Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Synthesis, structures, luminescent and molecular recognition properties of three new alkaline earth metal carboxyphosphonates with a 3D supramolecular structure

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Supplementary Materials

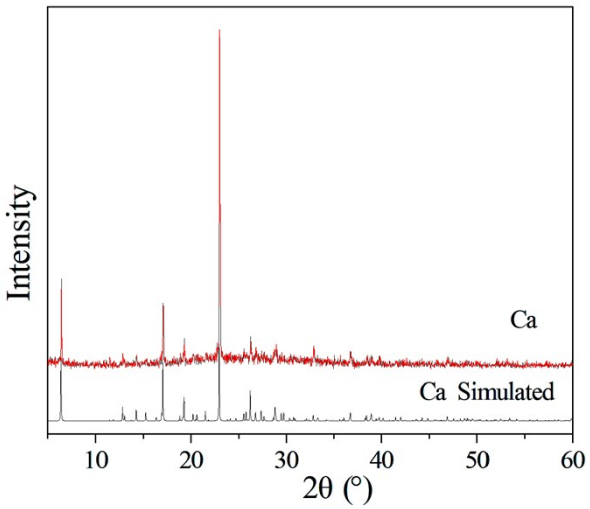


Fig S1. The simulated XRD pattern of compound **1** (down) and experimental powder XRD pattern of compound **1** (up)

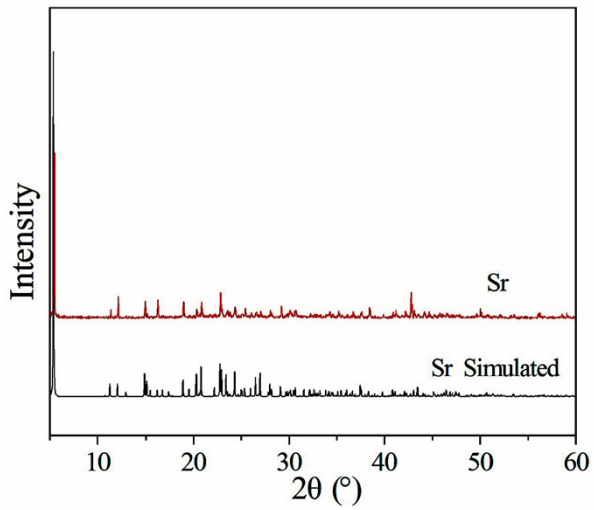


Fig S2. The simulated XRD pattern of compound **2** (down) and experimental powder XRD pattern of compound **2** (up)

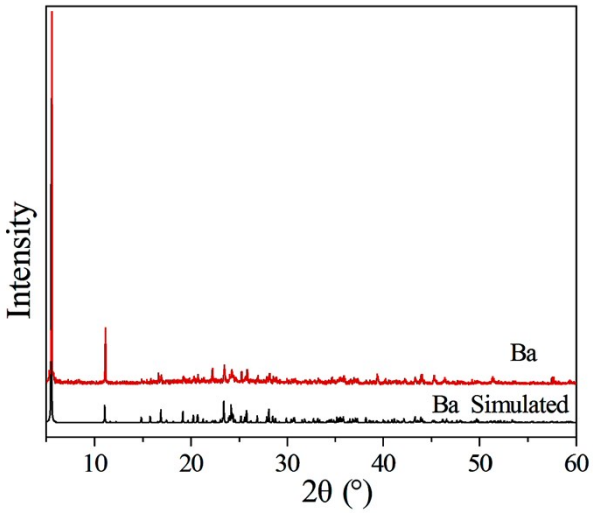


Fig S3. The simulated XRD pattern of compound **3** (down) and experimental powder XRD pattern of compound **3** (up)

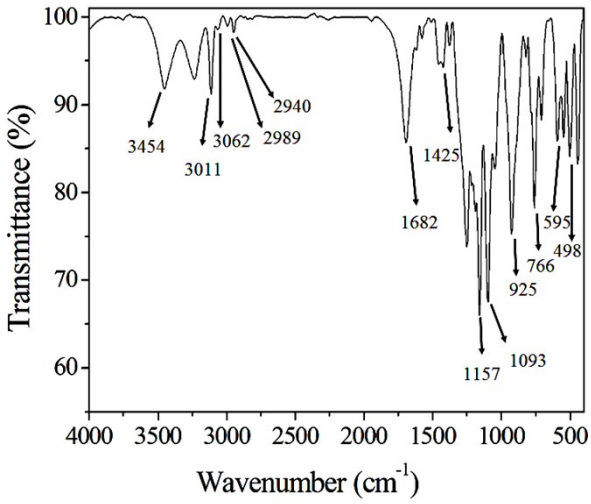


Fig S4. The IR spectrum of compound **1**.

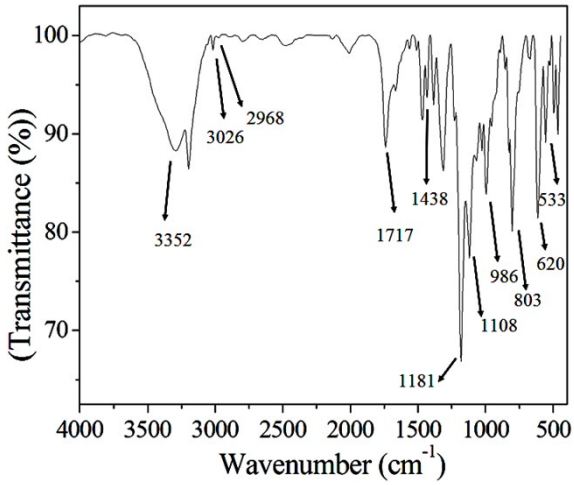


Fig S5. The IR spectrum of compound **2**.

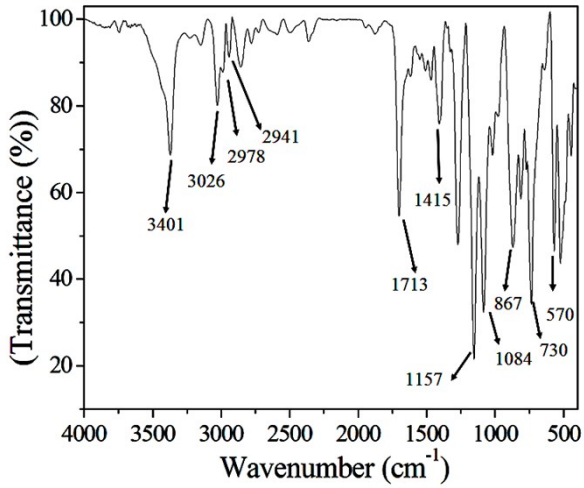


Fig S6. The IR spectrum of compound **3**.

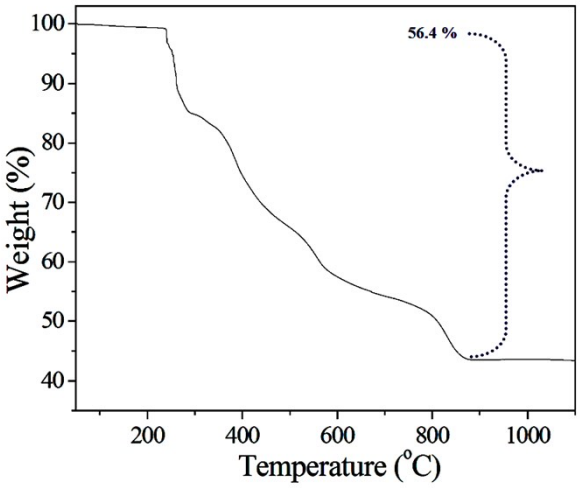


Fig S7. The TG curve of compound **1**.

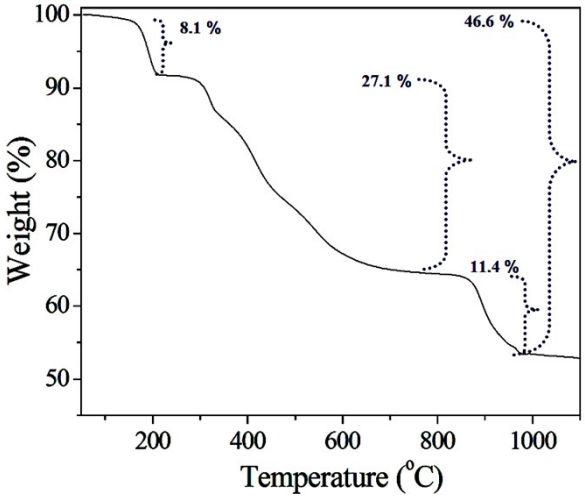


Fig S8. The TG curve of compound **2**.

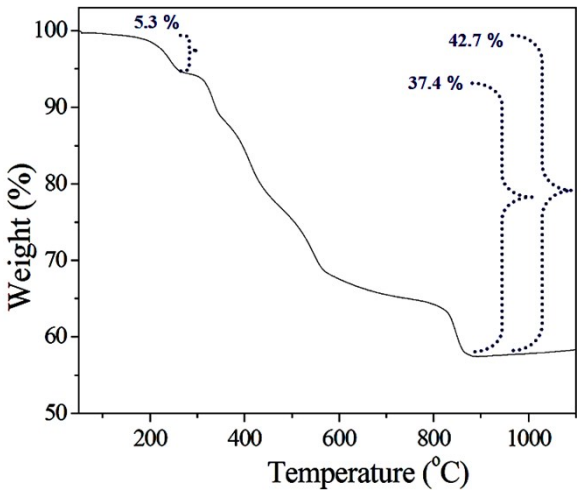


Fig S9. The TG curve of compound **3**.

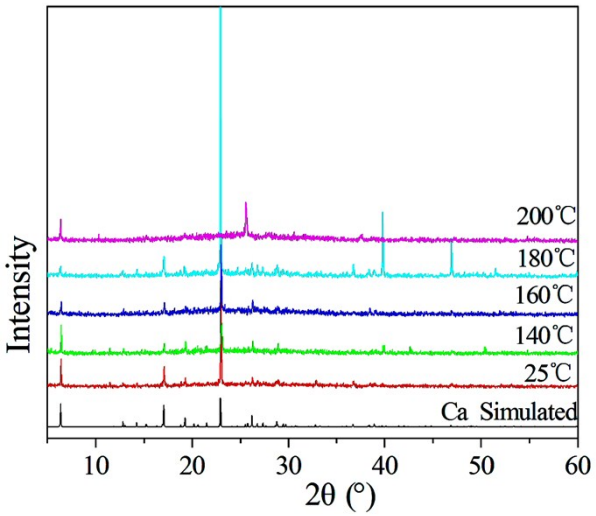


Fig S10. The PXRD patterns for compound **1** on heating from 25–200 ˚C.

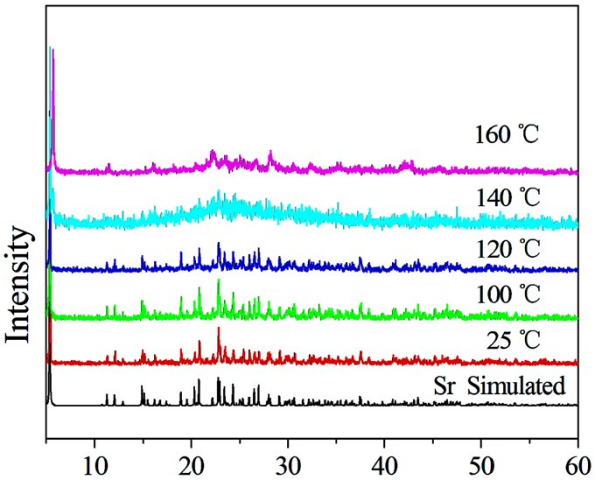


Fig S11. The PXRD patterns for compound **2** on heating from 25–160 ˚C.

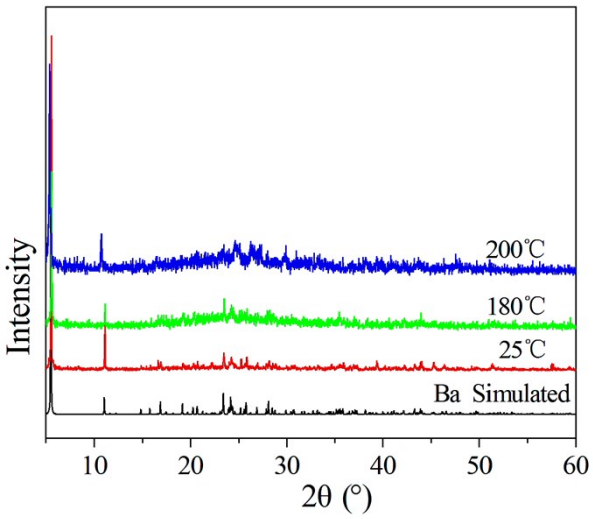
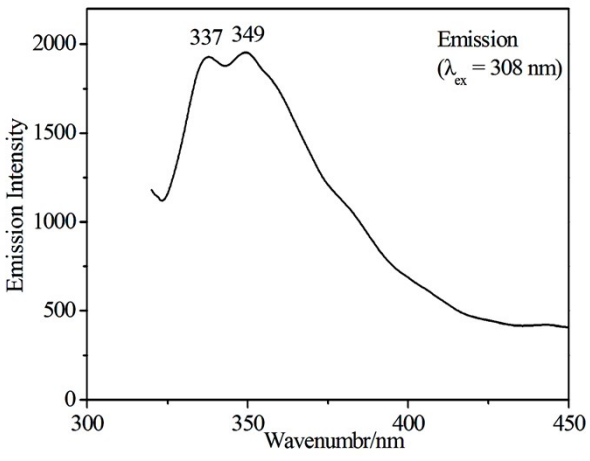


Fig S12. The PXRD patterns for compound **3** on heating from 25–200 ˚C.



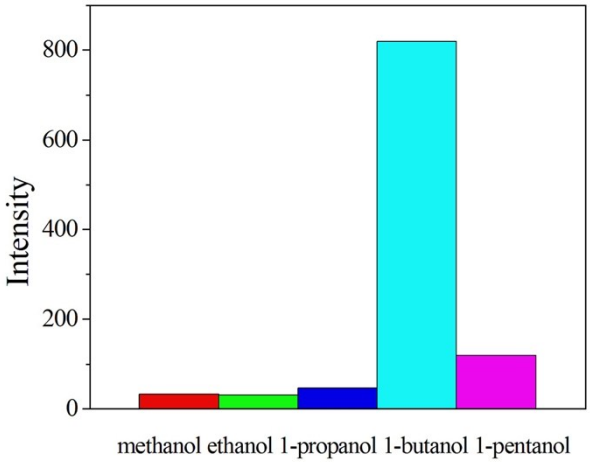


Fig S13. Solid–state emission spectrum of H_5L at room temperature.

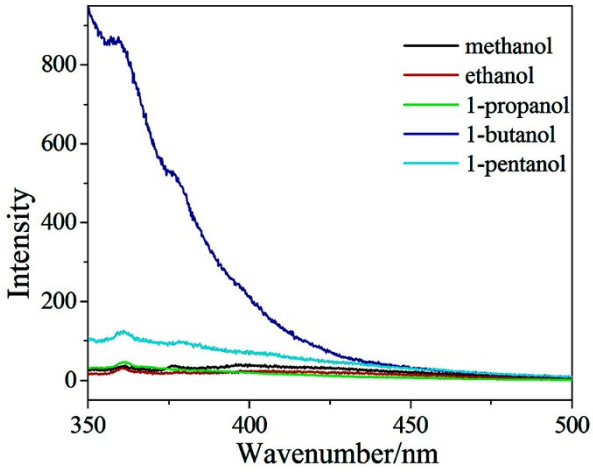


Fig S14. The emission spectra of alcohol solvents when excited at 325 nm.

Fig S15. The transition intensities of various alcohol solvents when excited at 325 nm.

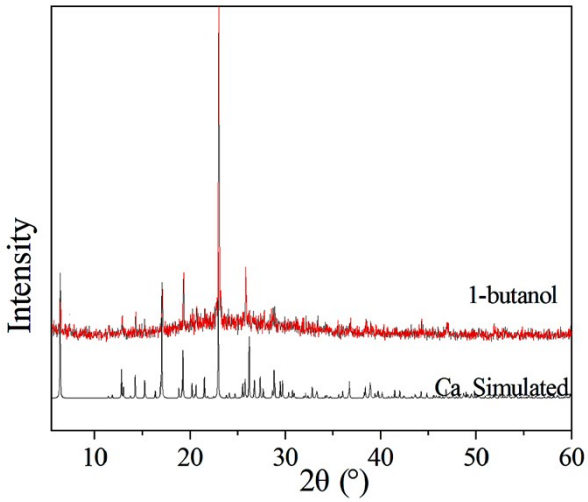


Fig S16. The simulated XRD pattern of compound **1** (down) and diffraction patterns obtained on compound **1** after the introduction of ethanol (up)

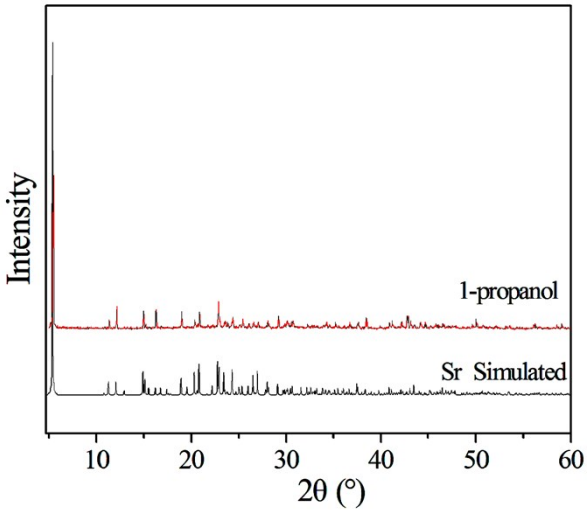


Fig S17. The simulated XRD pattern of compound **2** (down) and diffraction patterns obtained on compound **2** after the introduction of 1-propanol (up).

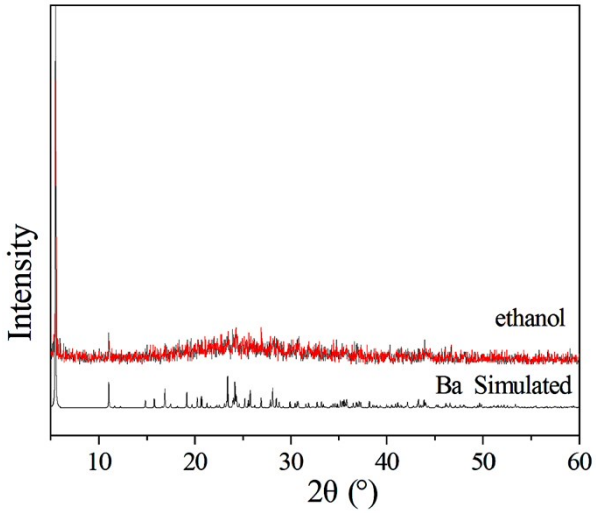


Fig S18. The simulated XRD pattern of compound **3** (down) and diffraction patterns obtained on compound **3** after the introduction of ethanol (up).

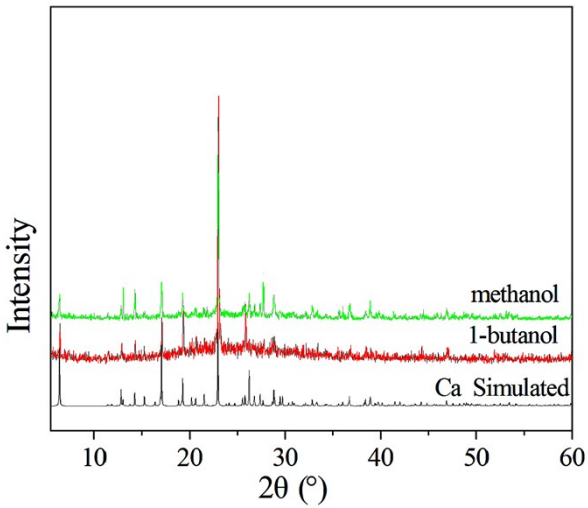


Fig S19. The simulated XRD pattern of compound **1** (down) and diffraction patterns obtained on compound **1** after the introduction of methanol and 1-butanol (up)

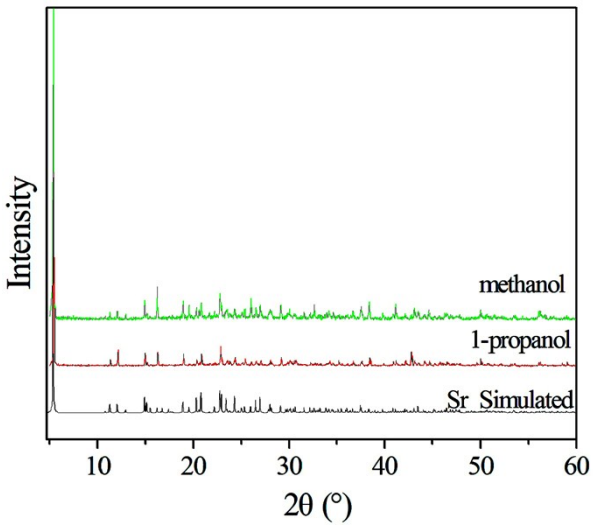


Fig S20. The simulated XRD pattern of compound **2** (down) and diffraction patterns obtained on compound **2** after the introduction of methanol and 1-propanol (up)

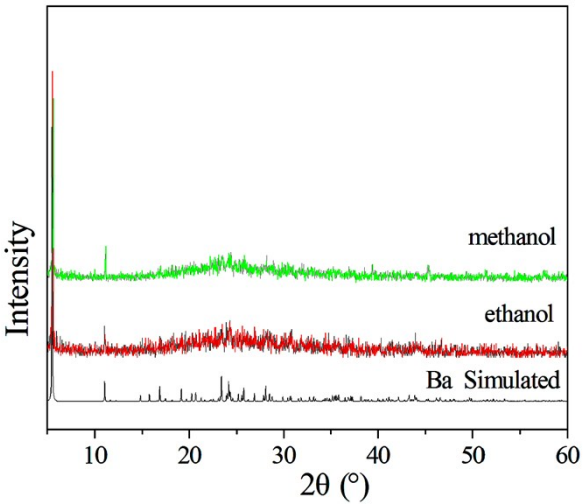


Fig S21. The simulated XRD pattern of compound **3** (down) and diffraction patterns obtained on compound **3** after the introduction of methanol and ethanol (up)

Table S1 Selected Bond Lengths (Å) and Angles (º) for Compound **1**[a]

Ca(1)–O(6)	2.2838(15)	P(1)–C(1)	1.832(2)
Ca(1)–O(3)#1	2.2850(16)	P(2)–O(5)	1.5058(15)
Ca(1)–O(2)#2 Ca(1)–	2.3079(16)	P(2)–O(6)	1.5069(16)
O(5)#2	2.3406(14)	P(2)–O(4)	1.5364(16)
Ca(1)–O(9)	2.4070(16)	P(2)–C(2)	1.841(2)
Ca(1)–O(7)#3	2.4109(17)	O(2)–Ca(1)#4	2.3079(16)
P(1)–O(3)	1.4895(16)	O(3)–Ca(1)#1	2.2850(16)
P(1)–O(2)	1.4956(16)	O(5)–Ca(1)#4	2.2850(16)
P(1)–O(1)	1.5713(17)	O(7)–Ca(1)#3	2.4109(17)
O(6)–Ca(1)–O(3)#1	90.29(6)	O(9)–Ca(1)–O(7)#3	85.01(6)
O(6)–Ca(1)–O(2)#2	88.14(6)	O(3)–P(1)–O(2)	117.82(10)
O(3)#1–Ca(1)–O(2)#2	99.42(6)	O(3)–P(1)–O(1)	110.55(10)
O(6)–Ca(1)–O(5)#2	175.85(6)	O(2)–P(1)–O(1)	106.29(9)
O(3)#1–Ca(1)–O(5)#2	88.16(6)	O(3)–P(1)–C(1)	104.06(9)
O(2)#2–Ca(1)–O(5)#2	88.32(6)	O(2)–P(1)–C(1)	110.77(10)
O(6)–Ca(1)–O(9)	98.79(6)	O(1)–P(1)–C(1)	106.58(10)
O(3)#1–Ca(1)–O(9)	87.43(6)	O(5)–P(2)–O(6)	115.42(9)
O(2)#2–Ca(1)–O(9)	170.27(6)	O(5)–P(2)–O(4)	111.64(9)
O(5)#2–Ca(1)–O(9)	84.98(6)	O(6)–P(2)–O(4)	112.78(9)
O(6)–Ca(1)–O(7)#3	92.99(6)	O(5)–P(2)–C(2)	108.78(9)
O(3)#1–Ca(1)–O(7)#3	172.14(7)	O(6)–P(2)–C(2)	103.17(10)
O(2)#2–Ca(1)–O(7)#3	87.83(7)	O(4)–P(2)–C(2)	103.95(9)
O(5)#2–Ca(1)–O(7)#3	89.03(6)		

[a] Symmetry transformations used to generate equivalent atoms: #1 –x + 2, –y + 1, –z + 1; #2 x – 1, y, z; #3 –x + 1, –y + 1, –z; #4 x + 1, y, z

Table S2 Selected Bond Lengths (Å) and Angles (º) for Compound **2**[a]

Sr(1)–O(2)#1	2.550(3)	P(1)–C(1)	1.842(4)
Sr(1)–O(1)	2.558(2)	P(2)–O(5)	1.504(3)
Sr(1)–O(3)#2	2.575(2)	P(2)–O(6)	1.507(3)
Sr(1)–O(6)#3	2.596(3)	P(2)–O(4)	1.564(3)
Sr(1)–O(10)	2.600(3)	P(2)–C(2)	1.8197(17)
Sr(1)–O(9)	2.629(3)	O(2)–Sr(1)#1	2.551(3)
Sr(1)–O(9)#4	2.632(3)	O(3)–Sr(1)#5	2.575(2)
P(1)–O(2)	1.511(3)	O(6)–Sr(1)#6	2.596(3)
P(1)–O(3)	1.521(3)	O(9)–Sr(1)#4	2.632(3)
P(1)–O(1)	1.528(3)		
O(2)#1–Sr(1)–O(1)	123.50(8)	O(3)#2–Sr(1)–O(9)#4	76.34(8)
O(2)#1-Sr(1)–O(3)#2	141.78(9)	O(10)–Sr(1)–O(9)#4	141.61(8)
O(1)–Sr(1)–O(3)#2	88.06(8)	O(6)#3–Sr(1)–O(9)#4	145.48(8)
O(2)#1–Sr(1)–O(10)	71.60(9)	O(9)–Sr(1)–O(9)#4 O(2)–	73.44(9)
O(1)–Sr(1)–O(10)	79.20(8)	P(1)–O(3) O(2)–	114.59(15)
O(3)#2–Sr(1)–O(10)	141.82(9)	P(1)–O(1) O(3)–	110.10(15)
O(6)#3–Sr(1)–O(10)	70.24(8)	P(1)–O(1) O(2)–	112.86(16)
O(2)#1–Sr(1)–O(6)#3	118.97(9)	P(1)–C(1) O(3)–	109.16(17)
O(1)–Sr(1)–O(6)#3	93.37(9)	P(1)–C(1) O(1)–	103.02(15)
O(3)#2–Sr(1)–O(6)#3	74.84(8)	P(1)–C(1) O(5)–	106.52(16)
O(2)#1–Sr(1)–O(9)	71.41(8)	P(2)–O(6) O(5)–	116.89(15)
O(1)–Sr(1)–O(9)	164.36(8)	P(2)–O(4) O(6)–	111.75(15)
O(3)#2–Sr(1)–O(9)	76.35(8)	P(2)–O(4) O(6)–	110.38(16)
O(10)–Sr(1)–O(9)	112.49(8)	P(2)–C(2) O(5)–	106.98(12)
O(6)#3–Sr(1)–O(9)	81.60(8)	P(2)–C(2) O(4)–	104.48(13)
O(2)#1–Sr(1)–O(9)#4	75.25(9)	P(2)–C(2)	105.42(12)
O(1)–Sr(1)–O(9)#4	104.26(8)		

[a] Symmetry transformations used to generate equivalent atoms: #1 x, y + 1, z + 1; #2 x + 1, y, z; #3 x, y 1, z; #4 x + 1, y +1, z + 1; #5 x 1, y, z; #6 x, y + 1, z

Table S3 Selected Bond Lengths (Å) and Angles (º) for Compound **3**[a]

Ba(1)–O(4)#1	2.733(6)	P(1)–C(1)	1.814(9)
Ba(1)–O(3)#1	2.781(6)	P(2)–O(6)	1.556(6)
Ba(1)–O(5)#2	2.804(6)	P(2)–O(4)	1.504(6)
Ba(1)–O(3)#3	2.876(6)	P(2)–O(5)	1.507(6)
Ba(1)–O(9)#4	2.880(6)	P(2)–C(2)	1.849(9)
Ba(1)–O(9)	2.911(6)	O(1)–Ba(1)#6	3.053(7)
Ba(1)–O(6)	2.956(6)	O(2)–Ba(1)#7	3.110(6)
Ba(1)–O(4)	3.003(6)	O(3)–Ba(1)#1	2.781(6)
Ba(1)–O(1)#3	3.053(7)	O(3)–Ba(1)#6	2.876(6)
Ba(1)–O(2)#5	3.110(6)	O(4)–Ba(1)#1	2.733(6)
P(1)–O(3)	1.494(6)	O(5)–Ba(1)#4	2.804(6)
P(1)–O(2)	1.508(6)	O(9)–Ba(1)#2	2.880(6)
P(1)–O(1)	1.566(6)		
O(4)#1–Ba(1)–O(3)#1	75.54(19)	O(5)–P(2)–O(6)	112.8(3)
O(4)#1–Ba(1)–O(5)#2	83.46(18)	O(5)–P(2)–C(2)	110.1(4)
O(3)#1–Ba(1)–O(5)#2	148.05(18)	O(6)–P(2)–C(2)	100.9(4)
O(4)#1–Ba(1)–O(3)#3	118.04(18)	O(4)–P(2)–C(2)	106.1(4)
O(3)#1–Ba(1)–O(3)#3	63.2(2)	O(4)#1–Ba(1)–O(4)	72.52(19)
O(5)#2–Ba(1)–O(3)#3	108.35(17)	O(3)#1–Ba(1)–O(4)	127.58(17)
O(3)#3–Ba(1)–O(9)#4	77.43(18)	O(5)#2–Ba(1)–O(4)	65.58(16)
O(3)#1–Ba(1)–O(9)#4	67.50(17)	O(9)#4–Ba(1)–O(4)	167.98(17)
O(5)#2–Ba(1)–O(9)#4	131.01(17)	O(3)#3–Ba(1)–O(4)	119.68(17)
O(4)#1–Ba(1)–O(9)#4	120.50(17)	O(9)–Ba(1)–O(4)	65.72(16)
O(4)#1–Ba(1)–O(9)	69.15(18)	O(6)–Ba(1)–O(4)	49.68(16)
O(3)#1–Ba(1)–O(9)	84.58(17)	O(4)#1–Ba(1)–O(1)#3	136.62(17)
O(5)#2–Ba(1)–O(9)	65.35(17)	O(3)#1–Ba(1)–O(1)#3	112.74(17)
O(3)#3–Ba(1)–O(9)	140.9(2)	O(5)#2–Ba(1)–O(1)#3	67.92(16)
O(9)#4–Ba(1)–O(9)	63.09(17)	O(3)#3–Ba(1)–O(1)#3	49.56(16)
O(4)#1–Ba(1)–O(6)	120.58(17)	O(9)#4–Ba(1)–O(1)#3	145.89(17)
O(3)#1–Ba(1)–O(6)	127.06(17)	O(9)–Ba(1)–O(1)#3	69.48(17)
O(5)#2–Ba(1)–O(6)	84.37(16)	O(6)–Ba(1)–O(1)#3	89.32(16)
O(3)#3–Ba(1)–O(6)	121.02(17)	O(4)–Ba(1)–O(1)#3	119.12(16)
O(9)–Ba(1)–O(6)	68.29(17)	O(4)#1–Ba(1)–O(2)#5	139.88(17)
O(9)#4–Ba(1)–O(6)	147.63(16)	O(3)#1–Ba(1)–O(2)#5	71.85(17)
O(3)–P(1)–O(2)	117.7(4)	O(5)#2–Ba(1)–O(2)#5	135.48(17)
O(3)–P(1)–O(1)	109.0(4)	O(3)#3–Ba(1)–O(2)#5	65.70(16)
O(2)–P(1)–O(1)	111.8(3)	O(9)#4–Ba(1)–O(2)#5	68.95(17)
O(3)–P(1)–C(1)	104.2(4)	O(9)–Ba(1)–O(2)#5	128.78(16)
O(2)–P(1)–C(1)	108.0(4)	O(6)–Ba(1)–O(2)#5	66.15(15)
O(1)–P(1)–C(1)	105.3(4)	O(4)–Ba(1)–O(2)#5	78.68(16)
O(4)–P(2)–O(5)	116.0(4)	O(1)#3–Ba(1)–O(2)#5	110.63(15)
O(4)–P(2)–O(6)	109.8(3)		

[a] Symmetry transformations used to generate equivalent atoms: #1 –x + 1, –y + 1, –z; #2 x – 1, y, z; #3 x, y + 1, z; #4 x + 1, y, z; #5 x + 1, y + 1, z; #6 x, y–1, z; #7 x – 1, y – 1, z