

Electronic supplementary information

A Series of Complexes Constructed by Different Calix[4]arene Derivatives

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Table S1. Selected bond distances (Å) and angles (°) for compounds **1-13**.

1			
Mn(1)-N(3)	2.204(3)	Mn(1)-N(2)	2.232(3)
Mn(1)-N(6)	2.240(3)	Mn(1)-N(4)	2.250(3)
Mn(1)-N(1)	2.281(3)	Mn(1)-N(5)	2.295(3)
N(3)-Mn(1)-N(2)	108.21(12)	N(3)-Mn(1)-N(6)	154.59(12)
N(2)-Mn(1)-N(6)	93.26(11)	N(3)-Mn(1)-N(4)	75.69(12)
N(2)-Mn(1)-N(4)	158.54(11)	N(6)-Mn(1)-N(4)	89.36(12)
N(3)-Mn(1)-N(1)	86.34(11)	N(2)-Mn(1)-N(1)	73.42(10)
N(6)-Mn(1)-N(1)	113.42(12)	N(4)-Mn(1)-N(1)	85.99(11)
N(3)-Mn(1)-N(5)	89.36(11)	N(2)-Mn(1)-N(5)	97.45(11)
N(6)-Mn(1)-N(5)	74.13(12)	N(4)-Mn(1)-N(5)	103.75(11)
N(1)-Mn(1)-N(5)	168.06(11)		
2			
Cd(1')-N(1)	1.564(6)	Cd(1')-N(5)	2.341(5)
Cd(1')-N(2)	2.449(5)	Cd(1')-N(4)	2.590(5)
Cd(1')-N(3)	2.605(5)	Cd(1)-N(4)	2.319(3)
Cd(1)-N(1)	2.326(4)	Cd(1)-N(6)	2.336(4)
Cd(1)-N(2)	2.349(4)	Cd(1)-N(3)	2.389(3)
Cd(1)-N(5)	2.403(3)		
N(1)-Cd(1')-N(5)	115.4(2)	N(1)-Cd(1')-N(2)	84.0(2)
N(5)-Cd(1')-N(2)	104.47(19)	N(1)-Cd(1')-N(4)	129.9(3)
N(5)-Cd(1')-N(4)	92.66(17)	N(2)-Cd(1')-N(4)	130.0(2)
N(1)-Cd(1')-N(3)	96.5(2)	N(5)-Cd(1')-N(3)	148.1(2)
N(2)-Cd(1')-N(3)	78.71(15)	N(4)-Cd(1')-N(3)	63.92(14)
N(4)-Cd(1)-N(1)	109.28(13)	N(4)-Cd(1)-N(6)	95.24(13)
N(1)-Cd(1)-N(6)	151.31(13)	N(4)-Cd(1)-N(2)	156.12(12)
N(1)-Cd(1)-N(2)	72.52(13)	N(6)-Cd(1)-N(2)	91.15(14)
N(4)-Cd(1)-N(3)	71.46(12)	N(1)-Cd(1)-N(3)	85.05(12)
N(6)-Cd(1)-N(3)	117.69(12)	N(2)-Cd(1)-N(3)	85.19(13)
N(4)-Cd(1)-N(5)	98.23(12)	N(1)-Cd(1)-N(5)	89.37(13)
N(6)-Cd(1)-N(5)	72.12(13)	N(2)-Cd(1)-N(5)	105.64(13)
N(3)-Cd(1)-N(5)	165.75(12)		
3			
Ni(1)-N(5)	2.037(7)	Ni(1)-N(6)	2.090(5)

Ni(1)-N(4)	2.097(5)	Ni(1)-N(1)	2.098(7)
Ni(1)-N(3)	2.105(5)	Ni(1)-N(2)	2.123(7)
N(5)-Ni(1)-N(6)	80.1(3)	N(5)-Ni(1)-N(4)	92.5(2)
N(6)-Ni(1)-N(4)	95.3(2)	N(5)-Ni(1)-N(1)	172.3(2)
N(6)-Ni(1)-N(1)	94.8(2)	N(4)-Ni(1)-N(1)	93.8(2)
N(5)-Ni(1)-N(3)	95.5(3)	N(6)-Ni(1)-N(3)	173.8(3)
N(4)-Ni(1)-N(3)	80.4(2)	N(1)-Ni(1)-N(3)	90.0(2)
N(5)-Ni(1)-N(2)	96.0(3)	N(6)-Ni(1)-N(2)	91.12(18)
N(4)-Ni(1)-N(2)	170.1(3)	N(1)-Ni(1)-N(2)	78.2(3)
N(3)-Ni(1)-N(2)	93.7(2)		

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Co(1)-N(1)	2.108(6)	Co(1)-N(2)	2.162(6)
N(1)-Co(1)-N(1) ^{#1}	95.9(2)	N(1)-Co(1)-N(2) ^{#1}	168.5(2)
N(1)-Co(1)-N(2)	76.8(2)	N(1) ^{#1} -Co(1)-N(2)	93.7(2)
N(2) ^{#1} -Co(1)-N(2) ^{#2}	94.64(19)		

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Co(1)-N(1)	2.1671(17)	Co(1)-N(3)	2.175(2)
Co(1)-N(2)	2.1852(18)		
N(1)-Co(1)-N(1) ^{#1}	98.65(11)	N(1)-Co(1)-N(3)	165.94(8)
N(1) ^{#1} -Co(1)-N(3)	92.57(9)	N(1)-Co(1)-N(3) ^{#1}	92.57(9)
N(1) ^{#1} -Co(1)-N(3) ^{#1}	165.94(8)	N(3)-Co(1)-N(3) ^{#1}	77.73(13)
N(1)-Co(1)-N(2)	79.22(7)	N(1) ^{#1} -Co(1)-N(2)	92.58(7)
N(3)-Co(1)-N(2)	91.90(8)	N(3) ^{#1} -Co(1)-N(2)	97.84(8)
N(1)-Co(1)-N(2) ^{#1}	92.58(7)	N(1) ^{#1} -Co(1)-N(2) ^{#1}	79.22(7)
N(3)-Co(1)-N(2) ^{#1}	97.84(8)	N(3) ^{#1} -Co(1)-N(2) ^{#1}	91.90(8)
N(2)-Co(1)-N(2) ^{#1}	167.50(11)		

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Zn(1)-N(1)	2.016(4)	Zn(1)-N(6')	2.03(3)
Zn(1)-N(5)	2.057(7)	Zn(1)-N(3)	2.067(6)
Zn(1)-N(4)	2.137(14)	Zn(1)-N(4')	2.22(2)
Zn(1)-N(5')	2.22(4)	Zn(1)-N(6)	2.300(9)
N(1)-Zn(1)-N(6')	109.3(9)	N(1)-Zn(1)-N(5)	115.6(4)
N(6')-Zn(1)-N(5)	84.0(9)	N(1)-Zn(1)-N(3)	113.0(3)
N(6')-Zn(1)-N(3)	81.4(10)	N(5)-Zn(1)-N(3)	131.4(5)
N(1)-Zn(1)-N(4)	96.4(5)	N(6')-Zn(1)-N(4)	150.9(10)

N(5)-Zn(1)-N(4)	97.3(6)	N(3)-Zn(1)-N(4)	76.0(5)
N(1)-Zn(1)-N(4')	104.3(6)	N(6')-Zn(1)-N(4')	146.2(10)
N(5)-Zn(1)-N(4')	78.3(6)	N(3)-Zn(1)-N(4')	89.0(6)
N(4)-Zn(1)-N(4')	19.1(6)	N(1)-Zn(1)-N(5')	96.4(11)
N(6')-Zn(1)-N(5')	85.6(15)	N(5)-Zn(1)-N(5')	19.8(9)
N(3)-Zn(1)-N(5')	150.4(11)	N(4)-Zn(1)-N(5')	105.3(14)
N(4')-Zn(1)-N(5')	87.1(14)	N(1)-Zn(1)-N(6)	94.4(3)
N(6')-Zn(1)-N(6)	19.3(8)	N(5)-Zn(1)-N(6)	79.0(4)
N(3)-Zn(1)-N(6)	98.6(4)	N(4)-Zn(1)-N(6)	169.1(5)
N(4')-Zn(1)-N(6)	155.1(6)	N(5')-Zn(1)-N(6)	74.6(13)
7			
Zn(1)-O(25)	1.941(2)	Zn(1)-O(6) ^{#1}	1.965(2)
Zn(1)-O(23)	1.983(2)	Zn(1)-O(1W)	2.182(3)
Zn(1)-O(19)	2.210(2)	Zn(2)-O(18)	1.953(2)
Zn(2)-O(9)	1.9670(19)	Zn(2)-N(1)	2.019(3)
Zn(2)-O(7) ^{#1}	2.030(2)	Zn(3)-O(25)	1.954(3)
Zn(3)-O(20)	1.972(2)	Zn(3)-O(5) ^{#1}	2.068(2)
Zn(3)-O(21) ^{#2}	2.145(2)	Zn(3)-O(22) ^{#2}	2.200(3)
Na(1)-O(12)	2.225(3)	Na(1)-O(2)	2.326(2)
Na(1)-O(1)	2.407(2)	Na(1)-O(3)	2.426(3)
Na(1)-O(4)	2.465(2)	Na(1)-O(8)	2.480(2)
Na(1)-O(10)	2.479(3)		
Na(2)-O(14)	2.297(2)	Na(2)-O(15)	2.369(2)
Na(2)-O(16)	2.302(2)	Na(2)-O(19)	2.306(2)
Na(2)-O(23)	2.308(3)	Na(2)-O(13)	2.334(3)
Na(3)-O(2W)	2.391(3)	Na(3)-O(10)	2.409(3)
Na(3)-O(12)	2.441(3)	Na(3)-O(18) ^{#1}	2.463(3)
Na(3)-O(8)	2.539(3)	Na(3)-O(7) ^{#1}	2.620(3)
O(25)-Zn(1)-O(6) ^{#1}	112.84(10)	O(25)-Zn(1)-O(23)	131.75(10)
O(6) ^{#1} -Zn(1)-O(23)	114.93(9)	O(25)-Zn(1)-O(1W)	93.47(11)
O(6) ^{#1} -Zn(1)-O(1W)	93.01(10)	O(23)-Zn(1)-O(1W)	90.47(9)
O(25)-Zn(1)-O(19)	88.11(10)	O(6) ^{#1} -Zn(1)-O(19)	97.58(9)
O(23)-Zn(1)-O(19)	79.48(8)	O(1W)-Zn(1)-O(19)	167.73(9)
O(18)-Zn(2)-O(9)	110.08(9)	O(18)-Zn(2)-N(1)	120.89(11)
O(9)-Zn(2)-N(1)	104.35(10)	O(18)-Zn(2)-O(7) ^{#1}	111.76(9)

O(9)-Zn(2)-O(7) ^{#1}	107.20(9)	N(1)-Zn(2)-O(7) ^{#1}	101.48(10)
O(25)-Zn(3)-O(20)	99.76(10)	O(25)-Zn(3)-O(5) ^{#1}	103.51(10)
O(20)-Zn(3)-O(5) ^{#1}	104.99(10)	O(25)-Zn(3)-O(21) ^{#2}	99.80(10)
O(20)-Zn(3)-O(21) ^{#2}	145.10(10)	O(5) ^{#1} -Zn(3)-O(21) ^{#2}	98.14(9)
O(25)-Zn(3)-O(22) ^{#2}	154.55(10)	O(20)-Zn(3)-O(22) ^{#2}	91.30(10)
O(5) ^{#1} -Zn(3)-O(22) ^{#2}	95.53(9)	O(21) ^{#2} -Zn(3)-O(22) ^{#2}	60.36(10)
O(12)-Na(1)-O(2)	150.78(8)	O(12)-Na(1)-O(1)	94.22(10)
O(2)-Na(1)-O(1)	92.57(8)	O(12)-Na(1)-O(3)	108.79(11)
O(2)-Na(1)-O(3)	83.00(8)	O(1)-Na(1)-O(3)	140.09(8)
O(12)-Na(1)-O(4)	69.46(8)	O(2)-Na(1)-O(4)	139.75(8)
O(1)-Na(1)-O(4)	78.29(8)	O(3)-Na(1)-O(4)	79.94(8)
O(12)-Na(1)-O(8)	86.33(9)	O(2)-Na(1)-O(8)	66.32(7)
O(1)-Na(1)-O(8)	83.20(8)	O(3)-Na(1)-O(8)	129.10(8)
O(4)-Na(1)-O(8)	148.02(9)	O(12)-Na(1)-O(10)	79.71(10)
O(2)-Na(1)-O(10)	80.98(9)	O(1)-Na(1)-O(10)	151.89(8)
O(3)-Na(1)-O(10)	66.62(7)	O(4)-Na(1)-O(10)	123.52(9)
O(8)-Na(1)-O(10)	69.11(8)	O(14)-Na(2)-O(16)	147.51(9)
O(14)-Na(2)-O(19)	71.66(8)	O(16)-Na(2)-O(19)	140.71(10)
O(14)-Na(2)-O(23)	141.02(8)	O(16)-Na(2)-O(23)	69.90(8)
O(19)-Na(2)-O(23)	71.21(8)	O(14)-Na(2)-O(13)	85.90(9)
O(16)-Na(2)-O(13)	89.13(8)	O(19)-Na(2)-O(13)	100.29(9)
O(23)-Na(2)-O(13)	112.02(9)	O(14)-Na(2)-O(15)	85.42(9)
O(16)-Na(2)-O(15)	82.16(8)	O(19)-Na(2)-O(15)	105.68(9)
O(23)-Na(2)-O(15)	93.48(9)	O(13)-Na(2)-O(15)	148.35(9)
O(2W)-Na(3)-O(10)	119.93(11)	O(2W)-Na(3)-O(12)	77.96(10)
O(10)-Na(3)-O(12)	77.04(9)	O(2W)-Na(3)-O(18) ^{#1}	104.13(10)
O(10)-Na(3)-O(18) ^{#1}	135.56(10)	O(12)-Na(3)-O(18) ^{#1}	120.59(11)
O(2W)-Na(3)-O(8)	153.59(12)	O(10)-Na(3)-O(8)	69.24(8)
O(12)-Na(3)-O(8)	80.67(8)	O(18) ^{#1} -Na(3)-O(8)	73.91(8)
O(2W)-Na(3)-O(7) ^{#1}	89.53(11)	O(10)-Na(3)-O(7) ^{#1}	80.69(8)
O(12)-Na(3)-O(7) ^{#1}	144.17(11)	O(18) ^{#1} -Na(3)-O(7) ^{#1}	94.92(8)
O(8)-Na(3)-O(7) ^{#1}	116.84(8)		
8			
Zn(1)-O(25)	1.947(3)	Zn(1)-O(6)	1.973(2)
Zn(1)-O(23) ^{#1}	1.986(2)	Zn(1)-O(1W)	2.161(3)

Zn(1)-O(19) ^{#1}	2.240(2)	Zn(2)-O(18)	1.950(2)
Zn(2)-O(9)	1.966(2)	Zn(2)-O(7) ^{#1}	2.016(2)
Zn(2)-N(1)	2.035(3)	Zn(3)-O(25)	1.959(3)
Zn(3)-O(20) ^{#1}	1.972(2)	Zn(3)-O(5)	2.107(2)
Zn(3)-O(22) ^{#2}	2.123(3)	Zn(3)-O(21) ^{#2}	2.237(3)
Na(1)-O(12)	2.229(3)	Na(1)-O(2)	2.318(2)
Na(1)-O(1)	2.415(2)	Na(1)-O(3)	2.424(2)
Na(1)-O(4)	2.474(3)	Na(1)-O(8)	2.482(3)
Na(1)-O(10)	2.506(3)	Na(2)-O(19)	2.299(3)
Na(2)-O(14)	2.300(3)	Na(2)-O(16)	2.303(2)
Na(2)-O(23)	2.311(2)	Na(2)-O(13)	2.343(3)
Na(2)-O(15)	2.369(2)	Na(3)-O(2W)	2.377(4)
Na(3)-O(10) ^{#1}	2.430(3)	Na(3)-O(12) ^{#1}	2.435(3)
Na(3)-O(18)	2.459(3)	Na(3)-O(8) ^{#1}	2.573(3)
Na(3)-O(7)	2.665(3)		
O(25)-Zn(1)-O(6)	112.41(10)	O(25)-Zn(1)-O(23) ^{#1}	132.32(9)
O(6)-Zn(1)-O(23) ^{#1}	114.80(10)	O(25)-Zn(1)-O(1W)	93.06(12)
O(6)-Zn(1)-O(1W)	93.46(11)	O(23) ^{#1} -Zn(1)-O(1W)	90.47(11)
O(25)-Zn(1)-O(19) ^{#1}	88.45(10)	O(6)-Zn(1)-O(19) ^{#1}	98.01(9)
O(23) ^{#1} -Zn(1)-O(19) ^{#1}	78.97(9)	O(1W)-Zn(1)-O(19) ^{#1}	166.89(10)
O(18)-Zn(2)-O(9)	111.16(9)	O(18)-Zn(2)-O(7) ^{#1}	113.63(10)
O(9)-Zn(2)-O(7) ^{#1}	107.34(10)	O(18)-Zn(2)-N(1)	118.42(11)
O(9)-Zn(2)-N(1)	103.50(10)	O(7) ^{#1} -Zn(2)-N(1)	101.67(10)
O(25)-Zn(3)-O(20) ^{#1}	101.81(10)	O(25)-Zn(3)-O(5)	102.26(10)
O(20) ^{#1} -Zn(3)-O(5)	103.90(10)	O(25)-Zn(3)-O(22) ^{#2}	153.10(11)
O(20) ^{#1} -Zn(3)-O(22) ^{#2}	94.83(10)	O(5)-Zn(3)-O(22) ^{#2}	93.94(10)
O(25)-Zn(3)-O(21) ^{#2}	96.74(11)	O(20) ^{#1} -Zn(3)-O(21) ^{#2}	149.70(11)
O(5)-Zn(3)-O(21) ^{#2}	95.20(10)	O(22) ^{#2} -Zn(3)-O(21) ^{#2}	60.12(11)
O(12)-Na(1)-O(2)	151.02(11)	O(12)-Na(1)-O(1)	95.61(11)
O(2)-Na(1)-O(1)	92.78(8)	O(12)-Na(1)-O(3)	106.68(11)
O(2)-Na(1)-O(3)	83.64(8)	O(1)-Na(1)-O(3)	139.89(8)
O(12)-Na(1)-O(4)	69.03(9)	O(2)-Na(1)-O(4)	139.95(8)
O(1)-Na(1)-O(4)	77.85(8)	O(3)-Na(1)-O(4)	79.64(8)
O(12)-Na(1)-O(8)	86.94(10)	O(2)-Na(1)-O(8)	66.51(8)
O(1)-Na(1)-O(8)	83.50(8)	O(3)-Na(1)-O(8)	129.61(9)

O(4)-Na(1)-O(8)	147.61(8)	O(12)-Na(1)-O(10)	79.36(11)
O(2)-Na(1)-O(10)	80.34(9)	O(1)-Na(1)-O(10)	152.21(9)
O(3)-Na(1)-O(10)	66.52(8)	O(4)-Na(1)-O(10)	123.99(10)
O(8)-Na(1)-O(10)	69.03(8)	O(19)-Na(2)-O(14)	71.70(8)
O(19)-Na(2)-O(16)	141.30(9)	O(14)-Na(2)-O(16)	146.90(9)
O(19)-Na(2)-O(23)	71.54(9)	O(14)-Na(2)-O(23)	141.47(10)
O(16)-Na(2)-O(23)	70.16(8)	O(19)-Na(2)-O(13)	100.81(9)
O(14)-Na(2)-O(13)	85.28(9)	O(16)-Na(2)-O(13)	88.86(9)
O(23)-Na(2)-O(13)	112.67(9)	O(19)-Na(2)-O(15)	105.47(9)
O(14)-Na(2)-O(15)	85.71(9)	O(16)-Na(2)-O(15)	82.14(9)
O(23)-Na(2)-O(15)	93.19(9)	O(13)-Na(2)-O(15)	147.86(9)
O(2W)-Na(3)-O(10) ^{#1}	122.21(13)	O(2W)-Na(3)-O(12) ^{#1}	78.59(12)
O(10) ^{#1} -Na(3)-O(12) ^{#1}	77.08(10)	O(2W)-Na(3)-O(18)	103.00(11)
O(10) ^{#1} -Na(3)-O(18)	134.25(11)	O(12) ^{#1} -Na(3)-O(18)	122.14(12)
O(2W)-Na(3)-O(8) ^{#1}	153.13(14)	O(10) ^{#1} -Na(3)-O(8) ^{#1}	68.74(8)
O(12) ^{#1} -Na(3)-O(8) ^{#1}	80.78(10)	O(18)-Na(3)-O(8) ^{#1}	73.98(8)
O(2W)-Na(3)-O(7)	90.16(12)	O(10) ^{#1} -Na(3)-O(7)	79.72(9)
O(12) ^{#1} -Na(3)-O(7)	143.04(12)	O(18)-Na(3)-O(7)	94.61(9)
O(8) ^{#1} -Na(3)-O(7)	116.59(9)		
9			
Co(1)-O(13)	2.041(2)	Co(1)-O(2W)	2.076(3)
Co(1)-O(10)	2.086(2)	Co(1)-O(12)	2.118(2)
Co(1)-O(1W)	2.120(2)	Co(1)-O(8)	2.138(2)
Co(1)-Na(1)	3.2360(16)	Co(2)-O(13)	2.072(2)
Co(2)-O(13) ^{#1}	2.073(2)	Co(2)-O(6) ^{#2}	2.093(2)
Co(2)-O(7) ^{#1}	2.103(2)	Co(2)-O(9)	2.124(2)
Co(2)-O(3W)	2.174(2)		
Na(1)-O(4)	2.269(3)	Na(1)-O(8)	2.312(3)
Na(1)-O(12)	2.385(3)	Na(1)-O(2)	2.368(3)
Na(1)-O(1)	2.386(3)	Na(1)-O(3)	2.389(3)
Na(1)-O(10)	2.778(3)		
O(13)-Co(1)-O(2W)	86.65(10)	O(13)-Co(1)-O(10)	99.63(10)
O(2W)-Co(1)-O(10)	173.03(10)	O(13)-Co(1)-O(12)	177.78(9)
O(2W)-Co(1)-O(12)	93.91(10)	O(10)-Co(1)-O(12)	79.94(10)
O(13)-Co(1)-O(1W)	87.92(10)	O(2W)-Co(1)-O(1W)	93.89(11)

O(10)-Co(1)-O(1W)	89.39(10)	O(12)-Co(1)-O(1W)	89.90(10)
O(13)-Co(1)-O(8)	96.28(9)	O(2W)-Co(1)-O(8)	93.74(11)
O(10)-Co(1)-O(8)	82.62(10)	O(12)-Co(1)-O(8)	85.83(9)
O(1W)-Co(1)-O(8)	171.49(10)	O(13)-Co(2)-O(13) ^{#1}	83.19(9)
O(13)-Co(2)-O(6) ^{#2}	178.01(9)	O(13) ^{#1} -Co(2)-O(6) ^{#2}	95.15(9)
O(13)-Co(2)-O(7) ^{#1}	89.22(9)	O(13) ^{#1} -Co(2)-O(7) ^{#1}	95.03(9)
O(6) ^{#2} -Co(2)-O(7) ^{#1}	92.01(9)	O(13)-Co(2)-O(9)	93.71(9)
O(13) ^{#1} -Co(2)-O(9)	92.06(9)	O(6) ^{#2} -Co(2)-O(9)	85.25(9)
O(7) ^{#1} -Co(2)-O(9)	172.61(9)	O(13)-Co(2)-O(3W)	94.93(9)
O(13) ^{#1} -Co(2)-O(3W)	177.64(9)	O(6) ^{#2} -Co(2)-O(3W)	86.76(9)
O(7) ^{#1} -Co(2)-O(3W)	83.50(10)	O(9)-Co(2)-O(3W)	89.48(10)
O(4)-Na(1)-O(8)	146.11(11)	O(4)-Na(1)-O(2)	143.47(10)
O(8)-Na(1)-O(2)	69.64(9)	O(4)-Na(1)-O(12)	69.92(9)
O(8)-Na(1)-O(12)	76.19(9)	O(2)-Na(1)-O(12)	144.27(10)
O(4)-Na(1)-O(1)	83.12(10)	O(8)-Na(1)-O(1)	97.52(9)
O(2)-Na(1)-O(1)	84.34(9)	O(12)-Na(1)-O(1)	90.16(9)
O(4)-Na(1)-O(3)	90.32(10)	O(8)-Na(1)-O(3)	105.37(10)
O(2)-Na(1)-O(3)	82.09(9)	O(12)-Na(1)-O(3)	117.65(10)
O(1)-Na(1)-O(3)	147.25(10)	O(4)-Na(1)-O(10)	97.39(10)
O(8)-Na(1)-O(10)	65.71(8)	O(2)-Na(1)-O(10)	110.18(9)
O(12)-Na(1)-O(10)	62.53(9)	O(1)-Na(1)-O(10)	150.06(9)
O(3)-Na(1)-O(10)	62.55(8)		
10			
Cu(1)-O(8) ^{#1}	1.938(2)	Cu(1)-O(12)	1.971(2)
Cu(1)-O(11) ^{#2}	1.979(2)	Cu(1)-O(7) ^{#3}	1.988(2)
Cu(1)-O(6) ^{#3}	2.156(2)	Cu(1)···Cu(1) ^{#2}	2.632(1)
Cu(2)-O(9)	1.896(2)	Cu(2)-O(5)	1.953(2)
Na(1)-O(9)	2.255(3)	Na(1)-O(1)	2.258(3)
Na(1)-O(3)	2.278(3)	Na(1)-O(5)	2.303(3)
Na(1)-O(2)	2.383(3)	Na(1)-O(4)	2.424(3)
O(8) ^{#1} -Cu(1)-O(12)	90.01(11)	O(8) ^{#1} -Cu(1)-O(11) ^{#2}	89.20(11)
O(12)-Cu(1)-O(11) ^{#2}	168.60(10)	O(8) ^{#1} -Cu(1)-O(7) ^{#3}	168.01(10)
O(12)-Cu(1)-O(7) ^{#3}	87.64(11)	O(11) ^{#2} -Cu(1)-O(7) ^{#3}	90.78(10)
O(8) ^{#1} -Cu(1)-O(6) ^{#3}	99.60(10)	O(12)-Cu(1)-O(6) ^{#3}	101.38(10)
O(11) ^{#2} -Cu(1)-O(6) ^{#3}	89.97(10)	O(7) ^{#3} -Cu(1)-O(6) ^{#3}	92.39(9)

O(9)-Cu(2)-O(5) ^{#1}	94.94(10)	O(9)-Cu(2)-O(5)	85.06(10)
11			
Cu(1)-O(21) ^{#1}	1.932(3)	Cu(1)-O(11)	1.950(3)
Cu(1)-O(8)	1.954(2)	Cu(1)-O(3W)	1.955(3)
Cu(2)-O(17) ^{#2}	1.954(3)	Cu(2)-O(17)	1.954(3)
Cu(2)-O(2W)	1.964(3)	Cu(2)-O(2W) ^{#2}	1.964(3)
Cu(2)-O(1W)	2.226(5)		
Cu(3)-O(25)	1.908(3)	Cu(3)-O(20)	1.955(2)
Cu(3)-O(24) ^{#2}	1.957(3)	Cu(3)-O(22)	1.987(3)
Cu(3)-O(12) ^{#3}	2.377(3)		
Cu(4)-O(25)	1.901(3)	Cu(4)-O(9)	1.935(3)
Cu(4)-O(5) ^{#3}	1.970(3)	Cu(4)-O(19)	1.990(3)
Na(1)-O(20)	2.360(3)	Na(1)-O(23)	2.377(3)
Na(1)-O(14)	2.419(3)	Na(1)-O(16)	2.445(3)
Na(1)-O(15)	2.481(3)	Na(1)-O(13)	2.540(3)
Na(1)-O(22)	2.709(3)		
Na(2)-O(11)	2.247(3)	Na(2)-O(2)	2.263(3)
Na(2)-O(4)	2.304(3)	Na(2)-O(8)	2.360(3)
Na(2)-O(1)	2.381(3)	Na(2)-O(3)	2.414(3)
O(21) ^{#1} -Cu(1)-O(11)	92.28(12)	O(21) ^{#1} -Cu(1)-O(8)	165.54(13)
O(11)-Cu(1)-O(8)	82.25(11)	O(21) ^{#1} -Cu(1)-O(3W)	90.02(12)
O(11)-Cu(1)-O(3W)	167.74(13)	O(8)-Cu(1)-O(3W)	92.63(12)
O(17) ^{#2} -Cu(2)-O(17)	179.9(2)	O(17) ^{#2} -Cu(2)-O(2W)	85.05(12)
O(17)-Cu(2)-O(2W)	94.94(12)	O(17) ^{#2} -Cu(2)-O(2W) ^{#2}	94.94(12)
O(17)-Cu(2)-O(2W) ^{#2}	85.05(12)	O(2W)-Cu(2)-O(2W) ^{#2}	167.09(18)
O(17) ^{#2} -Cu(2)-O(1W)	90.05(9)	O(17)-Cu(2)-O(1W)	90.05(9)
O(2W)-Cu(2)-O(1W)	96.45(9)	O(2W) ^{#2} -Cu(2)-O(1W)	96.45(9)
O(25)-Cu(3)-O(20)	90.50(11)	O(25)-Cu(3)-O(24) ^{#2}	95.23(11)
O(20)-Cu(3)-O(24) ^{#2}	172.83(11)	O(25)-Cu(3)-O(22)	172.02(12)
O(20)-Cu(3)-O(22)	81.91(11)	O(24) ^{#2} -Cu(3)-O(22)	92.16(11)
O(25)-Cu(3)-O(12) ^{#3}	91.30(12)	O(20)-Cu(3)-O(12) ^{#3}	82.70(11)
O(24) ^{#2} -Cu(3)-O(12) ^{#3}	101.43(11)	O(22)-Cu(3)-O(12) ^{#3}	90.18(11)
O(25)-Cu(4)-O(9)	159.98(14)	O(25)-Cu(4)-O(5) ^{#3}	96.98(12)
O(9)-Cu(4)-O(5) ^{#3}	92.41(13)	O(25)-Cu(4)-O(19)	89.60(11)
O(9)-Cu(4)-O(19)	88.29(12)	O(5) ^{#3} -Cu(4)-O(19)	157.78(12)

O(20)-Na(1)-O(23)	94.29(11)	O(20)-Na(1)-O(14)	67.54(9)
O(23)-Na(1)-O(14)	149.09(12)	O(20)-Na(1)-O(16)	156.65(11)
O(23)-Na(1)-O(16)	66.99(10)	O(14)-Na(1)-O(16)	135.39(10)
O(20)-Na(1)-O(15)	101.37(11)	O(23)-Na(1)-O(15)	119.50(11)
O(14)-Na(1)-O(15)	89.42(10)	O(16)-Na(1)-O(15)	77.93(10)
O(20)-Na(1)-O(13)	108.22(10)	O(23)-Na(1)-O(13)	86.78(11)
O(14)-Na(1)-O(13)	76.37(10)	O(16)-Na(1)-O(13)	85.43(10)
O(15)-Na(1)-O(13)	138.65(10)	O(20)-Na(1)-O(22)	60.85(9)
O(23)-Na(1)-O(22)	78.20(10)	O(14)-Na(1)-O(22)	110.66(10)
O(16)-Na(1)-O(22)	100.17(10)	O(15)-Na(1)-O(22)	61.03(9)
O(13)-Na(1)-O(22)	160.23(11)	O(11)-Na(2)-O(2)	136.66(13)
O(11)-Na(2)-O(4)	70.69(11)	O(2)-Na(2)-O(4)	151.87(13)
O(11)-Na(2)-O(8)	67.70(10)	O(2)-Na(2)-O(8)	69.82(11)
O(4)-Na(2)-O(8)	138.20(11)	O(11)-Na(2)-O(1)	110.41(12)
O(2)-Na(2)-O(1)	89.38(11)	O(4)-Na(2)-O(1)	84.24(11)
O(8)-Na(2)-O(1)	106.47(12)	O(11)-Na(2)-O(3)	88.17(11)
O(2)-Na(2)-O(3)	88.16(11)	O(4)-Na(2)-O(3)	86.15(11)
O(8)-Na(2)-O(3)	96.24(11)	O(1)-Na(2)-O(3)	154.73(13)
12			
Zn(1)-O(13)	1.978(3)	Zn(1)-O(5)	2.021(3)
Zn(1)-O(7) ^{#1}	2.080(3)	Zn(1)-O(1W)	2.112(5)
Zn(1)-O(9)	2.188(3)	Zn(1)-O(11)	2.322(4)
Zn(2)-O(12) ^{#2}	1.934(3)	Zn(2)-O(13)	1.951(4)
Zn(2)-O(10)	1.952(3)	Zn(2)-O(8) ^{#1}	1.967(3)
Na(1)-O(5)	2.294(3)	Na(1)-O(3)	2.299(3)
Na(1)-O(9)	2.324(3)	Na(1)-O(1)	2.354(3)
Na(1)-O(4)	2.367(3)	Na(1)-O(2)	2.413(3)
Na(1)-O(11)	2.860(4)		
O(13)-Zn(1)-O(5)	173.14(14)	O(13)-Zn(1)-O(7) ^{#1}	94.72(13)
O(5)-Zn(1)-O(7) ^{#1}	91.58(12)	O(13)-Zn(1)-O(1W)	93.04(17)
O(5)-Zn(1)-O(1W)	88.70(14)	O(7) ^{#1} -Zn(1)-O(1W)	98.36(16)
O(13)-Zn(1)-O(9)	94.20(15)	O(5)-Zn(1)-O(9)	82.95(11)
O(7) ^{#1} -Zn(1)-O(9)	91.29(12)	O(1W)-Zn(1)-O(9)	167.42(13)
O(13)-Zn(1)-O(11)	91.59(14)	O(5)-Zn(1)-O(11)	81.65(12)
O(7) ^{#1} -Zn(1)-O(11)	165.09(14)	O(1W)-Zn(1)-O(11)	94.78(17)

O(9)-Zn(1)-O(11)	74.76(13)	O(12) ^{#2} -Zn(2)-O(10)	114.73(14)
O(13)-Zn(2)-O(10)	105.82(16)	O(12) ^{#2} -Zn(2)-O(8) ^{#1}	102.19(12)
O(13)-Zn(2)-O(8) ^{#1}	101.82(15)	O(10)-Zn(2)-O(8) ^{#1}	114.69(14)
O(5)-Na(1)-O(3)	144.99(11)	O(5)-Na(1)-O(9)	74.34(11)
O(3)-Na(1)-O(9)	70.78(10)	O(5)-Na(1)-O(1)	68.77(10)
O(3)-Na(1)-O(1)	145.24(11)	O(9)-Na(1)-O(1)	139.83(11)
O(5)-Na(1)-O(4)	103.34(11)	O(3)-Na(1)-O(4)	90.45(10)
O(9)-Na(1)-O(4)	118.06(11)	O(1)-Na(1)-O(4)	86.11(10)
O(5)-Na(1)-O(2)	100.65(11)	O(3)-Na(1)-O(2)	81.37(10)
O(9)-Na(1)-O(2)	88.07(10)	O(1)-Na(1)-O(2)	83.67(10)
O(4)-Na(1)-O(2)	148.38(11)	O(5)-Na(1)-O(11)	66.02(12)
O(3)-Na(1)-O(11)	94.77(12)	O(9)-Na(1)-O(11)	62.81(10)
O(1)-Na(1)-O(11)	113.21(12)	O(4)-Na(1)-O(11)	60.75(10)
O(2)-Na(1)-O(11)	149.95(11)		

13

Pb(1)-O(13)	2.331(7)	Pb(1)-O(13) ^{#1}	2.540(8)
Pb(1)-O(7)	2.587(7)	Pb(1)-O(12) ^{#1}	2.588(8)
Pb(1)-O(8)	2.629(8)		
Pb(2')-O(8)	2.668(8)	Pb(2)-O(13)	2.296(7)
Pb(2)-O(9)	2.444(8)	Pb(2)-O(6) ^{#1}	2.532(9)
Pb(2)-O(10)	2.642(8)	Pb(2')-O(13)	2.322(9)
Na(1)-O(7)	2.249(9)	Na(1)-O(12)	2.253(8)
Na(1)-O(4)	2.372(7)	Na(1)-O(2)	2.407(7)
Na(1)-O(3)	2.414(7)	Na(1)-O(1)	2.463(7)
O(13)-Pb(1)-O(13) ^{#1}	71.0(3)	O(13)-Pb(1)-O(7)	83.0(3)
O(13) ^{#1} -Pb(1)-O(7)	77.7(3)	O(13)-Pb(1)-O(12) ^{#1}	74.4(3)
O(13) ^{#1} -Pb(1)-O(12) ^{#1}	96.9(3)	O(7)-Pb(1)-O(12) ^{#1}	157.2(3)
O(13)-Pb(1)-O(8)	76.8(3)	O(13) ^{#1} -Pb(1)-O(8)	121.6(2)
O(7)-Pb(1)-O(8)	50.7(3)	O(12) ^{#1} -Pb(1)-O(8)	119.6(3)
O(13)-Pb(1)-Pb(2')	37.9(2)	O(13) ^{#1} -Pb(1)-Pb(2')	107.38(18)
O(7)-Pb(1)-Pb(2')	80.4(2)	O(12) ^{#1} -Pb(1)-Pb(2')	80.2(2)
O(8)-Pb(1)-Pb(2')	46.65(18)	Pb(2')-Pb(2)-O(13)	73.2(2)
Pb(2')-Pb(2)-O(9)	137.9(2)	O(13)-Pb(2)-O(9)	82.8(3)
Pb(2')-Pb(2)-O(6) ^{#1}	128.4(3)	O(13)-Pb(2)-O(6) ^{#1}	78.9(3)
O(9)-Pb(2)-O(6) ^{#1}	77.8(3)	Pb(2')-Pb(2)-O(10)	90.4(3)

O(13)-Pb(2)-O(10)	83.8(3)	O(9)-Pb(2)-O(10)	52.5(3)
O(6) ^{#1} -Pb(2)-O(10)	129.0(3)	O(13)-Pb(2')-O(8)	76.2(3)
O(7)-Na(1)-O(12)	93.9(3)	O(7)-Na(1)-O(4)	148.6(3)
O(12)-Na(1)-O(4)	68.8(3)	O(7)-Na(1)-O(2)	69.8(3)
O(12)-Na(1)-O(2)	147.0(3)	O(4)-Na(1)-O(2)	137.6(3)
O(7)-Na(1)-O(3)	120.4(3)	O(12)-Na(1)-O(3)	84.5(3)
O(4)-Na(1)-O(3)	85.1(3)	O(2)-Na(1)-O(3)	80.1(2)
O(7)-Na(1)-O(1)	86.5(3)	O(12)-Na(1)-O(1)	124.3(3)
O(4)-Na(1)-O(1)	82.7(2)	O(2)-Na(1)-O(1)	84.3(2)
O(3)-Na(1)-O(1)	140.9(2)		

Symmetry codes for **4**: ^{#1} -x+y-1, -x+1, z; ^{#2} -y+1, x-y+2, z. For **5**: ^{#1} -x, y, -z+1/2. For **7**: ^{#1} -x+1, -y, -z; ^{#2} x+1, y+1, z. For **8**: ^{#1} -x-1, -y, z; ^{#2} x+1, y+1, z. For **9**: ^{#1} -x+2, -y, -z; ^{#2} x+1, y, z. For **10**: ^{#1} -x-2, -y, -z; ^{#2} -x-1, -y, -z; ^{#3} x+1, y, z. For **11**: ^{#1} x, y+1, z; ^{#2} -x+1, y, -z+3/2; ^{#3} x, y-1, z. For **12**: ^{#1} -x, y, -z+1/2; ^{#2} -x, -y+2, -z. For **13**: ^{#1} -x+2, -y+1, -z+2.

Table S2. Hydrogen-bonding parameters for **1-9**, **11** and **13** (in Å and deg)

	D-H...A	d(D-H)	d(D...A)	∠(D-H...A)
1				
O(2)-H(2)···O(1)	0.82	1.97	2.517(5)	123.5
O(3)-H(3)···O(2)	0.82	1.77	2.495(4)	146.5
O(4)-H(4)···O(3)	0.86	1.97	2.757(4)	151.9
O(5)-H(5A)···O(8)	0.82	1.99	2.741(4)	152.3
O(7)-H(7A)···O(6)	0.81(2)	1.79(3)	2.515(5)	148(6)
O(6)-H(6A)···O(5)	0.83(2)	1.71(4)	2.493(6)	156(7)
2				
O(2)-H(2A)···O(3)	0.83(2)	2.143(19)	2.920(7)	156(4)
O(4)-H(4A)···O(3)	0.82	1.99	2.743(6)	152.8
O(6)-H(6A)···O(8)	0.82	1.78	2.506(6)	146.3
O(1)-H(1A)···O(2)	0.83(2)	1.71(5)	2.487(6)	154(10)
O(7)-H(7)···O(8)	0.82	1.74	2.536(6)	162.8
3				
O(1)-H(1)···O(3)	0.82	1.88	2.559(9)	138.9
O(6)-H(6A)···O(8)	0.82	1.92	2.656(18)	149.1
O(7)-H(7A)···O(5)	0.82	1.80	2.413(16)	129.8

O(5)-H(5A)···O(8)	0.82	2.06	2.754(17)	142.8
4				
O(3)-H(3A)···O(4)	0.81(2)	1.988(19)	2.750(11)	156(2)
O(2)-H(2A)···O(3)	0.83(2)	1.85(10)	2.597(10)	150(20)
O(4)-H(4)···O(1)	0.82(2)	1.90(4)	2.712(13)	170(17)
C(2)-H(2)···O(3) ^{#1}	0.93	2.416(8)	3.34(1)	173(1)
5				
O(2)-H(2)···O(3)	0.82	1.85	2.5835(18)	148.1
O(1)-H(1)···O(4)	0.82	1.89	2.5678(17)	138.7
O(1W)-H(1WA)···O(4)	0.856(18)	2.36(3)	3.002(2)	132(3)
N(3)-H(3D)···O(1W) ^{#2}	0.97	2.16	3.083(3)	159.8
O(3)-H(3)···O(4)	0.735(14)	2.278(14)	3.0113(19)	175.1(17)
6				
O(1)-H(1A)···O(4)	0.82	1.95	2.668(6)	145.7
O(2)-H(2A)···O(3)	0.82	1.94	2.577(5)	133.8
O(4)-H(4)···O(3)	0.82	2.39	2.910(6)	121.6
O(5)-H(5)···O(8)	0.82	2.22	2.857(8)	134.3
O(6)-H(6A)···O(7)	0.82	1.82	2.486(8)	138.0
O(8)-H(8)···O(5)	0.82	2.30	2.857(8)	126.2
7				
O(1W)-H(1A)···O(3W)	0.828(18)	1.93(3)	2.690(5)	152(5)
O(1W)-H(1B)···O(24)	0.888(18)	1.94(3)	2.753(3)	152(4)
8				
O(1W)-H(1A)···O(5W)	0.866(19)	1.84(2)	2.697(5)	173(5)
O(1W)-H(1B)···O(24) ^{#1}	0.90(2)	1.96(3)	2.806(4)	155(5)
O(25)-H(25A)···O(4W) ^{#3}	0.71(6)	2.41(6)	3.104(10)	164(8)
O(25)-H(25A)···O(4W') ^{#3}	0.71(6)	2.46(6)	3.104(12)	151(8)
9				
O(13)-H(13)···O(7W)	0.813(19)	2.34(2)	3.147(10)	174(4)
O(1W)-H(1A)···O(11)	0.86	1.83	2.650(4)	156.5
O(1W)-H(1B)···O(7W)	0.70	2.21	2.754(10)	135.6
O(2W)-H(2A)···O(6) ^{#3}	0.97	1.82	2.775(4)	168.3
O(2W)-H(2B)···O(8)	0.82	2.54	3.076(4)	124.0
O(3W)-H(3A)···O(8W) ^{#1}	0.85	2.02	2.839(6)	162.2
O(3W)-H(3B)···O(5) ^{#2}	0.92	1.84	2.726(4)	160.2

O(4W)-H(4B)...O(6)	0.873(11)	2.04(3)	2.876(4)	160(6)
C(4)-H(4)...O1W ^{#4}	0.93	2.885(2)	3.536(5)	128(1)

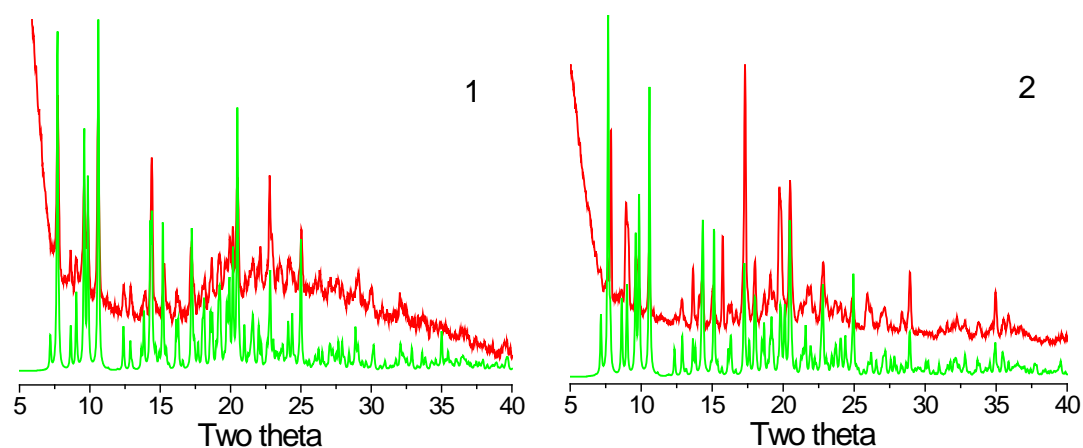
11

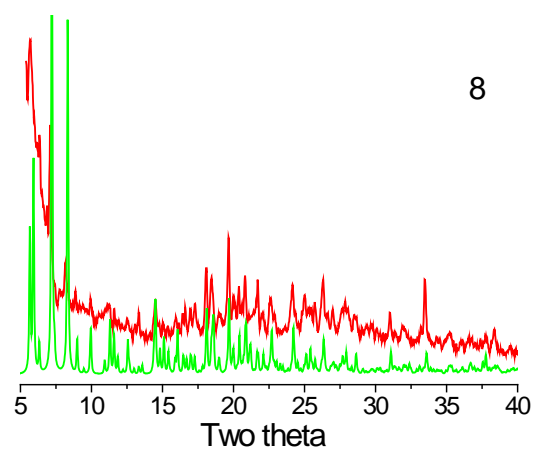
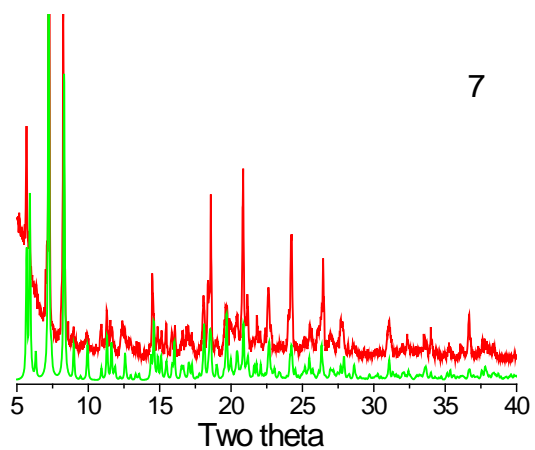
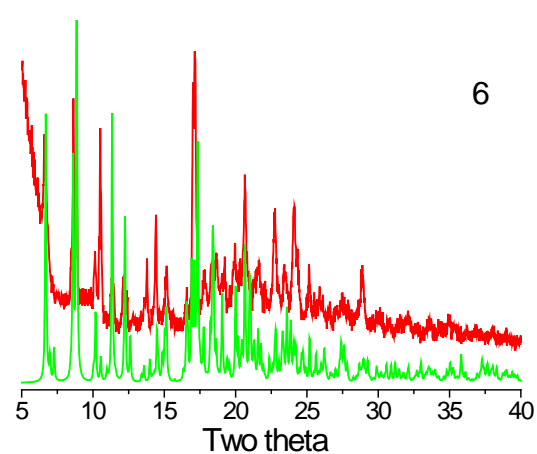
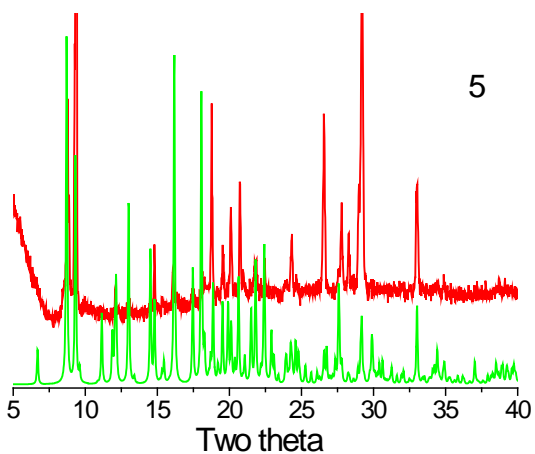
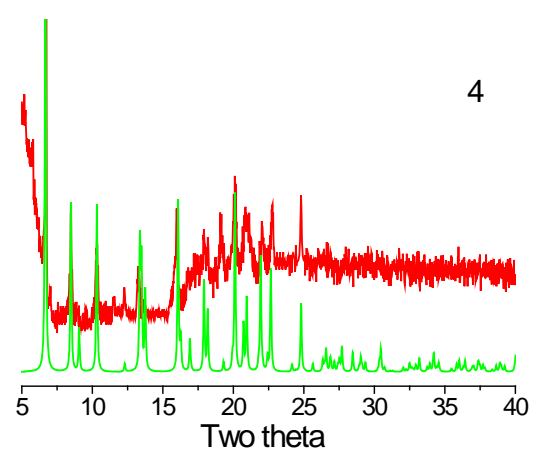
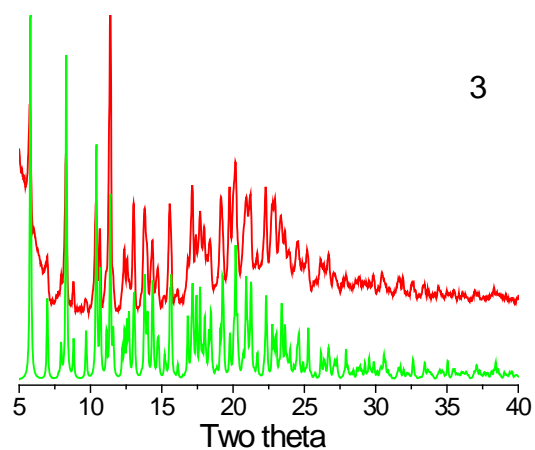
O(1W)-H(1C)...O(23)	0.89(2)	1.75(3)	2.633(4)	171(11)
O(1W)-H(1D)...O(25)	0.88(2)	2.22(4)	3.058(3)	158(9)
O(2W)-H(2B)...O(18)	0.872(18)	1.82(2)	2.650(4)	158(4)
O(2W)-H(2A)...O(25)	0.894(17)	2.02(3)	2.827(4)	150(3)
O(2W)-H(2A)...O(19)	0.894(17)	2.52(3)	3.127(4)	126(2)
O(3W)-H(3A)...O(2W)	0.843(18)	2.00(3)	2.807(4)	161(4)
O(7W)-H(7B)...O(4W) ^{#4}	0.92(2)	2.01(4)	2.871(11)	157(7)
O(7W)-H(7A)...O(6)	0.92(2)	2.02(5)	2.836(6)	148(8)

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C(14)-H(14B)...O(9) ^{#2}	0.96	2.505(8)	3.471(13)	174.0(6)
C(36)-H(36B)...O(8) ^{#2}	0.97	2.662(8)	3.449(15)	140(8)

Symmetry code for **4**: ^{#1} -1/3+x, 1/3+y, 1/3+z. For **5**: ^{#2} -x+1/2, -y+1/2, z-1/2. For **8**: ^{#1} -x-1, -y, -z; ^{#3} x, y+1, z. For **9**: ^{#1} -x+2, -y, -z; ^{#2} x+1, y, z; ^{#3} -x+1, -y, -z; ^{#4} 1+x, 1+y, 1+z. For **11**: ^{#4} -x+1, y+1, -z+3/2. For **13**: ^{#2} x, y+1, z.





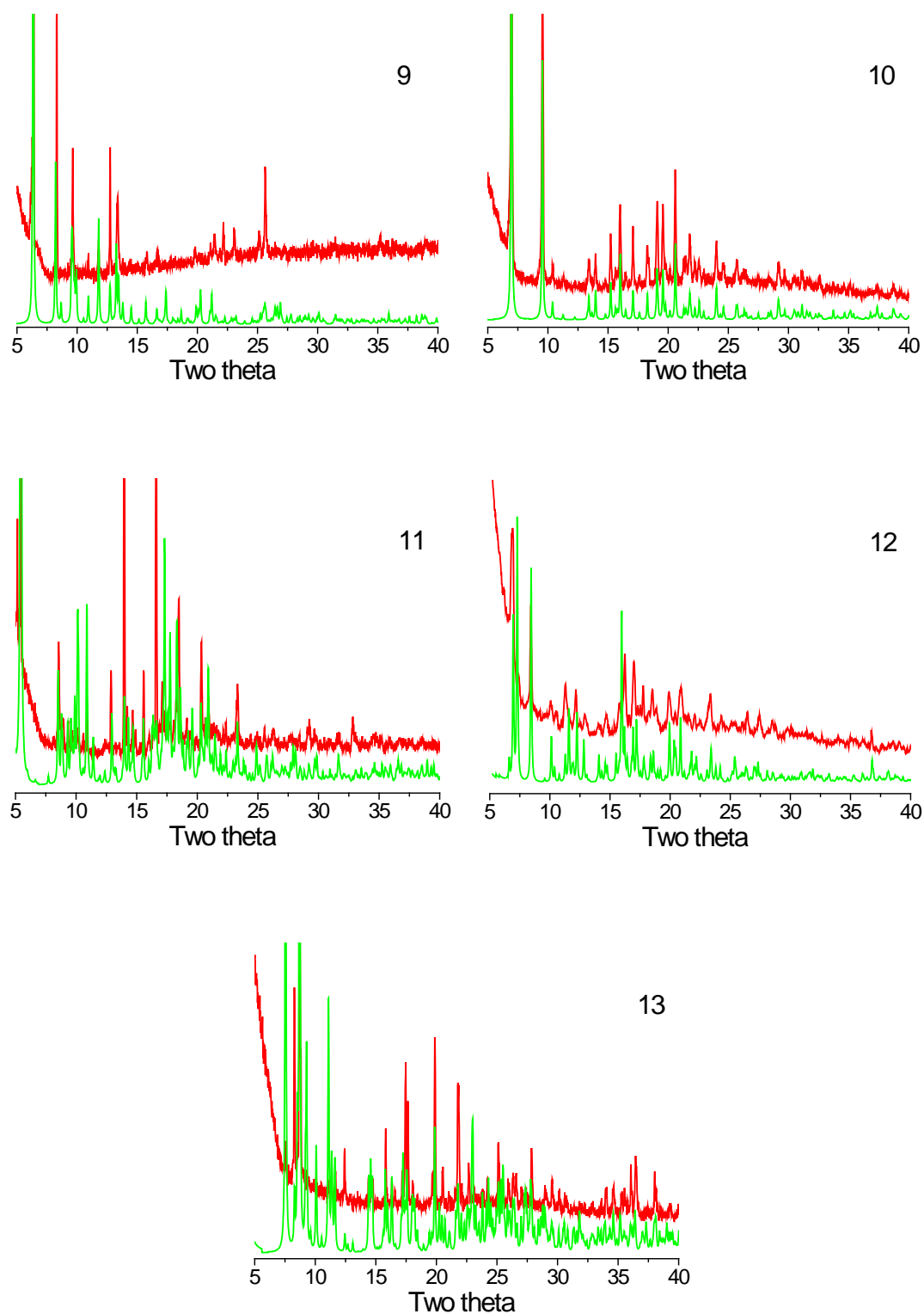


Fig. S1. The simulated (green) and experimental (red) XRPD patterns for the compounds **1-13** (the diffraction peaks of both simulated and experimental patterns match well in relevant positions, indicating that the phase purities of compounds **1-13** are good).

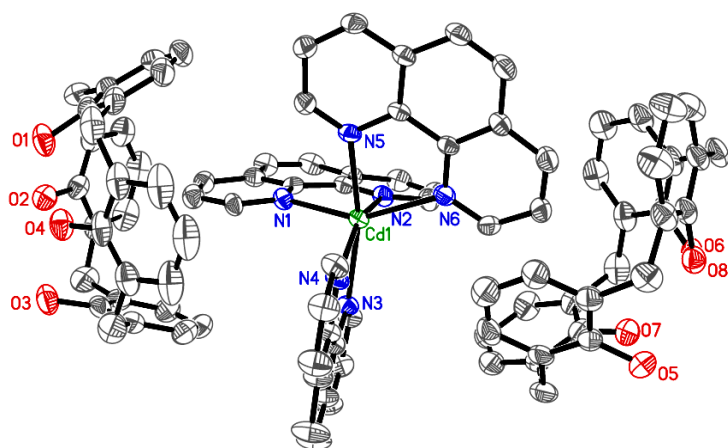


Fig. S2. The coordination environment of Cd(II) atom in **2**.

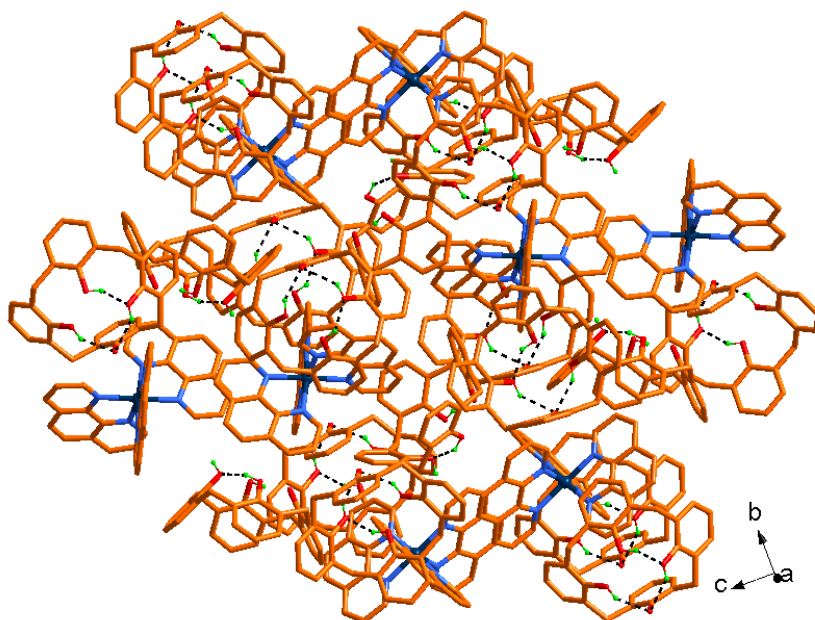


Fig. S3. The 3D supramolecular structure connected by C-H... π interactions in **3**.

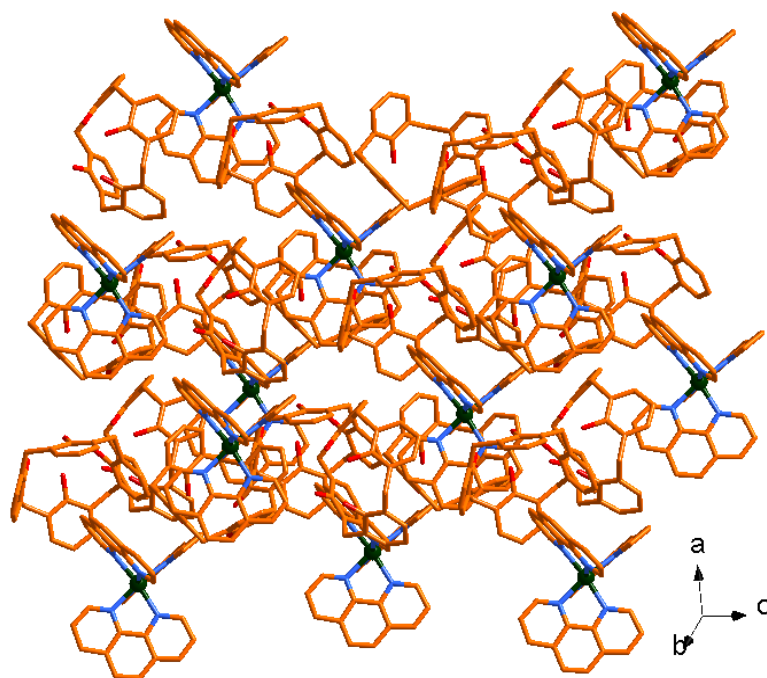


Fig. S4. The 3D supramolecular structure constructed by C-H...O and C-H... π interactions in **4**.

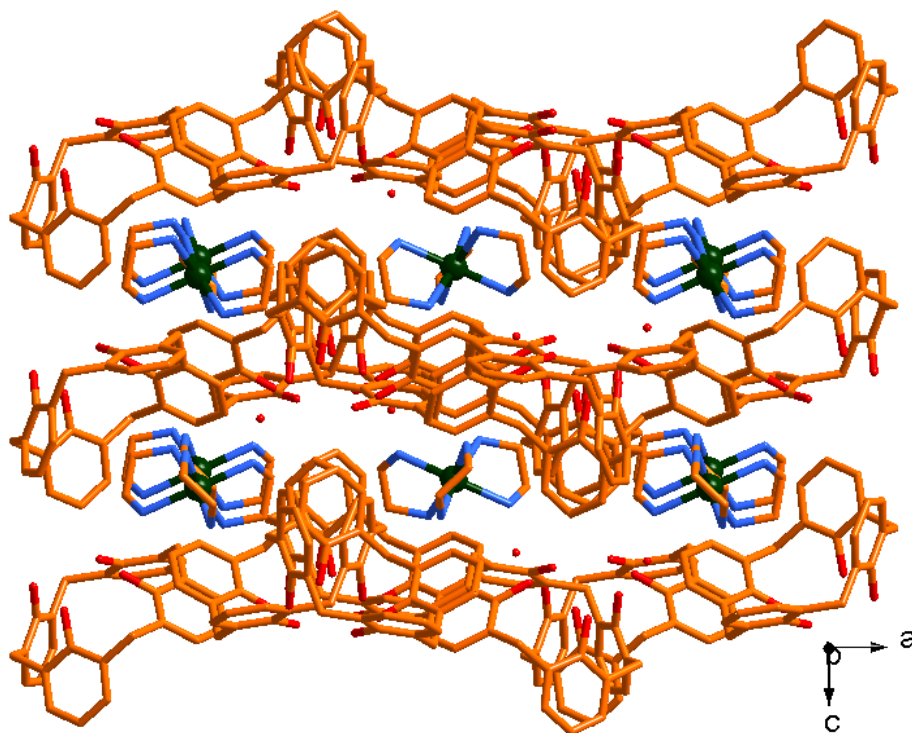


Fig. S5. The 3D supramolecular structure connected by intermolecular hydrogen-bonding interactions in **5**.

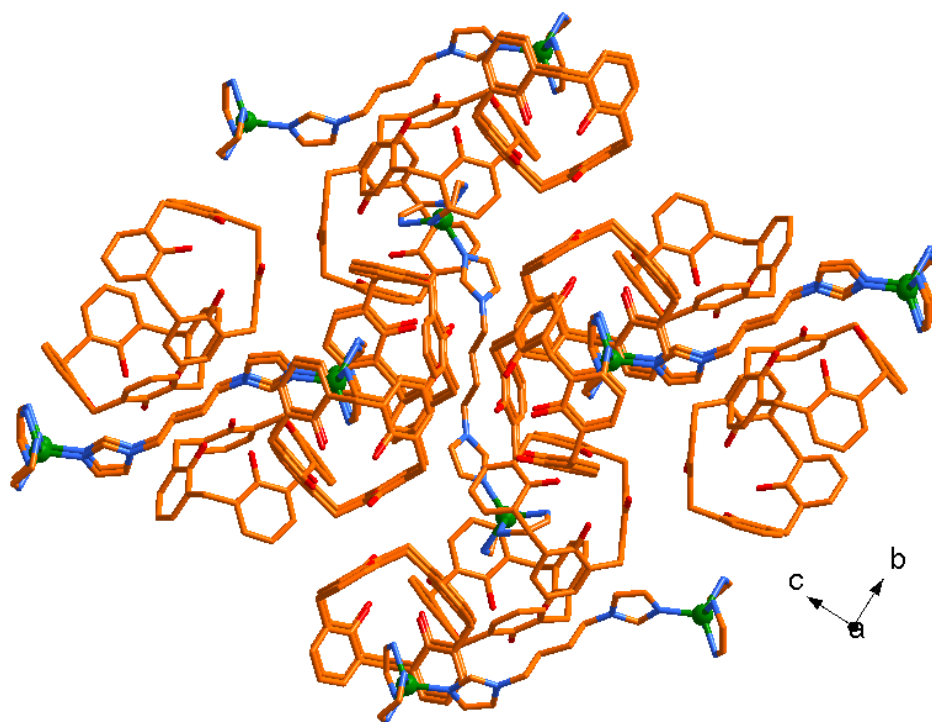


Fig. S6. The 3D supramolecular structure constructed by π - π interactions in **6**.

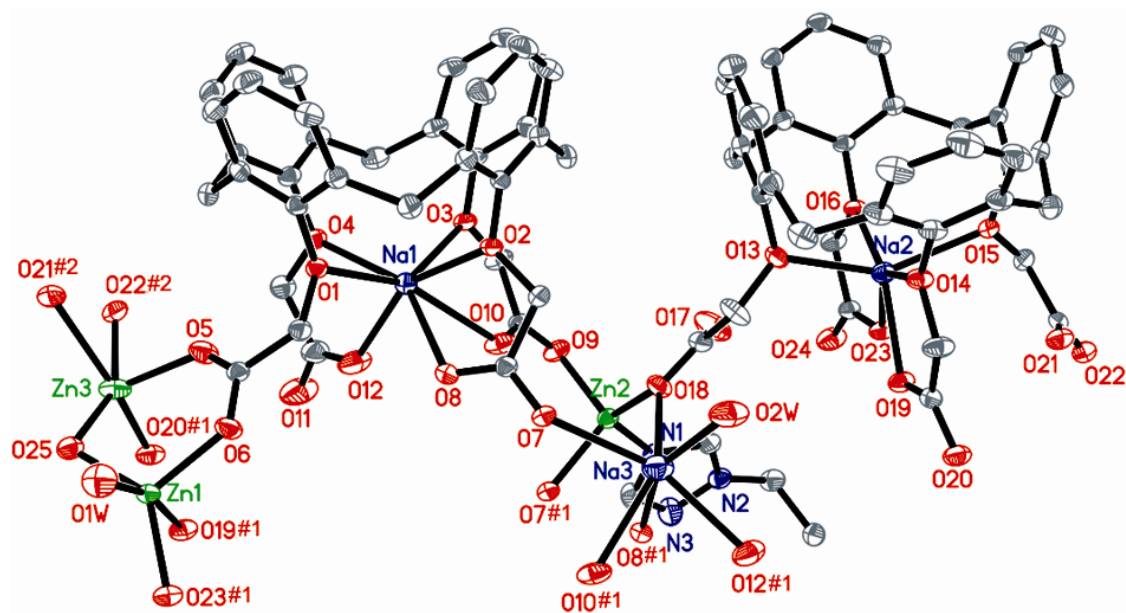


Fig. S7. ORTEP diagram showing the coordination environments of Zn(II) and Na(I) atoms in **8**. Symmetry codes: ^{#1} $-x+1, -y, -z$; ^{#2} $x+1, y+1, z$.

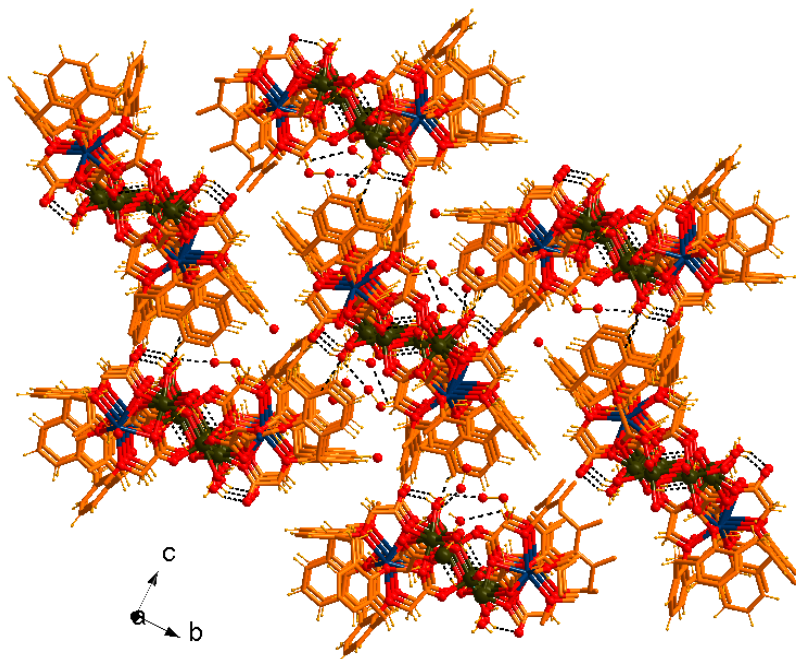


Fig. S8. The 3D supramolecular structure constructed by O-H...O and C-H...O interactions in **9**.

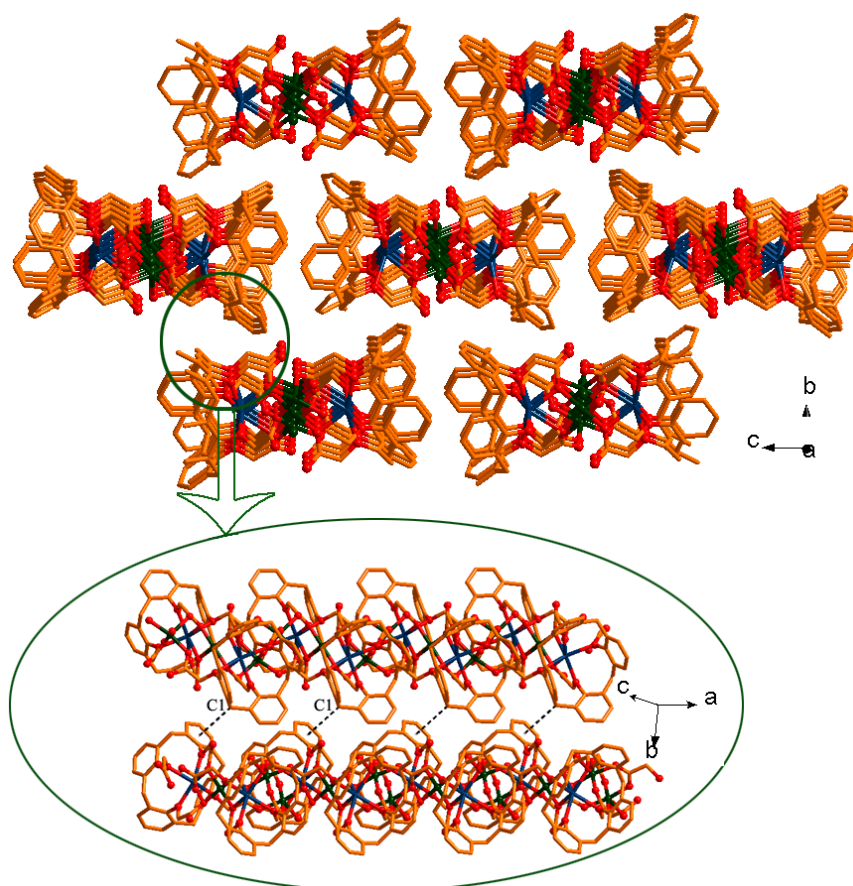


Fig. S9. The 3D supramolecular structure connected by C-H... π interactions in **10**.

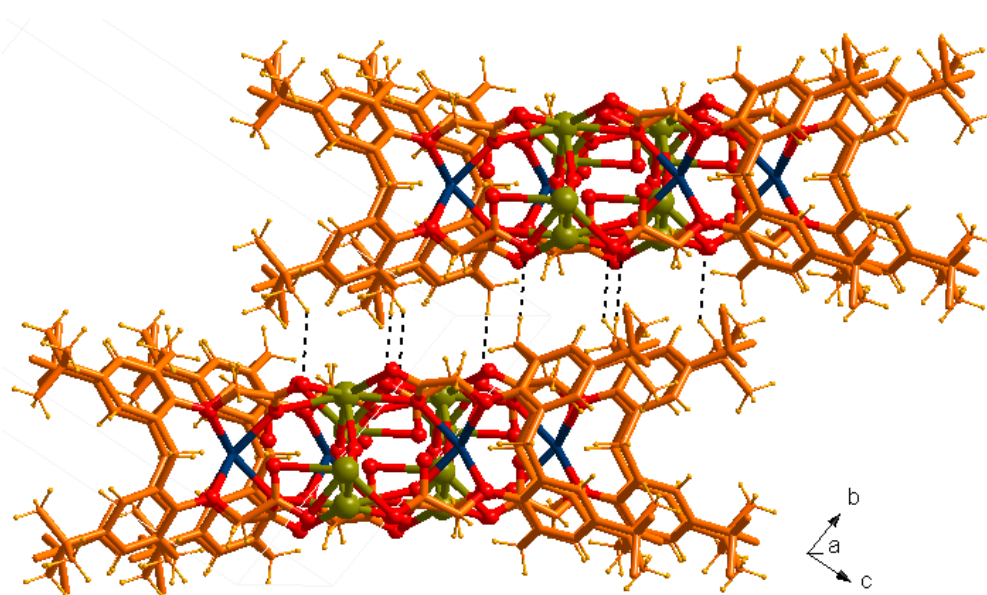


Fig. S10. The 1D supramolecular chain connected by C-H...O interactions in **13**.