

Supplementary information

## Experimental and computational exploration of the UV-visible properties of hexaniobate and hexatantalate ions

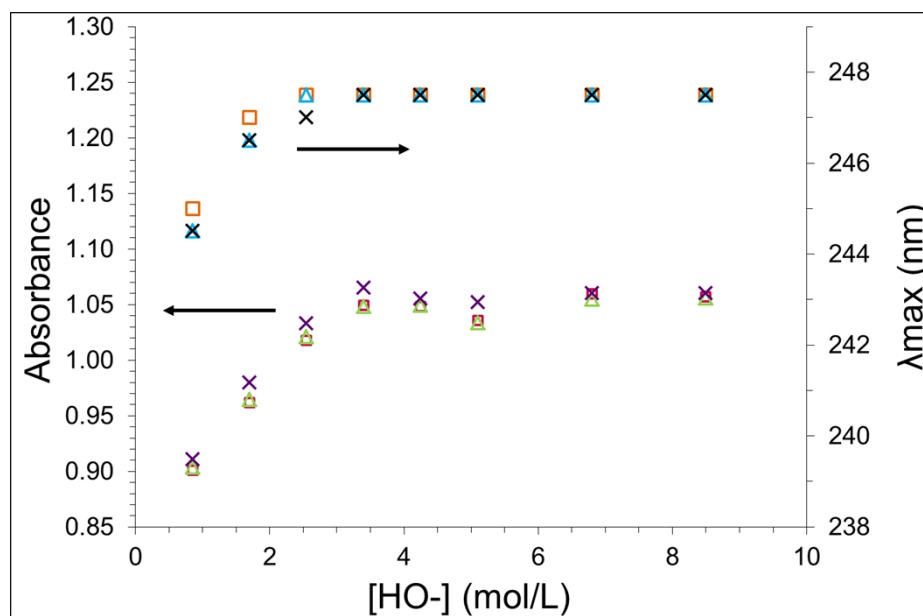
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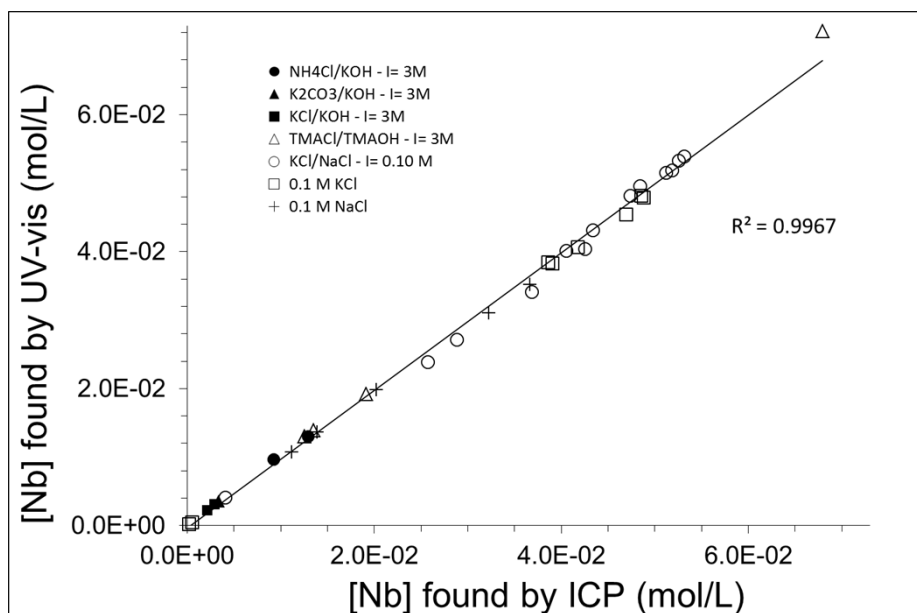
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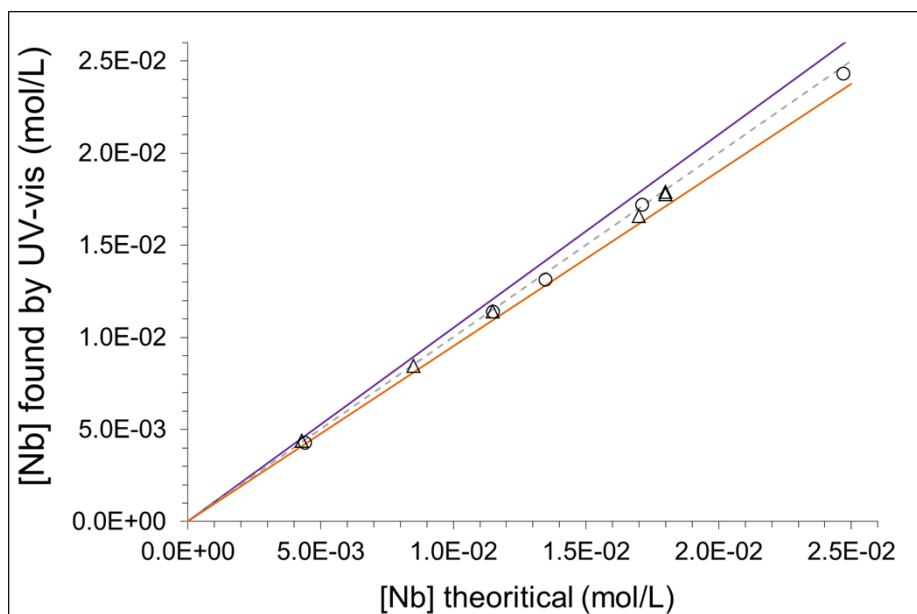
Gauthier J-P. Deblonde,<sup>\*a,b</sup> Aurélien Moncomble,<sup>c</sup> Gérard Cote,<sup>a</sup> Sarah Bélair<sup>b</sup>  
and Alexandre Chagnes<sup>a</sup>



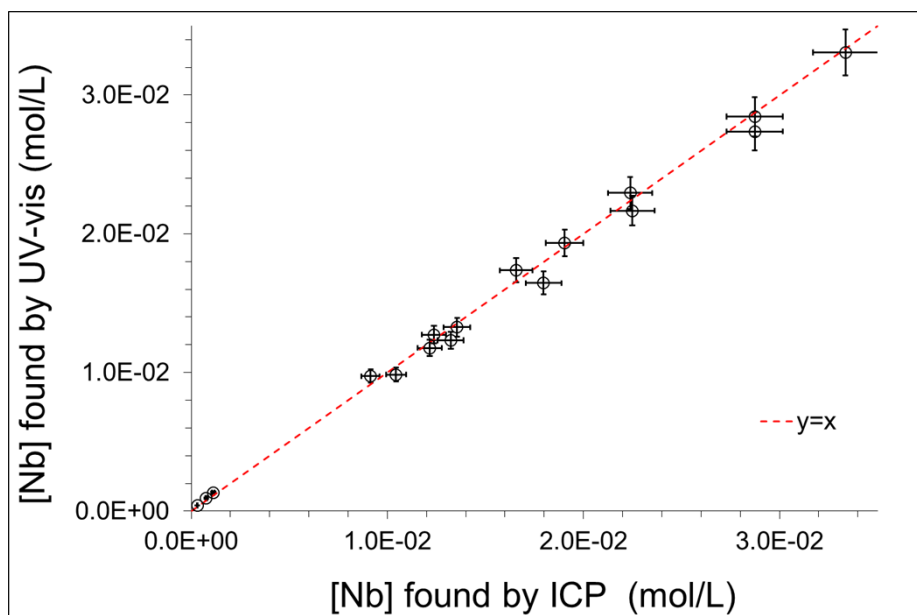
**Fig S1.** Absorbance (left axis, bottom points) and wavelength at maximum absorbance (right axis, top points) observed for hexaniobate solutions with different hydroxide concentrations. Equilibration time of 3h (squares), 11 days (triangles) and 35 days (crosses).  $T = 25\text{ }^{\circ}\text{C}$ .  $[\text{Nb}_6\text{O}_{19}]_{\text{total}} = 6.6 \times 10^{-5}\text{ M}$ .



**Fig S2.** Nb concentrations determined by ICP-AES and found by UV titration at 247.5 nm using  $\epsilon_{\text{Nb}_6\text{O}_{19}} = 15,900 \text{ L/mol/cm}$ . Samples were prepared by dissolving either  $\text{Na}_7\text{HfNb}_6\text{O}_{19} \cdot 15\text{H}_2\text{O}$  or  $\text{K}_8\text{Nb}_6\text{O}_{19} \cdot 16\text{H}_2\text{O}$  in 0.1 M NaCl (+), 0.1 M KCl ( $\square$ ), NaCl/KCl at  $I = 0.1 \text{ M}$  (o), TMACl/TMAOH at  $I = 3 \text{ M}$  ( $\Delta$ ), KCl/KOH at  $I = 3 \text{ M}$  ( $\blacksquare$ ),  $\text{K}_2\text{C}_2\text{O}_3/\text{KOH}$  at  $I = 3 \text{ M}$  ( $\blacktriangle$ ) and  $\text{NH}_4\text{Cl}/\text{KOH}$  at  $I = 3 \text{ M}$  ( $\bullet$ ).



**Fig S3.** Nb concentrations found by UV titration and theoretical concentration for samples of  $\text{Nb}(\text{HC}_2\text{O}_4)_5 \cdot n\text{H}_2\text{O}$  dissolved in water (o) and  $\text{NbCl}_5$  dissolved in HCl ( $\Delta$ ). UV titration performed in 4 M KOH using  $\epsilon_{\text{Nb}_6\text{O}_{19}} = 15,900 \text{ L/mol/cm}$  at 247.5 nm. The violet solid line, the grey dotted line, and the orange solid line correspond respectively to  $y = 1.05 \cdot x$ ,  $y = x$  and  $y = 0.95 \cdot x$ .



**Fig S4.** Nb concentrations determined by ICP-AES and found by UV titration for 17 industrial samples containing Nb and Ta (Nb/Ta= 80 mol/mol). UV titration performed in 4 M KOH using  $\epsilon_{\text{Nb}_6\text{O}_{19}} = 15,900 \text{ L/mol/cm}$  at 247.5 nm. The red dotted line corresponds to  $y=x$ .