

Table S1. Previously reported peaks and the peak assignments of infrared spectra of the Al-Fe³⁺ series of epidote.

Peak no. ^a	Refere nce	Observed peaks													Peak assignments					
		Langer and Raith (1974)						Petrusenko et al. (1992) ^b		Bradbury and Williams (2003)	Makreski et al. (2007)	White et al. (2017) ^d	Su et al. (2019)	Zheira et al. (2022)	Langer and Raith (1974)	Petrusenko et al. (1992) ^b	Bradbury and Williams (2003)	Makreski et al. (2007) ^c	White et al. (2017) ^d	Su et al. (2019)
		Sample	PF39	HU252	HU215	Wi51	Ep T	Ep	Czo	Nightengale, US	Dunje, Macedonia	NICOD OM ^c	Hamersley Basin, Austrarlia	Madagas car						
	Fe (apfu)	0	0.29	0.44	0.68	0.89	-	-	0.46	-	-	0.3-0.9	0.8	0.89-1.07						
												ca. 6450							2v(OH)	
													3762							O-H
													3360							O-H
													3641							O-H
													3397							O-H
1		3326	3338	3345	3360	3365	3380	3370	3351	3362s	3360s	3360-3375	3357	3379vs	v(OH)	v(OH)	v(OH)	v(OH)	v(OH)	O-H
2		1143	1126	1120	1110	1108	1118	1120	1121	1113m	1115m			1103w	v(Si-O)	v(Si-O) of Si ₂ O ₇	v3-SiO ₄	v(Si-O _{nb})		
3		1116	1106	1100wsh											v(Si-O)					
4				1090wsh	1079	1076	1080	1080		1076m	1075m			1076m	v(Si-O)	v(Si-O) of SiO ₄		v(Si-O _{nb})		
5		1047	1043	1039	1037	1035	1040	1045	1042	1038m	1036m			1034m	v(Si-O)	δ(OH)	v3-SiO ₄	v(Si-O _{nb}) + δ(OH)		
6		980sh	973wsh	977wsh	980wsh	975sh				970sh	970sh							antisym. v(Si-O _{nb})		
7		950	954	952	953	951	960	960	963	953vs	952vs			949vs	v(Si-O)	v(Si-O) of SiO ₄	v3-SiO ₄	antisym. v(Si-O _{nb})		
8		906	910wsh	905wsh	910wsh	900wsh				901sh	900sh			903wsh	δ(OH)			δ(OH)		
9		895	892	889	889	886	890	890	888	888s	885s		878	879s	v(Si-O)	v(Si-O) of SiO ₄	v1-SiO ₄	v(Si-O _{nb})		Si-O
10		869	865 sh	865 sh	862 sh	861			859	854vw	855vw			856wsh			v1(?)–SiO ₄	v(Si-O _{nb})		
11		849	843	843	840	836	840	850	841	831w	832vw			833w	v(Si-O)	v(Si-O) of SiO ₄	v1(?)–SiO ₄	v(Si-O _{nb})		
12			805	800wsh	802wsh	800wsh								798m						
13		741	733	731	723	718				722w	722w			714w				v(M-O)		
14		690sh	695wsh	697wsh	697wsh	697wsh								694wsh						
15		676	670	668sh	673wsh	670wsh		670	679	673sh, br	673sh, br			679sh	v(Si-O)	OH libration? v(M-O) or δ(Si-O)	δ(Si-O _b -Si)	δ(Si-O _b -Si)	δ(Si-O _b -Si)	δ(Si-O _b -Si)
16		650	649	648	649	648	650	650	660	646s	650vs			648s						
17		603	599	596sh	590wsh	585wsh				594sh	595sh			586sh						
18		575	575	571			570	570												
19		561	558	557	568	563				569w	570sh, br			559w						
20		527	544wsh	541	530wsh					539sh, br				540vw						
21			517	518	519	517	520	530		516s	520s			513s						
22		498	495wsh	495wsh																
23		487	477	474	467	460sh		470		469sh				462vw						
24		457	457	457	457	454	460	460		454m	455m			455m						
25			430wsh	430wsh	430wsh	410wsh				411sh					δ(O-Si-O), δ(Si-O-Si), v(M-O)			v(M-O)	δ(Si-O _b -Si)	v(M-O)
26		419	411	408	400	395	420	415		398s										
27		393	389	387	385sh	381				389sh										
28		363	360	359	355	351				371vw										
29		344	345sh	346wsh																
30		336sh	338	331sh																
31		320wsh	314	312		313														
32		305	299	295	300	297														
33					289	284														
34		274	268	265	260	256														

^a Adopted by Langer and Raith (1974).^b The OD stretching and libration modes are 2490 and 780 cm⁻¹, respectively.^c Frequencies and intensities are approximate because are not specified (Makreski et al., 2007).^d Result of short wave infrared spectroscopy.^e As the tentative assignments (Makreski et al., 2007).

Note : s: strong, w: weak, m: medium, sh: shoulder, v: very, br: broad, nb: non-bridging, b: bridging