



Thermodynamic modeling using BINGO-ANTIDOTE: A new strategy to investigate metamorphic rocks

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BINGO-ANTIDOTE is a new program, combining the achievements of the two petrological software packages XMAPTOOLS[1] and THERIAK-DOMINO[2]. XMAPTOOLS affords information about compositional zoning in mineral and local bulk composition of domains at the thin sections scale. THERIAK-DOMINO calculates equilibrium phase assemblages from given bulk rock composition, temperature T and pressure P. Primarily BINGO-ANTIDOTE can be described as an inverse THERIAK-DOMINO, because it uses the information provided by XMAPTOOLS to calculate the probable P-T equilibrium conditions of metamorphic rocks. Consequently, the introduced program combines the strengths of forward Gibbs free energy minimization models with the intuitive output of inverse thermobarometry models.

In order to get “best” P-T equilibrium conditions of a metamorphic rock sample and thus estimating the degree of agreement between the observed and calculated mineral assemblage, it is critical to define a reliable scoring strategy. BINGO uses the THERIAK_D ADD-ON[3] (Duesterhoeft and de Capitani, 2013) and is a flexible model scorer with 3+1 evaluation criteria. These criteria are the statistical agreement between the observed and calculated mineral-assemblage, -proportions (vol%) and -composition (mol). Additionally, a total likelihood, consisting of the first three criteria, allows the user an evaluation of the most probable equilibrium P-T condition. ANTIDOTE is an interactive user interface, displaying the 3+1 evaluation criteria as probability P-T-maps. It can be used with and without XMAPTOOLS. As a stand-alone program, the user is able to give the program macroscopic observations (i.e. mineral names and proportions), which ANTIDOTE converts to a readable BINGO input. In this manner, the use of BINGO-ANTIDOTE opens up thermodynamics to students and people with only a basic knowledge of phase diagrams and thermodynamic modeling techniques.

This presentation introduces BINGO-ANTIDOTE and includes typical examples of its functionality, such as the determination of P-T conditions of high-grade rocks. BINGO-ANTIDOTE is still under development and will soon be freely available online.

References:

[1] Lanari P., Vidal O., De Andrade V., Dubacq B., Lewin E., Grosch E. G. and Schwartz S. (2013) XMapTools: a MATLAB[®]-based program for electron microprobe X-ray image processing and geothermobarometry. *Comput. Geosci.* 62, 227–240.

[2] de Capitani C. and Petrakakis K. (2010) The computation of equilibrium assemblage diagrams with Theriak/Domino software. *Am. Mineral.* 95, 1006–1016.

[3] Duesterhoeft E. and de Capitani C. (2013) Theriak_D: An add-on to implement equilibrium computations in geodynamic models. *Geochem. Geophys. Geosyst.* 14, 4962–4967.