TABLE 9A. Atomic positional parameters and B_{eq} (Å^2) values for cordierite C005

Atom	*x/a*	*y/b*	*z/c*	B_{eq}
$Si_2$1	0.30792(2)	0.07805(3)	0	0.390(3)
$Si_1$6	0	0	¼	0.441(4)
$Si_2$3	0.36486(2)	0.23691(3)	½	0.388(4)
$Al_2$6	0.05055(2)	0.19245(3)	0	0.408(3)
$Al_1$1	¼	¼	0.25005(4)	0.487(3)
MgM*	0.16248(2)	0	¼	0.530(5)
$O_1$6	0.06208(3)	0.08413(5)	0.15114(6)	0.653(5)
$O_1$1	0.25328(3)	0.10318(5)	0.14144(6)	0.660(5)
$O_1$3	0.32664(3)	0.30963(5)	0.64171(6)	0.655(5)
$O_2$1	0.37794(5)	0.18492(9)	0	0.947(9)
$O_2$6	0.45664(4)	0.24873(9)	½	0.93(1)
$O_2$3	0.33579(5)	-0.07929(8)	0	0.93(1)
CH0†	½	0	½	7.29
CH1‡	½	0	¼	7.26
CH2§	0.45272	0	¼	5.86

*0.811(4) Mg + 0.199(4) Fe.
†0.07 Na.
‡ 0.20 O + C.
§ 0.08 O.

TABLE 9B. Atomic displacement parameters for cordierite C005

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
$Si_2$1	0.00535(9)	0.00402(9)	0.00546(9)	–0.00028(6)	0	0
$Si_1$6	0.0052(1)	0.0064(1)	0.0052(1)	0	0	0
$Si_2$3	0.0047(1)	0.0049(1)	0.0052(1)	–0.00059(6)	0	0
$Al_2$6	0.0047(1)	0.00545(9)	0.0054(1)	–0.00035(7)	0	0
$Al_1$1	0.00743(9)	0.00561(9)	0.0055(1)	–0.00119(7)	0	0
MgM	0.0058(1)	0.0060(1)	0.0084(2)	0	0	–0.00028(7)
$O_1$6	0.0073(2)	0.0096(2)	0.0079(2)	–0.0011(1)	–0.0002(1)	0.0033(1)
$O_1$1	0.0108(2)	0.0072(1)	0.0072(2)	–0.0007(1)	0.0036(1)	–0.0010(1)
$O_1$3	0.0088(2)	0.0088(2)	0.0074(2)	–0.0016(1)	0.0020(1)	–0.0021(1)
$O_2$1	0.0097(2)	0.0099(2)	0.0164(3)	–0.0055(2)	0	0
$O_2$6	0.0045(2)	0.0150(3)	0.0161(3)	–0.0022(2)	0	0
$O_2$3	0.0132(3)	0.0052(2)	0.0171(3)	0.0031(2)	0	0