

Supplemental Table OM6. Fractional atom coordinates, U_{eq} (Å²) values for fresnoite.

Site	Atom	x/a	y/b	z/c	U_{eq}	sof
Ti1	Ti	1	1	0.4740(2)	0.0113(3)	1
Ba1	Ba	0.67288(2)	0.17288(2)	1.00971(8)	0.01465(10)	0.969(7)
	Ca					0.031(7)
Si1	Si	0.87198(10)	0.37198(10)	0.4970(4)	0.0110(3)	1
O1	O	0.7078(4)	0.4233(5)	0.3658(7)	0.0257(8)	1
O2	O	0.8737(3)	0.3737(3)	0.8020(8)	0.0159(7)	1
O3	O	1	0.5	0.3801(12)	0.0249(13)	1
O4	O	1	1	0.7986(13)	0.0241(13)	1