Crystal Data and Results of Refinement for Kurokura Apatite Core and Rim:

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Sample and Crystal Data for Kurokura Core

Chemical formula	$Ca_{10}(PO_4)_6(F_{0.55}OH_{0.58}Cl_{0.87})$
Formula weight	1021.80 g/mol
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	hexagonal
Space group	P 63/m
Unit cell dimensions	a = 9.5213(4) Å α = 90°
	b = 9.5213(4) Å β = 90°
	c = 6.8496(3) Å γ = 120°
Volume	537.76(5) $Å^3$
Z	1
Density (calculated)	3.155 g/cm^3
Absorption coefficient	3.120 mm^{-1}
F(000)	507
Theta range for data collection	2.47 to 33.27°
Index ranges	-14<=h<=14, -14<=k<=14, -10<=l<=10
Reflections collected	12047
Independent reflections	733 [R(int) = 0.0249]
Absorption correction	multi-scan
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	733 / 0 / 51
Goodness-of-fit on F^2	1.102
Final R indices	730 data; I>2σ(I) R1 = 0.0158, wR2 = 0.0412
	all data R1 = 0.0158, wR2 = 0.0412
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0174P)^2+0.4357P]$ where $P=(F_o^2+2F_c^2)/3$
Extinction coefficient	0.1830(50)
Largest diff. peak and hole	0.415 and -0.364 $eÅ^{-3}$
R.M.S. deviation from mean	0.072 $eÅ^{-3}$

Sample and Crystal Data for Kurokura Rim

Chemical formula	$(PO_4)_6(F_{1.05}OH_{1.02}Cl_{0.04})$
Formula weight	1009.34 g/mol
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	hexagonal
Space group	P 63/m
Unit cell dimensions	a = 9.4082(9) Å α = 90°
	b = 9.4082(9) Å β = 90°
	c = 6.8853(7) Å γ = 120°
Volume	527.80(11) $Å^3$
Z	1
Density (calculated)	3.176 g/cm^3
Absorption coefficient	3.080 mm^{-1}
F(000)	501
Theta range for data collection	2.50 to 33.44°
Index ranges	-14<=h<=14, -14<=k<=14, -10<=l<=10
Reflections collected	11718
Independent reflections	726 [R(int) = 0.0098]
Absorption correction	multi-scan
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	726 / 0 / 49
Goodness-of-fit on F^2	1.505
Final R indices	720 data; I>2σ(I) R1 = 0.0143, wR2 = 0.0376
	all data R1 = 0.0145, wR2 = 0.0377
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0097P)^2+0.3046P]$ where $P=(F_o^2+2F_c^2)/3$
Extinction coefficient	0.0013(7)
Largest diff. peak and hole	0.511 and -0.391 $eÅ^{-3}$
R.M.S. deviation from mean	0.074 $eÅ^{-3}$