TABLE 5. (on deposit). Anisotropic displacement parameters ($Å^2$) for non-hydrogen atoms in the two analyzed fluor-elbaite samples.

		Standard SREF						Splite-site SREF					
Site	Sample	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
X	Cruzeiro	0.0247(5)	0.0247(5)	0.0150(6)	0	0	0.0124(3)	0.0233(4)	0.0233(4)	0.0149(5)	0	0	0.0116(2)
	Urubu	0.0310(11)	0.0310(11)	0.0219(14)	0	0	0.0155(5)	0.029(1)	0.029(1)	0.0212(12)	0	0	0.0143(5)
Y	Cruzeiro	0.00938(17)	0.00812(13)	0.01143(17)	-0.00053(6)	-0.00107(11)	0.00469(8)	0.00924(14)	0.00799(11)	0.01162(14)	-0.00057(5)	-0.00114(9)	0.00462(7)
	Urubu	0.0102(4)	0.0089(3)	0.0125(4)	-0.00057(11)	-0.0011(2)	0.00510(18)	0.0101(3)	0.0088(3)	0.0129(3)	-0.00058(10)	-0.0012(2)	0.00502(16)
Z	Cruzeiro	0.00620(11)	0.00732(11)	0.00530(9)	0.00059(8)	0.00008(8)	0.00369(9)	0.00626(9)	0.00734(9)	0.00525(7)	0.00060(6)	0.00007(6)	0.00378(7)
	Urubu	0.0079(2)	0.0093(3)	0.0070(2)	0.00068(19)	0.00048(18)	0.0048(2)	0.0079(2)	0.0093(2)	0.0067(2)	0.00076(17)	0.00047(16)	0.00472(18)
B	Cruzeiro	0.0069(3)	0.0058(4)	0.0064(4)	0.0007(3)	0.00036(17)	0.0029(2)	0.0071(3)	0.0062(4)	0.0064(3)	0.0004(3)	0.00020(14)	0.00311(18)
	Urubu	0.0093(9)	0.0088(12)	0.0079(11)	0.0008(9)	0.0004(4)	0.0044(6)	0.0098(8)	0.0108(11)	0.0073(10)	-0.0000(8)	-0.0000(4)	0.0054(5)
T	Cruzeiro	0.00502(9)	0.00484(9)	0.00526(8)	-0.00017(7)	0.00007(7)	0.00245(7)	0.00483(7)	0.00480(7)	0.00522(6)	-0.00018(6)	0.00011(6)	0.00240(6)
	Urubu	0.0066(2)	0.0062(2)	0.0069(2)	-0.00023(16)	0.00002(17)	0.00314(16)	0.0063(2)	0.00612(19)	0.00689(18)	-0.00027(14)	0.00008(15)	0.00302(14)
O1	Cruzeiro	0.0812(15)	0.0812(15)	0.0113(9)	0	0	0.0406(8)	Isotropic					
	Urubu	0.084(2)	0.084(2)	0.0113(17)	0	0	0.0419(12)	Isotropic					
O2	Cruzeiro	0.0264(5)	0.0044(4)	0.0122(4)	0.0009(3)	0.00043(15)	0.00222(18)	Isotropic					
	Urubu	0.0275(9)	0.0275(9)	0.014(1)	-0.0001(4)	0.0001(4)	0.024(1)	Isotropic					
O3	Cruzeiro	0.0201(5)	0.0093(2)	0.0054(3)	-0.00015(15)	-0.0003(3)	0.0101(2)	0.0198(4)	0.0092(2)	0.0052(2)	-0.00016(12)	-0.0003(2)	0.00988(19)
	Urubu	0.0207(10)	0.0103(6)	0.0058(8)	-0.0001(4)	-0.0002(7)	0.0104(5)	0.0206(9)	0.0104(6)	0.0053(7)	0.0000(3)	0.0000(6)	0.0103(5)
O4	Cruzeiro	0.0066(2)	0.0120(4)	0.0076(3)	-0.0007(3)	-0.00037(14)	0.00601(19)	0.00655(19)	0.0119(3)	0.0078(2)	-0.0011(2)	-0.00054(12)	0.00594(16)
	Urubu	0.0086(6)	0.0123(9)	0.0100(8)	-0.0003(7)	-0.0001(3)	0.0062(5)	0.0086(6)	0.0131(8)	0.0099(7)	-0.0006(6)	-0.0003(3)	0.0065(4)
O5	Cruzeiro	0.0129(4)	0.0062(2)	0.0077(3)	0.00045(14)	0.0009(3)	0.0064(2)	0.0133(3)	0.00624(18)	0.0075(3)	0.00030(11)	0.0006(2)	0.00663(16)
	Urubu	0.014(9)	0.0083(6)	0.0103(8)	0.0004(3)	0.0008(7)	0.0071(5)	0.0147(9)	0.0088(5)	0.0100(8)	0.0002(3)	0.0004(6)	0.0074(4)
O6	Cruzeiro	0.0070(2)	0.0083(2)	0.0049(2)	-0.00008(18)	0.00047(17)	0.0026(2)	0.00704(19)	0.0087(2)	0.00487(17)	-0.00028(15)	0.00028(14)	0.00274(16)
	Urubu	0.0084(6)	0.0099(6)	0.0063(5)	0.0002(4)	0.0003(4)	0.0030(5)	0.0084(5)	0.0104(5)	0.0061(5)	0.0000(4)	0.0001(4)	0.0034(4)
O7	Cruzeiro	0.0056(2)	0.0056(2)	0.0061(2)	-0.00107(17)	0.00043(17)	0.00138(18)	0.00556(18)	0.00548(18)	0.00601(18)	-0.00112(14)	0.00038(14)	0.00137(15)
	Urubu	0.0075(6)	0.0068(5)	0.0076(5)	-0.0012(4)	0.0001(4)	0.0023(5)	0.0073(5)	0.0072(5)	0.0074(5)	-0.0010(4)	0.0004(4)	0.0023(4)
O8	Cruzeiro	0.0056(2)	0.0103(3)	0.0077(2)	0.00325(19)	0.00092(18)	0.0045(2)	0.00556(19)	0.0103(2)	0.00750(17)	0.00329(15)	0.00114(15)	0.00449(17)
	Urubu	0.0077(6)	0.0115(6)	0.0108(6)	0.003(5)	0.0009(5)	0.0058(5)	0.0075(5)	0.0117(6)	0.0105(5)	0.0028(4)	0.0009(4)	0.0056(5)

Notes: Standard and Split-site SREF denote, respectively, structural refinements carried out with the O1 site at (0,0,*z*) and the O2 site at (*x*,2*x*,*z*), and with O1 at (*x*,*x*/2,*z*) and O2 at (*x*,*y*,*z*) to allow for positional disorder, as indicated by the high U_{eq} values (Burns et al. 1994).