Aqueous-Al

Test example for fitting multiple aqueous species independent (type F) and reaction constrained (type R). For one of the reactions (AlOH+2) the logK values are calculated using a logK function of water density (logK_dRHOw function and coefficients described in LogKFun) and literature parameters, and for a second one (NaAl(OH)4@) it uses the logK values from the input system file calculated in the initial step.

The test also uses the nested functionality to fix the calculated pH at each optimization step to the measured one by titrating NaOH and HCl.

Calcite-Strontianite Test example for fitting Calcite-Strontianite solid solution interaction parameters against excess Gibbs energy data, without using full equilibrium calculations (UseEqC set to -1 - no equilibrium, instead of 1 with equilibrium)

CSH-solid-solution

Test example for fitting G0 of end members and non ideal interaction parameters for a CSH solid-solution against measured Ca(aq), Si(aq), Ca/Si in solid, and mean silicate chain length (mChainL).

EuSorption

Test example for fitting G0 of sorption sites against Rd (partition coefficient) measured values form experiments with and without the presence of air.

TestPtizer

Test example for fitting Pitzer interaction parameters as a function of T and P against synthetic experimental data from Archer et al. (1992). Using 120% +- bounds from initial values for the parameters (PBPerc set to 120) – convergence problems – needs to be checked / updated.

Ti-in-Quartz

A. Test example for fitting Ti in quartz regular solid solution model parameters against experimental data of Thomas et al., (2010) and Wark and Watson (2006). TiQ_normal

B. Using the fitted parameters from TiQ_normal for doing invers modeling calculations determining the T &P of formation of quartz crystals based on their Ti content. TiQ_inverse. Results are found in Inv. Mod. Results tab of the Results window.