Electronic Supplementary Material (ESI) for CrystEngComm.

Electronic Supporting Information

Dependence of SBU length on the size of metal ion in alkaline earth MOFs derived from a flexible C_3-symmetric tricarboxylic acid

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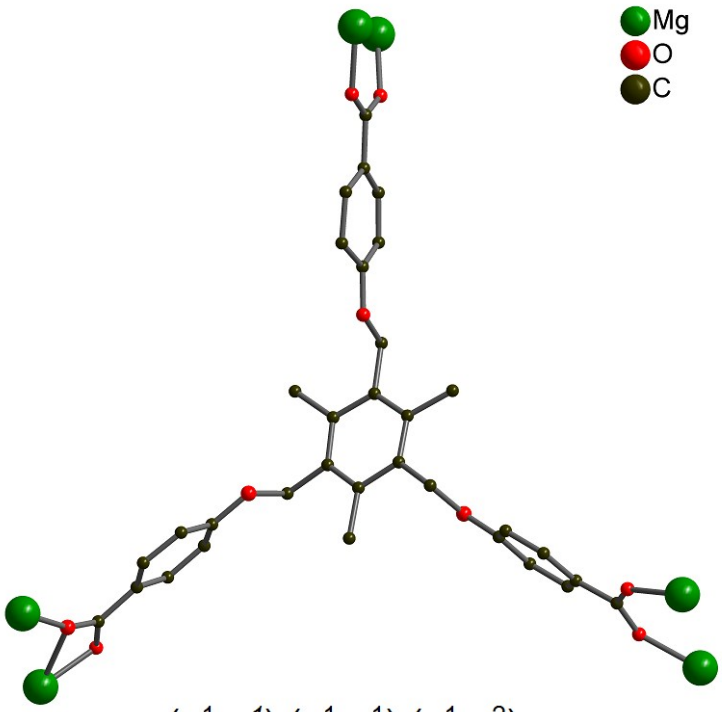
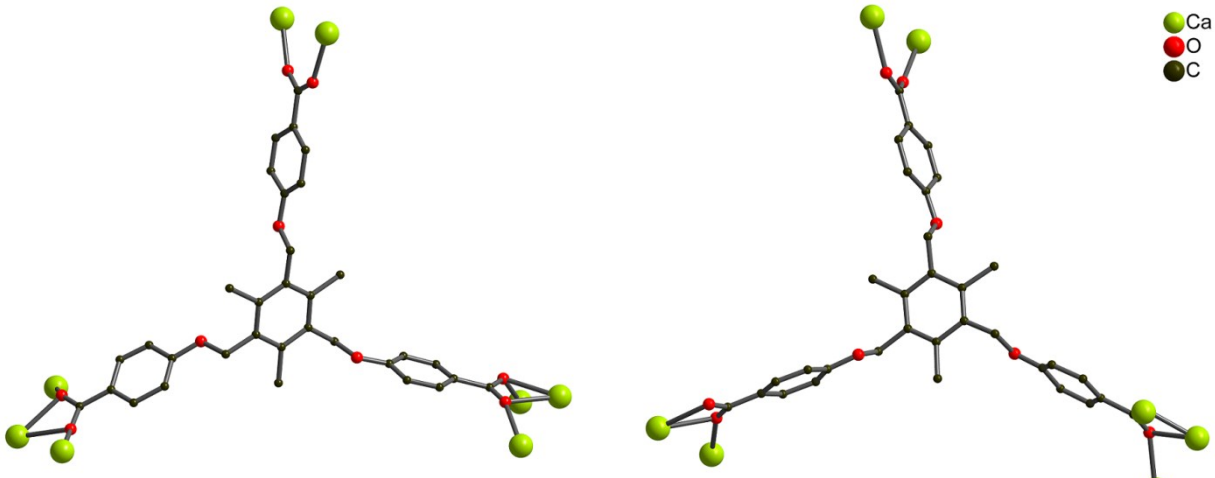


$(\eta^1\text{-}\eta^1)\text{-}(\eta^1\text{-}\eta^1)\text{-}(\eta^1\text{-}\eta^2)\text{-}\mu_6$

Fig. S1. Various coordination modes of the COO^- moieties in Mg-TCMTB.



$(\eta^1\text{-}\eta^1)\text{-}(\eta^1\text{-}\eta^2\text{-}\eta^1)\text{-}(\eta^1\text{-}\eta^2\text{-}\eta^1)\text{-}\mu_8$

$(\eta^1\text{-}\eta^1)\text{-}(\eta^1\text{-}\eta^2\text{-}\eta^1)\text{-}(\eta^1\text{-}\eta^2)\text{-}\mu_7$

Fig. S2. Various coordination modes of the COO^- moieties in Ca-TCMTB.

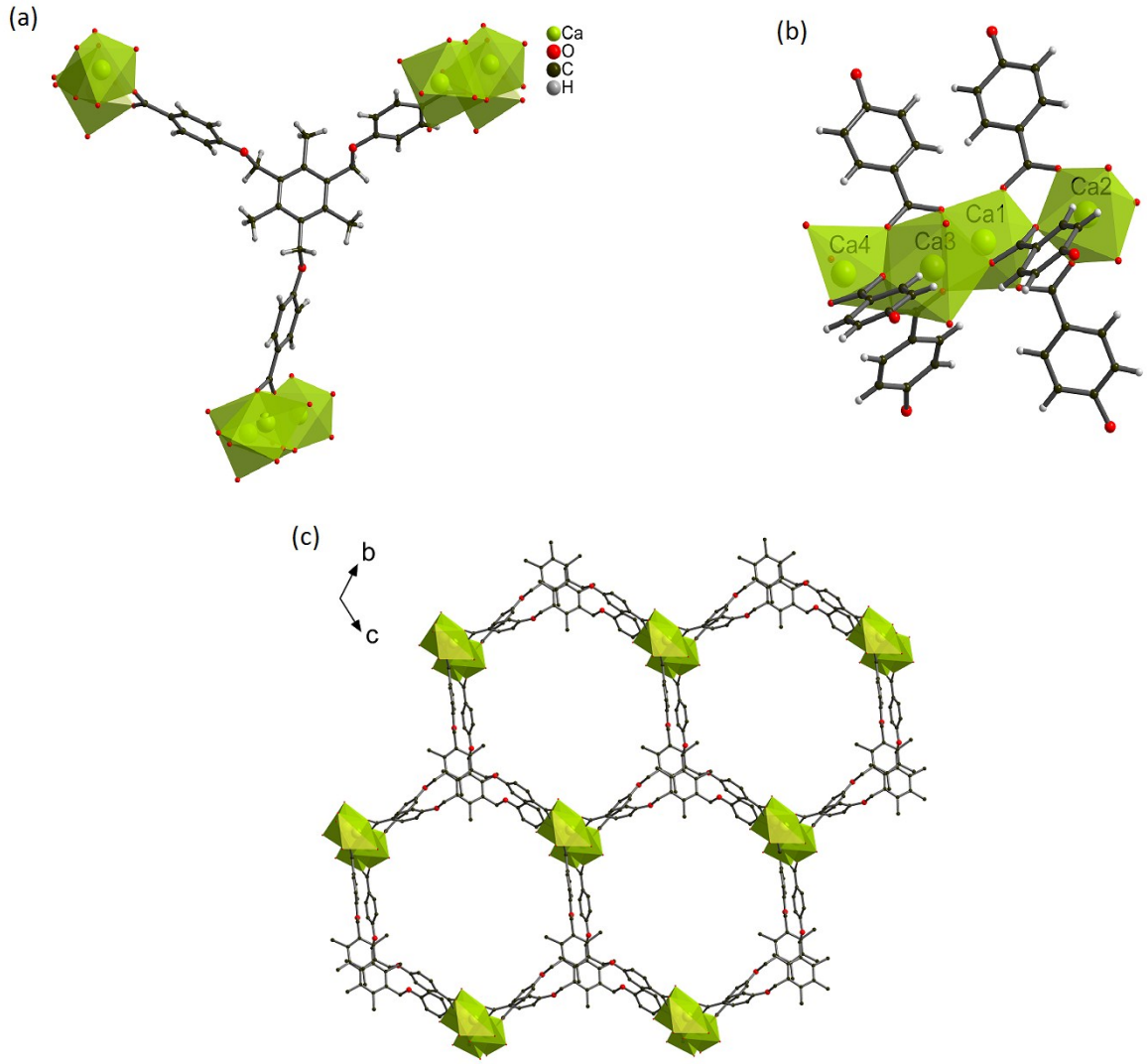


Fig S3. Crystal structure of Ca-TCMTB. (a) connectivity of $TCMTB^{3-}$ with Ca^{2+} ions; (b) polyhedral representation of the coordination environment of Ca^{2+}ions; (c) a view of the framework down to *a*-axis. (H-atoms and solvent molecules are omitted for clarity).

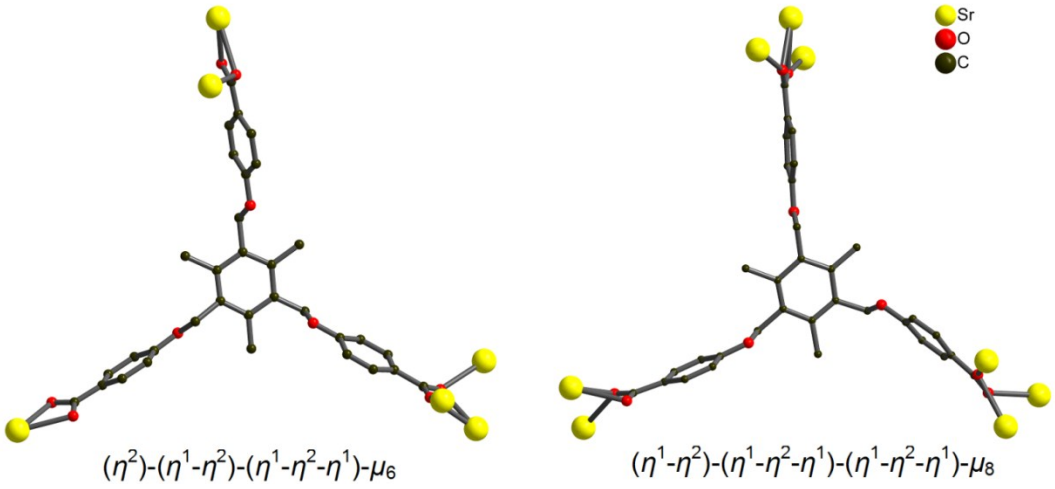


Fig. S4. Various coordination modes of the COO^- moieties in Sr-TCMTB.

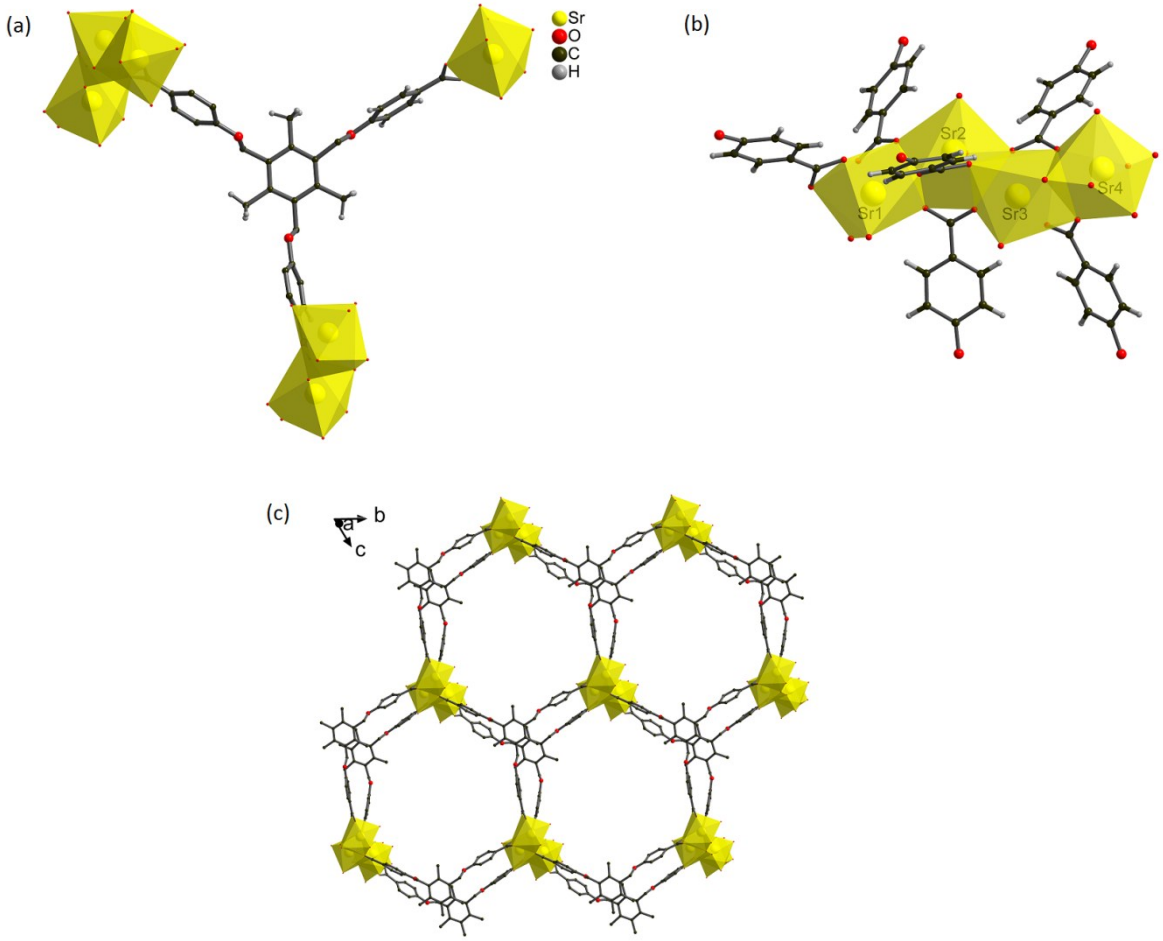


Fig S5. Crystal structure of Sr-TCMTB. (a) connectivity of $TCMTB^{3-}$; (b) coordination environment of Sr^{2+} ions; (c) 2D sheet viewed along *a*-axis (slightly off) showing hexagonal channels.

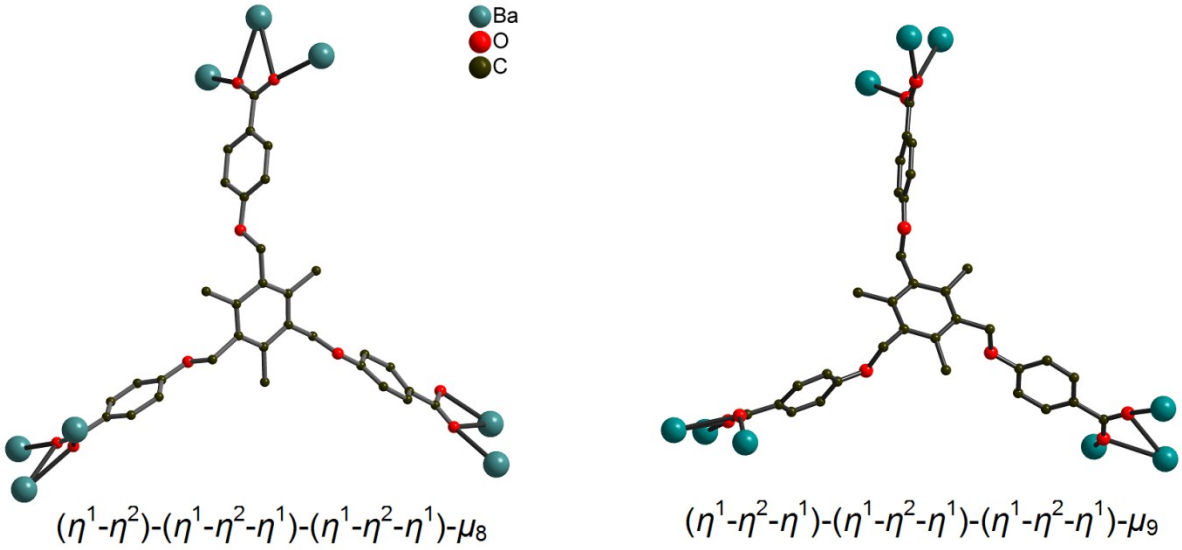


Fig. S6. Various coordination modes of the COO^- moieties in Ba-TCMTB.

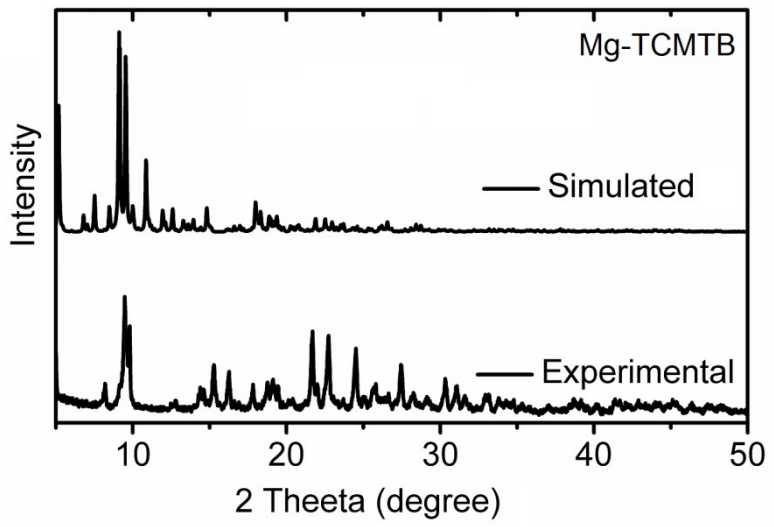


Fig S7. Experimental and simulated PXRD patterns of as-prepared Mg-TCMTB.

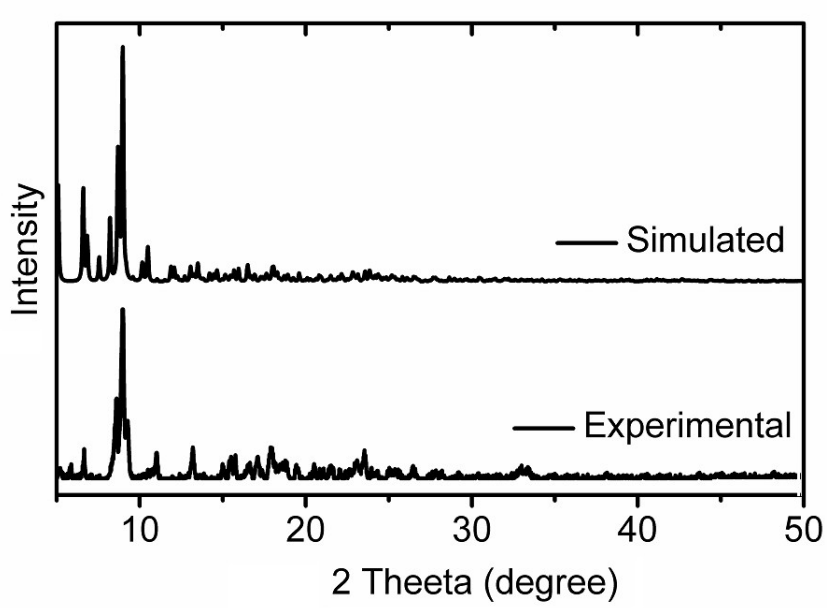


Fig S8. Experimental and simulated PXRD patterns of as-prepared Ca-TCMTB.

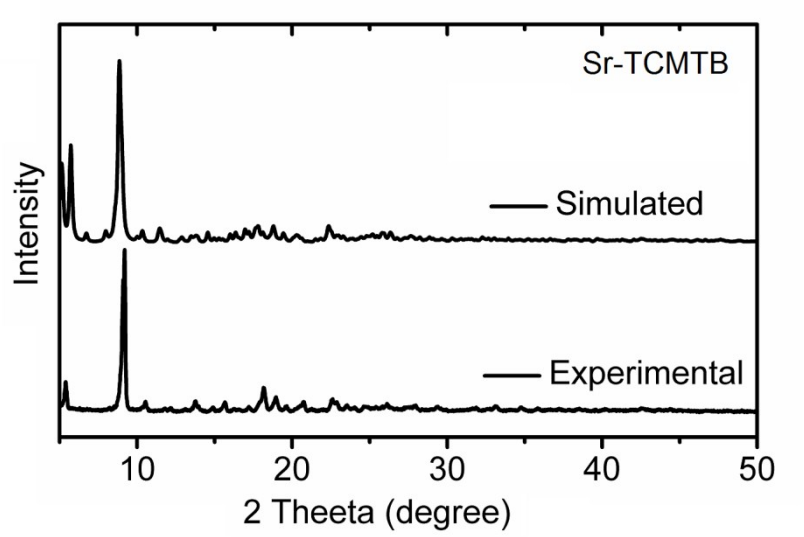


Fig S9. Experimental and simulated PXRD patterns of as-prepared Sr-TCMTB.

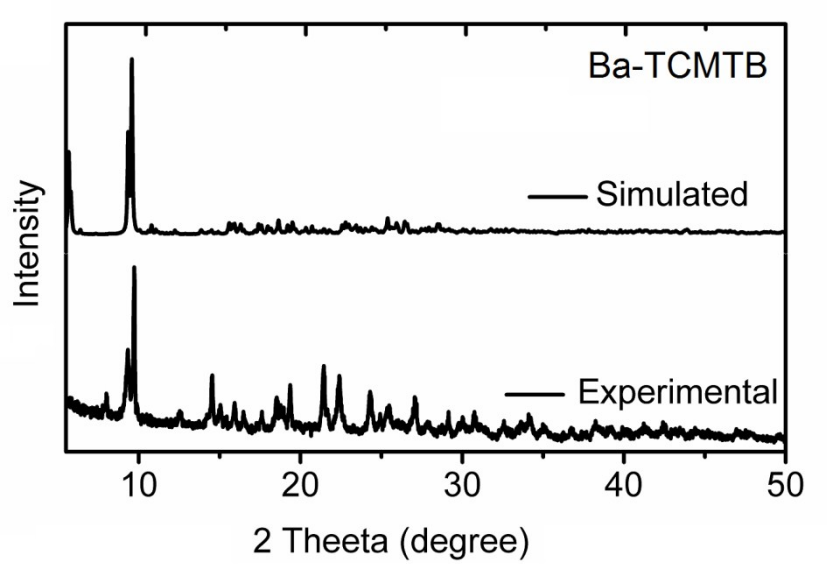


Fig S10. Experimental and simulated PXRD patterns of as-prepared Ba-TCMTB.

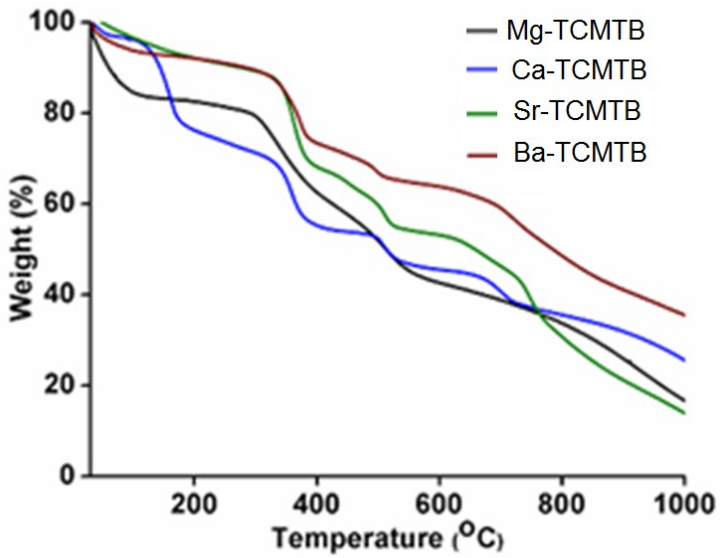


Fig S11. TGA profiles of the MOFs under N_2 atm at heating rate of 10 °C/minute.

FT-IR spectroscopic studies. FT-IR spectra have been recorded for ligand and the complexes which show the metal caboxylate bond formation (Figure S6). Disappearance of carbonyl group stretching frequency (1682 cm^{-1}) and appearance of two new peaks at lower wavenumbers (1610-1385 cm^{-1}) indicate the formation of metal-carboxylate bonds that corresponds to the anti-symmetric and symmetric C=O stretching of the carboxylate group ($-COO^-$).

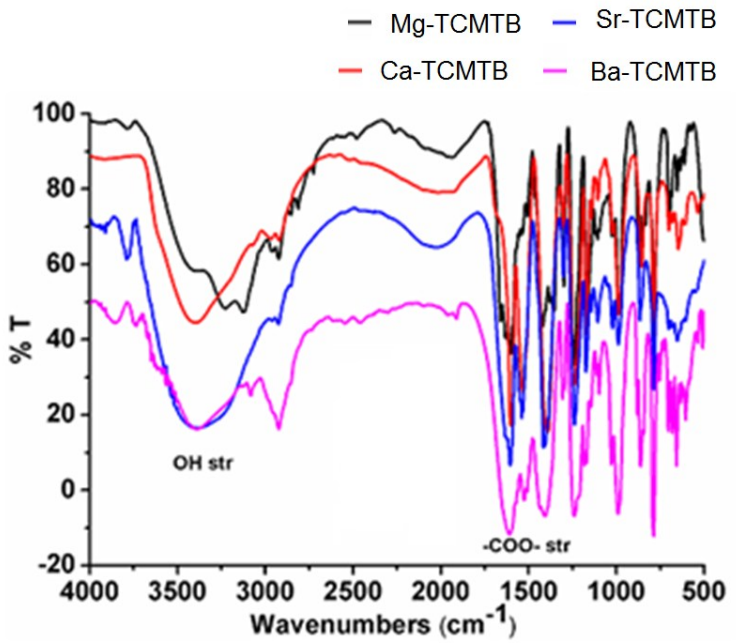


Fig S12. FT-IR spectra of the MOFs.

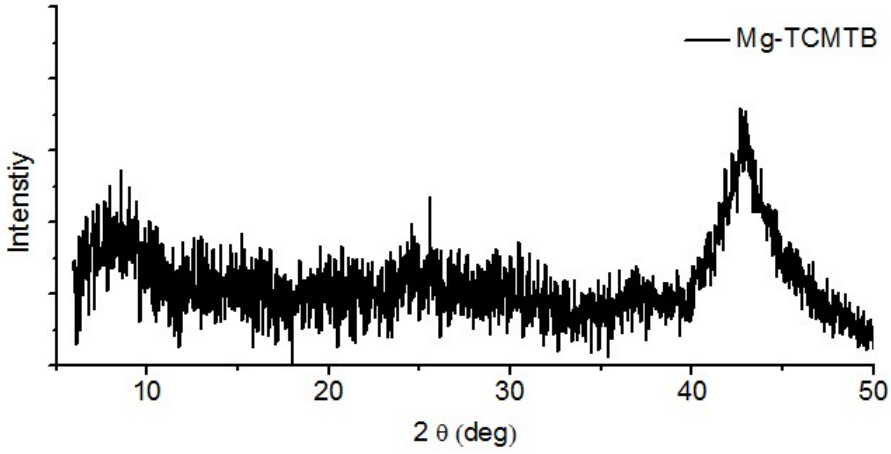


Fig S13. PXRD pattern of TGA analyzed Mg-TCMTB powder.

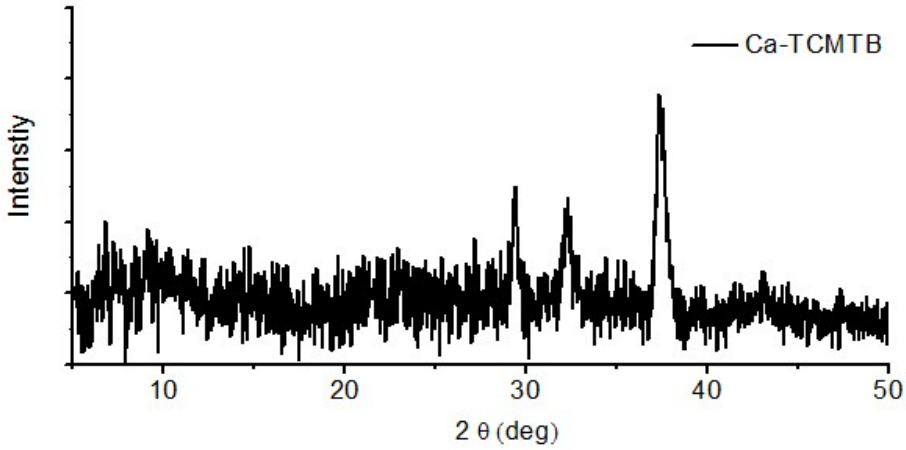


Fig S14. PXRD pattern of TGA analyzed Ca-TCMTB powder.

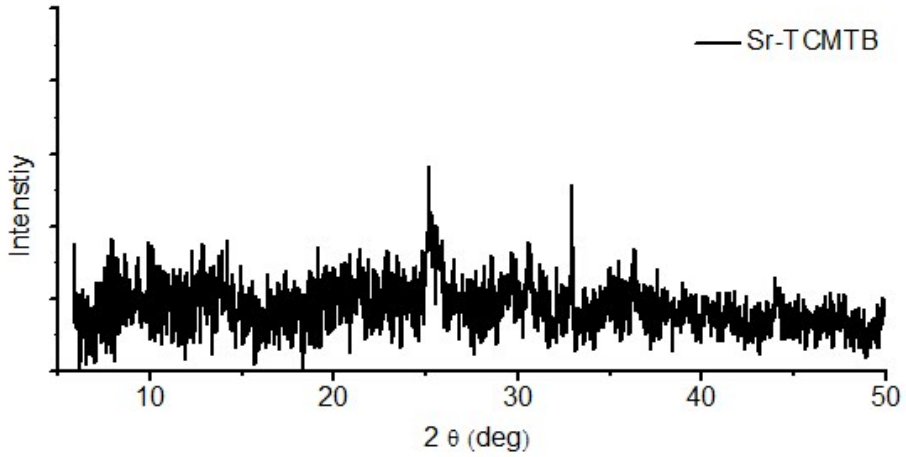


Fig S15. PXRD pattern of TGA analyzed Sr-TCMTB powder.

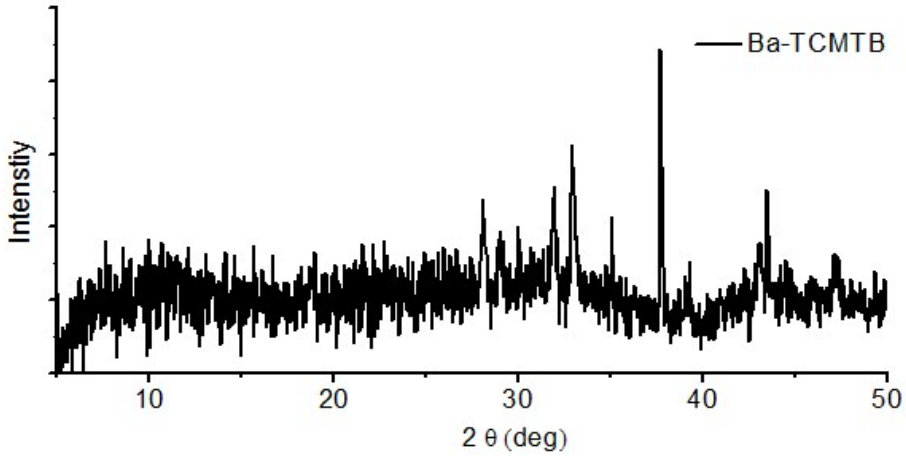


Fig S16. PXRD pattern of TGA analyzed Ba-TCMTB powder.

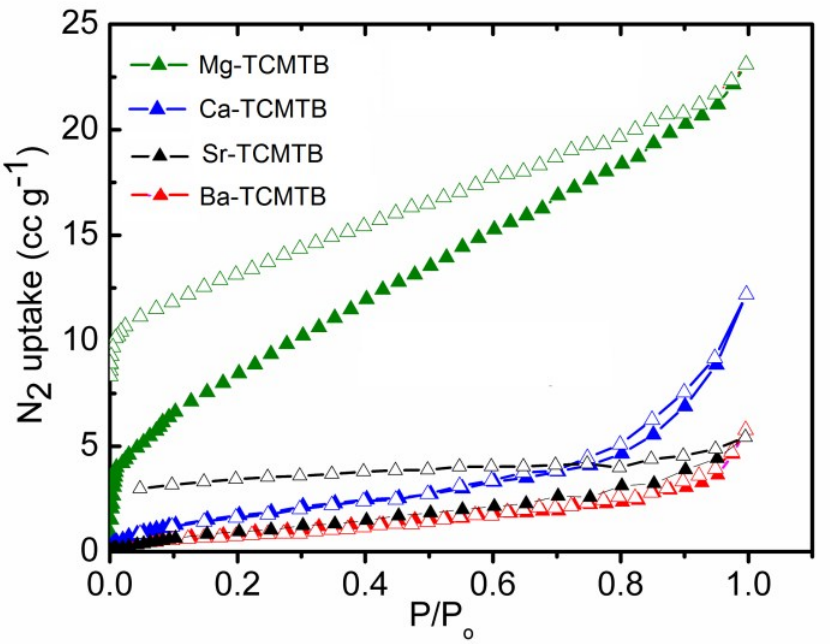


Fig S17. N_2 adsorption-desorption isotherms of the alkaline-earth metal MOFs at 77 K.

Absorption properties. The absorption spectra were recorded with a Varian Cary Bio 100 UV-vis spectrophotometer. The fluorescence spectral studies were performed on a Varian Cary Eclipse fluorescence spectrophotometer equipped with Xenon flash lamp light source and a 1 cm path length quartz cuvette keeping excitation slit width at 10 nm and emission slit width at 20 nm". 1 mg of each sample was dispersed in DMSO by sonication for 20 minutes.

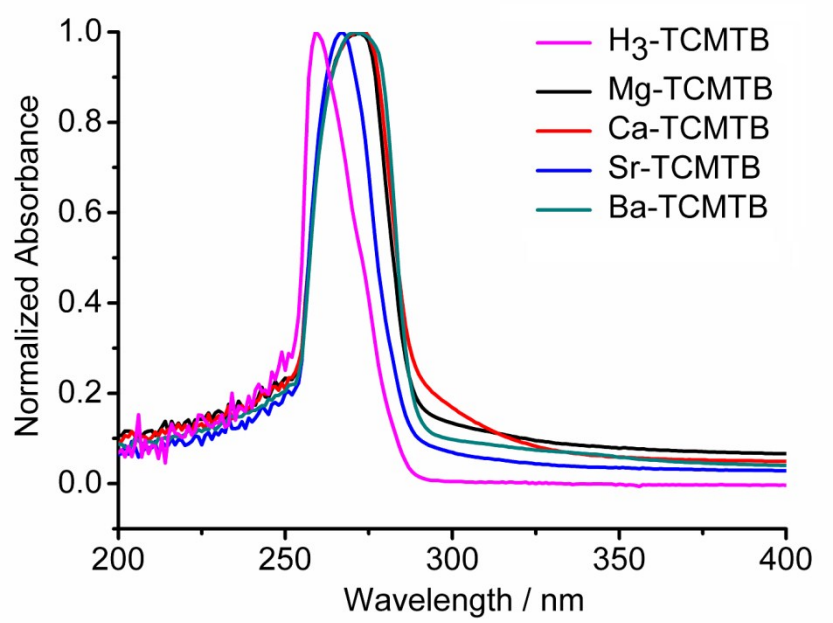


Fig S18. Absorption spectra of free ligand (Conc. = 1×10^{-5} M) and the MOFs in DMSO solution and suspension, respectively.

Table S1. Selected bond lengths (Å) and angles (°) for Mg-TCMTB.

Mg-O bond lengths			
Mg(1)-O(2)	2.031(4)	Mg(3)-O(2)	2.028(4)
Mg(1)-O(6)	2.048(3)	Mg(3)-O(1)	2.039(3)
Mg(1)-O(8)	2.092(3)	Mg(3)-O(2)	2.068(3)
Mg(2)-O(5)	1.994(3)	Mg(4)-O(1)	1.931(5)
Mg(2)-O(3)	2.030(4)	Mg(4)-O(1)	1.984(4)
Mg(2)-O(9)	2.169(4)	Mg(4)-O(2)	2.025(4)
Mg(2)-O(8)	2.196(3)	Mg(4)-O(2)	2.218(3)
Mg···Mg distances			
Mg(1)-Mg(2)	3.531(2)	Mg(3)-Mg(4)	3.543(2)
O-Mg-O bond angles			
O(2)-Mg(1)-O(6)	95.04(1)	O(14)-Mg(4)-O(1)	112.87(2)
O(2)-Mg(1)-O(8)	92.08(1)	O(14)-Mg(4)-O(2)	129.4(2)
O(6)1-Mg(1)-O(8)	91.58(1)	O(12)-Mg(4)-O(2)	110.98(2)
O(23)-Mg(1)-O(8)	88.21(1)	O(14)-Mg(4)-O(2)	94.37(2)
O(5)-Mg(2)-O(3)	97.45(2)	O(14)-Mg(4)-O(2)	159.59(1)
O(5)-Mg(2)-O(9)	154.41(1)	O(12)-Mg(4)-O(2)	91.15(1)
O(3)-Mg(2)-O(9)	93.54(1)	O(17)-Mg(4)-O(2)	60.65(1)
O(5)-Mg(2)-O(8)	95.53(1)	O(15)-Mg(3)-O(1)	92.33(2)
O(3)-Mg(2)-O(8)	95.15(1)	O(15)-Mg(3)-O(2)	89.89(1)
O(9)-Mg(2)-O(8)	60.40(1)	O(11)-Mg(3)-O(2)	88.52(1)

Table S2. Selected bond lengths (Å) and angles (°) for Ca-TCMTB.

Ca-O bond lengths					
Ca(1)-O(1)	2.297(6)	Ca(2)-O(1)	2.307(7)	Ca(3)-O(2)	2.379(6)
Ca(1)-O(3)	2.320(6)	Ca(2)-O(1)	2.371(6)	Ca(3)-O(2)	2.462(6)
Ca(1)-O(8)	2.394(6)	Ca(2)-O(2)	2.385(8)	Ca(3)-O(9)	2.468(6)
Ca(1)-O(2)	2.396(7)	Ca(2)-O(2)	2.413(8)	Ca(3)-O(2)	2.633(6)
Ca(1)-O(2)	2.452(5)	Ca(2)-O(2)	2.453(8)	Ca(4)-O(2)	2.454(7)
Ca(1)-O(2)	2.504(6)	Ca(3)-O(6)	2.336(6)	Ca(4)-O(2)	2.473(1)
Ca(1)-O(1)	2.675(6)	Ca(3)-O(2)	2.362(6)	Ca(4)-O(6)	2.521(7)
Ca(2)-O(2)	2.269(7)	Ca(3)-O(2)	2.368(5)	Ca(4)-O(5)	2.643(8)
Ca···Ca distances					
Ca(1)-Ca(3)	3.610(4)	Ca(1)-Ca(2)	4.145(3)	Ca(3)-Ca(1)	3.610(4)

Ca(4)-Ca(3)	3.545(3)				
O-Ca-O bond angles					
O(12)-Ca(1)-O(3)	103.7(2)	O(24)-Ca(1)-O(1)	159.5(2)	O(15)-Ca(3)-O(9)	123.76(2)
O(12)-Ca(1)-O(8)	91.7(2)	O(17)-Ca(1)-O(1)	118.75(2)	O(17)-Ca(3)-O(9)	87.4(2)
O(3)-Ca(1)-O(8)	164.5(2)	O(15)-Ca(1)-O(1)	50.74(2)	O(6)-Ca(3)-O(18)	74.4(2)
O(12)-Ca(1)-O(2)	158.5(2)	O(2)-Ca(2)-O(1)	98.0(3)	O(19)-Ca(3)-O(18)	156.8(2)
O(3)-Ca(1)-O(2)	88.7(2)	O(2)-Ca(2)-O(1)	86.2(2)	O(15)-Ca(3)-O(18)	120.0(2)
O(8)-Ca(1)-O(2)	76.99(2)	O(11)-Ca(2)-O(1)	90.4(2)	O(20)-Ca(3)-O(18)	84.5(2)
O(24)-Ca(1)-O(2)	81.6(2)	O(9)-Ca(3)-O(8)	51.85(2)	O(17)-Ca(3)-O(18)	51.54(2)
O(12)-Ca(1)-O(2)	125.9(2)	O(18)-Ca(3)-O(8)	102.1(2)	O(9)-Ca(3)-O(18)	74.3(2)
O(3)-Ca(1)-O(2)	95.2(2)	O(6)-Ca(3)-O(2)	159.2(2)	O(6)-Ca(3)-O(8)	122.1(2)
O(8)-Ca(1)-O(2)	74.42(2)	O(19)-Ca(3)-O(2)	83.1(2)	O(15)-Ca(3)-O(8)	72.01(2)
O(24)-Ca(1)-O(2)	149.5(2)	O(6)-Ca(3)-O(2)	125.8(2)	O(9)-Ca(4)-O(5)	119.0(2)
O(17)-Ca(1)-O(2)	69.13(2)	O(19)-Ca(3)-O(2)	148.1(2)	O(18)-Ca(4)-O(5)	100.2(3)
O(12)-Ca(1)-O(1)	80.1(2)	O(15)-Ca(3)-O(17)	71.2(2)	O(25)-Ca(4)-O(5)	155.6(3)
O(3)-Ca(1)-O(1)	86.3(2)	O(20)-Ca(3)-O(17)	94.7(2)	O(6)-Ca(4)-O(5)	51.4(2)
O(8)-Ca(1)-O(1)	95.42(2)	O(6)-Ca(3)-O(9)	72.8(2)	O(17)-Ca(3)-O(8)	72.09(2)

Table S3. Selected bond lengths (Å) and angles (°) for Sr-TCMTB.

Ca-O bond lengths					
Sr(1)-O(3)	2.548(1)	Sr(2)-O(8)	2.598(6)	Sr(3)-O(1)	2.748(8)
Sr(1)-O(9)	2.565(6)	Sr(2)-O(1)	2.510(6)	Sr(3)-O(2)	2.570(7)
Sr(1)-O(17)	2.599(7)	Sr(2)-O(2)	2.650(6)	Sr(3)-O(1)	2.645(6)
Sr(1)-O(5)	2.645(6)	Sr(2)-O(9)	2.704(7)	Sr(3)-O(1)	2.673(6)
Sr(1)-O(6)	2.711(7)	Sr(2)-O(2)	2.714(6)	Sr(4)-O(1)	2.549(7)
Sr(1)-O(2)	2.717(7)	Sr(3)-O(2)	2.531(6)	Sr(4)-O(1)	2.562(8)
Sr(2)-O(5)	2.513(6)	Sr(3)-O(8)	2.544(6)		
Sr···Sr distances					
Sr(1)-Sr(2)	3.8999(2)	Sr(2)-Sr(3)	3.8361(2)	Sr(3)-Sr(4)	3.859(2)
O-Sr-O bond angles					
O(3)-Sr(1)-O(9)	147.8(2)	O(8)-Sr(2)-O(9)	49.98(2)	O(5)-Sr(1)-O(2)	109.9(2)
O(3)-Sr(1)-O(17)	79.5(2)	O(17)-Sr(2)-O(9)	67.25(2)	O(6)-Sr(1)-O(2)	81.4(2)
O(9)-Sr(1)-O(17)	70.1(2)	O(11)-Sr(2)-O(2)	71.95(2)	O(11)-Sr(2)-O(5)	166.25(2)
O(3)-Sr(1)-O(5)	86.8(2)	O(5)-Sr(2)-O(2)	115.57(2)	O(18)-Sr(3)-O(1)	72.80(2)
O(9)-Sr(1)-O(5)	72.94(2)	O(8)-Sr(2)-O(2)	68.71(2)	O(8)-Sr(3)-O(1)	70.2(2)

O(17)-Sr(1)-O(5)	69.17(2)	O(17)-Sr(2)-O(2)	49.16(2)	O(15)-Sr(3)-O(1)	84.7(2)
O(3)-Sr(1)-O(6)	97.3(2)	O(9)-Sr(2)-O(2)	98.2(2)	O(18)-Sr(3)-O(1)	98.9(2)
O(9)-Sr(1)-O(6)	88.1(2)	O(18)-Sr(3)-O(8)	72.5(2)	O(8)-Sr(3)-O(1)	117.7(2)
O(11)-Sr(2)-O(8)	71.4(2)	O(18)-Sr(3)-O(2)	146.7(2)	O(15)-Sr(3)-O(1)	83.7(2)
O(5)-Sr(2)-O(8)	121.6(2)	O(8)-Sr(3)-O(2)	76.9(2)	O(11)-Sr(3)-O(1)	49.32(2)
O(11)-Sr(2)-O(17)	120.02(2)	O(17)-Sr(1)-O(6)	118.1(2)	O(18)-Sr(3)-O(1)	162.2(2)
O(5)-Sr(2)-O(17)	70.24(2)	O(5)-Sr(1)-O(6)	49.0(2)	O(8)-Sr(3)-O(1)	125.2(2)
O(8)-Sr(2)-O(17)	77.17(2)	O(3)-Sr(1)-O(2)	49.3(2)	O(15)-Sr(3)-O(1)	49.5(2)
O(11)-Sr(2)-O(9)	118.7(2)	O(9)-Sr(1)-O(2)	161.8(2)	O(11)-Sr(3)-O(1)	109.7(2)
O(5)-Sr(2)-O(9)	72.77(2)	O(17)-Sr(1)-O(2)	128.1(2)		

Table S4. Selected bond lengths (Å) and angles (°) for Ba-TCMTB.

Ba-O bond lengths					
Ba(1)-O(5)	2.693(3)	Ba(4)-O(2)	2.676(4)	Ba(6)-O(2)	2.794(3)
Ba(1)-O(34)	2.697(3)	Ba(4)-O(7)	2.686(3)	Ba(6)-O(2)	2.928(3)
Ba(1)-O(8)	2.792(3)	Ba(4)-O(1)	2.802(3)	Ba(7)-O(2)	2.658(3)
Ba(1)-O(9)	2.820(3)	Ba(4)-O(1)	2.881(3)	Ba(7)-O(3)	2.748(3)
Ba(1)-O(36)	2.849(3)	Ba(5)-O(3)	2.664(3)	Ba(7)-O(2)	2.858(3)
Ba(1)-O(35)	2.857(3)	Ba(5)-O(2)	2.693(3)	Ba(7)-O(2)	2.880(3)
Ba(2)-O(35)	2.734(3)	Ba(5)-O(1)	2.822(3)	Ba(8)-O(2)	2.719(3)
Ba(2)-O(6)	2.743(3)	Ba(5)-O(2)	2.827(3)	Ba(8)-O(3)	2.735(3)
Ba(2)-O(9)	2.750(3)	Ba(5)-O(2)	2.863(4)	Ba(8)-O(3)	2.776(3)
Ba(2)-O(5)	2.771(3)	Ba(5)-O(2)	2.865(4)	Ba(8)-O(3)	2.787(3)
Ba(2)-O(4)	2.896(3)	Ba(5)-O(2)	2.869(3)	Ba(9)-O(4)	2.755(3)
Ba(3)-O(4)	2.666(3)	Ba(5)-O(3)	2.982(3)	Ba(9)-O(3)	2.767(3)
Ba(3)-O(13)	2.704(3)	Ba(6)-O(3)	2.680(3)	Ba(9)-O(3)	2.771(3)
Ba(3)-O(7)	2.840(3)	Ba(6)-O(2)	2.727(3)	Ba(9)-O(8)	2.785(3)
Ba(3)-O(6)	2.855(3)	Ba(6)-O(2)	2.775(3)	Ba(9)-O(3)	2.912(3)
Ba···Ba distances					
Ba(2)-Ba(3)	4.3217(1)	Ba(3)-Ba(4)	4.2488(8)	Ba(4)-Ba(5)	4.1632(1)
Ba(6)-Ba(7)	4.3627(1)	Ba(9)-Ba(1)	4.2147(1)		

O-Ba-O bond angles

O(5)-Ba(1)-O(3)	169.75(9)	O(36)-Ba(1)-O(3)	45.75(8)	O(13)-Ba(3)-O(6)	100.47(9)
O(37)-Ba(1)-O(8)	155.81(9)	O(6)-Ba(2)-O(5)	111.90(9)	O(7)-Ba(3)-O(6)	46.23(8)
O(5)-Ba(1)-O(8)	117.82(9)	O(9)-Ba(2)-O(5)	71.85(9)	O(17)-Ba(4)-O(7)	133.74(1)
O(34)-Ba(1)-O(8)	72.19(9)	O(35)-Ba(2)-O(4)	114.36(9)	O(17)-Ba(4)-O(1)	76.44(1)
O(5)-Ba(1)-O(9)	71.93(9)	O(6)-Ba(2)-O(4)	69.48(9)	O(7)-Ba(4)-O(2)	149.74(1)
O(34)-Ba(1)-O(9)	117.51(9)	O(9)-Ba(2)-O(4)	96.54(9)	O(17)-Ba(4)-O(1)	69.15(1)
O(8)-Ba(1)-O(9)	46.73(9)	O(5)-Ba(2)-O(4)	45.42(8)	O(7)-Ba(4)-O(14)	118.26(8)
O(5)-Ba(1)-O(4)	114.68(9)	O(35)-Ba(2)-O(6)	149.19(8)	O(15)-Ba(4)-O(1)	69.40(9)
O(34)-Ba(1)-O(4)	66.02(9)	O(35)-Ba(2)-O(9)	67.00(8)	O(15)-Ba(4)-O(1)	112.96(9)
O(8)-Ba(1)-O(4)	66.72(8)	O(6)-Ba(2)-O(9)	143.76(8)	O(14)-Ba(4)-O(1)	45.83(8)
O(9)-Ba(1)-O(4)	77.52(8)	O(35)-Ba(2)-O(5)	69.71(9)	O(26)-Ba(5)-O(2)	96.22(1)
O(5)-Ba(1)-O(3)	68.99(9)	O(4)-Ba(3)-O(1)	171.46(9)	O(26)-Ba(5)-O(1)	80.93(9)
O(34)-Ba(1)-O(3)	110.51(9)	O(4)-Ba(3)-O(7)	98.53(9)	O(23)-Ba(5)-O(1)	174.31(9)
O(8)-Ba(1)-O(3)	89.73(9)	O(13)-Ba(3)-O(7)	73.86(8)	O(26)-Ba(5)-O(1)	113.51(1)
O(9)-Ba(1)-O(3)	64.43(8)	O(4)-Ba(3)-O(6)	71.15(9)	O(23)-Ba(5)-O(1)	117.52(9)
O(14)-Ba(5)-O(1)	68.17(9)	O(14)-Ba(5)-O(3)	113.37(8)	O(31)-Ba(7)-O(2)	103.68(9)
O(26)-Ba(5)-O(2)	160.32(1)	O(15)-Ba(5)-O(3)	95.45(9)	O(22)-Ba(7)-O(2)	100.49(9)
O(23)-Ba(5)-O(18)	70.24(1)	O(18)-Ba(5)-O(3)	132.33(1)	O(31)-Ba(7)-O(2)	66.51(9)
O(14)-Ba(5)-O(18)	111.19(9)	O(17)-Ba(5)-O(3)	167.28(1)	O(25)-Ba(7)-O(2)	45.54(8)
O(15)-Ba(5)-O(18)	85.83(1)	O(16)-Ba(5)-O(3)	64.68(8)	O(24)-Ba(8)-O(3)	92.72(9)
O(26)-Ba(5)-O(17)	142.04(1)	O(17)-Ba(4)-O(1)	92.65(1)	O(33)-Ba(8)-O(3)	70.83(9)
O(23)-Ba(5)-O(17)	114.57(1)	O(7)-Ba(4)-O(1)	73.46(8)	O(24)-Ba(8)-O(3)	68.22(9)
O(14)-Ba(5)-O(17)	66.30(9)	O(27)-Ba(6)-O(2)	70.04(8)	O(33)-Ba(8)-O(3)	94.35(9)
O(15)-Ba(5)-O(17)	72.42(1)	O(22)-Ba(6)-O(2)	114.02(9)	O(32)-Ba(8)-O(3)	46.60(9)
O(18)-Ba(5)-O(17)	45.02(1)	O(27)-Ba(6)-O(2)	141.08(8)	O(36)-Ba(9)-O(3)	141.86(8)
O(26)-Ba(5)-O(16)	106.35(1)	O(22)-Ba(6)-O(2)	66.87(1)	O(36)-Ba(9)-O(3)	66.36(9)
O(23)-Ba(5)-O(16)	74.21(9)	O(16)-Ba(6)-O(2)	148.83(8)	O(36)-Ba(9)-O(8)	68.12(8)
O(14)-Ba(5)-O(16)	111.28(8)	O(27)-Ba(6)-O(2)	68.12(9)	O(32)-Ba(9)-O(8)	149.94(9)
O(15)-Ba(5)-O(16)	45.79(9)	O(22)-Ba(6)-O(2)	46.20(9)	O(34)-Ba(9)-O(8)	71.22(9)
O(18)-Ba(5)-O(16)	84.20(1)	O(16)-Ba(6)-O(2)	72.10(9)	O(36)-Ba(9)-O(3)	100.80(9)
O(17)-Ba(5)-O(16)	103.16(9)	O(25)-Ba(6)-O(2)	112.73(9)	O(32)-Ba(9)-O(3)	68.38(9)
O(26)-Ba(5)-O(27)	46.09(1)	O(22)-Ba(7)-O(3)	166.44(9)	O(34)-Ba(9)-O(3)	45.45(9)
O(23)-Ba(5)-O(27)	67.13(9)	O(22)-Ba(7)-O(2)	66.82(1)	O(8)-Ba(9)-O(3)	111.15(9)

Table S5. Surface area of the alkaline-earth metal MOFs.

MOFs	SA_{BET} (m^2g^{-1})	SA_{Lang} (m^2g^{-1})
Mg-TCMTB	33.7	93.8
Ca-TCMTB	3.8	12.7
Sr-TCMTB	4.4	17.8
Ba-TCMTB	7.2	13.6

```
####################
1: Mg-TCMTB
####################

Topology for Mg1
-------------------
Atom Mg1 links by bridge ligands and  has
Common vertex with                                      R(A-A)          f
Mg 4    0.7953    0.8462    0.4615   ( 1 0 0)      5.284A          1
Mg 2    0.7060    1.3224    1.0177   ( 1 0 1)     19.002A          1
Mg 1    0.4894    1.3324    0.9682   ( 1 0 1)     19.020A          1
Mg 1    0.4894    0.3324    0.9682   ( 1-1 1)     19.020A          1
Mg 1    0.5106    0.8324   -0.4682   ( 0 0-1)     19.114A          1
Mg 1    0.5106    0.8324    1.5318   ( 0 0 1)     19.114A          1
Mg 2    0.2940    0.8224    1.4823   ( 0 0 1)     19.390A          1
Mg 2    0.2940    0.8224   -0.5177   ( 0 0-1)     19.485A          1
Mg 2    0.7060    0.3224    1.0177   ( 1-1 1)     19.600A          1
Mg 2    0.7060    1.3224    0.0177   ( 1 0 0)     20.059A          1
Mg 1    0.4894    1.3324   -0.0318   ( 1 0 0)     20.122A          1
Mg 1    0.4894    0.3324   -0.0318   ( 1-1 0)     20.122A          1
Mg 2    0.7060    0.3224    0.0177   ( 1-1 0)     20.626A          1
Common face with                                        R(A-A)
Mg 2    0.2940    0.8224    0.4823   ( 0 0 0)      3.531A          3
Topology for Mg2
-------------------
Atom Mg2 links by bridge ligands and  has
Common vertex with                                      R(A-A)          f
Mg 3    0.0045    0.8750    0.4936   ( 0 0 0)      5.222A          1
Mg 1    0.4894    0.3324    0.9682   ( 1-1 1)     19.002A          1
Mg 2    0.2940    0.8224    1.4823   ( 0 0 1)     19.114A          1
Mg 2    0.2940    0.8224   -0.5177   ( 0 0-1)     19.114A          1
Mg 1    0.5106    0.8324   -0.4682   ( 0 0-1)     19.390A          1
Mg 1    0.5106    0.8324    1.5318   ( 0 0 1)     19.485A          1
Mg 1    0.4894    1.3324    0.9682   ( 1 0 1)     19.600A          1
Mg 1    0.4894    0.3324   -0.0318   ( 1-1 0)     20.059A          1
Mg 2    0.7060    1.3224    1.0177   ( 1 0 1)     20.199A          1
Mg 2    0.7060    0.3224    1.0177   ( 1-1 1)     20.199A          1
Mg 1    0.4894    1.3324   -0.0318   ( 1 0 0)     20.626A          1
Mg 2    0.7060    1.3224    0.0177   ( 1 0 0)     21.152A          1
Mg 2    0.7060    0.3224    0.0177   ( 1-1 0)     21.152A          1
Common face with                                        R(A-A)
Mg 1    0.5106    0.8324    0.5318   ( 0 0 0)      3.531A          3
Topology for Mg3
-------------------
Atom Mg3 links by bridge ligands and  has
Common vertex with                                      R(A-A)          f
Mg 2    0.2940    0.8224    0.4823   ( 0 0 0)      5.222A          1
Mg 4    0.2047    1.3462    0.0385   ( 0 1 0)     18.960A          1
Mg 4    0.2047    1.3462    1.0385   ( 0 1 1)     18.989A          1
Mg 3    0.0045    0.8750    1.4936   ( 0 0 1)     19.114A          1
Mg 3    0.0045    0.8750   -0.5064   ( 0 0-1)     19.114A          1
Mg 4   -0.2047    0.8462   -0.5385   ( 0 0-1)     19.188A          1
Mg 3   -0.0045    0.3750    0.0064   ( 0-1 0)     19.407A          1
Mg 3   -0.0045    1.3750    0.0064   ( 0 0 0)     19.407A          1
Mg 3   -0.0045    0.3750    1.0064   ( 0-1 1)     19.683A          1
Mg 3   -0.0045    1.3750    1.0064   ( 0 0 1)     19.683A          1
Mg 4   -0.2047    0.8462    1.4615   ( 0 0 1)     19.687A          1
Mg 4    0.2047    0.3462    0.0385   ( 0 0 0)     20.648A          1
Mg 4    0.2047    0.3462    1.0385   ( 0 0 1)     20.674A          1
Common face with                                        R(A-A)
Mg 4   -0.2047    0.8462    0.4615   ( 0 0 0)      3.542A          3
Topology for Mg4
-------------------
Atom Mg4 links by bridge ligands and  has
Common vertex with                                      R(A-A)          f
Mg 1    0.4894    0.3324   -0.0318   ( 1-1 0)      5.284A          1
Mg 3    0.0045   -0.1250    0.4936   ( 0-1 0)     18.960A          1
Mg 3    0.0045   -0.1250   -0.5064   ( 0-1-1)     18.989A          1
Mg 4    0.2047    0.3462   -0.9615   ( 0 0-1)     19.114A          1
Mg 4    0.2047    0.3462    1.0385   ( 0 0 1)     19.114A          1
Mg 3   -0.0045    0.3750   -0.9936   ( 0-1-1)     19.188A          1
Mg 3   -0.0045    0.3750    1.0064   ( 0-1 1)     19.687A          1
Mg 4   -0.2047   -0.1538   -0.5385   ( 0-1-1)     20.538A          1
Mg 4   -0.2047    0.8462   -0.5385   ( 0 0-1)     20.538A          1
Mg 3    0.0045    0.8750    0.4936   ( 0 0 0)     20.648A          1
Mg 3    0.0045    0.8750   -0.5064   ( 0 0-1)     20.674A          1
Mg 4   -0.2047   -0.1538    0.4615   ( 0-1 0)     20.747A          1
Mg 4   -0.2047    0.8462    0.4615   ( 0 0 0)     20.747A          1
Common face with                                        R(A-A)
```

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c.2

Mg 3   -0.0045    0.3750    0.0064   ( 0-1 0)     3.542A        3
-------------------------
Structural group  analysis
-------------------------

-------------------------
Structural group No 1
-------------------------
Structure consists of 3D framework with Mg4O27N2C78H78
There are 2 interpenetrating  nets
FISE: Full interpenetration symmetry  elements
---------------------------------------------
1: -1
---------------------------------------------
PIC: [0,0,1][0,1,0][1,0,0]  (PICVR=1)

Zt=1; Zn=2

Class IIa  Z=2

Coordination sequences
----------------------
Mg1:  1  2   3   4   5   6    7    8    9   10
Num  14 44  98 170 266 380  518  674  854 1052
Cum  15 59 157 327 593 973 1491 2165 3019 4071
----------------------
Mg2:  1  2   3   4   5   6    7    8    9   10
Num  14 44  98 170 266 380  518  674  854 1052
Cum  15 59 157 327 593 973 1491 2165 3019 4071
----------------------
Mg3:  1  2   3   4   5   6    7    8    9   10
Num  14 44  98 170 266 380  518  674  854 1052
Cum  15 59 157 327 593 973 1491 2165 3019 4071
----------------------
Mg4:  1  2   3   4   5   6    7    8    9   10
Num  14 44  98 170 266 380  518  674  854 1052
Cum  15 59 157 327 593 973 1491 2165 3019 4071
----------------------
TD10=4071

Vertex symbols for selected  sublattice
--------------------------------------
Mg1 Point  symbol:{3^42.4^42.5^7}
Extended  point  symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.
--------------------------------------
Mg2 Point  symbol:{3^42.4^42.5^7}
Extended  point  symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.
--------------------------------------
Mg3 Point  symbol:{3^42.4^42.5^7}
Extended  point  symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.
--------------------------------------
Mg4 Point  symbol:{3^42.4^42.5^7}
Extended  point  symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.4.4.
--------------------------------------
Point symbol for net: {3^42.4^42.5^7}
14-c net; uninodal net

New topology, please, contact the authors (72725 types in 10 databases)
Elapsed time: 71.11  sec.
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############################
1:Ca-TCMTB
############################

Topology for Ca1
--------------------
Atom Ca1 links by bridge ligands and  has
Common vertex with                                    R(A-A)         f
Ca 3   -0.6711   -0.8252   -0.0895   (-1-1-1)     18.831A         1
Ca 2   -0.0901   -0.8176   -0.1990   (-1-1-1)     18.919A         1
Ca 2   -0.0901   -0.8176    0.8010   (-1-1 0)     18.982A         1
Ca 3    0.3289    1.1748    0.9105   ( 0 1 0)     19.384A         1
Ca 3    0.3289   -0.8252   -0.0895   ( 0-1-1)     19.929A         1
Ca 2   -0.0901    0.1824   -0.1990   (-1 0-1)     20.129A         1
Ca 1    0.1435    1.1229    0.7554   ( 0 1 0)     20.203A         1
Ca 1    0.1435   -0.8771    0.7554   ( 0-1 0)     20.203A         1
Ca 1    0.1435    0.1229   -0.2446   ( 0 0-1)     20.451A         1
Ca 1    0.1435    0.1229    1.7554   ( 0 0 1)     20.451A         1
Ca 1    0.1435   -0.8771   -0.2446   ( 0-1-1)     20.882A         1
Ca 1    0.1435    1.1229    1.7554   ( 0 1 1)     20.882A         1
Ca 2    0.9099    1.1824    0.8010   ( 0 1 0)     21.461A         1
Ca 2   -0.0901    0.1824    1.8010   (-1 0 1)     21.580A         1
Ca 3   -0.6711   -0.8252    0.9105   (-1-1 0)     22.128A         1
Ca 3    0.3289    1.1748    1.9105   ( 0 1 1)     22.383A         1
Ca 1   -0.8565   -0.8771    0.7554   (-1-1 0)     22.428A         1
Ca 1    1.1435    1.1229    0.7554   ( 1 1 0)     22.428A         1
Common edge with                                      R(A-A)
Ca 3    0.3289    0.1748   -0.0895   ( 0 0-1)     18.273A         2
Common face with                                      R(A-A)
Ca 3    0.3289    0.1748    0.9105   ( 0 0 0)      3.610A         3
Ca 2   -0.0901    0.1824    0.8010   (-1 0 0)      4.145A         3
Topology for Ca2
--------------------
Atom Ca2 links by bridge ligands and  has
Common vertex with                                    R(A-A)         f
Ca 3    1.3289    0.1748    0.9105   ( 1 0 0)      6.727A         1
Ca 3    1.3289    1.1748    0.9105   ( 1 1 0)     18.518A         1
Ca 3    0.3289   -0.8252   -0.0895   ( 0-1-1)     18.907A         1
Ca 1    1.1435    1.1229    1.7554   ( 1 1 1)     18.919A         1
Ca 1    1.1435    1.1229    0.7554   ( 1 1 0)     18.982A         1
Ca 3    1.3289    0.1748   -0.0895   ( 1 0-1)     19.909A         1
Ca 1    1.1435    0.1229    1.7554   ( 1 0 1)     20.129A         1
Ca 2    0.9099    0.1824   -0.1990   ( 0 0-1)     20.451A         1
Ca 2    0.9099    0.1824    1.8010   ( 0 0 1)     20.451A         1
Ca 3    1.3289    1.1748    1.9105   ( 1 1 1)     20.926A         1
Ca 1    0.1435   -0.8771    0.7554   ( 0-1 0)     21.461A         1
Ca 3    0.3289   -0.8252    0.9105   ( 0-1 0)     21.501A         1
Ca 1    1.1435    0.1229   -0.2446   ( 1 0-1)     21.580A         1
Common face with                                      R(A-A)
Ca 1    1.1435    0.1229    0.7554   ( 1 0 0)      4.145A         3
Topology for Ca3
--------------------
Atom Ca3 links by bridge ligands and  has
Common vertex with                                    R(A-A)         f
Ca 2   -0.0901    0.1824    0.8010   (-1 0 0)      6.727A         1
Ca 2   -0.0901   -0.8176    0.8010   (-1-1 0)     18.518A         1
Ca 1    1.1435    1.1229    1.7554   ( 1 1 1)     18.831A         1
Ca 2    0.9099    1.1824    1.8010   ( 0 1 1)     18.907A         1
Ca 1    0.1435   -0.8771    0.7554   ( 0-1 0)     19.384A         1
Ca 2   -0.0901    0.1824    1.8010   (-1 0 1)     19.909A         1
Ca 1    0.1435    1.1229    1.7554   ( 0 1 1)     19.929A         1
Ca 3    0.3289    0.1748    1.9105   ( 0 0 1)     20.451A         1
Ca 3    0.3289    0.1748   -0.0895   ( 0 0-1)     20.451A         1
Ca 3    0.3289    1.1748    1.9105   ( 0 1 1)     20.882A         1
Ca 3    0.3289   -0.8252   -0.0895   ( 0-1-1)     20.882A         1
Ca 2   -0.0901   -0.8176   -0.1990   (-1-1-1)     20.926A         1
Ca 2    0.9099    1.1824    0.8010   ( 0 1 0)     21.501A         1
Ca 1    1.1435    1.1229    0.7554   ( 1 1 0)     22.128A         1
Ca 1    0.1435   -0.8771   -0.2446   ( 0-1-1)     22.383A         1
Common edge with                                      R(A-A)
Ca 1    0.1435    0.1229    1.7554   ( 0 0 1)     18.273A         2
Common face with                                      R(A-A)
Ca 1    0.1435    0.1229    0.7554   ( 0 0 0)      3.610A         3
-------------------------
Structural group  analysis
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Structural group No 1
```

```
c.2

-------------------------
Structure consists of 3D framework with Ca3O24N2C72H68
There are 2 interpenetrating  nets
FISE: Full interpenetration symmetry  elements
---------------------------------------------
1: -1
---------------------------------------------
PIC: [0,1,0][0,0,1][1,0,0]  (PICVR=1)

Zt=1; Zn=2

Class IIa  Z=2

Coordination  sequences
----------------------
Ca1:  1   2   3   4    5    6    7    8    9   10
Num  21  79 175 311  485  699  951 1243 1573 1943
Cum  22 101 276 587 1072 1771 2722 3965 5538  7481
----------------------
Ca2:  1  2   3   4    5    6    7    8    9   10
Num  14 66 164 297  468  679  928 1217 1544 1911
Cum  15 81 245 542 1010 1689 2617 3834 5378 7289
----------------------
Ca3:  1  2   3   4    5    6    7    8    9   10
Num  17 71 173 308  483  696  949 1240 1571 1940
Cum  18 89 262 570 1053 1749 2698 3938 5509 7449
----------------------
TD10=7406

Vertex symbols for selected  sublattice
--------------------------------------
Ca1 Point  symbol:{3^70.4^120.5^20}
Extended  point  symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.
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Ca2 Point  symbol:{3^44.4^47}
Extended  point  symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.
--------------------------------------
Ca3 Point  symbol:{3^54.4^76.5^6}
Extended  point  symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.
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Point symbol for net: {3^44.4^47}{3^54.4^76.5^6}{3^70.4^120.5^20}
14,17,21-c net with stoichiometry (14-c)(17-c)(21-c); 3-nodal  net

New topology, please, contact the authors (72725 types in 10 databases)
Elapsed time: 42.09  sec.
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#######
1:Sr-TCMTB
#######

Topology for Sr1
--------------------
Atom Sr1 links by bridge ligands and  has
Common vertex with                                      R(A-A)          f
Sr 2     0.1137   -0.5685    0.3273   ( 0-1 0)      18.400A         1
Sr 3    -0.0706   -0.6942    1.3522   (-1-1 1)      19.400A         1
Sr 4    -0.3025   -0.6384    1.3449   (-1-1 1)      19.458A         1
Sr 1     0.2947   -0.7044    0.3965   ( 0-1 0)      19.681A         1
Sr 1     0.2947    1.2956    0.3965   ( 0 1 0)      19.681A         1
Sr 3    -0.0706    1.3058    0.3522   (-1 1 0)      19.781A         1
Sr 4    -0.3025    0.3616    1.3449   (-1 0 1)      19.916A         1
Sr 2     0.1137    0.4315    1.3273   ( 0 0 1)      20.409A         1
Sr 1     0.2947   -0.7044    1.3965   ( 0-1 1)      20.424A         1
Sr 1     0.2947    1.2956   -0.6035   ( 0 1-1)      20.424A         1
Sr 1     0.2947    0.2956   -0.6035   ( 0 0-1)      21.132A         1
Sr 1     0.2947    0.2956    1.3965   ( 0 0 1)      21.132A         1
Sr 2     0.1137    1.4315    0.3273   ( 0 1 0)      21.599A         1
Common edge with                                        R(A-A)
Sr 3    -0.0706    0.3058    0.3522   (-1 0 0)       6.297A         2
Sr 2     0.1137   -0.5685    1.3273   ( 0-1 1)      17.975A         2
Sr 3    -0.0706    0.3058    1.3522   (-1 0 1)      19.237A         2
Common face with                                        R(A-A)
Sr 2     0.1137    0.4315    0.3273   ( 0 0 0)       3.898A         3
Topology for Sr2
--------------------
Atom Sr2 links by bridge ligands and  has
Common vertex with                                      R(A-A)          f
Sr 4    -0.3025    0.3616    0.3449   (-1 0 0)       6.934A         1
Sr 1     0.2947    1.2956    0.3965   ( 0 1 0)      18.400A         1
Sr 4    -0.3025    1.3616    0.3449   (-1 1 0)      18.975A         1
Sr 2     0.1137    1.4315    0.3273   ( 0 1 0)      19.681A         1
Sr 2     0.1137   -0.5685    0.3273   ( 0-1 0)      19.681A         1
Sr 4    -0.3025    0.3616    1.3449   (-1 0 1)      19.730A         1
Sr 3    -0.0706    0.3058    1.3522   (-1 0 1)      19.758A         1
Sr 3    -0.0706    1.3058   -0.6478   (-1 1-1)      20.077A         1
Sr 1     0.2947    0.2956   -0.6035   ( 0 0-1)      20.409A         1
Sr 2     0.1137    1.4315   -0.6727   ( 0 1-1)      20.424A         1
Sr 2     0.1137   -0.5685    1.3273   ( 0-1 1)      20.424A         1
Sr 4    -0.3025   -0.6384    1.3449   (-1-1 1)      20.862A         1
Sr 3    -0.0706   -0.6942    1.3522   (-1-1 1)      21.462A         1
Sr 1     0.2947   -0.7044    0.3965   ( 0-1 0)      21.599A         1
Common edge with                                        R(A-A)
Sr 3    -0.0706    1.3058    0.3522   (-1 1 0)      17.390A         2
Sr 1     0.2947    1.2956   -0.6035   ( 0 1-1)      17.975A         2
Common face with                                        R(A-A)
Sr 3    -0.0706    0.3058    0.3522   (-1 0 0)       3.838A         3
Sr 1     0.2947    0.2956    0.3965   ( 0 0 0)       3.898A         3
Topology for Sr3
--------------------
Atom Sr3 links by bridge ligands and  has
Common vertex with                                      R(A-A)          f
Sr 4     0.6975   -0.6384    1.3449   ( 0-1 1)      19.319A         1
Sr 1     1.2947    1.2956   -0.6035   ( 1 1-1)      19.400A         1
Sr 4     0.6975   -0.6384    0.3449   ( 0-1 0)      19.440A         1
Sr 3     0.9294    1.3058    0.3522   ( 0 1 0)      19.681A         1
Sr 3     0.9294   -0.6942    0.3522   ( 0-1 0)      19.681A         1
Sr 2     1.1137    0.4315   -0.6727   ( 1 0-1)      19.758A         1
Sr 1     1.2947   -0.7044    0.3965   ( 1-1 0)      19.781A         1
Sr 2     1.1137   -0.5685    1.3273   ( 1-1 1)      20.077A         1
Sr 3     0.9294   -0.6942    1.3522   ( 0-1 1)      20.424A         1
Sr 3     0.9294    1.3058   -0.6478   ( 0 1-1)      20.424A         1
Sr 4     0.6975    1.3616    0.3449   ( 0 1 0)      20.653A         1
Sr 4     0.6975    0.3616    1.3449   ( 0 0 1)      20.664A         1
Sr 3     0.9294    0.3058    1.3522   ( 0 0 1)      21.132A         1
Sr 3     0.9294    0.3058   -0.6478   ( 0 0-1)      21.132A         1
Sr 2     1.1137    1.4315   -0.6727   ( 1 1-1)      21.462A         1
Common edge with                                        R(A-A)
Sr 1     1.2947    0.2956    0.3965   ( 1 0 0)       6.297A         2
Sr 2     1.1137   -0.5685    0.3273   ( 1-1 0)      17.390A         2
Sr 1     1.2947    0.2956   -0.6035   ( 1 0-1)      19.237A         2
Common face with                                        R(A-A)
Sr 2     1.1137    0.4315    0.3273   ( 1 0 0)       3.838A         3
Sr 4     0.6975    0.3616    0.3449   ( 0 0 0)       3.858A         3
Topology for Sr4
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c.2

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Atom Sr4 links by bridge ligands and  has
Common vertex with                                    R(A-A)        f
Sr 2    1.1137    0.4315    0.3273   ( 1 0 0)      6.934A        1
Sr 2    1.1137   -0.5685    0.3273   ( 1-1 0)     18.975A        1
Sr 3    0.9294    1.3058   -0.6478   ( 0 1-1)     19.319A        1
Sr 3    0.9294    1.3058    0.3522   ( 0 1 0)     19.440A        1
Sr 1    1.2947    1.2956   -0.6035   ( 1 1-1)     19.458A        1
Sr 4    0.6975    1.3616    0.3449   ( 0 1 0)     19.681A        1
Sr 4    0.6975   -0.6384    0.3449   ( 0-1 0)     19.681A        1
Sr 2    1.1137    0.4315   -0.6727   ( 1 0-1)     19.730A        1
Sr 1    1.2947    0.2956   -0.6035   ( 1 0-1)     19.916A        1
Sr 3    0.9294   -0.6942    0.3522   ( 0-1 0)     20.653A        1
Sr 3    0.9294    0.3058   -0.6478   ( 0 0-1)     20.664A        1
Sr 2    1.1137    1.4315   -0.6727   ( 1 1-1)     20.862A        1
Common face with                                      R(A-A)
Sr 3    0.9294    0.3058    0.3522   ( 0 0 0)      3.858A        3
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Structural group  analysis
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Structural group No 1
-------------------------
Structure consists of layers ( 1 0 0) with  Sr2O15N3C44H51

Coordination sequences
----------------------
Sr1:  1  2   3   4   5   6   7   8    9   10
Num  17 42  66  90 114 138 162 186  210  234
Cum  18 60 126 216 330 468 630 816 1026 1260
----------------------
Sr2:  1  2   3   4   5   6   7   8    9   10
Num  18 44  68  92 116 140 164 188  212  236
Cum  19 63 131 223 339 479 643 831 1043 1279
----------------------
Sr3:  1  2   3   4   5   6   7   8    9   10
Num  20 44  68  92 116 140 164 188  212  236
Cum  21 65 133 225 341 481 645 833 1045 1281
----------------------
Sr4:  1  2   3   4   5   6   7   8    9   10
Num  13 40  64  88 112 136 160 184  208  232
Cum  14 54 118 206 318 454 614 798 1006 1238
----------------------
TD10=1264

Vertex symbols for selected  sublattice
--------------------------------------
Sr1 Point  symbol:{3^70.4^61.5^5}
Extended  point  symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.
--------------------------------------
Sr2 Point  symbol:{3^77.4^76}
Extended  point  symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.
--------------------------------------
Sr3 Point  symbol:{3^90.4^91.5^9}
Extended  point  symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.
--------------------------------------
Sr4 Point  symbol:{3^51.4^27}
Extended  point  symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.
--------------------------------------
Point symbol for net: {3^51.4^27}{3^70.4^61.5^5}{3^77.4^76}{3^90.4^91.5^9}
13,17,18,20-c net with stoichiometry (13-c)(17-c)(18-c)(20-c); 4-nodal   net

New topology, please, contact the authors (72725 types in 10 databases)
Elapsed time: 17.24  sec.
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####################
1:Ba-TCMTB
####################

Topology for Ba1
-------------------
Atom Ba1 links by bridge ligands and  has
Common vertex with                                      R(A-A)          f
Ba 3    0.6102    0.6650    0.2962   ( 0 0 0)          7.171A          1
Ba 8    0.6387    0.7258   -0.1569   ( 0 0-1)          7.306A          1
Ba 9    0.7004    1.6147   -0.0235   ( 0 1-1)         18.489A          1
Ba 7    0.6554    1.6018   -0.2477   ( 0 1-1)         18.688A          1
Ba 9   -0.2996    0.6147   -0.0235   (-1 0-1)         18.731A          1
Ba 2   -0.2917    1.6865    0.1693   (-1 1 0)         18.811A          1
Ba 4   -0.3101    0.7171    0.3963   (-1 0 0)         19.024A          1
Ba 2    0.7083   -0.3135    0.1693   ( 0-1 0)         19.285A          1
Ba 7   -0.3446    1.6018   -0.2477   (-1 1-1)         19.406A          1
Ba 1   -0.4422    0.7403    0.0696   (-1 0 0)         19.519A          1
Ba 1    1.5578    0.7403    0.0696   ( 1 0 0)         19.519A          1
Ba 8   -0.3613    1.7258   -0.1569   (-1 1-1)         19.584A          1
Ba 3   -0.3898    0.6650    0.2962   (-1 0 0)         19.706A          1
Ba 4    0.6899   -0.2829    0.3963   ( 0-1 0)         19.741A          1
Ba 1   -0.4422    1.7403    0.0696   (-1 1 0)         20.042A          1
Ba 1    1.5578   -0.2597    0.0696   ( 1-1 0)         20.042A          1
Ba 8    0.6387    1.7258   -0.1569   ( 0 1-1)         20.082A          1
Ba 3    0.6102   -0.3350    0.2962   ( 0-1 0)         20.554A          1
Ba 9    1.7004    0.6147   -0.0235   ( 1 0-1)         21.135A          1
Ba 8    1.6387    0.7258   -0.1569   ( 1 0-1)         21.402A          1
Ba 3    1.6102   -0.3350    0.2962   ( 1-1 0)         21.691A          1
Ba 2    1.7083   -0.3135    0.1693   ( 1-1 0)         22.013A          1
Common edge with                                        R(A-A)
Ba 2   -0.2917    0.6865    0.1693   (-1 0 0)         17.024A          2
Ba 9   -0.2996    1.6147   -0.0235   (-1 1-1)         17.260A          2
Common face with                                        R(A-A)
Ba 2    0.7083    0.6865    0.1693   ( 0 0 0)          4.187A          3
Ba 9    0.7004    0.6147   -0.0235   ( 0 0-1)          4.215A          3
Topology for Ba2
-------------------
Atom Ba2 links by bridge ligands and  has
Common vertex with                                      R(A-A)          f
Ba 4    0.6899    0.7171    0.3963   ( 0 0 0)          7.408A          1
Ba 3    1.6102    0.6650    0.2962   ( 1 0 0)         18.304A          1
Ba 1    1.5578   -0.2597    0.0696   ( 1-1 0)         18.811A          1
Ba 9    1.7004    0.6147   -0.0235   ( 1 0-1)         19.109A          1
Ba 4    0.6899   -0.2829    0.3963   ( 0-1 0)         19.189A          1
Ba 1    0.5578    1.7403    0.0696   ( 0 1 0)         19.285A          1
Ba 3    1.6102   -0.3350    0.2962   ( 1-1 0)         19.298A          1
Ba 2    1.7083    0.6865    0.1693   ( 1 0 0)         19.519A          1
Ba 2   -0.2917    0.6865    0.1693   (-1 0 0)         19.519A          1
Ba 7    0.6554    1.6018   -0.2477   ( 0 1-1)         19.643A          1
Ba 9   -0.2996    1.6147   -0.0235   (-1 1-1)         19.758A          1
Ba 2    0.7083   -0.3135    0.1693   ( 0-1 0)         19.943A          1
Ba 2    0.7083    1.6865    0.1693   ( 0 1 0)         19.943A          1
Ba 2    1.7083   -0.3135    0.1693   ( 1-1 0)         20.042A          1
Ba 2   -0.2917    1.6865    0.1693   (-1 1 0)         20.042A          1
Ba 4   -0.3101    0.7171    0.3963   (-1 0 0)         20.144A          1
Ba 8    1.6387    0.7258   -0.1569   ( 1 0-1)         20.164A          1
Ba 8    0.6387    1.7258   -0.1569   ( 0 1-1)         20.424A          1
Ba 3    0.6102   -0.3350    0.2962   ( 0-1 0)         20.810A          1
Ba 3   -0.3898    0.6650    0.2962   (-1 0 0)         21.547A          1
Ba 1   -0.4422    1.7403    0.0696   (-1 1 0)         22.013A          1
Common edge with                                        R(A-A)
Ba 9    0.7004    0.6147   -0.0235   ( 0 0-1)          6.702A          2
Ba 1    1.5578    0.7403    0.0696   ( 1 0 0)         17.024A          2
Ba 9    0.7004    1.6147   -0.0235   ( 0 1-1)         18.046A          2
Common face with                                        R(A-A)
Ba 1    0.5578    0.7403    0.0696   ( 0 0 0)          4.187A          3
Ba 3    0.6102    0.6650    0.2962   ( 0 0 0)          4.321A          3
Topology for Ba3
-------------------
Atom Ba3 links by bridge ligands and  has
Common vertex with                                      R(A-A)          f
Ba 1    0.5578    0.7403    0.0696   ( 0 0 0)          7.171A          1
Ba 5    0.6640    0.6209    0.5229   ( 0 0 0)          7.263A          1
Ba 4   -0.3101    0.7171    0.3963   (-1 0 0)         17.446A          1
Ba 4    0.6899   -0.2829    0.3963   ( 0-1 0)         17.741A          1
Ba 2   -0.2917    0.6865    0.1693   (-1 0 0)         18.304A          1
Ba 2   -0.2917    1.6865    0.1693   (-1 1 0)         19.298A          1
Ba 3   -0.3898    0.6650    0.2962   (-1 0 0)         19.519A          1
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c.2

Ba 3	1.6102	0.6650	0.2962	(1 0 0)	19.519A	1
Ba 1	1.5578	0.7403	0.0696	(1 0 0)	19.706A	1
Ba 5	0.6640	-0.3791	0.5229	(0-1 0)	19.961A	1
Ba 6	0.7769	-0.3850	0.6304	(0-1 0)	20.067A	1
Ba 9	0.7004	1.6147	-0.0235	(0 1-1)	20.145A	1
Ba 9	-0.2996	1.6147	-0.0235	(-1 1-1)	20.148A	1
Ba 4	1.6899	-0.2829	0.3963	(1-1 0)	20.333A	1
Ba 1	0.5578	1.7403	0.0696	(0 1 0)	20.554A	1
Ba 2	0.7083	1.6865	0.1693	(0 1 0)	20.810A	1
Ba 5	1.6640	-0.3791	0.5229	(1-1 0)	21.430A	1
Ba 2	1.7083	0.6865	0.1693	(1 0 0)	21.547A	1
Ba 1	-0.4422	1.7403	0.0696	(-1 1 0)	21.691A	1
Common face with					R(A-A)	
Ba 4	0.6899	0.7171	0.3963	(0 0 0)	4.252A	3
Ba 2	0.7083	0.6865	0.1693	(0 0 0)	4.321A	3

Topology for Ba4

Atom Ba4 links by bridge ligands and has

Common vertex with					R(A-A)	f
Ba 2	0.7083	0.6865	0.1693	(0 0 0)	7.408A	1
Ba 6	0.7769	0.6150	0.6304	(0 0 0)	7.485A	1
Ba 3	1.6102	0.6650	0.2962	(1 0 0)	17.446A	1
Ba 3	0.6102	1.6650	0.2962	(0 1 0)	17.741A	1
Ba 5	1.6640	0.6209	0.5229	(1 0 0)	18.986A	1
Ba 1	1.5578	0.7403	0.0696	(1 0 0)	19.024A	1
Ba 5	0.6640	1.6209	0.5229	(0 1 0)	19.133A	1
Ba 2	0.7083	1.6865	0.1693	(0 1 0)	19.189A	1
Ba 6	-0.2231	0.6150	0.6304	(-1 0 0)	19.381A	1
Ba 4	-0.3101	0.7171	0.3963	(-1 0 0)	19.519A	1
Ba 4	1.6899	0.7171	0.3963	(1 0 0)	19.519A	1
Ba 1	0.5578	1.7403	0.0696	(0 1 0)	19.741A	1
Ba 9	0.7004	1.6147	-0.0235	(0 1-1)	19.849A	1
Ba 4	0.6899	1.7171	0.3963	(0 1 0)	19.943A	1
Ba 4	0.6899	-0.2829	0.3963	(0-1 0)	19.943A	1
Ba 4	-0.3101	1.7171	0.3963	(-1 1 0)	20.042A	1
Ba 4	1.6899	-0.2829	0.3963	(1-1 0)	20.042A	1
Ba 2	1.7083	0.6865	0.1693	(1 0 0)	20.144A	1
Ba 5	-0.3360	1.6209	0.5229	(-1 1 0)	20.196A	1
Ba 3	-0.3898	1.6650	0.2962	(-1 1 0)	20.333A	1
Ba 5	1.6640	-0.3791	0.5229	(1-1 0)	20.740A	1
Ba 6	0.7769	-0.3850	0.6304	(0-1 0)	20.812A	1
Ba 5	-0.3360	0.6209	0.5229	(-1 0 0)	20.885A	1
Ba 5	0.6640	-0.3791	0.5229	(0-1 0)	21.542A	1
Common face with					R(A-A)	
Ba 5	0.6640	0.6209	0.5229	(0 0 0)	4.164A	3
Ba 3	0.6102	0.6650	0.2962	(0 0 0)	4.252A	3

Topology for Ba5

Atom Ba5 links by bridge ligands and has

Common vertex with					R(A-A)	f
Ba 3	0.6102	0.6650	0.2962	(0 0 0)	7.263A	1
Ba 7	0.6554	0.6018	0.7523	(0 0 0)	7.273A	1
Ba 8	0.6387	-0.2742	0.8431	(0-1 0)	18.639A	1
Ba 4	-0.3101	0.7171	0.3963	(-1 0 0)	18.986A	1
Ba 4	0.6899	-0.2829	0.3963	(0-1 0)	19.133A	1
Ba 5	-0.3360	0.6209	0.5229	(-1 0 0)	19.519A	1
Ba 5	1.6640	0.6209	0.5229	(1 0 0)	19.519A	1
Ba 6	-0.2231	1.6150	0.6304	(-1 1 0)	19.751A	1
Ba 5	0.6640	-0.3791	0.5229	(0-1 0)	19.943A	1
Ba 5	0.6640	1.6209	0.5229	(0 1 0)	19.943A	1
Ba 3	0.6102	1.6650	0.2962	(0 1 0)	19.961A	1
Ba 7	0.6554	-0.3982	0.7523	(0-1 0)	20.035A	1
Ba 4	1.6899	-0.2829	0.3963	(1-1 0)	20.196A	1
Ba 7	-0.3446	0.6018	0.7523	(-1 0 0)	20.364A	1
Ba 7	1.6554	-0.3982	0.7523	(1-1 0)	20.604A	1
Ba 4	-0.3101	1.7171	0.3963	(-1 1 0)	20.740A	1
Ba 8	-0.3613	0.7258	0.8431	(-1 0 0)	20.802A	1
Ba 4	1.6899	0.7171	0.3963	(1 0 0)	20.885A	1
Ba 6	1.7769	-0.3850	0.6304	(1-1 0)	21.199A	1
Ba 3	-0.3898	1.6650	0.2962	(-1 1 0)	21.430A	1
Ba 4	0.6899	1.7171	0.3963	(0 1 0)	21.542A	1
Common edge with					R(A-A)	
Ba 6	-0.2231	0.6150	0.6304	(-1 0 0)	17.315A	2
Ba 6	0.7769	-0.3850	0.6304	(0-1 0)	18.607A	2
Ba 5	1.6640	-0.3791	0.5229	(1-1 0)	20.042A	2
Ba 5	-0.3360	1.6209	0.5229	(-1 1 0)	20.042A	2
Common face with					R(A-A)	
Ba 4	0.6899	0.7171	0.3963	(0 0 0)	4.164A	3
Ba 6	0.7769	0.6150	0.6304	(0 0 0)	4.252A	3

c.3

Topology for Ba6

Atom Ba6 links by bridge ligands and has

Common vertex with					R(A-A)	f
Ba 8	0.6387	0.7258	0.8431	(0 0 0)	7.466A	1
Ba 4	0.6899	0.7171	0.3963	(0 0 0)	7.485A	1
Ba 7	1.6554	0.6018	0.7523	(1 0 0)	17.887A	1
Ba 8	0.6387	-0.2742	0.8431	(0-1 0)	18.834A	1
Ba 7	1.6554	-0.3982	0.7523	(1-1 0)	19.000A	1
Ba 4	1.6899	0.7171	0.3963	(1 0 0)	19.381A	1
Ba 6	1.7769	0.6150	0.6304	(1 0 0)	19.519A	1
Ba 6	-0.2231	0.6150	0.6304	(-1 0 0)	19.519A	1
Ba 5	1.6640	-0.3791	0.5229	(1-1 0)	19.751A	1
Ba 6	0.7769	-0.3850	0.6304	(0-1 0)	19.943A	1
Ba 6	0.7769	1.6150	0.6304	(0 1 0)	19.943A	1
Ba 6	1.7769	-0.3850	0.6304	(1-1 0)	20.042A	1
Ba 6	-0.2231	1.6150	0.6304	(-1 1 0)	20.042A	1
Ba 3	0.6102	1.6650	0.2962	(0 1 0)	20.067A	1
Ba 4	0.6899	1.7171	0.3963	(0 1 0)	20.812A	1
Ba 7	0.6554	-0.3982	0.7523	(0-1 0)	20.908A	1
Ba 5	-0.3360	1.6209	0.5229	(-1 1 0)	21.199A	1
Ba 8	-0.3613	0.7258	0.8431	(-1 0 0)	21.673A	1
Ba 7	-0.3446	0.6018	0.7523	(-1 0 0)	21.911A	1
Common edge with					R(A-A)	
Ba 5	1.6640	0.6209	0.5229	(1 0 0)	17.315A	2
Ba 5	0.6640	1.6209	0.5229	(0 1 0)	18.607A	2
Common face with					R(A-A)	
Ba 5	0.6640	0.6209	0.5229	(0 0 0)	4.252A	3
Ba 7	0.6554	0.6018	0.7523	(0 0 0)	4.362A	3

Topology for Ba7

Atom Ba7 links by bridge ligands and has

Common vertex with					R(A-A)	f
Ba 5	0.6640	0.6209	0.5229	(0 0 0)	7.273A	1
Ba 9	0.7004	0.6147	0.9765	(0 0 0)	7.425A	1
Ba 6	-0.2231	0.6150	0.6304	(-1 0 0)	17.887A	1
Ba 8	1.6387	-0.2742	0.8431	(1-1 0)	18.620A	1
Ba 1	0.5578	-0.2597	1.0696	(0-1 1)	18.688A	1
Ba 8	-0.3613	0.7258	0.8431	(-1 0 0)	18.733A	1
Ba 9	0.7004	-0.3853	0.9765	(0-1 0)	18.962A	1
Ba 6	-0.2231	1.6150	0.6304	(-1 1 0)	19.000A	1
Ba 1	1.5578	-0.2597	1.0696	(1-1 1)	19.406A	1
Ba 7	-0.3446	0.6018	0.7523	(-1 0 0)	19.519A	1
Ba 7	1.6554	0.6018	0.7523	(1 0 0)	19.519A	1
Ba 2	0.7083	-0.3135	1.1693	(0-1 1)	19.643A	1
Ba 5	0.6640	1.6209	0.5229	(0 1 0)	20.035A	1
Ba 5	1.6640	0.6209	0.5229	(1 0 0)	20.364A	1
Ba 5	-0.3360	1.6209	0.5229	(-1 1 0)	20.604A	1
Ba 9	1.7004	-0.3853	0.9765	(1-1 0)	20.853A	1
Ba 6	0.7769	1.6150	0.6304	(0 1 0)	20.908A	1
Ba 6	1.7769	0.6150	0.6304	(1 0 0)	21.911A	1
Common face with					R(A-A)	
Ba 8	0.6387	0.7258	0.8431	(0 0 0)	4.127A	3
Ba 6	0.7769	0.6150	0.6304	(0 0 0)	4.362A	3

Topology for Ba8

Atom Ba8 links by bridge ligands and has

Common vertex with					R(A-A)	f
Ba 1	0.5578	0.7403	1.0696	(0 0 1)	7.306A	1
Ba 6	0.7769	0.6150	0.6304	(0 0 0)	7.466A	1
Ba 7	-0.3446	1.6018	0.7523	(-1 1 0)	18.620A	1
Ba 5	0.6640	1.6209	0.5229	(0 1 0)	18.639A	1
Ba 7	1.6554	0.6018	0.7523	(1 0 0)	18.733A	1
Ba 6	0.7769	1.6150	0.6304	(0 1 0)	18.834A	1
Ba 9	-0.2996	1.6147	0.9765	(-1 1 0)	19.250A	1
Ba 9	-0.2996	0.6147	0.9765	(-1 0 0)	19.383A	1
Ba 1	1.5578	-0.2597	1.0696	(1-1 1)	19.584A	1
Ba 8	-0.3613	1.7258	0.8431	(-1 1 0)	20.042A	1
Ba 8	1.6387	-0.2742	0.8431	(1-1 0)	20.042A	1
Ba 1	0.5578	-0.2597	1.0696	(0-1 1)	20.082A	1
Ba 2	-0.2917	0.6865	1.1693	(-1 0 1)	20.164A	1
Ba 2	0.7083	-0.3135	1.1693	(0-1 1)	20.424A	1
Ba 5	1.6640	0.6209	0.5229	(1 0 0)	20.802A	1
Ba 9	0.7004	-0.3853	0.9765	(0-1 0)	21.034A	1
Ba 1	-0.4422	0.7403	1.0696	(-1 0 1)	21.402A	1
Ba 6	1.7769	0.6150	0.6304	(1 0 0)	21.673A	1
Ba 9	1.7004	-0.3853	0.9765	(1-1 0)	21.694A	1
Common face with					R(A-A)	
Ba 7	0.6554	0.6018	0.7523	(0 0 0)	4.127A	3

c.4

Ba 9 0.7004 0.6147 0.9765 (0 0 0) 4.350A 3
Topology for Ba9

Atom Ba9 links by bridge ligands and has

Common vertex with					R(A-A)	f
Ba 7	0.6554	0.6018	0.7523	(0 0 0)	7.425A	1
Ba 1	0.5578	-0.2597	1.0696	(0-1 1)	18.489A	1
Ba 1	1.5578	0.7403	1.0696	(1 0 1)	18.731A	1
Ba 7	0.6554	1.6018	0.7523	(0 1 0)	18.962A	1
Ba 2	-0.2917	0.6865	1.1693	(-1 0 1)	19.109A	1
Ba 8	1.6387	-0.2742	0.8431	(1-1 0)	19.250A	1
Ba 8	1.6387	0.7258	0.8431	(1 0 0)	19.383A	1
Ba 9	1.7004	0.6147	0.9765	(1 0 0)	19.519A	1
Ba 9	-0.2996	0.6147	0.9765	(-1 0 0)	19.519A	1
Ba 2	1.7083	-0.3135	1.1693	(1-1 1)	19.758A	1
Ba 4	0.6899	-0.2829	1.3963	(0-1 1)	19.849A	1
Ba 9	0.7004	1.6147	0.9765	(0 1 0)	19.943A	1
Ba 9	0.7004	-0.3853	0.9765	(0-1 0)	19.943A	1
Ba 9	1.7004	-0.3853	0.9765	(1-1 0)	20.042A	1
Ba 9	-0.2996	1.6147	0.9765	(-1 1 0)	20.042A	1
Ba 3	0.6102	-0.3350	1.2962	(0-1 1)	20.145A	1
Ba 3	1.6102	-0.3350	1.2962	(1-1 1)	20.148A	1
Ba 7	-0.3446	1.6018	0.7523	(-1 1 0)	20.853A	1
Ba 8	0.6387	1.7258	0.8431	(0 1 0)	21.034A	1
Ba 1	-0.4422	0.7403	1.0696	(-1 0 1)	21.135A	1
Ba 8	-0.3613	1.7258	0.8431	(-1 1 0)	21.694A	1
Common edge with					R(A-A)	
Ba 2	0.7083	0.6865	1.1693	(0 0 1)	6.702A	2
Ba 1	1.5578	-0.2597	1.0696	(1-1 1)	17.260A	2
Ba 2	0.7083	-0.3135	1.1693	(0-1 1)	18.046A	2
Common face with					R(A-A)	
Ba 1	0.5578	0.7403	1.0696	(0 0 1)	4.215A	3
Ba 8	0.6387	0.7258	0.8431	(0 0 0)	4.350A	3

Structural group analysis

Structural group No 1

Structure consists of 3D framework with Ba9O67N17C177H108
There are 2 interpenetrating nets
FISE: Full interpenetration symmetry elements

1: -1

PIC: [1,0,0][0,1,0][0,0,1] (PICVR=1)

Zt=1; Zn=2

Class IIa Z=2

Coordination sequences

Ba1:	1	2	3	4	5	6	7	8	9	10
Num	26	107	242	479	689	990	1344	1922	2240	2763
Cum	27	134	376	855	1544	2534	3878	5800	8040	10803

Ba2:	1	2	3	4	5	6	7	8	9	10
Num	26	106	243	479	689	989	1345	1922	2240	2762
Cum	27	133	376	855	1544	2533	3878	5800	8040	10802

Ba3:	1	2	3	4	5	6	7	8	9	10
Num	21	98	241	423	696	965	1377	1735	2297	2722
Cum	22	120	361	784	1480	2445	3822	5557	7854	10576

Ba4:	1	2	3	4	5	6	7	8	9	10
Num	26	109	260	438	711	991	1420	1764	2322	2763
Cum	27	136	396	834	1545	2536	3956	5720	8042	10805

Ba5:	1	2	3	4	5	6	7	8	9	10
Num	27	121	248	440	684	1081	1354	1768	2231	3007
Cum	28	149	397	837	1521	2602	3956	5724	7955	10962

Ba6:	1	2	3	4	5	6	7	8	9	10
Num	23	115	247	435	685	1072	1356	1763	2232	2995
Cum	24	139	386	821	1506	2578	3934	5697	7929	10924

Ba7:	1	2	3	4	5	6	7	8	9	10

c.5

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Num  20 101 247 423  697  970 1388 1737 2298  2729
Cum  21 122 369 792 1489 2459 3847 5584 7882 10611
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Ba8:  1   2   3   4    5    6    7    8    9    10
Num  21 100 242 421  697  964 1374 1731 2298  2718
Cum  22 122 364 785 1482 2446 3820 5551 7849 10567
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Ba9:  1   2   3   4    5    6    7    8    9    10
Num  26 107 240 478  690  990 1342 1920 2242  2763
Cum  27 134 374 852 1542 2532 3874 5794 8036 10799
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TD10=10761

Vertex symbols for selected  sublattice
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Ba1 Point  symbol:{3^140.4^185}
Extended point symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.
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Ba2 Point  symbol:{3^140.4^176.5^9}
Extended point symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.
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Ba3 Point  symbol:{3^98.4^100.5^12}
Extended  point  symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.
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Ba4 Point  symbol:{3^129.4^178.5^18}
Extended  point  symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.
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Ba5 Point  symbol:{3^136.4^196.5^19}
Extended point symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.
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Ba6 Point  symbol:{3^105.4^141.5^7}
Extended  point  symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.
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Ba7 Point  symbol:{3^83.4^91.5^16}
Extended  point  symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.
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Ba8 Point  symbol:{3^94.4^100.5^16}
Extended  point  symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.
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Ba9 Point  symbol:{3^137.4^174.5^14}
Extended  point  symbol:[3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.
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Point symbol for net: {3^105.4^141.5^7}{3^129.4^178.5^18}{3^136.4^196.5^19}{3^137.4^174.5^14}{3^140.4^176.5^9}{
20,21,21,23,26,26,26,26,27-c net with stoichiometry (20-c)(21-c)(21-c)(23-c)(26-c)(26-c)(26-c)(26-c)(27-c);    9-n

New topology, please, contact the authors (72725 types in 10 databases)
Elapsed time: 377.81  sec.
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