Dear colleague,

Thanks you very much for your interest in our paper. Enclose an excel sheet corresponding to the calculations of enthalpy of formation for some end-members smectites (Table 14 of amer. J. Sci).

I provide you some details of computations ;

Cases A10 to B26 : enthalpies of formation from elements of some oxides involving in the calculations of enthalpy of formation of clay minerals from the estimated enthalpy of formation from constituent oxides

**Chemical composition of clay minerals (columns B to AT)**

Column A : Name of clay minerals

Columns B to G : Chemical composition of interlayer site

Column H : number of oxygen bound to interlayer cation

Columns I to N : Chemical composition of M2 site and sum

Column O : number of oxygen bound to M2 site

Columns P to U: Chemical composition of M1 site and sum

Column V : number of oxygen bound to M1 site

Columns W to AC: idem for M3 site

Column AD-AI : idem for M4 site

Column AJ-AM : idem for tetrahedral siteT1

Column AN-AQ : idem for tetrahedral siteT2

Column AR, AS, AT : number of oxygen bound to hydrogen respectively in Octahedral site Hi (internal), bruciic site Hb and external site ( He only for 7 Å)

Column AU checking of the stiochiometric formula

**Calculation of enthalpy of formation from oxides**

Parameters DO= cations for differents cation in different sites are given in case BT28-CC33 (see tables 4 and Table 11 for Li (interlayer and Brucitic), Mg (Interlayer) and Fe+3 (Tetrahedral)

Column BI to CB display calculated number of oxygen bound to site and calculated DHO= site for all the 10 sites :

Interlayer site : columns BI-BJ

M2 site : columns BK-BL

M1 site : columns BM-BN

M3 site : columns BO-BP

M4 site : columns BG-BR

T1 site colume BS-BT

T2 site : columns BU-BV

HI site : columns BW-BX

Hb site : columns BY-BZ

He site : Columns CA-CB

Columns CC, CD and CE displays the interactions energy between cations respectively in site Interlayer, M2 and M3 . these values are already included in column BJ, BL and BP). It helps to see the magnitude of mixing energy with a gien distribution.

**Calculation of the enthalpy of formation of clays**

Colume CF gives the enthalpy of formation of compounds that is the summation of product molar fraction of oxygen and difference of parameters DHO= site (equation 10)

Columns BA reported value of column CF

Column BB corrected value of DH°ox versus value of liquid water

Column BC enthalpy of formation of smectite calculated frm column BB and summation of enthalpy of formation of oxides).

The value given in column BC is the same as given in table 14.

I hope that there will be no problem in the processing of computation.

Please contact me if you have any problems. A new software is in preparation for all cations includings entropy, magnetic and configurations entropy, heat capacity and solubility products at different temperatures by the Van ‘ Hoff model.

Hoping to have some results and Best regards

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