

Tables and figures

Table 1. Pyroxene and related composition silicates, pyroxenoids [88M3, 91N1].

Silicate	Composition	End member	Classification group [91N1]
<i>I. Mg-Fe silicates</i>			
Enstatite (En)	$\text{Mg}_2\text{Si}_2\text{O}_6$		VIIID02
Ferrosilite (Fs)	$(\text{Fe},\text{Mg})_2(\text{SiO}_3)_2$	$\text{Fe}_2\text{Si}_2\text{O}_6$	VIIID02
Clinoenstatite (CEn)	$\text{Mg}_2\text{Si}_2\text{O}_6$		VIIID01a
Clinoferrosilite (CFs)	$(\text{Fe},\text{Mg})_2(\text{SiO}_3)_2$	$\text{Fe}_2\text{Si}_2\text{O}_6$	VIIID01a
Perovskite	MgSiO_3		
Ilmenite	MgSiO_3		
Akimotoite	$(\text{Mg},\text{Fe})\text{SiO}_3$		
<i>II. Mg-Mn silicates</i>			
Rhodonite (Rhd)	$(\text{Mn},\text{Fe},\text{Mg},\text{Ca})\text{SiO}_3$	MnSiO_3	VIIID13
Pyroxmangite (Pxm)	MnSiO_3		VIIID13
Pyroxferroite	$(\text{Fe},\text{Mg},\text{Ca})\text{SiO}_3$		VIIID13
Kanoite (Kan)	$(\text{Mn},\text{Mg})\text{SiO}_3$	$\text{MnMgSi}_2\text{O}_6$	VIIID01a
Donpeacorite	$(\text{Mn},\text{Mg})\text{MgSi}_2\text{O}_6$		VIIID02
AMgSi_2O_6 (A = Zn, Cr)	$\text{ZnMgSi}_2\text{O}_6, \text{CrMgSi}_2\text{O}_6$		
<i>III. Ca-, Ba-, Sr-, Zn-silicates</i>			
Wollastonite (Wo)	CaSiO_3		VIIID08
SrSiO_3	SrSiO_3		
BaSiO_3	BaSiO_3		
ZnSiO_3	ZnSiO_3		
AMgSi_2O_6 (A = Zn, Cr)	$\text{ZnMgSi}_2\text{O}_6, \text{CrMgSi}_2\text{O}_6$		
Diopside (Di)	$\text{CaMgSi}_2\text{O}_6$		VIIID01a
Hedenbergite (Hd)	$\text{CaFeSi}_2\text{O}_6$		VIIID01a
Johannsenite (Jo)	$\text{CaMnSi}_2\text{O}_6$		VIIID01a
Bustamite	$\text{CaMnSi}_2\text{O}_6$		VIIID08
Petedunnite	$\text{CaZnSi}_2\text{O}_6$		VIIID01a
Esseneite	CaFeAlSiO_6		VIIID01a
Calcium Tschermak's (CaTs)	$\text{CaAl}_2\text{SiO}_6$		
CaMSiO_6	M = Sc, Co, Ni		
CaScAlSiO_6	CaScAlSiO_6		
Pigeonite	$(\text{Mg},\text{Fe},\text{Ca})\text{SiO}_3$		VIIID01a
Augite	$(\text{Ca},\text{Mg},\text{Fe})_2\text{Si}_2\text{O}_6$		VIIID01a
Ferrobustamite	$\text{Ca}(\text{Fe},\text{Ca},\text{Mn})\text{Si}_2\text{O}_6$		VIIID08
$\text{BaCuSi}_2\text{O}_6$	$\text{BaCuSi}_2\text{O}_6$		

Table 1 (cont.)

Silicate	Composition	End member	Classification group [91N1]
<i>IV. Na-silicates</i>			
Aegirine (Ae) (Acmite)	NaFeSi ₂ O ₆		VIIID01a
Kosmochlor (Ko) (Ureyite)	NaCrSi ₂ O ₆		VIIID01a
Na ₂ ZnSi ₂ O ₆ (Chkalovite) ^{a)}	Na ₂ ZnSi ₂ O ₆		
NaMSi ₂ O ₆	M = Sc, Ti, V, Cr, Mn, In, Ga		
Jadeite (Jd)	Na(Al, Fe)Si ₂ O ₆	NaAlSi ₂ O ₆	VIIID01a
Jervisite	(Na,Ca,Fe)(Sc,Mg,Fe)Si ₂ O ₆	NaScSi ₂ O ₆	VIIID01a
Natalyite	Na(V,Cr)Si ₂ O ₆		VIIID01a
Na ₂ BaSi ₂ O ₆	Na ₂ BaSi ₂ O ₆		
Na ₂ SiO ₃	Na ₂ SiO ₃		
<i>V. Ca-Na silicates</i>			
Omphacite	(Ca,Na)(Mg,Fe,Al)Si ₂ O ₆		VIIID01a
<i>VI. Li-silicates</i>			
Spodumene	LiAlSi ₂ O ₆		VIIID01a
LiMSi ₂ O ₆	M = Sc, Ti, Cr, Fe, Ni, Ga, Sn		
Virgilite	LiAlSi ₂ O ₆		VIIID01b
Li ₂ SiO ₃	Li ₂ SiO ₃		
<i>VII. Other silicates</i>			
CoSiO ₃			
Alamosite	PbSiO ₃		VIIID17
ZnZnSi ₂ O ₆	Zn ₂ Si ₂ O ₆		
Cs ₅ CoSiO ₆	Cs ₅ CoSiO ₆		
HAlSi ₂ O ₆	HAlSi ₂ O ₆		
(KH) ₂ Si ₂ O ₆	(KH) ₂ Si ₂ O ₆		
CdSiO ₃	CdSiO ₃		
<i>VIII. Group VIIID01b</i>			
Lorenzenite (Ramsayite)	Na ₄ Ti ₄ [Si ₂ O ₆] ₂ O ₆		VIIID01b
Vinogradovite	(Na,Ca) ₄ Ti ₄ Si ₈ O ₂₆ (H ₂ O,K) ₃		VIIID01b
Paravinogradovite	(Na,□) ₂ [(Ti ⁴⁺ ,Fe ³⁺) ₄ {Si ₂ O ₆ } ₂ {Si ₃ AlO ₁₀ }(OH) ₄].H ₂ O		VIIID01b
Aërinite	Ca ₄ (Al,Fe,Mg) ₁₀ Si ₁₂ O ₃₆ (OH) ₁₂ CO ₃ ·12H ₂ O		VIIID01b
Lintisite	Na ₃ LiTi ₂ [Si ₂ O ₆] ₂ O ₂ ·2H ₂ O		
Joesmithite	(Ca,Pb) ₃ (Mg,Fe) ₅ Si ₆ Be ₂ O ₂₂ (OH) ₂		VIIID01b
Nchwaningite	Mn ²⁺ ₂ SiO ₃ (OH) ₂ ·H ₂ O		

^{a)} The name chkalovite was given also for Na₂BeSi₂O₆ (group VIIIB02b)

Table 2. Atomic coordinates and thermal parameters.a) $\text{Fe}_2\text{Si}_2\text{O}_6$, orthoferrosilite, having space group Pbca [82S1].

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$B_{\text{eq}} [\text{\AA}^2]$
Fe1	0.37574(3)	0.65397(4)	0.87456(9)	0.409
Fe2	0.37775(3)	0.48566(5)	0.3664(1)	0.573
SiA	0.27231(4)	0.3390(1)	0.0494(2)	0.317
SiB	0.47315(4)	0.3342(1)	0.7893(2)	0.328
O1A	0.1849(3)	0.3392(3)	0.0384(4)	0.479
O1B	0.5610(1)	0.3368(3)	0.7859(4)	0.472
O2A	0.3120(1)	0.4962(3)	0.0575(5)	0.593
O2B	0.4330(1)	0.4805(3)	0.6922(5)	0.518
O3A	0.3025(1)	0.2355(3)	−0.1832(5)	0.611
O3B	0.4475(1)	0.2023(3)	0.5871(4)	0.516

b) $\text{Mg}_{0.613}\text{Fe}_{0.387}\text{SiO}_3$, clinopyroxene, having space group $\text{P2}_1/\text{c}$ [98A3].

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$B_{\text{eq}} [\text{\AA}^2]$
M1	0.2512(5)	0.6539(4)	0.2201(8)	1.01
M2	0.2570(4)	0.0153(3)	0.2202(6)	1.28
SiA	0.0431(3)	0.3401(7)	0.2899(6)	0.79
SiB	0.5531(3)	0.8359(6)	0.2354(6)	0.73
O1A	0.8691(10)	0.3376(16)	0.1821(18)	0.97
O2A	0.1239(10)	0.4993(12)	0.3283(20)	0.81
O3A	0.1047(7)	0.2729(2)	0.6053(14)	1.11
O1B	0.3750(9)	0.8388(15)	0.1287(16)	0.72
O2B	0.6244(11)	0.9819(13)	0.3869(20)	1.21
O3B	0.6048(7)	0.7006(9)	0.4625(14)	0.99

c) FeSiO_3 , clinoferrosilite at 1050°C, having $\text{C2}/\text{c}$ -type structure [84S4].

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$B_{\text{eq}} [\text{\AA}^2]$
Fe1	0.0	0.9014	0.25	2.03(10)
Fe2	0.0	0.2625(6)	0.25	2.84(12)
Si	0.2962(5)	0.0852(8)	0.2708(7)	1.90(10)
O1	0.1241(13)	0.0903(19)	0.1587(16)	3.28(28)
O2	0.3747(14)	0.2398(13)	0.3616(19)	2.23(25)
O3	0.3589(15)	0.0134(12)	0.0445(20)	2.40(30)

d) MgSiO_3 , protoenstatite at 1080°C, having space group Pbcn [82M5].

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$B_{\text{eq}} [\text{\AA}^2]$
M1	0.0	0.1006(5)	0.75	2.16
M2	0.0	0.2625(5)	0.25	2.65
Si	0.2928(2)	0.0897(2)	0.0739(3)	1.33
O1	0.1200(5)	0.0942(6)	0.0770(10)	1.85
O2	0.3773(6)	0.2463(7)	0.0677(11)	2.53
O3	0.3481(5)	0.9836(9)	0.3079(11)	2.95

Table 2 (cont.)e) CaSiO_3 pseudowollastonite (two layers), having monoclinic space group $C2/c$ [99Y3].

Atom	x	y	z
Ca1	0.0870(1)	0.2403(1)	0.4989(1)
Ca2	0.25	0.25	0
Si1	0.1278(1)	0.4530(1)	0.2445(1)
Si2	0	0.8400(1)	0.25
O1	0.1275(1)	0.4045(2)	0.0965(2)
O2	0.2290(1)	0.3991(2)	0.3863(2)
O3	0.1109(1)	0.6929(2)	0.2478(2)
O4	0.0497(1)	0.9436(2)	0.3939(2)
O5	0	0.3592(3)	0.25

f) MgSiO_3 perovskite, having orthorhombic structure [89R2].

Atom	x	y	z	$B_{\text{eq}} [\text{\AA}^2]$
Mg	0.9856(10)	0.0564(6)	$\frac{1}{4}$	0.75(7)
Si	0	$\frac{1}{2}$	0	0.25
O1	0.1015(17)	0.4673(13)	$\frac{1}{4}$	0.45(12)
O2	0.9662(10)	0.2983(8)	0.0524(9)	0.47(8)

g) MgSiO_3 ilmenite, having space group $R\bar{3}$ [82H1].

Atom	Site	Symmetry	x	y	z	$B_{\text{eq}} [\text{\AA}^2]$
Mg	2g	3	0	0	0.35970(12)	0.59
Si	2g	3	0	0	0.15768(10)	0.42
O	6l	1	0.3214(5)	0.0361(4)	0.24077(11)	0.48

h) Omphacite $(\text{Ca}_{0.516}\text{Na}_{0.484})(\text{Mg}_{0.392}\text{Fe}^{2+}_{0.077}\text{Fe}^{3+}_{0.137}\text{Al}_{0.398}\text{Ti}_{0.005})(\text{Si}_{1.918}\text{Al}_{0.082})\text{O}_6$, having space group $P2/n$ [75M2].

Atom	x	y	z	$B_{\text{eq}} [\text{\AA}^2]$	Site occupancy
O11	0.3634(4)	0.3382(5)	0.1232(7)	0.73(7)	1.0 for all O
O12	0.3621(4)	0.1767(5)	0.6475(8)	0.74(6)	
O21	0.6138(4)	0.5090(5)	0.3091(8)	0.76(7)	
O22	0.6063(4)	0.9974(5)	0.8054(8)	0.80(7)	
O31	0.6057(4)	0.2663(4)	0.0037(8)	0.65(6)	1 for all Si
O32	0.5981(4)	0.2398(4)	0.4984(8)	0.70(7)	
Si1	0.5393(2)	0.3465(2)	0.2273(3)	0.37(3)	
Si2	0.5376(2)	0.1621(2)	0.7310(3)	0.36(3)	
M11	0.2500	0.3480(2)	0.7500	0.32(5)	Al 0.868(9), Fe 0.132
M1	0.2500	0.1580(3)	0.2500	0.43(5)	Mg 0.815(9), Fe 0.185
M2	0.2500	0.5521(3)	0.2500	0.86(6)	Ca 0.314(13), Na 0.686
M21	0.2500	0.9502(2)	0.7500	0.82(5)	Ca 0.716, Na 0.284

Table 2 (cont.)i) $\text{LiAlSi}_2\text{O}_6$ -II, having tetragonal structure P4_32_12 or its enantiomorph P4_12_12 [68L2].

Atom	x	y	z	$B_{\text{eq}} [\text{\AA}^2]$
Si1	0.3324(3)	0.1221(3)	0.2384(3)	0.26(3)
Si2	0.4182(3)	0.4182	0	0.23(4)
O1	0.4436(10)	0.1190(9)	0.3926(7)	1.50(10)
O2	0.1254(8)	0.1154(8)	0.2999(7)	1.08(9)
O3	0.3628(9)	0.3024(10)	0.1454(8)	2.01(11)
Li	0.0644(38)	0.1880(38)	0.4964(31)	1.79(37)

j) $\text{LiAlSi}_2\text{O}_6$ -III, having hexagonal structure, space group P6_222 (or P6_422) [68L1].

Atom	x	y	z	$B_{\text{eq}} [\text{\AA}^2]$
Si, Al	1/2	0	0	0.29(5)
O	0.2055(8)	(0.4110)	1/2	1.65(10)
Li	0	0	0	1.45(88)

Table 3. Crystal structure and lattice parameters.

Silicate	T [K]	Space group	Lattice parameters				Refs.
			a [Å]	b [Å]	c [Å]	β	
$\text{Mg}_2\text{Si}_2\text{O}_6$ (OEn)	RT	Pbca	18.210(10)	8.812(5)	5.178(4)		69M1
	RT	Pbca	18.225(1)	8.815(1)	5.175(1)		66S2
	RT	Pbca	18.216(2)	8.813(1)	5.179(1)		77H2
	RT	Pbca	18.2230(30)	8.8190(6)	5.1812(13)		79G1
	RT	Pbca	18.227(4)	8.819(2)	5.179(1)		82S1
	RT	Pbca	18.225(2)	8.8128(6)	5.180(1)		84O1
	RT	Pbca	18.225(2)	8.818(1)	5.178(1)		86H3
	296	Pbca	18.235(3)	8.818(1)	5.179(1)		86G3
	298	Pbca	18.227(1)	8.818(1)	5.181(0)		95Z1
MgSiO_3 (PEn)	RT	Pbcn	9.250(5)	8.740(5)	5.320(5)		59S1
	1353	Pbcn	9.306(6)	8.892(7)	5.349(4)		82M5, 84M3
	1533		9.302(6)	8.914(6)	5.362(4)		84M3
	1633		9.349(6)	8.929(6)	5.361(4)		84M3
MgSiO_3 (natural sample)	1373	$\text{P2}_1\text{cn}$	9.304(4)	8.902(2)	5.351(5)		71S3
MgSiO_3 (LCEn)	RT	$\text{P2}_1/\text{c}$	9.606(1)	8.8131(7)	5.170(2)	108.35(1)°	84O1
	RT	$\text{P2}_1/\text{c}$	9.620(5)	8.835(5)	5.188(5)	108°20(10)°	60M1
$\text{Mg}_2\text{Si}_2\text{O}_6$ (LCEn)	RT		9.609(2)	8.814(2)	5.175(2)	108.37(2)°	77H2
	RT		9.607(1)	8.815(1)	5.169(1)	108.34(1)°	66S2
MgSiO_3 (HPCEn)	RT	$\text{C2}/\text{c}$	9.201(3)	8.621(1)	4.908(1)	101.50(3)°	92A1
MgSiO_3 (ilmenite)	RT	R3 or $\text{R}\bar{3}$	4.7284(4)		13.5591(16)		77I2, 82H1
			4.722(3)		13.560(12)		96R2
MgSiO_3 (perovskite) s.c.	RT		4.774(1)	4.928(2)	6.893(2)		87K3
	s.c.		4.7786(9)	4.9293(9)	6.9003(8)		89R2
	s.c.	Pbnm	4.7787(4)	4.9313(4)	6.9083(8)		87H6
	powder	Pbnm	4.7754(4)	4.9292(4)	6.8969(5)		78I1

Table 3 (cont.)

Silicate	<i>T</i> [K]	Space group	Lattice parameters				Refs.
			<i>a</i> [Å]	<i>b</i> [Å]	<i>c</i> [Å]	β	
MgSiO ₃ (perovskite) (cont.)							
powder	RT		4.780(1)	4.933(1)	6.902(1)		78Y1
powder	RT		4.783(7)	4.953(8)	6.886(7)		86K4
powder	RT		4.790(4)	4.943(4)	6.897(6)		76L2
	RT		4.777(2)	4.927(1)	6.89772(9)		90R3
(<i>p</i> = 1.0 GPa)	RT		4.768(3)	4.922(2)	6.8898(15)		90R3
(<i>p</i> = 2.2 GPa)			4.762(1)	4.918(1)	6.8767(9)		90R3
(<i>p</i> = 3.0 GPa)			4.758(2)	4.911(3)	6.8680(14)		90R3
(<i>p</i> = 3.5 GPa)			4.754(6)	4.911(2)	6.8653(12)		90R3
(<i>p</i> = 5.0 GPa)			4.746(2)	4.899(3)	6.8538(16)		90R3
MgSiO ₃ (garnet)	RT	I4 ₁ /a	11.501(1)		11.480(2)		89A1
MnMg[Si ₂ O ₆]	473	P2 ₁ /c	9.758(3)	8.897(1)	5.283(1)	108.74(2)°	97A2
	543	C2/c	9.796(5)	8.880(8)	5.315(3)	109.26(4)°	97A2
Enstatite							
[Mg _{(x-12)/3} Sc ₄][Li _{4/3} Si _{(x-4)/3}]O _x							
x = 124 (En-IV-10)	RT	P2/a	9.429(2)	8.748(2)	27.038(8)	93.25(2)°	77T1,
x = 112 (En-IV-9)	RT	I2/a	9.432(2)	8.756(1)	48.792(14)	92.25(2)°	84T1
x = 100 (En-IV-8)	RT	P2/a	9.429(2)	8.741(1)	21.808(6)	91.20(2)°	
[Mg _{(x-7.5)/3} Sc ₃][Mg _{2/3} Si _{(x-4)/3}]O _x							
x = 124 (En-IV'-10)	RT	P2/a	9.424(2)	8.738(2)	27.021(8)	93.24(2)°	84T2
x = 112 (En-IV'-9)	RT	I2/a	9.424(1)	8.740(1)	48.808(6)	92.38(1)°	
x = 100 (En-IV'-8)	RT	P2/a	9.434(1)	8.731(1)	21.791(4)	91.30(1)°	
Fe ₂ Si ₂ O ₆	RT	Pbca	18.427(4)	9.076(2)	5.237(1)		82S1
FeSiO ₃	297	Pbca	18.418(2)	9.078(1)	5.2366(4)		76S1
	673	Pbca	18.484(1)	9.124(1)	5.2593(3)		76S1
	873	Pbca	18.527(1)	9.145(1)	5.2756(4)		76S1
	1073	Pbca	18.569(1)	9.160(1)	5.2974(4)		76S1
	1173	Pbca	18.596(1)	9.1685(5)	5.3113(3)		76S1
		P2 ₁ /c	9.7075(5)	9.0807(4)	5.2347(5)	108.46(1)°	97H3
(<i>p</i> = 1.87 GPa)		C2/c	9.540(1)	8.996(3)	5.008(1)	103.01(1)°	97H3
	1323	C2/c	9.928(1)	9.179(1)	5.338(1)	110.20(1)°	84S4
(Mg _{0.56} Fe _{0.44}) ₂ Si ₂ O ₆	RT	Pbca	18.312(4)	8.917(2)	5.217(1)		93H1
Mg _{0.305} Fe _{0.68} Ca _{0.015} SiO ₃	293	Pbca	18.363(5)	8.990(3)	5.232(4)		73S1
Mg _{0.613} Fe _{0.387} SiO ₃	RT	P2 ₁ /c	9.6519(7)	8.9075(7)	5.2004(3)	108.590(1)°	98A3
Mg _{0.31} Fe _{0.67} Ca _{0.015} SiO ₃	293	P2 ₁ /c	9.691(3)	8.993(3)	5.231(2)	108.61(2)°	74S1
Mg _{1.425} Cr _{0.611} Si _{1.964} O ₆	RT	P2 ₁ /c	9.713(2)	8.910(2)	5.238(2)	109.41(2)°	89A2
Mg _{0.79} Fe _{0.21} SiO ₃ (akimotoite)		R $\bar{3}$	4.78(5)		13.6(1)		99T2
Co ₂ Si ₂ O ₆	RT	Pbca	18.296(4)	8.923(1)	5.204(1)		82S1
Mg _{0.776} Co _{0.224} SiO ₃	293	Pbca	18.233(7)	8.836(6)	5.188(3)		78H1
Mg(Cu _{0.56} Mg _{0.44})Si ₂ O ₆	RT	Pbca	18.221(4)	8.890(1)	5.2260(7)		97T1
Mg _{0.7} Co _{0.1} Li _{0.1} Sc _{0.1} SiO ₃	298		9.253(1)	8.7716(9)	5.3350(5)		85M2
(protopyroxene)	1413		9.320(4)	8.898(5)	5.346(3)		85M2
MnSiO ₃ (CPx)	RT		9.864(2)	9.179(2)	5.298(1)	71°47(1)'	72A2
MnSiO ₃ (Rhd)	RT	P $\bar{1}$	7.616(1)	11.853(2)	6.706(1)	$\alpha=92.44(2)^\circ$ $\beta=94.40(2)^\circ$ $\gamma=105.70(1)^\circ$	89R1

Table 3 (cont.)

Silicate	<i>T</i> [K]	Space group	Lattice parameters				Refs.
			<i>a</i> [Å]	<i>b</i> [Å]	<i>c</i> [Å]	β	
MnSiO ₃ (Rhd)	RT	P $\bar{1}$	7.633(5)	11.868(9)	6.716(5)	$\alpha=92^\circ41(6)'$ $\beta=94^\circ38(6)'$ $\gamma=105^\circ40(4)'$	85T2
	RT	P $\bar{1}$	7.614	11.848	6.699	$\alpha=92^\circ39'$ $\beta=94^\circ24'$ $\gamma=105^\circ41'$	72I2
	RT		7.614(3)	11.856(6)	6.703(2)	$\alpha=92.40(4)^\circ$ $\beta=94.25(4)^\circ$ $\gamma=105.73(4)^\circ$	86H3
	RT		7.616(3)	11.851(5)	6.707(2)	$\alpha=92^\circ33(6)'$ $\beta=94^\circ21(6)'$ $\gamma=105^\circ40(6)'$	72A2
MnSiO ₃ (Pxm)	RT		6.717(2)	7.601(2)	17.429(11)	$\alpha=113.79(3)^\circ$ $\beta=82.35(5)^\circ$ $\gamma=94.73(5)^\circ$	86H3
	RT		6.721(2)	7.603(3)	17.455(6)	$\alpha=113^\circ10(6)'$ $\beta=82^\circ16(6)'$ $\gamma=94^\circ08(6)'$	72A2
MnSiO ₃ (garnet)	RT	I4 ₁ /a	11.774(1)		11.636(2)		86F2
MgSiO ₃ (garnet)	RT		11.769(3)		11.624(3)		72A2
Mg _{0.925} Mn _{0.075} SiO ₃	293	Pbca	18.270(6)	8.833(6)	5.195(3)		78H1
Mg _{1.41} Mn _{0.56} Ca _{0.03} Si ₂ O ₆ (donpeacorite)	RT	Pbca	18.384(11)	8.878(7)	5.226(3)		84P2
Mg _{1.43} Mn _{0.54} Ca _{0.03} Si ₂ O ₆ (donpeacorite)	RT	Pbca	18.3668(3)	8.8725(2)	5.2289(1)		05S1
Mg _{1.562} Mn _{0.175} Ca _{0.263} Si ₂ O ₆	RT	Pbca	18.246(3)	8.839(2)	5.196(1)		77H2
Mn _{0.143} Mg _{0.857} SiO ₃ (OPx)	RT		18.290(3)	8.849(1)	5.206(1)		86H3
Mn _{0.286} Mg _{0.714} SiO ₃ (OPx)	RT		18.350(2)	8.879(1)	5.221(1)		86H3
Mn _{0.714} Mg _{0.286} SiO ₃ (Pxm)	RT		6.672(2)	7.528(2)	17.350(3)	$\alpha=113.77(2)^\circ$ $\beta=81.96(2)^\circ$ $\gamma=94.63(2)^\circ$	86H3
Mn _{0.428} Mg _{0.572} SiO ₃ (Kan)	RT		9.724(3)	8.911(2)	5.247(2)	108.60(3) $^\circ$	86H3
Mn _{0.50} Mg _{0.50} SiO ₃ (Kan)	RT		9.732(2)	8.934(1)	5.245(2)	108.52(2) $^\circ$	86H3
Co _{1/3} Ni _{1/3} Zn _{1/3} SiO ₃	RT	Pbca	18.209(1)	8.915(1)	5.2182(4)		90T2
Kanoite ¹⁾	RT	P2 ₁ /c	9.739	8.939	5.260	108.56 $^\circ$	77K1
Kanoite, MnMg[Si ₂ O ₆]	473	P2 ₁ /c	9.758(3)	8.897(1)	5.283(1)	108.74(2) $^\circ$	97A2
	543	C2/c	9.796(5)	8.880(8)	5.315(3)	109.26(4) $^\circ$	97A2
Pyroxferroite (Fe _{0.84} Ca _{0.13} Mg _{0.02} Mn _{0.02})SiO ₃	RT	Tricl.	6.62	7.54	17.35	$\alpha=114.4^\circ$ $\beta=82.7^\circ$ $\gamma=94.5^\circ$	70C2
CaSiO ₃ (pseudowollastonite 4-layers)	RT	C $\bar{1}$	6.853(3)	11.895(5)	19.674(13)	$\alpha=90.12(3)^\circ$ $\beta=90.55(3)^\circ$ $\gamma=90.00(3)^\circ$	81Y1
CaSiO ₃ (pseudowollastonite)	RT	triclinic	6.856(12)	11.901(8)	19.672(22)	$\alpha=90.06(9)^\circ$ $\beta=90.36(14)^\circ$ $\gamma=89.93(14)^\circ$	98R3
CaSiO ₃ (pseudowollastonite 4-layers)	RT	C2/c	6.8394(5)	11.8704(9)	19.6313(7)	90.667(6) $^\circ$	99Y2

Table 3 (cont.)

Silicate	<i>T</i> [K]	Space group	Lattice parameters				Refs.
			<i>a</i> [Å]	<i>b</i> [Å]	<i>c</i> [Å]	β	
CaSiO ₃ (pseudowollastonite 2-layers)	RT	C2/c	11.8322(6)	6.8624(8)	10.5297(5)	111.245(8) ^o	99Y3
CaSiO ₃ (high pressure)	RT	P $\bar{1}$	6.695(5)	9.257(7)	6.666(6)	$\alpha=86^{\circ}38(3)'$ $\beta=76^{\circ}08(3)'$ $\gamma=70^{\circ}23(3)'$	69T1
Wollastonite 3T	RT		23.2(1)	7.30(3)	7.06(3)	$\alpha=90^{\circ}$ $\beta=95.5(2)^{\circ}$ $\gamma=94.6(2)^{\circ}$	83H1
Wollastonite 4T	RT		31.2(11)	7.30(3)	7.06(3)	$\alpha=90^{\circ}$ $\beta=95.5(2)^{\circ}$ $\gamma=96.8(2)^{\circ}$	83H1
Wollastonite 5T	RT		38.6(1)	7.30(3)	7.06(3)	$\alpha=90^{\circ}$ $\beta=95.5(2)^{\circ}$ $\gamma=98.0(2)^{\circ}$	83H1
Ca ₃ [Si ₃ O ₉]-wollastonite 2M	RT	P2 ₁ /c	15.409(3)	7.332(1)	7.063(1)	95.30(2) ^o	84H2
CaSiO ₃ (perovskite)	RT	P4/m32/m	3.567(1)				86M2
CaTi _{0.51} Si _{0.49} O ₃ (perovskite)	RT		5.225(5)	7.389(2)	5.225(3)		98S3
CaTi _{0.77} Si _{0.23} O ₃ (perovskite)	RT		5.322(5)	7.556(2)	5.366(4)		98S3
ϵ -CaSiO ₃	RT		9.485(8)				75L3
δ -CaSiO ₃	RT	P $\bar{1}$	6.695(5)	9.257(7)	6.666(6)	$\alpha=86.63(5)^{\circ}$ $\beta=76.13(5)^{\circ}$ $\gamma=70.38(5)^{\circ}$	69T1
α -SrSiO ₃	RT	C2	12.323(5)	7.139(2)	10.873(5)	111.58(4) ^o	82M1
δ -SrSiO ₃	RT	P $\bar{1}$	6.874(2)	6.894(2)	9.717(3)	$\alpha=85.01(3)^{\circ}$ $\beta=110.57(3)^{\circ}$ $\gamma=104.01(2)^{\circ}$	82M1
δ^+ -SrSiO ₃	RT	P2 ₁ /c	7.452(4)	6.066(2)	13.497(7)	117.09(4) ^o	82M1
SrSiO ₃ : Eu ³⁺ , Bi ³⁺ (sintering at atm. pressure) (high <i>T</i> , high <i>p</i>)	RT	hex	7.123(5)		10.005(5)	120 ^o	93L2
SrSiO ₃ (perovskite) (at 35 GPa and 1450(50) K)	RT	P6 ₃ /mmc	8.532(5)	10.792(5)	36.364(5)	90.326 ^o	93L2
BaSiO ₃ (high- <i>T</i> form)	RT		5.0688(3)		12.4175(7)		05Y1
CaMgSi ₂ O ₆	RT	C2/c	4.54	5.56	12.27		60L1
	RT	C2/c	9.748(1)	8.924(1)	5.251(1)	105 ^o 40.4'	63N1, 69G1
	RT	C2/c	9.746(4)	8.899(5)	5.251(6)	105.63(6) ^o	69C1, 79O2
Diopside ²⁾	RT		9.7456(7)	8.9198(8)	5.2516(5)	105.86(1) ^o	81L1
Diopside ²⁾ (<i>p</i> = 5.3 GPa)	RT		9.612(2)	8.765(1)	5.1793(2)	105.32(1) ^o	81L1
Diopside ³⁾	RT	C2/c	9.719(2)	8.838(2)	5.287(1)	106.05(2) ^o	02D1
CaFeSi ₂ O ₆	RT		9.844	9.028	5.246	104.8 ^o	70V1
	RT		9.845	9.024	5.245	104.8 ^o	73C1
	RT		9.845	9.021	5.246	104.7 ^o	88K1
	RT	C2/c	9.841	9.027	5.247	104.8 ^o	69N1
	RT	C2/c	9.838	9.038	5.244	105.0 ^o	88G2
Hedenbergite ⁴⁾	RT		9.840	9.024	5.250	104.2 ^o	91K2
Mg _{0.39} Fe _{0.52} Ca _{0.09} SiO ₃	RT	P2 ₁ /c	9.706(2)	8.950(1)	5.246(1)	108.59(1) ^o	70M2
Mg _{0.33} Fe _{0.57} Ca _{0.10} SiO ₃	RT		9.731(5)	8.953(5)	5.256(5)	108.5(2) ^o	69M2

Table 3 (cont.)

Silicate	<i>T</i> [K]	Space group	Lattice parameters				Refs.
			<i>a</i> [Å]	<i>b</i> [Å]	<i>c</i> [Å]	β	
Ca _{0.15} Mg _{1.85} Si ₂ O ₆ (clinopyroxene)	RT	P2 ₁ /c	9.651(2)	8.846(2)	5.202(1)	108.38(2) ^o	02T1
Ca _{0.80} Mg _{1.20} Si _{1.99} O ₆	RT	C2/c	9.727(3)	8.912(1)	5.245(1)	106.36(3) ^o	90B1
Ca _{0.82} Fe _{0.15} Mn _{0.03} SiO ₃ (Fs _{0.18} Wo _{0.82})	RT	A $\bar{1}$	7.862	7.253	13.967	$\alpha=89^{\circ}44'$ $\beta=95^{\circ}28'$ $\gamma=103^{\circ}29'$	77Y2
Fs _{0.65} Wo _{0.35}	RT	C2/c	9.812(1)	9.049(1)	5.233(1)	105.34(1) ^o	75O1
Fs _{0.75} Wo _{0.25}	RT	C2/c	9.781(2)	9.072(2)	5.246(2)	106.55(2) ^o	75O1
Fs _{0.80} Wo _{0.20}	RT	C2/c	9.760(6)	9.057(8)	5.234(3)	106.28(5) ^o	75O1
Fs _{0.85} Wo _{0.15}	RT	C2/c	9.779(1)	9.088(1)	5.285(1)	107.39(1) ^o	75O1
En _{0.39} Fs _{0.52} Wo _{0.09}	RT	C2/c	9.858(4)	9.053(2)	5.329(3)	109.42(1) ^o	72B1
CaFe _{0.8} Mg _{0.2} Si ₂ O ₆	RT	C2/c	9.815(1)	8.977(1)	5.2416(6)	104.910(9) ^o	86W3
Ca _{2.90} Mn _{0.10} Fe _{0.02} Si _{2.99} O ₉ (Mn-Wo)	RT	C $\bar{1}$	10.121(2)	11.070(1)	7.312(1)	$\alpha=99.51(1)^{\circ}$ $\beta=100.51(1)^{\circ}$ $\gamma=83.43(1)^{\circ}$	78O3
Ca _{2.90} Mg _{0.03} Mn _{0.02} Fe _{0.11} Si _{2.97} O ₉ (Fe-Wo)	RT	C $\bar{1}$	10.104(1)	11.054(1)	7.305(1)	$\alpha=99.53(1)^{\circ}$ $\beta=100.56(1)^{\circ}$ $\gamma=83.44(1)^{\circ}$	78O3
Ca _{0.742} Mg _{0.016} Fe _{0.100} Al _{1.384} Si _{1.534} O ₆	RT	C2/c	9.719(1)	8.814(2)	5.305(1)	106.04(1) ^o	98O1
Mg _{0.475} Fe _{0.475} Ca _{0.05} SiO ₃	RT		9.696(1)	8.942(1)	5.227(1)	108.75(1) ^o	69M2
CaMnSi ₂ O ₆	RT		9.978(9)	9.156(9)	5.293(5)	105.5 ^o	67F1
CaCoSi ₂ O ₆	RT	C2/c	9.806(1)	8.950(1)	5.243(1)	105.45(1) ^o	75G3, 87G1
CaNiSi ₂ O ₆	RT		9.797(1)	8.954(1)	5.243(1)	105.40(2) ^o	77S2
	RT		9.737(2)	8.899(2)	5.231(1)	105.92(1) ^o	77S2
	RT	C2/c	9.734(2)	8.891(2)	5.228(1)	105.87(2) ^o	75G3, 87G1
CaZnSi ₂ O ₆ (2 GPa, 900°C)	RT		9.728(2)	8.891(2)	5.228(1)	105.83(2) ^o	88O1
CaAl ₂ SiO ₆ (CaTs)	RT	C2/c	9.803(6)	8.975(7)	5.243(7)	105.75(7) ^o	87E1
CaAl ₂ SiO ₆	RT	C	9.609(3)	8.652(2)	5.274(2)	106.06(2) ^o	74O1
	RT	P3c1 or P $\bar{3}$ c1	9.943(2)		8.228(3)		73K1
CaFeAlSiO ₆	RT	C2/c	9.781(2)	8.782(1)	5.365(1)	105.80(3) ^o	83A2
	RT	C2/c	9.7797(16)	8.7819(14)	5.3685(5)	105.78(1) ^o	86G2
Esseneite ⁵⁾	RT	C2/c	9.79(1)	8.822(9)	5.37(1)	105.81(9) ^o	87C3
Ca _{1.49} Mg _{0.03} Mn _{1.11} Fe _{0.36} Si ₃ O ₉ (bustamite)	RT	I $\bar{1}$	9.864(3)	10.790(5)	7.139(5)	$\alpha=99.53(4)^{\circ}$ $\beta=99.71(3)^{\circ}$ $\gamma=83.83(3)^{\circ}$	78O3
Ca _{0.94} Mg _{0.13} Mn _{1.79} Fe _{0.13} Si ₃ O ₉ (Mn-bustamite)	RT	I $\bar{1}$	9.807(4)	10.680(4)	7.091(2)	$\alpha=99.58(2)^{\circ}$ $\beta=99.99(3)^{\circ}$ $\gamma=83.79(3)^{\circ}$	78O3
Ca _{2.33} Mg _{0.06} Mn _{0.36} Fe _{0.22} Si ₃ O ₉ (Ca-bustamite)	RT	I $\bar{1}$	9.994(3)	10.946(3)	7.231(3)	$\alpha=99.30(3)^{\circ}$ $\beta=100.56(3)^{\circ}$ $\gamma=83.29(2)^{\circ}$	78O3
Ferrobustamite ⁶⁾	RT		9.777	8.940	5.260	104.8 ^o	89K1
ZnSiO ₃	RT	C2/c	9.787(3)	9.161(2)	5.296(1)	111.42(3) ^o	75M3
ZnSiO ₃ (clinopyroxene)	RT	C2/c	9.7891(18)	9.1785(8)	5.3006(6)	111 ^o 28'	71S4
	RT	C2/c	9.781(1)	9.179(1)	5.2933(9)	111 ^o 27'	89L1

Table 3 (cont.)

Silicate	<i>T</i> [K]	Space group	Lattice parameters				Refs.
			<i>a</i> [Å]	<i>b</i> [Å]	<i>c</i> [Å]	β	
ZnSiO ₃ (orth.)	RT	Pbca	18.204(5)	9.087(3)	5.278(2)		75M3
ZnSiO ₃ (ilmenite)	RT		4.746(1)		13.755(2)		74I2
	RT		4.7469(2)		13.7536(8)		89L1
ZnMgSi ₂ O ₆	RT	Pbca	18.201(5)	8.916(2)	5.209(2)		75M3
CaZnSi ₂ O ₆	RT	C2/c	9.803(7)	8.975(7)	5.243(7)	105.75(7)°	87E1
Petedunnite ⁷⁾	RT	C2/c	9.82(3)	9.00(1)	5.27(2)	105.6(2)°	87E1
CaScAlSiO ₆	RT	C2/c	9.884(2)	8.988(1)	5.446(1)	105.86(1)°	78O1, 78O4
	RT	C2/c	9.887(3)	8.996(2)	5.446(1)	105.89(3)°	78O2, 83O2
Ca _{1.00} Sc _{0.84} Ti _{0.27} Al _{1.16} Si _{0.73} O ₆	RT	C2/c	9.925(5)	8.949(2)	5.460(1)	105.77(4)°	79O3
0.9CaScAlSiO ₆ – 0.1CaTiAl ₂ Si ₂ O ₆	RT	C2/c	9.900(3)	8.977(2)	5.452(2)	105.86(3)°	83O2
0.8CaScAlSiO ₆ – 0.2CaTiAl ₂ Si ₂ O ₆	RT	C2/c	9.894(2)	8.947(1)	5.453(1)	105.81(2)°	83O2
0.7CaScAlSiO ₆ – 0.3CaTiAl ₂ Si ₂ O ₆	RT	C2/c	9.889(4)	8.913(2)	5.450(2)	105.73(2)°	83O2
0.9CaFeGaSiO ₆ –0.1CaGa ₂ SiO ₆	RT	C2/c	9.903(2)	8.821(2)	5.410(1)	105.441(8)°	97A1
BaCuSi ₂ O ₆	RT	I4m2	7.042(3)		11.133(3)		89F2
Na ₂ SiO ₃	RT	Cmc2 ₁	10.482	6.064	4.826		67M1
	RT	orth.	10.43	6.02	4.81		52G1
	RT	orth.	10.52	6.075	4.825		56S1
	340		10.506(2)	6.065(1)	4.821(1)		96R3
	568		10.543(5)	6.088(3)	4.845(3)		96R3
	712		10.566(5)	6.102(3)	4.862(3)		96R3
	955		10.578(5)	6.109(3)	4.894(3)		96R3
	1158		10.586(7)	6.112(4)	4.928(4)		96R3
	1290		10.599(4)	6.118(2)	4.942(3)		96R3
NaScSi ₂ O ₆	298	C2/c	9.8372(10)	9.0550(5)	5.3488(6)	107.175(5)°	94O1
	RT	C2/c	9.8438(4)	9.0439(4)	5.3540(2)	107.215(2)°	73H2
NaTiSi ₂ O ₆	RT	C2/c	9.692(2)	8.874(2)	5.301(2)	106.85(1)°	82O2
	100		6.627(1)	8.845(2)	5.2895(4)	$\alpha=90.180(1)^\circ$ $\beta=102.230(1)^\circ$ $\gamma=47.034(1)^\circ$	03N1
	300	C2/c	9.6955(3)	8.8851(2)	5.2968(2)	106.720(2)°	03N1
NaVSi ₂ O ₆	RT	C2/c	9.6339(4)	8.7413(2)	5.2960(3)	109.905(2)°	04V1
NaCrSi ₂ O ₆	RT	C2/c	9.550(16)	8.712(7)	5.273(8)	107.44(16)°	79O2
	RT		9.579	8.722	5.267	107.4°	73C1
NaMnSi ₂ O ₆	302	C2/c	9.513(1)	8.621(1)	5.354(1)	105.14(1)°	87O3
NaFeSi ₂ O ₆	RT		9.666(3)	8.804(2)	5.305(1)	107.44(2)°	97B1
	295	C2/c	9.658(1)	8.795(1)	5.294(1)	107.42°	69C1
	14	C2/c	9.68(1)	8.83(1)	5.30(1)	107.3(2)°	89B1
NaAlSi ₂ O ₆	RT		9.423	8.564	5.223	107.6°	73C1, 77R1
	RT	C2/c	9.418(1)	8.562(2)	5.219(1)	107.58(1)°	66P2
NaInSi ₂ O ₆	RT	C2/c	9.8997(5)	9.1310(3)	5.3656(3)	107.226(2)°	90O1
	RT		9.902	9.131	5.359	107.2°	77R1

Table 3 (cont.)

Silicate	<i>T</i> [K]	Space group	Lattice parameters				Refs.
			<i>a</i> [Å]	<i>b</i> [Å]	<i>c</i> [Å]	β	
NaGaSi ₂ O ₆	RT	C2/c	9.557(5)	8.679(4)	5.260(1)	107.68(2) ^o	95O2
NaCr _{0.2} Sc _{0.8} Si ₂ O ₆	RT	C2/c	9.776(3)	8.988(2)	5.324(2)	107.13(4) ^o	79O1
NaCr _{0.5} Sc _{0.5} Si ₂ O ₆	RT	C2/c	9.690(5)	8.878(4)	5.304(2)	107.17(5) ^o	79O1
(<i>p</i> = 5 GPa)	RT	C2/c	9.699(2)	8.873(4)	5.310(1)	107.30(2) ^o	81O1
NaCr _{0.6} Sc _{0.4} Si ₂ O ₆	RT	C2/c	9.677(3)	8.848(2)	5.299(2)	107.27(3) ^o	79O1
(<i>p</i> = 5 GPa)	RT	C2/c	9.674(3)	8.840(4)	5.302(2)	107.34(3) ^o	81O1
NaIn _{0.8} Sc _{0.2} Si ₂ O ₆	RT	C2/c	9.8907(5)	9.1164(2)	5.3623(3)	107.204(2) ^o	90O1
NaIn _{0.65} Sc _{0.35} Si ₂ O ₆	RT	C2/c	9.8811(5)	9.1043(2)	5.3592(3)	107.188(2) ^o	90O1
NaIn _{0.60} Sc _{0.40} Si ₂ O ₆	RT	C2/c	9.8782(5)	9.1008(3)	5.3582(3)	107.191(2) ^o	90O1
NaIn _{0.55} Sc _{0.45} Si ₂ O ₆	RT	C2/c	9.8734(5)	9.0947(2)	5.3570(3)	107.187(2) ^o	90O1
NaIn _{0.50} Sc _{0.50} Si ₂ O ₆	RT	C2/c	9.8701(4)	9.0901(2)	5.3559(2)	107.179(2) ^o	90O1
NaIn _{0.40} Sc _{0.60} Si ₂ O ₆	RT	C2/c	9.8659(5)	9.0848(2)	5.3553(3)	107.178(2) ^o	90O1
NaIn _{0.20} Sc _{0.80} Si ₂ O ₆	RT	C2/c	9.8516(5)	9.0698(2)	5.3521(3)	107.175(2) ^o	90O1
NaMg _{0.5} Si _{0.5} Si ₂ O ₆	RT	P2/n	9.418(1)	8.647(1)	5.274(1)	108.13(2) ^o	88A1
Na ₂ BaSi ₂ O ₆	RT	P2 ₁	11.440(5)	4.758(2)	5.670(2)	91.42(4) ^o	73G2
Na ₂ ZnSi ₂ O ₆ (chkalovite)	RT	Fdd2	21.54	7.139	7.413		80S3
Na ₂ BeSi ₂ O ₆	RT	Fdd2	21.129	6.881	21.188		75S2
Na ₂ Cr ₂ Si ₂ O ₆	RT	C2/c	9.560(16)	8.746(8)	5.270(6)	107.38(10) ^o	65F1
(Na _{0.56} Ca _{0.36} Mg _{0.08})Si _{0.27} Mg _{0.73} - Si ₂ O ₆ (CPx)	RT	C2/c	9.5792(13)	8.7588(12)	5.2610(6)	107.199(3) ^o	05Y2
(NaPx ₁₆ En ₈₄)							
Na _{0.20} Ca _{0.80} Cr _{0.20} Mg _{0.80} Si ₂ O ₆	RT	C2/c	9.705(2)	8.895(1)	5.252(1)	106.10(2) ^o	83O1
Na _{0.25} Ca _{0.75} Cr _{0.25} Mg _{0.75} Si ₂ O ₆	RT	C2/c	9.691(3)	8.868(2)	5.249(1)	106.13(2) ^o	79O2
Na _{0.45} Ca _{0.55} Cr _{0.45} Mg _{0.55} Si ₂ O ₆	RT	C2/c	9.645(3)	8.821(3)	5.254(2)	106.47(2) ^o	87O2
Na _{0.50} Ca _{0.50} Cr _{0.50} Mg _{0.50} Si ₂ O ₆	RT	C2/c	9.633(4)	8.808(2)	5.254(2)	106.45(4) ^o	79O2
Na _{0.75} Ca _{0.25} Cr _{0.75} Mg _{0.25} Si ₂ O ₆	RT	C2/c	9.594(3)	8.748(3)	5.256(2)	106.94(2) ^o	79O2
Na _{0.99} Ca _{0.01} Fe _{0.99} Mg _{0.01} Si ₂ O ₆	RT		9.658(2)	8.795(2)	5.294(1)	107.42(2) ^o	63N1
Na _{0.70} Ca _{0.30} Fe _{0.84} Mg _{0.16} Si ₂ O ₆	RT		9.698	8.848	5.284	106.78 ^o	69N1
(Na _{0.86} Ca _{0.09})(Fe ²⁺ ,Fe ³⁺) _{0.93} Ti _{0.03} - Mn _{0.03} Si ₂ O ₆ ⁸⁾ (aegirine)	RT		9.664	8.813	5.277	107.61 ^o	04S1
(Na _{0.99} Ca _{0.01})(Fe ²⁺ ,Fe ³⁺) _{1.0} Si ₂ O ₆ ⁹⁾			9.658	8.811	5.285	107.62 ^o	04S1
Na _{0.4} Ca _{0.6} Sc _{0.2} Cr _{0.2} Mg _{0.6} Si ₂ O ₆	RT		9.725(3)	8.922(2)	5.271(2)	106.29(3) ^o	83O1
Na _{0.6} Ca _{0.4} Sc _{0.4} Cr _{0.2} Mg _{0.4} Si ₂ O ₆	RT		9.751(3)	8.942(2)	5.290(2)	106.50(3) ^o	83O1
Na _{0.8} Ca _{0.2} Sc _{0.6} Cr _{0.2} Mg _{0.2} Si ₂ O ₆	RT		9.758(3)	8.966(3)	5.311(3)	106.85(4) ^o	83O1
Omphacite ¹⁰⁾	RT	P2/n	9.585(3)	8.776(3)	5.260(3)	106.85(3) ^o	75M1
Omphacite ¹¹⁾	RT	P2/n	9.596(5)	8.771(4)	5.265(6)	106.93(8) ^o	66C1, 68C1
Ca _{0.52} Mg _{0.39} Al _{0.40} Fe _{0.21} Si ₂ O ₆	RT	P2/n	9.585(3)	8.776(3)	5.260(3)	106.85(3) ^o	72M1
Omphacite ¹²⁾	RT	C2/c	9.646(6)	8.824(5)	5.270(6)	106.59(8) ^o	69C1
Di _{0.80} Jd _{0.20} ¹³⁾	RT		9.680(1)	8.859(1)	5.250(1)	106.25(2) ^o	80W1
Di _{0.60} Jd _{0.40}	RT		9.610(1)	8.790(1)	5.248(1)	106.60(2) ^o	80W1
Di _{0.50} Jd _{0.50}	RT		9.570(1)	8.749(1)	5.246(1)	106.79(2) ^o	80W1
Ae _{1.00} (synthetic)	RT		9.666(3)	8.804(2)	5.305(1)	107.44(2) ^o	97B1
Ae _{0.99} Di _{0.01} (natural)	RT		9.658(2)	8.795(2)	5.294(1)	107.42(2) ^o	63N1
Ae _{0.70} Hd _{0.14} Di _{0.16} (synthetic)	RT		9.698	8.848	5.284	106.78 ^o	69N1
Ae _{0.65} Hd _{0.11} Di _{0.19} Oth _{0.05} (natural) ^{13a)}	RT		9.681(5)	8.811(4)	5.306(9)	107.38(5) ^o	97B1

Table 3 (cont.)

Silicate	<i>T</i> [K]	Space group	Lattice parameters				Refs.
			<i>a</i> [Å]	<i>b</i> [Å]	<i>c</i> [Å]	β	
Hd _{0.84} Di _{0.12} Jo _{0.04} (natural) ^{13b)}	RT		9.826(3)	9.010(3)	5.252(1)	105.00(3)°	97B1
Di _{0.75} En _{0.10} CaTs _{0.15}	RT		9.707(1)	8.863(1)	5.267(1)	106.27(1)°	94T2
Di _{0.65} En _{0.20} CaTs _{0.15}	RT		9.700(1)	8.861(1)	5.258(1)	106.47(1)°	94T2
Di _{0.70} CaTs _{0.30}	RT		9.687(1)	8.832(1)	5.268(1)	106.18(1)°	94T2
Jervisite ¹⁴⁾	RT	C2/c	9.853(11)	9.042(10)	5.312(7)	106°37(7)'	82M4
Joesmithite ¹⁵⁾	RT	P2/a	9.88(2)	17.87(2)	5.97(5)	105°40(10)'	68M2, 68M3
Natalyite ¹⁶⁾	RT	C2/c	9.58(1)	8.72(1)	5.27(1)	107.16°	85R1, 87H1
Vinogradovite ¹⁷⁾	RT	I2/c	24.242(4)	8.691(7)	5.219(1)	92.4°	90M1, 84R1
Paravinogradovite ¹⁸⁾	RT	A2/a	5.219(1)	8.691(7)	25.01(4)	104.43(8)°	84R1
	RT	P1	5.246(1)	8.734(3)	12.968(5)	$\alpha=70.32(1)^\circ$ $\beta=79.01(1)^\circ$ $\gamma=80.90(2)^\circ$	03K1
Na ₄ Ti ₄ [Si ₂ O ₆] ₂ O ₆	RT	Pbcn	8.7128(10)	5.2327(5)	14.487(2)		87S4
PbSiO ₃	RT	P2/n	11.23	7.08	12.26	113°15'	68B1
Cs ₅ CoSiO ₆	RT	P2 ₁ /n	6.7057(7)	10.808(2)	16.461(2)	94.89(1)°	01H1
KHSiO ₃	RT	Cmca	11.537(7)	9.694(6)	11.245(9)		84D2
(H,D)AlSi ₂ O ₆	298	P4 ₃ 2 ₁ 2 or P4 ₁ 2 ₁ 2	7.586(5)		8.402(5)		90V1
Li ₂ SiO ₃	302		9.381(6)	5.399(3)	4.667(3)		96R3
	665		9.460(4)	5.445(2)	4.677(2)		96R3
	1062		9.544(4)	5.496(2)	4.704(2)		96R3
	1284		9.595(6)	5.520(3)	4.720(3)		96R3
	1474		9.623(14)	5.553(9)	4.747(7)		96R3
(Li ₂ SiO ₃) _x	RT	Cmc2 ₁	9.392(2)	5.397(2)	4.660(1)		77H3
LiScSi ₂ O ₆	RT		9.8033(7)	8.9581(7)	5.3515(4)	110.281(4)°	77H1
LiTiSi ₂ O ₆	RT		9.688(1)	8.797(2)	5.317(1)	108.99(2)°	88O2
LiVSi ₂ O ₆	RT		9.642(13)	8.581(8)	5.314(9)	109.73(11)°	71B2
	RT	C2/c	9.634(4)	8.586(2)	5.304(2)	109.69(3)°	04V1
	RT	A2/a	5.219(1)	8.691(7)	25.01(4)	104.43(8)°	84R1
LiCrSi ₂ O ₆	RT		9.546(3)	8.583(1)	5.255(1)	110.04(3)°	71B2
LiFeSi ₂ O ₆	RT		9.666	8.669	5.294	110.2°	69C1
	RT	P2 ₁ /c	9.6655(2)	8.6611(2)	5.2933(1)	110.18(1)°	98L1
	RT		9.682(1)	8.679(1)	5.299(1)	110.14(1)°	71B2
	1.4	P2 ₁ /c	9.6329(6)	8.6857(6)	5.2672(3)	109.90(3)°	98L1
	35	P2 ₁ /c	9.6221(2)	8.6730(1)	5.2663(1)	109.98(1)°	98L1
	213	P2 ₁ /c	9.642	8.694	5.281	110.03°	84B4
	295	C2/c	9.675	8.668	5.297	110.22°	84B4
Li _{0.85} Mg _{0.09} Fe ²⁺ _{0.06} Fe ³⁺ _{0.85-} Mg _{0.15} Si ₂ O ₆ (ferrian magnesian spodumene)	RT	P2 ₁ /c	9.638(3)	8.709(2)	5.258(2)	109.83(3)°	03C1
LiNiSi ₂ O ₆	RT		9.423(1)	8.847(1)	5.251(1)	110.52(2)°	88O2
LiAlSi ₂ O ₆	RT	C2	9.449(3)	8.386(1)	5.215(1)	110.10(2)°	66A1, 69C1
LiAlSi ₂ O ₆ -II (β-spodumene)	RT	P4 ₃ 2 ₁ 2 or P4 ₁ 2 ₁ 2	7.541(1)		9.156(2)		68L2

Table 3 (cont.)

Silicate	<i>T</i> [K]	Space group	Lattice parameters				Refs.
			<i>a</i> [Å]	<i>b</i> [Å]	<i>c</i> [Å]	β	
LiAlSi ₂ O ₆ -II (β-spodumene)	RT		7.534(5)		9.158(9)		69C2
LiAlSi ₂ O ₆ -III	RT	P6 ₂ 22 or P6 ₄ 22	5.217(1)		5.464(2)		68L1
Li ₂ Al ₂ Si ₁₃ O ₁₀	RT	P6 ₂ 22 or P6 ₄ 22	5.238(1)		5.472(1)		70L1
LiGaSi ₂ O ₆	RT	C2/c	9.561(1)	8.569(1)	5.268(1)	110.244(3) ^o	94S1
	273	P2 ₁ /c	9.5394(4)	8.5756(2)	5.2508(3)	110.124(2) ^o	95S1
LiInSi ₂ O ₆	RT		9.805	9.051	5.376	110.47 ^o	83G2
Li _{0.91} Na _{0.09} GaSi ₂ O ₆	RT	C2/c	9.5519(8)	8.5847(4)	5.2678(5)	109.950(4) ^o	96O1
Li _{0.75} Na _{0.25} GaSi ₂ O ₆	RT	C2/c	9.5468(7)	8.5995(3)	5.2689(4)	109.678(3) ^o	96O1
Li _{0.64} Na _{0.36} GaSi ₂ O ₆	RT	C2/c	9.5467(6)	8.6217(3)	5.2698(3)	109.338(3) ^o	96O1
Li _{0.25} Na _{0.75} GaSi ₂ O ₆	RT	C2/c	9.5492(5)	8.6753(3)	5.2698(3)	108.152(3) ^o	96O1
Li _{0.10} Na _{0.90} GaSi ₂ O ₆	RT	C2/c	9.5512(5)	8.6890(2)	5.2686(3)	107.824(2) ^o	96O1
Virgilite	RT	P6 ₂ 22 or P6 ₄ 22	5.132(1)		5.454(1)		78F2
Li _{0.61} (Si _{2.37} Al _{0.60} Fe _{0.02} P _{0.01})O ₆							
Lintisite	RT	C2/c	28.583(4)	8.600(1)	5.219(1)	91.03(2) ^o	90M1
Na ₃ LiTi ₂ [Si ₂ O ₆] ₂ O ₂ ·2H ₂ O							
Mineral X ¹⁹⁾	RT	1	24.066	8.720	5.128	92.6 ^o	86K1
Mn ²⁺ ₂ SiO ₃ (OH) ₂ ·H ₂ O	RT	Pca2 ₁	12.672(9)	7.217(3)	5.341(2)		95N1
(Nchwangingite)							
Lorenzenite (Ramsayite) ^{20),a)}	RT	Pnca	14.487(2)	8.7128(10)	5.2327(5)		87S4
Aerinite ²¹⁾	RT	Mono- clinic	14.690(15)	16.872(15)	5.170(15)	94°45'	88A4

- 1) Mn_{1.040}Mg_{0.885}Fe²⁺_{0.087}Fe³⁺_{0.012}Ca_{0.024}Si_{1.973}O₆;
- 2) Ca_{0.99}Mg_{0.98}Fe_{0.02}Na_{0.02}Al_{0.01}Si_{1.99}O₆;
- 3) (Ca_{0.98}Na_{0.03})(Mg_{0.68}Fe²⁺_{0.07}Fe³⁺_{0.03}Al_{0.16}Ti_{0.04})(Si_{1.77}Al_{0.23})O₆
- 4) Ca_{0.98}Fe_{0.99}Mg_{0.01}Na_{0.02}Al_{0.01}Si₂O₆;
- 5) (Ca_{1.01}Na_{0.01})(Fe³⁺_{0.72}Mg_{0.16}Al_{0.04}Ti_{0.03}Fe²⁺_{0.02})(Si_{1.19}Al_{0.81})O₆;
- 6) Ca_{0.93}Fe_{0.61}Mn_{0.34}Mg_{0.08}Na_{0.01}Zn_{0.02}Al_{0.003}Si₂O₆;
- 7) (Ca_{0.92}Na_{0.06}Mn_{0.02})(Zn_{0.37}Mn_{0.18}Fe²⁺_{0.19}Fe³⁺_{0.12}Mg_{0.14})(Si_{1.94}Al_{0.06})O₆;
- 8) Including V_{0.002}, Mg_{0.006}, Al_{0.007};
- 9) Including V_{0.002};
- 10) (Ca_{0.516}Na_{0.484}Mg_{0.392}Fe²⁺_{0.077}Fe³⁺_{0.137}Al_{0.398}Ti_{0.005})(Si_{1.918}Al_{0.082})O₆;
- 11) (Ca_{0.51}Na_{0.48}Mg_{0.44}Fe²⁺_{0.10}Fe³⁺_{0.10}Al_{0.39}Ti_{0.01})(Si_{1.96}Al_{0.04})O₆;
- 12) (Ca_{0.583}Na_{0.325}Mg_{0.582}Fe²⁺_{0.116}Fe³⁺_{0.123}Al_{0.233}Ti_{0.002})(Si_{1.995}Al_{0.005})O₆;
- 13) Ae - aegirine, Di - diopside, Jd - jadeite, Hd - hedenbergite, CaTs - Calcium-Tschermak, Jo - johannsenite, En - enstatite;
- 13a) {Na_{0.65}Ca_{0.34}}[Fe³⁺_{0.64}Fe²⁺_{0.11}Mg_{0.19}Al_{0.04}Ti_{0.01}](Si_{1.98}Al_{0.01})O₆.
- 13b) Ca_{0.99}[Fe²⁺_{0.84}Mg_{0.12}Mn_{0.04}]Si₂O₆;
- 14) (Na_{0.43}Ca_{0.31}Fe²⁺_{0.14}□_{0.12})(Sc_{0.66}Fe²⁺_{0.15}Mg_{0.19})Si₂O₆;
- 15) (Pb_{0.6}Ca_{0.6}Ba_{0.1}Mn_{0.8})Ca_{4.0}Fe³⁺_{2.0}(Mg_{6.3}Fe³⁺_{1.4}Fe²⁺_{0.8}Al_{0.3})(Si_{13.8}Be_{0.1})(OH)_{14.9}O_{39.7};
- 16) (Na_{0.92}Ca_{0.07})(V_{0.54}Cr_{0.36}Mg_{0.07}Al_{0.03})Si_{1.99}O₆;
- 17) (Na_{7.64}Ca_{0.36})(Ti_{7.3}Nb_{0.7})O₈[Si₂O₆]₄[(Si_{2.78}Al_{1.22})O₁₀]₂[(H₂O)_{5.34}K_{1.38}];
- 18) (Na_{2.293}K_{0.169})(Ti_{3.386}Fe_{0.471}Nb_{0.034}Mg_{0.029})(Si_{6.626}Al_{1.098}Be_{0.276})O₂₂(OH)₄(H₂O)_{1.12};
- 19) Na₃K_{0.1}Ti_{2.2}Nb_{0.2}Fe_{0.1}Al_{0.8}Si₄O_{15.6}·H₂O;
- 20) Na₄Ti₄[Si₂O₆]₂O₆; ^{a)} In original paper space group Pbca was considered, related to Pnca by $a \rightarrow b$, $b \rightarrow c$, $c \rightarrow a$;
- 21) Ca₄(Al, Fe, Mg)₁₀Si₁₂O₃₆(OH)₁₂CO₃·H₂O.

Table 4. Elastic properties.a) Bulk moduli, K , and shear moduli, G , as well as their derivatives.

Silicate ¹⁾	K_o [GPa]	K_o'	G_o [GPa]	p [GPa]	Method	Refs.
MgSiO ₃ (OEn)	102.8(2)	10.2(1.2)			Diamond anvil	95Z1
MgSiO ₃ (OEn)	107.6(1.5)		76.8(7)		Brillouin	99J1
MgSiO ₃ (OEn)	107.8		75.7		Brillouin	78W1
MgSiO ₃ (OEn)	109(2)	7.0(4)	74.9	10.0	ultrasonic	98F1
MgSiO ₃ (OEn)	102.3(1.2)	9.2(6)		8.5	X-ray	94A1, 02A1
MgSiO ₃ (OEn)	105.8(5)	8.5(3)		9.0	X-ray	02A1
MgSiO ₃ (OPx)	104(2)	$K_o' = 10.9(5)$ $K_o'' =$ $-1.6(2) \text{ GPa}^{-1}$	$G_o = 74.8(1.5)$ $G_o' = 1.4(1)$	10.0	Shear wave	98F1
Orthopyroxene (natural)	105	10.9(3)		8.5	Shear wave	86W2
MgSiO ₃ –P2 ₁ /c LCEn	111.1(3.3)	6.6(1.1)			X-ray	94A1
MgSiO ₃ –P2 ₁ /c CEn	108.5(6.4)	4.5(1.3)		12	Diamond anvil	99S1
MgSiO ₃ –C2/c HPCEn	106.4(17.4)	5.4(2.7)		12	Diamond anvil	99S1
MgSiO ₃ (HPCEn)	106.9(25.9)	5.3(3.0)		12	Diamond anvil	99S1
MgSiO ₃ (HPCEn)	104.1(5.7)	6.6 ²⁾		9.0	X-ray	94A1
MgSiO ₃ (perovskite) s.c.	246					90Y1
MgSiO ₃ (perovskite) s.c.	247	4				87K3
MgSiO ₃ (perovskite) s.c.	254	4				90R3
MgSiO ₃ (perovskite) p.	258	4 ²⁾				82Y1
MgSiO ₃ (perovskite)	265	4 ²⁾				86J1
MgSiO ₃ (perovskite)	264		177			98S3
MgSiO ₃ (perovskite)	260 (predicted)					87M2
Mg _{0.9} Fe _{0.1} SiO ₃ (perovskite) p.	266	3.9				87K2
(Fe,Mg)SiO ₃ (perovskite)	272	4				89M2
MgSiO ₃ (ilmenite)	212	4.3	132		Brillouin	85W1
MgSiO ₃ (ilmenite)	212	5.6(1.0)				96R2
FeSiO ₃ (OFs)	95.1(3.0)	10.6(1.1)		5.4	X-ray	97H2
FeSiO ₃ (OFs)	98	9.1(4)			Brillouin	84B2
Mg _{0.8} Fe _{0.2} SiO ₃	103.5		74.8			72F2
Mg _{0.8} Fe _{0.2} SiO ₃	109.4(8)	$K_o' = 10.8(8)$ $K_o'' =$ $-1.6(2) \text{ GPa}^{-1}$	$G_o = 75.2(4)$ $G_o' = 2.06(7)$ $G_o'' =$ $-0.12(0) \text{ GPa}^{-1}$			93W2
Mg _{0.59} Fe _{0.41} SiO ₃	98.0(1.8)	10.0(8)		7.5	X-ray	97H2
Mg _{0.29} Fe _{0.71} SiO ₃	102.2(1.3)	8.0(5)		7.3	X-ray	97H2
Orthopyroxene ³⁾	109.2(2.3)	9.05(1.0)		6	X-ray	97H2
Orthopyroxene ⁴⁾	112.4(1.1)	7.4(4)		8.6	X-ray	97H2
CaSiO ₃ (PWo)	86(1)	3.8(4)		9.94	X-ray	99Y3

Table 4a (cont.)

Silicate	K_o [GPa]	K_o'	G_o [GPa]	p [GPa]	Method	Refs.
CaSiO ₃ (perovskite)	281(4)	4.0(2)		134		89M1, 89M2
CaSiO ₃ (perovskite)	232(8)	4.8(3)		13	Multianvil cell	96W1
CaSiO ₃ (perovskite)	212(7)		112(5)		Predicted	98S3
CaSi _{0.49} Ti _{0.51} O ₃	188(2)		109(1)		Ultrasound	98S3
CaSi _{0.23} Ti _{0.77} O ₃	182(3)		107(1)		Ultrasound	98S3
Diopside s.c.	112				Brillouin	61A1
Diopside s.c. ⁵⁾	113		67		Brillouin	79L1
Diopside s.c.	122.2	4.0 ²⁾		6.0	X-ray	89M3
Diopside s.c.	104.1(9)	6.2(3)		10	X-ray	97Z1
Diopside	105.1(9)	6.8(1)		40.8	X-ray	00T3
Diopside	105	6.2		5	Simulation	84M1
Chrome-diopside ⁶⁾	116.5(9) ⁷⁾		72.8(4) ⁸⁾		Resonant ultrasound spectroscopy	03I1
Di ₇₂ Hd ₉ Jd ₃ Ko ₃ MgTs ₁₂ ⁹⁾	117.2(7) ⁷⁾		72.2(2) ⁸⁾		Impulsive stimulated scattering	98C4
Ca _{0.8} Mg _{1.2} Si ₂ O ₆	107.3(1.4)	5.7(3)		1.51	X-ray	00T3
Hedenbergite s.c.	120		61		Brillouin	88K1
Hedenbergite s.c.	117(1)	4.3(4)		10	X-ray	97Z1
Hedenbergite p.	119(2)	4.0 ²⁾		10	X-ray	89Z1, 92Z1
Hd _{0.60} Di _{0.40}	82.7(1)	4				92Z1
Mg _{1.54} Li _{0.23} Sc _{0.23} Si ₂ O ₆ (Pbcn)	130(3)	4		10	X-ray	99Y1
Mg _{1.54} Li _{0.23} Sc _{0.23} Si ₂ O ₆ (P2 ₁ cn)	111(1)	4		10	X-ray	99Y1

¹⁾ OEn – orthoenstatite, Hd – hedenbergite, OFs – orthoferrosilite, Di – diopside, Jd – jadeite, Ko – Kosmochlor, MgTs – Magnesium Tschermak's, PWo – pseudowollastonite, s.c. – single crystal, p. – powder;

²⁾ Fixed value;

³⁾ (Mg_{0.85}Fe_{0.13}Ca_{0.02})(Si_{0.96}Al_{0.04})O₃;

⁴⁾ (Mg_{0.83}Fe_{0.12}Ca_{0.006}Al_{0.04})(Si_{0.97}Al_{0.03})O₃;

⁵⁾ Ca_{0.99}Na_{0.02}Mg_{0.98}Al_{0.01}Fe_{0.02}Si_{1.99}O₆;

⁶⁾ (Ca_{0.956}Na_{0.026}K_{0.0002})(Mg_{0.928}Fe_{0.032}Cr_{0.024}Al_{0.010}Ti_{0.0019}Mn_{0.0014})Si₂O₆;

⁷⁾ Isotropic bulk modulus;

⁸⁾ isotropic shear modulus;

⁹⁾ Ca_{0.7596}Na_{0.1050}Mg_{0.8513}Mn_{0.0026}Fe_{0.0907}Cr_{0.0275}Ti_{0.0129}Al_{0.2833}Si_{1.8756}O₆.

Table 4 (cont.)

b) Linear compressibilities and pressure derivatives of axial ratios.

Silicate	Linear compressibilities [GPa^{-1}] $\cdot 10^5$				Pressure derivatives [GPa^{-1}] $\cdot 10^5$		Refs.
	β_a	β_b	β_c	β_β	$d/dp(b/a)$	$d/dp(c/a)$	
MgSiO ₃ (perovskite) s.c.	131	120	156				90Y1
MgSiO ₃ (perovskite) s.c.	141	107	157		35	−23	87K3
MgSiO ₃ (perovskite) s.c.	130(5)	104(4)	124(4)				90R3
MgSiO ₃ (perovskite) p.	158	119	110		40	70	82Y1
MgSiO ₃ (perovskite) (predicted)	123	118	153		13	−43	87M2
(Fe,Mg)SiO ₃ p.	129	105	133				89M2
CaMgSi ₂ O ₆	2.22(8)	330(10)	260(10)				92Z1
CaMgSi ₂ O ₆	236(4)	317(4)	250(4)				97Z1
CaFeSi ₂ O ₆	193(5)	338(6)	242(8)				97Z1
CaFeSi ₂ O ₆	258(3)	327.4(7)	259.7(3)				92Z1
Hd _{0.6} Di _{0.4}	190(20)	310(20)	220(20)				92Z1
CaSiO ₃ (two layers) (pseudowollastonite)	11.8320 − 0.0560 p + 0.000885 p^2	6.8621 − 0.0341 p + 0.000615 p^2	10.5300 − 0.0221 p + 0.000488 p^2	111.25 − 0.0444 p + 0.000671 p^2			99Y3

Table 4 (cont.)

c) Elastic constants.

Silicate	Elastic constants c_{ij} [GPa]												Refs.
	c_{11}	c_{22}	c_{33}	c_{44}	c_{55}	c_{66}	c_{12}	c_{13}	c_{23}	c_{15}	c_{25}	c_{35}	c_{46}
Orthoenstatite	224.7(2.3)	177.9(2.2)	213.6(3.6)	77.6(1.9)	75.9(1.1)	81.6(1.6)	72.4(4.2)	54.1(11.0)	52.7(4.6)				78W1
Orthoenstatite MgSiO ₃	233(1)	171(1)	216(1)	83(1)	79(1)	77(1)	73(2)	56(2)	50(3)				99J1
Protoenstatite	213	152	246	81	44	67							83V1
Enstatite (calculated)	181	200	153	79	66	81							98C3
Protoenstatite (calculated)	193	151	202	71	43	58							94G3
Ferrosilite	198	136	175	59	58	49	84	72	55				84B2
Mg _{0.8} Fe _{0.2} SiO ₃	228.6	160.5	210.4	81.74	75.48	77.66	71.0	54.8	46.0				72F2
Mg _{0.8} Fe _{0.2} SiO ₃	231.0(4)	169.8(2)	215.7(3)	82.8(2)	76.5(3)	78.1(1)	78.9(4)	61.4(6)	49.1(4)				93W2
Mg _{0.845} Fe _{0.155} SiO ₃	229.9	165.4	205.7	83.1	76.4	78.5	70.1	57.3	49.6				69K1
Diopside ¹⁾	223(2)	171(2)	235(2)	74(1)	67(1)	66(2)	77(3)	81(2)	57(2)	17(1)	7(2)	43(1)	79L1
Chrome-diopside ²⁾	228.1(1.0)	181.1(6)	245.4(1.3)	78.9(3)	68.2(2)	78.1(2)	78.8(5)	70.2(7)	61.1(7)	7.9(5)	5.9(5)	39.7(4)	03I1
CaMgSi ₂ O ₆ (computed)	210	166	242	80	70	58	64	87	72	26	11	49	84M1
Di ₇₂ Hd ₉ Id ₃ Ko ₃ MgTs ₁₂	237.8(9)	183.6(9)	229.5(9)	76.5(9)	73.0(4)	81.6(1.0)	83.5(1.3)	80.0(1.1)	59.9(1.6)	9.0(6)	9.5(1.0)	48.1(6)	98C4
Hedenbergite	222(6)	176(5)	249(5)	55(3)	63(2)	60(4)	69(14)	79(9)	86(10)	12(3)	13(7)	26(3)	88K1

1) Ca_{0.99}Na_{0.02}Mg_{0.98}Al_{0.01}Fe_{0.02}Si_{1.99}O₆.2) (Ca_{0.956}Na_{0.026}K_{0.0002})(Mg_{0.928}Fe_{0.032}Cr_{0.024}Al_{0.010}Ti_{0.0019}Mn_{0.0014})Si_{2.008}O₆.

Table 5. Thermal expansivities.

Silicate	Temperature range [K]	Thermal expansivities α [10^{-6}K^{-1}]				Refs.
		$\alpha_a^{1)}$	α_b	α_c	α_v	
MgSiO ₃ (OEn)					36	62S1
MgSiO ₃ (OEn)					24	66S1
MgSiO ₃ (OEn)		16.4	14.5	16.8	47.7	72F2
MgSiO ₃ (OEn)		5.5	9.6	8.2	23.5	94Y1
MgSiO ₃ (OEn)	300...900	8.0(5)	13.0(6)	10.9(6)	32.2(1.1)	97H1
MgSiO ₃ (OEn)	298...1000				28.6(2.9) + 0.72(10) · 10 ⁻² T [K ⁻²]	95Z1
FeSiO ₃ (OFs)		11.2	10.9	16.8	39.3	76S1
FeSiO ₃ (OFs)		6.7	13.9	6.1	29.0	94Y1, 94Y2
FeSiO ₃ (OFs)	300...900	10.4(1.0)	6.8(1.5)	10.1(1.4)	27.5(1.3)	97H1
Mg _{0.85} Fe _{0.15} SiO ₃ (OPx)					20.8	82D2
Mg _{0.305} Fe _{0.68} Ca _{0.015} SiO ₃ (OPx)		13.5	14.5	15.4	43.8	73S1
MgSiO ₃ (CEn)					40.5	62S1
MgSiO ₃ (CEn)					22	66S1
MgSiO ₃ (CPx)	300...900	7.6(6)	16.6(5)	5.2(7)	29.9(1.1)	97H1
FeSiO ₃ (CPx)	300...900	2.7(0.9)	7.5(1.3)	10.2(1.2)	20.3(1.5)	97H1
Mg _{0.95} Fe _{0.05} SiO ₃ (CPx)		8.2	13.4	11.5	33.3	84P1
Mg _{0.305} Fe _{0.68} Ca _{0.015} SiO ₃		8.3	10.4	13.8	32.7	74S1
Fe _{0.85} Ca _{0.15} SiO ₃		8.9	13.3	15.2	37.6	73O1
MgSiO ₃ –C2/c HPCPx					20.1(4.4) + 2.10(1.1) · 10 ⁻² T [K ⁻²]	99S1
MgSiO ₃ (ilmenite)	298...876	7.07		9.96	24.4	88A3
MgSiO ₃ (perovskite) ²⁾	77...298	8.4(9)	≡0	5.9(5)	14.5(9)	89R2
	298...381				22(8)	
Mg _{0.9} Fe _{0.1} SiO ₃ (perovskite)	300...1300				48	86K4
Diopside (natural)	293...1098	5.5 ³⁾	15.9	5.1		33K1
	673...1273	6.9 ³⁾	17.5	6.4		
Diopside (natural)	473...1073	7.4 ⁴⁾			48	42R1
Diopside (natural)	298...1098	7.7	17.3	7.0		73D1
Diopside ⁵⁾		10 ⁶ α ₀ = 0.186	10 ⁶ α ₀ = 13.880	10 ⁶ α ₀ = -2.152	10 ⁶ α ₀ = 9.263	98R3
		10 ⁹ α ₁ = 11.49	10 ⁹ α ₁ = 4.29	10 ⁹ α ₁ = 21.04	10 ⁹ α ₁ = 42.70	
		10 ¹² α ₂ = -0.810	10 ¹² α ₂ = 3.795	10 ¹² α ₂ = -6.094	10 ¹² α ₂ = -7.215	

(cont.)

Table 5 (cont.)

Silicate	Temperature range [K]	Thermal expansivities α [10^{-6}K^{-1}]				Refs.
		$\alpha_a^{1)}$	α_b	α_c	α_v	
Pseudowollastonite ⁵⁾		$10^6\alpha_0 = 1.112$ $10^9\alpha_1 = 13.27$ $10^{12}\alpha_2 = -0.276$	$10^6\alpha_0 = 5.771$ $10^9\alpha_1 = 8.89$ $10^{12}\alpha_2 = -0.189$	$10^6\alpha_0 = 2.722$ $10^9\alpha_1 = 3.09$ $10^{12}\alpha_2 = 5.753$	$10^6\alpha_0 = 2.051$ $10^9\alpha_1 = 41.012$ $10^{12}\alpha_2 = -2.290$	98R3
Di _{0.15} En _{0.85}	440...1040	1.08(12) ⁶⁾	1.34(15) ⁶⁾	0.46(16) ⁶⁾	$\alpha_v = 2.7(4)^{6)}$, $\alpha_\beta = 3.0(5)^{6)}$	03T3
Di _{0.52} En _{0.46} CaTs _{0.02}	440...1040	0.92(16) ⁶⁾	1.35(9) ⁶⁾	0.72(11) ⁶⁾	$\alpha_v = 2.8(4)^{6)}$, $\alpha_\beta = 3.5(1.7)^{6)}$	03T3
Di _{0.60} En _{0.40}	440...1040	1.07(1) ⁶⁾	1.35(6) ⁶⁾	0.86(2) ⁶⁾	$\alpha_v = 3.1(2)^{6)}$, $\alpha_\beta = 4.24(8)^{6)}$	03T3
Di _{0.70} En _{0.30}	440...1440	1.06(2) ⁶⁾	1.56(7) ⁶⁾	0.89(1) ⁶⁾	$\alpha_v = 3.27(11)^{6)}$, $\alpha_\beta = 4.83(17)^{6)}$	03T3

1) For clinopyroxenes (CPx) the α_a represents the thermal expansion coefficients between (100) planes;

2) There are some theoretical models which predicted thermal expansion coefficients of MgSiO₃ perovskite (values in 10^{-6}K^{-1}) namely [87H4]: 13 at 298 K and 21 at 1000 K; [87W3]: 18 at 300 K and 29 at 800 K; [87C2]: 11 at 298...400 K and 13 at 1000 K; [89H3]: 23 at 298 K and 33 at 1000 K;

3) Along a^* ;

4) Average value;

5) $\alpha = \alpha_0 + \alpha_1 T + \alpha_2 T^2$ [K^{-1}];

6) Thermal coefficients $\alpha_{a_i} = (1/a_{i0})(\partial a_i / \partial T)$ where a_{i0} is the initial lattice parameter or volume.

Table 6. Atomic charges.

a) Net atomic charges of ions in some pyroxenes.

Atom	Mg ₂ Si ₂ O ₆ [80S1]	Fe ₂ Si ₂ O ₆ [82S1]	Co ₂ Si ₂ O ₆ [82S1]	LiAlSi ₂ O ₆ [80S1]	CaMgSi ₂ O ₆ [80S1]	Mg _{0.88} Fe _{0.12} SiO ₃ [96C1]
M1	+1.84(4)	+1.41(12)	+1.29(11)	+2.4(1)	+1.44(1)	+2.78 (Fe)
M2	+1.79(4)	+1.10(13)	+0.61(12)	+0.7(1)	+1.39(2)	+2.07 (Fe)
SiA	+2.20(4)	+2.21(11)	+1.79(9)			
SiB	+2.36(4)	+2.16(11)	+2.76(9)	2.4(1)	2.56(1)	
O1A	-1.51	-1.04	-1.10			
O1B	-1.37	-1.19	-1.14	-1.3	-1.33	
O2A	-1.36	-1.09	-1.12			
O2B	-1.43	-1.20	-1.16	-1.4	-1.28	
O3A	-1.31	-0.92	-0.84			
O3B	-1.22	-1.18	-1.10	-1.3	-1.35	

Table 6 (cont.)

b) Charges of oxygens in $\text{LiAlSi}_2\text{O}_6$ spodumene calculated from [03P1] by application of various models (see references).

Method	[40P1]	[73B2]	[89H4]	[94B1]
O1	−2.17	−2.00	−1.97	−1.75
O2	−1.67	−1.89	−1.92	−1.74
O3	−2.17	−2.15	−2.11	−1.73

Table 7. The site occupancies of some pyroxenes.

Sample	Site	Site occupancy	K_D	Refs.
$\text{Fe}_{1.732}\text{Mg}_{0.268}\text{Si}_2\text{O}_6$ ¹⁾	M1	0.76Fe + 0.24Mg	0.10	69S2
	M2	0.97Fe + 0.03Mg		
$\text{Fe}_{1.516}\text{Mg}_{0.484}\text{Si}_2\text{O}_6$ ¹⁾	M1	0.56Fe + 0.44Mg	0.053	69S2
	M2	0.96Fe + 0.04Mg		
$\text{Fe}_{0.78}\text{Mg}_{1.22}\text{Si}_2\text{O}_6$ ¹⁾	M1	0.07Fe + 0.93Mg	0.03	69S2
	M2	0.72Fe + 0.28Mg		
$\text{Fe}_{0.544}\text{Mg}_{1.456}\text{Si}_2\text{O}_6$ ¹⁾	M1	0.04Fe + 0.96Mg	0.04	69S2
	M2	0.51Fe + 0.49Mg		
$\text{Fe}_{1.064}\text{Mg}_{0.936}\text{Si}_2\text{O}_6$ ^{2,3)}	M1	0.16Fe + 0.84Mg	0.02	67E2
	M2	0.91Fe + 0.09Mg		
$\text{Fe}_{1.064}\text{Mg}_{0.936}\text{Si}_2\text{O}_6$ ^{2,3,4)}	M1	0.29Fe + 0.71Mg	0.116	67E2
	M2	0.78Fe + 0.22Mg		
$\text{Fe}_{1.064}\text{Mg}_{0.936}\text{Si}_2\text{O}_6$ ^{2,3,5)}	M1	0.31Fe + 0.69Mg	0.142	67E2
	M2	0.76Fe + 0.24Mg		
$\text{Fe}_{0.79}\text{Mg}_{1.21}\text{Si}_2\text{O}_6$	M1	0.190Fe + 0.810Mg	0.154	74G1, 75G2
	M2	0.604Fe + 0.396Mg		
$\text{Fe}_{1.70}\text{Mg}_{0.26}\text{Ca}_{0.04}\text{Si}_2\text{O}_6$	M1	0.25Mg ²⁺ + 0.75Fe ²⁺	0.126	71B3
	M2	0.96Fe ²⁺ + 0.04Ca ²⁺		
$\text{Fe}_{1.70}\text{Mg}_{0.26}\text{Ca}_{0.04}\text{Si}_2\text{O}_6$	M1	0.24Mg + 0.76Fe		87R1
	M2	0.94Fe + 0.02Mg + 0.04Ca		
$\text{Mn}_{0.150}\text{Mg}_{1.850}\text{Si}_2\text{O}_6$ (Pbca)	M1	0.023(4)Mn + 0.977Mg	0.162	78H1
	M2	0.127Mn + 0.873Mg		
$\text{Mn}_{0.90}\text{Mg}_{1.10}\text{Si}_2\text{O}_6$	M1	0.118Mn + 0.882Mg	0.037	74G1
	M2	0.782Mn + 0.218Mg		
$\text{Co}_{0.448}\text{Mg}_{1.552}\text{Si}_2\text{O}_6$ (Pbca)	M1	0.129(3)Co + 0.871Mg	0.316	78H1
	M2	0.319Co + 0.681Mg		
$\text{Co}_{0.74}\text{Mg}_{1.26}\text{Si}_2\text{O}_6$	M1	0.265Co + 0.735Mg	0.398	74G1, 75G2
	M2	0.475Co + 0.525Mg		
$\text{Ni}_{0.38}\text{Mg}_{1.62}\text{Si}_2\text{O}_6$	M1	0.211Ni + 0.789Mg	1.32	74G1, 75G2
	M2	0.169Ni + 0.831Mg		
$\text{Zn}_{0.45}\text{Mg}_{1.55}\text{Si}_2\text{O}_6$	M1	0.067Zn + 0.933Mg	0.116	74G1, 75G2
	M2	0.383Zn + 0.617Mg		
$\text{Zn}_{1.0}\text{Mg}_{1.0}\text{Si}_2\text{O}_6$	M1	0.36Zn + 0.64Mg	0.316	75M3
	M2	0.64Zn + 0.36Mg		
$\text{Co}_{1/3}\text{Ni}_{1/3}\text{Zn}_{1/3}\text{SiO}_3$ (Pbca)	M1	0.273(14)Co + 0.530(18)Ni + 0.197(12)Zn	0.398	90T2
	M2	0.394(14)Co + 0.137(18)Ni + 0.469(12)Zn		

Table 7 (cont.)

Sample	Site	Site occupancy	K_D	Refs.
Orthopyroxene ⁶⁾	M1	0.993(2)Mg + 0.003(2)Fe ²⁺ + 0.003Fe ³⁺ + 0.001Cr		92S5
	M2	0.862(2)Mg + 0.130(2)Fe ²⁺ + 0.005Mn + 0.003Ca		
	T	1.996Si + 0.004Al		
Orthopyroxene ⁷⁾	M1	0.922(3)Mg + 0.055(2)Fe ²⁺ + 0.006Fe ³⁺ + 0.014Al + 0.001Ti + 0.002Mn		92S5
	M2	0.212(3)Mg + 0.740(3)Fe ²⁺ + 0.026Mn + 0.022Ca		
	T	1.978Si + 0.022Al		
Orthopyroxene ⁸⁾	M1	0.818(2)Mg + 0.097(2)Fe ²⁺ + 0.012Fe ³⁺ + 0.066Al + 0.004Ti + 0.001Cr + 0.002Mn		92S5
	M2	0.139(3)Mg + 0.831(3)Fe ²⁺ + 0.021Mn + 0.009Ca		
	T	1.913Si + 0.087Al		
Orthopyroxene ⁹⁾	M1	0.847(3)Mg + 0.138(3)Fe ²⁺ + 0.008Al + 0.004Ti + 0.003Mn		92S5
	M2	0.079(3)Mg + 0.864(3)Fe ²⁺ + 0.020Mn + 0.037Ca		
	T	1.984Si + 0.016Al		
Esseneite ¹⁰⁾ (C2/c)	M1	0.58(3)Fe + 0.42(3)Al		87C3
	M2	0.97Ca + 0.03Fe		
	T	0.54(3)Si + 0.46(3)Al		
Ferrian spodumene Li _{0.85} Fe _{0.91} Mg _{0.24} Si ₂ O ₆	M1	0.15Mg + 0.85Fe ³⁺		03C1
	M2	0.85Li + 0.09Mg + 0.06Fe ²⁺		
	T			
Ca _{1.00} Sc _{0.84} Ti _{0.27} Al _{1.16} Si _{0.73} O ₆ (C2/c)	M1	0.84Sc + 0.16Ti		79O3
	M2	1.00Ca		
	T	0.11Ti + 1.16Al + 0.73Si		
CaFe _{0.910} Al _{0.590} Si _{0.500} O ₆	M1	0.179(1)Al + 0.821Fe ³⁺		86G2
	M2	1.00Ca		
	T	0.500Si + 0.411Al + 0.089Fe ³⁺		
CaNiSi ₂ O ₆ ¹¹⁾	M1	1.00Ni		90R1
	M2	1.00Ca		
CaNi _{0.8} Mg _{0.2} Si ₂ O ₆ ¹¹⁾	M1	0.26(1)Mg + 0.74(1)Ni		90R1
	M2	1.00(1)Ca		
CaNi _{0.5} Mg _{0.5} Si ₂ O ₆ ¹¹⁾	M1	0.55(1) Mg + 0.45(1) Ni		90R1
	M2	1.00(1)Ca		
CaNi _{0.25} Mg _{0.75} Si ₂ O ₆ ¹¹⁾	M1	0.78(1) Mg + 0.22(1) Ni		90R1
	M2	1.00(1)Ca		
CaMgSi ₂ O ₆ ¹¹⁾	M1	1.00 Mg		90R1
	M2	0.89(2) Ca + 0.11(2) Mg		
Ca _{0.742} Fe _{0.100} Mg _{0.016} Al _{1.384} - Si _{1.534} O ₆ (C2/c)	M1	0.016Mg + 0.888Al + 0.075Fe ²⁺ + 0.021□		98O1
	M2	0.742Ca + 0.087(2)Fe ²⁺ + 0.171□		
	T	0.500Al + 1.500Si		
Ca-rich clinopyroxene ¹²⁾				76M2
Thermal treated at:				
1350°C	3 GPa	3.75 h	0.250(24)	
1250°C	2 GPa	7.0 h	0.253(24)	
927°C		152.25 h	0.162(22)	
927°C		152.25 h	0.139(22)	
802°C		96 h	0.096(15)	
802°C disordered from 675 °C			0.123(20)	
675°C		302.5 h	0.066(13)	

Table 7 (cont.)

Sample	Site	Site occupancy	K_D	Refs.
Rhodonites:				
MnSiO ₃	M1	1.0Mn		88P1
	M2	1.0Mn		
	M3	1.0Mn		
	M4	1.0Mn		
	M5	1.0Mn		
Mn _{0.81} Fe _{0.07} Mg _{0.06} Ca _{0.05} SiO ₃	M1	0.93Mn + 0.07(1)Mg		88P1
	M2	0.93Mn + 0.07(1)Mg		
	M3	0.91Mn + 0.09(1)Mg		
	M4	0.78Mn + 0.22(1)Mg		
	M5	0.83Mn + 0.17Mg		
Mn _{0.75} Mg _{0.15} Ca _{0.10} SiO ₃	M1	0.89Mn + 0.11(1)Mg		88P1
	M2	0.86Mn + 0.14(1)Mg		
	M3	0.86Mn + 0.14(1)Mg		
	M4	0.53Mn + 0.47(1)Mg		
	M5	0.40Mn + 0.60Mg		
Mn _{0.685} Mg _{0.315} SiO ₃	M1	0.696Mn + 0.304(6)Mg		88P1
	M2	0.746Mn + 0.254(6)Mg		
	M3	0.634Mn + 0.366(6)Mg		
	M4	0.481Mn + 0.519(6)Mg		
	M5	0.868Mn + 0.132Mg		
Mn _{0.62} Mg _{0.38} SiO ₃	M1	0.615Mn + 0.385(5)Mg		88P1
	M2	0.687Mn + 0.313(5)Mg		
	M3	0.572Mn + 0.428(5)Mg		
	M4	0.350Mn + 0.650(5)Mg		
	M5	0.876Mn + 0.124Mg		
Mn _{3.73} Mg _{0.73} Ca _{0.51} Fe _{0.03} Si ₅ O ₁₅ (C1)	M1	0.89(1)Mn + 0.11Mg		78P1
	M2	0.86(1)Mn + 0.14Mg		
	M3	0.86(1)Mn + 0.14Mg		
	M4	0.53(1)Mn + 0.47Mg		
	M5	0.40(1)Mn + 0.60Mg		
Pyroxmangites:				
Mn _{0.97} Mg _{0.02} Ca _{0.01} SiO ₃	M1	0.973Mn + 0.027(2)Mg		88P1
	M2	0.952Mn + 0.048(7)Mg		
	M3	0.962Mn + 0.038(7)Mg		
	M4	0.967Mn + 0.033(7)Mg		
	M5	0.999Mn + 0.001(7)Mg		
	M6	0.921Mn + 0.079(7)Mg		
	M7	1.000Mn + 0.0Mg		
Mn _{0.82} Fe _{0.07} Mg _{0.09} Ca _{0.02} SiO ₃	M1	0.97Mn + 0.03(1)Mg		88P1
	M2	0.81Mn + 0.19(1)Mg		
	M3	0.83Mn + 0.17(1)Mg		
	M4	0.89Mn + 0.11(1)Mg		
	M5	0.88Mn + 0.12(1)Mg		
	M6	0.81Mn + 0.19(1)Mg		
	M7	0.91Mn + 0.09Mg		

Table 7 (cont.)

Sample	Site	Site occupancy	K_D	Refs.
$\text{Mn}_{0.51}\text{Mg}_{0.49}\text{SiO}_3$	M1	0.516Mn + 0.484(5)Mg		88P1
	M2	0.351Mn + 0.649(6)Mg		
	M3	0.451Mn + 0.549(5)Mg		
	M4	0.452Mn + 0.548(5)Mg		
	M5	0.788Mn + 0.212(5)Mg		
	M6	0.253Mn + 0.747(5)Mg		
	M7	0.777Mn + 0.223Mg		
$\text{Mn}_{0.15}\text{Mg}_{0.85}\text{SiO}_3$	M1	0.04Mn + 0.96(1)Mg		88P1
	M2	0.00Mn + 1.00(1)Mg		
	M3	0.05Mn + 0.95(1)Mg		
	M4	0.03Mn + 0.97(1)Mg		
	M5	0.30Mn + 0.70(1)Mg		
	M6	-0.02Mn + 1.02(1)Mg		
	M7	0.27Mn + 0.73Mg		
$\text{Ca}_{0.43}\text{Mn}_{0.69}\text{Mg}_{0.82}\text{Si}_2\text{O}_6$ (Mn-diopside C2/c)	M1	0.06Mn + 0.94Mg		81G2
	M2	0.87(2)Ca + 0.13Mn		
$\text{Ca}_{0.43}\text{Mn}_{0.69}\text{Mg}_{0.82}\text{Si}_2\text{O}_6$ (Kanoite P2 ₁ /c)	M1	0.10(1)Mn + 0.90Mg		81G2
	M2	0.86(1)Mn + 0.14Mg		
$\text{Ca}_{0.0245}\text{Mn}_{0.5415}\text{Mg}_{1.4325}\text{-Ti}_{0.0015}\text{Al}_{0.0030}\text{Si}_{1.9969}\text{O}_6$ (Donpeacorite, untreated)	M1	0.9882Mg + 0.0103Mn + 0.0015Ti		05S1
	M2	0.4443Mg + 0.5312Mn + 0.0245Ca		
$\text{Ca}_{0.0245}\text{Mn}_{0.5415}\text{Mg}_{1.4325}\text{-Ti}_{0.0015}\text{Al}_{0.0030}\text{Si}_{1.9969}\text{O}_6$ (treated at 904 °C)	M1	0.9371Mg + 0.0614Mn + 0.0015Ti		05S1
	M2	0.4955Mg + 0.4480Mn + 0.0245Ti		
Omphacites P2/n:				
$\text{NaMg}_{0.5}\text{Si}_{0.5}\text{Si}_2\text{O}_6$	M1	Mg		88A1
	M11	Si		
	M2	Na		
	M21	Na		
	T1	Si		
	T2	Si		
Omphacite ¹³⁾	M1	0.815(9)Mg + 0.185Fe		75M2
	M11	0.868(9)Al + 0.132Fe		
	M2	0.314(3)Ca + 0.686Na		
	M21	0.716Ca + 0.284Na		
Augite-jadeite ¹⁴⁾	M1	0.867Mg + 0.071Al + 0.062Fe ²⁺		98B1
	M11	0.251Mg + 0.688Al + 0.061Fe ²⁺		
	M2	0.500Ca + 0.500Na		
	M21	0.740Ca + 0.260Na		
Augite-jadeite ¹⁵⁾	M1	0.903Mg + 0.012Al + 0.085Fe ²⁺		98B1
	M11	0.075Mg + 0.880Al + 0.041Fe ²⁺ + 0.004Fe ³⁺		
	M2	0.336Ca + 0.664Na		
	M21	0.767Ca + 0.233Na		
Augite-jadeite ¹⁶⁾	M1	0.824Mg + 0.089Al + 0.087Fe ²⁺		98B1
	M11	0.010Mg + 0.973Al + 0.011Fe ²⁺ + 0.006Fe ³⁺		
	M2	0.236Ca + 0.764Na		
	M21	0.697Ca + 0.303Na		

Table 7 (cont.)

Sample	Site	Site occupancy	K_D	Refs.
Augite-jadeite ¹⁷⁾	M1	0.552Mg + 0.401Al + 0.045Fe ²⁺ + 0.002Fe ³⁺		98B1
	M11	0.266Mg + 0.669Al + 0.053Fe ²⁺ + 0.012Fe ³⁺		
	M2	0.402Ca + 0.598Na		
	M21	0.514Ca + 0.486Na		
Augite-jadeite ¹⁸⁾	M1	0.764Mg + 0.126Al + 0.110Fe ²⁺		98B1
	M11	0.972Al + 0.028Fe ²⁺		
	M2	0.211Ca + 0.789Na		
	M21	0.691Ca + 0.309Na		
Other compositions ¹⁹⁾				

1) Very slow cooled;

2) Natural samples;

3) Impurities as Al, Si, Ca were observed, in addition to Mg;

4) Thermal treated at 1000° C;

5) Thermal treated at 1100° C.

6) $\text{Ca}_{0.003}\text{Mn}_{0.005}\text{Fe}_{0.134}\text{Mg}_{1.857}\text{Cr}_{0.001}\text{Al}_{0.005}\text{Si}_{1.996}\text{O}_6$;7) $\text{Ca}_{0.022}\text{Mn}_{0.028}\text{Fe}_{0.802}\text{Mg}_{1.134}\text{Al}_{0.036}\text{Ti}_{0.001}\text{Si}_{1.978}\text{O}_6$;8) $\text{Ca}_{0.009}\text{Mn}_{0.023}\text{Fe}_{0.941}\text{Mg}_{0.962}\text{Cr}_{0.001}\text{Al}_{0.153}\text{Ti}_{0.004}\text{Si}_{1.913}\text{O}_6$;9) $\text{Ca}_{0.037}\text{Mn}_{0.023}\text{Fe}_{1.00}\text{Mg}_{0.929}\text{Cr}_{0.001}\text{Al}_{0.024}\text{Ti}_{0.004}\text{Si}_{1.984}\text{O}_6$;10) $(\text{Ca}_{1.01}\text{Na}_{0.01})(\text{Fe}^{3+}_{0.72}\text{Mg}_{0.16}\text{Al}_{0.04}\text{Ti}_{0.03}\text{Fe}^{2+}_{0.002})(\text{Si}_{1.19}\text{Al}_{0.81})\text{O}_6$;11) Synthetic clinopyroxenes, at $T = 1350^\circ\text{C}$;12) $\text{Ca}_{0.634}\text{Na}_{0.093}\text{Mg}_{0.885}\text{Ti}_{0.023}\text{Cr}_{0.004}\text{Mn}_{0.005}\text{Fe}^{2+}_{0.134}\text{Fe}^{3+}_{0.048}\text{Al}_{0.350}\text{Si}_{1.822}\text{O}_6$;13) $\text{Ca}_{0.516}\text{Na}_{0.484}\text{Mg}_{0.392}\text{Fe}^{2+}_{0.077}\text{Fe}^{3+}_{0.137}\text{Al}_{0.398}\text{Ti}_{0.005}\text{Si}_{1.918}\text{Al}_{0.082}\text{O}_6$;14) $(\text{Na}_{0.380}\text{Ca}_{0.620})(\text{Fe}^{2+}_{0.061}\text{Al}_{0.380}\text{Mg}_{0.559})\text{Si}_2\text{O}_6$;15) $(\text{Na}_{0.448}\text{Ca}_{0.552})(\text{Fe}^{3+}_{0.002}\text{Fe}^{2+}_{0.063}\text{Al}_{0.446}\text{Mg}_{0.489})\text{Si}_2\text{O}_6$;16) $(\text{Na}_{0.534}\text{Ca}_{0.466})(\text{Fe}^{3+}_{0.003}\text{Fe}^{2+}_{0.049}\text{Al}_{0.531}\text{Mg}_{0.417})\text{Si}_2\text{O}_6$;17) $(\text{Na}_{0.542}\text{Ca}_{0.458})(\text{Fe}^{3+}_{0.007}\text{Fe}^{2+}_{0.049}\text{Al}_{0.535}\text{Mg}_{0.409})\text{Si}_2\text{O}_6$;18) $(\text{Na}_{0.549}\text{Ca}_{0.451})(\text{Fe}^{2+}_{0.069}\text{Al}_{0.549}\text{Mg}_{0.382})\text{Si}_2\text{O}_6$;19) For Mg-Fe ordering in orthopyroxenes see: [70V2, 89S2, 93H1, 93S6, 97K2, 01V1], in $\text{Mg}(\text{Cu},\text{Mg})\text{Si}_2\text{O}_6$ orthopyroxene [97T1], in $\text{Wo}_{0.43}\text{En}_{0.46}\text{Es}_{0.11}$ clinopyroxene [01B1] and $(\text{Mg},\text{Fe})\text{SiO}_3$ clinopyroxene [97K2, 97W2], in ferrobustamite [79Y2] etc.

Table 8. Data obtained from neutron diffraction studies.

Sample	T [K]	Magnetic structure	T_N [K]	Refs.
$\text{Fe}_2\text{Si}_2\text{O}_6$	1.5	Ferromagnetic within octahedral band and antiferromagnetically coupled to neighbouring bands: $p_{\text{Fe}}(\text{M1}) = 4.3(1) \mu_B$; $p_{\text{Fe}}(\text{M2}) = 3.3(1) \mu_B$ (values extrapolated to 0 K); $T < 8 \text{ K}$: $p_{\text{Fe}}(\text{M2})$ deviates slightly from \mathbf{b} -axis; $p_{\text{Fe}}(\text{M1}) \parallel \mathbf{b}$ -axis;	38	88G2
$\text{Fe}_2\text{Si}_2\text{O}_6$	4.2	Ferromagnetic within octahedral band and antiferromagnetically coupled to neighbouring bands: $p_{\text{Fe}}(\text{M1}), p_{\text{Fe}}(\text{M2}) \parallel \mathbf{b}$ -axis; $p_{\text{Fe}}(\text{M1}) = 4.2 \mu_B$; $p_{\text{Fe}}(\text{M2}) = 3.3 \mu_B$	45	86W3
$\text{Fe}_{0.87}\text{Mg}_{0.13}\text{SiO}_3$	4.2	Ferromagnetic within octahedral band and antiferromagnetically coupled to neighbouring bands $\langle p_{\text{Fe}}(\text{M1}) \rangle = \langle p_{\text{Fe}}(\text{M2}) \rangle = 3.70(25) \mu_B^{1)}$; $p_{\text{Fe}}(\text{M1}), p_{\text{Fe}}(\text{M2}) \parallel \mathbf{b}$ -axis;	26	86W3
$\text{CaFeSi}_2\text{O}_6$	1.5	The spins are ferromagnetically coupled within one chain and antiferromagnetically coupled to those of adjacent chains; $p_{\text{Fe}}(\text{M1}) = 4.33(4) \mu_B$ (values extrapolated to 0 K). The moments are in the (ac) -plane, 132° away from the \mathbf{c} -axis in (ac) -plane	38	88G2
$\text{CaFe}_{0.8}\text{Mg}_{0.2}\text{Si}_2\text{O}_6$	3	Collinear antiferromagnetic ordering $p_x = 3.17(10) \mu_B$; $p_z = 2.64(7) \mu_B$; $p_o = 3.36(10) \mu_B$ making 45° with \mathbf{a} -axis	35	86W3
$\text{CaCoSi}_2\text{O}_6$	2	$p_x = 1.91(23) \mu_B$; $p_z = -2.23(12) \mu_B$; $p_{\text{Co}} = 3.30(15) \mu_B$; \mathbf{p} and \mathbf{a} make an angle of 41°	9.75	96D3
$\text{NaFeSi}_2\text{O}_6$	1.5 2.0 4.0	Antiferromagnetic ordering $p = 3.59(5) \mu_B$; $\phi = 14.0(4)^\circ$ $p = 3.16(5) \mu_B$; $\phi = 14.0(4)^\circ$ $p = 3.40(5) \mu_B$; $\phi = 18.4(7)^\circ$. The moments lie within planes parallel to (ac) -plane. They make an angle ϕ with \mathbf{c} -axis	8	89B1
$\text{LiFeSi}_2\text{O}_6$	1.4	$\mathbf{p} \parallel \mathbf{c}$ -axis with a small component along \mathbf{a} , which indicates a spin canting in (ac) -plane; $p_x = 0.76(9) \mu_B$; $p_z = 4.88(3) \mu_B$	19.5	98L1

¹⁾ Only mean value per site $\langle p_{\text{Fe}}(\text{M1}) \rangle = \frac{1}{2} [0.76 p_{\text{Fe}}(\text{M1}) + 0.94 p_{\text{Fe}}(\text{M2})] = 3.22 \mu_B$ was obtained which corresponds to an average moment $\langle p_{\text{Fe}}(\text{M1}) \rangle = \langle p_{\text{Fe}}(\text{M2}) \rangle = 3.70(25) \mu_B$ similar as the average moment in ferrosilite.

Table 9. Magnetic properties.

Sample	T [K]	$T_N(T_C)$ [K]	$T_M^{(2)}$ [K]	Θ [K]	C [K cm ³ mol ⁻¹]	p_{eff} [μ _B /atom]	Refs.
MnSiO ₃ (triclinic)				-45		5.91	64S2
FeSiO ₃ (OPx) ³⁾	4.2	38(1)	40(1)	27.4(5.0)	3.6	5.4	86W3, 86W4
FeSiO ₃ (OPx)		37.0(5)					69S2
FeSiO ₃ (OPx)		40 (T_N)		30 (50 K < T < 190 K)			88G2
		8 (T_F)		138 (190 K < T < 300 K)			
FeSiO ₃ (OPx)		39(1) (⁵⁷ Fe NGR) ⁴⁾					86R1
		41(1) (magnetic)					
FeSiO ₃ (CPx) ¹⁾		38(1)		9.4 ($T \geq 50$ K)		4.09(18)	01E1
Mg _{0.09} Fe _{0.91} SiO ₃ (CPx) ¹⁾		32(2)		-38.8 ($T \geq 200$ K)		3.05(13)	01E1
Mg _{0.13} Fe _{0.87} SiO ₃ (CPx)		26(2)		-145.5 ($T \geq 200$ K)		3.59(16)	01E1
Mg _{0.13} Fe _{0.87} SiO ₃ (OPx)		27(1)					87R1
Mg _{0.13} Fe _{0.87} SiO ₃ (OPx) ³⁾	4.2	26(1) (magnetic)	29(1)	34(5) ($T \geq 200$ K)	3.4	5.24(13)	86W3, 86W4
		27(1) (⁵⁷ Fe NGR) ⁴⁾					
Mg _{0.134} Fe _{0.866} SiO ₃ (OPx)		18(1)					69S2
Mg _{0.20} Fe _{0.80} SiO ₃ (OPx)		28					93L1
Mg _{0.22} Fe _{0.78} SiO ₃ (CPx)		21(4)		-57.7 ($T \geq 190$ K)			01E1
Mg _{0.242} Fe _{0.758} SiO ₃ (OPx)		11(1)					69S2
Mg _{0.39} Fe _{0.61} SiO ₃				-80.6 ($T \geq 190$ K)			01E1
Mg _{0.80} Fe _{0.20} SiO ₃ (OEn)				35.8 (77 K ≤ T ≤ 400 K)		5.31...5.57	01V1
Mg _{0.88} Fe _{0.12} SiO ₃ (OEn)				36.5 (77 K ≤ T ≤ 400 K)		5.26...5.53	01V1
Mg _{0.90} Fe _{0.10} SiO ₃ (OEn)		< 5(2)					92P1
Mg _{0.9} Fe _{0.1} SiO ₃ (perovskite)		5					92J1
CaFeSi ₂ O ₆		38		35(3) ($T > 100$ K)		4.98	85C2, 88G2
CaFe _{0.8} Mg _{0.2} Si ₂ O ₆ (C2/c)		35					86W3
Hd ₈₄ Di ₁₂ Jo ₄ ⁵⁾		31(1)		21(1) ($T < 80$ K)	3.05	4.94	97B1
Hedenbergite ⁶⁾		33(1)					03E1
Hedenbergite ⁷⁾		27(1)					03E1
Ca _{0.96} Mg _{0.19} Fe _{0.82} Mn _{0.02} Si ₂ O ₆		29(2) (⁵⁷ Fe NGR) ⁴⁾		21		5.43	88R1
		23(1) (magnetic)					
Ca _{0.96} Mg _{0.31} Fe _{0.66} Mn _{0.02} Al _{0.06} Si _{1.99} O _{6.02}		29(1)					86S3
Ca _{0.97} Mg _{0.06} Fe _{0.79} Mn _{0.17} Al _{0.01} Si ₂ O _{6.01}		28(1)					86S3
CaCoSi ₂ O ₆		9.75		-28	3.82		96D3
CaCo _{0.75} Ni _{0.25} Si ₂ O ₆		13.2		-3	2.68		96D3
CaCo _{0.50} Ni _{0.50} Si ₂ O ₆		15.6		4	2.14		96D3
CaCo _{0.25} Ni _{0.75} Si ₂ O ₆		18.3		12	1.52		96D3
CaNiSi ₂ O ₆		21.7		31	0.96		96D3
NaFeSi ₂ O ₆		5.0(3)		-39 ($T > 60$ K)	4.36	5.9	88B1
NaFeSi ₂ O ₆ (synthetic)		8		-46	4.4	5.93	89B1
Natural acmite ⁸⁾ (aegirine)				-22	3.8		89B1
LiFeSi ₂ O ₆		19.5(5)		-33 ($T > 40$ K)	4.60	6.1	88B1
LiFeSi ₂ O ₆		17.5		-25.8 ($T > 100$ K)		5.81	00R2
LiTiSi ₂ O ₆		210 (TSP) ⁹⁾					0211

Table 9 (cont.)

Sample	T [K]	$T_N (T_C)$ [K]	$T_M^{2)}$ [K]	Θ [K]	C [K cm ³ mol ⁻¹]	p_{eff} [μ _B /atom]	Refs.
NaTiSi ₂ O ₆		230 (T_{SP}) ⁹⁾	186	−255	0.375		02I1, 04I1
LiVSi ₂ O ₆		22	115				04I1
LiVSi ₂ O ₆		21.6	110	−290			04V1
NaVSi ₂ O ₆		19	53				04I1
NaVSi ₂ O ₆		17.4	48	−78			04V1
LiCrSi ₂ O ₆		11	18	−28.7			04I1, 05Y1
NaCrSi ₂ O ₆		3	3.6	−0.3			05V1
NaCrSi ₂ O ₆		3.4	< 3	−1.8 ($T > 10\text{K}$)	1.73		04I1
Ac ₈₁ Di ₁₉		15(1)		−36(2)		6.12	88D1
Ae ₆₅ Hd ₁₁ Di ₁₉ Oth ₅ ¹⁰⁾		7.5(5)		−19(1) ($T < 60\text{K}$)	3.34	5.17	97B1

¹⁾ Magnetization in a field $\mu_0 H = 14\text{ T}$ is $\sigma = 1.45(5) \cdot 10^4\text{ emu/g}$ for FeSiO₃ and $1.49(5) \cdot 10^4\text{ emu/g}$ for Mg_{0.09}Fe_{0.91}SiO₃ at 40 K;

²⁾ Temperature for maximum susceptibility;

³⁾ Critical field for magnetic transition to a parallel spin alignment $\mu_0 H_c = 5.0(5)\text{ T}$ for FeSiO₃ and $3.5(3)\text{ T}$ for Mg_{0.13}Fe_{0.87}SiO₃.

⁴⁾ T_N determined from ⁵⁷Fe NGR data and magnetic measurements;

⁵⁾ Ca_{0.99}[Fe²⁺_{0.84}Mg_{0.12}Mn_{0.04}]Si₂O₆;

⁶⁾ Ca_{1.0}Fe²⁺_{0.74}Mg_{0.16}Mn_{0.03}Al_{0.03}Fe³⁺_{0.02}Si_{2.0}O₆;

⁷⁾ Ca_{1.0}Fe²⁺_{0.68}Mg_{0.20}Mn_{0.15}Al_{0.05}Fe³⁺_{0.04}Si_{1.92}O₆;

⁸⁾ $\langle \text{Na}_{0.8}\text{Ca}_{0.01}\text{Mn}_{0.01} \rangle \{ \text{Fe}^{3+}_{0.74}\text{Ti}_{0.03}\text{Al}_{0.12}\text{Fe}^{2+}_{0.07} \} [\text{Si}_{1.99}\text{Al}_{0.01}]\text{O}_6$;

⁹⁾ T_{SP} – Spin Peierls transition;

¹⁰⁾ $\{ \text{Na}_{0.65}\text{Ca}_{0.34} \} [\text{Fe}^{3+}_{0.64}\text{Fe}^{2+}_{0.11}\text{Mg}_{0.19}\text{Al}_{0.04}\text{Ti}_{0.01}](\text{Si}_{1.98}\text{Al}_{0.01})\text{O}_6$.

Table 10. Data obtained by ^{57}Fe NGR studies.

Sample	Site	NN ⁽¹⁾	T [K]	$\delta^{(2)}$ [mm/s]	ΔQ [mm/s]	B_{hf} [T]	DH [mm/s]	$\eta^{(2b)}$	$\theta^{(2c)}$	$\phi^{(2d)}$	A [%]	$\mu_0 H$ [T]	$B_i^{(2e)}$ [T]	Refs.
FeSiO_3 (OPx)	M1		4.2	1.31	3.13	7.0	0.44	0.40	49					86W4
	M2			1.26	1.98	31.9	0.44	0.35	85					
	M1		77	1.303	3.11		0.141							
	M2			1.259	1.975		0.140							
FeSiO_3 (OPx)	M1		4.2	1.31 ⁽³⁾	$\pm 3.14^{(4)}$	6.8	0.42	0.59	47					86R1
	M2			1.26 ⁽³⁾	2.24	31.4	0.44	0.29	78					
	M1		46	1.31	3.12		0.29							
	M2			1.26	1.97		0.31							
$\text{Fe}_{0.87}\text{Mg}_{0.13}\text{SiO}_3$ (OPx)	M1		77	1.30	3.11		0.28							86W4
	M2			1.26	1.97		0.28							
	M1		300	1.18	2.50		0.35							
	M2			1.13	1.90		0.35							
	M1		47	1.30	3.05		0.142							
	M2			1.259	1.98		0.151							
	M1		77	1.289	3.09		0.139							
	M2			1.249	2.00		0.147							
$\text{Fe}_{0.40}\text{Mg}_{0.60}\text{SiO}_3$ (OPx)	M1		300	1.178	2.40		0.163							86S1
	M2			1.124	1.90		0.153							
	M1		77	1.36	2.57		0.45				21			
	M2			1.27	2.12		0.34				79			
$\text{Fe}_{0.27}\text{Mg}_{1.65}\text{Al}_{0.03}\text{-Si}_{2.02}\text{O}_6$ (OPx)	M1		300	1.16	2.25		0.34							93V1
	M2			1.14	2.04		0.31							
	M1		80	1.276(5)	3.10(1)		0.27(1)				5			
	M2			1.273(5)	2.15(1)		0.31(1)				95			
$\text{Fe}_{0.10}\text{Mg}_{0.9}\text{SiO}_3$ (OPx)	M1		300	1.078(5)	2.51(1)		0.47(1)				5			92P1
	M2			1.143(5)	2.10(1)		0.29(1)				95			
	M2m		4	1.49(2)	2.1(1)	12.1(7)	1.2	0.1(1)	12(5)	0(10)	100			
	M1		77	1.295(4)	3.08(1)		0.35(1)				20(1)			
	M2			1.270(1)	2.17(1)		0.35(1)				80(1)			
	M1		295	1.179(2)	2.51(1)		0.38(1)				20(1)			
	M2			1.147(2)	2.22(2)		0.38(1)				80(1)			

Table 10 (cont.)

Sample	Site	NN ⁽¹⁾	T [K]	$\delta^{(2)}$ [mm/s]	ΔQ [mm/s]	B_{hf} [T]	DH [mm/s]	η	θ	φ	A [%]	$\mu_0 H$ [T]	B_i [T]	Refs.
FeSiO ₃ (CPx)	M1	3Fe	4.2	1.30(2)	3.03(4)	8.3(5)		0.5(2)			51(5)			01E1
	M2	3Fe		1.24(2)	2.03(4)	32.2(5)		0.4(2)			49(5)			
Fe _{0.91} Mg _{0.09} SiO ₃ (CPx)	M1	3Fe	0.3	1.32(2)	3.08(4)	7.6(5)		0.3(2)			34(5)			01E1
	M1	1Mg, 2Fe		1.32(2)	3.08(4)	11.9(5)		0.3(2)			8(5)			
	M2	3Fe		1.25(2)	1.96(4)	32.8(5)		0.3(2)			28(5)			
	M2	1Mg, 2Fe		1.25(2)	1.96(4)	25.3(5)		0.3(2)			30(5)			
Fe _{0.87} Mg _{0.13} SiO ₃ (CPx)	M1	3Fe	4.2	1.31(2)	2.89(4)	7.8(5)		0.3(2)			35(5)			01E1
	M1	1Mg, 2Fe		1.31(2)	2.89(4)	13.1(5)		0.3(2)			9(5)			
	M2	3Fe		1.28(2)	1.83(4)	31.9(5)		0.2(2)			24(5)			
	M2	1Mg, 2Fe		1.28(2)	1.83(4)	24.1(5)		0.2(2)			26(5)			
Fe _{0.78} Mg _{0.22} SiO ₃ (CPx)	M2	2Mg, 1Fe		1.28(2)	1.83(4)	18.0(5)		0.2(2)			6(5)			
	M1	3Fe	0.3	1.31(2)	3.01(4)	8.4(5)		0.5(2)			27(5)			01E1
	M1	1Mg, 2Fe		1.31(2)	3.01(4)	12.8(5)		0.5(2)			19(5)			
	M1	2Mg, 1Fe		1.31(2)	3.01(4)	14.6(5)		0.5(2)			7(5)			
Fe _{0.61} Mg _{0.39} SiO ₃ (CPx)	M2	3Fe		1.22(2)	2.03(4)	29.9(5)		0.1(2)			16(5)			
	M2	1Mg, 2Fe		1.22(2)	2.03(4)	23.7(5)		0.1(2)			11(5)			
	M2	2Mg, 1Fe		1.22(2)	2.03(4)	19.1(5)		0.1(2)			20(5)			
	M1	3Fe	0.3	1.30(2)	2.91(4)	8.5(5)		0.4(2)			18(5)			01E1
Fe _{0.09} Mg _{0.91} SiO ₃ (CPx)	M1	1Mg, 2Fe		1.30(2)	2.91(4)	9.3(5)		0.4(2)			18(5)			
	M1	2Mg, 1Fe		1.30(2)	2.91(4)	11.7(5)		0.4(2)			4(5)			
	M2	3Fe		1.27(2)	2.04(4)	24.7(5)		0.1(2)			23(5)			
	M2	1Mg, 2Fe		1.27(2)	2.04(4)	19.7(5)		0.1(2)			11(5)			
Fe _{0.09} Mg _{0.91} SiO ₃ (CPx)	M2	2Mg, 1Fe		1.30(2)	2.04(4)	15.2(5)		0.1(2)			26(5)			
	M1	—	0.3	1.30(2)	2.94(4)						29(5)			01E1
	M2	—		1.30(2)	2.04(4)						35(5)			
	M2	—		1.21(2)	2.19(4)	13.6(5)		0.0 ³⁾			36(5)			
Fe _{0.09} Mg _{0.91} SiO ₃ (CPx)	M1	—	4.2	1.30(2)	2.98(4)						23(5)			01E1
	M2	—		1.28(2)	2.19(4)						47(5)			
	M2	—		1.33(2)	1.90(4)	12.5(5)		0.0 ³⁾			30(5)			
	M2	—		1.290	2.550						44.7			94F2
Fe _{0.10} Mg _{0.90} SiO ₃ (perovskite)	Fe ²⁺ 1		77	1.285	1.774		0.530				38.1			
	Fe ²⁺ 2			0.417	1.237		0.638				13.5			
	Fe ³⁺			0.526	2.290		0.390				3.5			
	Fe ⁿ⁺						0.518							

Table 10 (cont.)

Sample	Site	NN ⁽¹⁾	T [K]	$\delta^{(2)}$ [mm/s]	ΔQ [mm/s]	B_{hf} [T]	DH [mm/s]	η	θ	φ	A [%]	$\mu_0 H$	B_i [T]	Refs.
Fe _{0.10} Mg _{0.90} SiO ₃ (perovskite)	Fe ²⁺ 1		298	1.172	2.190		0.430				13.77			94F2
	Fe ²⁺ 2			1.142	1.566		0.542				63.36			
	Fe ³⁺			0.414	0.985		0.402				12.19			
	Fe ⁿ⁺			0.542	1.602		0.593				10.70			
Fe _{0.05} Mg _{0.95} SiO ₃ (perovskite)	Fe ²⁺ 1		181	1.221	2.220		0.510				32.76			94F2
	Fe ²⁺ 2			1.205	1.624		0.458				52.78			
	Fe ³⁺			0.425	1.099		0.399				11.57			
	Fe ⁿ⁺			0.726	1.500		0.485				2.89			
Fe _{0.05} Mg _{0.95} SiO ₃ (perovskite)	Fe ²⁺ 1		298	1.140	2.023		0.542				20.14			94F2
	Fe ²⁺ 2			1.132	1.521		0.455				61.99			
	Fe ³⁺			0.427	0.927		0.396				10.86			
	Fe ⁿ⁺			0.554	1.540		0.564				7.00			
Fe _{0.05} Mg _{0.95} SiO ₃ (perovskite)	Fe ²⁺		80	1.251(15)	2.09(2)						93.4			98M1
	Fe ³⁺			0.405(3)	1.25(5)						3.8			
	Fe ⁿ⁺			0.934(3)	1.53(5)						2.8			
	Fe ²⁺		293	1.137(15)	1.60(2)						84			
CaFeSi ₂ O ₆	Fe ³⁺			0.306(3)	1.04(5)						6.3			85C2
	Fe ⁿ⁺			0.714(3)	1.31(5)						9.8			
	Fe ²⁺ (M1)		4.2	1.21(2)	2.68(3)	18.8(2)	0.42(4)	0.06	74(5)	0	100			
	Fe ²⁺ (M1)		296	1.07(1)	2.26(2)		0.31(2)				100			
Hedenbergite ⁽⁶⁾ (natural)	Fe ²⁺ (M1)		5	1.28(5)	2.8(2)	17.1(6)		0.02(50)	74(22)		100			97B1
	Fe ²⁺ (M1)		77	1.29(1)	2.72(3)		0.29(8)				100			
	Hedenbergite ⁽⁷⁾ (natural)		4.2	1.34	2.64	14...19		0.02	75	0				
	Hedenbergite ⁽⁸⁾		77	1.30	2.70		0.32							
Hedenbergite ⁽⁸⁾			4.2	1.31	2.77	17.6		0.0	73					86S3
			295	1.19	2.24									
			295	1.19	2.24			0.5				4.5	H X=-0.7, H Y=-0.4, H Z=-1.6	
			295	1.19	2.24			0.7				7.5	H X=-2.1, H Y=-1.4, H Z=-3.1	

Table 10 (cont.)

Sample	Site	NN ⁽¹⁾	T [K]	δ^2 [mm/s]	ΔQ [mm/s]	B_{hf} [T]	DH [mm/s]	η	θ	φ	A [%]	$\mu_0 H$	B_i [T]	Refs.
Hedenbergite ⁹⁾			4.2	1.31	2.68	17.4		0.0	74					86S3
			78	1.30	2.72			0.3				7.5	$H\ X=-3.0,$ $H\ Y=-5.6,$ $H\ Z=-2.1$	
			295	1.18	2.20			1.0				7.5	$H\ X=-1.3,$ $H\ Y=-1.9,$ $H\ Z=-1.3$	
Hedenbergite ¹⁰⁾			4.2	1.31(1)	2.57(4)	18.0(2)		0.71(15)	81(3)	39(8)				03E1,
			10	1.31(1)	2.57(4)	17.7(2)		0.78(15)	84(3)	39(8)				03E2
			15	1.32(1)	2.59(4)	17.8(2)		0.74(15)	82(3)	39(8)				
			20	1.32(1)	2.56(4)	17.5(2)		0.78(15)	85(3)	38(8)				
			24	1.32(1)	2.55(4)	16.7(2)		0.78(15)	84(3)	38(8)				
			36	1.311(5)	2.72(1)		0.31(1)							
			80	1.304(5)	2.74(1)		0.27(1)							
			200	1.244(5)	2.50(1)		0.29(1)							
			300	1.179(5)	2.19(1)		0.29(1)							
			521	1.024(5)	1.60(1)		0.26(1)							
			800	0.804(5)	1.11(1)		0.24(1)							
Hedenbergite ¹⁰⁾ (at 6T)			4.2	1.31(1)	2.64(4)	16.8(2)		0.66(15)	75	50		6	$H\ X=-37$	03E1,
			80	1.30(2)	2.75(4)		0.34(2)	0.81(15)					$H\ Y=-21$	03E2
								$V_{\text{zz}}(-)$					$H\ Z=-42$	
Hedenbergite ¹¹⁾			290	1.17(2)	2.25(4)		0.32(2)	0.99(15)					$H\ X=-7$	
								$V_{\text{zz}}(-)$					$H\ Y=-4$	
													$H\ Z=-15$	
			8	1.31(1)	2.62(4)	18.5(2)		0.77(15)	84(3)	38(8)				03E1,
			15	1.32(1)	2.60(4)	18.2(2)		0.77(15)	84(3)	38(8)				03E2
			20	1.32(1)	2.53(4)	17.7(2)		0.78(15)	87(3)	37(8)				
			25	1.31(1)	2.61(4)	16.1(2)		0.81(15)	90(3)	37(8)				
	Fe ²⁺		36	1.304(5)	2.72(1)		0.26(1)				86			
	Fe ³⁺			0.550(5)	0.67(1)		0.29(1)				14			
	Fe ²⁺		80	1.294(5)	2.76(1)		0.24(1)				86			
	Fe ³⁺			0.510(5)	0.66(1)		0.28(1)				14			
	Fe ²⁺		200	1.240(5)	2.52(1)		0.25(1)				88			

Table 10 (cont.)

Sample	Site	NN ⁽¹⁾	T [K]	δ^3 [mm/s]	ΔQ [mm/s]	B_{hf} [T]	DH [mm/s]	η	θ	φ	A [%]	$\mu_0 H$ [T]	B_i [T]	Refs.
Hedenbergite ⁽¹⁾ (cont.)	Fe ³⁺		200	0.500(5)	0.69(1)		0.33(1)				12			
	Fe ²⁺		301	1.180(5)	2.21(1)		0.26(1)				90			
	Fe ³⁺			0.340(5)	0.68(1)		0.22(1)				10			
	Fe ²⁺		500	1.046(5)	1.69(1)		0.26(1)				97			
	Fe ³⁺			0.230(5)	0.91(1)		0.22(1)				3			
Hedenbergite ⁽¹⁾ (at 6T)			4.2	1.31(1)	2.67(4)	17.3(2)		0.64(15)	76	48		6		03E1, 03E2
			83	1.29(2)	2.76(4)		0.33(2)	0.70(15)						$H\parallel X = -33$ $H\parallel Y = -41$ $H\parallel Z = -21$ $H\parallel X = -10$ $H\parallel Y = -11$ $H\parallel Z = -5$
			277	1.17(2)	2.29(4)		0.30(2)	0.80(15)						
								$V_z(+)$						
CaFe ³⁺ AlSiO ₆ (2GPa, 1375°C)	M1(Fe ³⁺)		RT	0.302(6)	0.95(1)		0.50(1)				85(2)			97A1
	T(Fe ³⁺)			0.24(1)	1.51(2)		0.27(1)				15(2)			
	M1(Fe ²⁺)		RT	1.15(1)	1.99(1)						2(2)			83A2
	M1(Fe ³⁺)			0.35(1)	0.99(2)						87(2)			
	T(Fe ³⁺)			0.22(1)	1.58(2)						11(2)			
CaFe _{0.9} Ga _{0.1} SiO ₆ (1 atm, 1200°C)	M1(Fe ³⁺)		RT	0.359(6)	0.82(1)		0.54(1)				65(2)			97A1
	T(Fe ³⁺)			0.327(6)	1.41(1)		0.44(2)				35(2)			
	M1(Fe ²⁺)		RT	1.21(2)	1.89(4)		0.39(9)				2(2)			97A1
	M1(Fe ³⁺)			0.41(2)	0.95(3)		0.65(5)				90(2)			
	T(Fe ³⁺)			0.21(2)	1.76(1)		0.27(2)				8(2)			
CaMg _{0.95} Fe _{0.05} Al _{0.05} - Si _{1.95} O ₆	M1(Fe ²⁺)		RT	1.10(2)	1.75(4)		0.43(1)				13 (3)			97A1
	M1(Fe ³⁺)			0.38(3)	0.90(3)		0.75(3)				77(3)			
	T(Fe ³⁺)			0.21(2)	1.80(1)		0.46(2)				10(3)			
	M1(Fe ²⁺)		4.2	1.30(1)	2.53(2)		0.40(2)				71(2)			03D1
	M2(Fe ²⁺)			1.29(1)	2.15(2)		0.40(2)				24(2)			
Diopside ⁽²⁾ (0.01 Fe apfu)	Fe ³⁺			0.40(5)	0.55 ⁽³⁾		1.04(2)				5(2)			
	M1(Fe ²⁺)		300	1.16(1)	1.87(2)		0.31(2)				68(2)			
	M2(Fe ²⁺)			1.15(1)	2.14(2)		0.31(2)				23(2)			
			300	0.25(5)	0.55 ⁽³⁾		0.52(2)				10(2)			

Table 10 (cont.)

Sample	Site	NN ⁽¹⁾	T [K]	$\delta^{(2)}$ [mm/s]	ΔQ [mm/s]	B_{hf} [T]	DH [mm/s]	η	θ	φ	A [%]	$\mu_0 H$	B_i [T]	Refs.
Diopside ⁽¹²⁾ (0.01 Fe apfu) (cont.)	M1(Fe ²⁺)		700	0.87(1)	1.08(2)		0.33(2)				63(2)			
	M2(Fe ²⁺)			0.87(1)	1.76(2)		0.33(2)				21(2)			
Diopside ⁽¹⁴⁾ (0.30 Fe apfu)	Fe ³⁺			0.25(5)	0.55 ⁽¹³⁾		0.67(2)				16(2)			03D1
	M1(Fe ²⁺)		80	1.29(1)	2.63(2)		0.37(2)				69(2)			
	M2(Fe ²⁺)			1.26(1)	2.96(2)		0.37(2)				11(2)			
	Fe ³⁺			0.53(5)	0.55 ⁽¹³⁾		0.41(2)				20(2)			
	M1(Fe ²⁺)		300	1.17(1)	1.96(2)		0.35(2)				69(2)			
	M2(Fe ²⁺)			1.09(1)	2.50(2)		0.35(2)				10(2)			
Diopside ⁽¹⁴⁾ (at 6T)	Fe ³⁺			0.43(5)	0.55 ⁽¹³⁾		0.51(2)				21(2)			03D1
	M1(Fe ²⁺)		800	0.77(1)	0.97(2)		0.32(2)				71(2)			
	M2(Fe ²⁺)			0.69(1)	1.27(2)		0.32(2)				11(2)			
	Fe ³⁺			0.11(5)	0.55 ⁽¹³⁾		0.55				18(2)			
	M1(Fe ²⁺)		80				0.37	0.86(5)			70(3)	6	$H \parallel X = -3.4(5)^{(15)}$ $H \parallel Y = -1.2(5)$ $H \parallel Z = -3.0(5)$	
	M2(Fe ²⁺)						0.35	0.97(5)			10(3)		$H \parallel X = -3.4(5)$ $H \parallel Y = -3.5(5)$ $H \parallel Z = -3.6(5)$	
	Fe ³⁺						0.67	0.96(5)			20(3)		$H \parallel X = -5.5(5)$ $H \parallel Y = -5.5(5)$ $H \parallel Z = -5.5(5)$	

Table 10 (cont.)

Sample	Site	NN ⁽¹⁾	T [K]	$\delta^{(2)}$ [mm/s]	ΔQ [mm/s]	B_{hf} [T]	DH [mm/s]	η	θ	φ	A [%]	$\mu_0 H$	B_i [T]	Refs.
Rhodonite ⁽⁶⁾	M4(Fe ²⁺)		295	1.076	1.27		0.35(1)				28			75D1
	M5(Fe ²⁺)			1.20	1.93		0.37(1)				12.6			
	M1(Fe ²⁺)			1.208	2.29		0.24(1)				} 59.4			
	M2(Fe ²⁺)			1.21	2.51		0.24(1)							
	M3(Fe ²⁺)			1.21	2.70		0.24(1)							
NaFeSi ₂ O ₆ (aegirine)			5	0.50(1)	0.01(1)	46.1(5)	0.92(1)							88B1
NaFeSi ₂ O ₆			295	0.39(1)	0.33(1)		0.30(1)							89B1
(synthetic aegirine)			1.5	0.52(3)	0.20(8)	51.9(5)								
Na _{1.06} Ca _{0.06} Mg _{0.04} - Fe _{1.01} Al _{0.06} Si _{1.91} O ₆ (aegirine)	Fe ³⁺		296	0.41(1)	0.29(2)						95			98D1
	Fe ²⁺		4.2	0.48		46.7					5			
				1.27	3.10	22.0					85(1)			
	M1(Fe ³⁺)		30	0.504(5)	0.34(1)						8(1)			
	M1(Fe ²⁺)			1.28(2)	3.07(3)						3(1)			
	M1(Fe ²⁺)			1.30(2)	2.26(3)						4(1)			
	T(Fe ³⁺)			0.32(2)	0.18(3)						87(1)			
	M1(Fe ³⁺)		298	0.384(5)	0.34(1)						5(1)			
	M1(Fe ²⁺)			1.14(2)	2.77(3)						5(1)			
	M1(Fe ²⁺)			1.08(2)	1.87(3)						3(1)			
	T(Fe ³⁺)			0.17(2)	0.17(3)						52			88D1
Ae _{0.81} Di _{0.19}	M1	3Fe ³⁺	2	0.36(2) ^(2a)	0.18(2)	46.2(2)	0.40(2)				36			
	M1	1Fe ³⁺		0.35(2) ^(2a)	0.11(2)	44.5(3)	0.40(2)				11			
	M1	1Fe ³⁺		0.37(3) ^(2a)	0.02(2)	42.2(3)	0.42(3)				100			
			80	0.38(1) ^(2a)	0.35(2)		0.30(2)				100			
Aegirine ⁽⁷⁾			300	0.28(1) ^(2a)	0.34(2)		0.27(2)				87			97B1
	M1	Fe ³⁺	77	0.473(4)	0.34(7)		0.30(1)				8			
	M1	Fe ²⁺		1.31(5)	2.1(2)		0.376(4)				5			
	M1	Fe ²⁺		1.25(8)	3.1(2)		0.258(6)				38.5(3.8)			78A1
Omphacite ⁽⁸⁾	Fe ²⁺		295	1.19(5)	2.96(5)		0.31(3)				22.1(2.2)			
	Fe ²⁺			1.16(5)	2.31(5)		0.31(3)				21.3(2.1)			
	Fe ²⁺			1.15(5)	1.94(5)		0.31(3)				18.1(1.8)			
	Fe ³⁺			0.43(5)	0.56(5)		0.31(3)							

Table 10 (cont.)

Sample	Site	NN ⁽¹⁾	T [K]	$\delta^{(2)}$ [mm/s]	ΔQ [mm/s]	B_{hf} [T]	DH [mm/s]	η	θ	ϕ	A [%]	$\mu_0 H$	B_i [T]	Refs.
Omphacite ¹⁹⁾	Fe ²⁺		295	1.17(5)	2.84(5)		0.42(3)				27.8(2.8)			78A1
	Fe ²⁺			1.15(5)	2.13(5)		0.42(3)				27.8(2.8)			
	Fe ²⁺			1.19(5)	1.77(5)		0.42(3)				7.7(7)			
	Fe ³⁺			0.41(5)	0.43(5)		0.43(3)				36.7(3.7)			
Omphacite ²⁰⁾	Fe ²⁺		295	1.19(5)	2.55(5)		0.47				25.2			78A1
	Fe ²⁺			1.20(5)	1.95(5)		0.35				53.5			
	Fe ³⁺			0.52(5)	0.41(5)		0.49				21.3			
	Fe ³⁺			0.43(2)	0.46(2)		0.36(3)				23(2)			
Hd _{0.80} Ae _{0.20}	Fe ²⁺		RT	1.19(2)	2.13(2)		0.35(1)				70(2)			82D3
	Fe ²⁺			1.19(2)	2.69(2)		0.35(1)				7(2)			
	Fe ³⁺			0.41(2)	0.35(1)		0.31(1)				79(2)			
	Fe ²⁺			1.14(2)	1.83(3)		0.36(2)				3.4(2.0)			
Hd _{0.20} Ae _{0.80}	Fe ²⁺		RT	1.13(2)	2.18(2)		0.36(2)				5.9(2.0)			82D3
	Fe ²⁺			1.15(2)	2.77(2)		0.36(2)				11.7(2.0)			
	Fe ³⁺			0.40(2)	0.43(3)		0.37(2)				34(2)			
	Fe ²⁺			1.17(2)	2.07(2)		0.39(2)				47(2)			
Hd _{0.50} Ae _{0.27} Ko _{0.24}	Fe ³⁺		RT	1.17(2)	2.70(3)		0.39(2)				19(2)			82D3
	Fe ³⁺			0.40(2)	0.35(2)		0.32(1)				64(1)			
	Fe ²⁺			1.15(2)	1.77(4)		0.36(2)				12(2)			
	Fe ²⁺			1.15(2)	2.80(3)		0.36(2)				24(2)			
LiFeSi ₂ O ₆ (single crystal)	Fe ³⁺ (M1)		10	0.474(6)	0.57(9)	49.81(4)	0.35(1)		125.4(5)	47.4(8)				98L1
	Fe ³⁺ (M1)		15	0.477(6)	0.5(x ²) ¹⁾	44.78(4)	0.45(1)		125.9(7)	40(1)				
	Fe ³⁺ (M1)		18	0.48(1)	0.5(x ²) ¹⁾	36.97(7)	0.67(2)		125(2)	37(2)				
	Fe ³⁺ (M1)		25	0.5(1)	0.2(x ²) ¹⁾	—	0.3(3)			44(x ²) ¹⁾				
LiFeSi ₂ O ₆ (powder)	Fe ³⁺ (M1)		295	0.36(4)	0.3(x ²) ¹⁾	—	0.31(9)			41(20)				98L1
	Fe ³⁺ (M1)		11	0.474(3)	0.55(7)	53.21(2)	0.394(6)		126.3(5)					
LiFeSi ₂ O ₆ (powder)	Fe ³⁺ (M1)		5	0.49(1)	0.01(1)	54.0(5)	0.40(1)				100			88B1
			295	0.39(1)	0.31(1)		0.28(1)				100			

- 1) Number of next-neighbour atoms;
- 2) Relative to α -Fe if no other notations were used;
- 2a) ^{57}Co source in Rh matrix. The δ values relative to α -Fe is 0.18(1) mm/s.
- 2b) Asymmetry parameter;
- 2c) Angle between EFG principal axis and direction of hyperfine field;
- 2d) Zenithal angle between EFG and the direction of hyperfine field;
- 2e) Components of the anisotropic reduction field for external field $\mu_0 H$.
- 3) δ values constrained determined at 46 K;
- 4) Two possibilities of sign for V_{zz} at M1 site;
- 5) Fixed value;
- 6) $\text{Ca}_{0.99}\text{Fe}^{2+}_{0.84}\text{Mg}_{0.12}\text{Mn}_{0.04}\text{Si}_2\text{O}_6$;
- 7) $\text{Ca}_{0.96}\text{Fe}_{0.82}\text{Mg}_{0.19}\text{Mn}_{0.02}\text{Si}_2\text{O}_6$;
- 8) $\text{Ca}_{0.97}\text{Mn}_{0.17}\text{Fe}_{0.79}\text{Mg}_{0.06}\text{Al}_{0.01}\text{Si}_{1.99}\text{O}_{6.01}$;
- 9) $\text{Ca}_{0.96}\text{Mn}_{0.02}\text{Fe}_{0.66}\text{Mg}_{0.31}\text{Al}_{0.06}\text{Si}_{1.99}\text{O}_{6.02}$;
- 10) $\text{Ca}_{1.0}\text{Fe}^{2+}_{0.74}\text{Mg}_{0.16}\text{Mn}_{0.03}\text{Al}_{0.03}\text{Fe}^{3+}_{0.02}\text{Si}_{2.00}\text{O}_6$;
- 11) $\text{Ca}_{1.0}\text{Fe}^{2+}_{0.68}\text{Mg}_{0.20}\text{Mn}_{0.15}\text{Al}_{0.05}\text{Fe}^{3+}_{0.04}\text{Si}_{1.92}\text{O}_6$;
- 12) Natural sample, Jaipur, India;
- 13) Fixed value;
- 14) Natural sample, Zillertal, Tyrol, Austria;
- 15) Field reduction;
- 16) $\text{Ca}_{0.204}\text{Fe}_{0.22}\text{Mn}_{0.566}\text{Mg}_{0.01}\text{SiO}_3$;
- 17) $(\text{Na}_{0.65}\text{Ca}_{0.34})(\text{Fe}^{3+}_{0.64}\text{Fe}^{2+}_{0.11}\text{Mg}_{0.19}\text{Al}_{0.04}\text{Ti}_{0.01})(\text{Si}_{1.98}\text{Al}_{0.01})\text{O}_6$;
- 18) $(\text{Na}_{0.54}\text{Ca}_{0.45})(\text{Fe}^{3+}_{0.14}\text{Fe}^{2+}_{0.33}\text{Mg}_{0.05}\text{Al}_{0.44}\text{Ti}_{0.05})(\text{Si}_{1.95}\text{Al}_{0.05})\text{O}_6$;
- 19) $(\text{Na}_{0.48}\text{Ca}_{0.52})(\text{Fe}^{3+}_{0.14}\text{Fe}^{2+}_{0.08}\text{Mg}_{0.39}\text{Al}_{0.40}\text{Ti}_{0.01})(\text{Si}_{1.92}\text{Al}_{0.08})\text{O}_6$;
- 20) $(\text{Na}_{0.19}\text{Ca}_{0.82})(\text{Fe}^{3+}_{0.06}\text{Fe}^{2+}_{0.08}\text{Mg}_{0.72}\text{Al}_{0.14})(\text{Si}_{1.97}\text{Al}_{0.03})\text{O}_6$;
- 21) When error exceeds the parameter value an "x" is marked instead;
- 22) $(\text{Ca}_{0.98}\text{Na}_{0.03})(\text{Mg}_{0.68}\text{Fe}^{2+}_{0.07}\text{Fe}^{3+}_{0.03}\text{Al}_{0.16}\text{Ti}_{0.04})(\text{Si}_{1.77}\text{Al}_{0.23})\text{O}_6$;
- 23) $(\text{Na}_{0.86}\text{Ca}_{0.09})(\text{Fe}^{2+}_{0.93}\text{Fe}^{3+}_{0.03}\text{Ti}_{0.03}\text{Mn}_{0.03}\text{Si}_{2.00}\text{O}_6$ including $V_{0.002}$, $\text{Mg}_{0.006}$, $\text{Al}_{0.007}$;
- 24) $(\text{Na}_{0.99}\text{Ca}_{0.01})(\text{Fe}^{2+}_{1.00}\text{Fe}^{3+}_{1.00}\text{Si}_{2.00}\text{O}_6$ including $V_{0.002}$.

Table 11. Data obtained from NMR spectroscopy: Isotropic chemical shift, δ_i , the principal values of the chemical shielding tensor, δ_{11} , δ_{22} , δ_{33} , the shielding anisotropy $\Delta\delta = \delta_{33} - 1/2(\delta_{11} + \delta_{22})$ and the asymmetry parameter $\eta = (\delta_{22} - \delta_{11})(\delta_{33} - \delta_i)^{-1}$ [83S1].

Silicate	Site	Chemical shift [ppm] ¹⁾					ΔQ [MHz]	η	DH [ppm]	Relative intensity A [%]	Refs.
		δ_i	δ_{11}	δ_{22}	δ_{33}	$\Delta\delta$					
²⁹Si											
MgSiO ₃ (synthetic)		−81	−40	−70	−132	−77		0.59			83S1
Enstatite		−83	−41	−76	−133	−74		0.70			83S1
CaSiO ₃ (wollastonite)		−89	−24	−85	−158	−104		0.88			83S1
CaMgSi ₂ O ₆ (synthetic)		−84	−31	−73	−148	−96		0.66			83S1
CaMgSi ₂ O ₆ (crystal)		−84.7							≤ 1		86K3
CaAl ₂ SiO ₆		− 79.0							6.0		86K3
		− 88.1									
Diopside	Si(0Al)[0Al]+ Si(1Al)[1Al]	−84.4							45 ²⁾	100	02F1
Di _{0.95} CaTs _{0.05}	Si(1Al)[0Al]+ Si(2Al)[1Al]	−80.7							71 ²⁾	2	02F1
	Si(0Al)[0Al]+ Si(1Al)[1Al]	−84.5							59 ²⁾	95	
Di _{0.75} CaTs _{0.25}	Si(0Al)[1Al]	−88.7							79 ²⁾	3	
	Si(2Al)[0Al]	−78.1							71 ²⁾	2	02F1
	Si(1Al)[0Al]+ Si(2Al)[1Al]	−81.0							95 ²⁾	21	
	Si(0Al)[0Al]+ Si(1Al)[1Al]	−84.6							106 ²⁾	67	
Di _{0.50} CaTs _{0.50}	Si(0Al)[1Al]	−88.8							111 ²⁾	10	
	Si(2Al)[0Al]	−78.3							86 ²⁾	6	02F1
	Si(1Al)[0Al]+ Si(2Al)[1Al]	−81.3							117 ²⁾	37	
	Si(0Al)[0Al]+ Si(1Al)[1Al]	−85.0							143 ²⁾	46	
Di _{0.25} CaTs _{0.75}	Si(0Al)[1Al]	−89.0							137 ²⁾	11	
	Si(2Al)[0Al]	−78.3							70 ²⁾	11	02F1
	Si(1Al)[0Al]+ Si(2Al)[1Al]	−81.6							115 ²⁾	41	
	Si(0Al)[0Al]+ Si(1Al)[1Al]	−85.2							147 ²⁾	41	
CaTs _{1.00}	Si(0Al)[1Al]	−89.2							120 ²⁾	7	
	Si(1Al)[0Al]+ Si(2Al)[1Al]	−81.9							94 ²⁾	70	82F1
	Si(0Al)[0Al]+ Si(1Al)[1Al]	−85.6							154 ²⁾	25	
	Si(0Al)[1Al]	−89.7							81 ²⁾	5	
Diopside (glass)		−81.1							17.1		86K3

Table 11 (cont.)

Silicate	Site	Chemical shift [ppm] ¹⁾					ΔQ [MHz]	η	DH [ppm]	Relative intensity A [%]	Refs.
		δ_1	δ_{11}	δ_{22}	δ_{33}	$\Delta\delta$					
$\text{Di}_{0.90}\text{CaTs}_{0.10}$ (glass)		−81.0							13.9		86K3
$\text{Di}_{0.80}\text{CaTs}_{0.20}$ (glass)		−81.1							14.7		86K3
$\text{Di}_{0.60}\text{CaTs}_{0.40}$ (glass)		−81.1							12.7		86K3
$\text{Di}_{0.40}\text{CaTs}_{0.60}$ (glass)		−81.4							11.2		86K3
$\text{Di}_{0.20}\text{CaTs}_{0.80}$ (glass)		−83							11.1		86K3
$\text{CaAl}_2\text{SiO}_6$ (glass)		−83.5							11.2		86K3
CaSiO_3		−89	−24	−85	−158	−104		0.88			83S1
CaSiO_3	in 1 : 1 : 1 ratio	−87.7									90S2
		−88.9									
		−89.3									
SrSiO_3 (synthetic)		−85	−30	−71	−154	−104		0.59			83S1
BaSiO_3 (synthetic)		−80	−29	−71	−140	−90		0.70			83S1
Na_2SiO_3		−76.8									93X1
$\text{Na}_2\text{BaSi}_2\text{O}_6$		−77.8									93X1
		−75.2									
$\text{NaAlSi}_2\text{O}_6$ (jadeite) natural		−91.8									93X1
$\text{LiAlSi}_2\text{O}_6$ (natural)		−92	−53	−81	−142	−75		0.56			83S1
CdSiO_3		−83.7									00C4
		−79.9									
$\text{Cd}_7[\text{Ga}_6\text{Si}]\text{O}_{21}$		−74.1									00C4
		−76.2									
		−79.4									
²⁷Al											
$\text{CaAl}_2\text{SiO}_6$ (crystal)		60.5									86K3
CaTs (glass)		64									86K3
$\text{Di}_{0.20}\text{CaTs}_{0.80}$ (glass)		64									86K3
$\text{Di}_{0.40}\text{CaTs}_{0.60}$ (glass)		61									86K3
$\text{Di}_{0.60}\text{CaTs}_{0.40}$ (glass)		62									86K3
$\text{Di}_{0.80}\text{CaTs}_{0.20}$ (glass)		59									86K3
$\text{Di}_{0.90}\text{CaTs}_{0.10}$ (glass)		56									86K3
²³Na											
Na_2SiO_3		23(3) ⁴⁾									93X1
$\text{NaAlSi}_2\text{O}_6$		11(1)					3.30(10)	0.25(5)			93X1
$\text{Na}_2\text{BaSi}_2\text{O}_6$		Na1- 25(1)					2.10(10)	0.75(5)	1.0		93X1
		Na2- 5.4(1.0)					2.96(10)	0.10(5)	1.5		93X1

Table 11 (cont.)²⁵Mg

CaMgSi ₂ O ₆ ⁵⁾	8.0(5)	0.75(10)	18.0(5)	00K1
--	--------	----------	---------	------

- 1) δ for ²⁹Si relative to TMS; for ²⁷Al relative to 1M AlCl₃ solution; for ²³Na relative to dilute aqueous NaCl;
 2) in Hz; ³⁾ Two peaks of equal intensity; ⁴⁾ Probably contains multiple Na sites, average value estimated;
 5) Relative to 1M aqueous Mg(NO₃)₂.

Table 12. Debye temperatures and enthalpies of ordering.

a) Debye temperature.

Samples	Θ_D [K]				Refs.
	Thermal expansion	Elastic constant	Heat capacity	⁵⁷ Fe NGR data ¹⁾ (lattice temperature)	
MgSiO ₃ (OPx)	812	729...753			94Y1
FeSiO ₃ (OPx)	562	539...581			94Y1
Fe _{0.05} Mg _{1.95} Al _{0.05} Si _{1.96} O ₆				380(20) (M2) 360(20) (M1)	93V1
Fe _{0.27} Mg _{1.65} Al _{0.03} Si _{2.02} O ₆				330 (M2) 310 (M1)	
Fe _{0.2} Mg _{0.8} SiO ₃ (OPx)	775	700...724			94Y1
Fe _{0.4} Mg _{0.6} SiO ₃ (OPx)	721				94Y1
Fe _{0.5} Mg _{0.5} SiO ₃ (OPx)	686	654			94Y1
Fe _{0.75} Mg _{0.25} SiO ₃ (OPx)	641				94Y1
Fe _{0.83} Mg _{0.17} SiO ₃ (OPx)	618				94Y1
MgSiO ₃ (perovskite)			980(15) 1030(20)		93A1
Fe _{0.05} Mg _{0.95} SiO ₃ (perovskite)				365(52) (Fe ²⁺) 476(90) (Fe ³⁺)	98M1
Fe _{0.05} Mg _{0.95} SiO ₃ (perovskite)				392(15) (Fe ²⁺) 1441(336) (Fe ³⁺)	94F2
Hedenbergite ^{10*)}				330(20) (<i>T</i> < 600 K) 440(10) (<i>T</i> > 600 K)	03E1
Hedenbergite ^{11*)}				370(20) (<i>T</i> < 600 K) 490(20) (<i>T</i> > 600 K)	03E1
CaAl ₂ SiO ₆			820(50)		84H1
NaTiSi ₂ O ₆			450		02I1
LiVSi ₂ O ₆			532		04V1
NaVSi ₂ O ₆			482		04V1

* Compositions given in Table 10; ¹⁾ See also [91D1]

b) Enthalpies of Mg-Fe ordering in orthopyroxenes.

Reference	82G1	83C1	88A2	89S1	92S3	94Y2	96G1	97K2	00C1
ΔH_{exch}^0 [kJ mol ⁻¹]	12.986	31.49	10.005	7.892	11.773	7.751	22.778	17.5(7)	18.0(4)

Table 13. Dielectric constants.

Silicate	ϵ'_a	$\tan \delta$	ϵ'_b	$\tan \delta$	ϵ'_c	$\tan \delta$	$\langle \epsilon' \rangle$	ν [MHz]	Refs.
LiAlSi ₂ O ₆	8.142(4)	0.0007	8.463(20)	0.0002				1	92S1
(α -spodumene)	$\epsilon'_{11} = 7.70(5)$		$\epsilon'_{22} = 8.463(20)$		$\epsilon'_{33} = 11.12(5)$		8.96	1	92S1
	8.05	0.001	7.82	0.0004	9.31	0.003	8.39	1	72W1
	8.30	(undefined orientation)						1	81O2
	7.8	(undefined orientation) (natural)						1	81O2
	7.25	0.0002 (powder)					7.25	300	88C2
	8.45	(powder)					8.45	0.5	53T1
LiAlSi ₂ O ₆	6.4	0.004					6.4	1	63L1
(β -spodumene)	6.3...6.5						6.4	1	81K1
	5.7...5.9	0.012					5.8	$9.37 \cdot 10^3$	72M2
	5.65						5.65		88O3
LiAlSi ₂ O ₆ (amorphous)	8.07	0.047					8.07	1	92S1
CaMgSi ₂ O ₆	8.741(20)	0.0016	7.31(10)	0.0007	7.664(60)	0.0019		1	92S1
(crystalline)	$\epsilon'_{11} = 9.69$		$\epsilon'_{22} = 7.31$		$\epsilon'_{33} = 7.29$		8.10	1	92S1
	7.90							0.5	53T1
	8.60	(undefined orientation)						1	81O2
	7.9	0.0256 (undefined orientation)						1	81O2
CaMgSi ₂ O ₆ (amorphous)	8.893	0.0021					8.893	1	92S1

Table 14. Luminescence properties for the polymorph: CaSiO₃ and SrSiO₃ doped crystals.

Phase	$\lambda_{\max}^a)$ [nm]	$\lambda/2^b)$ [nm]	$I^c)$ [%]	$T_{50}^d)$ [K]	Refs.
α -CaSiO ₃ : Pb ²⁺ (5 at %)	light-blue	broad	6 ^{e)}		82M2
β -CaSiO ₃ : Pb ²⁺ (5 at %)	346	45	32 ^{e)}	430	
δ -CaSiO ₃ : Pb ²⁺ (5 at %)	341	37	26 ^{e)}	440	
α -SrSiO ₃ : Pb ²⁺ (5 at %)	light-blue	broad	weak		
δ -SrSiO ₃ : Pb ²⁺ (5 at %)	337	37	11 ^{e)}	330	
δ' -SrSiO ₃ : Pb ²⁺ (5 at %)	331	37	6 ^{e)}	320	
β -Ca _{1-x} Pb _x SiO ₃					
x = 0.01	336	33	21 ^{e)}		
x = 0.03	337	34	31 ^{e)}		
x = 0.05	346	45	32 ^{e)}		
x = 0.07	348, 355	54	29 ^{e)}		

Table 14. (cont.)

Phase	$\lambda_{\max}^{\text{a)}}$ [nm]	$\lambda/2^{\text{b)}}$ [nm]	$I^{\text{c)}}$ [%]	$T_{50}^{\text{d)}}$ [K]	Refs.
$\beta\text{-Ca}_{1-x}\text{Pb}_x\text{SiO}_3$ (cont.)					82M2
$x = 0.10$	349, 356	54	24 ^{e)}		
$x = 0.20$	350, 359	55	16 ^{e)}		
$\alpha\text{-CaSiO}_3$: Eu^{2+} (1 at %)	507	70...80	$\cong 1$	420	83A1
$\delta\text{-CaSiO}_3$: Eu^{2+} (1 at %) (4.5 GPa, 1000°C)	472	83	22	420	
$\alpha\text{-SrSiO}_3$: Eu^{2+} (1 at %)	498	75...80	<1	380	
$\delta\text{-SrSiO}_3$: Eu^{2+} (1 at %) (3.5 GPa, 1000°C)	503	63	6	300	
$\delta'\text{-SrSiO}_3$: Eu^{2+} (1 at %) (6 GPa, 1000°C)	466	58	37	360	
SrSiO_3 : $\text{Eu}^{3+}, \text{Bi}^{3+}$ (sol-gel)	16260 ^{f)}	428 ^{f)}	82		93L2
SrSiO_3 : $\text{Eu}^{3+}, \text{Bi}^{3+}$ (sintering at atmospheric pressure)	16260 ^{f)}	428 ^{f)}	40		
SrSiO_3 : $\text{Eu}^{3+}, \text{Bi}^{3+}$ (high pressure, high temperature)	15504 ^{f)}	2420 ^{f)}	10		

a) λ_{\max} : peak position of the emission band at 300 K;b) $\lambda/2$: half-width of emission band;c) I : relative emission intensity;d) T_{50} : quenched temperature at which the intensity of luminescence is half of that at 77 K;e) Excitation at 254 nm and 300 K; ^{f)} in cm^{-1} .**Table 15.** Refractive indices.

Silicate	n_α	n_β	n_γ	$2 V^0$		Refs.
				Exp.	Calc.	
Kanoite ¹⁾ , $\text{P2}_1/\text{c}$ at 25°C	1.699(1)	1.702(1)	1.724(5)	54.5	39.7	97A2
Kanoite ²⁾ , $\text{P2}_1/\text{c}$	1.715(2)	1.717(2)	1.728(2)	40...42		biaxial, positive 77K1
Pyroxferroite ($\text{Fe}_{0.84}\text{Ca}_{0.13}\text{Mg}_{0.02}\text{-Mn}_{0.02}\text{SiO}_3$)	1.748	1.750	1.768	34...40		biaxial, positive 70C2
Donpeacorite ³⁾	1.677(2)	1.684(2)	1.692(2)	88		biaxial, negative 84P2
Peteddunnite ⁴⁾	1.68(1)	1.69(1)	1.70(1)	80(5)		87E1
Esseneite ⁵⁾	1.795(5)	1.815(5)	1.825(5)	77(5)		biaxial, negative 87C3
$\text{CaAl}_2\text{SiO}_6$	1.597(2)(ω)		1.603(2)(ϵ)			uniaxial, positive 73K1
Diopside ⁶⁾	1.747(5)	1.750(5)	1.762(5)			73D2
Diopside ⁷⁾	1.690(2)	1.700(2)	1.712(2)			02D1
$\text{NaCrSi}_2\text{O}_6$	1.740(1)	1.756(1)	1.762(1)	60...70		biaxial, negative 65F1
Natalyite ⁸⁾	1.741(2)	1.762(3)	1.762(3)	8-12		biaxial, negative 85R1, 87H1
Joesmithite ⁹⁾	1.747(5)	1.765(5)	1.78(1)			biaxial, positive 68M2, 68M3
Aërintine ¹⁰⁾	1.510(5)	1.560(5)	1.580(5)		63	biaxial, negative 88A4

Table 15 (cont.)

Silicate	n_α	n_β	n_γ	$2 \nu^0$		Refs.
				Exp.	Calc.	
Vinogradovite ¹¹⁾	1.745	1.770	1.775	41		biaxial, negative 56S2
Paravinogradovite ¹²⁾	1.707(2)	1.741(2)	1.755(2)	64(1)	64	biaxial, negative 03K1
Nchwaningite ¹³⁾	1.681(2)	1.688(2)	1.690(2)	54.4(4)		biaxial, negative 95N1

1) $\text{MnMgSi}_2\text{O}_6$;2) $\text{Mn}_{1.040}\text{Mg}_{0.885}\text{Fe}^{2+}_{0.087}\text{Fe}^{3+}_{0.012}\text{Ca}_{0.024}\text{Si}_{1.993}\text{O}_6$;3) $\text{Mg}_{1.41}\text{Mn}_{0.56}\text{Ca}_{0.03}\text{Si}_2\text{O}_6$;4) $(\text{Ca}_{0.92}\text{Na}_{0.06}\text{Mn}_{0.02})(\text{Zn}_{0.37}\text{Mn}_{0.18}\text{Fe}^{2+}_{0.19}\text{Fe}^{3+}_{0.12}\text{Mg}_{0.14})(\text{Si}_{1.94}\text{Al}_{0.06})\text{O}_6$;5) $(\text{Ca}_{1.01}\text{Na}_{0.01})(\text{Fe}^{3+}_{0.72}\text{Mg}_{0.16}\text{Al}_{0.04}\text{Ti}_{0.03}\text{Fe}^{2+}_{0.02})(\text{Si}_{1.19}\text{Al}_{0.81})\text{O}_6$;6) $\text{Ca}_{1.0}\text{Mg}_{0.3}\text{Ti}_{0.48}\text{Al}_{0.13}(\text{Al}_{0.74}\text{Si}_{1.26})\text{O}_6$;7) $(\text{Ca}_{0.98}\text{Na}_{0.03})(\text{Mg}_{0.68}\text{Fe}^{2+}_{0.07}\text{Fe}^{3+}_{0.03}\text{Al}_{0.16}\text{Ti}_{0.04})(\text{Si}_{1.77}\text{Al}_{0.23})\text{O}_6$;8) $(\text{Na}_{0.92}\text{Ca}_{0.07})(\text{V}_{0.54}\text{Cr}_{0.36}\text{Mg}_{0.07}\text{Al}_{0.03})\text{Si}_{1.99}\text{O}_6$;9) $(\text{Pb}_{0.6}\text{Ca}_{0.6}\text{Ba}_{0.1}\text{Mn}_{0.8})\text{Ca}_{0.4}\text{Fe}^{3+}_{2.0}(\text{Mg}_{6.3}\text{Fe}^{3+}_{1.4}\text{Fe}^{2+}_{0.8}\text{Al}_{0.3})(\text{Si}_{13.8}\text{Be}_{0.1})(\text{OH})_{14.9}\text{O}_{39.7}$;10) $(\text{Ca}_{4.04}\text{Na}_{0.16}\text{K}_{0.02})(\text{Fe}^{2+}_{0.91}\text{Mn}_{0.03}\text{Mg}_{1.47})(\text{Al}_{6.36}\text{Fe}^{3+}_{1.72})(\text{Si}_{11.59}\text{P}_{0.19})\text{O}_{36.21}(\text{OH})_{12.11}(\text{CO}_2)_{0.99} \cdot 12.11\text{H}_2\text{O}$;11) Composition: SiO_2 -40.70, TiO_2 -33.60; Al_2O_3 -6.20, MgO -0.36, CaO -1.00, Na_2O -12.00, K_2O -1.8, H_2O -4.80;12) $(\text{Na}_{2.293}\text{K}_{0.169})(\text{Ti}_{3.386}\text{Fe}_{0.471}\text{Nb}_{0.034}\text{Mg}_{0.029})(\text{Si}_{6.626}\text{Al}_{1.098}\text{Be}_{0.276})\text{O}_{22}(\text{OH})_4(\text{H}_2\text{O})_{1.12}$;13) $\text{Mn}^{2+}_2\text{SiO}_3(\text{OH})_2 \cdot \text{H}_2\text{O}$.