Chemical Thermodynamics for Process Simulation
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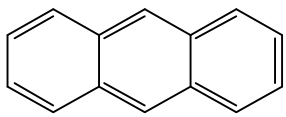
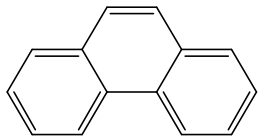
Example 08.01 Solubility of Anthracene and Phenanthrene in Benzene

problem:

Calculate the solubility of anthracene (1) and phenanthrene (2) in benzene at θ=20°C. For the calculation it should be assumed that the binary systems show ideal mixture behavior (γ_i=1).



anthracene



phenanthrene

general constants and definitions:

$kPa := 1000Pa \qquad dm := 0.1m \qquad R := 8.31433 \frac{J}{K \cdot mol}$

input data

$ncomp := 2 \qquad i := 1..ncomp$

$T := (273.15 + 20)K$

$T_m := \begin{pmatrix} 489.6 \\ 369.4 \end{pmatrix} K \qquad \Delta h_m := \begin{pmatrix} 28860 \\ 18640 \end{pmatrix} \frac{J}{mol}$

Solution

First calculate the logarithm of the activity of the pure solid component at 20°C:

$$\ln a_i := \frac{-\Delta h_{m_i}}{R \cdot T} \cdot \left(1 - \frac{T}{T_{m_i}}\right) \qquad \ln a = \begin{pmatrix} -4.751 \\ -1.579 \end{pmatrix}$$

In an ideal liquid mixture, the activity in the liquid phase is equal to the mole fraction (solubility).

$$x_i := e^{\ln a_i} \qquad x = \begin{pmatrix} 0.0086 \\ 0.2063 \end{pmatrix}$$

Both components are chemically very similar but show a large difference in solubility. This is mainly due to the significant difference in melting temperature and to a smaller extent because of the different heats of fusion.