

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

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Supplementary Table 4 Macroscopic W_{ij} 's and their decomposition into microscopic interaction parameters w 's for the KFMASHTO biotite activity model of this study, with end-members given in Table 1. For macroscopic W_{phlann} and W_{phleas} (**bold**), corresponding micro- w 's have been quantified using *Castep* (Table 5). V = vacancy, Fe3 = Fe³⁺.

		n	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21
		macro- W	W	W	W	W	W	W	W	W	W	W	W	W	W	W	W	W	W	W	W	W	W
		i	phl	phl	phl	phl	ann	ann	ann	eas	eas	obi	phl	ann	eas	obi	pyp	phl	ann	eas	obi	pyp	tbio
		j	ann	eas	obi	pyp	eas	obi	pyp	obi	pyp	pyp	tbio	tbio	tbio	tbio	tbio	fbio	fbio	fbio	fbio	fbio	fbio
		kJ/mol	-2.4	18.8	-0.1	117	-5	-0.4	108	-5	120	120	0	-30									
		multipli-	1	1/4	1	1/4	1/4	1	1/4	1/4	1	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1	1/4	1	1/4
		cator																					
Site	micro- w	same site mixing																					
A	w_{KV}					4			4		1	4					4						
M1	w_{MgFe}	1		1										4		4							
	w_{MgAl}		4												4								
	w_{MgV}				4												4						
	w_{MgFe3}						4			4								4					4
	w_{FeAl}							4			4												
	w_{FeV}								4			4											
	w_{FeFe3}												4						4		4		
	w_{AlV}										1												
	w_{AlFe3}																			1			
	w_{VFe3}																					1	
M2	w_{MgFe}	1					4	1						2					4				
	w_{MgAl}				4						1	4					2					1	

[illegible]