

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

(Contributions to Mineralogy and Petrology, in press)

Department of Chemistry and Physics of Materials, University of Salzburg

Jakob-Haringerstrasse 2a, A-5020 Salzburg, Austria

E-mail: edgar.dachs@plus.ac.at

Supplementary Table 6 Predicted versus measured compositions of selected minerals from test samples. Calculations were done with *Perple_X* (program *Werami*) with thermodynamic standard state data of biotite endmembers and the activity model Bio(D) from this study (Tables 2, 3), compared to calculations with *Perple_X*-implemented biotite models Bi(W) (White et al. 2014) and Bio(TCC) (Tajčmanova et al. 2009). Other solid-solution models used are given in the text, bulk-rock compositions are given in supplementary Table 5.

sample / ref. assemblage	P kbar	T °C	biotite model	Si	Al ^{IV}	Al ^{VI}	biotite composition							other compositions				
							Al ^{VI} _{ex}	Ti	Fe ²⁺	Fe ³⁺	Mg	K	X _{Fe²⁺}	chl ²⁾ X _{Fe²⁺}	chl/bio K _D	phe Si	X _{Fe²⁺}	chl/phe K _D
16 / M70¹⁾	4	350																
bio-chl-phe- plag-qtz-cal			measured	2.77	1.23	0.31	0.08	0.12	1.41	0.09	0.85	0.84	0.62	0.60	0.89	3.21	0.41	2.17
			Bio(D)	2.68	1.32	0.26	0.00	0.04	1.53	0.07	1.10	1.00	0.58	0.55	0.89	3.12	0.44	1.55
			Bi(W)	2.94	1.06	0.05		0.04	1.82	0.01	1.08	1.00	0.63	0.43	0.44	3.04	0.40	1.11
			Bio(TCC)	2.92	1.08	0.06		0.06	1.71	0.02	1.15	1.00	0.60	0.52	0.74	3.05	0.42	1.49
18 / M70¹⁾	4	410	measured	2.69	1.31	0.25	-0.06	0.11	1.43	0.07	0.97	0.87	0.60	0.56	0.88	3.19	0.35	2.35
bio-chl-phe- plag-qtz-cal			Bio(D)	2.75	1.25	0.21	0.00	0.04	1.65	0.06	1.01	0.99	0.62	0.60	0.94	3.17	0.51	1.47
			Bi(W)	2.95	1.05	0.04		0.04	1.88	0.01	1.01	1.00	0.65	0.47	0.48	3.11	0.42	1.24
			Bio(TCC)	2.91	1.09	0.07		0.06	1.79	0.02	1.04	1.00	0.63	0.56	0.75	3.10	0.48	1.40
980A / T01¹⁾, F80¹⁾	4	560												stau X _{Fe²⁺}	plag X _{Ca}		grt X _{Ca}	X _{Mn}
grt-bio-stau- phe-and-qtz			measured			0.52		0.09		nd			0.52	0.84	0.35	0.89	0.06	0.12
			Bio(D)	2.48	1.52	0.56	0.04	0.12	1.24	0.04	0.99	0.97	0.56	0.80	0.37	0.88	0.05	0.29
			Bi(W)	2.65	1.35	0.29		0.08	1.38	0.06	1.18	1.00	0.54	0.77	0.38	0.86	0.05	0.29
			Bio(TCC)	2.50	1.50	0.47		0.07	1.30	0.04	1.04	1.00	0.56	0.76	0.37	0.86	0.05	0.34
X567 / PdW01¹⁾	2	665												crd X _{Fe²⁺}	plag X _{Ca}		grt X _{Ca}	X _{Mn}
crd-bio-kfsp- plag-qtz±grt			measured	2.53	1.47	0.48	0.01	0.19	1.73	nd	0.48	0.89	0.78	0.65	0.36	0.92	0.03	0.01
			Bio(D)	2.55	1.45	0.48	0.03	0.19	1.73	0.05	0.53	0.97	0.77	0.68	0.37	0.95	0.02	0.04
			Bio(Did) ³⁾	2.49	1.51	0.55	0.04	0.25	1.72	0.04	0.42	0.97	0.81	0.63	0.32			
			Bi(W)	2.65	1.35	0.26		0.12	2.07	0.09	0.46	1.00	0.82	0.67	0.38			
		730	Bio(TCC)	2.46	1.54	0.48		0.25	1.81	0.06	0.40	1.00	0.82	0.67	0.37			

16Slo12 / L20 ¹⁾	9	630											stau	phe		
													X _{Fe} ²⁺	Si	X _{Fe} ²⁺	
bio+stau+ru			measured	2.71	1.29	0.54	0.24	0.08	0.91	nd	1.34	0.82	0.40	0.62	3.08	0.44
incl. in grt			Bio(D)	2.63	1.37	0.47	0.10	0.11	1.17	0.00	1.21	0.97	0.49	0.72	3.08	0.40
phe ₁ in			Bi(W)	2.78	1.22	0.22		0.10	1.29	0.00	1.38	1.00	0.48	0.72	3.08	0.41
matrix			Bio(TCC)	2.61	1.39	0.39		0.17	1.35	0.00	1.09	1.00	0.55	0.77	3.06	0.46
	7	630	Bio(D)	2.58	1.42	0.52	0.10	0.14	1.30	0.00	1.00	0.97	0.56	0.79	3.03	0.48
			Bi(W)	2.73	1.27	0.27		0.11	1.48	0.00	1.15	1.00	0.56	0.78	3.04	0.47
			Bio(TCC)	2.52	1.48	0.48		0.18	1.44	0.00	0.89	1.00	0.62	0.80	3.01	0.50

¹⁾ M70: Mather (1970); F80: Ferry (1980); T01: Tinkham et al. (2001); PdW01: Pitra and de Waal (2001); L20: Li et al. (2020).

²⁾ mineral abbreviations: chl: chlorite; bio: biotite; phe: phengite; stau: staurolite; plag: plagioclase; kfsp: kalifeldspar; grt: garnet; ru: rutile; crd: cordierite; qtz: quartz; $K_D = (\text{Fe/Mg})^{\text{chl}}/(\text{Fe/Mg})^{\text{bio}}$; nd: not determined.

³⁾ simplified version of Bio(D) assuming ideal Fe-Mg mixing.