Lattice parameters (Angstrom or degree) and unit-cell volume (Angstrom**3) in Fluorapatite

a	b	c	alpha	beta	gamma	V
9.36903	9.36903	6.88384	90.0000	90.0000	120.0000	523.2997
0.00010	-	0.00006	-	-	-	0.0094

Structure parameters, g, x, y, z, B/Angstrom**2, and U/Angstrom**2, in Fluorapatite

Atom	Site		100*B/nm**2 neq	*	g	=	100*U/nm**2 n	x	y	z	B	U
O1	6h	x y 1/4	6		1.0000		6.0000	0.32418	0.48536	0.25000	0.736	0.00932
			-		-		-	0.00033	0.00034	-	0.069	0.00087
O2	6h	x y 1/4	6		1.0000		6.0000	0.59179	0.46983	0.25000	0.736	0.00933
			-		-		-	0.00035	0.00037	-	0.070	0.00088
O3	12i	x y z	12		1.0000		12.0000	0.33915	0.25727	0.06979	0.831	0.01053
			-		-		-	0.00027	0.00027	0.00027	0.050	0.00064
P	6h	x y 1/4	6		1.0000		6.0000	0.39731	0.36788	0.25000	0.553	0.00700
			-		-		-	0.00016	0.00016	-	0.026	0.00033
Ca1	4f	1/3 2/3 z	4		1.0000		4.0000	0.33333	0.66667	0.00133	0.647	0.00820
			-		-		-	-	-	0.00023	0.024	0.00030
Ca2	6h	x y 1/4	6		1.0000		6.0000	0.24179	-0.00796	0.25000	0.530	0.00671
			-		-		-	0.00012	0.00015	-	0.019	0.00024
F	2a	0 0 1/4	2		1.0000		2.0000	0.00000	0.00000	0.25000	1.421	0.01800
			-		-		-	-	-	-	0.091	0.00116

neq: multiplicity of the Wyckoff position (number of equivalent points per unit cell)
n: number of equivalent atoms per unit cell

Atomic displacement parameters, 10**6*betaij, 10**6*Uij/Angstrom**2, Beq/Angstrom**2, and Ueq/Angstrom**2, in Fluorapatite

Atom	beta11	beta22	beta33	beta12	beta13	beta23	10**8*Uij/nm**2 U11	U22	U33	U12	U13	U23	100*Beq/nm**2 Beq	100*Ueq/nm**2 Ueq	NCON
O1	2795	2795	3883	1398	0	0	9322	9322	9322	4661	0	0	-	-	2
	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
O2	2796	2796	3885	1398	0	0	9327	9327	9327	4663	0	0	-	-	2
	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
O3	3156	3156	4384	1578	0	0	10525	10525	10525	5263	0	0	-	-	0
	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
P	2099	2099	2916	1050	0	0	7001	7001	7001	3501	0	0	-	-	2
	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
Ca1	2457	2457	3414	1229	0	0	8195	8195	8195	4098	0	0	-	-	16
	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
Ca2	2013	2013	2797	1007	0	0	6715	6715	6715	3357	0	0	-	-	2
	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
F	5398	5398	7499	2699	0	0	18002	18002	18002	9001	0	0	-	-	16
	-	-	-	-	-	-	-	-	-	-	-	-	-	-	

```
  Isotropic Debye-Waller factor = exp(-B*(sin(theta)/lambda)**2) = exp(-8*pi**2*U*(sin(theta)/lambda)**2)
Anisotropic Debye-Waller factor = exp(-(h**2*beta11 + k**2*beta22 + l**2*beta33 + 2*h*k*beta12 + 2*h*l*beta + 2*k*l*beta23))
                                = exp(-2*pi**2*(h**2*(a*)**2*U11 + k**2*(b*)**2*U22 + l**2*(c*)**2*U33 +
                                  2*h*k*(a*)*(b*)*U12 + 2*h*l*(a*)*(c*)*U13 + 2*k*l*(b*)*(c*)*U23))
Beq, Ueq: equivalent isotropic atomic displacement parameters calculated from anisotropic atomic displacement parameters
```

NCON	beta11	beta22	beta33	beta12	beta13	beta23
1				0		0
* 2					0	0
3				0	0	
4				0	0	0
5	A	A			0	0
6	A	A			B	B
7	A	A			B	-B
8	A	A		0	0	0
9		A	A	0	0	
10		A	A	B	B	
11		A	A	-B	B	
12		A	A	0	0	0
13		A		A/2		0
14		A		A/2	0	0
15		A		A/2	B	2B
* 16	A	A		A/2	0	0
17	A	A	A	0	0	0
18	A	A	A	B	B	B

This table appears in
W. J. A. M. Peterse and J. H. Palm, Acta Crystallogr., 20 (1966) 147.

These constraints have to be imposed on anisotropic atomic displacement parameters for the first coordinate triplet of each site in "International Tables for Crystallography," Vol. A.

If two or more discriptions are available for a space group, select the following setting in accordance with STRUCTURE TIDY:
(1) monoclinic: unique axis b,
(2) trigonal (R lattice): hexagonal axes (triple cell),
(3) tetragonal and cubic: a center of symmetry at the origin.

Chemical species in the unit cell, and density for Fluorapatite

Ne	Atom	N	* At.wt.	/ 6.02214E23	= Mass
8.000	O-	24.00000	15.99940		6.376230E-22 g
15.000	P	6.00000	30.97376		3.085988E-22 g
20.000	Ca2+	10.00000	40.07800		6.655108E-22 g
9.000	F-	2.00000	18.99840		6.309518E-23 g

```
---------------------------------------------------------------------------
                                                        Total = 1.674828E-21 g
            d = Total/V = 1.674828E-21 / 5.232997E-22 =  3.200513 g/cm**3
                          Total number of electrons = F(000) =    500.000
```