Table 5. Site occupancies, interatomic distances and polyhedral volume (run H4181)

Parameter	T	M1	M2	M3
Mg (%)	0	87.1(4)	94.4(4)	84.6(4)
Si (%)	95.1(5)	0	0	0
Fe (%)	4.9(5)	12.9(4)	5.6(4)	13.7(4)
Vacancy (from *b*/*a*)	-	-	-	1.7
Average T-O (Å)	1.6543(8)	-	-	-
Average M-O (Å)	-	2.0794(7)	2.0896(9)	2.0982(6)
Polyhedral volume ($Å^3$)	2.313	11.902	12.073	12.204

Table 6. Water contents of wadsleyite single crystals

E	Number	Water content (wt% H_2O)		
	of analyses	Paterson (1982)*	Libowitzky and Rossman (1997)*	Deon et al. (2010)*
[100]	4	0.055(1)	0.060(2)	0.066(2)
[010]	4	0.035(1)	0.042(1)	0.058(1)
[001]	3	0.101(6)	0.111(7)	0.132(9)
Total		0.191(6)	0.213(7)	0.256(9)

Note: Numbers in parentheses are one standard deviation on the last digit.

*: Calibrations used to determine the water contents.

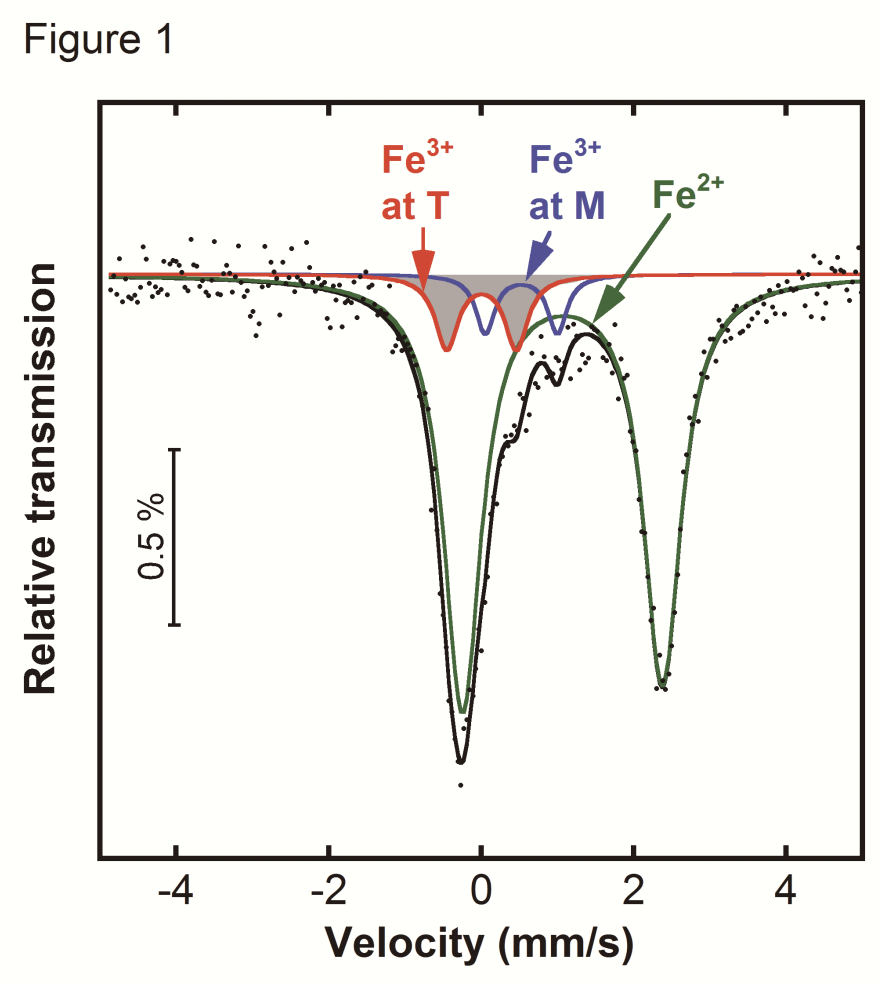

Figure 1. Room temperature Mössbauer spectrum of one orientation of the wadsleyite single crystal. Doublets corresponding to Fe^{3+} at the T site are shaded gray.

Figure 3

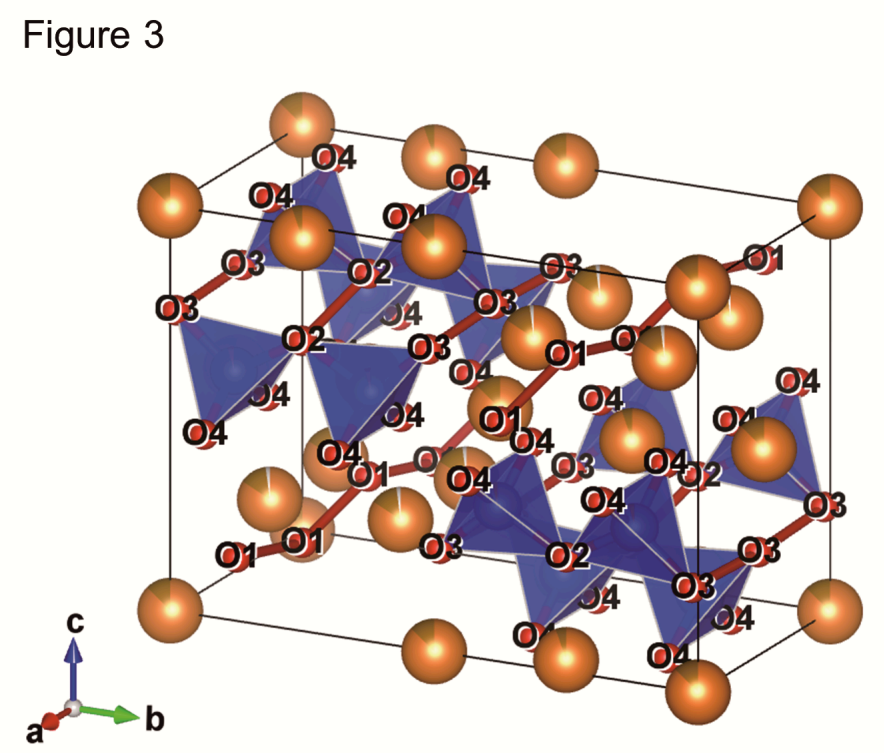

Figure 3. Crystal structure of wadsleyite from the [411] direction. Oxygens are labelled as O1, O2, O3 and O4. Bold lines represent candidates for the 3477 cm^{-1} band (O2···O2 (2.908 Å) and O3···O3 (2.858 Å)) and for the 3614 cm^{-1} band (O1···O1 (2.905 Å)). The crystal structure was drawn using the program VESTA (Momma and Izumi 2011).