



# Theriak-Domino: A Fast, Automatic, and Easy-To-Use Phase Diagram Calculator Based on Free Energy Minimization



**GEOCANADA 2010**  
WORKING WITH THE EARTH  
Calgary, Alberta - May 10-14, 2010

## This short course

will be held at the University of Calgary as the first part of a metamorphic "extravaganza," May 8-16, 2010 in conjunction with the GeoCanada 2010 conference in Calgary

The events include:

- a two-day, pre-meeting short course on Theriak-Domino Sat & Sun, May 8-9, 2010
- a two-day special session, "Interplay between Thermodynamics, Kinetics and Deformation in Metamorphism" - to be held during the main meeting, Mon to Wed, May 10-12, 2010
- a 3.5-day, post-meeting field trip, "Barrovian and Buchan Metamorphism and Their Tectonic Juxtapositions in Southeastern British Columbia" - Thu to Sun, May 13-16, 2010

The enrollment for the short course will be limited to

**30**

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**Mineralogical Association of Canada**  
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Date: Sat & Sun, May 8-9, 2010  
Prior to the GeoCanada 2010 conference

Location: Department of Geoscience, University of Calgary

Instructor: Christian de Capitani, University of Basel, Switzerland  
Website: <http://titan.minpet.unibas.ch/minpet/theriak/>  
E-mail: [christian.decapitani@unibas.ch](mailto:christian.decapitani@unibas.ch)

Local organizer: David Pattison, University of Calgary, Canada  
E-mail: [pattison@ucalgary.ca](mailto:pattison@ucalgary.ca)

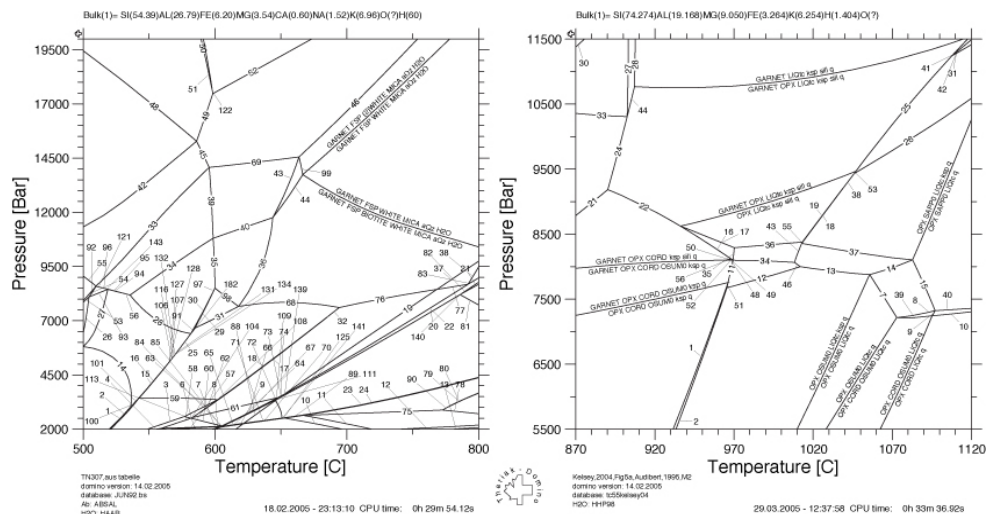
Registration: Will occur through the GeoCanada 2010 website at [www.geocanada2010.ca](http://www.geocanada2010.ca)

Theriak-Domino is an automated phase equilibrium modelling software package of great power and relative ease of use. It is complementary to two other well-known phase equilibrium modelling software packages, 'THERMOCALC' (Powell & Holland, 1998) and 'Perplex' (Connolly, 1990). Theriak-Domino offers choices of the Berman (1996) and Holland-Powell (1998) thermodynamic databases and their subsequent modifications. It can run on PC or Mac computers.

Like Perplex and THERMOCALC, Theriak-Domino can calculate isochemical phase diagram sections (pseudosections), T-X/P-X/X-X diagrams, binary and ternary diagrams, molar contours, isopleths, modes, and various rock-physical properties for user-specified bulk compositions and P-T conditions. The output consists of smooth-line, publication-quality diagrams in postscript (.ps) format.

Theriak-Domino is an automated program based on free energy minimization. This approach allows rapid, unattended calculation of phase diagrams, thereby permitting experimentation with respect to different thermodynamic mixing models, bulk compositions, chemical systems, fractionation, and other variables.

The equilibrium assemblage diagrams below (Fig. 1) were calculated and plotted without user intervention that might be a source of errors.



"Examples of equilibrium assemblage diagrams involving complex solid solutions, fluids and melts for metapelitic bulk compositions at moderate (Fig. 1a) and high grade (Fig. 1b)." Calculation and plotting of these "ready-to-use" diagrams was carried out with a 1.33 GHz PowerBook G4 running OSX in around 30 minutes. The THERIAK-DOMINO software is capable of porting most thermodynamic data and models developed for THERMOCALC (Holland & Powell, 1998). The right figure reproduces satisfactorily Fig. 5 in Kelsey et al. (2004).