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Supplementary materials

New Ce (III) Sulfate-Tartrate-Based MOFs: An Insight into Controllable Self-Assembly of Acentric Metal-Organic Complexes

Jin–Li Qi, Yue–Qing Zheng,* Wei Xu, Hong–Lin Zhu, Jian–Li Lin, Hai–Sheng Chang

Crystal Engineering Division
Center for Applied Solid State Chemistry Research
Ningbo University, Ningbo, 315211 P.R. China
* Corresponding author. Phone: Int. +574/87600747; Fax: Int. +574/87600792
E–mail address: *zhengcm@nbu.edu.cn*

Table S1. Selected Interatomic Distances (Å) and Bond Angles (deg) for **1**[a]

Ce–O1	2.492(3)	Ce–O4$^{\#2}$	2.659(4)	Ce–O7	2.563(4)
Ce–O2$^{\#1}$	2.475(3)	Ce–O5$^{\#3}$	2.514(4)	Ce–O8	2.594(4)
Ce–O3	2.535(4)	Ce–O6$^{\#2}$	2.473(4)	Ce–O9	2.535(4)
O1–Ce–O2$^{\#1}$	129.0(1)	O2$^{\#1}$–Ce–O7	126.7(1)	O4$^{\#2}$–Ce–O8	133.1(1)
O1–Ce–O3	61.1(1)	O2$^{\#1}$–Ce–O8	73.2(1)	O4$^{\#2}$–Ce–O9	65.9(1)
O1–Ce–O4$^{\#2}$	120.3(1)	O2$^{\#1}$–Ce–O9	82.1(1)	O5$^{\#3}$–Ce–O6$^{\#2}$	93.1(1)
O1–Ce–O5$^{\#3}$	70.2(1)	O3–Ce–O4$^{\#2}$	127.1(1)	O5$^{\#3}$–Ce–O7	72.0(1)
O1–Ce–O6$^{\#2}$	72.8(1)	O3–Ce–O5$^{\#3}$	131.3(1)	O5$^{\#3}$–Ce–O8	123.5(1)
O1–Ce–O7	76.2(1)	O3–Ce–O6$^{\#2}$	72.3(1)	O5$^{\#3}$–Ce–O9	82.7(1)
O1–Ce–O8	106.6(1)	O3–Ce–O7	96.5(1)	O6$^{\#2}$–Ce–O7	148.7(1)
O1–Ce–O9	148.5(1)	O3–Ce–O8	74.3(1)	O6$^{\#2}$–Ce–O8	141.5(2)
O2$^{\#1}$–Ce–O3	70.6(1)	O3–Ce–O9	143.5(2)	O6$^{\#2}$–Ce–O9	126.0(1)
O2$^{\#1}$–Ce–O4$^{\#2}$	76.8(1)	O4$^{\#2}$–Ce–O5$^{\#3}$	76.7(1)	O7–Ce–O8	53.7(1)
O2$^{\#1}$–Ce–O5$^{\#3}$	153.1(1)	O4$^{\#2}$–Ce–O6$^{\#2}$	60.8(1)	O7–Ce–O9	80.5(1)
O2$^{\#1}$–Ce–O6$^{\#2}$	78.1(1)	O4$^{\#2}$–Ce–O7	136.4(1)	O8–Ce–O9	74.9(2)

Hydrogen bonding contacts

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠(D–H···A)
O3–H3A···O12A	0.86	1.81	2.560	144
O3–H3A···O12B	0.86	1.84	2.690	171
O4–H4A···O6$^{\#2}$	0.85	1.77	2.617	173
O9–H91···O11	0.81	2.18	2.833	139
O9–H92···O1$^{\#1}$	0.83	1.98	2.808	173
O10–H10···O8	0.84	1.97	2.801	170
O11–H11···O7$^{\#4}$	0.85	2.28	3.067	153
O12A–H121···O9$^{\#5}$	0.82	2.14	2.760	132
O12A–H122···O10	0.82	2.31	3.005	143
O12A–H122···O11$^{\#5}$	0.82	2.34	2.990	137
O12B–H123···O7$^{\#5}$	0.79	2.15	2.904	160
O12B–H124···O9$^{\#5}$	0.76	2.59	3.354	176

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

Table S2. Selected Interatomic Distances (Å) and Bond Angles (deg) for **2**[a]

Ce–O1	2.483(4)	Ce–O4$^{\#2}$	2.653(4)	Ce–O7	2.564(5)
Ce–O2$^{\#1}$	2.475(4)	Ce–O5$^{\#3}$	2.513(5)	Ce–O8	2.600(5)
Ce–O3	2.539(5)	Ce–O6$^{\#2}$	2.474(5)	Ce–O9	2.555(5)
O1–Ce–O2$^{\#1}$	128.8(1)	O2$^{\#1}$–Ce–O7	126.7(2)	O4$^{\#2}$–Ce–O8	132.9(1)
O1–Ce–O3	61.5(1)	O2$^{\#1}$–Ce–O8	73.2(2)	O4$^{\#2}$–Ce–O9	66.0(2)
O1–Ce–O4$^{\#2}$	120.3(2)	O2$^{\#1}$–Ce–O9	81.8(1)	O5$^{\#3}$–Ce–O6$^{\#2}$	93.4(2)
O1–Ce–O5$^{\#3}$	70.2(2)	O3–Ce–O4$^{\#2}$	127.2(1)	O5$^{\#3}$–Ce–O7	72.0(2)
O1–Ce–O6$^{\#2}$	72.7(2)	O3–Ce–O5$^{\#3}$	130.7(2)	O5$^{\#3}$–Ce–O8	123.5(2)
O1–Ce–O7	76.5(2)	O3–Ce–O6$^{\#2}$	72.0(2)	O5$^{\#3}$–Ce–O9	83.2(2)
O1–Ce–O8	106.8(2)	O3–Ce–O7	96.5(2)	O6$^{\#2}$–Ce–O7	148.9(2)
O1–Ce–O9	149.0(2)	O3–Ce–O8	74.7(2)	O6$^{\#2}$–Ce–O8	141.3(2)
O2$^{\#1}$–Ce–O3	71.0(1)	O3–Ce–O9	143.5(2)	O6$^{\#2}$–Ce–O9	126.0(2)
O2$^{\#1}$–Ce–O4$^{\#2}$	76.7(1)	O4$^{\#2}$–Ce–O5$^{\#3}$	76.9(1)	O7–Ce–O8	53.7(2)
O2$^{\#1}$–Ce–O5$^{\#3}$	153.2(1)	O4$^{\#2}$–Ce–O6$^{\#2}$	60.9(1)	O7–Ce–O9	80.4(2)
O2$^{\#1}$–Ce–O6$^{\#2}$	77.9(2)	O4$^{\#2}$–Ce–O7	136.3(2)	O8–Ce–O9	74.5(2)

Hydrogen bonding contacts

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠(D–H···A)
O3–H3A···O12A	0.86	1.83	2.579	144
O3–H3A···O12B	0.86	1.84	2.695	170
O4–H4A···O6$^{\#2}$	0.85	1.77	2.618	173
O9–H91···O11	0.82	2.14	2.795	137
O9–H92···O1$^{\#1}$	0.82	2.00	2.818	173
O10–H10···O8	0.83	1.99	2.809	170
O11–H11···O7$^{\#4}$	0.82	2.26	3.031	158
O12A–H121···O9$^{\#5}$	0.83	2.13	2.756	132
O12A–H122···O10	0.82	2.30	2.996	143
O12A–H122···O11$^{\#5}$	0.82	2.37	3.014	137
O12B–H123···O7$^{\#5}$	0.79	2.11	2.874	161
O12B–H124···O9$^{\#5}$	0.76	2.56	3.320	175

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

Table S3. Selected Interatomic Distances (Å) and Bond Angles (deg) for **3**[a]

Ce–O1	2.468(4)	Ce–O4$^{\#2}$	2.643(4)	Ce–O7	2.623(5)
Ce–O2$^{\#1}$	2.472(4)	Ce–O5$^{\#3}$	2.525(4)	Ce–O8	2.569(4)
Ce–O3	2.527(4)	Ce–O6$^{\#2}$	2.479(4)	Ce–O9	2.567(5)
O1–Ce–O2$^{\#1}$	129.2(1)	O2$^{\#1}$–Ce–O7	124.7(1)	O4$^{\#2}$–Ce–O8	130.7(1)
O1–Ce–O3	61.0(1)	O2$^{\#1}$–Ce–O8	71.1(1)	O4$^{\#2}$–Ce–O9	65.3(1)
O1–Ce–O4$^{\#2}$	120.7(1)	O2$^{\#1}$–Ce–O9	83.7(1)	O5$^{\#3}$–Ce–O6$^{\#2}$	92.9(1)
O1–Ce–O5$^{\#3}$	69.7(1)	O3–Ce–O4$^{\#2}$	127.4(1)	O5$^{\#3}$–Ce–O7	75.5(1)
O1–Ce–O6$^{\#2}$	73.4(1)	O3–Ce–O5$^{\#3}$	130.7(2)	O5$^{\#3}$–Ce–O8	127.0(1)
O1–Ce–O7	77.4(2)	O3–Ce–O6$^{\#2}$	72.7(1)	O5$^{\#3}$–Ce–O9	81.5(2)
O1–Ce–O8	108.5(2)	O3–Ce–O7	94.3(2)	O6$^{\#2}$–Ce–O7	150.7(1)
O1–Ce–O9	146.9(1)	O3–Ce–O8	73.2(1)	O6$^{\#2}$–Ce–O8	138.9(2)
O2$^{\#1}$–Ce–O3	71.4(1)	O3–Ce–O9	145.1(1)	O6$^{\#2}$–Ce–O9	125.6(1)
O2$^{\#1}$–Ce–O4$^{\#2}$	75.3(1)	O4$^{\#2}$–Ce–O5$^{\#3}$	77.0(1)	O7–Ce–O8	53.8(1)
O2$^{\#1}$–Ce–O5$^{\#3}$	152.1(1)	O4$^{\#2}$–Ce–O6$^{\#2}$	60.7(1)	O7–Ce–O9	79.9(2)
O2$^{\#1}$–Ce–O6$^{\#2}$	76.8(1)	O4$^{\#2}$–Ce–O7	138.3(2)	O8–Ce–O9	75.9(2)

Hydrogen bonding contacts

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠(D–H···A)
O3–H3A···O11A	0.82	1.94	2.612	139
O3–H3A···O11B	0.82	1.87	2.615	151
O4–H4A···O6$^{\#2}$	0.82	1.80	2.615	173
O9–H91···O10A	0.82	2.15	2.745	130
O9–H92···O1$^{\#1}$	0.78	2.16	2.840	146
O10A–H101···O7$^{\#1}$	0.86	1.91	2.714	157
O10A–H102···O8$^{\#4}$	0.82	1.90	2.713	176
O10B–H103···O7$^{\#1}$	0.85	2.16	3.013	179
O10B–H104···O8$^{\#4}$	0.85	2.29	3.142	179
O11A–H111···O7$^{\#5}$	0.83	2.16	2.989	179
O11A–H112···O10A$^{\#6}$	0.84	2.64	3.452	164
O11A–H113···O9$^{\#5}$	0.80	2.05	2.817	160
O11A–H114···O10B$^{\#4}$	0.81	2.15	2.944	165

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

Table S4. Selected Interatomic Distances (Å) and Bond Angles (deg) for **4**[a]

Ce–O1	2.472(3)	Ce–O4$^{\#2}$	2.643(3)	Ce–O7	2.627(3)
Ce–O2$^{\#1}$	2.472(3)	Ce–O5$^{\#3}$	2.527(3)	Ce–O8	2.572(3)
Ce–O3	2.527(3)	Ce–O6$^{\#2}$	2.478(3)	Ce–O9	2.567(3)
O1–Ce–O2$^{\#1}$	129.4(1)	O2$^{\#1}$–Ce–O7	124.5(1)	O4$^{\#2}$–Ce–O8	131.0(1)
O1–Ce–O3	61.2(1)	O2$^{\#1}$–Ce–O8	71.2(1)	O4$^{\#2}$–Ce–O9	65.4(1)
O1–Ce–O4$^{\#2}$	120.8(1)	O2$^{\#1}$–Ce–O9	83.6(1)	O5$^{\#3}$–Ce–O6$^{\#2}$	93.2(1)
O1–Ce–O5$^{\#3}$	69.8(1)	O3–Ce–O4$^{\#2}$	127.3(1)	O5$^{\#3}$–Ce–O7	75.6(1)
O1–Ce–O6$^{\#2}$	73.6(1)	O3–Ce–O5$^{\#3}$	131.0(1)	O5$^{\#3}$–Ce–O8	126.9(1)
O1–Ce–O7	77.4(1)	O3–Ce–O6$^{\#2}$	72.5(1)	O5$^{\#3}$–Ce–O9	81.4(1)
O1–Ce–O8	108.1(1)	O3–Ce–O7	94.5(1)	O6$^{\#2}$–Ce–O7	150.9(1)
O1–Ce–O9	146.7(1)	O3–Ce–O8	73.0(1)	O6$^{\#2}$–Ce–O8	138.6(1)
O2$^{\#1}$–Ce–O3	71.3(1)	O3–Ce–O9	144.9(1)	O6$^{\#2}$–Ce–O9	125.8(1)
O2$^{\#1}$–Ce–O4$^{\#2}$	75.4(1)	O4$^{\#2}$–Ce–O5$^{\#3}$	76.9(1)	O7–Ce–O8	53.6(1)
O2$^{\#1}$–Ce–O5$^{\#3}$	152.0(1)	O4$^{\#2}$–Ce–O6$^{\#2}$	60.8(1)	O7–Ce–O9	79.7(1)
O2$^{\#1}$–Ce–O6$^{\#2}$	76.7(1)	O4$^{\#2}$–Ce–O7	138.1(1)	O8–Ce–O9	76.0(1)

Hydrogen bonding contacts

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠(D–H···A)
O3–H3A···O11A	0.82	1.96	2.630	139
O3–H3A···O11B	0.82	1.86	2.608	151
O4–H4A···O6$^{\#2}$	0.82	1.79	2.607	174
O9–H91···O10A	0.82	2.17	2.770	130
O9–H92···O1$^{\#1}$	0.81	2.14	2.835	145
O10A–H101···O7$^{\#1}$	0.82	1.93	2.711	159
O10A–H102···O8$^{\#4}$	0.82	1.90	2.721	174
O10B–H103···O7$^{\#1}$	0.85	2.18	3.029	175
O10B–H104···O8$^{\#4}$	0.83	2.30	3.128	179
O11A–H111···O7$^{\#5}$	0.81	2.15	2.961	176
O11A–H112···O10A$^{\#6}$	0.82	2.61	3.416	165
O11A–H113···O9$^{\#5}$	0.79	2.07	2.827	160
O11A–H114···O10B$^{\#4}$	0.83	2.13	2.939	164

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

Table S5. Selected Interatomic Distances (Å) and Bond Angles (deg) for **5** [a]

Ce1–O1	2.459(4)	Ce1–O13$^{\#3}$	2.488(4)	Ce2–O6	2.416(5)
Ce1–O3	2.611(4)	Ce1–O14$^{\#4}$	2.455(5)	Ce2–O9	2.496(4)
Ce1–O7	2.570(4)	Ce1–O15	2.526(5)	Ce2–O11	2.604(5)
Ce1–O8	2.595(4)	Ce2–O2$^{\#5}$	2.391(4)	Ce2–O12	2.572(4)
Ce1–O8$^{\#1}$	2.561(4)	Ce2–O4	2.645(4)	Ce2–O16	2.688(5)
Ce1–O10$^{\#2}$	2.509(4)	Ce2–O5$^{\#6}$	2.417(4)	Ce2–O17	2.596(5)
O1–Ce1–O3	62.8(1)	O8–Ce1–O14$^{\#4}$	127.2(1)	O4–Ce2–O12	132.0(1)
O1–Ce1–O7	79.4(2)	O8–Ce1–O15	117.1(2)	O4–Ce2–O16	132.8(1)
O1–Ce1–O8	121.0(1)	O8$^{\#1}$–Ce1–O10$^{\#2}$	96.0(1)	O4–Ce2–O17	129.5(1)
O1–Ce1–O8$^{\#1}$	130.5(1)	O8$^{\#1}$–Ce1–O13$^{\#3}$	148.4(2)	O5$^{\#6}$–Ce2–O6	126.4(2)
O1–Ce1–O10$^{\#2}$	133.3(2)	O8$^{\#1}$–Ce1–O14$^{\#4}$	71.0(2)	O5$^{\#6}$–Ce2–O9	82.3(2)
O1–Ce1–O13$^{\#3}$	68.9(2)	O8$^{\#1}$–Ce1–O15	75.8(1)	O5$^{\#6}$–Ce2–O11	144.6(2)
O1–Ce1–O14$^{\#4}$	72.7(2)	O10$^{\#2}$–Ce1–O13$^{\#3}$	72.9(2)	O5$^{\#6}$–Ce2–O12	149.9(2)
O1–Ce1–O15	121.9(2)	O10$^{\#2}$–Ce1–O14$^{\#4}$	139.5(2)	O5$^{\#6}$–Ce2–O16	82.5(2)
O3–Ce1–O7	77.3(1)	O10$^{\#2}$–Ce1–O15	68.1(2)	O5$^{\#6}$–Ce2–O17	81.7(2)
O3–Ce1–O8	72.1(1)	O13$^{\#3}$–Ce1–O14$^{\#4}$	97.9(2)	O6–Ce2–O9	81.9(2)
O3–Ce1–O8$^{\#1}$	74.9(1)	O13$^{\#3}$–Ce1–O15	72.5(2)	O6–Ce2–O11	74.2(2)
O3–Ce1–O10$^{\#2}$	142.6(1)	O14$^{\#4}$–Ce1–O15	71.5(2)	O6–Ce2–O12	74.9(2)
O3–Ce1–O13$^{\#3}$	131.4(1)	O2$^{\#5}$–Ce2–O4	70.6(2)	O6–Ce2–O16	136.4(2)
O3–Ce1–O14$^{\#4}$	72.6(2)	O2$^{\#5}$–Ce2–O5$^{\#6}$	83.1(2)	O6–Ce2–O17	136.3(2)
O3–Ce1–O15	139.2(2)	O2$^{\#5}$–Ce2–O6	78.5(2)	O9–Ce2–O11	72.0(1)
O7–Ce1–O8	54.3(1)	O2$^{\#5}$–Ce2–O9	141.3(2)	O9–Ce2–O12	125.1(1)
O7–Ce1–O8$^{\#1}$	116.1(1)	O2$^{\#5}$–Ce2–O11	131.9(2)	O9–Ce2–O16	139.2(2)
O7–Ce1–O10$^{\#2}$	74.7(1)	O2$^{\#5}$–Ce2–O12	81.1(2)	O9–Ce2–O17	68.5(2)
O7–Ce1–O13$^{\#3}$	90.0(2)	O2$^{\#5}$–Ce2–O16	73.2(2)	O11–Ce2–O12	54.1(1)
O7–Ce1–O14$^{\#4}$	145.8(2)	O2$^{\#5}$–Ce2–O17	143.5(2)	O11–Ce2–O16	101.3(2)
O7–Ce1–O15	142.0(2)	O4–Ce2–O5$^{\#6}$	64.2(2)	O11–Ce2–O17	66.6(2)
O8–Ce1–O8$^{\#1}$	62.7(2)	O4–Ce2–O6	62.2(1)	O12–Ce2–O16	68.5(2)
O8–Ce1–O10$^{\#2}$	71.6(1)	O4–Ce2–O9	70.8(1)	O12–Ce2–O17	96.2(2)
O8–Ce1–O13$^{\#3}$	134.9(1)	O4–Ce2–O11	125.4(1)	O16–Ce2–O17	72.0(2)

Hydrogen bonding contacts

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠(D–H···A)
O3–H3A···O7$^{\#8}$	0.83	2.05	2.869	173
O4–H4A···O16$^{\#7}$	0.83	2.32	3.133	171
O15–H15A···O17$^{\#4}$	0.84	2.06	2.886	166
O15–H15B···O9$^{\#1}$	0.84	2.07	2.877	161
O16–H16A···O1$^{\#10}$	0.84	2.16	2.954	158
O16–H16B···O6$^{\#6}$	0.84	2.49	3.041	124
O17–H17A···O13$^{\#6}$	0.84	2.09	2.923	169
O17–H17B···O15$^{\#2}$	0.85	2.01	2.854	171

[a] Symmetry transformations used to generate equivalent atoms: #1 = –*x*, –*y*+1, –*z*; #2 = –*x*+1, –*y*+1, –*z*; #3 = *x*+1, *y*, *z*+1; #4 = *x*, *y*, *z*+1; #5 = *x*, –*y*+1/2, *z*–1/2; #6 = *x*+1, *y*, *z*; #7 = *x*–1, *y*, *z*; #8 = *x*, –*y*+1/2, *z*+1/2; #9 = *x*, *y*, *z*+1; #10 = *x*, *y*, *z*–1

Figure captions

Figure S1. PXRD patterns measured, simulated along with the i.r. spectrum for **1**.

Figure S2. PXRD patterns measured, simulated along with the i.r. spectrum for **2**.

Figure S3. PXRD patterns measured, simulated along with the i.r. spectrum for **3**.

Figure S4. PXRD patterns measured, simulated along with the i.r. spectrum for **4**.

Figure S5. PXRD patterns measured, simulated along with the i.r. spectrum for **5**.

Figure S6. 2D $^{2}_{\infty}[Ce_2(H_2O)_2(L\text{-tar})_2]$ network, 3D $^{3}_{\infty}\{^{2}_{\infty}[M_2(H_2O)_2(L\text{-tar})_2](SO_4)\}$ framework along with the corresponding topological nets in **2**.

Figure S7. 2D $^{2}_{\infty}[Ce_2(H_2O)_2(L\text{-tar})_2]$ network, 3D $^{3}_{\infty}\{^{2}_{\infty}[M_2(H_2O)_2(L\text{-tar})_2](SO_4)\}$ framework along with the corresponding topological nets in **3**.

Figure S8. 2D $^{2}_{\infty}[Ce_2(H_2O)_2(L\text{-tar})_2]$ network, 3D $^{3}_{\infty}\{^{2}_{\infty}[M_2(H_2O)_2(L\text{-tar})_2](SO_4)\}$ framework along with the corresponding topological nets in **4**.

Figure S9. TG curves for **1**-**5**.

Figure S1.

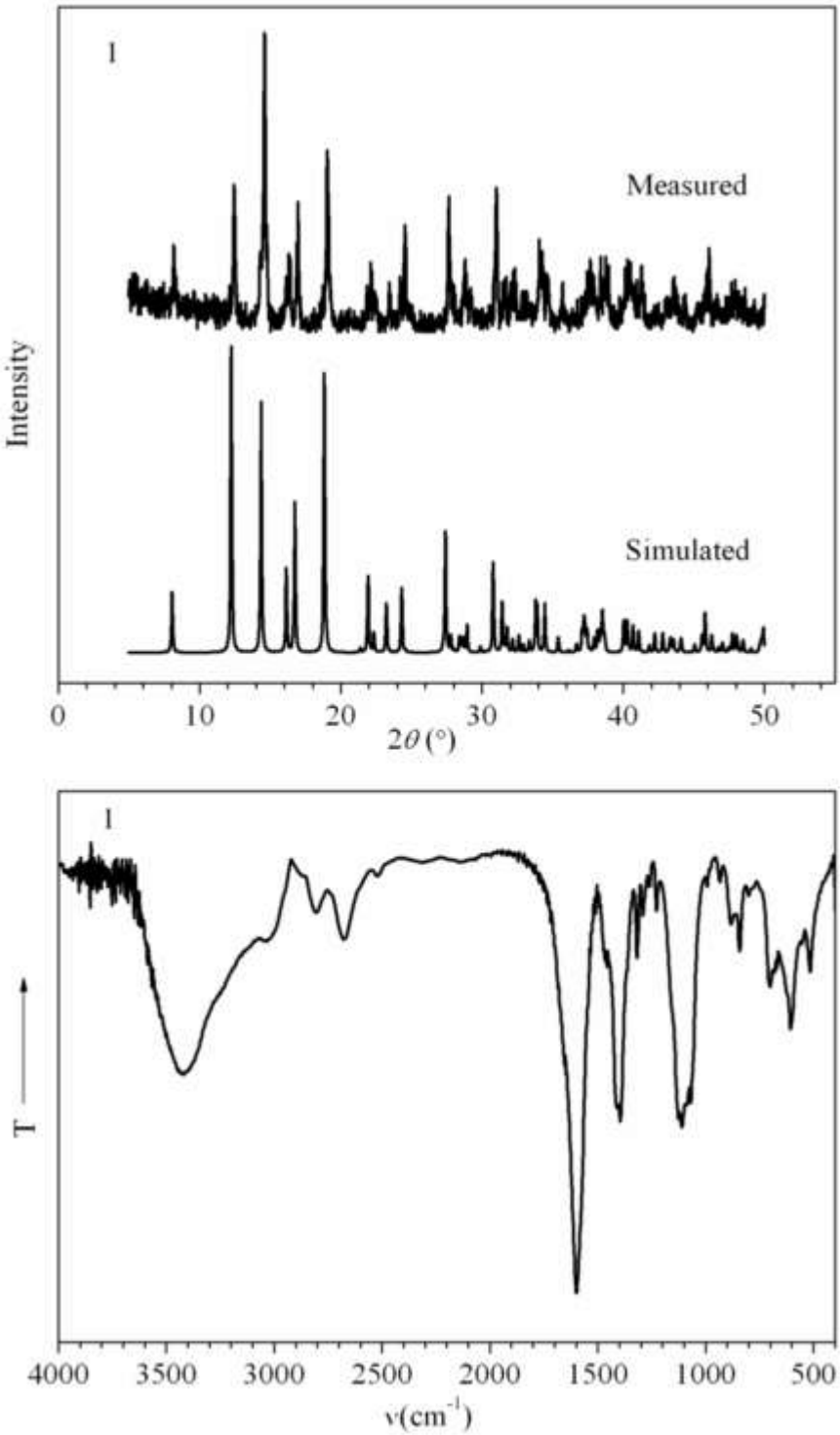

Figure S2.

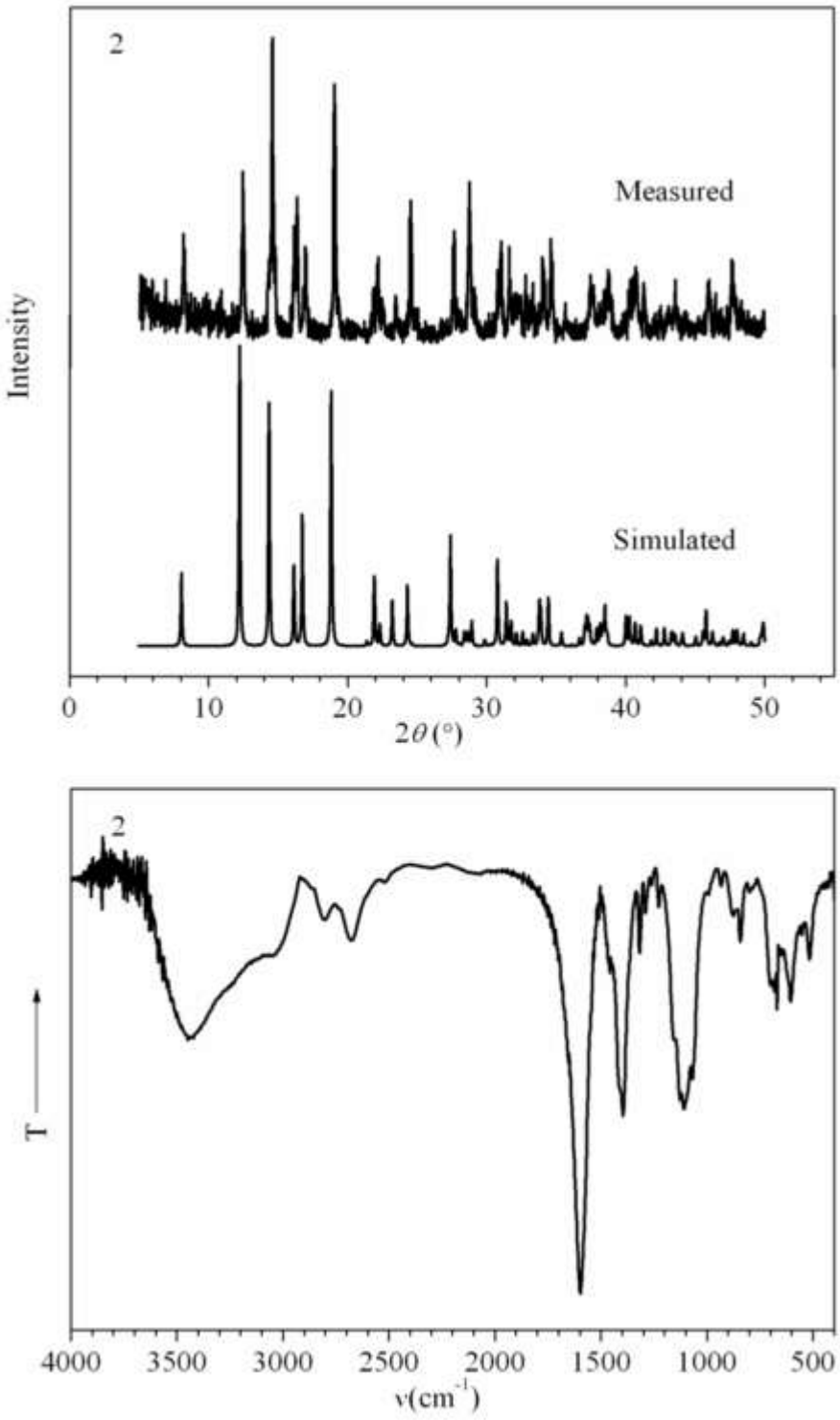

Figure S3.

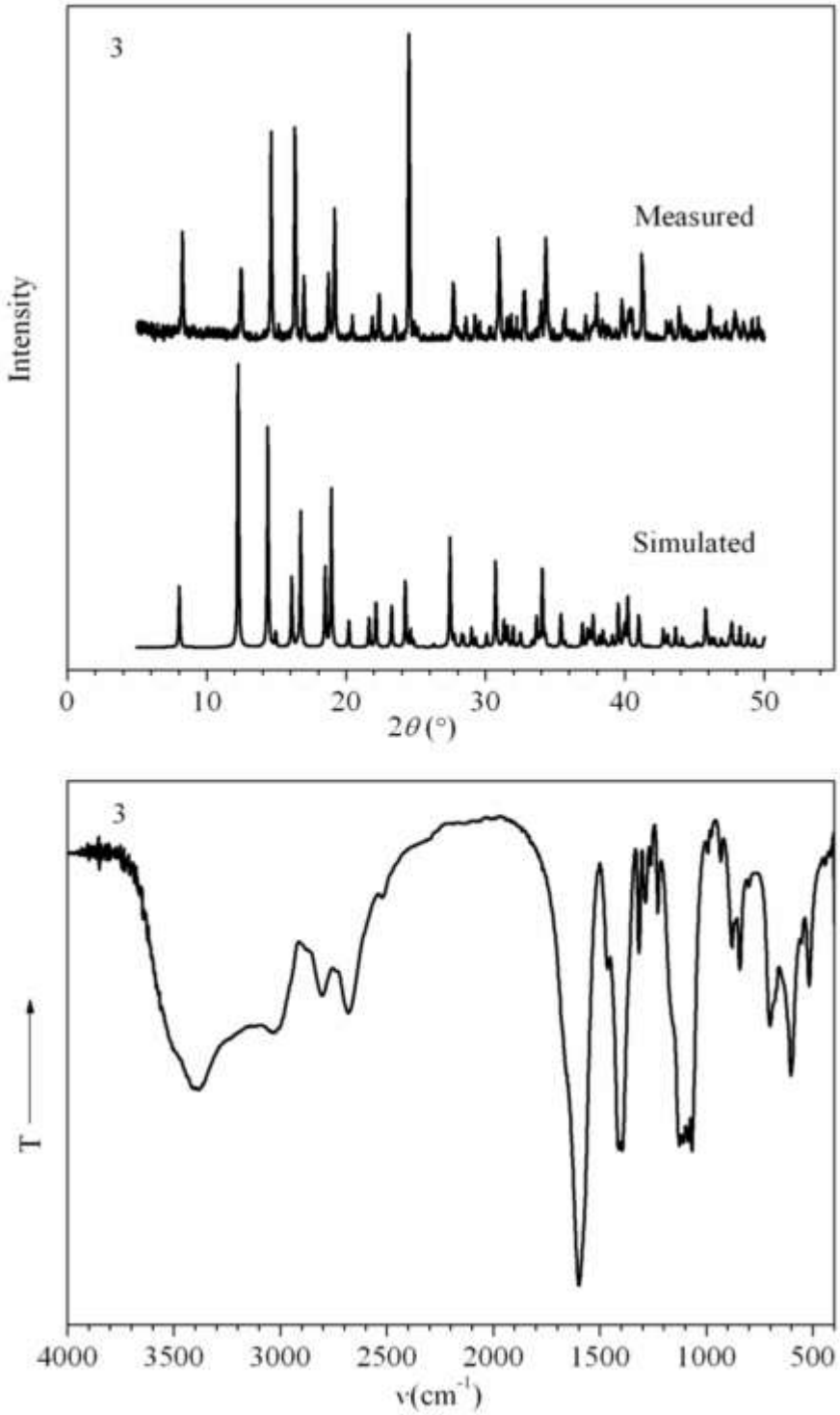

Figure S4.

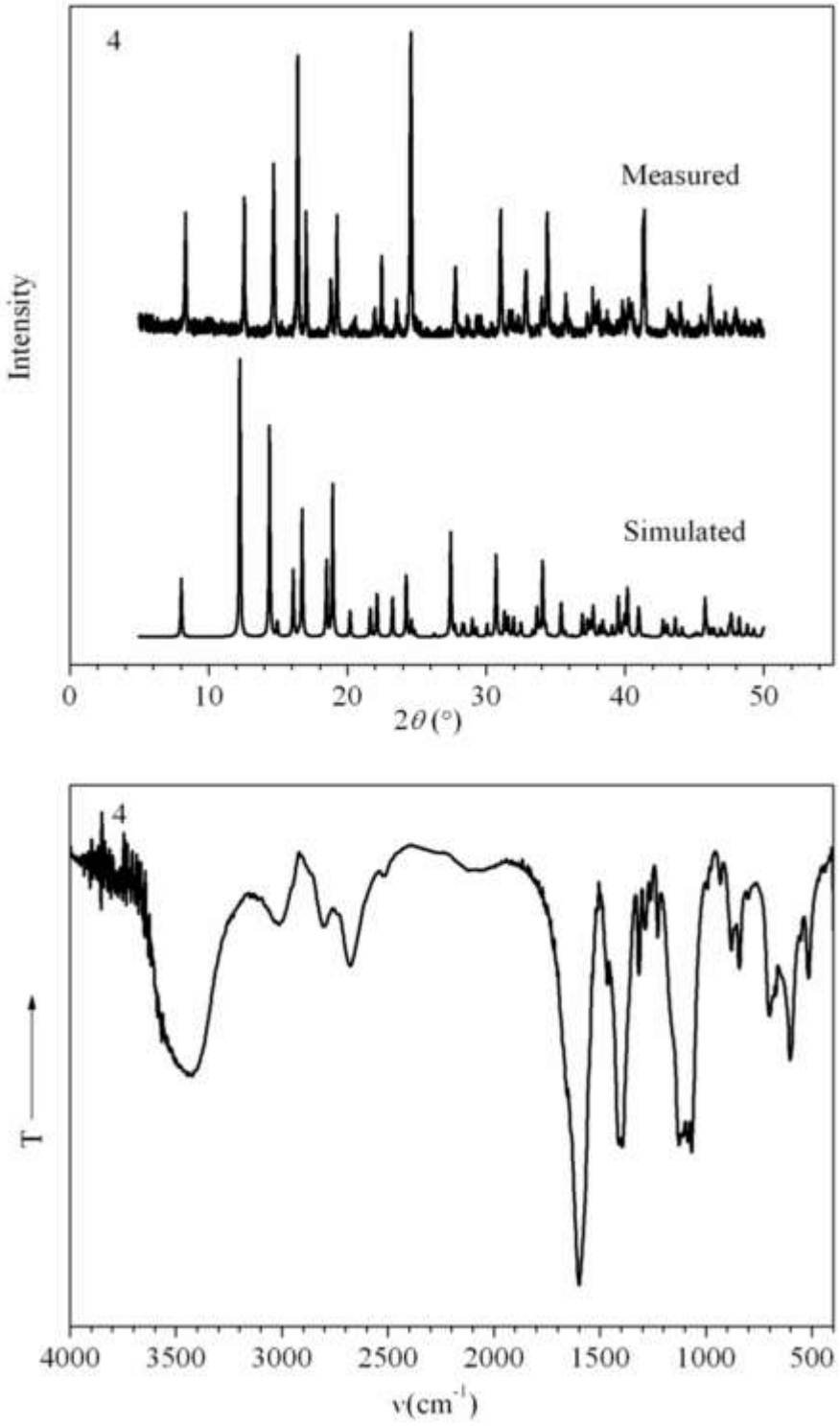

Figure S5.

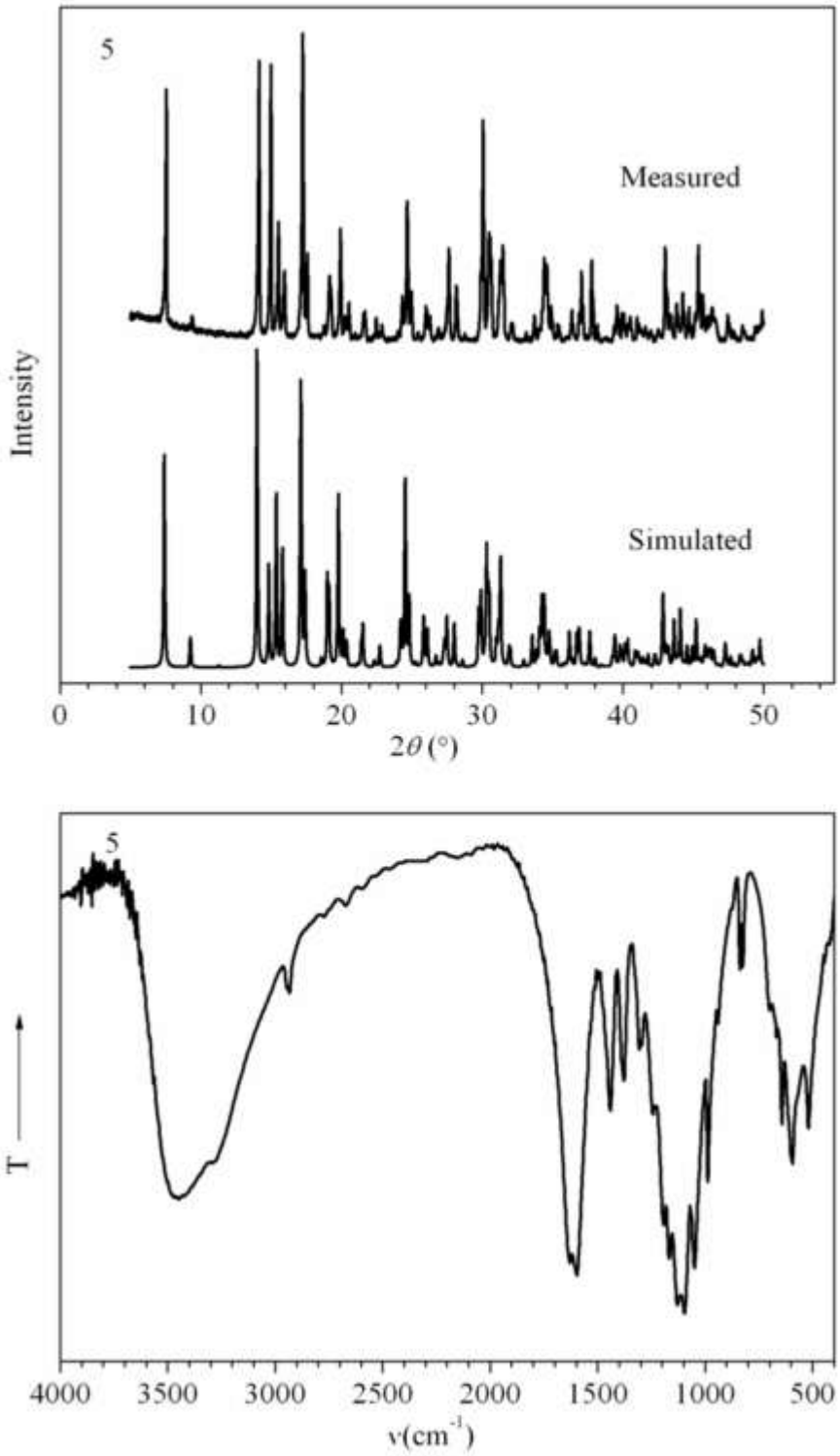

Figure S6.

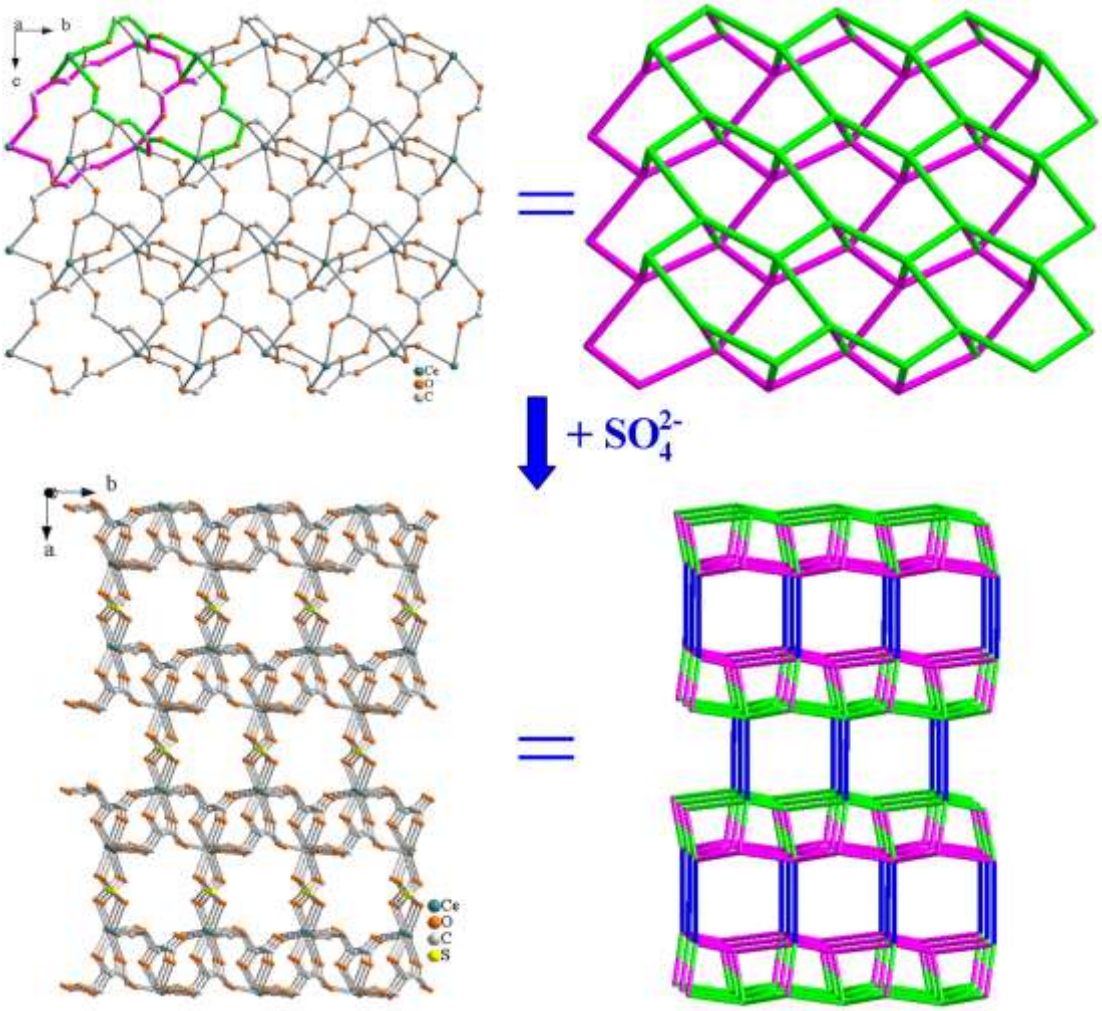

Figure S7.

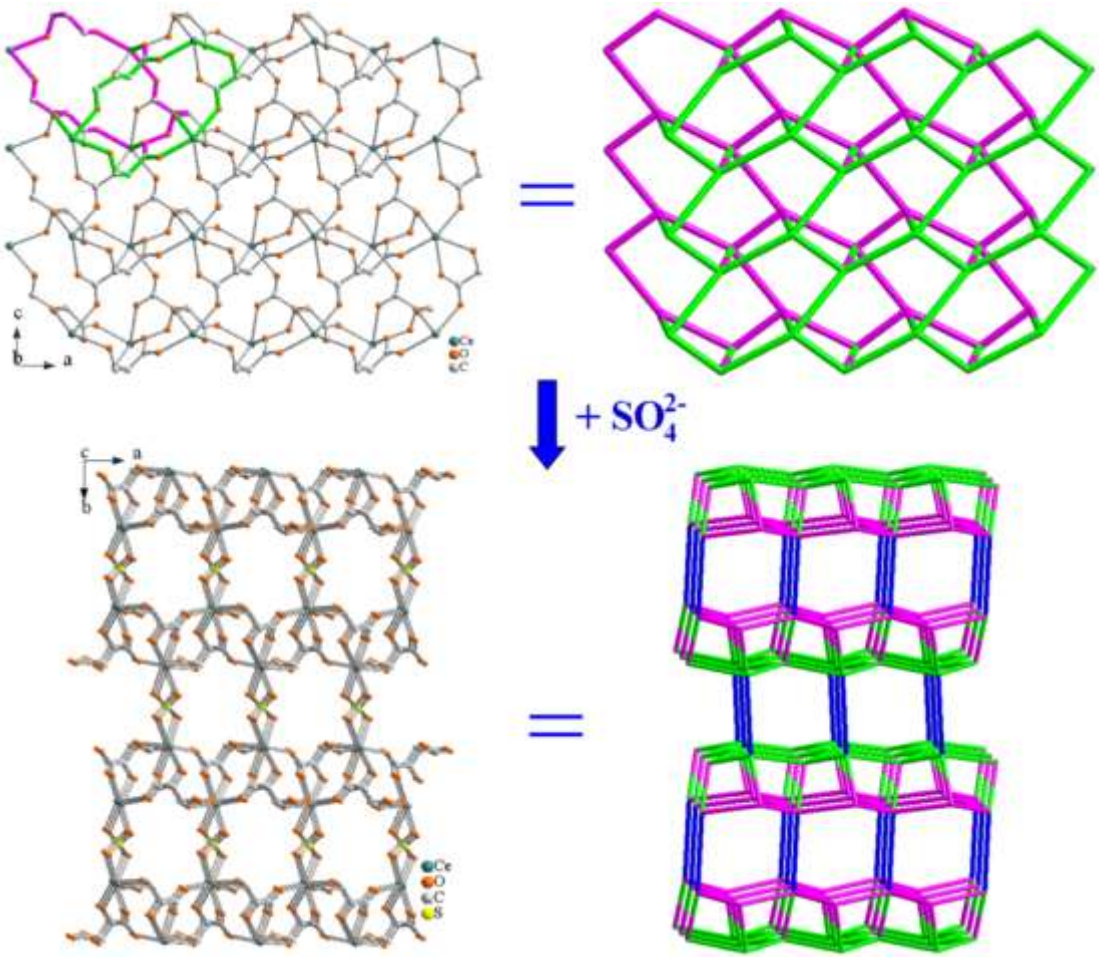

Figure S8.

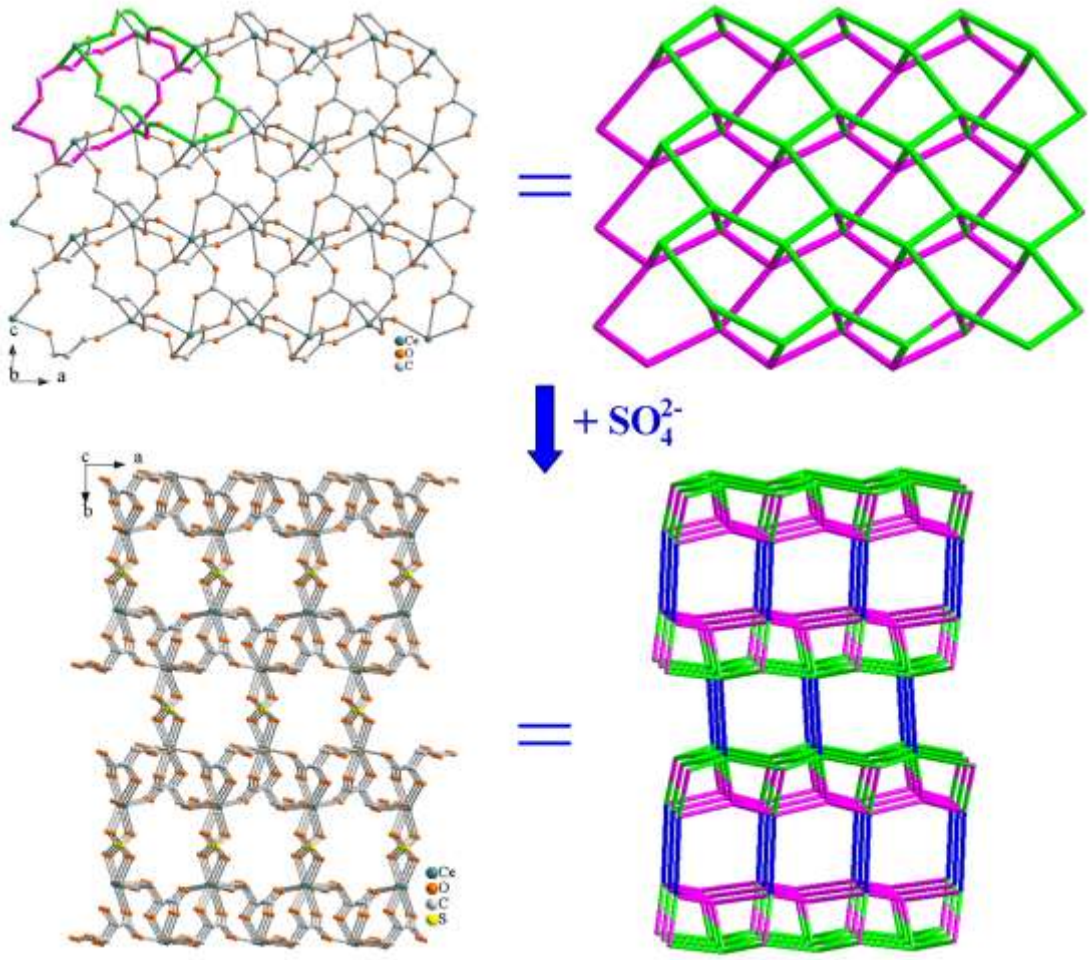

Figure S9.