{As}, ρO_{As}-H_{As}
	288.16	0.06		ρCe-O_{bulk}, ρCe-O_{surf}
	426.67		0.06	$v_{as}Ce\text{-}O_{bulk}$ (L)
	690.32	0.06		vAs-OH_{As} (⊥),$v_{s}As\text{-}O_{As}$
	2618.69	0.08		vO_{As}-H_{As} (‖)
	2623.41	0.06		vO_{As}-H_{As} (‖)
{100}-4OAs-2O_{surf}	51.37		0.05	*Breathing mode of surface and arsenate
	56.09		0.05	*Breathing mode of surface and arsenate
	157.03	0.15		*Breathing mode of surface and arsenate
	270.89	0.08		$v_{s}Ce\text{-}O_{bulk}$ (L), $v_{s}Ce\text{-}O_{surf}$ (T), δAs-O_{As}
	272.05	0.06	0.06	$v_{s}Ce\text{-}O_{bulk}$ (L), $v_{s}Ce\text{-}O_{surf}$ (T)
	273.71	0.20		$v_{s}Ce\text{-}O_{bulk}$ (L), $v_{as}Ce\text{-}O_{surf}$ (T)
	276.47	0.20		$v_{s}Ce\text{-}O_{bulk}$ (L)
	288.14		0.05	Complex vCe-O, scAs-O_{As}, scO_{As}-As-OH_{As}
	297.88	0.20		$v_{s}Ce\text{-}O_{surf}$ (L)
	316.32		0.06	$v_{s}Ce\text{-}O_{surf}$ (L), scAs-O_{As}
	338.03		0.06	$v_{as}Ce\text{-}O_{bulk}$ (T), $v_{as}Ce\text{-}O_{surf}$ (T), δAs-O_{As}
	382.99		0.08	$v_{as}Ce\text{-}O_{bulk}$ (T), $v_{as}Ce\text{-}O_{surf}$ (T), scAs-O_{As}, ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	395.57		0.08	$v_{as}Ce\text{-}O_{bulk}$ (T), $v_{as}Ce\text{-}O_{surf}$ (T), scAs-O_{As}, ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	400.60		0.12	$v_{as}Ce\text{-}O_{surf}$ (L), ρAs-O_{As}, ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	414.63		0.05	$v_{s}Ce\text{-}O_{surf}$ (T), $v_{s}Ce\text{-}O_{bulk}$ (T), ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	414.88		0.13	$v_{s}Ce\text{-}O_{surf}$ (T), $v_{s}Ce\text{-}O_{bulk}$ (T), ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	416.07		0.07	$v_{s}Ce\text{-}O_{surf}$ (T), $v_{s}Ce\text{-}O_{bulk}$(T), scAs-O_{As}, ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	420.86		0.23	$v_{s}Ce\text{-}O_{surf}$ (T), $v_{s}Ce\text{-}O_{bulk}$(T), scAs-O_{As}, ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	424.38		0.18	$v_{as}Ce\text{-}O_{surf}$ (T), $v_{s}Ce\text{-}O_{bulk}$(T), ρO_{As}-H_{As}
	427.06		0.16	$v_{as}Ce\text{-}O_{surf}$ (T), $v_{s}Ce\text{-}O_{bulk}$(T), ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	439.15		0.07	$v_{as}Ce\text{-}O_{bulk}$ (L)
	448.10		0.09	$v_{as}Ce\text{-}O_{bulk}$ (L)
	470.36	0.06		$v_{s}Ce\text{-}O_{surf}$ (T), ρO_{As}-H_{As}
	474.74		0.05	$v_{s}Ce\text{-}O_{surf}$ (T), ρO_{As}-H_{As}
	476.39		0.06	$v_{s}Ce\text{-}O_{surf}$ (T), ρO_{As}-H_{As}
	489.76		0.11	$v_{s}Ce\text{-}O_{surf}$ (T), scO_{As}-As-OH_{As}
	522.07		0.05	ρCe-O_{surf} (T), ρCe-O_{bulk}(T)
	523.76		0.07	$v_{s}Ce\text{-}O_{surf}$ (T), $v_{as}O_{As}$-H_{As}
	569.45		0.10	$v_{s}Ce\text{-}O_{surf}$ (T), $v_{s}Ce\text{-}O_{bulk}$(T)
	571.30		0.06	$v_{s}Ce\text{-}O_{surf}$ (T), $v_{s}Ce\text{-}O_{bulk}$(T)
	757.46		0.09	ρO_{surf}-H_{surf}, $v_{as}As\text{-}O_{As}$
	757.47		0.20	ρO_{surf}-H_{surf}, $v_{as}As\text{-}O_{As}$
	847.81		0.06	$v_{s}As\text{-}O_{As}$, ρO_{surf}-H_{surf}
	848.06	0.13		$v_{s}As\text{-}O_{As}$ (‖), ρO_{surf}-H_{surf}
	894.25	1.00		$v_{as}As\text{-}O_{As}$, ρO_{surf}-H_{surf}
	1028.39		0.18	$v_{s}As\text{-}O_{As}$, ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	1028.49		0.28	$v_{s}As\text{-}O_{As}$, ρO_{As}-H_{As}, ρO_{surf}-H_{surf}
	1063.63		0.35	δO_{As}-As-O_{As}, ρO_{As}-H_{As}, ρO_{surf}-H_{surf}

	1065.01		0.55	$\delta As\text{-}OH_{As}$, $\rho O_{As}\text{-}H_{As}$, $\rho O_{surf}\text{-}H_{surf}$
	2767.42	0.07	0.42	$vO_{surf}\text{-}H_{surf}$
	2771.93	0.06	0.25	$vO_{surf}\text{-}H_{surf}$
	3545.13		0.37	$vO_{As}\text{-}H_{As}$, $vO_{surf}\text{-}H_{surf}$
	3545.16		0.16	$vO_{As}\text{-}H_{As}$, $vO_{surf}\text{-}H_{surf}$
	3690.00		0.71	$vO_{surf}\text{-}H_{surf}$
	3690.82		0.60	$vO_{surf}\text{-}H_{surf}$
	268.26	0.07		$v_sCe\text{-}O_{bulk}$ (L), $v_sCe\text{-}O_{surf}$ (L)
	272.75	0.15		$\delta As\text{-}O_{As}$, $v_sCe\text{-}O_{bulk}$ (L), $v_sCe\text{-}O_{surf}$ (T)
	273.14	0.05		$v_{as}Ce\text{-}O$ (T), $\delta As\text{-}O_{As}$
	277.12	0.25		$v_sCe\text{-}O_{bulk}$ (L), $v_sCe\text{-}O_{surf}$ (L)
	280.95	0.05		$v_sCe\text{-}O_{bulk}$ (T), $v_sCe\text{-}O_{surf}$ (T)
{111}-4OAs-3O$_{surf}$	508.90	0.02		$v_{as}Ce\text{-}O_{bulk}$ (T), $v_{as}Ce\text{-}O_{surf}$ (T)
	683.24	0.01		$v_{as}O_{As}\text{-}As\text{-}OH_{As}$, $v_sAs\text{-}O_{As}$, $\rho O_{surf}\text{-}H_{surf}$
	752.20	0.02		$v_{as}As\text{-}O_{As}$, $\rho O_{surf}\text{-}H_{surf}$
	779.20	0.01		$v_{as}As\text{-}O_{As}$, $v_{as}As\text{-}OH_{As}$, $\rho O_{surf}\text{-}H_{surf}$
	3162	0.04		$vO_{surf}\text{-}H_{surf}$
	3481.31	0.02		$vO_{surf}\text{-}H_{surf}$
	173.54		0.05	*Breathing mode of the surface
	175.90		0.11	*Breathing mode of the surface
	220.04		0.05	*Breathing mode of the surface
	227.12		0.08	*Breathing mode of the surface
	234.09	0.07		$v_sCe\text{-}O_{surf}$ (L), $\rho Ce\text{-}O_{bulk}$
	238.86	0.13		$\rho Ce\text{-}O_{bulk}$ (L)
	239.63		0.06	$\rho Ce\text{-}O_{bulk}$ (L), $\rho O_{As}\text{-}H_{As}$
	245.63		0.05	$v_sCe\text{-}O_{surf}$ (L), $v_sCe\text{-}O_{bulk}$ (L), $\rho O_{As}\text{-}H_{As}$
	256.26		0.06	$\rho Ce\text{-}O_{surf}$, $\rho Ce\text{-}O_{bulk}$
	263.22	0.15	0.11	$\rho Ce\text{-}O_{surf}$, $\rho Ce\text{-}O_{bulk}$
	266.46	0.22	0.05	$v_sCe\text{-}O_{bulk}$ (L)
	269.77	0.09		$v_sCe\text{-}O_{bulk}$ (L), $\rho Ce\text{-}O_{surf}$
	273.88		0.12	$\rho Ce\text{-}O_{surf}$, $\rho Ce\text{-}O_{bulk}$, $\rho O_{As}\text{-}H_{As}$
	274.27		0.09	$\rho Ce\text{-}O_{surf}$, $\rho Ce\text{-}O_{bulk}$, $\rho O_{As}\text{-}H_{As}$, $\delta As\text{-}O_{As}$
	282.07	0.10		$\rho Ce\text{-}O_{surf}$, $\rho Ce\text{-}O_{bulk}$, $\delta As\text{-}O_{As}$
	289.47	0.13		$\rho Ce\text{-}O_{surf}$, $\rho Ce\text{-}O_{bulk}$, $\delta As\text{-}O_{As}$
	292.22	0.08		$v_sCe\text{-}O_{bulk}$ (L), $\rho O_{As}\text{-}H_{As}$, $tAs\text{-}O_{As}$
	305.83	0.11		$v_{as}Ce\text{-}O_{bulk}$ (T), $\delta As\text{-}O_{As}$, $\delta O_{As}\text{-}As\text{-}OH_{As}$
	339.56		0.10	$v_{as}Ce\text{-}O_{bulk}$ (L), $scAs\text{-}O_{As}$, $\delta As\text{-}O_{As}$
	343.39		0.07	$v_{as}Ce\text{-}O_{bulk}$ (L), $tAs\text{-}O_{As}$
	356.89		0.11	$v_{as}Ce\text{-}O_{surf}$ (L), $v_{as}Ce\text{-}O_{bulk}$ (L), $tAs\text{-}O_{As}$
	365.94		0.08	$v_{as}Ce\text{-}O_{surf}$ (L), $v_{as}Ce\text{-}O_{bulk}$ (L), $\rho As\text{-}O_{As}$
	365.95		0.06	$v_{as}Ce\text{-}O_{surf}$ (L), $v_{as}Ce\text{-}O_{bulk}$ (L), $\rho As\text{-}O_{As}$
	419.44		0.18	$v_sCe\text{-}O_{surf}$ (T), $v_sCe\text{-}O_{bulk}$ (T)
	422.24		0.08	$v_sCe\text{-}O_{surf}$ (T), $v_sCe\text{-}O_{bulk}$ (T)
	434.55		0.14	$v_sCe\text{-}O_{surf}$ (L), $v_sCe\text{-}O_{bulk}$ (L), $\delta As\text{-}O_{As}$
{110}-4OAs-3O$_{surf}$	440.64		0.06	$v_sCe\text{-}O_{surf}$ (L), $v_sCe\text{-}O_{bulk}$ (L), $\delta As\text{-}O_{As}$
	442.90		0.16	$v_sCe\text{-}O_{surf}$ (L), $v_sCe\text{-}O_{bulk}$ (L)
	445.32		0.05	$v_sCe\text{-}O_{surf}$ (T), $v_sCe\text{-}O_{bulk}$ (L)
	446.98		0.06	Complex vCe-O
	462.35		0.06	$v_sCe\text{-}O_{bulk}$ (T), $\omega As\text{-}O_{As}$
	468.11	0.07		$v_sCe\text{-}O_{bulk}$ (T), $v_sCe\text{-}O_{surf}$ (L)
	470.94	0.46		$v_sCe\text{-}O_{bulk}$ (T), $v_sCe\text{-}O_{surf}$ (L)
	563.30		0.09	$v_sCe\text{-}O_{bulk}$ (T), $v_sCe\text{-}O_{surf}$ (L)
	574.85		0.05	Complex vCe-O
	671.15	0.23	0.09	Complex $vCe\text{-}O_{surf}$, $vCe\text{-}O_{bulk}$
	692.96		0.45	$vAs\text{-}OH_{As}$, $\rho O_{surf}\text{-}H_{surf}$, $v_sAs\text{-}O_{As}$
	718.22	0.05		$v_{as}As\text{-}O_{As}$, $\rho O_{surf}\text{-}H_{surf}$
	718.37		0.13	$v_{as}As\text{-}O_{As}$, $\rho O_{surf}\text{-}H_{surf}$
	778.45	0.19	0.09	$v_sAs\text{-}O_{As}$, $\rho O_{surf}\text{-}H_{surf}$, $vAs\text{-}OH_{As}$
	783.06		0.11	$v_{as}O_{As}\text{-}As\text{-}OH_{As}$, $\rho O_{surf}\text{-}H_{surf}$, $v_{as}As\text{-}O_{As}$
	798.10		0.53	$v_{as}O_{As}\text{-}As\text{-}OH_{As}$, $\rho O_{surf}\text{-}H_{surf}$, $v_sAs\text{-}O_{As}$
	810.54	0.04	0.20	$v_{as}As\text{-}O_{As}$, $\rho O_{surf}\text{-}H_{surf}$
	945.24		0.50	$v_{as}O_{As}\text{-}As\text{-}OH_{As}$, $\rho O_{surf}\text{-}H_{surf}$, $v_{as}As\text{-}O_{As}$
	945.241		0.34	$v_{as}O_{As}\text{-}As\text{-}OH_{As}$, $\rho O_{surf}\text{-}H_{surf}$, $v_{as}As\text{-}O_{As}$
	953.09		1.00	$v_{as}As\text{-}O_{As}$, $\rho O_{surf}\text{-}H_{surf}$
	953.74		0.25	$v_{as}As\text{-}O_{As}$, $\rho O_{surf}\text{-}H_{surf}$
	1001.78	0.01	0.22	$v_sAs\text{-}O_{As}$
	1003.48		0.06	$v_sAs\text{-}O_{As}$, $\rho O_{surf}\text{-}H_{surf}$, $\rho O_{As}\text{-}H_{As}$
	3185.39		0.10	$\rho O_{surf}\text{-}H_{surf}$, $vO_{As}\text{-}H_{As}$
	3185.41		0.11	$\rho O_{surf}\text{-}H_{surf}$, $vO_{As}\text{-}H_{As}$
	3207.16	0.13	0.11	$vO_{surf}\text{-}H_{surf}$
	3208.93		0.08	$vO_{surf}\text{-}H_{surf}$
	86.77	0.05		*Breathing mode of surface and Arsenate
	149.73	0.12		*Breathing mode of surface
	152.63	0.09		*Breathing mode of surface and Arsenate
{100}-4OAs-3O$_{surf}$	269.94	0.42		$v_sCe\text{-}O_{bulk}$ (L)
	270.96	0.38		$v_sCe\text{-}O_{bulk}$ (L), $v_sCe\text{-}O_{surf}$ (T)
	416.81	0.10		$v_{as}Ce\text{-}O_{bulk}$ (T), $v_sCe\text{-}O_{surf}$ (T), $\rho O_{surf}\text{-}H_{surf}$
	626.06	0.09		$\rho O_{surf}\text{-}H_{surf}$, $v_sAs\text{-}O_{As}$, $vAs\text{-}OH_{As}$

	791.28	0.13	ν_{as}As-O_{As}, ρO_{surf}-H_{surf}
	825.51	0.13	ν_{as}As-O_{As}, ρO_{surf}-H_{surf}
	846.98	0.07	ν_{s}As-O_{As}, $\nu_{as}O_{As}$-As-OH_{As}, ρO_{surf}-H_{surf}
	859.28	0.02	ν_{as}As-O_{As}, ρO_{surf}-H_{surf}, ρO_{As}-H_{As}
	1005.87	0.04	ρO_{As}-H_{As}
	3348.4	0.13	νO_{surf}-H_{surf}
	3756.3	0.02	νO_{surf}-H_{surf}

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