Quantifying geological uncertainty in metamorphic phase equilibria modelling; a Monte Carlo assessment and implications for tectonic interpretations

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APPENDIX A – SETUP CONDITIONS AND SOLID-SOLUTION MODELS UTILISED FOR PSEUDOSECTION MODELLING

In both case studies, pseudosection construction was performed using Theriak-Domino version 01.08.09 (de Capitani, 1994) and the internally consistent thermodynamic dataset ds55 (Holland and Powell 1998, updated to August 2004) in the MnO–Na_2O–CaO–K_2O–FeO–MgO–Al_2O_3–SiO_2–H_2O–TiO_2–O_2 (MnNCKFMASHTO) compositional system using the following *a*–*x* relations: garnet (White et al., 2005), orthopyroxene (White et al., 2002), silicate melt, biotite, ilmenite–hematite, spinel–magnetite (White et al., 2007), staurolite, cordierite (Mahar et al., 1997; Holland and Powell, 1998), ternary feldspar (Baldwin et al., 2005), epidote (Holland and Powell, 1998), chlorite (Holland et al., 1998), chloritoid (White et al., 2000), and muscovite–paragonite (Coggon and Holland, 2002). Andalusite, kyanite, sillimanite, rutile, quartz, and H_2O were treated as pure phases. Calculation of uncertainties on the *P*–*T* conditions of isopleths and modal proportion contours was performed using THERMOCALC version 3.37 (Powell and Holland, 1988) with the same thermodynamic dataset and solid solution models. For point-counted bulk compositions, bulk-rock H_2O content was calculated directly from the proportion of hydrous phases present, with the contribution from biotite adjusted from stoichiometric proportions to account for the incorporation of Ti by a deprotonation substitution (Waters and Charnley, 2002; White et al., 2007). For OD68-12, the resulting calculated H_2O content is low, consistent with the preservation of a high-temperature assemblage (White and Powell, 2002). Al_2O_3–FeO–MgO compatibility diagrams were calculated using THERMOCALC with the same thermodynamic dataset and solid-solution models described above.

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