Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supported and Inserted Monomeric Niobium Oxide Species on/in Silica: A Molecular Picture

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Supplementary Material

Table S1. Calculated frequencies for selected models (A, B, C, D, and E) with one Nb per unit cell grafted on the silica surface model. (Values in cm^{-1})

Model	Frequency	Vibrational Mode
A-V	3784	NbO-H stretching
	1009 – 1000	Nb=O
	936 – 843	Nb–O–Si stretching
	723	NbO–H stretching (O stretching)
	614 – 609	Nb–O–Si stretching
B-G	3347	NbO-H stretching (H bonded)
	1015 – 969	Nb=O
	912	Nb–O–Si stretching
	861 – 726	NbO-H bending
	711	NbO-H stretching (O stretching)
C	3784 – 3770	NbO-H stretching (H bonded)
	1016 – 918	Nb–O–Si stretching
	870	Nb–O–Si stretching
	722	NbO-H bending
	664 – 659	NbO-H stretching (O stretching)
	642	NbO-H stretching (O stretching)
D	1019	Nb–O–Si stretching
	964	Nb=O
	895 – 841	Nb–O–Si stretching
	637 – 616	Nb–O–Si stretching
E	3770	NbO-H stretching (H bonded)
	1036 – 1018	Nb–O–Si stretching
	922	Nb–O–Si stretching

	882 – 857	Nb–O–Si stretching
	674	NbO-H bending
	630 – 607	NbO-H stretching
	602	NbO-H stretching
SiO_2 surface	3851	SiO-H stretching

Table S2. Calculated frequencies for selected double unit cell surface models with two Nb species. (Values in cm^{-1})

Model	Frequency	Vibration Mode
Structure-1	3770	NbO-H stretching (NbO_5)
	1066	Nb–O–Si stretching (NbO_6) ; Nb=O
	986	Nb–O–Si stretching (NbO_6)
	983	Nb–O–Si stretching (NbO_5); Nb=O
	970	Si–O–Si stretching (NbO_6)
	937 – 918	Nb–O–Si stretching (NbO_6)
	905	Nb=O (NbO_5)
	905	Nb=O (NbO_6)
	879	Nb–O–Si stretching (NbO_5)
	757	Si–O–Si stretching (NbO_5)
	693	NbO-H stretching (O stretching) (NbO_5)
	690	NbO-H stretching (O stretching) (NbO_5); Nb-O-Si (Si bending)
	674 – 602	Nb-O-Si bending (Si bending) (NbO_5, NbO_6)
	597	Nb–O–Si stretching (NbO_6)
	593	NbO-H (H bending; O stretching) (NbO_5)
	578 – 542	Nb–O–Si stretching (NbO_5)
	562 – 557	Nb–O–Si stretching (NbO_6)
Structure-2	3269	NbO-H stretching (NbO_4)
	1071 – 1055	Nb–O–Si stretching (NbO_6)

	1027 – 974	Nb–O–Si stretching (NbO_6)
	947 – 941	Nb–O–Si stretching (NbO_6)
	933 – 915	Nb–O–Si stretching (NbO_6)
	918 – 906	Nb–O–Si stretching (NbO_4)
	901 – 648	Nb–O–Si stretching (NbO_6)
	890	Nb=O
	835 – 780	Nb–O–Si stretching (NbO_4)
	808	NbO-H bending (NbO_4)
	674	NbO-H (O stretching; H bending) (NbO_4)
	671	NbO-H bending (NbO_4)
Structure-3	3769	NbO-H stretching (NbO_4)
	3650	NbO-H stretching (NbO_4)
	1068 – 1047	Nb–O–Si stretching (NbO_6)
	1033 – 992	Nb–O–Si stretching (NbO_6)
	958 – 934	Nb–O–Si stretching (NbO_6)
	937 – 850	Nb–O–Si stretching (NbO_4)
	902	Nb=O
	900	Nb=O; Nb–O–Si stretching (NbO_6)
	671	NbO-H stretching (O stretching) (NbO_4)
	661	NbO-H (O stretching; H bending) (NbO_4)
	657	Nb–O–Si stretching (NbO_6)
	601	NbO-H (O stretching) (NbO_4)
Structure-4	2263	NbO-H stretching (NbO_4)
	1107	NbO-H bending (NbO_4)
	1066 – 1035	Nb–O–Si stretching (NbO_6)
	989 – 957	Nb–O–Si stretching (NbO_6)
	951	NbO-H bending (NbO_4)
	936 – 910	Nb–O–Si stretching (NbO_6)
	925	Nb–O–Si stretching (NbO_4)
	895	Nb=O

	893 - 878	Nb–O–Si stretching (NbO_6)
	849 – 846	Nb–O–Si stretching (NbO_4)
	745	NbO-H (O stretching) (NbO_4)
	652	Nb–O–Si stretching (NbO_6)
	618	Nb–O–Si bending (NbO_6)
	615	Nb–O–Si stretching (NbO_4)
Structure-5	3708 – 3332	NbO-H stretching (H bonded) (NbO_4)
	1077 – 1030	Nb–O–Si stretching (NbO_6)
	998 – 975; 958 – 948; 941 – 926	Nb–O–Si stretching (NbO_6, NbO_4)
	919	Nb–O–Si stretching (NbO_6)
	909	NbO-H bending (NbO_4)
	906 – 874	NbO-H bending (NbO_4); Nb–O–Si stretching (NbO_6)
		Nb–O–Si stretching (NbO_4)
	832	Nb=O
	825	NbO-H stretching (O stretching) (NbO_4)
	753 – 684	NbO-H bending (NbO_4)
	679	
Structure-6	3747 – 2523	NbO-H stretching (NbO_4)
	1070 – 1039	Nb–O–Si stretching (NbO_6)
	1019	NbO-H bending (NbO_4)
	988 – 972	Nb–O–Si stretching (NbO_6)
	950	NbO-H bending (NbO_4)
	949	NbO-H bending (NbO_4); Nb–O–Si stretching (NbO_6)
		Nb–O–Si stretching (NbO_6)
	944 – 940	Nb–O–Si stretching (NbO_6)
	913 – 901	Nb–O–Si stretching (NbO_4)
	903 – 836	Nb=O
	893	NbO-H stretching (O stretching) (NbO_4)
	770 – 738	Nb–O–Si stretching (NbO_6)

	650 613	Nb–O–Si stretching (NbO_4)
Structure-7	1067 – 1061 1043 1010 988 – 972 971 – 930 929 920 910 – 904 888 – 873 852 830 647	Nb–O–Si stretching (NbO_6) Nb–O–Si stretching (NbO_6 Nb–O–Si stretching (NbO_6; NbO_4) Nb–O–Si stretching (NbO_6) Nb–O–Si stretching (NbO_6) Nb–O–Si stretching (NbO_6) Nb–O–Si stretching (NbO_4) Nb=O (Nb O_6) Nb–O–Si stretching (NbO_6) Nb–O–Si stretching (NbO_6) Nb–O–Si stretching (NbO_4) Nb–O–Si stretching (NbO_6)
Structure 8	3724 3648 1064 – 1040 1038 1021 1003 988 – 984 968 – 943 941 – 920 900 892 885 – 881 874 815 – 774 695 666 – 594	NbO-H stretching (NbO_4) NbO-H stretching (NbO_4) Nb–O–Si stretching (NbO_6) Nb–O–Si stretching (NbO_6) Nb–O–Si bending (NbO_4) Nb–O–Si stretching (NbO_4) Nb–O–Si stretching (NbO_6) Nb–O–Si stretching (NbO_6) Nb–O–Si stretching (NbO_6) Nb–O– Si stretching (NbO_6) Nb=O (NbO_6); Nb–O–Si stretching (NbO_4) Nb–O–Si stretching (NbO_4) Nb=O (NbO_6); Nb–O–Si stretching (NbO_4) Nb–O–Si stretching (NbO_4) NbO-H (O stretching) (NbO_4) NbO-H (O stretching; H bending) (NbO_4)

	648	Nb–O–Si stretching (NbO_6)
	619	Nb–O–Si stretching (NbO_4)

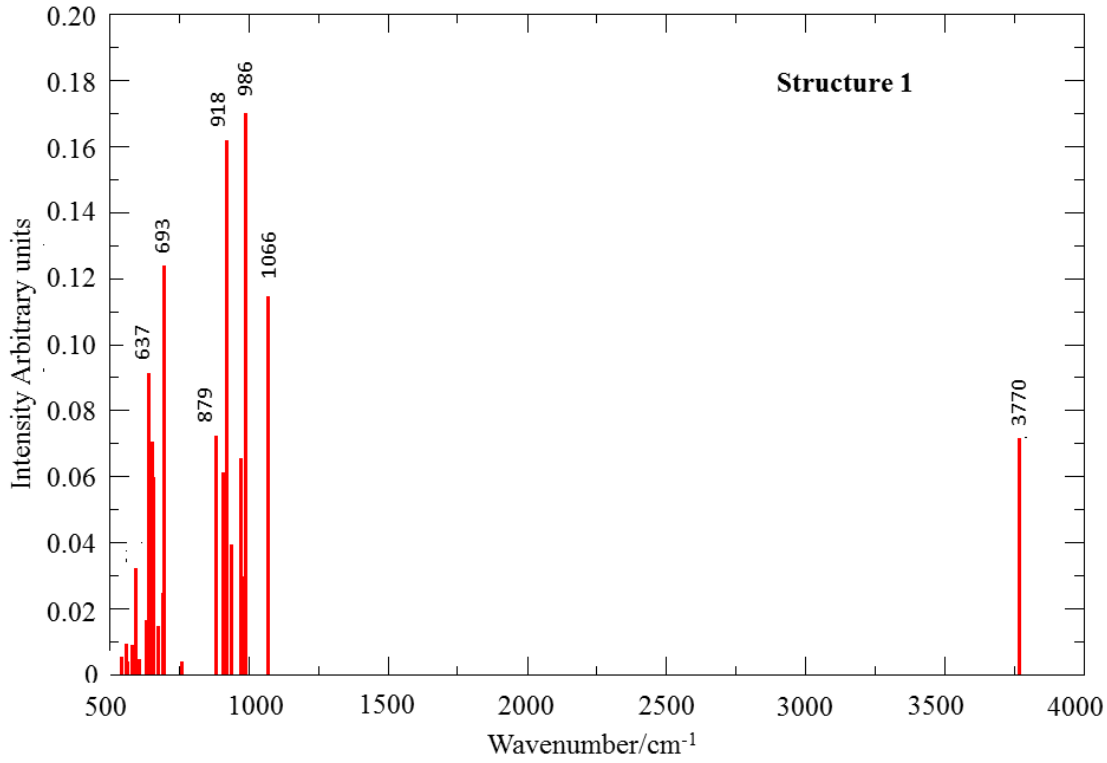

Figure S1. Calculated Infrared spectrum for Structure 1.