

APPENDIX 3

1. The calculation procedure after Triboulet (1992) assumes conversion of microprobe analyses of amphiboles (in wt.%) to 23 oxygens (Papike et al., 1974) as follows: four Si atoms on the T2 site, remaining silica with Al^{IV} to T1 (Si + Al^{IV} = 4), remaining Al, Ti, Fe³⁺, Fe²⁺, Mn and Mg to M4 (Ca+Na^{M4} = 2), left over Na and K to A site (A = 1 pfu) with vacancy.

Next step involved calculations of particular vectors activities of amphiboles edenite, tremolite, pargasite, hastingsite) and comparison with appearing as mutual parageneses of chlorite and epidote and their activities [ln(K_d)], regarding: XAl³⁺, XMg and XFe³⁺ values.

2. Conventional thermobarometry proposed by Bhadra and Bhattacharya (2007) contributes two empirical equations:

$$P_1[kbar] = [-9.326 + 0.01462T - RT \ln K_{ideal} - 98.698X_{Na}^A - 33.213X_K^A - 20.338X_{Na}^{M4} - 39.101X_{Fe^{2+}}^{M13} + 100.392X_{Al}^{M2} + 131.03X_{Fe^{2+}}^{M2} + 82.479X_{Fe^{3+}}^{M2} - 118.653X_{Al}^{T1} - 2RT \ln \gamma_{Ab}] / (-\Delta V)$$

$$P_2[kbar] = [-1.869 + 0.0076T - RT \ln K_{ideal} - 102.692X_{Na}^A - 35.251X_K^A - 15.969X_{Na}^{M4} - 40.499X_{Fe^{2+}}^{M13} + 93.069X_{Al}^{M2} + 130.75X_{Fe^{2+}}^{M2} + 74.226X_{Fe^{3+}}^{M2} - 104.402X_{Al}^{T1} - 2RT \ln \gamma_{Ab}] / (-\Delta V)$$

where:

$$K_{ideal} = \left[\frac{16(X_{Na}^A)(X_{Al}^{T1})}{(X_{\square}^A)(X_{Si}^{T1})(X_{Ab})} \right]^2, \quad RT \ln \gamma_{Ab} = W_{C1}(1 - X_{Ab})^2$$

and W_{C1} ~ 1.0 (Holland and Powell, 1992).

3. Calibrated geothermobarometer after Zenk and Schulz (2004) involves the following equations:

$$T[K] = \frac{4701}{1.825 - \ln\left(\frac{8}{15.5} - \frac{Si_{Am}}{sum_{Kat}} + 0.07531\right)} \quad \text{and}$$

$$P[kbar] = \frac{-425 - 1719 \left(\frac{XAl_M}{Fe^{3+}} + 2.75T[K] + 1.987T[K]\ln(XAl_M) \right) + 1}{XAl_M + \frac{2.763}{2.763}} \cdot \frac{1000}{1000}$$

where $XAl_M = (Si_{Am} + Al_{Am} - 8)/2.763$ and sum_{Kat} is the sum of cations using 13eCNK recalculation method.

++++++

- [1] **Mg-Chl + 4SiO₂ + 4Cal + 5H₂O = Ep (Ps₃₀₋₄₀) + Act + 4CO₂ + 7.5H₂⁺**
 $[Mg_4Fe^{2+}Al(Si_3Al)O_{10}(OH)_8 + 4SiO_2 + 4CaCO_3 + 5H_2O = Ca_2Fe_{0.3}^{3+}Al_2O(SiO_4)(Si_2O_7)(OH) + Ca_2(Mg_4Fe_{0.7}^{2+})Si_8O_{22}(OH)_2 + 4CO_2 + 7.5H_2^+]$
- [2] **Ep (Ps₃₀₋₄₀) + Act + 2Ab + 2Rt + CO₂ + H₂O = Mg-Hbl + Olg + Ab(2) + Ilm + Ttn(IIA) + Cal + 8H₂O**
 $[Ca_2Fe_{0.3}^{3+}Al_2O(SiO_4)(Si_2O_7)(OH) + Ca_2(Mg_4Fe_{0.7}^{2+})Si_8O_{22}(OH)_2 + 2NaAlSi_3O_8 + 2TiO_2 + CO_2 + H_2O = Ca_2Mg_4Al(AlSi_7O_{22})(OH)_2 + (Na_{0.8}Ca_{0.2})AlSi_4O_8 + NaAlSi_3O_8 + FeTiO_3 + CaTiSiO_5 + CaCO_3 + 8H_2O]$
- [3] **20Ca₂Fe_{0.3}³⁺Al₂O(SiO₄)(Si₂O₇)(OH) + 8H₂O = 20Ca₂Fe_{0.2-0.1}³⁺Al₂O(SiO₄)(Si₂O₇)(OH) + 2Fe²⁺Fe₂³⁺O₄ + 8H₂⁺**

Stoichiometric variance of Fe²⁺ might be due to the increasing temperature and growing oxygen fugacity (fO₂), which caused substantial acceleration of the oxidation rate from Fe²⁺ to Fe³⁺. During metamorphism the whole iron content could be oxidized so that the reaction may be simplified:

- [3'] **10Ep(Ps₃₀₋₄₀) + 4H₂O = 10Ep(Ps₁₀₋₂₀) + Mag + 4H₂⁺**
 $[10Ca_2Fe_{0.3}Al_2O(SiO_4)(Si_2O_7)(OH) + 4H_2O = 10Ca_2Fe_{0.2-0.1}Al_2O(SiO_4)(Si_2O_7)(OH) + Fe_3O_4 + 4H_2^+]$
- [4] **Mg-Chl + Act + Czo + 3Ep + Rt = 3.5Ts + 3Cal + Ilm + 2SiO₂ + 3.5H₂⁺**
 $[Mg_4Al(Si_3Al)O_{10}(OH)_8 + Ca_2Mg_3Fe_{0.6}Si_8O_{22}(OH)_2 + Ca_2Al_3Si_3O_{12}(OH) + 3Ca_2Al_2Fe(Si_2O_7)(SiO_4)O(OH) + TiO_2 = 3.5Ca_2(Mg_2Al_2)(AlSi_6O_{22})(OH)_2 + 3CaCO_3 + FeTiO_3 + 2SiO_2 + 3.5H_2^+]$
- [5] **Mg-Hbl + 4Rt + 2Cal + 4H₂O = Mg-Chl + 4Ttn(IIIA) + 2CO₂ + H₂⁺**
 $[Ca_2Mg_4Al(AlSi_7O_{22})(OH)_2 + 4TiO_2 + 2CaCO_3 + 4H_2O = Mg_4Al(Si_3Al)O_{10}(OH)_8 + 4CaTiSiO_5 + 2CO_2 + H_2^+]$

