AM-95-584

Site preference of rare earth elements in fluorapatite

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For deposit: Tables 4 and 5

American Mineralogist, 80, 3-4, 329-335.

Site Preference of Rare Earth Elements in Fluorapatite

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DEPOSITED MATERIALS:

TABLE 4: Anisotropic thermal parameters

TABLE 5: Lists of observed and calculated structure factors

TABLE 4: Anisotropic thermal parameters ($x10^2$ $Å^2$)

Anisotropic temperature factors have the form
$\exp[-¼(B_{11}h^2a^{*2} + ... + 2B_{23}klb^*c^*\cos\alpha^*)]$

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
			La-FAp			
Ca1	101(2)	B_{11}	61(2)	$B_{11}/2$	0	0
Ca2	80(2)	107(2)	64(1)	54(1)	0	0
P	52(2)	60(2)	54(2)	31(1)	0	0
O1	101(5)	125(5)	112(5)	83(5)	0	0
O2	84(5)	66(5)	198(7)	29(4)	0	0
O3	116(4)	240(5)	93(3)	111(4)	-37(3)	-69(4)
F	110(8)	B_{11}	695(22)	$B_{11}/2$	0	0
			Nd-FAp			
Ca1	98(3)	B_{11}	71(2)	$B_{11}/2$	0	0
Ca2	74(3)	93(3)	66(2)	47(2)	0	0
P	49(3)	55(3)	54(2)	28(2)	0	0
O1	91(8)	126(8)	105(7)	79(7)	0	0
O2	85(8)	85(8)	199(10)	43(6)	0	0
O3	124(6)	252(8)	85(5)	124(6)	-40(5)	-66(5)
F	102(11)	B_{11}	677(30)	$B_{11}/2$	0	0
			Gd-FAp			
Ca1	92(1)	B_{11}	57(1)	$B_{11}/2$	0	0
Ca2	64(1)	72(1)	59(1)	35(1)	0	0
P	47(1)	52(1)	46(1)	28(1)	0	0
O1	97(4)	124(4)	98(4)	85(3)	0	0
O2	78(4)	66(4)	172(5)	29(3)	0	0
O3	106(3)	225(4)	86(3)	104(3)	-38(2)	-69(3)
F	100(5)	B_{11}	539(14)	$B_{11}/2$	0	0
			Dy-FAp			
Ca1	91(2)	B_{11}	55(2)	$B_{11}/2$	0	0
Ca2	62(1)	67(1)	57(1)	33(1)	0	0
P	43(2)	47(2)	45(1)	27(1)	0	0
O1	82(5)	114(5)	104(5)	76(4)	0	0
O2	70(5)	56(4)	169(6)	24(4)	0	0
O3	96(3)	194(4)	80(3)	91(3)	-33(3)	-59(3)
F	94(7)	B_{11}	497(16)	$B_{11}/2$	0	0