# Thermo-Calc Software

Database name:	TCS Pure Radionuclides Database	Database acronym:	NUMT2
Database owner:	Thermo-Calc Software AB	Database version:	2.1
Database segment:	Nuclear Materials		

#### **Brief Description**

NUMT2 is suitable for calculations in nuclear materials. Database for about 600 condensed and gas phase substances, including pure radio nuclides.

## **Applications**

This database can be applied to a wide range of nuclear related applications, which can be modelled adequately, or to a first approximation, using pure substances. However, it can also be coupled with other pure substance databases (e.g. SSUB) and/or solution databases (e.g. NUOX, SSOL and TCFE) to increase the range of applications which can be studied.

## **Included Elements**

Ag	Al	Am	В	Ва	Bi	С	Ca	Cd	Ce	Cl	Со	Cr	Cs	Eu	F	Fe
Н	I	In	Kr	La	Mg	Mn	Мо	Na	Nb	Nd	Ni	0	Pd	Pr	Pu	Rh
Ru	Sb	Si	Sn	Sr	Тс	Te	U	Xe	Zr							

## **Included** Phases

Total amount of different phases is 248 and it includes a gas mixture phase. Hence, for vaporization calculations, the database can also be used in conjunction with any other database (such as NUOX) which requires the gas phase species. It is compatible with PURE (the SGTE Pure Elements Database), SSUB (the SGTE Substances Database), SSOL (the SGTE Solutions Database), and NUOX (the UES Nuclear Oxides Database).

## **Assessed Systems**

NUMT2 contains critically-assessed thermodynamic data for pure substances, which were of relevance to calculations for various nuclear applications. The current version has been both updated and expanded. It contains pure radionuclides in the following 15-element framework: Ba, Ce, Cs, I, La, Mo, Pd, Pr, Pu, Rh, Ru, Sr, Te, U and Zr.

It should be stressed that this current database is still only intended as a supplement to other pure substance databases (such as SSUB) for applications in nuclear materials related systems. The reference state of the Gibbs Energy function is the enthalpy of the elements in their standard states at 298.15 K [i.e., G-H(SER)].

## Limits

As in the spirit of the CALPHAD method, predictions can be made for multicomponent systems by extrapolation into multicomponent space of data critically evaluated and assessed based on binary, ternary and in some cases higher order systems. However, critical calculations must always be verified by equilibrium experimental data; it is the user's responsibility to verify the calculations but Thermo-Calc Software AB is interested to know about any significant deviations in order to improve any future release.

## **Scientific Models & References**

See the Thermo-Calc Software reference list and reference library at: <u>http://www.thermocalc.com/resources/</u>

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