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NEA-TDB update book on U, Np, Pu, Am and Tc: overview, systematic trends and datagaps of relevance to nuclear waste disposal

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Within the scope of the OECD Nuclear Energy Agency (NEA) Thermochemical Database (TDB) Project, a comprehensive critical review of thermodynamic data available for inorganic compounds and aqueous complexes of U, Np, Pu, Am and Tc with focus on the relevance to waste disposal safety has been completed, and was released by October 2020. The review work covers all new studies available since the release of the previous NEA–TDB update volume [1] and up to 2015, extending in some cases with publications up to 2017. The volume provides selected thermodynamic data for more than 150 new aqueous species and solid compounds, over a total of almost 800. This represents a vast amount of critically reviewed, high quality self-consistent thermodynamic data for a number of relevant inorganic systems of U, Np, Pu, Am and Tc. In this framework, the objective of this contribution is three-fold:

(i) to summarize the most significant modifications and improvements achieved in this review with respect to previous volumes;

(ii) to make use of the large body of high quality thermodynamic data to explore and to gain further insight on systematic trends along series of analogous chemical elements / oxidation states. Particular focus is given to the actinide systems U, Np, Pu and Am reviewed in this update book, but extending to Th as critically reviewed in the corresponding NEA–TDB volume. The exercise targets equilibrium constants of aqueous species and amorphous solid phases, thermodynamic formation functions of crystalline solid compounds and (SIT) ion interaction coefficients;

(iii) to identify thermodynamic datagaps in systems of relevance in the context of nuclear waste disposal, *i.e.* with focus on reducing and alkaline systems, temperature conditions < 100 °C and relevant inorganic ligands (hydroxide, carbonate, silicate, etc.). The role / relevance of amorphous solid phases in the context of nuclear waste disposal (especially for M(IV) systems, with M = Th, U, Np, Pu and Tc) and the feasibility of providing a thermodynamic description of their chemical behaviour will be also discussed.

[1] R. Guillaumont, T. Fanghänel, J. Fuger, I. Grenthe, V. Neck, D. A. Palmer, M. H. Rand. OECD NEA Data Bank (2003)