

Oberti et al. On the symmetry and crystal chemistry of britholite: new structural and microanalytical data

Table 5 Atomic coordinates and anisotropic displacement factors

A - Sample CAPR

ATOM	x/a	y/b	z/c	b ₁₁	b ₂₂	b ₃₃	b ₁₂	b ₁₃	b ₂₃
REE1	1/3	2/3	-.00476	0.0036	0.0036	0.0031	0.0018	0.0000	0.0000
REE1a	2/3	1/3	.00001	0.0029	0.0029	0.0044	0.0015	0.0000	0.0000
REE2	0.23780	-0.01160	1/4	0.0042	0.0029	0.0036	0.0020	-0.0001	0.0002
Si	0.39898	0.37182	0.25126	0.0027	0.0024	0.0036	0.0015	-0.0009	-0.0009
O1	0.32287	0.48860	0.25320	0.0084	0.0052	0.0068	0.0054	-0.0013	0.0025
O2	0.59402	0.46955	0.25691	0.0034	0.0034	0.0162	0.0009	-0.0013	-0.0002
O3	0.31684	0.24308	0.42176	0.0160	0.0043	0.0059	0.0061	0.0044	0.0016
O3a	0.35805	0.26045	0.05956	0.0086	0.0061	0.0030	0.0052	-0.0011	-0.0016
O4	0 0	0.23594	0.0075	0.0075	0.0617	0.0037	0.0000	0.0000	

B - Sample LOS

ATOM	x/a	y/b	z/c	b ₁₁	b ₂₂	b ₃₃	b ₁₂	b ₁₃	b ₂₃
REE1	1/3	2/3	-0.00389	0.0059	0.0059	0.0110	0.0030	0.0000	0.0000
REE1a	2/3	1/3	0.00603	0.0070	0.0070	0.0099	0.0035	0.0000	0.0000
REE2	0.23645	-0.01330	1/4	0.0071	0.0057	0.0094	0.0032	0.0013	0.0001
Si	0.40069	0.37279	0.25636	0.0066	0.0058	0.0092	0.0035	-0.0050	-0.0021
O1	0.32457	0.48677	0.25890	0.0119	0.0092	0.0134	0.0070	0.0065	-0.0015
O2	0.59287	0.46930	0.24393	0.0069	0.0079	0.0224	0.0026	0.0000	0.0011
O3	0.31198	0.24449	0.41744	0.0166	0.0095	0.0176	0.0077	0.0048	0.0012
O3a	0.36497	0.26497	0.06334	0.0105	0.0082	0.0094	0.0057	-0.0024	-0.0021
O4	0 0	0.17714	0.0110	0.0110	0.0952	0.0055	0.0000	0.0000	