Thermodynamic calculator for clay minerals

This calculator currently works for 10 Å clays, but at present, I do not know how the cations are distributed among sites for 7 and 14 Å clays. Currently, the calculator is only for computing the enthalpy of formation of a mineral at standard state.

Example mineral: nontrite (K) – K0.34Fe3+1.67Al0.67Si3.66O10(OH)2

Input cells D3 – D75:

Start by entering the chemical formula into A1 (optional). Enter the number of moles into C1.

The number of moles of cations can be entered directly for the interlayer sites (e.g. 0.34 in cell D3). For the octahedral sites, the M2 sites get filled first with up to 2 moles of cations and the remainder gets placed into the M1 sites. For nontrite, no cations will go into the M1 site, because the M2 site will use up all of the Al and Fe. The tetrahedral sites take 4 moles of cations, and all of the Si goes into the tetrahedral sites, leaving 4 – 3.66 = 0.34 moles of Al for the tetrahedral site, and 0.67 – 0.34 = 0.33 moles Al for the M2 site. For an example where the M1 site receives cations (M2 overflow), consider Saponite Fe with the octahedral sites as Mg2Fe+2. Given that there are 3 moles, and the M2 site can only take 2 moles, the Mg will occupy (2/3)\*2 = 1.33 moles and the Fe will occupy (1/3)\*2 = 0.67 moles. The M1 sites will take the remaining 2 – 1.33 = 0.67 moles of Mg and 1 – 0.67 = 0.33 moles of Al. Si, Al and Fe are equally shared amongst T1 and T2 sites. For the example of nontrite, the T1 and T2 sites will both receive 1.83 Si and 0.17 Al.

The hydrogen sites get filled by the number of moles of H in the hydroxide. For example, with nontrite, there will be 2 moles of H in the Hi site.

To verify that the mineral is charge balanced, cell G78 will be highlighted green if the charge on all oxygen atoms is satisfied and highlighted red otherwise.

Columns:

Sheet 1 (input): A lot of the computations are done in this sheet, but to compute the enthalpy of formation of the oxide in the mineral (Eq. 10) requires knowledge of the site specific interaction terms that are computed through matrix operations in sheets “site Mtx”, with mixing energy between cations in the I, M2 and M3 sites in sheets “I mix”, “M2 mix” and “M3 mix”.

D: number of moles of cation in given site.

E: Charge of cation (z).

F: Half charge of cation (x = z/2).

G: number of moles of cation bonded to oxygen (n\*x).

H: enthalpy of cation in clay (ΔHO=Mz+(clay)) from minimization of Blanc et al. (2105).

I: Enthalpy of formation of oxide. Oxides of major elements taken from Blanc et al. (2015) and all other oxides taken from Appendix B in Faure (1998).

J: Computation of first term in Eq. 14.

K: Computation Eq. 14, which is column J + mixing energy

L: number of moles of cation bonded to one oxygen in the oxide.

M: First term in Eq. 9.

O: Sum of first term in Eq. 9

P: Eq. 10 (second term in Eq. 9)

Q: Water correction term that is mentioned nowhere in Blanc et al. (2015). I discovered this term through a communication with P. Viellard.

R: The output: ΔHof of the mineral