Free Energy of Hydration of Niobium Oxide

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FREE ENERGY OF HYDRATION OF NIOBIUM OXIDE (U)

SUMMARY

Some of the glasses being formulated by SRTC researchers contain niobium oxide. In this report, the free energy of hydration of the oxide is calculated ($\Delta G^\circ_{\text{hydration}} = +12.26 \text{ kJ/mol}$, or $+2.93 \text{ kcal/mol}$), from the free energies of formation of the oxide, the hydroxide, and water. This value can be used in calculations of the free energy of hydration of glasses containing niobium.

CALCULATION

There is very little information about niobium in glass, primarily due to its rarity and cost. Potentially, niobium could exist as either Nb_2O_3 , NbO_2 , or Nb_2O_5 in borosilicate glasses. However, based on the discussion in Volf,¹ it is clear that the +5 oxide is much more likely to be the form in glass. This is supported by the aqueous chemistry of Nb, where Nb^{+4} is not stable in aqueous environments, and Nb^{+3} is only stable at low Eh and pH.^{2,3} Thus, the calculation has been based on Nb_2O_5 .

The hydration reaction is

The free energies of formation of the reactants and product are⁴

<u>Compound</u>	<u>ΔG°_f (kJ/mol)</u>
Nb_2O_5	-1766.0
H_2O	-228.572
$\text{Nb}(\text{OH})_5$	-1448.3

Thus, the free energy of the hydration reaction is $2 \times (-1448.3) - 5 \times (-228.572) - (-1766.0) \text{ kJ/mol}$, or $+12.26 \text{ kJ/mol}$. Dividing by 4.184 kJ/kcal yields a value of $+2.93 \text{ kcal/mol}$. This value should be used for calculations of the free energy of hydration of glasses.

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