

## SOFTWARE NOTICE

### PTMAFIC: Software for thermobarometry and activity calculations with mafic and ultramafic assemblages

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#### ABSTRACT

PTMAFIC is a PC-compatible computer program for thermobarometric calculation in mafic and ultramafic rocks. The program includes 14 geothermometers and 11 geobarometers, each with up to ten calibrations chosen from all those published up to 1991. For the principal minerals of these rocks (e.g., amphiboles, garnet, olivine, plagioclase, pyroxenes, spinels) PTMAFIC can provide stoichiometric parameters such as cation site allocations, mole fractions, and mole percents of the end-members and thermodynamic parameters such as Margules parameters ( $W$ ), activities ( $a$ ), and activity coefficients ( $\gamma$ ) according to different models.

#### INTRODUCTION

Despite the undoubted advantages of mafic rocks for discovering the predominant  $P$ - $T$  conditions of the initial metamorphic stages of an orogeny (e.g., Brodie and Rutter, 1985), the software developed for the calculation of  $P$ - $T$  conditions by geothermobarometry has been designed mainly for pelitic systems. PTMAFIC has been written to make up partially for the lack of geothermobarometric programs for these rocks.

The purpose of PTMAFIC is to ease thermobarometric calculations for petrologists concerned with mafic and ultramafic systems. The program contains multiple geothermometers and geobarometers applicable to a wide range of  $P$ - $T$  conditions, from granulite and eclogite facies to the upper part of greenschist facies. The different calibrations of each of these thermobarometers published up to 1991 have been collected.

#### PROGRAM DESCRIPTION

The program consists of two closely related parts that can be used independently. The first part, located in only one option of the main menu, allows the user to calculate, for each of the most petrologically significant minerals, parameters such as cation site allocations, mole fractions at the different structural positions, mole percents of the end-members, and different models of thermodynamic activities. The second part of the program, that concerning thermobarometric calculations, is contained in two menus: one for geothermometry and the other for geobarometry. In each menu the different geothermometers (14 in all) and geobarometers (11 in all) appear in alphabetical order of the constituent minerals. According to the mineral assemblage in question, the user can therefore recognize the geothermometers or geobarometers that can be used. For each of these, different results will be obtained according to the calibrations updated by the author of the program.

#### Activities

Some of the most significant minerals included in this option of PTMAFIC are

1. Amphibole. The cation site allocations are calculated ac-

ording to the procedures of Holland and Richardson (1979) and Hawthorne (1983). The activities of the end-members are calculated according to the models by Holland and Richardson (1979), Triboulet and Audren (1988), and Kohn and Spear (1989, 1990). The distribution coefficients of  $T$ - and  $P$ -dependent reactions between different amphibole end-members, are calculated after Holland and Richardson (1979), Trzcieski et al. (1984), and Triboulet and Audren (1988).

2. Garnet. Activities and activity coefficients of the end-members (almandine, grossular, pyrope, and spessartine) are calculated after Ganguly and Perkins (1974), Perkins (1979), Hodges and Spear (1982), Newton and Perkins (1982), Saxena and Erikson (1983), and Ganguly and Saxena (1984) with the modifications by Perkins and Chipera (1985a, 1985b), Moecher et al. (1988), and Hoinkes (1986).

3. Plagioclase. Activities of the end-member are calculated following the models of Orville (1972), Kerrick and Darken (1975), Newton et al. (1980), Newton (1983), Hodges and Royden (1984), and Paria et al. (1988).

4. Pyroxenes. The program distributes the cations at the M1 and M2 tetrahedral sites, following the model by Wood and Banno (1973), and calculates the mole percent of the pyroxene end-members (jadeite, hypersthene, wollastonite and enstatite, ferrosilite, wollastonite). Calculation of activities for the different end-members (diopside, enstatite, ferrosilite, and hedenite) is carried out following models by Wood and Banno (1973), Herzberg and Chapman (1976), Gasparik and Newton (1984), and Chatterjee and Terhart (1985).

5. Spinel. The program calculates the Margules parameters ( $W$ ), activities, and activity coefficients for magnesium-chromium spinel and magnesium-aluminum spinel, according to the models by Herzberg and Chapman (1976), Oka et al. (1984), and Chatterjee and Terhart (1985).

#### Thermobarometry

The program includes 24 thermobarometers. They are listed below in alphabetical order together with a brief description and the calibrations included. Mineral abbreviations are standardized following Kretz (1983).

1. Al-in-amphibole barometer; empirical calibrations of Hammarstrom and Zen (1986) and Hollister et al. (1987) and experimental calibration of Johnson and Rutherford (1989).

2. Amp-Chl-Ep-Pl thermobarometer; based on the  $Fe^{3+}$ -Al exchange between Amp and Ep, coexisting with Chl and Pl; experimental calibration by Maruyama et al. (1986).

3. Amp-Grt thermometer; based on the Fe-Mg exchange between the two phases; empirical calibrations by Graham and Powell (1984) and Perchuk et al. (1985).

4. Amp-Grt-Pl-Qtz barometer; based on the empirical calibration of the reactions  $An + Ab + Tr = Grs + Prp + Prg + Qtz$ ,  $An + Ab + Fe-Act = Grs + Alm + Fe-Prg + Qtz$ ,  $An +$

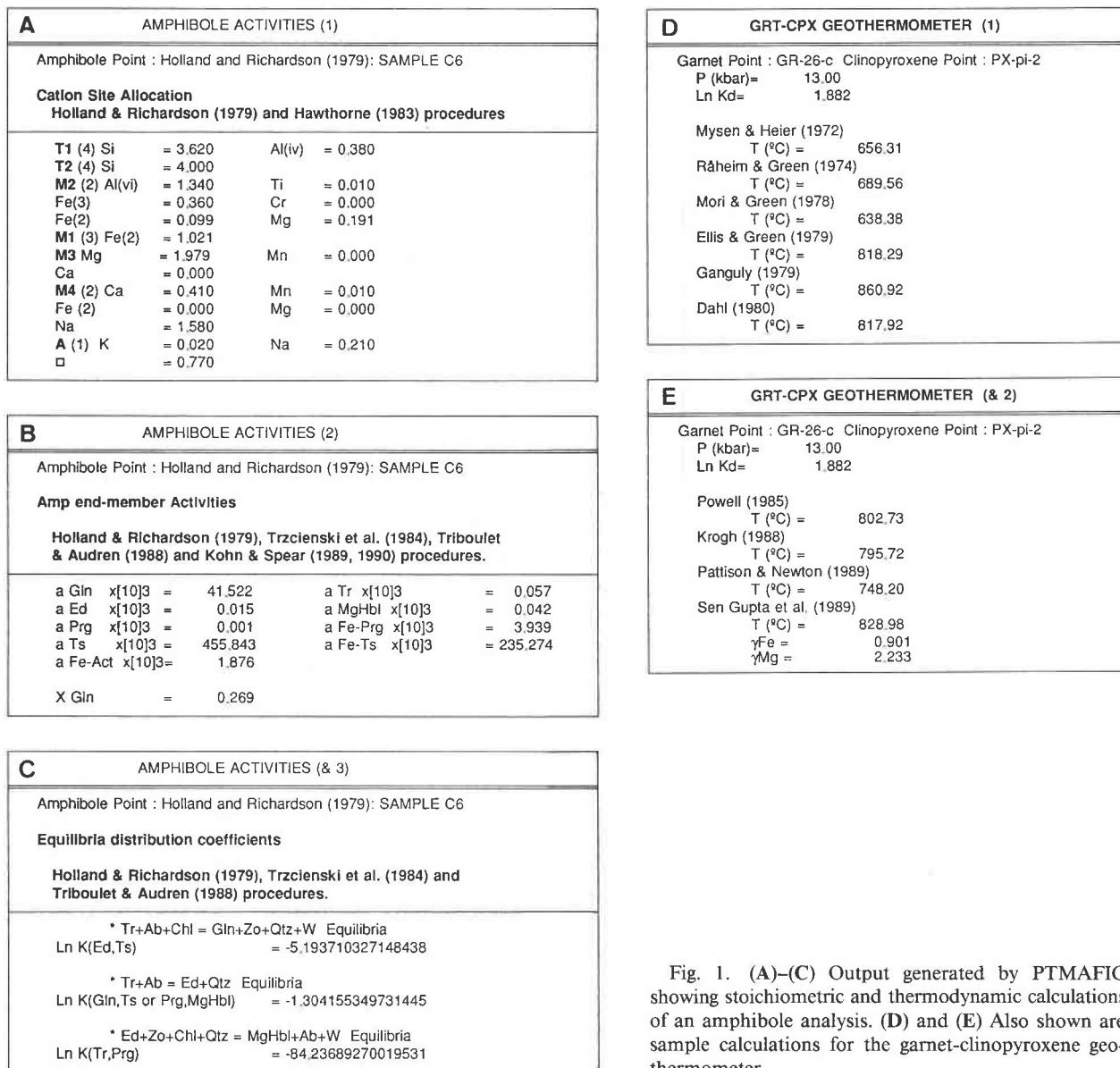


Fig. 1. (A)–(C) Output generated by PTMAFIC showing stoichiometric and thermodynamic calculations of an amphibole analysis. (D) and (E) Also shown are sample calculations for the garnet-clinopyroxene geothermometer.

Tr = Grs + Prp + Ts + Qtz, and An + Fe-Act = Grs + Alm + Fe-Ts + Qtz by Kohn and Spear (1989, 1990).

5. Amp-Pl thermometer; according to the NaSi = CaAl exchange between the two phases, for instance in Ed + Qtz = Tr + Ab and Prg + Qtz = Hbl + Ab reactions; empirical calibrations by Spear (1980) and Fershtater (1991), experimental calibration by Plyusnina (1982), and mixed calibration by Blundy and Holland (1990).

6. Cpx-Ol thermometer; based on the following Fe-Mg exchange reaction: Ol (Fo) + Hd = Ol (Fa) + Di; calibration by Powell and Powell (1974).

7. Cpx-Ol-Spl thermometer; based on the equilibrium Di + Spl = Ca-Ts + Ol (Fo); experimental calibration by Herzberg and Chapman (1976).

8. Cpx-Opx thermometer; according to the miscibility gap and the distribution of Ca and Na between both pyroxenes; empirical

calibration by Wood and Banno (1973); experimental calibrations by Nehru and Wyllie (1974) and Herzberg and Chapman (1976); mixed calibration by Brey and Köhler (1990).

9. Cpx-Pl-Qtz barometer; according to the equilibrium An = Ca-Ts + Qtz, proposed as an empirical barometer by Ellis (1980).

10. Grt-Cpx thermometer; based on the Fe-Mg exchange between the two phases; calibrations: experimental by Råheim and Green (1974), Ellis and Green (1979), and Pattison and Newton (1989); empirical by Mysen and Heier (1972), Mori and Green (1978), and Dahl (1980); mixed by Ganguly (1979), Powell (1985), Krogh (1988), and Sen Gupta et al. (1989).

11. Grt-Cpx-Opx-Pl-Qtz barometer; based on the empirical calibration of the reactions: Alm + Hd + Qtz = Fs + Pl and Prp + Di + Qtz = En + Pl obtained by Paria et al. (1988).

12. Grt-Cpx-Pl-Qtz barometer; based on the equilibria An + Di = Grs + Prp + Qtz and An + Hd = Grs + Alm + Qtz; with

empirical calibrations by Perkins and Newton (1981), Newton and Perkins (1982), Moecher et al. (1988), and Powell and Holland (1988); semiempirical calibration by Eckert et al. (1991).

13. Grt-Ilm thermometer; based on the Fe-Mn exchange between the two minerals; experimental calibrations by Pownceby et al. (1987a, 1987b, 1991).

14. Grt-Ms thermometer; according to the Fe-Mg exchange between the two minerals; calibrations included are experimental by Krogh and Råheim (1978), empirical by Hynes and Forest (1988), and mixed by Green and Hellman (1982).

15. Grt-Ol-Pl barometer; resulting from the experimental calibration of the reaction  $Ol (Fa) + Pl = Grs + Alm$  proposed by Bohlen et al. (1983).

16. Grt-Opx barometer; based on the Al content of the orthopyroxene coexisting with garnet, according to the equilibrium  $En + Mg-Ts = Prp$ ; empirical calibrations by Nickel and Green (1985) and Brey et al. (1986); semiempirical calibration by Brey and Köhler (1990).

17. Grt-Opx thermometer; based on the Fe-Mg exchange between the two phases; empirical calibrations by Wood and Banno (1973), Dahl (1980), and Sen and Bhattacharya (1984); experimental calibration by Harley (1984).

18. Grt-Opx-Pl-Qtz barometer; based on the equilibria  $An + En = Grs + Pyr + Qtz$  and  $An + Fs = Grs + Alm + Qtz$ ; empirical calibrations by Perkins and Newton (1981), Newton and Perkins (1982), and Powell and Holland (1988); experimental calibration by Bohlen et al. (1983); semiempirical calibrations by Perkins and Chipera (1985a, 1985b), Moecher et al. (1988) and Eckert et al. (1991).

19. Grt-Rt-Pl-Ilm barometer; according to the equilibrium  $Grt(Alm, Grs) + Rt = Ilm + An + Qtz$  (GRIPS); experimental calibration by Bohlen and Liotta (1986).

20. Ol-Spl thermometer; based on the Mg-Fe exchange between the two minerals; empirical calibrations by Fabriès (1979) and Roeder et al. (1979); experimental calibration by Ballhaus et al. (1991a, 1991b).

21. Opx thermometer; according to the solubility of Ca-Al and Cr-Al; empirical calibration by Witt-Eickschen and Seck (1991) and semiempirical calibration by Brey and Köhler (1990).

22. Opx-Ol thermometer; according to the Ni-Mg distribution between the two phases; experimental calibrations by Berger and Vannier (1978) and Povdin (1988).

23. Opx-Ol-Spl thermometer; based on the reaction  $En + Sp = Mg-Ts + Ol (Fo)$ ; experimental calibration by Fujii (1976); empirical calibrations by Gasparik and Newton (1984) and Witt-Eickschen and Seck (1991).

24. Phengite barometer; based on the Si content of the phengite coexistent with  $Qtz/Coes + Tlc + Ky$ ; experimental calibration by Massone and Schreyer (1989).

#### CHARACTERISTICS AND REQUIREMENTS OF THE PROGRAM

The program is written in a compiled version of Basic (TurboBasic) for PC-compatible computers, with a microprocessor of the 80086 family (from 80286 to 80486), color monitor, CGA graphics card or higher (up to VGA), and either MSDOS (version 3.0 or later) or DRDOS operating systems. Several text files, with specific instructions on how to use the program (README.TXT), and a complete list of the bibliographic references (REFERN.TXT) are included.

The program has been designed so that no consultation of a reference manual is required during use, and the menus and result screens are intended to be self-explanatory. Data are in-

troduced into the program by means of the keyboard. All the input operations require the analysis of the minerals to be given in ions per formula unit, so the user will need to have previously normalized the analysis. For some minerals the program offers the possibility of introducing Fe as  $Fe^{2+}$  and  $Fe^{3+}$  (e.g., amphiboles and pyroxenes).

The numerical results of the calculations are always displayed on one or several screens, which may be printed by screen dumps. Figure 1A–1E shows several examples of results created by the program.

#### HOW TO OBTAIN THE PROGRAM

PTMAFIC is available by writing to the author at the following address: Departamento de Geodinámica (Facultad de Ciencias), Av. Fuentenuueva s/n, 18071-Granada, Spain [Tel/Fax: 34-(9)58-243352]. As no financing has yet been found for publication and distribution to the program, the software has a price of U.S.\$35.00. Please send a check (made payable to J.I. Soto Hermoso) or money order, including name and address for shipping. To avoid computer virus problems, please do not send blank diskettes.

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## ERRATUM

**The composition of lizardite *IT* and the formation of magnetite in serpentinites**, by David S. O'Hanley and M. Darby Dyar (v. 78, p. 391–404). In Figure 7D–7F, the arrows should be pointing in the opposite direction. This change does not affect either the data (given in Table 4) or the interpretation of the data given in the text.