Example phase diagrams calculated with THERMOCALC

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The main examples in the following pages are the ones for which there is the Mathematica code, and also the THERMOCALC datafiles to calculate them here. Figs 1–7 are from White et al. (2001) (not the same figure numbering)

Fig. 1 . *P-T* projection for NKASH (solid lines), with connection to KASH (dashed lines) (Holland and Powell, 2000). Note that the solidus is a univariant line down pressure to a singularity, and is a cotectic to lower pressure. The line representing the top of the alkali feldspar solvus terminates at a singularity immediately beyond the cotectic.

Fig. 2 . (a) *P-T* projection for KFMASH. Note that the solidus is made up of univariant lines at pressures below about 7 kbars, but involves higher variance equilibria at highre pressure. The solidus is at 50–100° higher temperature than in NKASH, Fig. 1. (b) Details of the equilibria around (1) and (2) in (a). (Datafile TH DKB1)

Fig. 3 . *P-T* projection for NCKFMASH. The heavy univariant lines each correspond to KFMASH invariant points, with each line running from a CKFMASH invariant point at higher temperature, to a NKFMASH point at lower temperature. Light lines are the KFMASH univariant reactions. (Datafile TH DNCK1)

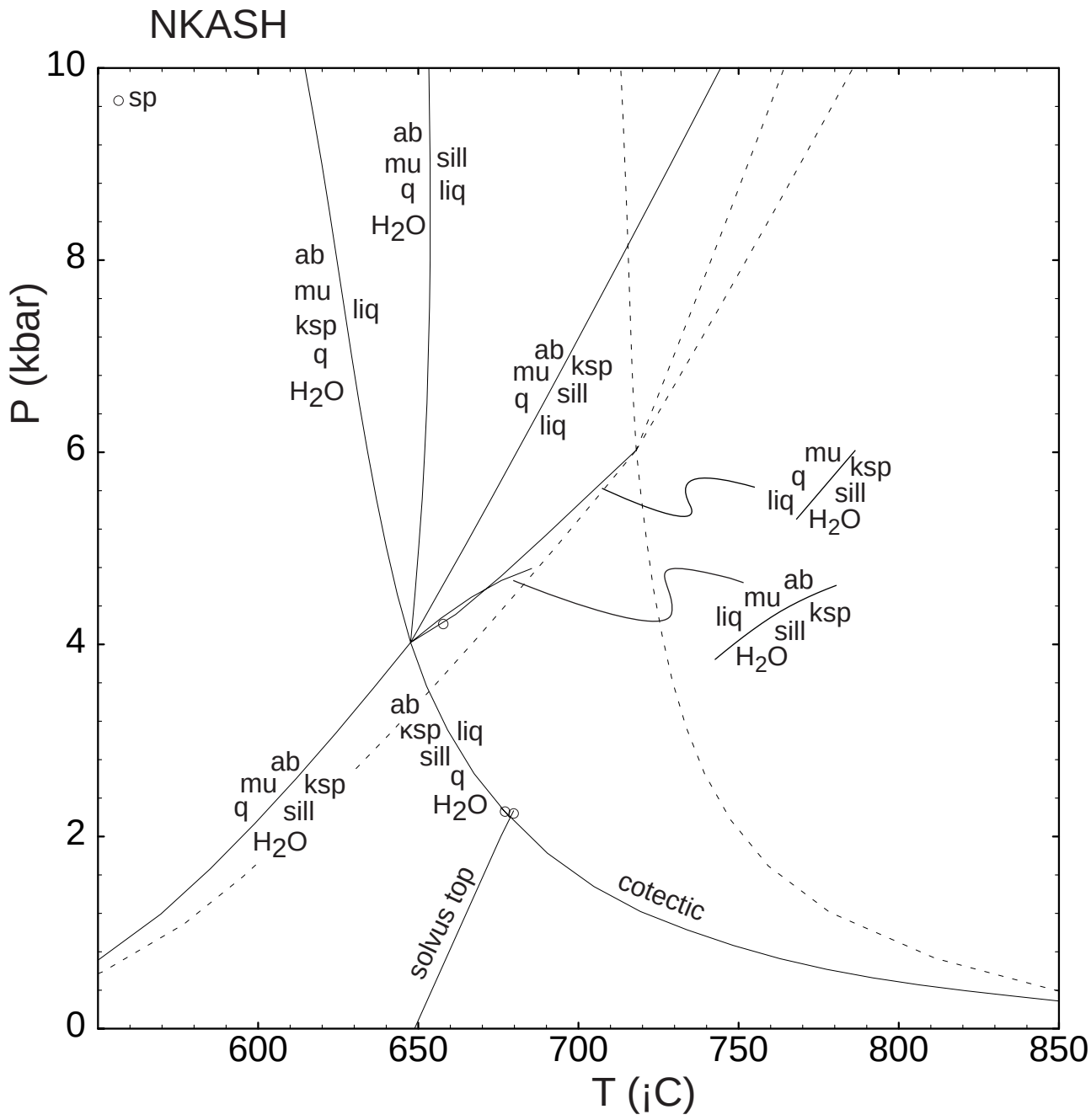
Fig. 4 . (a) *P-T* pseudosection for the average pelite composition used in Powell *et al.* (1998), with representative Na_2O and CaO added, and with H_2O sufficient to just saturate the mineral assemblages immediately sub-solidus at 6 kbar. The bulk composition in mole % is Al_2O_3 = 30.66, FeO = 23.74, MgO = 12.47, CaO = 0.97, Na_2O = 1.94, K_2O = 9.83, and H_2O = 20.39; quartz is taken to be in excess. (b) Summary information for (a), including the solidus and melt mode contours as proportions. (Datafile TH DNCK2)

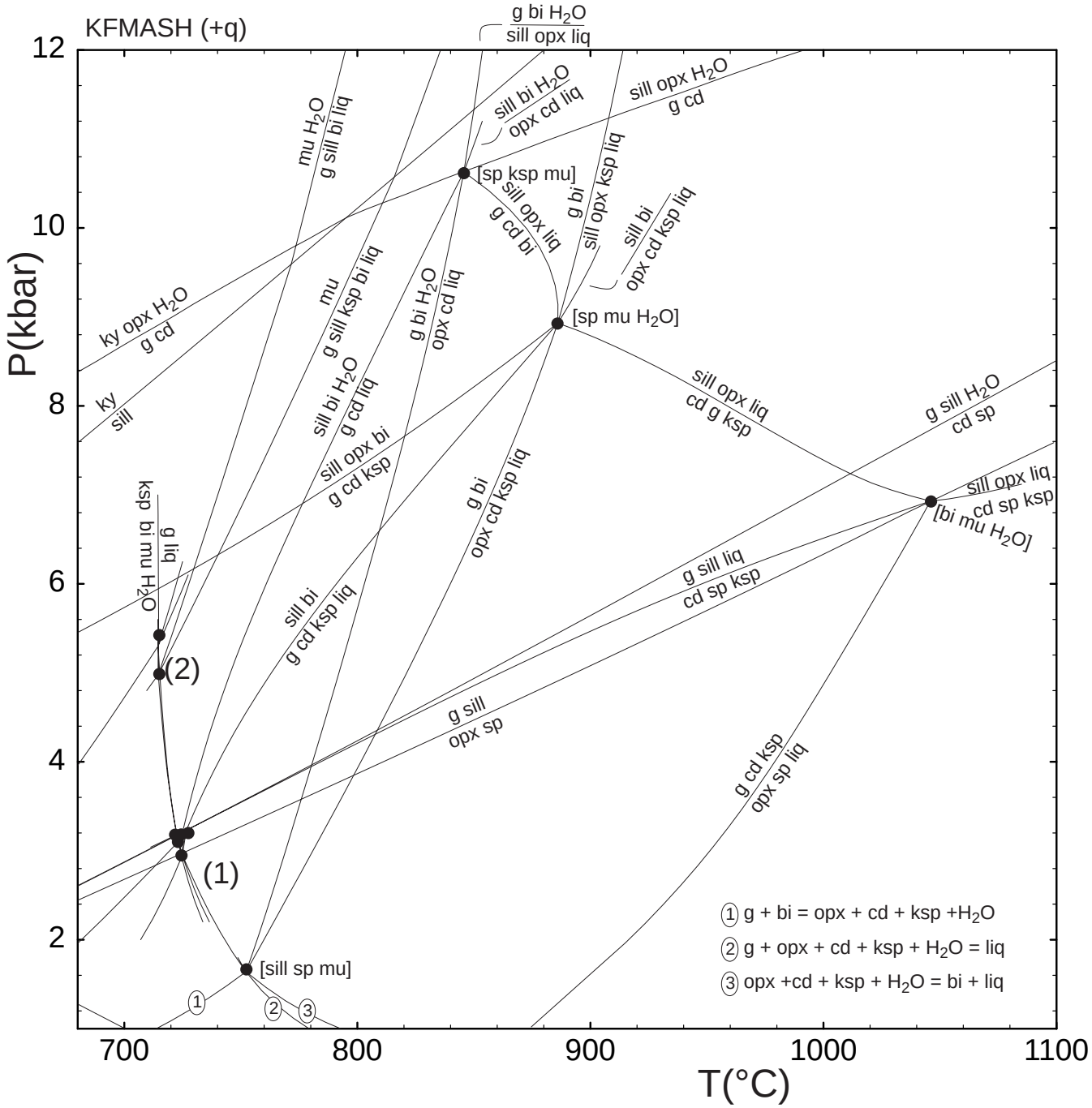
Fig. 5 . *P-T* pseudosection in KFMASH for the bulk composition in Fig. 3, but without CaO and Na_2O. Note the similarities with the *P-T* pseudosection in NCKFMASH in the supra-solidus region in Fig. 3. (Datafile TH DKB2)

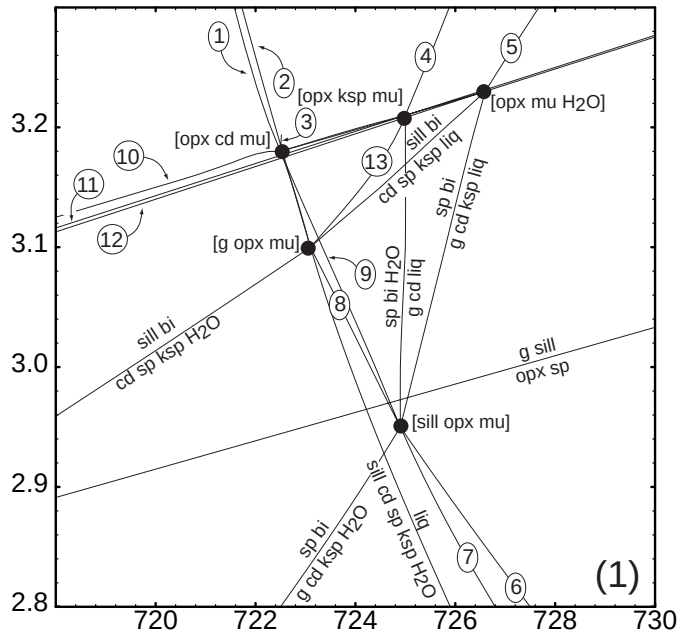
Fig. 6 . (a) T-X_{H_2O} pseudosection at 5 kbar for the bulk composition used in Fig. 3, with the x axis representing variation in the H_2O content in this bulk composition. At $x = 0$, the bulk composition is anhydrous, with Al_2O_3 = 38.51, FeO = 29.82, MgO = 15.66, CaO = 1.22, Na_2O = 2.44, K_2O = 12.35, while at $x = 1$, Al_2O_3 = 28.20, FeO = 21.83, MgO = 11.47, CaO = 0.89, Na_2O = 1.79, K_2O = 9.04, and H_2O = 21.61. (b) Summary information for (a), including the solidus, H2O-saturation line and melt mode contours. (Datafile TH DNCK3A)

Fig. 7 . *T-X* pseudosection at 5 kbar for a composition range representing mixtures of the residue ($x = 0$) and melt ($x = 1$) formed at 760°C and 5 kbars in the bulk composition used in Fig. 3. The melt composition is Al_2O_3 = 22.31, FeO = 1.57, MgO = 0.47, CaO = 1.00, Na_2O = 5.47, K_2O = 12.76 and H_2O = 56.42. (Datafile TH DNCK3B)

rp 28·4·01


NKASH
sp
ab
mu
q
H2O
sill
liq
ab
mu
ksp
q
H2O
liq
ab
mu
q
ksp
sill
liq
mu
q
ksp
liq
sill
H2O
ab
mu
liq
ksp
sill
H2O
ab
ksp
liq
sill
q
H2O
ab
mu
ksp
q
sill
H2O
solvus top
cotectic
P (kbar)
T (¡C)
0
2
4
6
8
10
600
650
700
750
800
850


KFMASH (+q)
P(kbar)
T(°C)
12
10
8
6
4
2
700
800
900
1000
1100
g bi H2O
sill opx liq
mu H2O
g sill bi liq
sill bi H2O
opx cd liq
sill opx H2O
g cd
[sp ksp mu]
sill opx liq
g cd bi
g bi
sill opx ksp liq
sill bi
opx cd ksp liq
[sp mu H2O]
ky opx H2O
g cd
ky
sill
mu
g sill ksp bi liq
g bi H2O
opx cd liq
sill bi H2O
g cd liq
sill opx bi
g cd ksp
sill opx liq
cd g ksp
g sill H2O
cd sp
sill opx liq
cd sp ksp
[bi mu H2O]
ksp bi mu H2O
g liq
g bi
opx cd ksp liq
g sill liq
cd sp ksp
sill bi
g cd ksp liq
(2)
g sill
opx sp
g cd ksp
opx sp liq
(1)
[sill sp mu]
① g + bi = opx + cd + ksp +H2O
② g + opx + cd + ksp + H2O = liq
③ opx +cd + ksp + H2O = bi + liq



① g + sill + ksp + bi + H_2O = liq

② sill + ksp + bi + H_2O = cd + liq

③ g + sill + ksp + H_2O = sp + liq

④ sill + bi + H_2O = g + cd + liq

⑤ sill + bi = g + cd + ksp + liq

⑥ g + cd + ksp + H_2O = bi + liq

⑦ cd + sp + ksp + H_2O = g + liq

⑧ cd + sp + ksp + H_2O = bi + liq

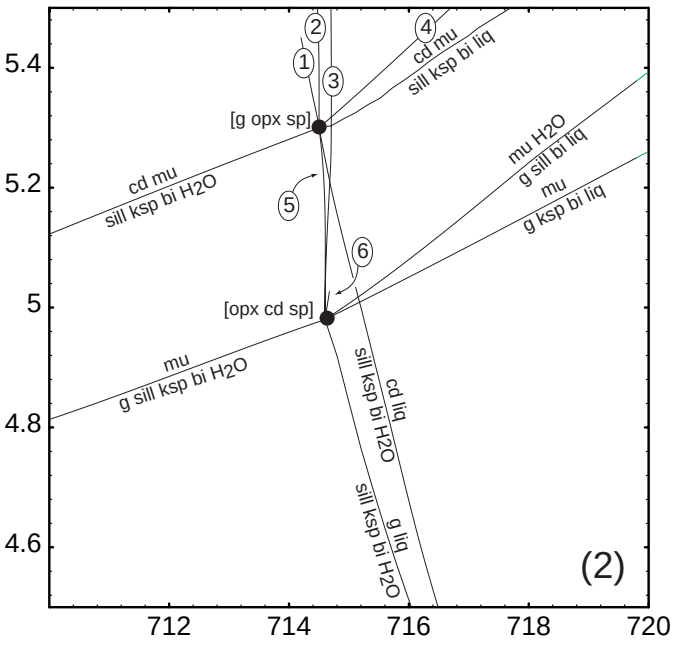
⑨ sp + bi + ksp + H_2O = g + liq

⑩ g + sill + ksp + H_2O = sp + bi

⑪ g + sill + H_2O = cd + sp

⑫ g + sill + bi = cd + sp + ksp

⑬ sill + bi + H_2O = cd + sp + liq



① cd + ksp + mu + H_2O = bi + liq

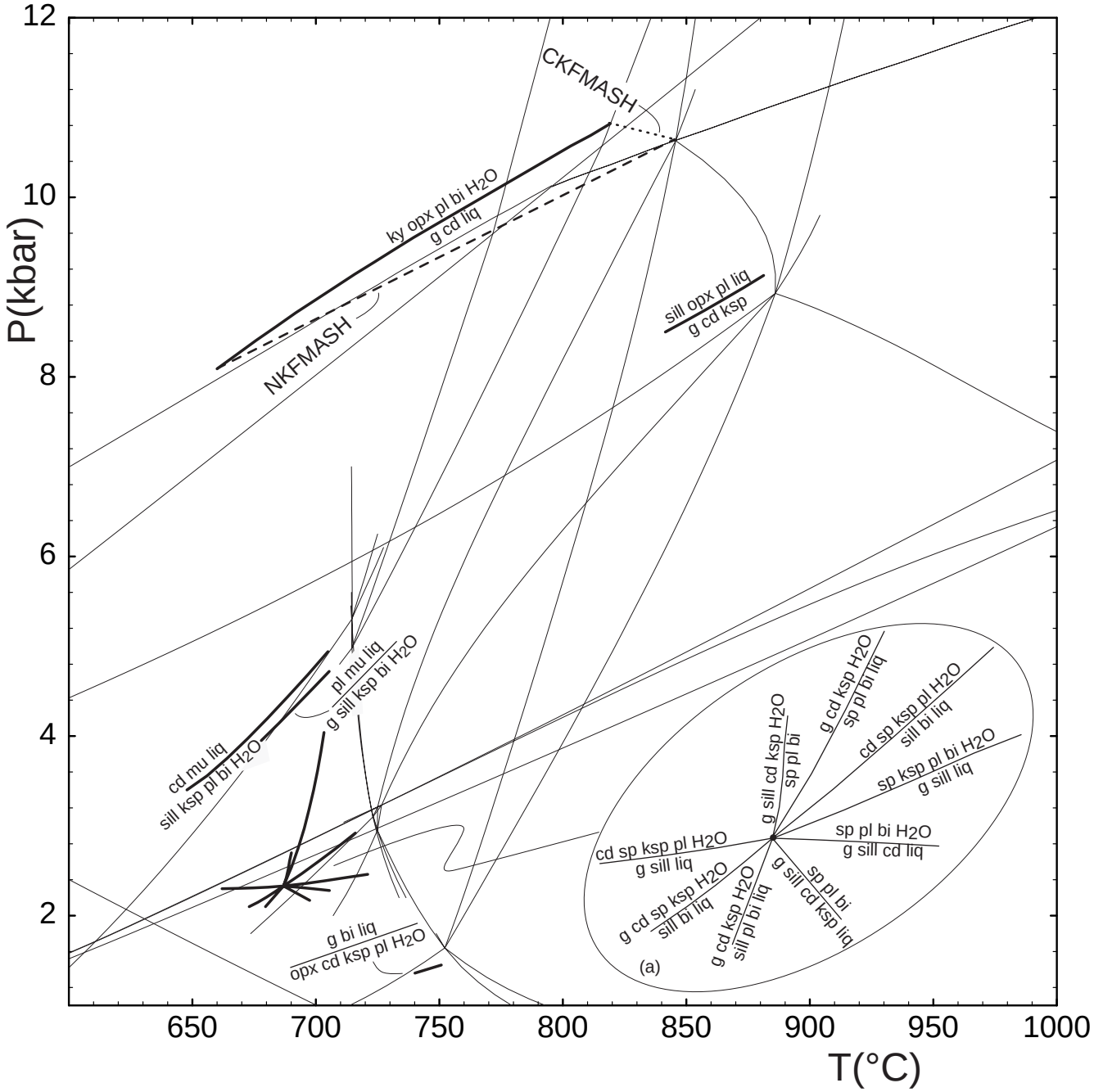
② sill + ksp + mu + H_2O = cd + liq

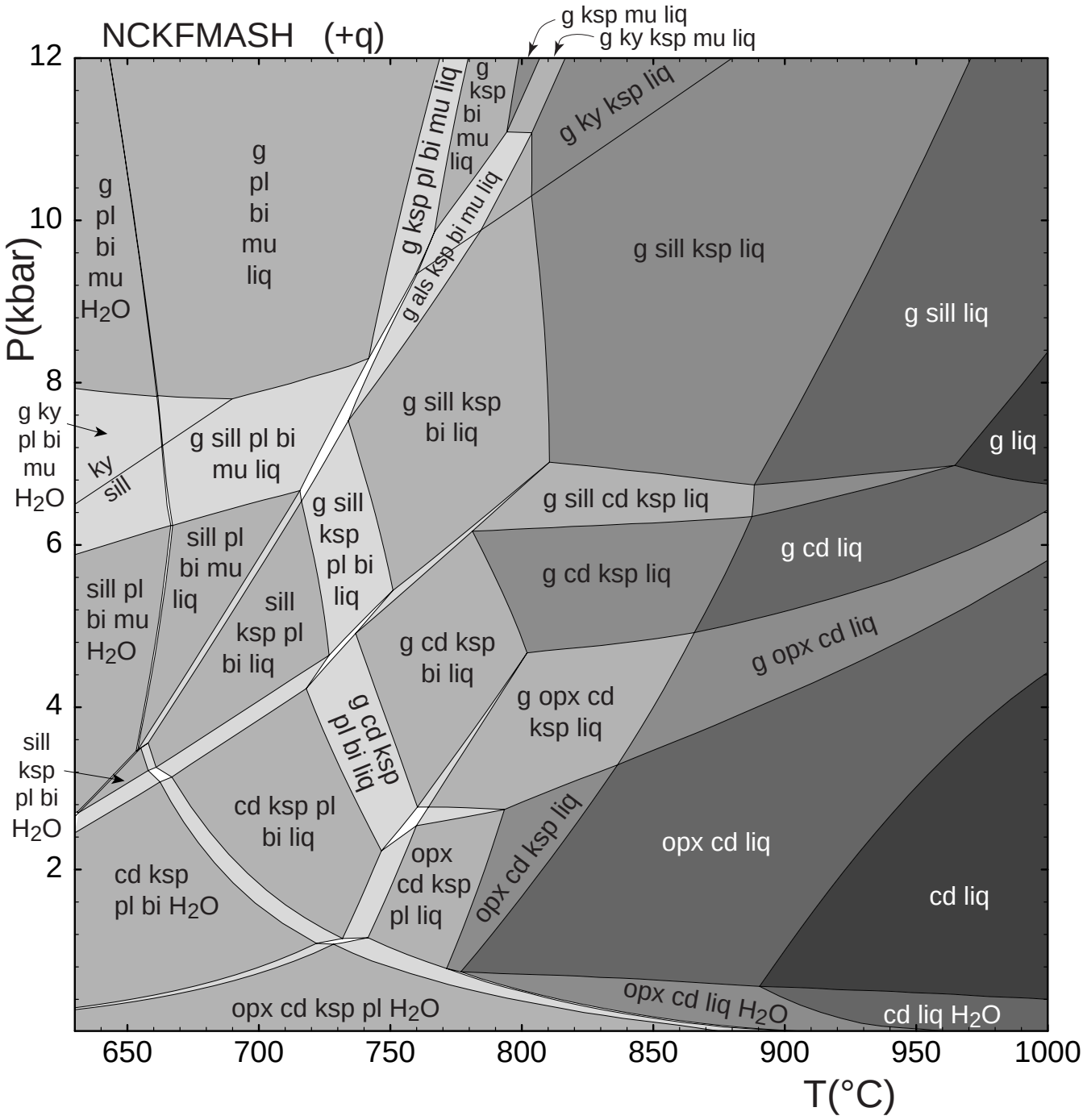
③ ksp + bi + mu + H_2O = g + liq

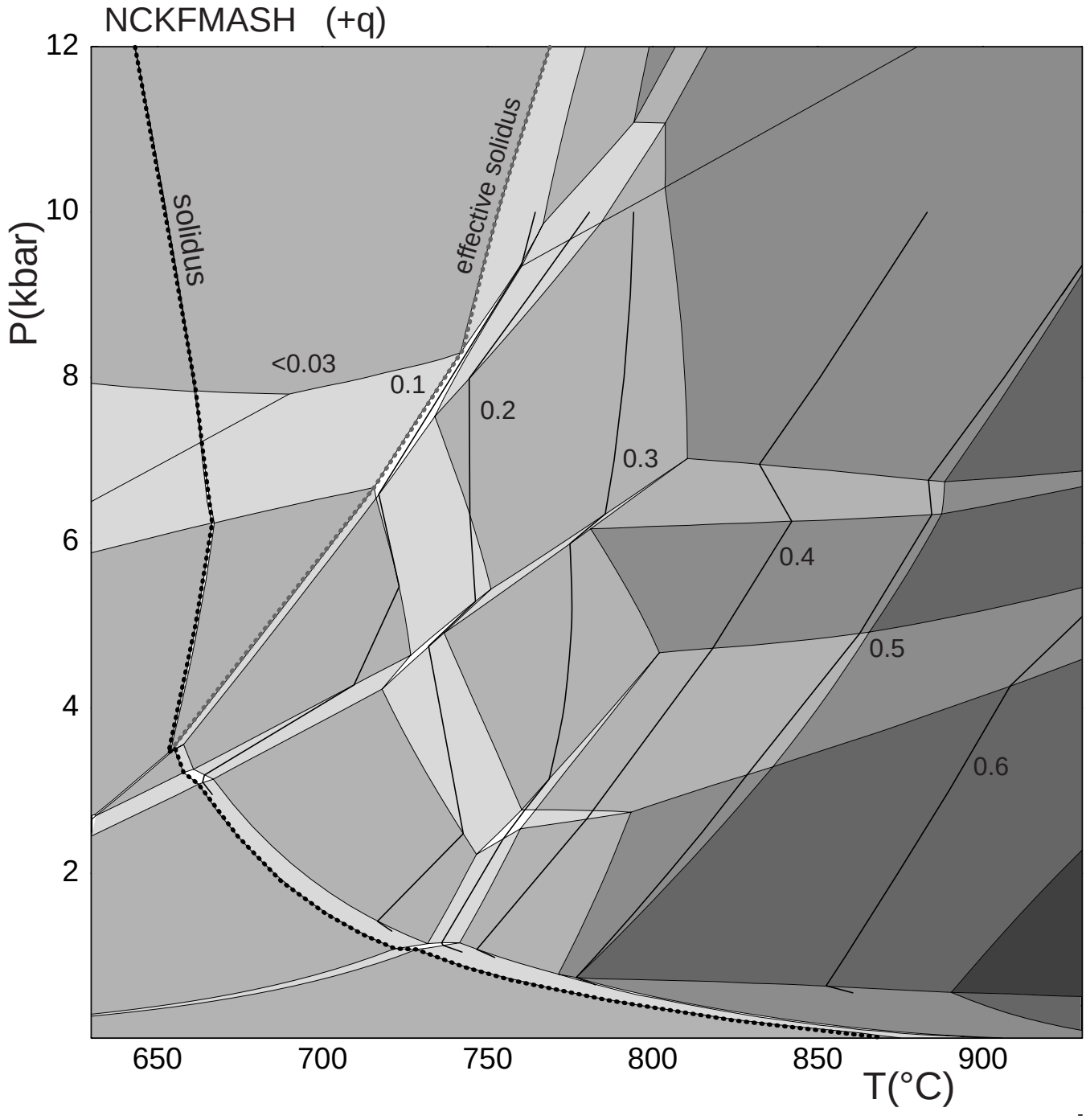
④ cd + mu + H_2O = sill + bi + liq

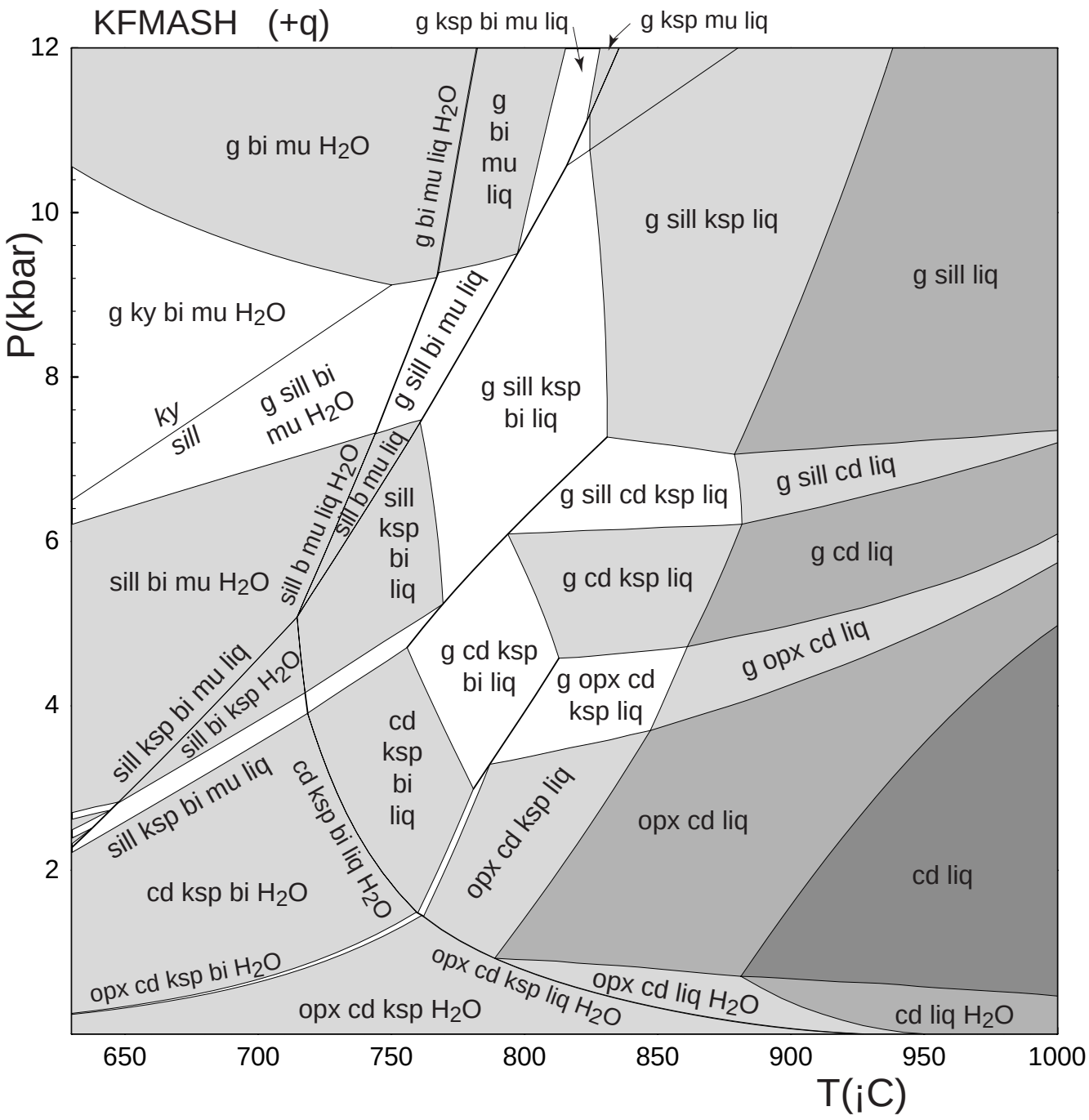
⑤ sill + ksp + bi + mu + H_2O = liq

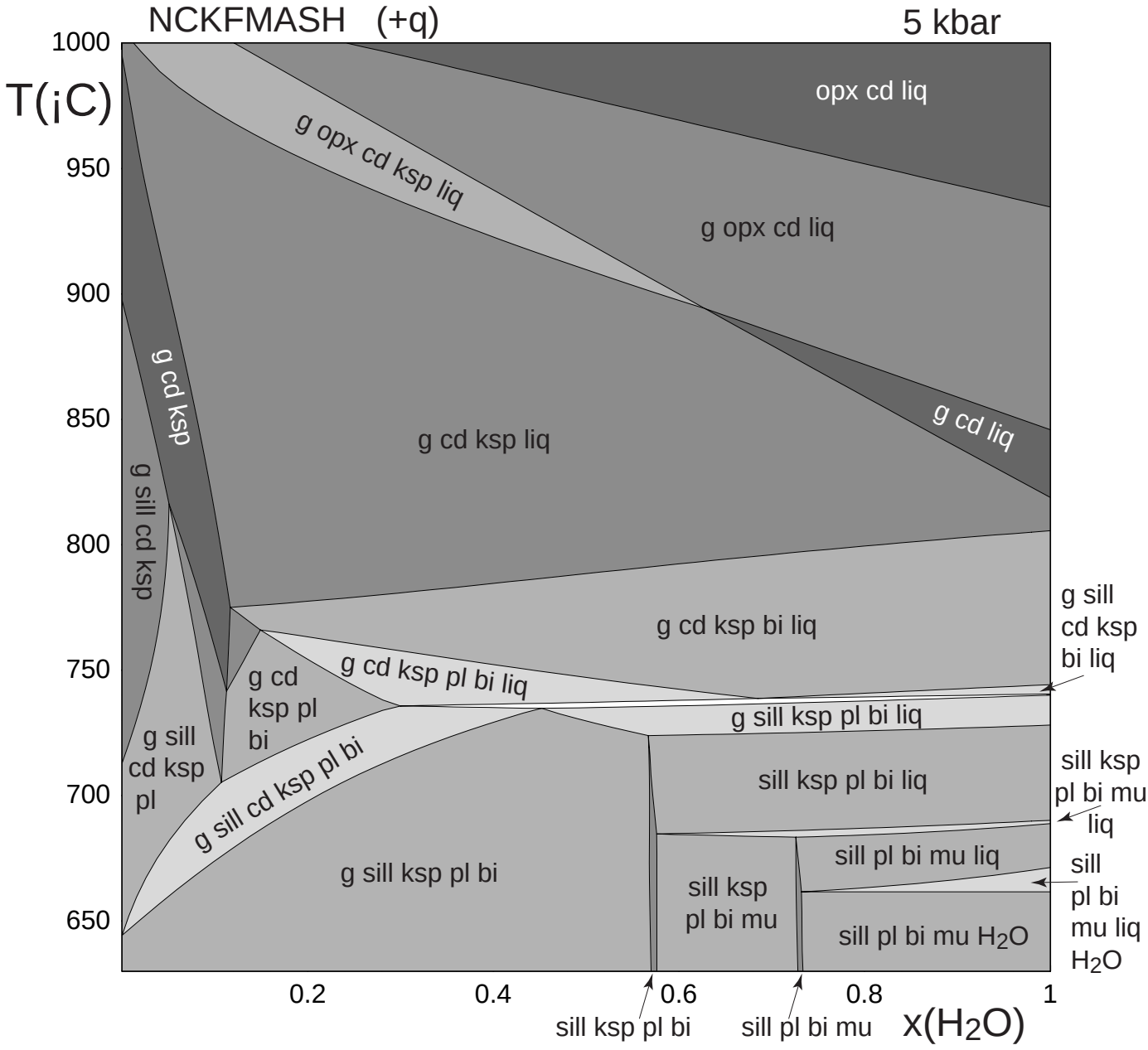
⑥ ksp + mu + H_2O = g + sill + liq

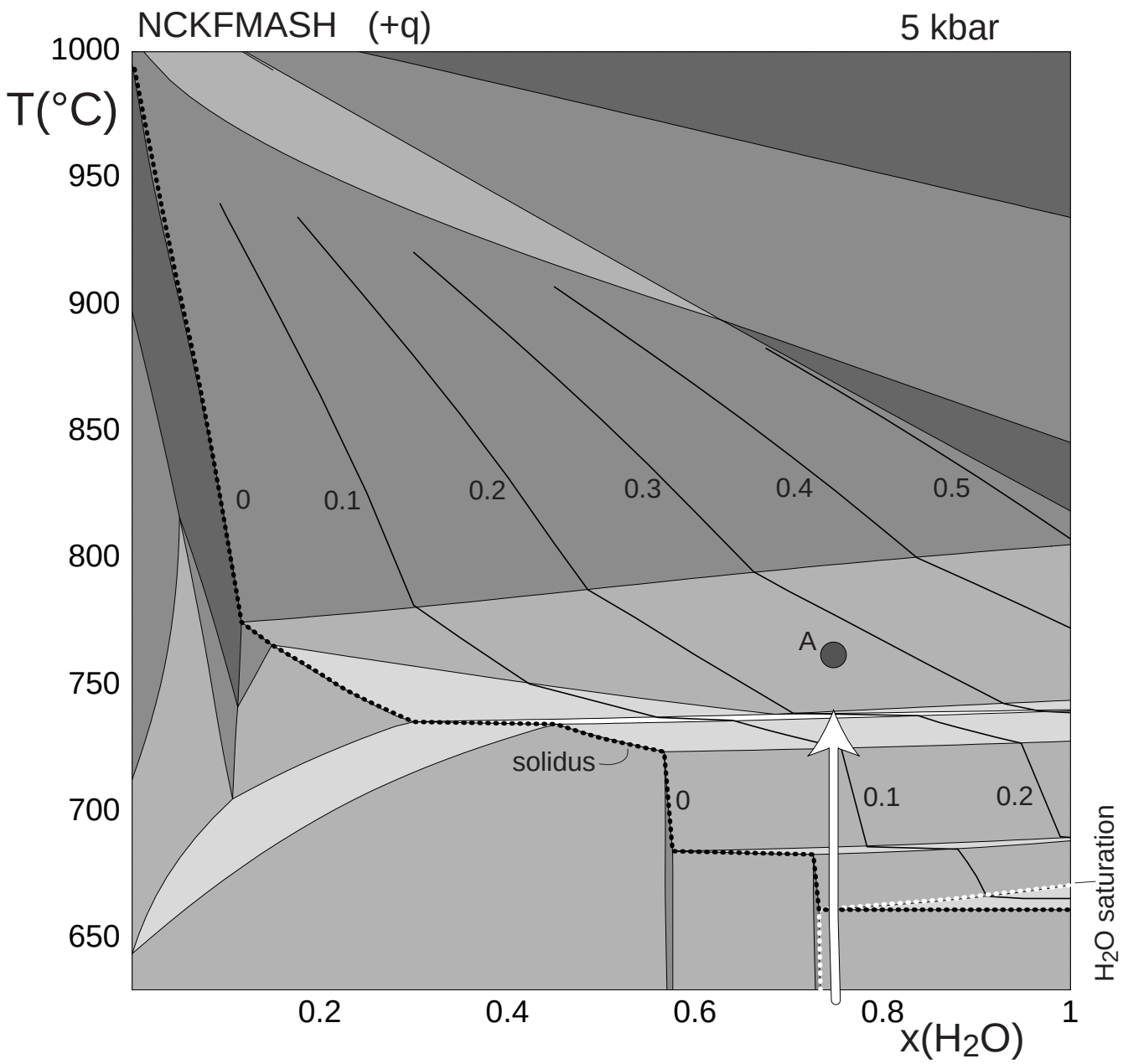

P(kbar)
T(°C)
12
10
8
6
4
2
650
700
750
800
850
900
950
1000
CKFMASH
NKFMASH
ky opx pl bi H2O
g cd liq
sill opx pl liq
g cd ksp
pl mu liq
g sill ksp bi H2O
cd mu liq
sill ksp pl bi H2O
g bi liq
opx cd ksp pl H2O
g sill cd ksp H2O
sp pl bi
g cd ksp H2O
sp pl bi liq
cd sp ksp pl H2O
sill bi liq
sp ksp pl bi H2O
g sill liq
sp pl bi H2O
g sill cd liq
cd sp ksp pl H2O
g sill liq
g cd sp ksp H2O
sill bi liq
g cd ksp H2O
sill pl bi liq
sp pl bi
g sill cd ksp liq
(a)

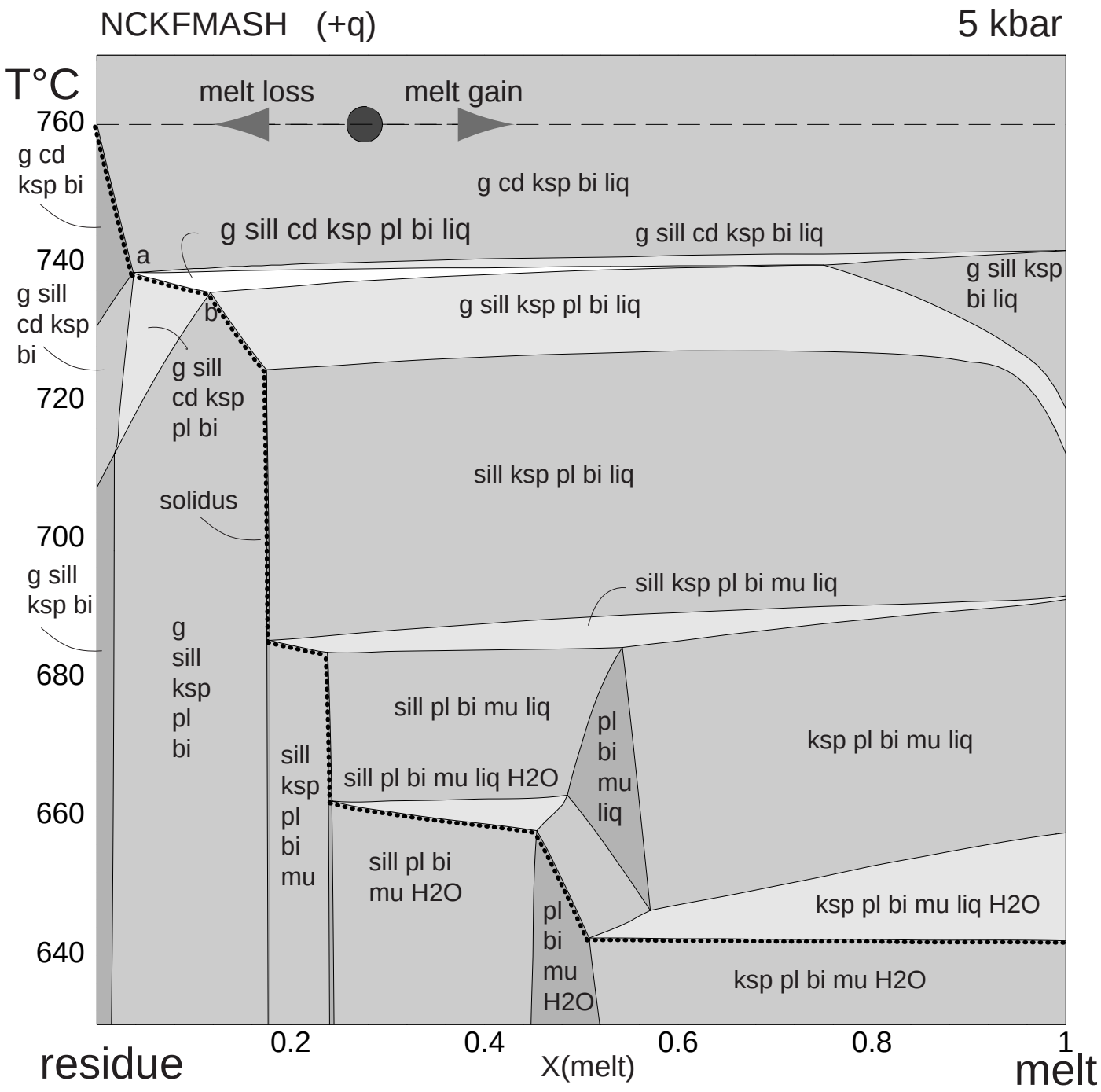

NCKFMASH (+q)
g ksp mu liq
g ky ksp mu liq
g pl bi mu H2O
g pl bi mu liq
g ksp pl bi mu liq
g ksp bi mu liq
g ky ksp liq
g sill ksp liq
g sill liq
g liq
g ky pl bi mu H2O
ky
sill
g sill pl bi mu liq
g sill ksp bi liq
g sill cd ksp liq
g cd liq
g cd ksp liq
sill pl bi mu liq
sill pl bi mu H2O
sill ksp pl bi liq
g sill ksp pl bi liq
g cd ksp bi liq
g opx cd liq
g opx cd ksp liq
g cd ksp pl bi liq
sill ksp pl bi H2O
cd ksp pl bi liq
opx cd ksp liq
opx cd liq
cd ksp pl bi H2O
opx cd ksp pl liq
cd liq
opx cd ksp pl H2O
opx cd liq H2O
cd liq H2O
P(kbar)
T(°C)
12
10
8
6
4
2
650
700
750
800
850
900
950
1000


NCKFMASH (+q)
P(kbar)
T(°C)
12
10
8
6
4
2
650
700
750
800
850
900
solidus
effective solidus
<0.03
0.1
0.2
0.3
0.4
0.5
0.6

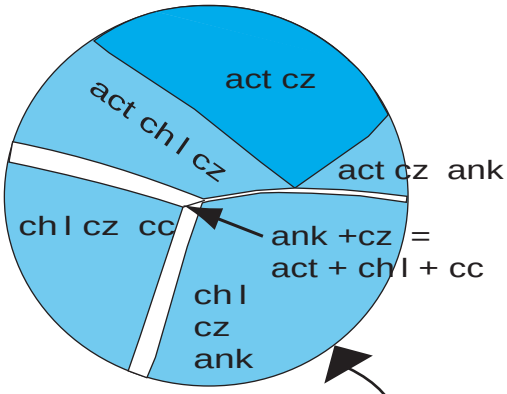

KFMASH (+q)
g ksp bi mu liq
g ksp mu liq
g bi mu H2O
g bi mu liq H2O
g bi mu liq
g sill ksp liq
g sill liq
g ky bi mu H2O
ky
sill
g sill bi mu H2O
g sill bi mu liq
g sill ksp bi liq
g sill cd liq
g sill cd ksp liq
sill b mu liq H2O
sill b mu liq
sill ksp bi liq
g cd liq
sill bi mu H2O
g cd ksp liq
g cd ksp bi liq
g opx cd liq
g opx cd ksp liq
sill ksp bi mu liq
sill bi ksp H2O
cd ksp bi liq
sill ksp bi mu liq
cd ksp bi liq H2O
opx cd ksp liq
opx cd liq
cd liq
cd ksp bi H2O
opx cd ksp bi H2O
opx cd ksp liq H2O
opx cd liq H2O
opx cd ksp H2O
cd liq H2O
P(kbar)
T(¡C)
12
10
8
6
4
2
650
700
750
800
850
900
950
1000

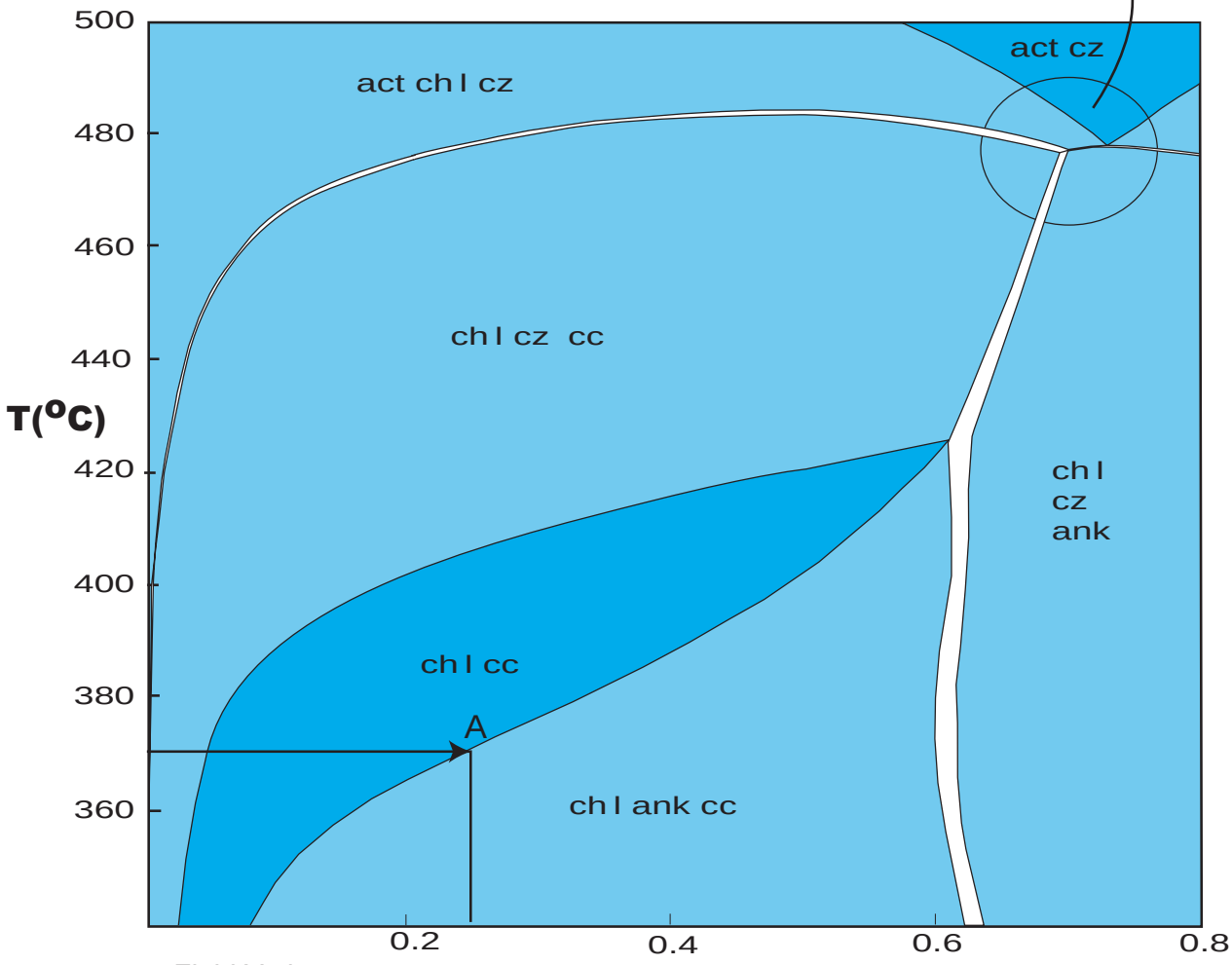

NCKFMASH (+q)
5 kbar
T(¡C)
1000
950
900
850
800
750
700
650
opx cd liq
g opx cd ksp liq
g opx cd liq
g cd liq
g cd ksp
g sill cd ksp
g cd ksp liq
g cd ksp bi liq
g cd ksp pl bi liq
g cd ksp pl bi
g sill cd ksp pl
g sill cd ksp pl bi
g sill ksp pl bi liq
sill ksp pl bi liq
sill pl bi mu liq
g sill ksp pl bi
sill ksp pl bi mu
sill pl bi mu H2O
g sill cd ksp bi liq
sill ksp pl bi mu liq
sill pl bi mu liq H2O
0.2
0.4
0.6
0.8
1
sill ksp pl bi
sill pl bi mu
x(H2O)


NCKFMASH (+q)
5 kbar
T(°C)
1000
950
900
850
800
750
700
650
0
0.1
0.2
0.3
0.4
0.5
A
solidus
0
0.1
0.2
H2O saturation
0.2
0.4
0.6
0.8
1
x(H2O)

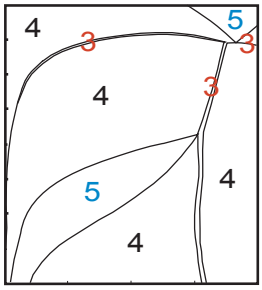

NCKFMASH (+q)
5 kbar
T°C
melt loss
melt gain
760
740
720
700
680
660
640
g cd ksp bi
g cd ksp bi liq
g sill cd ksp pl bi liq
g sill cd ksp bi liq
a
g sill ksp bi liq
g sill cd ksp bi
b
g sill ksp pl bi liq
g sill cd ksp pl bi
sill ksp pl bi liq
solidus
g sill ksp bi
sill ksp pl bi mu liq
g sill ksp pl bi
sill pl bi mu liq
sill ksp pl bi mu
sill pl bi mu liq H2O
pl bi mu liq
ksp pl bi mu liq
sill pl bi mu H2O
pl bi mu H2O
ksp pl bi mu liq H2O
ksp pl bi mu H2O
0.2
0.4
0.6
0.8
1
residue
X(melt)
melt

T -x(CO_2) Pseudosection at 2.5 Kbar for NCaFMASCH + q + ab + fluid





Field Variance



Bulk Rock Composition

Al_2O_3 : CaO : MgO : FeO

16.85 32.08 29.21 21.85

T- x(CO_2) pseudosection for NCaFMASCH +ab+cc +qtz +fluid. Path A demonstrates the effect of an infiltrating fluid on the mineral assemblages at Bronz ewing. The temperature of infiltration is constrained by the presence of ankerite as an alteration mineral.

calculated by fiona elmer