

Edgar Dachs and Artur Benisek (2024): "A new activity model for biotite and its application"

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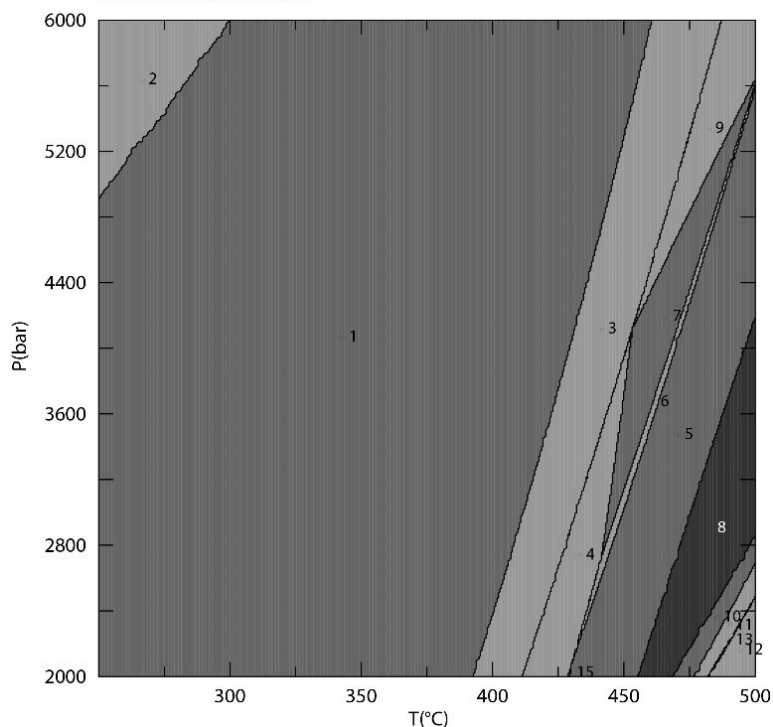
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Online Resource 7 *Perple_X* raw pseudosections of test samples.

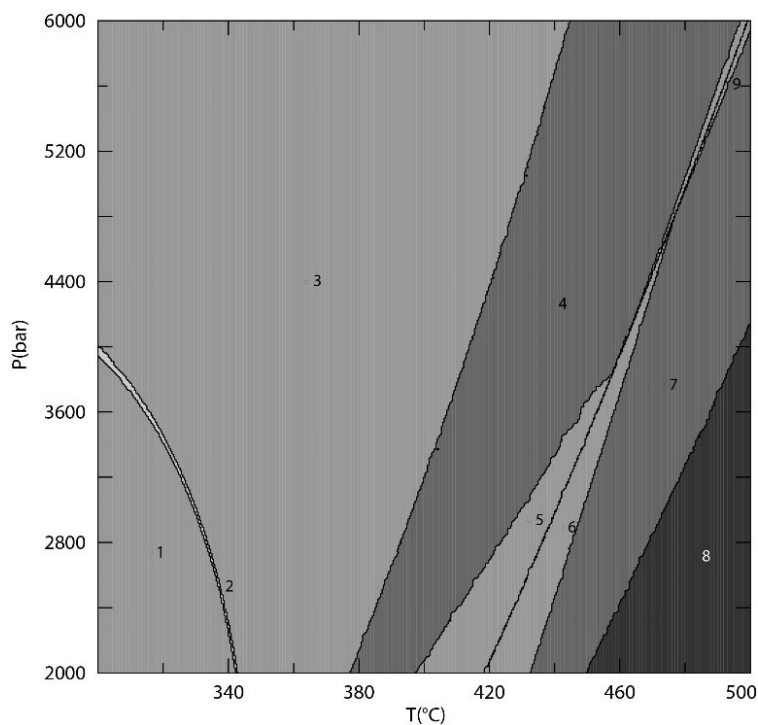
Mather (1970), 16, Bio(D)



- 1 - Bio Chl Phe Ep Carb sph ab q CH4
- 2 - Bio Chl Phe Ep Carb Carb sph ab q CH4
- 3 - Bio Chl Phe Ep Carb sph ab q H2O CH4
- 4 - Bio Chl Phe Pl Carb sph ab q H2O CH4
- 5 - Bio Phe Pl Carb sph q ru H2O CH4
- 6 - Bio Chl Phe Pl Carb sph q ru H2O CH4
- 7 - Bio Chl Phe Pl Carb sph q H2O CH4
- 8 - Bio Phe Pl Carb q ru H2O CH4
- 9 - Bio Chl Phe Pl Ep Carb sph q H2O CH4
- 10 - Bio Phe Pl Kfsp Carb q ru H2O CH4
- 11 - Bio Phe Pl Kfsp Carb q ru H2O CO2 CH4
- 12 - Bio feldspar Pl Kfsp Carb q ru H2O CO2 CH4

Fig. S1a *Perple_X* raw-pseudosection for sample 16 (Mather, 1970), computed with Bio(D). Bulk composition is given in supplementary Table 5. H₂O and CO₂ contents were 2.2 and 1.57 wt.%, O₂ was assumed to be 0.015 wt.%.

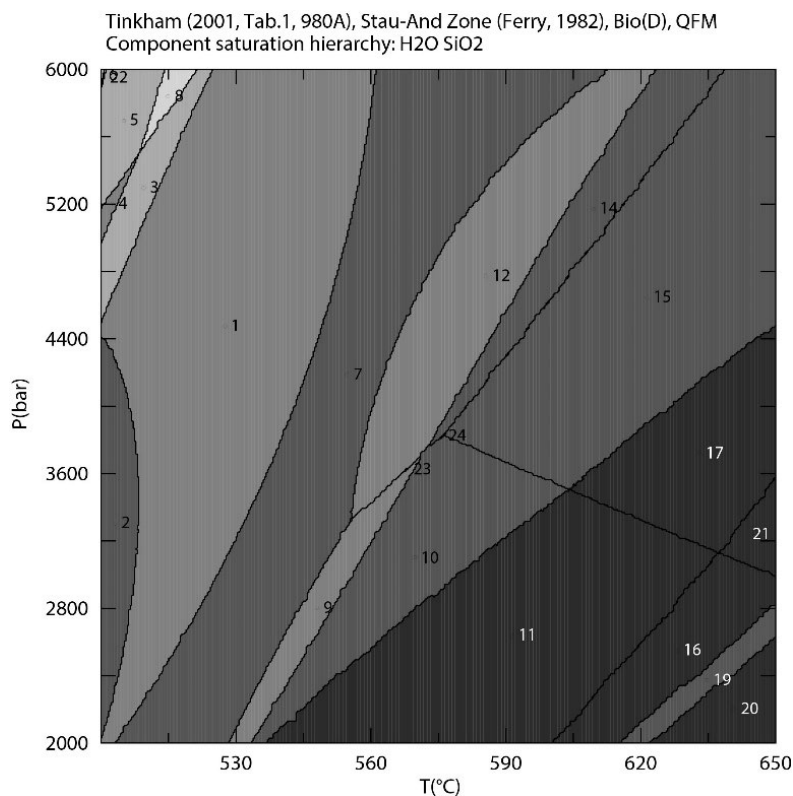
$K_D = (Fe/Mg)_{Chl}/(Fe/Mg)_{Bio} = 0.89$ in this sample and is shown in Fig. 8 as function of P and T.



- 1 - Chl Phe Pl Ep Carb sph ab q H2O CH4
- 2 - Bio Chl Phe Pl Ep Carb sph ab q H2O CH4
- 3 - Bio Chl Phe Ep Carb sph ab q H2O CH4
- 4 - Bio Phe Ep Carb sph ab q H2O CH4
- 5 - Bio Phe Pl Ep Carb sph ab q H2O CH4
- 6 - Bio Pl Kfsp Ep Carb sph ab q H2O CH4
- 7 - Bio Pl Kfsp Ep Carb sph ab q H2O
- 8 - Bio Pl Kfsp Carb sph ab q H2O

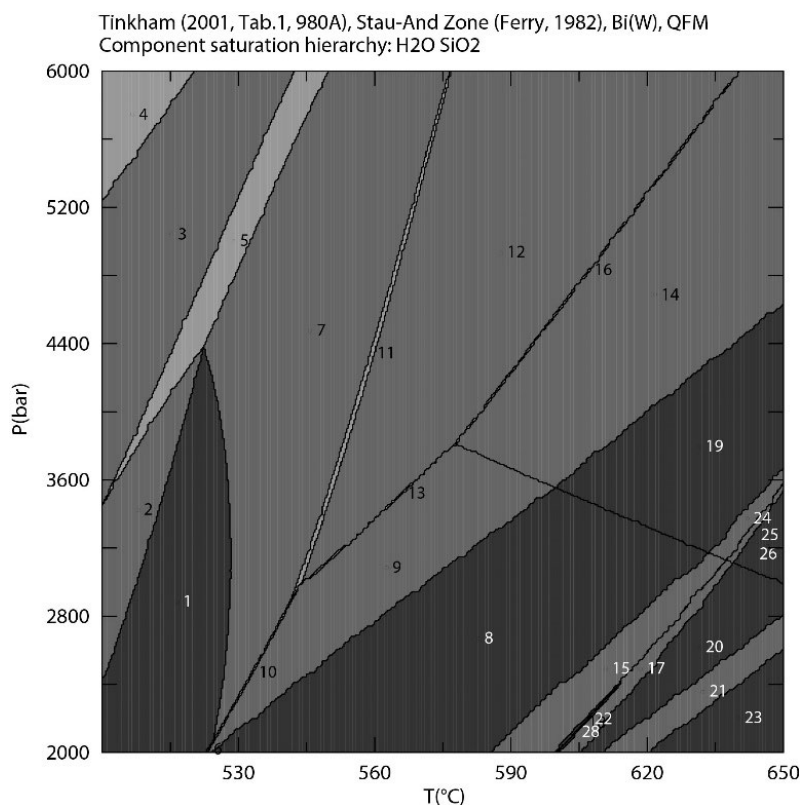
Fig. S1b *Perple_X* raw-pseudosection for sample 18 (Mather, 1970), computed with Bio(D). Bulk composition is given in supplementary Table 5. H₂O content was 0.7 wt.%, CO₂ and O₂ contents were assumed to be 0.3 and 0.015 wt.%.

$K_D = (Fe/Mg)_{Chl}/(Fe/Mg)_{Bio} = 0.88$ in this sample.



- 1 - Bio Grt Chl Phe Ilm Pl
- 2 - Bio Chl Phe Ilm Pl
- 3 - Bio Grt Chl Phe Ilm Pl ru
- 4 - Bio Grt Chl Phe Pl ru
- 5 - Bio Grt Chl Phe Ep Pl ru
- 6 - Bio Grt Chl Phe Ep Pl sph
- 7 - Bio Grt Phe Ilm Pl
- 8 - Bio Grt Chl Phe Ep Ilm Pl ru
- 9 - Bio Grt Phe Ilm Pl and
- 10 - Bio Grt Phe Pl and
- 11 - Bio Phe Pl and
- 12 - Bio Grt St Phe Ilm Pl
- 13 - Bio Grt St Phe Pl sil
- 14 - Bio Grt St Phe Pl
- 15 - Bio Grt Phe Pl sil
- 16 - Bio Pl Kfsp and
- 17 - Bio Phe Pl sil
- 18 - Bio Phe Pl Kfsp and
- 19 - Bio Crd Pl Kfsp and
- 20 - Bio Crd Pl Kfsp
- 21 - Bio Pl Kfsp sil

Fig. S2a *Perple_X* raw-pseudosection for sample 980A (Tinkham 2001, Tab. 1), computed with Bio(D) and imposing $\log f_{O_2}$ -conditions of the QFM buffer. Mineral-chemical data can be found in Ferry (1980). Bulk composition used is given in supplementary Table 5.



- 1 - Bio Chl Phe Ilm Pl
- 2 - Bio Chl Phe Ilm Pl ru
- 3 - Bio Grt Chl Phe Pl ru
- 4 - Bio Grt Chl Phe Ep Pl ru
- 5 - Bio Grt Chl Phe Ilm Pl ru
- 6 - Bio Chl Phe Ilm Pl and
- 7 - Bio Grt Chl Phe Ilm Pl
- 8 - Bio Phe Ilm Pl and
- 9 - Bio Grt Phe Ilm Pl and
- 10 - Bio Grt Chl Phe Ilm Pl and
- 11 - Bio Grt Chl St Phe Ilm Pl
- 12 - Bio Grt St Phe Ilm Pl
- 13 - Bio Grt St Phe Ilm Pl and
- 14 - Bio Grt Phe Ilm Pl sil
- 15 - Bio Phe Ilm Pl and ru
- 16 - Bio Grt St Phe Ilm Pl sil
- 17 - Bio Ilm Pl Kfsp and ru
- 18 - Bio Phe Pl and ru
- 19 - Bio Phe Ilm Pl sil
- 20 - Bio Ilm Pl Kfsp and
- 21 - Bio Crd Ilm Pl Kfsp and
- 22 - Bio Pl Kfsp and ru
- 23 - Bio Crd Ilm Pl Kfsp
- 24 - Bio Phe Ilm Pl sil ru
- 25 - Bio Ilm Pl Kfsp sil ru
- 26 - Bio Ilm Pl Kfsp sil
- 27 - Bio Phe Ilm Pl Kfsp and ru
- 28 - Bio Phe Pl Kfsp and ru

Fig. S2b *Perple_X* raw-pseudosection for sample 980A (Tinkham 2001, Tab. 1), computed with Bi(W) and imposing $\log f_{O_2}$ -conditions of the QFM buffer.

Tinkham (2001, Tab.1, 80A), Stau-And Zone (Ferry, 1982), Bio(TCC), QFM
Component saturation hierarchy: H₂O SiO₂

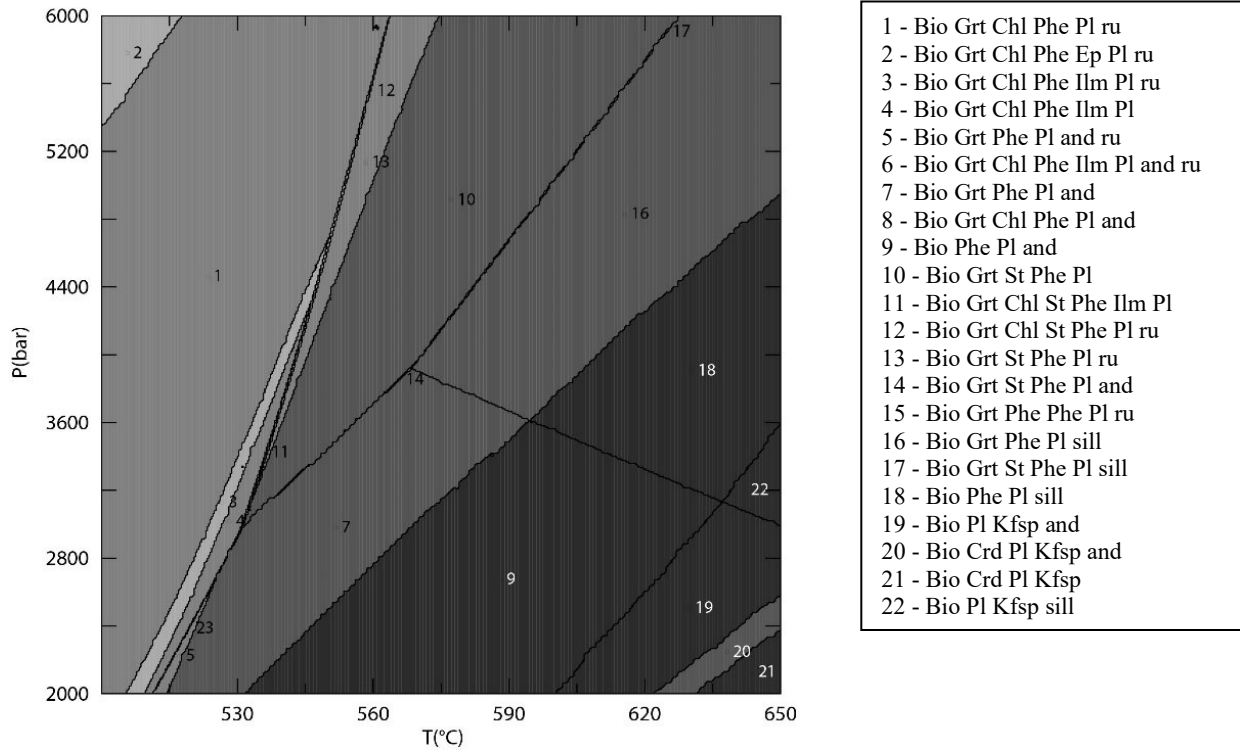


Fig. S2c *Perple_X* raw-pseudosection for sample 980A (Tinkham 2001, Tab. 1), computed with Bio(TCC) and imposing log_fO₂-conditions of the QFM buffer.

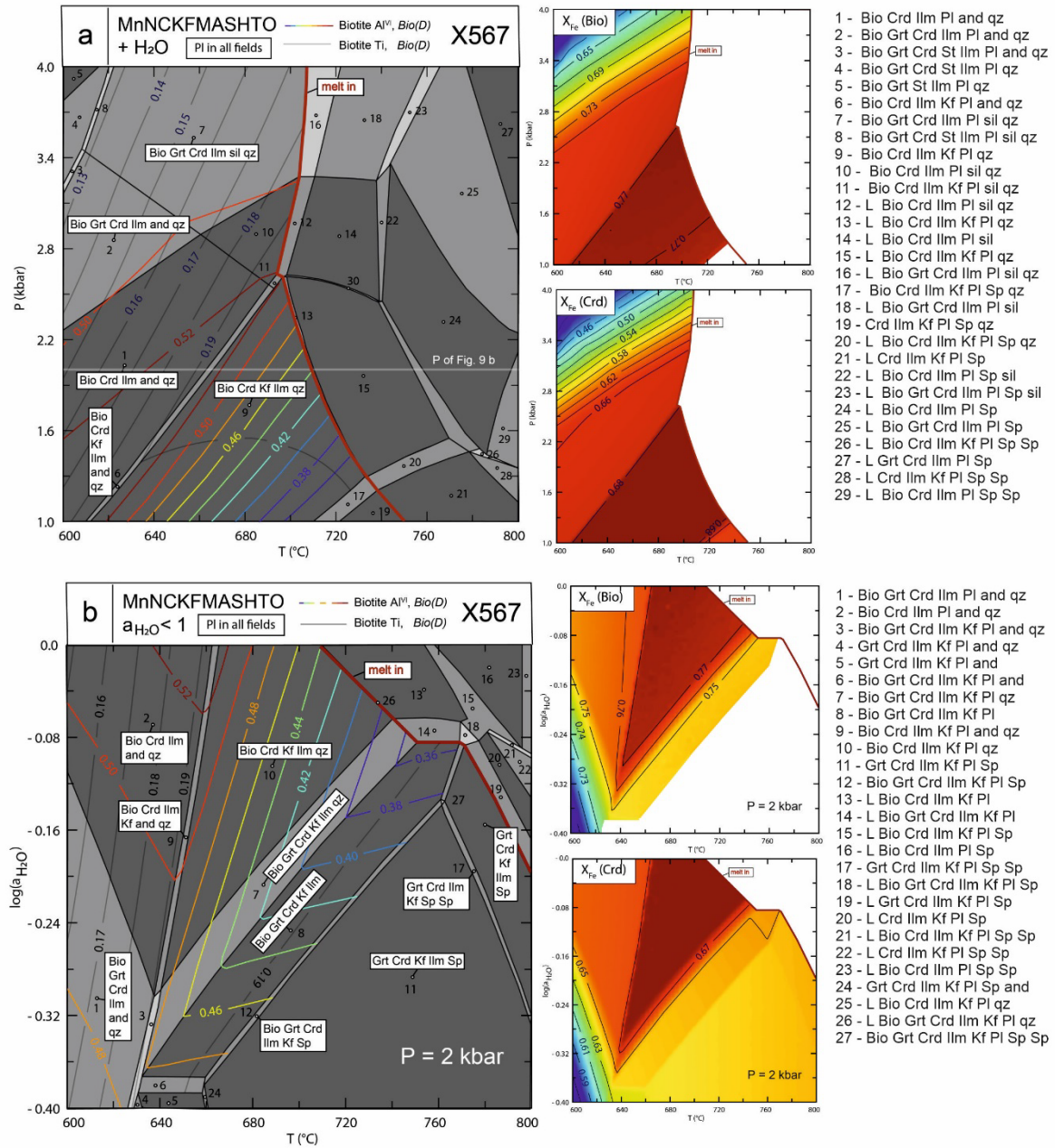


Fig. S3 a) P-T pseudosection for water-saturated conditions, **b)** log(a_{H₂O})-T pseudosection for reduced water-activity conditions at 2 kbar for sample X567 (Pitra and de Waal 2001; bulk-rock composition is given in supplementary Table 5). Calculations were done with *Perple_X* using Bio(D) as activity model for biotite and imposing logf_{O₂}-conditions of the QFM buffer. Coloured/dark-grey isopleths are the Al^{VI}-, respectively the Ti content in biotite, X_{Fe} in biotite and in cordierite are shown in separate colour density plots. Phase-fields are numbered using the following mineral abbreviations: and andalusite, Bio biotite, Crd cordierite, Grt garnet, Ilm ilmenite, Pl plagioclase, Kfsp kalifeldspar, L melt, sil sillimanite, Sp spinel.

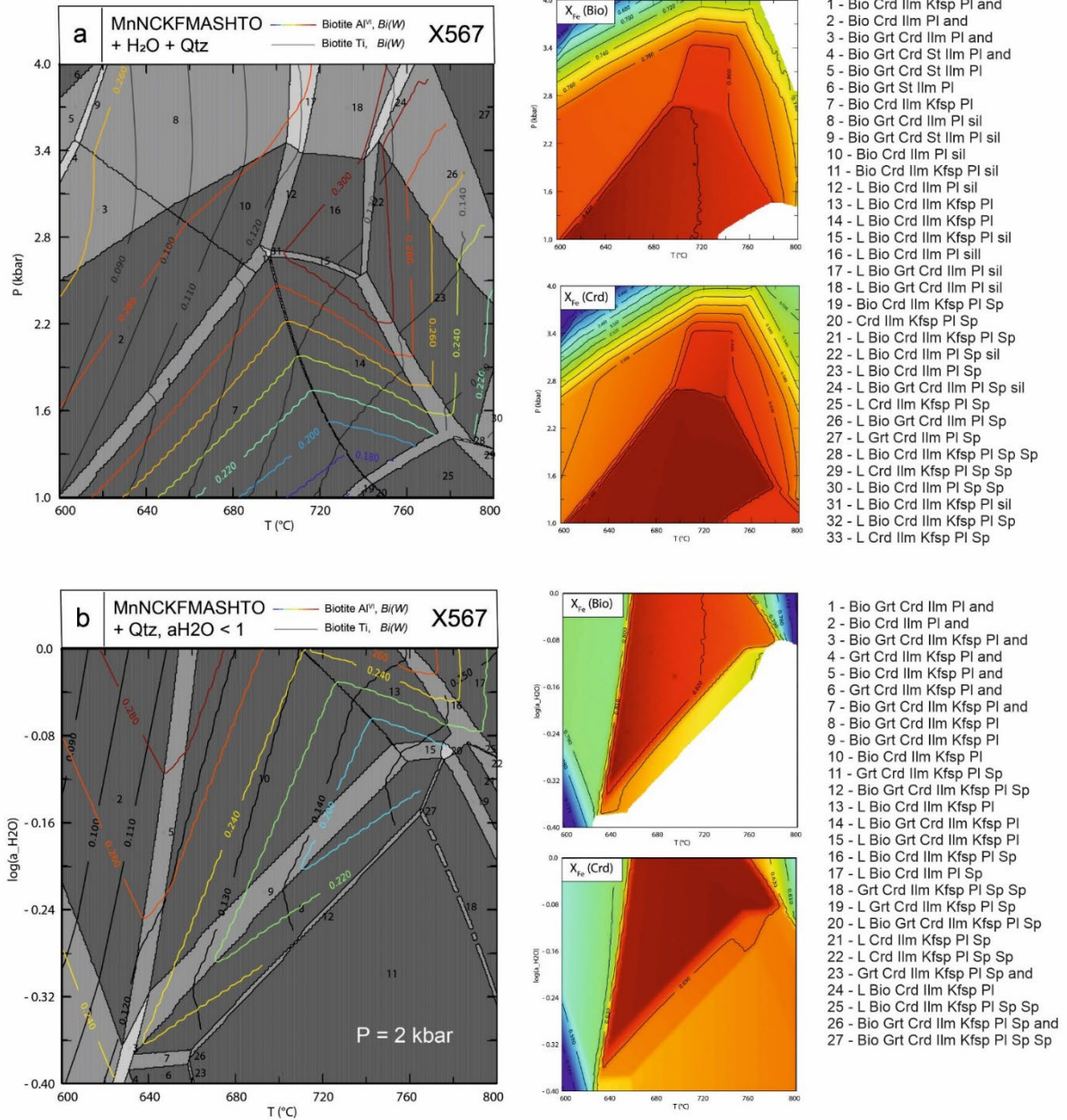


Fig. S4 b) P-T pseudosection for water-saturated conditions, **b)** log(a_{H2O})-T pseudosection for reduced water-activity conditions at 2 kbar for sample X567 (Pitra and de Waal, 2001; bulk-rock composition is given in supplementary Table 5). Calculations were done with *Perple_X* using Bi(W) as activity model for biotite and imposing logf_{O2}-conditions of the QFM buffer. Coloured/dark-grey isopleths are the Al^{VI}-, respectively the Ti content in biotite, X_{Fe} in biotite and in cordierite are shown in separate colour density plots. Phase-fields are numbered using the following mineral abbreviations: and andalusite, Bio biotite, Crd cordierite, Grt garnet, Ilm ilmenite, Pl plagioclase, Kfsp kalifeldspar, L melt, sil sillimanite, Sp spinel.

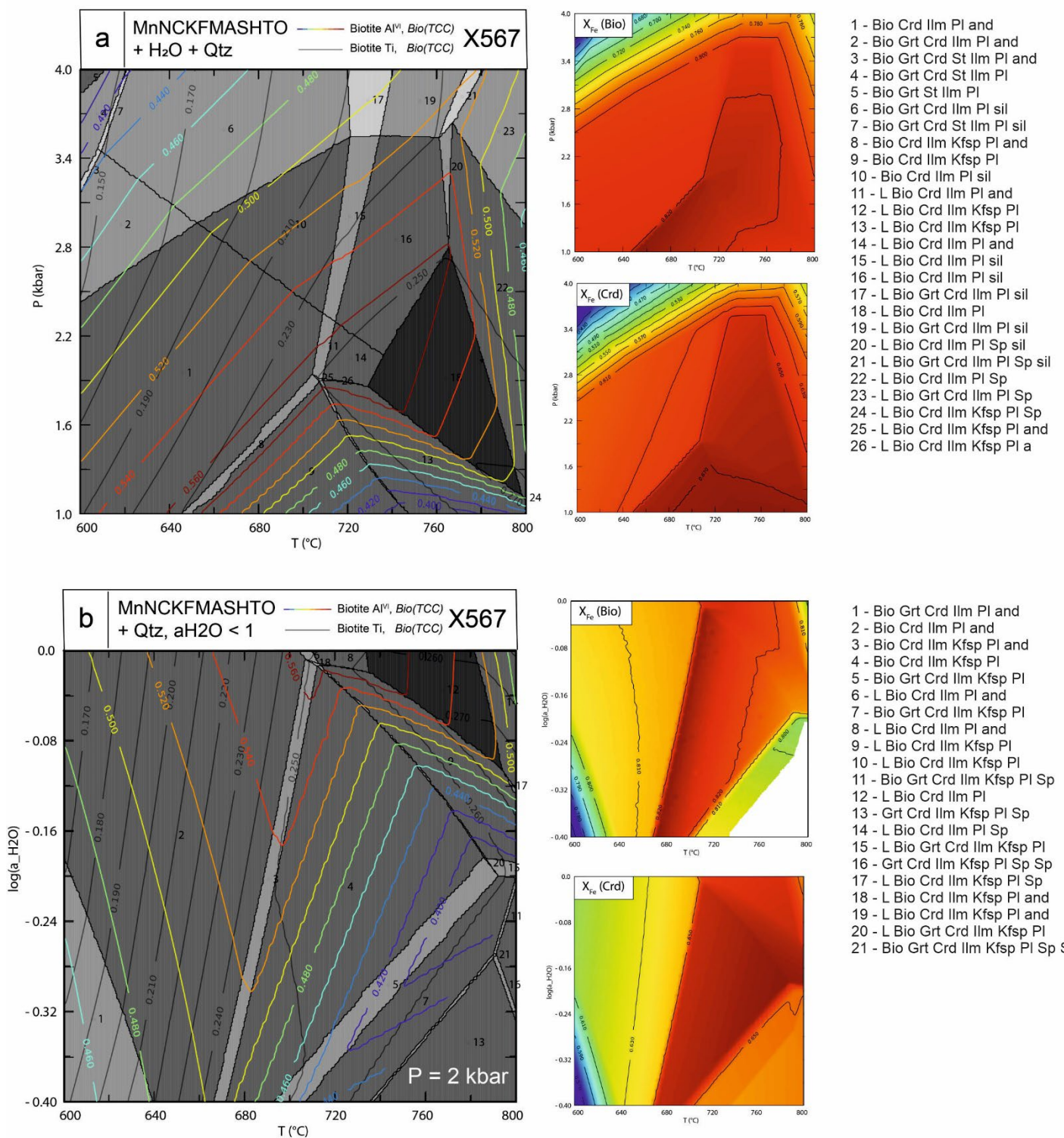
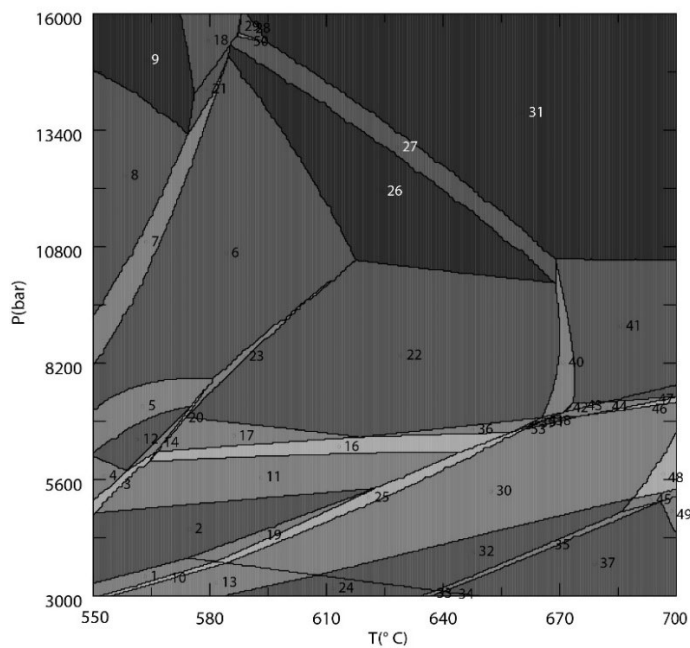


Fig. S5: a) P-T pseudosection for water-saturated conditions, **b)** log(a_{H2O})-T pseudosection for reduced water-activity conditions at 2 kbar for sample X567 (Pitra and de Waal, 2001; bulk-rock composition is given in supplementary Table 5). Calculations were done with *Perple_X* using Bio(TCC) as activity model for biotite and imposing logf_{O2}-conditions of the QFM buffer. Coloured/dark-grey isopleths are the Al^{VI}-, respectively the Ti content in biotite, X_{Fe} in biotite and in cordierite are shown in separate colour density plots. Phase-fields are numbered using the following mineral abbreviations: and andalusite, Bio biotite, Crd cordierite, Grt garnet, Ilm ilmenite, Pl plagioclase, Kfsp kalifeldspar, L melt, sil sillimanite, Sp spinel.

Li et al. (2020), 16Slo12, bulk XRFA1, Bio(D)



- | | |
|--|-----------------------------------|
| 1 - Bio St Phe Ilm Pl and | 28 - Grt Chl Phe ky r |
| 2 - Bio St Phe Ilm Pl | 29 - Grt Chl Ctd Phe ky ru |
| 3 - Bio Grt Chl St Phe Ilm Pl | 30 - Bio Grt Phe Ilm Pl sil |
| 4 - Grt Chl St Phe Ilm Pl | 31 - Grt Phe ky ru |
| 5 - Grt Chl St Phe Ilm ru | 32 - Bio Phe Ilm Pl sil |
| 6 - Grt Chl St Phe ru H ₂ O | 33 - Bio Phe Ilm Kfsp Pl and |
| 7 - Grt Chl St Ctd Phe ru | 34 - Bio Ilm Kfsp Pl and |
| 8 - Grt Chl Ctd Phe ru | 35 - Bio Phe Ilm Kfsp Pl sil |
| 9 - Grt Ctd Phe ru | 36 - Bio Grt St Phe Pl ru |
| 10 - Bio Grt St Phe Ilm Pl and | 37 - Bio Ilm Kfsp Pl sil |
| 11 - Bio Grt St Phe Ilm Pl | 38 - Bio Grt Phe Ilm sil |
| 12 - Grt Chl St Phe Ilm | 39 - Bio Grt St Phe Ilm sil |
| 13 - Bio Grt Phe Ilm Pl and | 40 - Bio Grt St Phe ky ru |
| 14 - Bio Grt Chl St Phe Ilm | 41 - Bio Grt Phe ky ru |
| 15 - Bio Grt Chl St Phe Ilm Pl ru | 42 - Bio Grt St Phe Ilm ky ru |
| 16 - Bio Grt St Phe Ilm Pl ru | 43 - Bio Grt Phe Ilm ky ru |
| 17 - Bio Grt St Phe Ilm ru | 44 - Bio Grt Phe Ilm sil ru |
| 18 - Grt Ctd Phe ky ru | 45 - L Bio Phe Ilm Pl sil |
| 19 - Bio St Phe Ilm Pl sil | 46 - Bio Grt Phe Ilm Pl sil ru |
| 20 - Bio Grt Chl St Phe Ilm ru | 47 - Bio Grt Phe sil ru |
| 21 - Grt St Ctd Phe ru | 48 - L Bio Grt Phe Ilm Pl sil |
| 22 - Bio Grt St Phe ru | 49 - L Bio Ilm Kfsp Pl sil |
| 23 - Bio Grt Chl St Phe ru | 50 - Grt Chl St Phe ky ru |
| 24 - Bio Phe Ilm Pl and | 51 - Bio Grt St Phe sil ru |
| 25 - Bio Grt St Phe Ilm Pl sil | 52 - Bio Grt St Phe Ilm Pl sil ru |
| 26 - Grt St Phe ru | 53 - Bio Grt St Phe Pl sil ru |
| 27 - Grt St Phe ky ru | 54 - Bio Grt St Phe Ilm sil ru |

Fig. S6 *Perple_X* raw-pseudosection for sample 16Slo12 (Li et al 2021), computed with Bio(D). H₂O present in all fields.