

Table 6. Anisotropic atomic displacement parameters ( $\text{\AA}^2$ )

Atom	$\underline{U}(1,1)$	$\underline{U}(2,2)$	$\underline{U}(3,3)$	$\underline{U}(1,2)$	$\underline{U}(1,3)$	$\underline{U}(2,3)$
Pb1	0.0121 (5)	0.0167 (5)	0.0153 (7)	0.0051 (4)	0.0009 (6)	0.0006 (6)
Pb2	0.0158 (5)	0.0087 (4)	0.0150 (7)	0.0062 (3)	-0.0001 (5)	-0.0011 (6)
Pb3	0.0188 (5)	0.0178 (5)	0.0130 (6)	0.0118 (4)	0.0003 (6)	0.0010 (6)
Ba	0.012 (1)	0.012	0.016 (2)	0.006	0	0
Ca1	0.008 (5)	0.008	0.027 (11)	0.004	0	0
Ca2	0.022 (4)	0.022	0.031 (9)	0.011	0	0
Ca3	0.009 (3)	0.009	0.012 (7)	0.004	0	0
Fe	0.009 (2)	0.009	0.017 (5)	0.004	0	0
Mn	0.012 (3)	0.012	0.020 (6)	0.006	0	0
Si1	0.002 (4)	0.002	0.010 (9)	0.001	0	0
Si2	0.004 (3)	0.015 (3)	0.007 (5)	0.005 (2)	0.001 (3)	-0.001 (4)
Si3	0.006 (3)	0.009 (3)	0.020 (6)	0.005 (2)	-0.001 (4)	0.001 (4)
Si4	0.002 (4)	0.002	0.014 (9)	0.001	0	0
Si5	0.011 (3)	0.015 (3)	0.008 (5)	0.011 (2)	0.000 (3)	-0.003 (3)
Si6	0.011 (3)	0.018 (3)	0.006 (5)	0.011 (2)	-0.002 (4)	-0.003 (4)
Cl	0.026 (8)	0.026	0.036 (16)	0.013	0	0

The form of the anisotropic displacement parameter is  $\exp[-2\pi^2\{\underline{h}^2\underline{a}^2\underline{U}(1,1) + \underline{k}^2\underline{b}^2\underline{U}(2,2) + \underline{l}^2\underline{c}^2\underline{U}(3,3) + 2\underline{h}\underline{k}\underline{a}\underline{b}\underline{U}(1,2) + 2\underline{h}\underline{l}\underline{a}\underline{c}\underline{U}(1,3) + 2\underline{k}\underline{l}\underline{b}\underline{c}\underline{U}(2,3)\}]$ , where  $\underline{a}$ ,  $\underline{b}$ , and  $\underline{c}$  are reciprocal lattice constants. Esds are in parenthesis.