Characterization of decavanadate and decaniobate solutions by Raman spectroscopy

Manuel Aureliano*, C. André Ohlin, Michele O. Vieira, M. Paula M. Marques, William H. Casey, Luís A.E. Batista de Carvalho

Supporting information

Contents

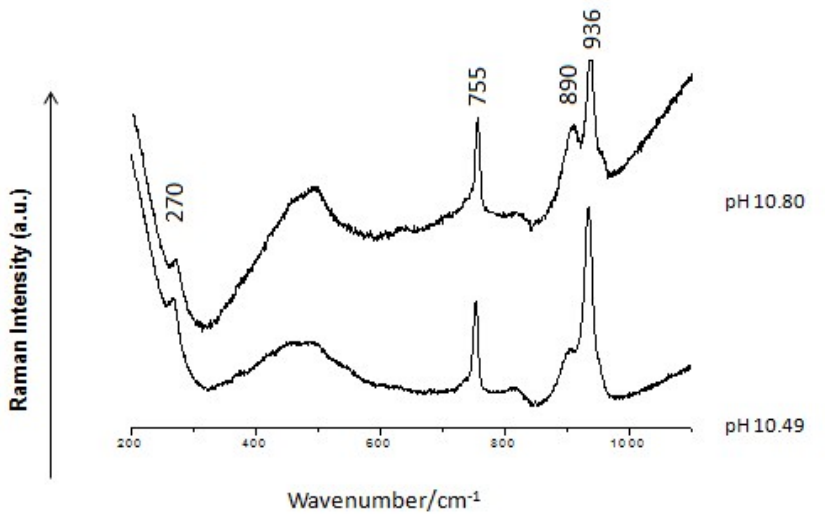

Figure S1. Raman spectra (200 to 1100 cm^{-1}) of 50 mM Nb_{10} solutions (pH 10.49 and 10.80), after two weeks at 40 ºC.

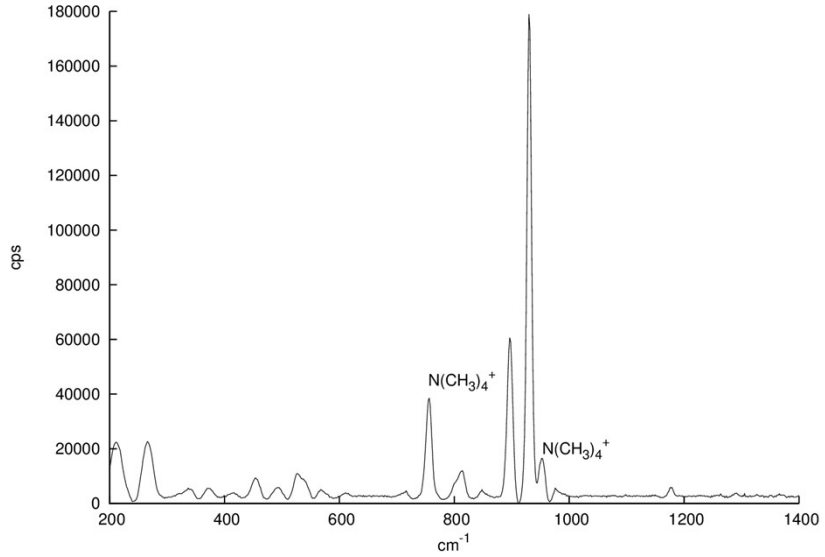

Figure S2. Raman spectrum of $[N(CH_3)_4]_6[Nb_{10}O_{28}]\cdot 6H_2O$ powder. Collected on a Bayspec Agility Raman spectrometer equipped with a 785 nm laser at 300 mW.

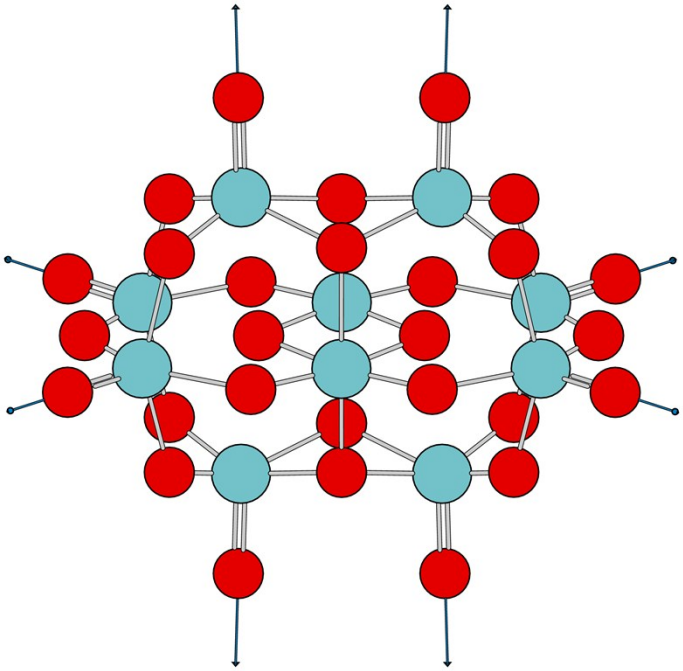

Figure S3. Illustration of computed 956.86 cm^{-1} mode of $[Nb_{10}O_{28}]^{6-}$.

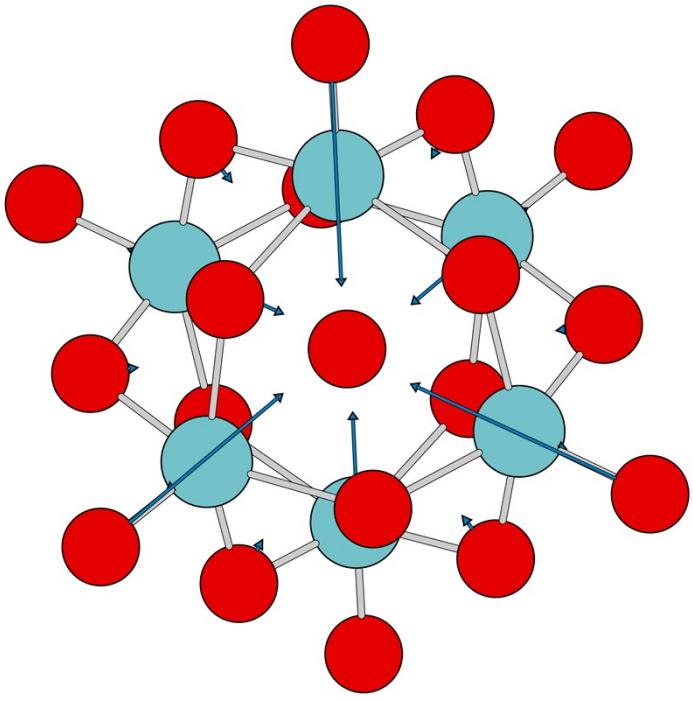

Figure S4. Illustration of computed 855.78 cm^{-1} mode of $[Nb_6O_{19}]^{8-}$.

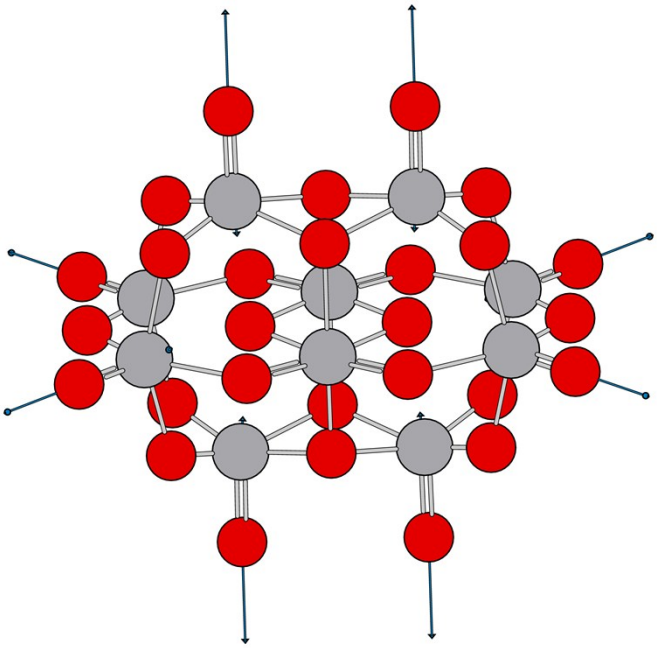

Figure S5. Illustration of computed 1058.63 cm^{-1} mode of $[V_{10}O_{28}]^{6-}$.

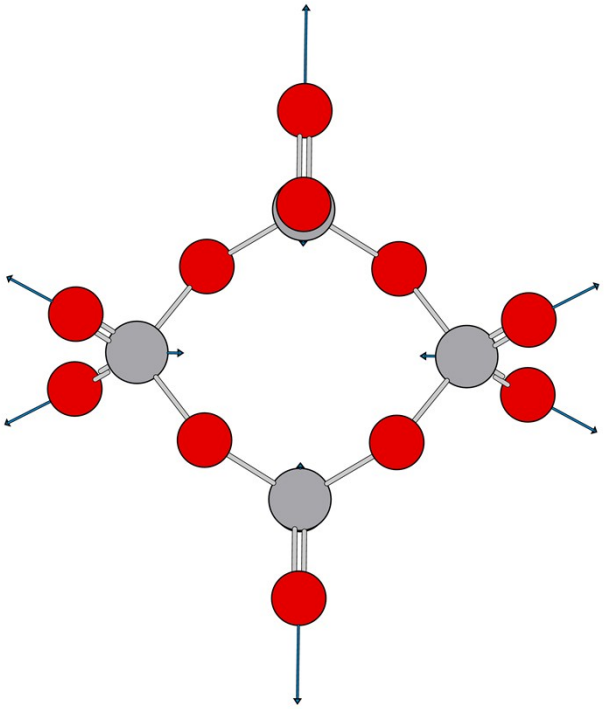

Figure S6. Illustration of computed 1001.55 cm^{-1} mode of $[V_4O_{12}]^{4-}$.

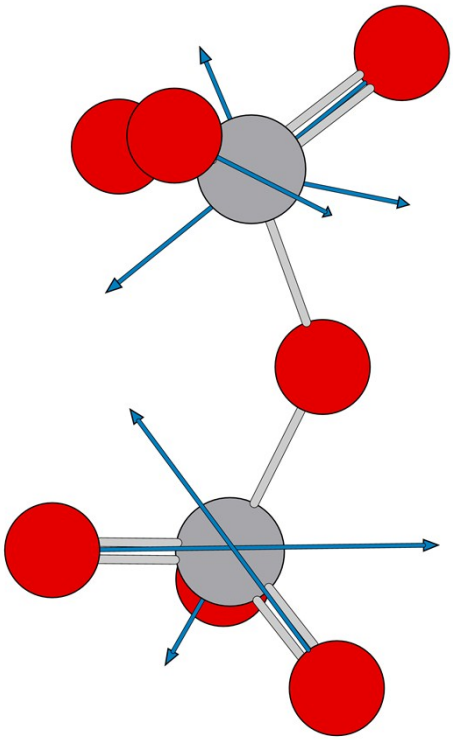

Figure S7. Illustration of computed 906.49 cm^{-1} mode of $[V_2O_7]^{4-}$.

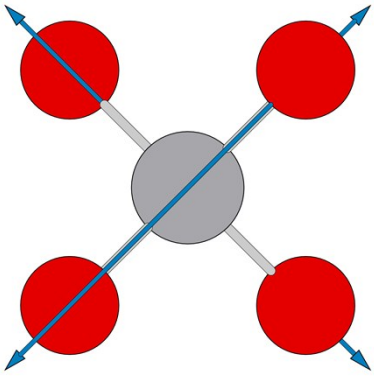

Figure S8. Illustration of computed 855.88 cm^{-1} mode of $[VO_4]^{3-}$.

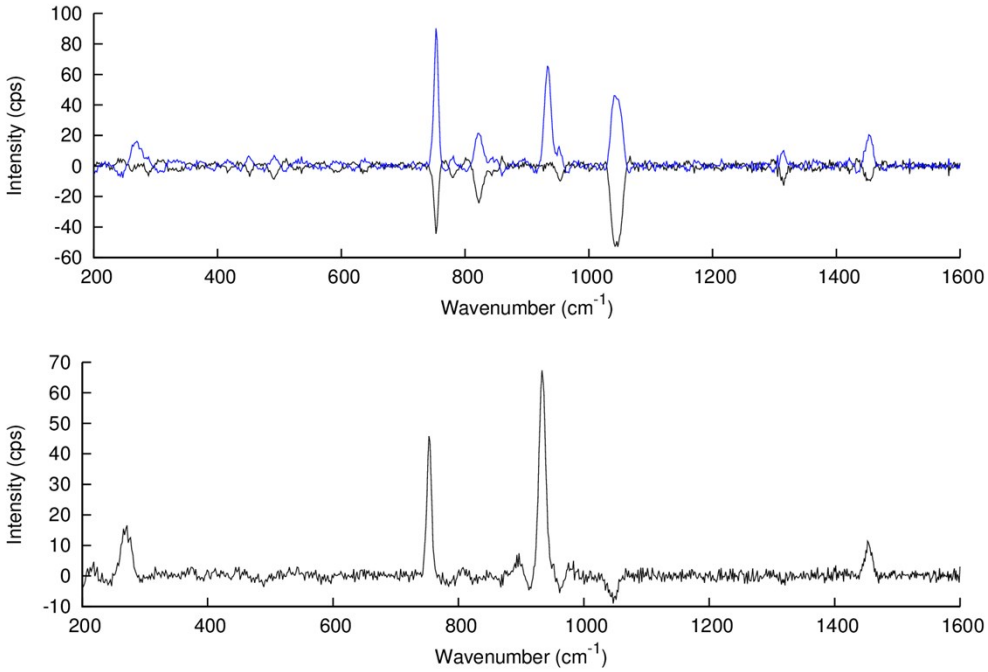

Figure S9. Top: spectra of 10 mM Nb_{10} in 0.1 M MES buffer at pH 6.13. (blue) and 0.1 M MES buffer at pH 6.13 without niobate (black). Bottom: Difference spectrum between background buffer spectrum and sample spectrum.

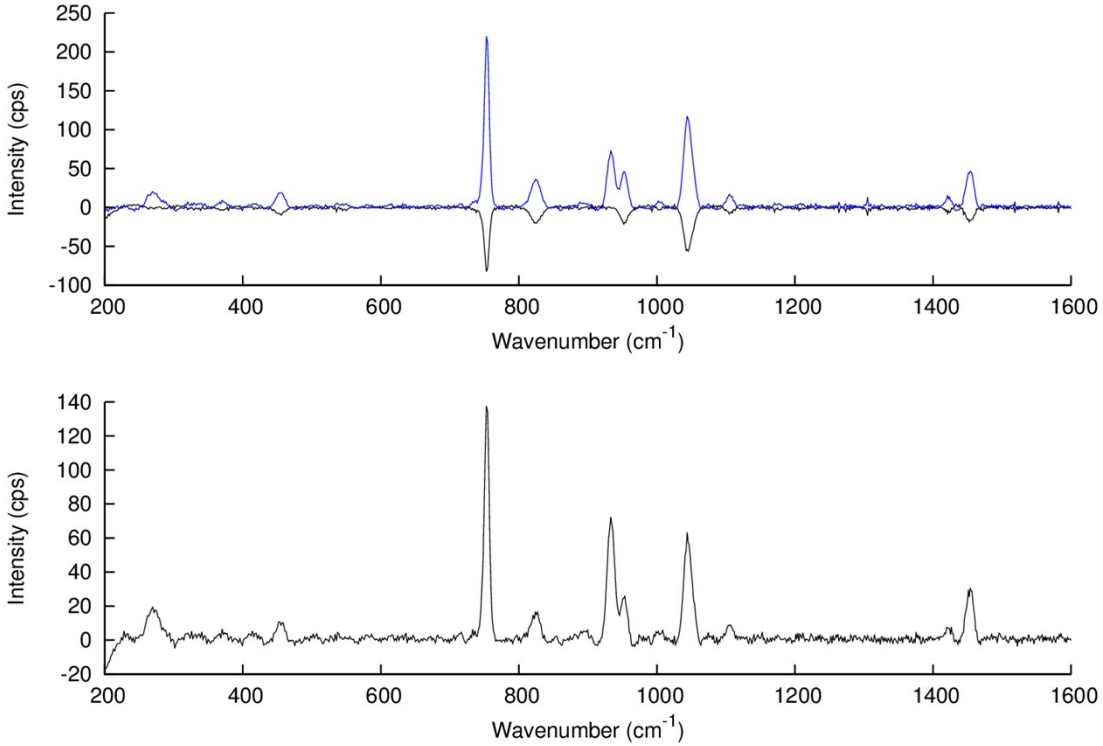

Figure S10. Top: spectra of 10 mM Nb_{10} in 0.1 M PIPES buffer at pH 7.28. (blue) and 0.1 M PIPES buffer at pH 7.31 without niobate (black). Bottom: Difference spectrum between background buffer spectrum and sample spectrum.

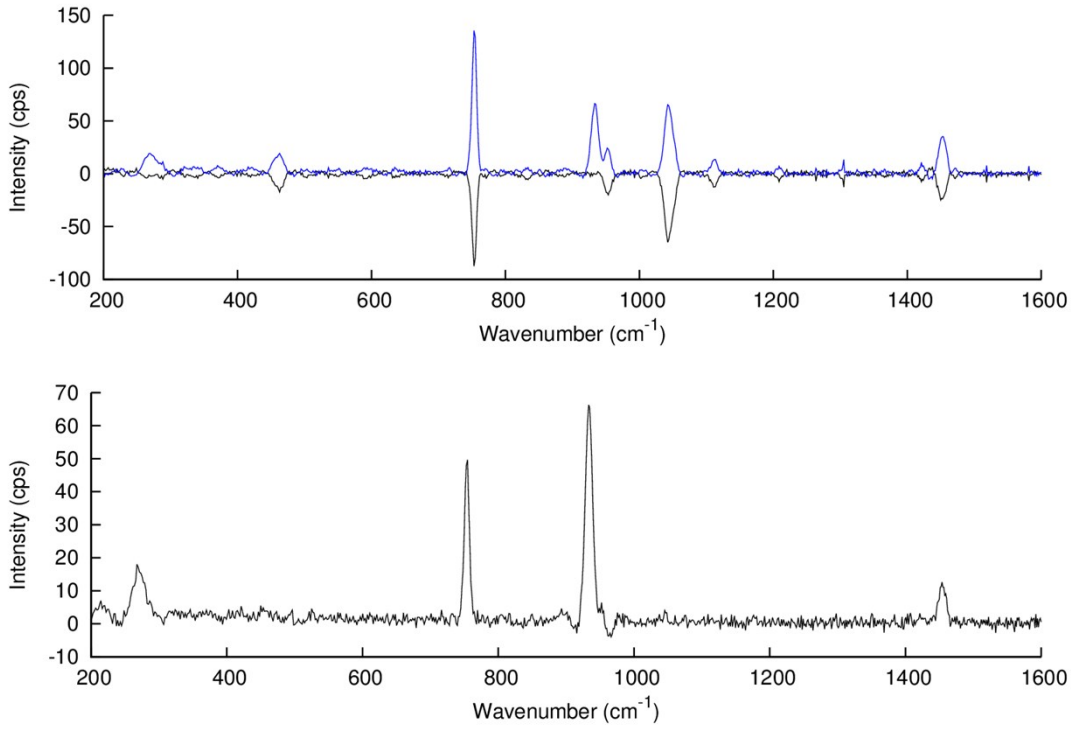

Figure S11. Top: spectra of 10 mM Nb_{10} in 0.1 M HEPES buffer at pH 8.18. (blue) and 0.1 M HEPES buffer at pH 8.11 without niobate (black). Bottom: Difference spectrum between background buffer spectrum and sample spectrum.

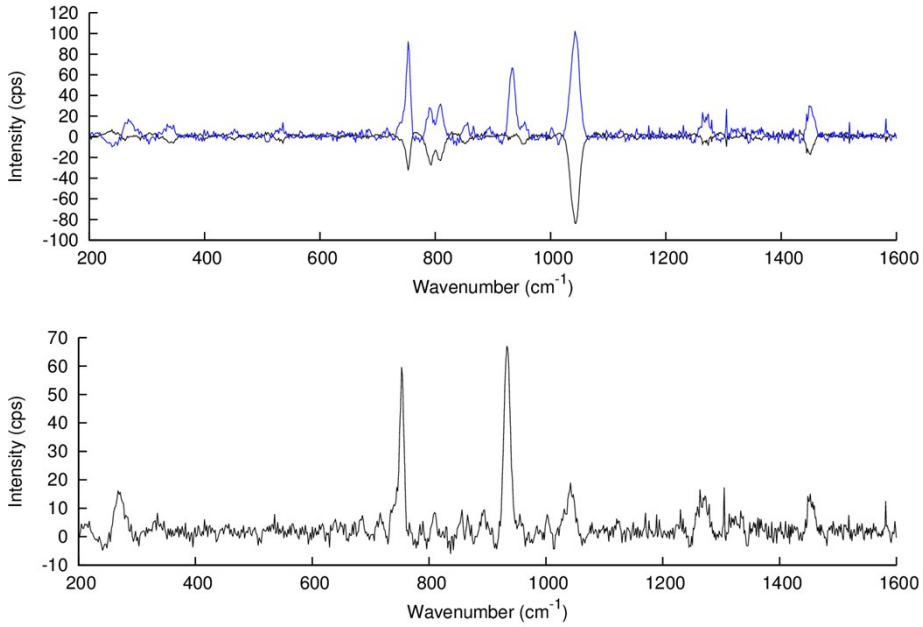

Figure S12. Top: spectra of 10 mM Nb_{10} in 0.1 M CHES buffer at pH 9.05. (blue) and 0.1 M CHES buffer at pH 9.04 without niobate (black). Bottom: Difference spectrum between background buffer spectrum and sample spectrum.

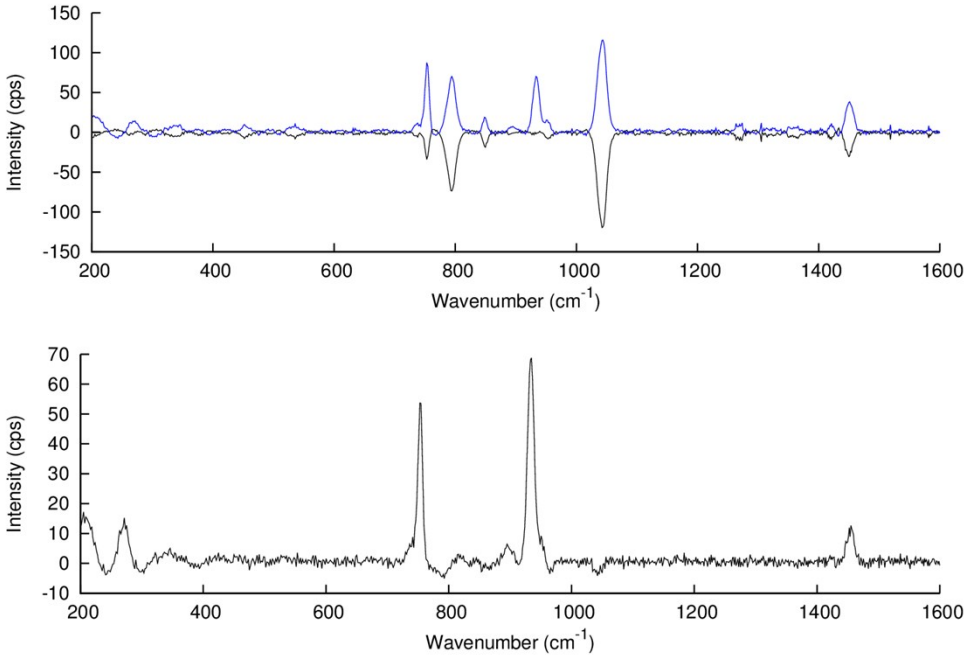

Figure S13. Top: spectra of 10 mM Nb_{10} in 0.1 M CAPS buffer at pH 10.08. (blue) and 0.1 M CAPS buffer at pH 10.13 without niobate (black). Bottom: Difference spectrum between background buffer spectrum and sample spectrum.

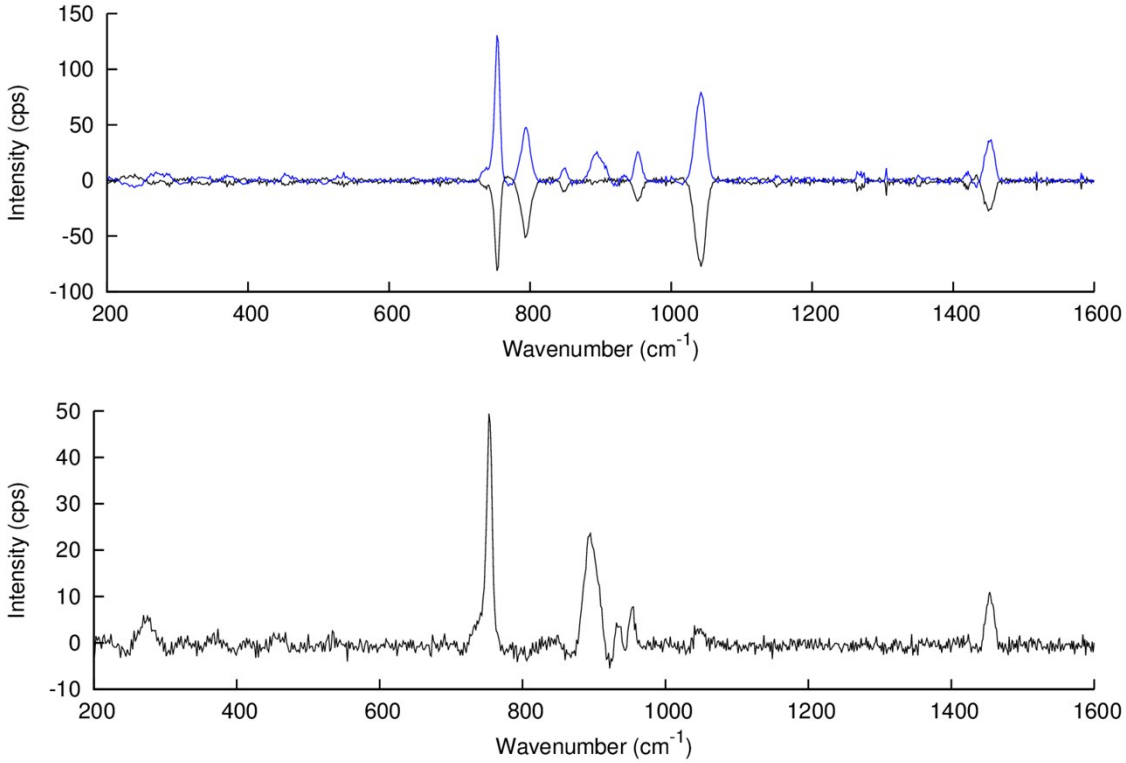

Figure S14 Top: spectra of 10 mM Nb_{10} in 0.1 M CAPS buffer at pH 11.12. (blue) and 0.1 M CAPS buffer at pH 11.38 without niobate (black). Bottom: Difference spectrum between background buffer spectrum and sample spectrum.

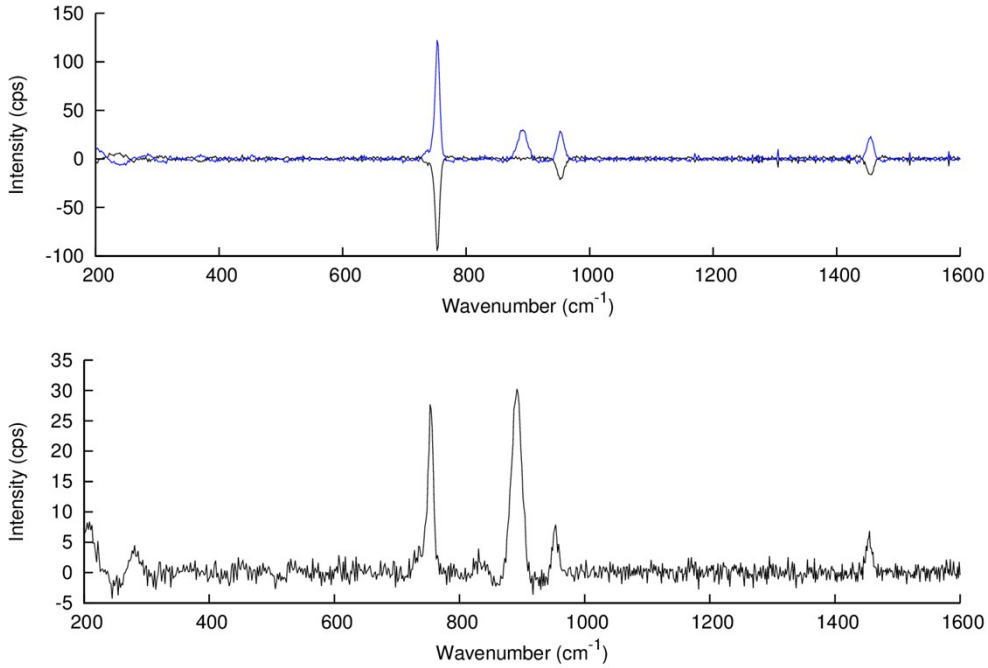

Figure S15. Top: spectra of 10 mM Nb_{10} in 0.1 M $[N(CH_3)_4]OH$. (blue) and 0.1 M $[N(CH_3)_4]OH$ buffer at pH 12.80 without niobate (black). Bottom: Difference spectrum between background buffer spectrum and sample spectrum.

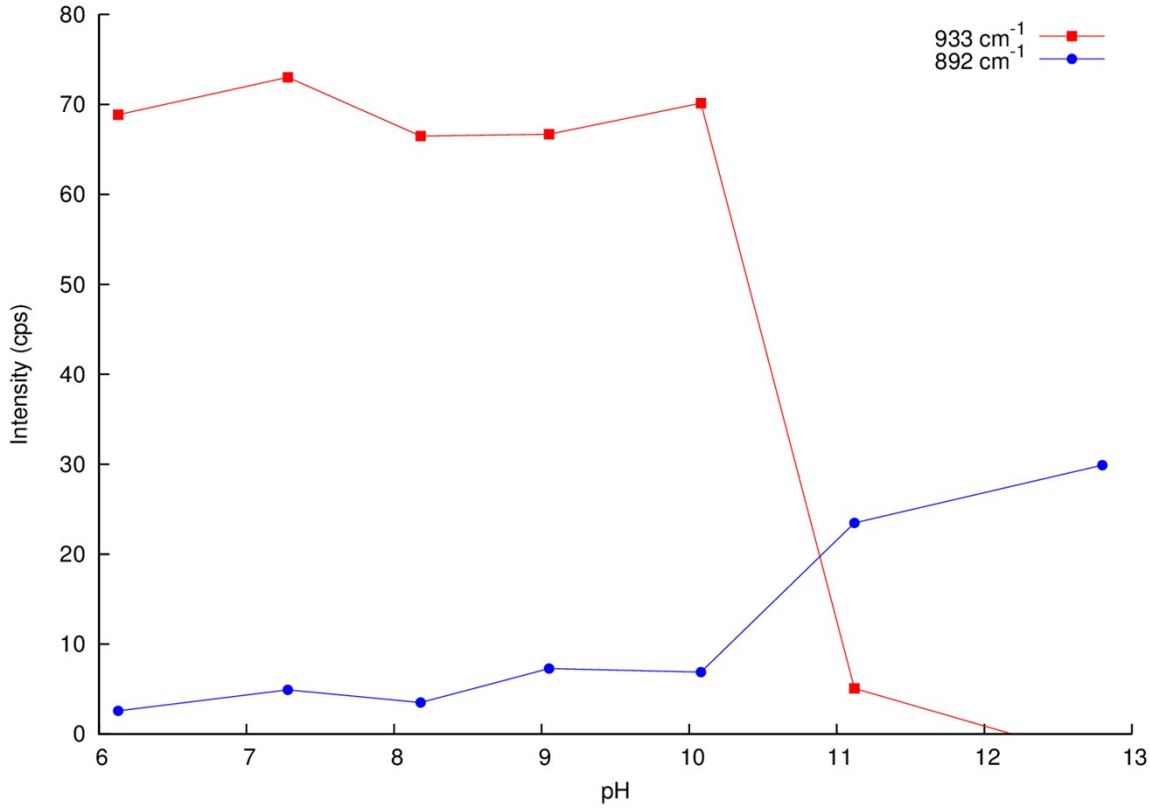

Figure S16. Intensity of the main Raman bands of Nb_{10} (933 cm^{-1}) and Nb_6 (892 cm^{-1}) as a function of pH.