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Updated and extended activity–composition models for thermodynamic calculations in metapelitic systems

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The recent publication of an improved and updated internally consistent thermodynamic dataset (ds6; Holland and Powell, 2011, Journal of Metamorphic Geology 29, 333–383) including a new equation of state for solids greatly enhances the potential to undertake quantitative calculations on rocks in expanded chemical systems and under a wider range of P–T conditions than was previously possible. However, to be compatible with the new dataset requires that many of the existing activity–composition (a–X) relationships for solid solution phases be modified, a task that is ongoing and non-trivial. Here we report on progress primarily related to the modification and refinement of a–X models for minerals appropriate to metapelitic phase equilibria. Aspects of the models have been calibrated using large dataset ($n > 1000$) of naturally occurring mineral pairs compiled from the literature. The natural dataset has enabled an examination of the fundamentally important partitioning of Fe and Mg for consistency with the new dataset, as well as providing the framework for including Mn in the models for relevant phases. Many of the models for commonly-occurring metapelitic minerals have been updated and expanded with greater consideration of order-disorder, ferric iron and titanium along with a re-assessment of the values for the non-ideal mixing parameters (W). For example, chlorite now involves Fe–Mg order-disorder and a ferric iron endmember, cordierite has been made non-ideal and staurolite now includes both ferric iron and titanium endmembers. These improvements will provide a much more consistent set of models than currently available and permit quantitative modelling of metapelitic rocks in the comprehensive MnNCKFMASHTO system.