

DEPOSIT ITEMS

(Deposit figures at bottom.)

Table 1. Chemical compositions of wadsleyite single crystals (run H4181)

Crystal	Number	Si [*]	Fe ^{3+*}	Mg [*]	Fe ^{2+*}	Ni [*]	Fe/(Mg + Fe)
of analyses							
1	20	1.001(2)	0.022(6)	1.784(5)	0.173(7)	0.007(1)	0.099(2)
2	20	1.000(2)	0.022(6)	1.787(3)	0.172(6)	0.007(1)	0.098(1)
3	20	1.001(3)	0.022(6)	1.785(6)	0.174(7)	0.007(1)	0.099(2)
4	20	1.002(2)	0.022(6)	1.783(4)	0.173(7)	0.007(1)	0.099(2)
Average		1.001(3)	0.022(6)	1.785(4)	0.173(7)	0.007(1)	0.099(2)

Notes: Numbers in parentheses are one standard deviation on the last digit. The compositions were determined by a combination of electron-microprobe analysis and Mössbauer spectroscopy.

*: Cations per 4 oxygen atoms.

Table 2. Hyperfine parameters determined from room-temperature Mössbauer spectra

Orientation [*]	Doublet assignment	Center shift (mm/s)	Quadrupole splitting (mm/s)	FWHM [#] (mm/s)	Relative area (%)
1	^{VI} Fe ²⁺	1.08(1)	2.61(1)	0.61(2)	89(4)
	^{VI} Fe ³⁺	0.53(4)	0.80(8)	0.41(14)	7(3)
	^{IV} Fe ³⁺	0.06(3)	1.00(5)	0.25(13)	4(3)
	Σ Fe ³⁺	-	-	-	11(4)
2	^{VI} Fe ²⁺	1.06(1)	2.62(2)	0.60(3)	85(5)
	^{VI} Fe ³⁺	0.53(5)	0.95(10)	0.30(16)	6(3)
	^{IV} Fe ³⁺	0.01(4)	0.91(9)	0.36(18)	9(5)
	Σ Fe ³⁺	-	-	-	15(5)
3	^{VI} Fe ²⁺	1.06(1)	2.63(1)	0.57(1)	87(3)
	^{VI} Fe ³⁺	0.51(4)	0.77(8)	0.48(13)	10(3)
	^{IV} Fe ³⁺	0.05(3)	0.98(5)	0.19(13)	3(2)
	Σ Fe ³⁺	-	-	-	13(3)
Average	^{VI} Fe ²⁺	-	-	-	87(4)
	^{VI} Fe ³⁺	-	-	-	8(3)
	^{IV} Fe ³⁺	-	-	-	5(3)
	Σ Fe ³⁺	-	-	-	13(4)

Notes: Numbers in parentheses are two standard deviations on the last digit based on the statistics of the fit.

*: Mössbauer spectra were collected along each of three orthogonal directions of the crystal.

#: full width at half-maximum.

Table 3. Unit-cell and collection parameters

Parameter	H4181
a (Å)	5.7135(3)
b (Å)	11.4873(6)
c (Å)	8.2829(5)
V (Å ³)	543.63(5)
b/a	2.0105
2θ max (°)	70
No. of reflections	9806
No. of unique reflections	681