

Table 3 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 117–226. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
M2B	16(6)	11(6)	23(5)	−2(3)	−6(6)	−2(5)
Z1	11.3(4)	11.3(3)	7.9(3)	−0.36(12)	−0.7(2)	5.64(19)
M1B	21.4(9)	12.1(9)	10.1(10)	−1.5(6)	−0.7(3)	6.0(5)
Ce1	21.4(9)	12.1(9)	10.1(10)	−1.5(6)	−0.7(3)	6.0(5)
M2A	66(3)	239(10)	14.8(15)	−43(3)	−21.6(13)	120(5)
M3	1.3(14)	1.3(14)	82(5)	0	0	0.7(7)
M1A	26.3(8)	6.2(8)	8.1(8)	−0.7(5)	−0.3(3)	3.1(4)
Zr2	26.3(8)	6.2(8)	8.1(8)	−0.7(5)	−0.3(3)	3.1(4)
X2C	57(6)	149(17)	75(7)	10(10)	−32(5)	36(9)
M4	10(2)	10(2)	8(3)	0	0	4.8(12)
Si1	13.5(7)	11.8(10)	15.8(7)	3.7(10)	5.2(6)	7.0(10)
Si2	15.4(10)	9.9(10)	11.7(11)	−1.4(8)	−0.2(8)	8.2(8)
Si3	7.5(9)	11.5(10)	9.8(11)	−1.8(8)	−0.6(8)	3.1(8)
Si4	6.2(7)	18.6(11)	9.4(6)	−1.5(10)	1.3(5)	2.1(9)
N3	27(3)	35(2)	22(2)	−12.8(17)	−8(3)	18(3)
N4	36(11)	43(8)	32(7)	−20(6)	−19(8)	33(10)
N1	33(2)	45(3)	76(2)	−34(2)	24(2)	−15.0(11)
Sr1	33(2)	45(3)	76(2)	−34(2)	24(2)	−15.0(11)
O1	28(3)	12(3)	26(4)	−5(2)	−8(3)	13(2)
O2	12(3)	60(6)	98(5)	40(5)	10(3)	13(4)
O3	18(2)	21(3)	14.6(18)	0(3)	3.5(16)	9(3)
O4	77(5)	33(4)	8(3)	3(3)	7(3)	45(4)
O5	15(3)	24(2)	23(2)	7.8(16)	3(2)	12(3)
O6	23(3)	32(4)	22(4)	−8(3)	−6(3)	7(3)
O7	18(3)	23(3)	9(3)	3(2)	1(2)	6(2)
O8	27(4)	14(3)	26(4)	−6(3)	4(3)	10(3)
O9	22(2)	40(4)	19(2)	−2(3)	10.5(17)	10(3)
O10	16(3)	19(3)	35(2)	2(3)	1(3)	13(2)
O11	21(2)	47(4)	17(2)	−6(4)	−5.8(17)	12(3)
O12	32(3)	23(3)	18(4)	1(3)	4(3)	20(3)
O14	14(6)	14(6)	4(7)	0	0	7(3)
X1A	130(30)	130(30)	34(19)	0	0	63(13)
X2A	31(5)	31(5)	87(11)	0	0	16(2)
X2B	10(3)	10(3)	6(4)	0	0	4.9(15)
X1B	130(40)	130(40)	40(30)	0	0	70(20)