**Amphibole Chemometers**

|  |  |  |  |
| --- | --- | --- | --- |
| Reference | Melt parameter | Output name | T-dependent? |
| **Amphibole-only Chemometry. *Function “calculate\_amp\_only\_melt\_comps”***  Returns all equations by default (need to specify T to get T-dependent equations) | | | |
| Ridolfi (2021) | ΔNNO | deltaNNO\_Ridolfi21 | **✗** |
| H2O | H2O\_Ridolfi21 | **✗** |
| Zhang et al. (2017) | SiO2 (Eq 1) | SiO2\_Eq1\_Zhang17 | **✗** |
| SiO2 (Eq 2) | SiO2\_Eq2\_Zhang17 | **✗** |
| SiO2 (Eq 3) | SiO2\_Eq3\_Zhang17 | **🗸** |
| SiO2 (Eq 4) | SiO2\_Eq4\_Zhang17 | **✗** |
| TiO2 (Eq 5) | TiO2\_Eq5\_Zhang17 | **🗸** |
| TiO2 (Eq 6) | TiO2\_Eq6\_Zhang17 | **✗** |
| FeO (Eq 7) | FeO\_Eq7\_Zhang17 | **✗** |
| FeO (Eq 8) | FeO\_Eq8\_Zhang17 | **✗** |
| MgO (Eq 9) | MgO\_Eq9\_Zhang17 | **✗** |
| CaO (Eq 10) | CaO\_Eq10\_Zhang17 | **✗** |
| CaO (Eq 11) | CaO\_Eq11\_Zhang17 | **✗** |
| K2O (Eq 12) | K2O\_Eq12\_Zhang17 | **✗** |
| K2O (Eq 13) | K2O\_Eq13\_Zhang17 | **✗** |
| Al2O3 (Eq 14) | Al2O3\_Eq14\_Zhang17 | **✗** |
| Putirka (2016) | SiO2 (Eq 10) | SiO2\_Eq10\_Put2016 | **🗸** |

**Amphibole Thermobarometers**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Reference | Name in Thermobar | T-dependent? | P-dependent? | H2O-dependent? |
| **Amphibole-Liquid Barometry. *Function “calculate\_amp\_liq\_press”*** | | | | |
| Putirka (2016) | P\_Put2016\_eq7a | **✗** |  | **🗸** |
| P\_Put2016\_eq7b | **✗** | **🗸1\*** |
| P\_Put2016\_eq7c | **✗** | **✗** |
| **Amphibole-Liquid Thermometry. *Function “calculate\_amp\_liq\_temp”*** | | | | |
| Putirka (2016) | T\_Put2016\_eq4b |  | **✗** | **🗸** |
| T\_Put2016\_eq4a\_amp\_sat | **✗** | **🗸1\*** |
| T\_Put2016\_eq9 | **✗** | **🗸1\*** |
| **Amphibole-only Barometry. *Function “calculate\_amp\_only\_press”*** | | | | |
| Medard & Pennec (2022)**\*2** | P\_Medard2022\_RidolfiSites  P\_Medard2022\_LeakeSites  P\_Medard2022\_MutchSites | **✗** |  | **✗** |
| Ridolfi and Renzulli (2012)  &  Ridolfi (2021) | P\_Ridolfi2012\_1a | **✗** |  | **✗** |
| P\_Ridolfi2012\_1b | **✗** | **✗** |
| P\_Ridolfi2012\_1c | **✗** | **✗** |
| P\_Ridolfi2012\_1d | **✗** | **✗** |
| P\_Ridolfi2012\_1e | **✗** | **✗** |
| **P\_Ridolfi2021\*3** | **✗** | **✗** |
| Mutch et al. (2016) | P\_Mutch2016 | **✗** | **✗** |
| Ridolfi et al. (2010) | P\_Ridolfi2010 | **✗** | **✗** |
| Hammerstrom & Zen (1986) | P\_Hammarstrom1986\_eq1 | **✗** | **✗** |
| P\_Hammarstrom1986\_eq2 | **✗** | **✗** |
| P\_Hammarstrom1986\_eq3 | **✗** | **✗** |
| Hollister et al. (1987) | P\_Hollister1987 | **✗** | **✗** |
| Johnson & Rutherford (1989) | P\_Johnson1989 | **✗** | **✗** |
| Blundy et al. (1990) | P\_Blundy1990 | **✗** | **✗** |
| Schmidt (1992) | P\_Schmidt1992 | **✗** | **✗** |
| Anderson & Smith, 1995 | P\_Anderson1995 | **🗸** | **✗** |
| Krawczynski et al. (2012) | P\_Kraw2012 | **✗** | **✗** |
| **Amphibole-only Thermometry. *Function “calculate\_amp\_only\_temp”*** | | | | |
| Putirka (2016) | T\_Put2016\_eq5 |  | **✗** | **✗** |
| T\_Put2016\_eq6 | **✗** | **✗** |
| T\_Put2016\_SiHbl | **✗** | **✗** |
| T\_Put2016\_eq8 | **🗸** | **✗** |
| Ridolfi and Renzuli, 2012 | T\_Ridolfi2012 | **🗸** | **✗** |
| **Amphibole-Plagioclase Thermometry. Function “*calculate\_amp\_plag\_temp*”** | | | | |
| Holland and Blundy, 1994 | T\_HB1994\_A  T\_HB1994\_B |  | **🗸** | **✗** |

**🗸1\*** H2O-dependence because of parameterization in terms of hydrous fractions, not a specific H2O-term

\*2 We provide 3 options for how to calculate AlVI

\*3 EquationP=” **P\_Ridolfi2021”** uses an algorithm to combine results of eq1a-1e

**Clinopyroxene-Liquid Thermobarometers**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Reference | Name in Thermobar | T-dependent? | P-dependent? | H2O-dependent? |
| **Clinopyroxene-Liquid Barometry. *Function “calculate\_cpx\_liq\_press”*** | | | | |
| Putirka (1996) | P\_Put1996\_eqP1 | **🗸** |  | **✗** |
| P\_Put1996\_eqP2 | **🗸** | **✗** |
| Putirka (2003) | P\_Put2003 | **🗸** | **✗** |
| Putirka (2008) | P\_Put2008\_eq30 | **🗸** | **🗸** |
| P\_Put2008\_eq31 | **🗸** | **🗸** |
| P\_Put2008\_eq32c | **🗸** | **🗸** |
| Masotta et al. (2013) *recalibration of Putirka eqs. for alkali systems* | P\_Mas2013\_eqPalk1tex | **🗸** | **✗** |
| P\_Mas2013\_eqPalk2 | **🗸** | **✗** |
| P\_Mas2013\_eqalk32c | **🗸** | **🗸** |
| Masotta et al. (2013) | P\_Mas2013\_Palk2012 | **✗** | **🗸** |
| Neave & Putirka (2017) | P\_Neave2017 | **🗸** | **✗** |
| Petrelli et al. (2020) | P\_Petrelli2020\_Cpx\_Liq\*1 | **✗** | **🗸** |
| Jorgenson et al. (2022) | P\_Jorgenson2022\_Cpx\_Liq\*1 | **✗** | **✗** |
| **Clinopyroxene-Liquid Thermometry. *Function “calculate\_cpx\_liq\_temp”*** | | | | |
| Putirka (1996) | T\_Put1996\_eqT1 |  | **✗** | **✗** |
| T\_Put1996\_eqT2 | **🗸** | **✗** |
| Putirka (1999) | T\_Put1999 | **🗸** | **✗** |
| Putirka (2003) | T\_Put2003 | **🗸** | **✗** |
| Putirka (2008) | T\_Put2008\_eq33 | **🗸** | **🗸** |
| Masotta et al. (2013)  *Recalibration of Putirka eqs. for alkali systems* | T\_Mas2013\_eqTalk1 | **✗** | **✗** |
| T\_Mas2013\_eqTalk2 | **🗸** | **✗** |
| T\_Mas2013\_eqalk33 | **🗸** | **🗸** |
| Masotta et al. (2013) | T\_Mas2013\_Talk2012 | **✗** | **🗸** |
| Brugman & Till (2019) | T\_Brug2019 | **✗** | **✗** |
| Petrelli et al. (2020) | T\_Petrelli2020\_Cpx\_Liq\*1 |  | **✗** | **🗸** |
| Jorgenson et al. (2022) | T\_Jorgenson2022\_Cpx\_Liq\*1 |  | **✗** | **✗** |

**Clinopyroxene-only Thermobarometers**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Reference | Name in Thermobar | T-dependent? | P-dependent? | H2O-dependent? |
| **Clinopyroxene-only Barometry. *Function “calculate\_cpx\_only\_press”*** | | | | |
| Putirka (2008) | P\_Put2008\_eq32a | **🗸** |  | **✗** |
| P\_Put2008\_eq32b | **🗸** | **🗸** |
| Petrelli et al. (2020)  \*our adaptations | P\_Petrelli2020\_Cpx\_only\*1 | **✗** | **✗** |
| P\_Petrelli2020\_Cpx\_only\_withH2O\* | **✗** | **🗸** |
| Wang et al. (2021) | P\_Wang2021\_eq1 | **✗** | **✗** |
| Jorgenson et al. (2022) | P\_Jorgenson2022\_Cpx\_only\*1 | **✗** | **✗** |
| **Clinopyroxene-only Thermometry. *Function “calculate\_cpx\_only\_temp”*** | | | | |
| Putirka (2008) | T\_Put2008\_eq32d |  | **🗸** | **✗** |
| T\_Put2008\_eq32d\_subsol | **🗸** | **✗** |
| Wang et al. (2021) | T\_Wang2021\_eq2 |  | **✗** | **🗸** |
| Jorgenson et al. (2022) | T\_Jorgenson2022\_Cpx\_only\*1 |  | **✗** | **✗** |

**Liquid-only thermometry**

Function: “calculate\_liq\_only\_temp”

|  |  |  |  |
| --- | --- | --- | --- |
| Reference | Name in Thermobar | P-dependent? | H2O-dependent? |
| **Olivine-Sat Liquids** | | | |
| Putirka (2008) | T\_Put2008\_eq13 | **✗** | **✗** |
| T\_Put2008\_eq14 | **✗** | **🗸** |
| T\_Put2008\_eq15 | **🗸** | **🗸** |
| Helz & Thornber, (1987) | T\_Helz1987\_MgO | **✗** | **✗** |
| Shea et al. (2022) | T\_Shea2022\_MgO | **✗** | **✗** |
| Montierth (1995) | T\_Montierth1995\_MgO | **✗** | **✗** |
| Sugawara (2000) | T\_Sug2000\_eq1 | **✗** | **✗** |
| T\_Sug2000\_eq3\_ol | **🗸** | **✗** |
| T\_Sug2000\_eq6a | **🗸** | **✗** |
| T\_Sug2000\_eq6a\_H7a | **🗸** | **🗸** |
| Beattie (1993) | T\_Beatt93\_ BeattDMg | **🗸** | **✗** |
| T\_Beatt93\_BeattDMg\_HerzCorr | **🗸** | **✗** |
| Putirka (2008) | T\_Put2008\_eq19\_BeattDMg | **🗸** | **✗** |
| T\_Put2008\_eq21\_BeattDMg | **🗸** | **🗸** |
| T\_Put2008\_eq22\_BeattDMg | **🗸** | **🗸** |
| **Cpx-Sat Liquids** | | | |
| Putirka (2008) | T\_Put2008\_eq34\_cpx\_sat | **🗸** | **🗸** |
| Putirka (1999) | T\_Put1999\_cpx\_sat | **🗸** | **✗** |
| Sugawara (2000) | T\_Sug2000\_eq3\_cpx | **🗸** | **✗** |
| T\_Sug2000\_eq3\_pig | **🗸** | **✗** |
| T\_Sug2000\_eq6b | **🗸** | **✗** |
| T\_Sug2000\_eq6b\_H7b | **🗸** | **🗸** |
| **Opx-Sat Liquids** | | | |
| Putirka (2008) | T\_Put2008\_eq28b\_opx\_sat | **🗸** | **🗸** |
| Sugawara (2000) | T\_Sug2000\_eq3\_opx | **🗸** | **✗** |
| Beattie (1993) | T\_Beatt1993\_opx | **🗸** | **✗** |
| **Amp-Sat Liquids** | | | |
| Putirka (2008) | T\_Put2016\_eq3\_amp\_sat | **✗** | **🗸**\* |
| Molina (2015) | T\_Molina2015\_amp\_sat | **✗** | **✗** |
| **Fspar-Sat Liquids** | | | |
| Putirka (2005) | T\_Put2005\_eqD\_plag\_sat | **🗸** | **🗸** |
| Putirka (2008) | T\_Put2008\_eq26\_plag\_sat | **🗸** | **🗸** |
| T\_Put2008\_eq24c\_kspar\_sat | **🗸** | **🗸** |
| **Ol-Cpx-Plag Sat Liquids** | | | |
| Putirka (2008) | T\_Put2008\_eq16 | **🗸** | **✗** |
| Helz & Thornber (1987) | T\_Helz1987\_CaO | **✗** | **✗** |

**Orthopyroxene Thermobarometers**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Reference | Name in Thermobar | T-dependent? | P-dependent? | H2O-dependent? |
| **Orthopyroxene-Liquid Barometry. *Function “calculate\_opx\_liq\_press”*** | | | | |
| Putirka (2008) | P\_Put2008\_eq29a | **🗸** |  | **🗸** |
| P\_Put2008\_eq29b | **🗸** | **🗸** |
| Putirka Supplement New “Global” calibrations | P\_Put\_Global\_Opx | **✗** | **✗** |
| P\_Put\_Felsic\_Opx | **✗** | **✗** |
| **Orthopyroxene-Liquid Thermometry. *Function “calculate\_opx\_liq\_temp”*** | | | | |
| Putirka (2008) | T\_Put2008\_eq28a |  | **🗸** | **🗸** |
| T\_Put2008\_eq28b\_opx\_sat | **🗸** | **🗸** |
| **Orthopyroxene-only Barometry. Function “calculate\_opx\_only\_press”** | | | | |
| Putirka (2008) | P\_Put2008\_eq29c | **🗸** |  | **✗** |

**Orthopyroxene-Clinopyroxene Thermobarometers**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Reference | Name in Thermobar | T-dependent? | P-dependent? | H2O-dependent? |
| **Orthopyroxene-Clinopyroxene Barometry. *Function “calculate\_cpx\_opx\_press”*** | | | | |
| Putirka (2008) | P\_Put2008\_eq38 | **✗** |  | **✗** |
| P\_Put2008\_eq39 | **🗸** | **✗** |
| **Orthopyroxene-Clinopyroxene Thermometry. *Function “calculate\_cpx\_opx\_press”*** | | | | |
| Putirka (2008) | T\_Put2008\_eq36 |  | **🗸** | **✗** |
| T\_Put2008\_eq37 | **🗸** | **✗** |
| Brey and Kohler (1990) | T\_Brey1990 | **🗸** | **✗** |
| Wells (1977) | T\_Wells1977 | **✗** | **✗** |
| Wood and Banno (1973) | T\_Wood1973 | **✗** | **✗** |

**Feldspar Thermometers, Barometers and Hygrometers**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Phase | Reference | Name in Thermobar | T-dependent? | P-dependent? | H2O-dependent? |
| **Feldspar-Liquid thermometry. *Function “calculate\_fspar\_liq\_temp”*** | | | | | |
| **Plag-Liq** | Putirka (2008) | T\_Put2008\_eq23 |  | **🗸** | **🗸** |
| T\_Put2008\_eq24a | **🗸** | **🗸** |
| **Kspar-Liq** | Putirka (2008) | T\_Put2008\_eq24b |  | **🗸** | **✗** |
| **Feldspar-Liquid barometry. *Function “calculate\_fspar\_liq\_press”*** | | | | | |
| **Plag-Liq** | Putirka (2008) | P\_Put2008\_eq25 | **🗸** |  | **✗** |
| **Feldspar-Liquid hygrometry. *Function “calculate\_fspar\_liq\_hygr”*** | | | | | |
| **Plag-Liq** | Putirka (2008) | H\_Put2008\_eq25b | **🗸** | **🗸** |  |
| Putirka (2005) | H\_Put2005\_eqH | **🗸** | **✗** |
| Waters & Lange (2015) | H\_Waters2015 | **🗸** | **🗸** |
| Masotta et al. (2019) | H\_Masotta2019 | **🗸** | **✗** |
| **Plagioclase-Alkali Feldspar thermometry. Function “calculate\_plag\_kspar\_temp”** | | | | | |
| **Plag-Kspar** | Putirka (2008) | T\_Put2008\_eq27a |  | **🗸** | **✗** |
| T\_Put2008\_eq27b | **🗸** | **✗** |
| T\_Put\_Global\_  2Fspar | **🗸** | **✗** |

**Garnet Thermometers and Barometers**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Reference | Name in Thermobar | T-dependent? | P-dependent? | H2O-dependent? |
| **Garnet-only thermometry. *Function “calculate\_gt\_only\_temp”*** | | | | |
| Ryan et al. (1996) | T\_Ryan1996 |  | **✗** | **✗** |
| Canil et al. (1999) | T\_Canil1999 | **✗** | **✗** |
| Sudholz et al. (2021) | T\_Sudholz2021 | **✗** | **✗** |
| **Garnet-only barometry *Function “calculate\_gt\_only\_press”*** | | | | |
| Ryan et al. (1996) | P\_Ryan1996 | **🗸** |  | **✗** |

**Other Garnet Functions**

|  |  |
| --- | --- |
| Garnet classification of Griffin et al. (2002) | “garnet\_CARP\_class\_Griffin2002” |
| Cr-pyrope classification of Grutter et al. (2004) | “garnet\_class\_Grutter2004” |
| Ca-Cr classification of Cr-pyrope of Griffin et al. (2002) | “garnet\_ca\_cr\_class\_Griffin2002” |
| Y-Zr Classification of Cr-pyrope of Griffin et al. (2002) | “y\_zr\_classification\_Griffin2002” |
| Ol Mg# from Cr-pyrope (Gaul et al. 2000) | “calculate\_ol\_mg” |
| Calculate Al2O3 of whole-rock from Cr-pyrope (after O’Reilly et al. 2006) | “calculate\_al2O3\_whole\_rock” |

**Olivine Thermometers and Hygrometers**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Reference | Name in Thermobar | T-dependent? | P-dependent? | H2O-dependent? |
| **Olivine-Liquid thermometry. *Function “calculate\_ol\_liq\_temp”*** | | | | |
| Putirka (2008) | T\_Put2008\_eq19 |  | **🗸** | **✗** |
| T\_Put2008\_eq21 | **🗸** | **🗸** |
| T\_Put2008\_eq22 | **🗸** | **🗸** |
| Beattie (1993) | T\_Beatt93\_ol | **🗸** | **✗** |
| T\_Beatt93\_ol\_HerzCorr | **🗸** | **✗** |
| Sisson and Grove (1992) | T\_Sisson1992 | **🗸** | **✗** |
| Pu et al. (2017) | T\_Pu2017 | **✗** | **✗** |
| Pu et al. (2021) | T\_Pu2021 | **🗸** | **✗** |
| **Olivine-Liquid hygrometers. *Function “calculate\_ol\_liq\_hygr”*** | | | | |
| Gavrilenko et al. (2016) | H\_Gavr2016 | **✗** | **✗** |  |
| **Olivine-Spinel thermometry. *Function “calculate\_ol\_sp\_temp”*** | | | | |
| Coogan et al. (2014) | T\_Coogan2014 |  | **✗** | **✗** |
| Wan et al. (2008) | T\_Wan2008 | **✗** | **✗** |