CryMinal – the Software for Simulation of Equilibrium Crystallization

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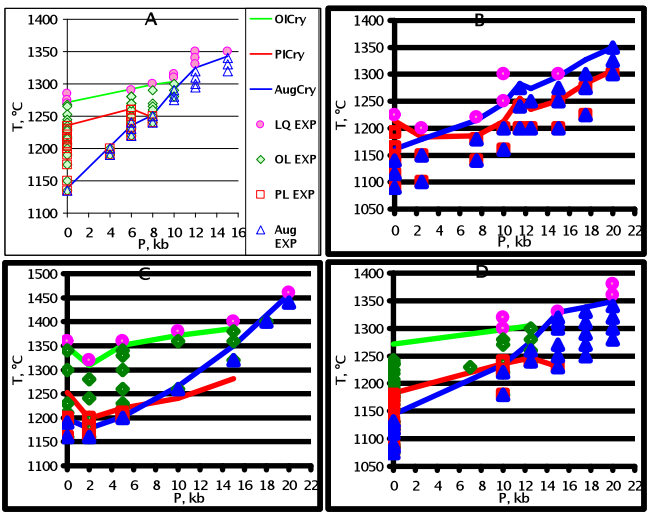
CryMinal created for simulation of mafic magmas equilibrium **Cry**stallization using sum of **Minal**s (end-members) mole fractions as target function. Concentrations of minals in the minerals are calculated using equilibrium constants. As an example, here is the equation for enstatite $MgSiO_3$ (En) minal:

$$X_{En}=\exp((A+\beta P)/T+B+D\lg fO_2+\Sigma J_i X_i+\ln\alpha^*_{MgO}+\ln\alpha^*_{SiO2}),$$

where X_{En} is the value of the enstatite mole fraction, P is the pressure in kb, T is the absolute temperature in Kelvins, fO_2 is the oxygen fugacity, X_i is the mole fraction of i-th component of the melt. A, β, C, D, E, F, and J_i are the coefficients for corresponding variables, B is the constant, a^*– activity of the initial components in the melt according to network modifiers - network formers model of silicate melt.

The figure shows the comparison of calculated and experimental liquidus temperature (T_L). In experimental series, we see a deviation from the monotonous increase of T_L with increasing pressure. In the calculations, these deviations are reproduced by changes fO_2.



P-T diagram for liquidus relations in experimental series: A – [1]; B – [2]; C – [3]; D – [4].

[1] Bender *et al* (1978), *Earth and Planet. Sci. Lett.* **41**, 277-302 [2] Takahahshi *et al* (1998), *Earth and Planet. Sci. Lett.* **162**, 63-80 [3] Falloon *et al* (1999), *J. Petrol.*, **40**, 255-277 [4] Thy, (1991), *Lithos*, **26**, 223-243