

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

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**Supplementary Table 1a** Thermodynamic data of *phl*, *ann*, *east*, *tbio* and *fbio* to be inserted into *Perple\_X* thermodynamic data file <hp62ver.dat>

phlD    EoS = 8 | H= -6209867. from Dachs and Benisek (2019), required for Bio(D)  
MgO(3)Al<sub>2</sub>O<sub>3</sub>(.5)SiO<sub>2</sub>(3)K<sub>2</sub>O(.5)H<sub>2</sub>O(1)  
GH = -6308534   S0 = 330.93   V0 = 14.964  
c1 = 920.883   c2 = -.8451119E-1   c3 = 2105320   c5 = -9802.57  
b1 = .38E-4   b5 = 500.325   b6 = 513000   b7 = -.143E-4   b8 = 7.33  
end

annD    EoS = 8 | H= -5131546 from Dachs and Benisek (2021), required for Bio(D)  
Al<sub>2</sub>O<sub>3</sub>(.5)SiO<sub>2</sub>(3)K<sub>2</sub>O(.5)FeO(3)H<sub>2</sub>O(1)  
GH = -5257643   S0 = 422.93   V0 = 15.48  
c1 = 748.96   c2 = -.0581675E-1   c3 = -921630   c5 = -6095.58  
b1 = .38E-4   b5 = 416.5931   b6 = 513000   b7 = -.143E-4   b8 = 7.33  
end

annDid   EoS = 8 | H= -5133636.5 from Dachs and Benisek (2024), required for Bio(Did), ideal Fe-Mg mixing  
Al<sub>2</sub>O<sub>3</sub>(.5)SiO<sub>2</sub>(3)K<sub>2</sub>O(.5)FeO(3)H<sub>2</sub>O(1)  
GH = -5259733   S0 = 422.93   V0 = 15.48  
c1 = 748.96   c2 = -.0581675E-1   c3 = -921630   c5 = -6095.58  
b1 = .38E-4   b5 = 416.5931   b6 = 513000   b7 = -.143E-4   b8 = 7.33  
end

eastD    EoS = 8 | H= -6352012 from Dachs and Benisek (2019), required for Bio(D)  
MgO(2)Al<sub>2</sub>O<sub>3</sub>(1.5)SiO<sub>2</sub>(2)K<sub>2</sub>O(.5)H<sub>2</sub>O(1)  
GH = -6439816   S0 = 294.5   V0 = 14.65  
c1 = 852.5   c2 = -.586602E-1   c3 = -404300   c5 = -8426.84  
b1 = .38E-4   b5 = 509.0324   b6 = 530000   b7 = -.143E-4   b8 = 7.33  
end

tbioD    EoS = 8 | tbioD: H= -6131113 from Dachs and Benisek (2024), required for Bio(D)  
Al<sub>2</sub>O<sub>3</sub>(.5)SiO<sub>2</sub>(3)K<sub>2</sub>O(.5)MgO(2)TiO<sub>2</sub>(1)  
GH = -6228924   S0 = 328.06   V0 = 14.808  
c1 = 798.37   c2 = -.597056E-1   c3 = 58239.6   c5 = -7792.34  
b1 = .38E-4   b5 = 416.5931   b6 = 632800   b7 = -.143E-4   b8 = 9.08  
end

fbioD    EoS = 8 | H= -5933628 from Dachs and Benisek (2024), required for Bio(D)  
Al<sub>2</sub>O<sub>3</sub>(1)SiO<sub>2</sub>(2)K<sub>2</sub>O(.5)MgO(2)FeO(1)H<sub>2</sub>O(1)O<sub>2</sub>(.25)  
GH = -6023579   S0 = 301.693   V0 = 15.414  
c1 = 777.684   c2 = -.396494E-1   c3 = -2838850   c5 = -6422.47  
b1 = .38E-4   b5 = 416.5931   b6 = 513000   b7 = -.143E-4   b8 = 7.33  
end

Supplementary Table Table 1b Solution model Bio(D) to be inserted into *Perple\_X* data file  
<solution\_model.dat>

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begin\_model

Fe-Mg-Al(Ts)-Al(ex)-Ti-Fe3+-Mn Biotite: Dachs and Benisek (2024)

688 format, E. Dachs Jun/2024.

Polytope 1 = [V][V][T']  
Polytope 2 = [K][M,T][M]

where

T = Al on M1, T' = Al on M2  
M = Mg, Fe

|              | 1 | 2  | 3  | 4  | H |  |
|--------------|---|----|----|----|---|--|
|              | A | M1 | M2 | T1 |   |  |
| Mutliplicity | 1 | 1  | 2  | 2  | 2 |  |

|             | endmember        |         |     |      |      |      | type               |
|-------------|------------------|---------|-----|------|------|------|--------------------|
| polytope 1: | 1: pyp           | V       | V   | AlAl | SiSi | OH   | independent orphan |
|             | mnbi             | K       | Mn  | MnMn | AlSi | OH   |                    |
| polytope 2: | 2: ffbio         | K       | Fe3 | FeFe | AlAl | OH   | dependent          |
|             | 3: fbio          | K       | Fe3 | MgMg | AlAl | OH   |                    |
|             | 4: sid           | K       | Al  | FeFe | AlAl | OH   | dependent          |
|             | 5: east          | K       | Al  | MgMg | AlAl | OH   |                    |
|             | 6: ffbio         | K       | Fe  | FeTi | AlSi | O    | dependent          |
|             | 7: tbio          | K       | Mg  | MgTi | AlSi | O    |                    |
|             | 8: ann           | K       | Fe  | FeFe | AlSi | OH   |                    |
|             | 9: phl           | K       | Mg  | MgMg | AlSi | OH   |                    |
|             | ordered species: | 10: obi | K   | Fe   | MgMg | AlSi | OH                 |

Bio(D) | model name  
abbreviation Bio  
full\_name biotite

688 | model type: 688 format standard model

2 | number of polytopes  
| polytope names and composite composition space subdivision schemes

[V][V][T'] 0 0.5 .1 0 |  
[K][M,T][M] by difference

-----  
Polytope 1 - 1 simplex  
1 | number of simplices  
2 1 | number of vertices on each simplex  
prl mnbi | endmembers on the vertices

X\_Mn 0 0.5 .1 0 | X(1,1) is bulk Fe/M  
X\_Prl by difference

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|-----
Polytope 2 - 2x4 simplices
2      number of simplices
2 4    number of vertices on each simplex
      endmembers on the vertices

ffbio  fbioD
sid     eastD
ftbio  tbioD
annD    phlD

| First 2-simplex
X_Mg  0  1  .1  0      | X(1,1) is bulk Fe/M
X_Fe  by difference

| Second 2-simplex
X_FeTs 0  1  .1  0      | X(2,1) is Fe3/[T+M] on M1, M on M2
X_AlTs  0  1  .1  0      | X(2,2) is Al/[T+M] on M1, M on M2
X_TiTs  0  1  .1  0      | X(2,3) is MTi/[M+MTi] on M2, M on M1
X_MBio  by difference

begin_ordered_endmembers
obi = 2/3 phlD + 1/3 annD  enthalpy_of_ordering = -2.0d3
end_ordered_endmembers

begin_dependent_endmembers
sid = 1 annD + 1 eastD - 1 obi
ftbio = 1 tbioD + 1/2 annD + 1/2 obi - 1 phlD
ffbio = 1 fbioD + 1 annD - 1 obi
end_dependent_endmembers

begin_excess_function
W(phlD annD annD) -8800. | excess parameters from Dachs and Benisek (2021, 2024)
W(phlD phlD annD) 14300.
W(phlD eastD) 19000.
W(phlD obi) -100.
W(phlD prl) 116800
W(annD eastD) -5000.
W(annD obi) -400.
W(annD prl) 108200
W(annD tbioD) -30000.
W(eastD obi) -5000.
W(eastD prl) 120000
W(obi prl) 120000
W(prl tbioD) 120000
W(prl fbioD) 120000
end_excess_function

5      | number of identsites in configurational entropy model
A
2 1 1
z(K,A) = 1 phlD + 1 eastD + 1 annD + 1 obi + 1 tbioD + 1 fbioD + 1 mnbi
z(Vac,A) = 1 prl

M1      | site name
6 1 1   | number of species, effective multiplicity, true multiplicity
z(Al,M1) = 1 eastD
z(Mg,M1) = 1 phlD + 1 tbioD
z(Fe3,M1) = 1 fbioD
z(Mn,M1) = 1 mnbi
z(Fe,M1) = 1 annD + 1 obi
z(Vac,M1) = 1 prl

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M2 | site name  
5 2 2 | number of species, effective multiplicity, true multiplicity  
z(Fe,M2) = 1 annD  
z(Al,M2) = 1 prl  
z(Ti,M2) = 1/2 tbioD  
z(Mn,M2) = 1 mnbi  
z(Mg,M2) = 1 eastD + 1 obi + 1 phlD + 1/2 tbioD + 1 fbioD

T1 | site name  
2 2 2 | number of species, effective multiplicity, true multiplicity  
z(Si,T1) = 1/2 phlD + 1/2 annD + 1/2 obi + 1 prl + 1/2 tbioD + 1/2 mnbi  
z(Al,T1) = 1 eastD + 1/2 phlD + 1/2 annD + 1/2 obi + 1/2 tbioD + 1 fbioD + 1/2 mnbi

OH | site name  
2 2 2 | 2 species on H, 2 site per formula unit.  
z(O,OH) = 1 tbioD  
z(OH,OH) = 1 eastD + 1 phlD + 1 annD + 1 obi + 1 prl + 1 fbioD + 1 mnbi

[Si2O10(OH)2] | formula suffix, enter "none" for no suffix.

end\_of\_model

**Supplementary Table 1c** Solution model Bio(Did) (ideal Fe-Mg mixing) to be inserted into *Perple\_X* data file  
<solution\_model.dat>

begin\_model

Fe-Mg-Al(Ts)-Al(ex)-Ti-Fe3+-Mn Biotite: Dachs and Benisek (2024)  
simplified version of Bio(D) with ideal Fe-Mg mixing.

688 format, E. Dachs Jun/2024.

Polytope 1 = [V][V][T']  
Polytope 2 = [K][M,T][M]

where

T = Al on M1, T' = Al on M2  
M = Mg, Fe

|              |          |    |       |      |      |    |                    |
|--------------|----------|----|-------|------|------|----|--------------------|
|              | 1        | 2  | 3     | 4    | H    |    |                    |
|              | A        | M1 | M2    | T1   |      |    |                    |
| <hr/>        |          |    |       |      |      |    |                    |
| Mutliplicity | 1        | 1  | 2     | 2    | 2    |    |                    |
| <hr/>        |          |    |       |      |      |    |                    |
| endmember    |          |    | type  |      |      |    |                    |
| <hr/>        |          |    | <hr/> |      |      |    |                    |
| polytope 1:  | 1: pyp   | V  | V     | AlAl | SiSi | OH | independent orphan |
|              | mnbi     | K  | Mn    | MnMn | AlSi | OH |                    |
| polytope 2:  | 2: ffbio | K  | Fe3   | FeFe | AlAl | OH | dependent          |
|              | 3: fbio  | K  | Fe3   | MgMg | AlAl | OH |                    |
|              | 4: sid   | K  | Al    | FeFe | AlAl | OH | dependent          |
|              | 5: east  | K  | Al    | MgMg | AlAl | OH |                    |
|              | 6: ftbio | K  | Fe    | FeTi | AlSi | O  | dependent          |

|         |   |    |      |      |    |
|---------|---|----|------|------|----|
| 7: tbio | K | Mg | MgTi | AlSi | O  |
| 8: ann  | K | Fe | FeFe | AlSi | OH |
| 9: phl  | K | Mg | MgMg | AlSi | OH |

ordered species: 10: obi      K      Fe      MgMg      AlSi      OH      ordered

Bio(Did)                      | model name  
 abbreviation Bio  
 full\_name biotite

688                              | model type: 688 format standard model

2                                | number of polytopes  
                                  | polytope names and composite composition space subdivision schemes

[V][V][T] 0 0.5 .1 0 |  
 [K][M,T][M] by difference

                                 | Polytope 1 - 1 simplex  
 1                                | number of simplices  
 2 1                              | number of vertices on each simplex  
 prl mnbi                      | endmembers on the vertices

X\_Mn 0 0.5 .1 0              | X(1,1) is bulk Fe/M  
 X\_Prl by difference

                                 | -----  
                                  | Polytope 2 - 2x4 simplices  
 2                                | number of simplices  
 2 4                              | number of vertices on each simplex  
                                  | endmembers on the vertices

ffbio fbioD  
 sid eastD  
 ftbio tbioD  
 annDid phlD

                                 | First 2-simplex  
 X\_Mg 0 1 .1 0                | X(1,1) is bulk Fe/M  
 X\_Fe by difference

                                 | Second 2-simplex  
 X\_FeTs 0 1 .1 0              | X(2,1) is Fe3/[T+M] on M1, M on M2  
 X\_AlTs 0 1 .1 0              | X(2,2) is Al/[T+M] on M1, M on M2  
 X\_TiTs 0 1 .1 0              | X(2,3) is MTi/[M+MTi] on M2, M on M1  
 X\_MBio by difference

begin\_ordered\_endmembers  
 obi = 2/3 phlD + 1/3 annDid    enthalpy\_of\_ordering = -2.0d3  
 end\_ordered\_endmembers

begin\_dependent\_endmembers  
 sid = 1 annDid + 1 eastD - 1 obi  
 ftbio = 1 tbioD + 1/2 annDid + 1/2 obi - 1 phlD  
 ffbio = 1 fbioD + 1 annDid - 1 obi  
 end\_dependent\_endmembers

begin\_excess\_function  
 W(phlD eastD) 19000.              | excess parameters from Dachs and Benisek (2021, 2024)  
 W(phlD prl) 116800  
 W(annDid eastD) -5000.  
 W(annDid prl) 108200  
 W(annDid tbioD) -30000.  
 W(eastD obi) -5000.  
 W(eastD prl) 120000

W(eastD tbioD) 0.  
W(obi prl) 120000  
W(prl tbioD) 120000  
W(prl fbioD) 120000  
end\_excess\_function

5 | number of identsites in configurational entropy model

A

2 1 1

$z(K,A) = 1 \text{ phlD} + 1 \text{ eastD} + 1 \text{ annDid} + 1 \text{ obi} + 1 \text{ tbioD} + 1 \text{ fbioD} + 1 \text{ mnbi}$

$z(\text{Vac},A) = 1 \text{ prl}$

M1 | site name

6 1 1 | number of species, effective multiplicity, true multiplicity

$z(\text{Al},M1) = 1 \text{ eastD}$

$z(\text{Mg},M1) = 1 \text{ phlD} + 1 \text{ tbioD}$

$z(\text{Fe3},M1) = 1 \text{ fbioD}$

$z(\text{Mn},M1) = 1 \text{ mnbi}$

$z(\text{Fe},M1) = 1 \text{ annDid} + 1 \text{ obi}$

$z(\text{Vac},M1) = 1 \text{ prl}$

M2 | site name

5 2 2 | number of species, effective multiplicity, true multiplicity

$z(\text{Fe},M2) = 1 \text{ annDid}$

$z(\text{Al},M2) = 1 \text{ prl}$

$z(\text{Ti},M2) = 1/2 \text{ tbioD}$

$z(\text{Mn},M2) = 1 \text{ mnbi}$

$z(\text{Mg},M2) = 1 \text{ eastD} + 1 \text{ obi} + 1 \text{ phlD} + 1/2 \text{ tbioD} + 1 \text{ fbioD}$

T1 | site name

2 2 2 | number of species, effective multiplicity, true multiplicity

$z(\text{Si},T1) = 1/2 \text{ phlD} + 1/2 \text{ annDid} + 1/2 \text{ obi} + 1 \text{ prl} + 1/2 \text{ tbioD} + 1/2 \text{ mnbi}$

$z(\text{Al},T1) = 1 \text{ eastD} + 1/2 \text{ phlD} + 1/2 \text{ annDid} + 1/2 \text{ obi} + 1/2 \text{ tbioD} + 1 \text{ fbioD} + 1/2 \text{ mnbi}$

OH | site name

2 2 2 | 2 species on H, 2 site per formula unit.

$z(\text{O},\text{OH}) = 1 \text{ tbioD}$

$z(\text{OH},\text{OH}) = 1 \text{ eastD} + 1 \text{ phlD} + 1 \text{ annDid} + 1 \text{ obi} + 1 \text{ prl} + 1 \text{ fbioD} + 1 \text{ mnbi}$

[Si2O10(OH)2] | formula suffix, enter "none" for no suffix.

end\_of\_model