# Thermodynamics computer exercise 1

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## Problem 1.

**Prepare in Microsoft Excel worksheet a table with the data for Fe and Ni at 300-1500 K with a 50 K interval. Collect the data (in J/mol) using the Tsim and HSC software. Plot in Excel, the for Fe and Ni data against temperature. If there is a difference between both databases, explain briefly.**

In figure 1 and 2, the temperature dependence of the values for iron and nickel were plotted using two different databases, HSC and Tsim. The databases slightly disagree about the location and magnitude of the ‘peaks’. The plotting resolution of 50 K maybe insufficient for capturing the exact location or size of the peak, if it is very sharp. The coarse resolution may cause even a small discrepancy between the two databases to appear moderately large in areas where the curve is sharp. Another reason for the observed difference is that the databases are constructed from different experiments, which leads to variation in results.

Fig. 1. The temperature of the of iron according to the HSC and Tsim software.

Fig. 2. The temperature of the of nickel according to the HSC and Tsim software.

## Problem 2

**Using HSC software calculate the enthalpy (in J/mol) for Fe, Ni and Pb. Consider the temperature range between 300 and 2000K with a 50K or lower interval. (i) Using this database, give the melting point (in K), the density (g/cc) and the molecular weight (g/g-mol). (ii) Plot in Excel, the H­T data against temperature.**