

Table S3. Anisotropic displacement parameters U^{ij} for stracherite

atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ba1	0.02367(17)	0.02367(17)	0.01528(19)	0	0	0.01184(8)
Ca1	0.0104(2)	0.0105(3)	0.0257(10)	0.0000(4)	0.00001(18)	0.00525(14)
Ca1A	0.0104(2)	0.0105(3)	0.0257(10)	0.0000(4)	0.00001(18)	0.00525(14)
T1	0.0071(3)	0.0071(3)	0.0126(4)	0	0	0.00353(13)
T2	0.0119(8)	0.0119(8)	0.0070(12)	0	0	0.0060(4)
O1	0.0354(11)	0.0354(11)	0.0140(13)	0	0	0.0177(6)
O2	0.0123(6)	0.0123(6)	0.022(3)	-0.0005(11)	0.0005(11)	0.0080(7)
O2A	0.0123(6)	0.0123(6)	0.022(3)	-0.0005(11)	0.0005(11)	0.0080(7)
O3	0.0358(9)	0.0220(10)	0.0224(9)	0.0024(7)	0.0012(4)	0.0110(5)
O4	0.0312(10)	0.0312(10)	0.0136(12)	0	0	0.0156(5)
F1	0.0304(12)	0.0304(12)	0.0204(16)	0	0	0.0152(6)