

**Table S2 Anisotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for Iv-153–178. The Anisotropic displacement factor exponent takes the form:  $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$ .**

Atom	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>23</sub>	U <sub>13</sub>	U <sub>12</sub>
M1B	12.2(5)	21.3(5)	10.2(5)	0.50(17)	1.0(3)	6.1(3)
Ce1	12.2(5)	21.3(5)	10.2(5)	0.50(17)	1.0(3)	6.1(3)
M2A	60(2)	60(2)	15.6(14)	19.9(11)	−19.9(11)	−44(2)
M2B	60(2)	60(2)	16(2)	19.9(14)	−19.9(14)	−43.7(11)
M3	28.7(15)	28.7(15)	67(3)	0	0	14.4(8)
M4	7(4)	7(4)	19(6)	0	0	4(2)
O1	15.6(16)	15.6(16)	35(2)	0.4(9)	−0.4(9)	9.4(19)
O2	33(2)	25(3)	17(2)	−11.1(18)	−5.5(9)	12.5(13)
O3	39(2)	24(3)	15(2)	3.7(18)	1.9(9)	12.0(13)
O4	19.6(16)	19.6(16)	18(2)	2.0(9)	−2.0(9)	8.3(19)
O5	20.7(18)	29.0(19)	21.1(15)	−0.4(14)	0.1(13)	−2.1(16)
O6	21.1(17)	21.1(17)	23(2)	−4.6(10)	4.6(10)	6(2)
O7	35(2)	29.2(19)	26.5(17)	7.7(14)	0.3(14)	17.7(17)
O8	20.5(16)	29.6(18)	15.5(13)	−3.3(13)	−1.3(12)	13.4(14)
O9	50(6)	50(6)	51(10)	0	0	25(3)
O10	48(3)	14(3)	107(5)	−11(3)	−5.3(16)	7.2(14)
Si1	17.2(6)	10.1(8)	11.1(7)	−1.1(6)	−0.5(3)	5.0(4)
Si3	14.8(6)	19.4(9)	21.1(8)	−6.3(7)	−3.1(3)	9.7(4)
Si5	10.4(6)	17.0(6)	12.6(5)	0.6(4)	−0.2(4)	6.9(5)
Z1	13.2(4)	14.2(3)	9.7(3)	−0.56(12)	−1.1(2)	6.60(19)
N1A	24.8(14)	24.8(14)	20.6(19)	6.0(9)	−6.0(9)	6.7(17)
N1B	25(4)	25(4)	22(6)	13(3)	−13(3)	−3(5)
N5	38(4)	38(4)	91(19)	0	0	18.8(19)
N4	71(2)	26.3(11)	61.1(19)	−19.8(7)	−39.7(14)	35.3(11)
Sr1	71(2)	26.3(11)	61.1(19)	−19.8(7)	−39.7(14)	35.3(11)
X1	160(11)	160(11)	101(9)	−10(3)	10(3)	123(12)
X2A	50(6)	50(6)	51(10)	0	0	25(3)
X2C	40(10)	40(10)	56(17)	0	0	20(5)