APPENDIX 1. Crystal data and results of structure analysis for synthetic F-OH apatites.

Appendix 1a. Sample and crystal data for DHAPS68.

Crystal size	0.125 x 0.131 x 0.142 mm	
Space group	P 6_3/m	
Unit cell dimensions	a = 9.3818(3) Å	
	c = 6.8908(2) Å	
Volume	525.26(4) Å^3	
Density (calculated)	3.187 g/cm^3	
Absorption coefficient	3.090 mm^{-1}	
F(000)	500	
Theta range	2.51 to 33.44°	
Index ranges	-14<=h<=14, -14<=k<=14, -10<=l<=10	
Reflections collected	11433	
Independent reflections	716 [R(int) = 0.0137]	
Coverage	97.7%	
Average Redundancy	15.968	
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	716 / 0 / 43	
Final R indices	713 data; I>2σ(I)	R1 = 0.0140, wR2 = 0.0346
	all data	R1 = 0.0142, wR2 = 0.0347
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0101P)^2+0.3179P]$ where $P=(F_o^2+2F_c^2)/3$	
Extinction coefficient	0.0340(20)	
Largest diff. peaks	0.521 and -0.264 eÅ^{-3}	

Appendix 1b. Sample and crystal data for DHAPS69.

Crystal size	0.099 x 0.100 x 0.100 mm	
Space group	P 6_3/m	
Unit cell dimensions	a = 9.3970(4) Å	
	c = 6.8905(3) Å	
Volume	526.94(5) Å^3	
Z	1	
Density (calculated)	3.172 g/cm^3	
Absorption coefficient	3.079 mm^{-1}	
F(000)	500	
Theta range	2.50 to 33.35°	
Index ranges	-14<=h<=14, -14<=k<=14, -10<=l<=10	
Reflections collected	11585	
Independent reflections	718 [R(int) = 0.0122]	
Coverage	98.2%	
Average Redundancy	16.135	
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	718 / 0 / 43	
Goodness-of-fit on F^2	1.304	
Final R indices	715 data; I>2σ(I)	R1 = 0.0124, wR2 = 0.0321
	all data	R1 = 0.0125, wR2 = 0.0322
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0115P)^2+0.2353P]$ where $P=(F_o^2+2F_c^2)/3$	
Extinction coefficient	0.0295(13)	
Largest diff. peaks	0.477 and -0.264 eÅ^{-3}	

Table 1c. Sample and crystal data for DHAPS70.

Crystal size	0.074 x 0.095 x 0.800 mm	
Space group	P 6_3/m	
Unit cell dimensions	a = 9.3991(8) Å	
	c = 6.8887(6) Å	
Volume	527.04(10) Å^3	
Z	1	
Density (calculated)	3.171 g/cm^3	
Absorption coefficient	3.078 mm^{-1}	
F(000)	499	
Theta range	2.50 to 33.45°	
Index ranges	-14<=h<=14, -14<=k<=14, -10<=l<=10	
Reflections collected	11788	
Independent reflections	717 [R(int) = 0.0119]	
Coverage	97.0%	
Average Redundancy	16.441	
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	717 / 0 / 43	
Goodness-of-fit on F^2	1.272	
Final R indices	711 data; I>2σ(I)	R1 = 0.0116, wR2 = 0.0292
	all data	R1 = 0.0118, wR2 = 0.0293
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0108P)^2+0.1958P]$ where $P=(F_o^2+2F_c^2)/3$	
Extinction coefficient	0.0168(11)	
Largest diff. peaks	0.410 and -0.229 eÅ^{-3}	

Table 1d. Sample and crystal data for DHAPS77.

Crystal size	0.110 x 0.120 x 0.122 mm
Space group	P 6_3/m
Unit cell dimensions	a = 9.4055(6) Å
	c = 6.8902(5) Å
Volume	527.87(8) Å^3
Z	1
Density (calculated)	3.164 g/cm^3
Absorption coefficient	3.073 mm^{-1}
F(000)	499
Theta range	2.50 to 33.30°
Index ranges	-14<=h<=14, -14<=k<=14, -10<=l<=10
Reflections collected	11696
Independent reflections	719 [R(int) = 0.0205]
Coverage	98.6%
Average Redundancy	16.267
Absorption correction	multi-scan
Max. and min. transmission	0.7290 and 0.7060
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	719 / 0 / 43
Goodness-of-fit on F^2	1.250
Final R indices	716 data; I>2σ(I) R1 = 0.0123, wR2 = 0.0279
	all data R1 = 0.0125, wR2 = 0.0280
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0072P)^2+0.2454P]$ where $P=(F_o^2+2F_c^2)/3$
Extinction coefficient	0.0820(20)
Largest diff. peaks	0.389 and -0.322 eÅ^{-3}

Table 1e. Sample and crystal data for DHAPS84.

Crystal size	0.208 x 0.310 x 0.343 mm
Space group	P 6_3/m
Unit cell dimensions	a = 9.3857(2) Å
	c = 6.8885(2) Å
Volume	525.52(3) Å^3
Z	1
Density (calculated)	3.183 g/cm^3
Absorption coefficient	3.088 mm^{-1}
F(000)	500
Theta range	2.51 to 33.38°
Index ranges	-14<=h<=14, -14<=k<=14, -10<=l<=10
Reflections collected	11562
Independent reflections	712 [R(int) = 0.0130]
Coverage	97.4%
Average Redundancy	16.239
Absorption correction	multi-scan
Max. and min. transmission	0.5660 and 0.4170
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	712 / 0 / 43
Goodness-of-fit on F^2	1.261
Final R indices	709 data; I>2σ(I) R1 = 0.0118, wR2 = 0.0285
	all data R1 = 0.0119, wR2 = 0.0286
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0085P)^2+0.2486P]$ where $P=(F_o^2+2F_c^2)/3$
Extinction coefficient	0.0200(10)
Largest diff. peak and hole	0.475 and -0.217 eÅ^{-3}

Table 1f. Sample and crystal data for DHAPS85.

Crystal size	0.326 x 0.331 x 0.402 mm
Space group	P 6_3/m
Unit cell dimensions	a = 9.3967(3) Å
	c = 6.8893(2) Å
Volume	526.81(4) Å^3
Z	1
Density (calculated)	3.171 g/cm^3
Absorption coefficient	3.080 mm^{-1}
F(000)	499
Theta range	2.50 to 33.40°
Index ranges	-14<=h<=14, -14<=k<=14, -10<=l<=10
Reflections collected	11529
Independent reflections	721 [R(int) = 0.0128]
Coverage	98.4%
Average Redundancy	15.990
Absorption correction	multi-scan
Max. and min. transmission	0.4330 and 0.3710
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	721 / 0 / 43
Goodness-of-fit on F^2	1.333
Final R indices	718 data; I>2σ(I) R1 = 0.0129, wR2 = 0.0324
	all data R1 = 0.0130, wR2 = 0.0324
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0098P)^2+0.2711P]$ where $P=(F_o^2+2F_c^2)/3$
Extinction coefficient	0.0286(12)
Largest diff. peaks	0.512 and -0.295 eÅ^{-3}

Table 1g. Sample and crystal data for DHAPS86.

Crystal size	0.197 x 0.268 x 0.339 mm
Space group	P 6_3/m
Unit cell dimensions	a = 9.3829(3) Å
	c = 6.8898(2) Å
Volume	525.30(4) Å^3
Z	1
Density (calculated)	3.185 g/cm^3
Absorption coefficient	3.090 mm^{-1}
F(000)	500
Theta range	2.51 to 33.23°
Index ranges	-14<=h<=14, -14<=k<=14, -10<=l<=10
Reflections collected	12830
Independent reflections	715 [R(int) = 0.0134]
Coverage	98.8%
Average redundancy	17.944
Absorption correction	multi-scan
Max. and min. transmission	0.5810 and 0.4210
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	715 / 0 / 43
Goodness-of-fit on F^2	1.294
Final R indices	713 data; I>2σ(I) R1 = 0.0119, wR2 = 0.0298
	all data R1 = 0.0120, wR2 = 0.0299
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0088P)^2+0.2613P]$ where $P=(F_o^2+2F_c^2)/3$
Extinction coefficient	0.0144(10)
Largest diff. peak and hole	0.443 and -0.254 eÅ^{-3}

Table 1h. Sample and crystal data for DHAPS87.

Crystal size	0.302 x 0.346 x 0.371 mm
Space group	P 6_3/m
Unit cell dimensions	a = 9.3777(6) Å
	c = 6.8896(5) Å
Volume	524.71(8) Å^3
Z	1
Density (calculated)	3.190 g/cm^3
Absorption coefficient	3.094 mm^{-1}
F(000)	500
Theta range	2.51 to 33.30°
Index ranges	-14<=h<=14, -14<=k<=14, -10<=l<=10
Reflections collected	11324
Independent reflections	713 [R(int) = 0.0157]
Coverage	98.2%
Average Redundancy	15.882
Absorption correction	multi-scan
Max. and min. transmission	0.4550 and 0.3930
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	713 / 0 / 43
Goodness-of-fit on F^2	1.244
Final R indices	710 data; I>2σ(I) R1 = 0.0122, wR2 = 0.0297
	all data R1 = 0.0123, wR2 = 0.0297
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0082P)^2+0.3016P]$ where $P=(F_o^2+2F_c^2)/3$
Extinction coefficient	0.0491(14)
Largest diff. peaks	0.431 and -0.279 eÅ^{-3}