Electronic supplementary information (ESI)

Alkali Earth MO_x (x=6, 7, 9, 12) PolyhedraTuned Cadmium Selenites with Different Dimensions and Diverse SeO_3^{2-} Coordinations

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Table S1. Atomic coordinates (Å×10^4) and equivalent isotropic displacements parameters (Å^2×10^3) for **1**-**4**. $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

(1)

atoms	x	y	z	U(eq)
Cd(1)	8659(1)	2100(1)	4084(1)	35(1)
Cd(2)	3335(1)	-311(1)	1846(1)	37(1)
Cd(3)	2434(1)	4045(1)	3575(1)	34(1)
Se(1)	665(1)	2166(1)	6653(1)	32(1)
Se(2)	7067(1)	1754(1)	1236(1)	30(1)
Se(3)	5174(1)	6669(1)	3092(1)	31(1)
Se(4)	1299(1)	3480(1)	902(1)	33(1)
Mg(1)	5000	0	5000	18(1)
Mg(2)	5000	5000	0	21(1)
O(1)	-261(12)	563(10)	6552(12)	52(2)
O(2)	-229(11)	3510(9)	5624(9)	39(2)
O(3)	2822(9)	1806(9)	5197(8)	35(2)
O(4)	6205(11)	349(9)	671(8)	37(2)
O(5)	5347(10)	3389(9)	1662(8)	35(2)
O(6)	6857(10)	1101(9)	3017(8)	36(2)
O(7)	4567(11)	6885(9)	1567(8)	36(2)
O(8)	3577(10)	5733(9)	4473(8)	36(2)
O(9)	-927(10)	4029(10)	1970(9)	42(2)
O(10)	2226(10)	4994(9)	1189(8)	36(2)
O(11)	1720(11)	2178(9)	2261(8)	37(2)
O(12)	5893(10)	1357(8)	6186(8)	33(1)

(2)

atoms	x	y	z	U(eq)
Cd(1)	4199(1)	4602(1)	1562(1)	11(1)
Cd(2)	476(1)	109(1)	3023(1)	13(1)
Se(2)	4144(1)	1844(1)	3778(1)	10(1)
Se(1)	623(1)	2978(1)	620(1)	11(1)
Se(3)	7512(1)	4715(1)	4561(1)	10(1)
Cd(1')	7496(1)	2472(1)	2331(1)	12(1)
O(6)	4917(3)	3007(2)	634(3)	15(1)
O(7)	8793(3)	3334(2)	829(3)	18(1)
O(5)	5821(4)	3938(2)	3705(3)	25(1)
O(8)	5780(3)	1417(2)	3252(3)	15(1)
O(4)	1586(3)	4204(2)	1253(3)	20(1)
O(9)	3305(3)	552(2)	3774(3)	13(1)
O(1)	8141(3)	4166(2)	6278(3)	18(1)
O(3)	235(3)	3138(2)	-1220(3)	15(1)
O(2)	8867(4)	4134(2)	3779(3)	21(1)
Ca(1)	7496(1)	2472(1)	2331(1)	12(1)

(3)

atoms	x	y	z	U(eq)
Cd(1)	7746(2)	3529(1)	3065(1)	21(1)
Se(1)	12207(2)	2959(1)	5843(1)	21(1)
Se(2)	2296(2)	5076(1)	2833(1)	20(1)
Sr(1)	12603(2)	3840(1)	9706(1)	16(1)
O(1)	11800(20)	2946(5)	7582(8)	35(2)
O(2)	12902(17)	1852(5)	5668(8)	27(2)
O(3)	8618(16)	2993(5)	5194(8)	27(2)
O(4)	2926(16)	3941(5)	2789(8)	26(2)
O(5)	-1423(17)	5025(5)	2906(10)	33(2)
O(6)	2642(18)	5335(5)	1130(8)	29(2)

(4)

atom	x	y	z	U(eq)
Cd(1)	4488(1)	2500	6221(1)	12(1)
Se(1)	3671(1)	7500	8693(1)	13(1)
Se(2)	4279(1)	2500	1782(1)	13(1)
Ba(1)	2831(1)	7500	3797(1)	12(1)
O(1)	3528(2)	5111(7)	7192(6)	18(1)
O(2)	4456(3)	152(8)	3320(6)	25(1)
O(3)	3292(4)	2500	1658(10)	34(2)
O(4)	2818(4)	7500	9922(9)	28(1)

Table S2. Selected bond distances (Å) for **1**-**4**.

(1)

Cd(1)-O(1)#3	2.340(9)	Cd(3)-O(2)	2.342(8)	Mg(2)-O(7)	2.125(7)
Cd(1)-O(8)#6	2.341(8)	Cd(3)-O(11)	2.379(7)	Mg(2)-O(7)#8	2.125(7)
Cd(1)-O(12)	2.477(7)	Cd(3)-O(2)#1	2.386(8)	Se(1)-O(2)	1.708(7)
Cd(1)-O(9)#10	2.446(8)	Cd(3)-O(3)	2.412(7)	Se(1)-O(1)	1.708(8)
Cd(1)-O(2)#10	2.497(8)	Cd(3)-O(10)	2.418(7)	Se(1)-O(3)	1.714(7)
Cd(1)-O(6)	2.426(7)	Mg(1)-O(6)	2.154(7)	Se(2)-O(6)	1.692(6)
Cd(1)-O(8)#6	2.341(8)	Mg(1)-O(12)	2.087(7)	Se(2)-O(5)	1.701(7)
Cd(2)-O(11)	2.210(8)	Mg(1)-O(3)	2.065(7)	Se(2)-O(4)	1.719(7)
Cd(2)-O(4)#2	2.259(7)	Mg(1)-O(3)#3	2.065(7)	Se(3)-O(8)	1.700(7)
Cd(2)-O(12)#3	2.294(7)	Mg(1)-O(12)#3	2.087(7)	Se(3)-O(7)	1.714(7)
Cd(2)-O(4)	2.323(8)	Mg(1)-O(6)#3	2.154(7)	Se(3)-O(12)#6	1.753(7)
Cd(2)-O(7)#4	2.363(7)	Mg(2)-O(10)#8	2.087(7)	Se(4)-O(9)	1.667(7)
Cd(2)-O(1)#5	2.392(8)	Mg(2)-O(10)	2.087(7)	Se(4)-O(10)	1.706(7)
Cd(3)-O(8)	2.245(7)	Mg(2)-O(5)#8	2.088(7)	Se(4)-O(11)	1.741(7)
Cd(3)-O(5)	2.305(7)	Mg(2)-O(5)	2.088(7)		

(2)

Cd(1)-O(4)	2.191(3)	Cd(2)-O(4)#6	2.339(3)	Se(1)-O(3)	1.685(3)
Cd(1)-O(8)#1	2.208(8)	Cd(2)-O(7)#4	2.405(3)	Se(1)-O(4)	1.712(3)
Cd(1)-O(5)	2.219(3)	Cd(1')-O(8)	2.304(2)	Se(2)-O(8)	1.693(2)
Cd(1)-O(6)	2.286(3)	Cd(1')-O(7)	2.304(3)	Se(2)-O(6)#3	1.687(3)
Cd(1)-O(9)#1	2.513(2)	Cd(1')-O(6)	2.362(3)	Se(2)-O(9)	1.719(3)
Cd(1)-O(9)#2	2.522(3)	Cd(1')-O(1)#2	2.363(3)	Se(3)-O(1)	1.685(3)
Cd(2)-O(3)#3	2.274(3)	Cd(1')-O(3)#9	2.411(3)	Se(3)-O(5)	1.693(3)
Cd(2)-O(2)#4	2.287(3)	Cd(1')-O(2)	2.510(3)	Se(3)-O(2)	1.701(3)
Cd(2)-O(1)#5	2.318(3)	O(1)-Ca(1)#3	2.363(3)		
Cd(2)-O(9)	2.336(2)	Se(1)-O(7)#7	1.678(3)		

(3)

Cd(1)-O(3)	2.211(7)	Sr(1)-O(2)#5	2.569(7)	Sr(1)-O(5)#9	3.057(9)
Cd(1)-O(4)	2.258(7)	Sr(1)-O(6)#6	2.633(8)	Se(1)-O(1)	1.684(8)
Cd(1)-O(5)#1	2.298(7)	Sr(1)-O(6)#7	2.640(8)	Se(1)-O(3)	1.702(7)
Cd(1)-O(1)#2	2.313(8)	Sr(1)-O(2)#8	2.722(8)	Se(1)-O(2)	1.712(7)
Cd(1)-O(2)#2	2.371(8)	Sr(1)-O(6)#9	2.752(8)	Se(2)-O(5)	1.679(8)
Cd(1)-O(4)#1	2.438(7)	Sr(1)-O(3)#8	2.843(8)	Se(2)-O(6)	1.691(7)
Sr(1)-O(1)	2.454(7)	Sr(1)-O(4)#7	2.953(8)	Se(2)-O(4)	1.740(7)

(4)

Cd(1)-O(1)#8	2.245(4)	Ba(1)-O(1)#3	2.902(4)	Ba(1)-O(3)	3.214(4)
Cd(1)-O(1)	2.245(4)	Ba(1)-O(1)#4	2.902(4)	Ba(1)-O(3)#7	3.214(4)
Cd(1)-O(2)#9	2.296(4)	Ba(1)-O(1)#5	2.978(4)	Se(1)-O(4)	1.663(6)
Cd(1)-O(2)#10	2.296(4)	Ba(1)-O(1)	2.978(4)	Se(1)-O(1)	1.701(4)
Cd(1)-O(2)	2.430(5)	Ba(1)-O(4)#6	3.039(3)	Se(1)-O(1)#5	1.701(4)
Cd(1)-O(2)#8	2.430(5)	Ba(1)-O(4)#3	3.039(3)	Se(2)-O(3)	1.640(6)
Ba(1)-O(4)#1	2.758(6)	Ba(1)-O(2)#7	3.078(4)	Se(2)-O(2)#8	1.709(4)
Ba(1)-O(3)#2	2.761(6)	Ba(1)-O(2)#8	3.078(4)	Se(2)-O(2)	1.709(4)

Symmetry codes: for: **1** :#1 -x, -y+1, -z+1; #2 -x+1, -y, -z; #3 -x+1, -y, -z+1; #4 x, y-1, z; #5 -x, -y, -z+1; #6 -x+1, -y+1 ,-z+1; #7 x, y+1, z; #8 -x+1, -y+1, -z; #9 x-1, y, z; #10 x+1, y, z. For **2** : #1 -x+1,y+1/2,-z+1/2; #2 x,-y+1/2,z-1/2; #3 x,-y+1/2,z+1/2; #4 -x+1,y-1/2,-z+1/2; #5 x-1,-y+1/2,z-1/2; #6 -x,y-1/2,-z+1/2; #7 x-1,y,z; #8 -x,y+1/2,-z+1/2; #9 x+1,-y+1/2,z+1/2; #10 x+1,y,z.For **3** : #1 x+1, y, z; #2 x-1/2, -y+1/2, z-1/2; #3 x-1, y, z-1; #4 x, y, z-1; #5 x-1/2, -y+1/2, z+1/2; #6 -x+2, -y+1, -z+1; #7 x+1, y, z+1; #8 x+1/2, -y+1/2, z+1/2; #9 -x+1, -y+1, -z+1; #10 x-1, y, z; #11 x+1/2, -y+1/2, z-1/2. For **4** : #1 x, y, z-1; #2 -x+1/2, -y+1, z+1/2; #3 -x+1/2, -y+1, z-1/2; #4 -x+1/2, y+1/2, z-1/2; #5 x, -y+3/2, z; #6 -x+1/2, -y+2, z-1/2; #7 x, y+1, z; #8 x, -y+1/2, z; #9 -x+1, y+1/2, -z+1; #10 -x+1, -y, -z+1; #11 -x+1/2, -y+2, z+1/2; #12 x, y-1, z; #13 x, y, z+1.

Table S3. Energy-Dispersive Spectrometry (EDS) for 1-4.

(1)

Point 1				Point 2			
Element	Weight %	Atomic %	Formula	Element	Weight %	Atomic %	Formula
O K	17.15	55.61		O K	12.61	56.06	
Mg K	3.11	5.80	1.0	Mg K	3.10	5.59	1.0
Se L	39.25	22.41	3.86	Se L	41.33	22.36	4.0
Cd L	40.49	16.18	2.79	Cd L	42.96	16.60	2.97
Totals	100			Totals	100		
Point 3							
Element	Weight %	Atomic %	Formula	Average ratio: $Mg_{1.0}Cd_{2.9}Se_{3.9}$			
O K	4.79	21.21					
Mg K	3.44	10.06	1.0				
Se L	44.50	39.08	3.88				
Cd L	47.27	29.65	2.95				
Totals	100						

(2)

Point 1				Point 2			
Element	Weight %	Atomic %	Formula	Element	Weight %	Atomic %	Formula
O K	28.12	52.58		O K	37.95	64.46	
Ca K	5.73	5.39	0.7	Ca K	4.74	4.13	0.7
Se L	32.96	23.06	2.99	Se L	29.45	18.43	3.11
Cd L	33.19	18.97	2.46	Cd L	27.86	12.98	2.20
Totals	100			Totals	100		
Point 3							
Element	Weight %	Atomic %	Formula				
O K	28.51	68.77		Average ratio: $Ca_{0.7}Cd_{2.3}Se_{3.1}$			
Ca K	5.29	4.89	0.7				
Se L	32.99	22.07	3.16				
Cd L	33.21	15.58	2.23				
Totals	100						

(3)

Point 1				Point 2			
Element	Weight %	Atomic %	Formula	Element	Weight %	Atomic %	Formula
O K	25.34	65.40		O K	22.9	62.39	
Se L	32.67	17.07	2.15	Se L	32.84	18.13	2.01
Sr L	20.36	9.58	1.21	Sr L	21.00	10.44	1.16
Cd L	21.63	7.95	1.0	Cd L	23.26	9.03	1.0
Totals	100			Totals	100		
Point 3							
Element	Weight %	Atomic %	Formula				
O K	26.98	67.43		Average ratio: $Sr_{1.1}Cd_{1.0}Se_{2.0}$			
Se L	31.93	16.18	1.96				
Sr L	17.83	8.13	0.98				
Cd L	23.25	8.26	1.0				
Totals	100						

(4)

Point 1				Point 2			
Element	Weight %	Atomic %	Formula	Element	Weight %	Atomic %	Formula
O K	27.83	70.98		O K	12.46	47.87	
Se L	28.77	14.89	2.20	Se L	33.33	25.86	2.22
Cd L	18.59	6.76	1.0	Cd L	21.36	11.64	1.0
Ba L	24.78	7.37	1.09	Ba L	32.85	14.64	1.26
Totals	100			Totals	100		
Point 3							
Element	Weight %	Atomic %	Formula	Average ratio: $Ba_{1.2}Cd_{1.0}Se_{2.1}$			
O K	13.35	50.02					
Se L	30.79	23.37	1.85				
Cd L	23.71	12.61	1.0				
Ba L	32.15	14.00	1.11				
Totals	100						

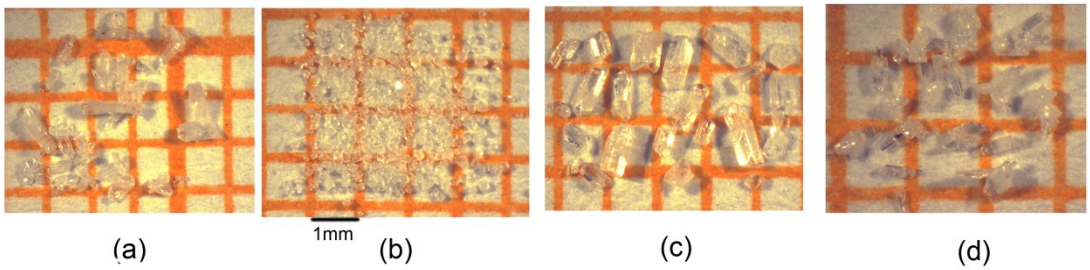


Fig. S1. The morphology for 1(a), 2(b), 3(c) and 4(d).

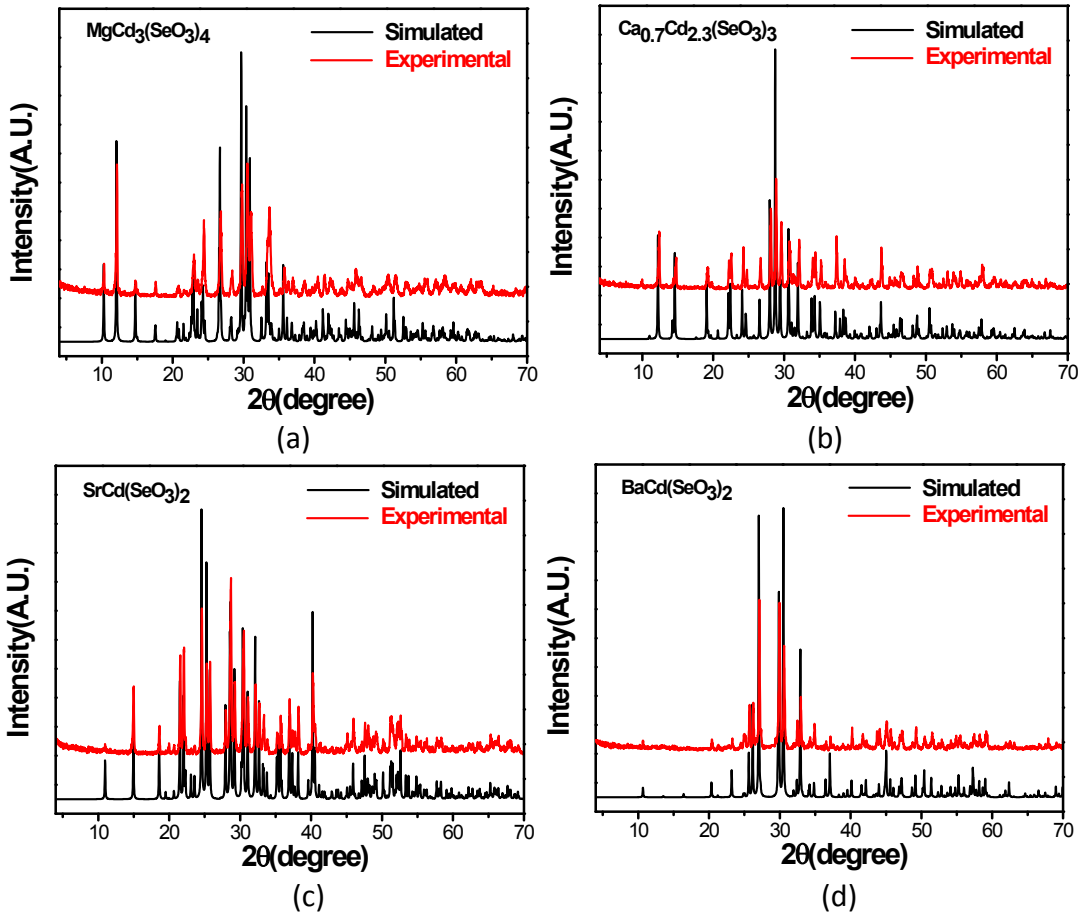
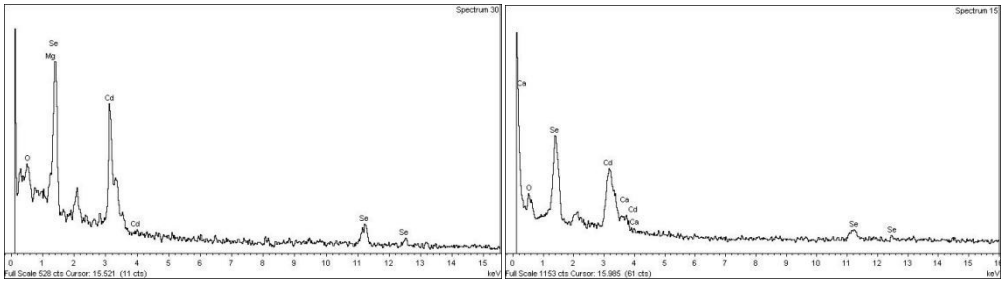


Fig. S2. Experimental and simulated PXRD powder patterns of 1(a), 2(b), 3(c) and 4(d).



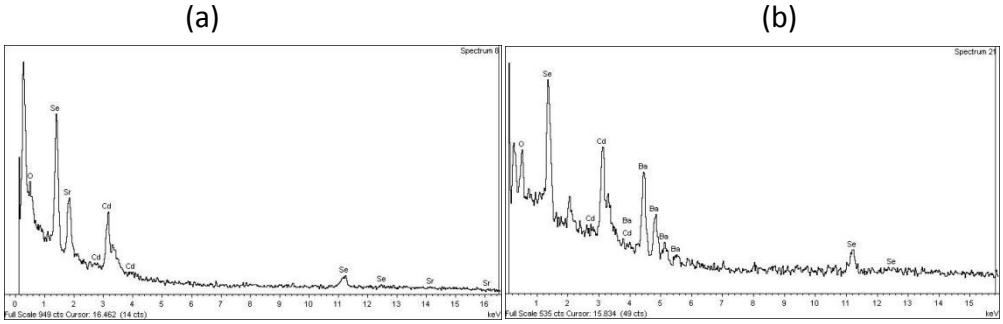


Fig. S3. Energy-Dispersive Spectrometry (EDS) plot of 1(a), 2(b), 3(c) and 4(d).

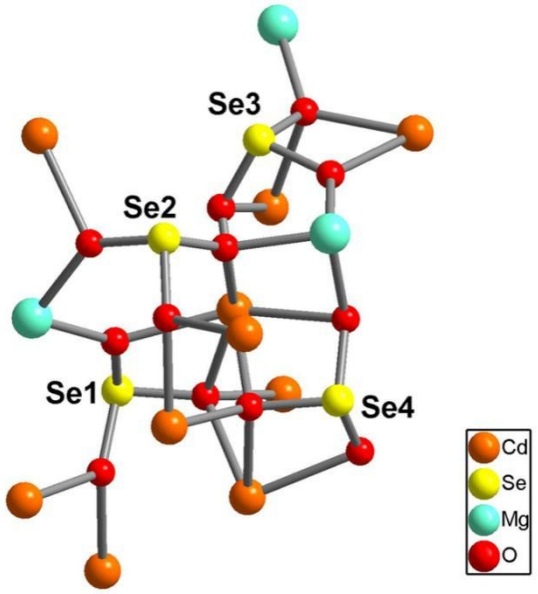


Fig. S4. The coordinate environments of the SeO_3^{2-} in **1**.

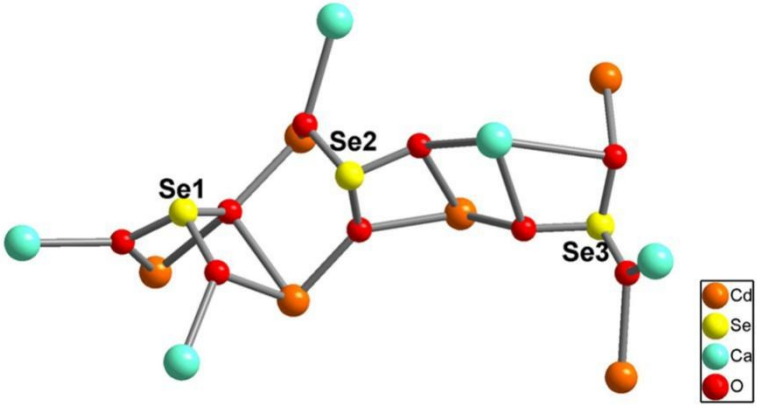


Fig. S5. The coordinate environments of the SeO_3^{2-} in **2**.

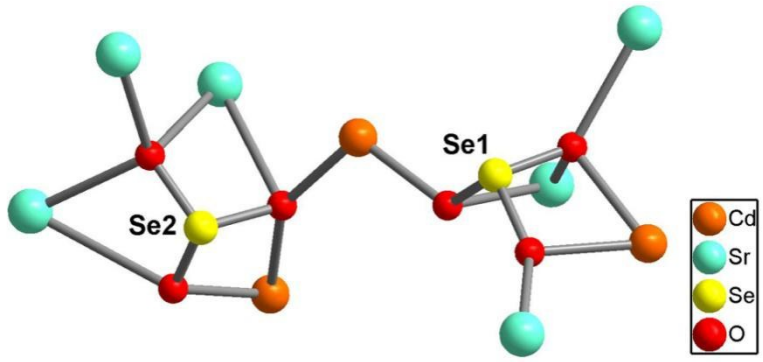


Fig. S6. The coordinate environments of the SeO_3^{2-} in **3**.

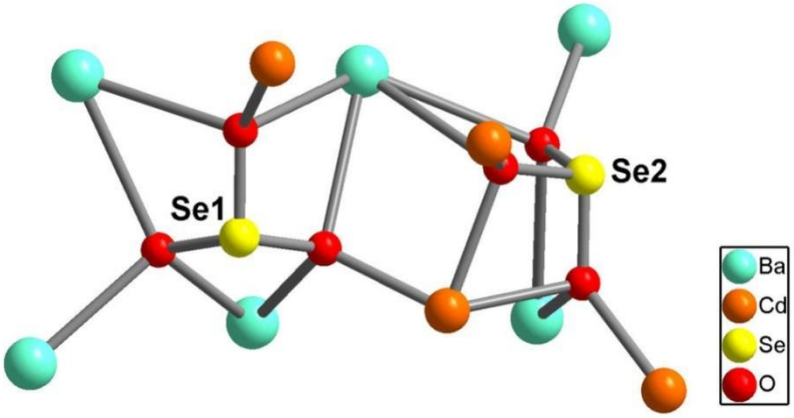
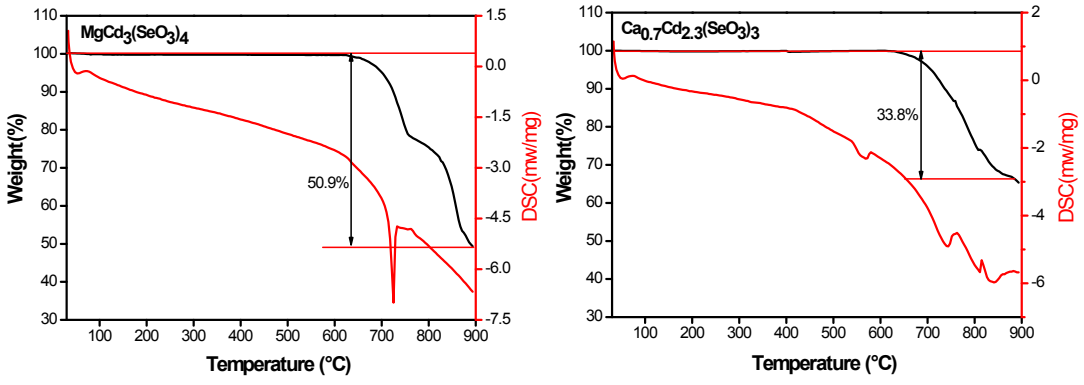
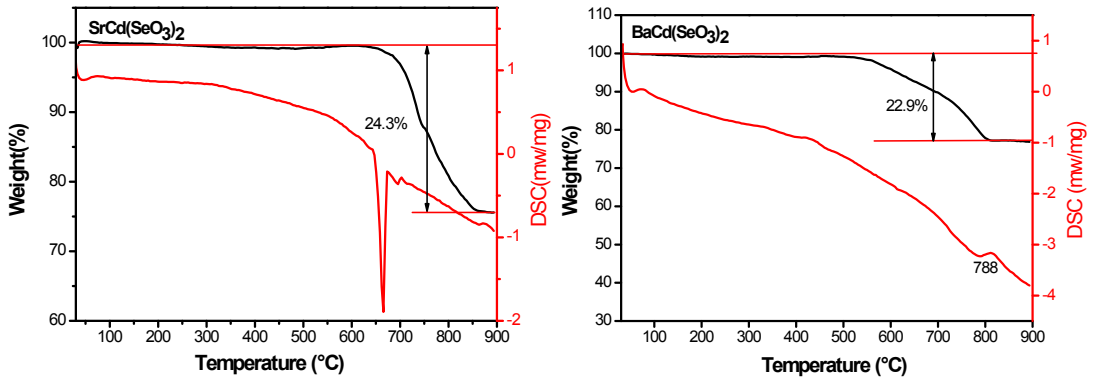


Fig. S7. The coordinate environments of the SeO_3^{2-} in **4**.

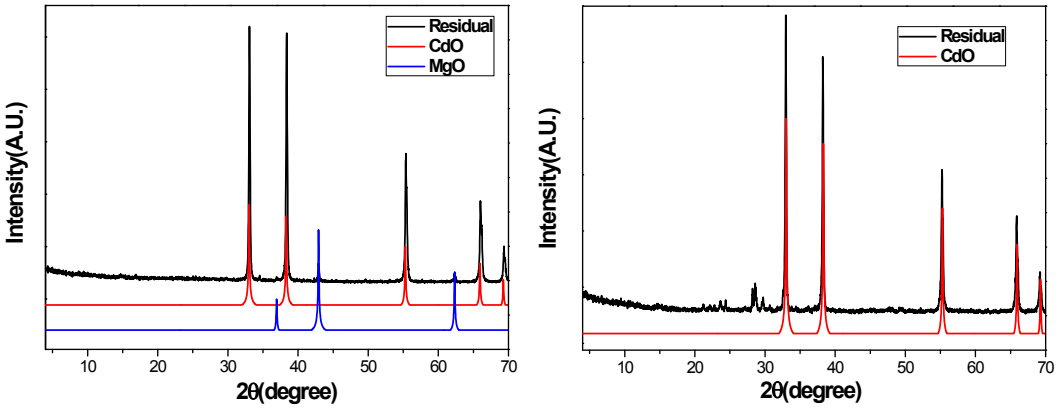


(a) (b)

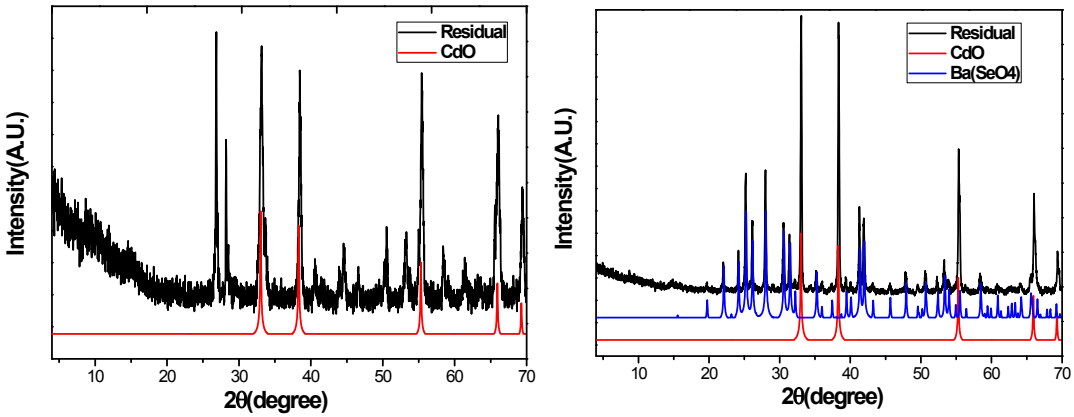


(c) (d)

Fig. S8. TGA and DSC curves of 1(a), 2(b), 3(c) and 4(d).



(a) (b)



(c) (d)

Fig. S9. PXRD powder patterns for the residual of 1(a), 2(b), 3(c) and 4(d).

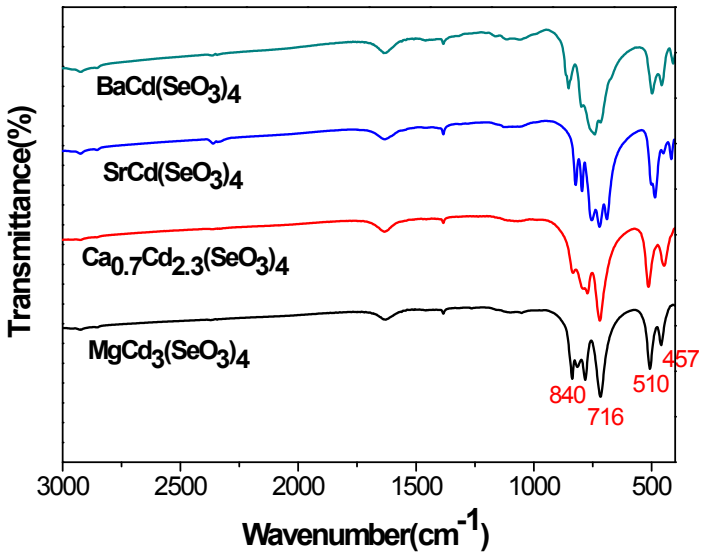


Fig. S10. IR spectrum of 1-4.