Identification of the transcription errors and methodological problems summarized above is intended to assist future users of the subregular model. Application of this model requires considerable care and attention to detail because of the large number of steps and equations involved. It is recommended that users consider the points raised here and confirm their own procedures can reproduce the values reported by Elprince et al. (1980) and Chu and Sposito (1981), subject to the corrections noted above.

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References


Reply to “Comments on Application of the Subregular Model for Prediction of Ternary Cation Exchange”

Chu and Sposito (1981) developed a thermodynamic theory of ternary cation-exchange systems whose principal results are closed-form equations for rational activity coefficients \(f_i\) and exchange equilibrium constants \(K_{ij}\):

\[
Z_i Z_j \ln f_i = -Z_i (1 - E_i) \ln K_{jic} - Z_k E_k \ln K_{jkc}
\]

\[
\ln K_{ij} = \int_{(E_i=0,E_j=0,E_k=0)}^{(E_i=0,E_j=1,E_k=0)} \left( \ln K_{jic} dE_j - \frac{Z_i}{Z_k} \ln K_{jkc} dE_k \right)
\]

any path

where \(ijk\) is any cyclic permutation of \(123\), \(E_i\) is the exchanger-phase charge fraction of cation \(i\) whose valence is \(Z_i\), and subscript \(c\) denotes a conditional equilibrium constant. Equations [1] and [2] reduce to well-known expressions for binary systems, and the path independence of Eq. [2] with an example of Na\(^+\)\textrightarrow Ca\(^{2+}\) exchange on specimen montmorillonite. The large magnitude of the standard deviation in the estimate of \(c_0\) could simply reflect the large scatter in the data of Elprince et al. (1980, Fig. 3), or it could signify that the ternary subregular model does not provide a good description of ternary exchange systems, can find a review of studies carried out exclusively.

Chu and Sposito (1981, Table 1) in the course of applying it to the data of Elprince et al. (1980, Fig. 3), or it could signify that the ternary subregular model does not provide a good description of ternary exchange systems, can find a review of studies carried out exclusively.

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Bond and Verburg (1997), as well as others experienced in the thermodynamics of cation-exchange systems, can find a review of studies carried out exclusively.