

## **Effect of thermodynamic database selection on the estimated aqueous uranium speciation**

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Comparisons of the completeness and accuracy of the thermodynamic databases for aqueous uranyl complexes involving common inorganic anions ( $\text{OH}^-$ ,  $\text{SO}_4^{2-}$ ,  $\text{PO}_4^{3-}$ ,  $\text{CO}_3^{2-}$ ,  $\text{SO}_4^{2-}$ ,  $\text{Cl}^-$ ,  $\text{F}^-$ ,  $\text{I}^-$ ,  $\text{Br}^-$ ) and some organic ligands have been made between a number of publicly-available thermodynamic databases (MINTEQA2, LLNL, WATEQ4F, ThermoChimie, NEA-TDB, and PSI/Nagra).

Although the stability of the stronger bioavailable uranyl-phosphate complexes remains uncertain, the available thermodynamic data suggests that the proportion and toxicity of most uranyl-phosphate complexes will be negligible when the pH exceeds 8.5 and the inorganic phosphate concentration (as  $\text{PO}_4^{3-}$ ) is less than 2 mg/L.

Detailed information:

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