

Supporting Information

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Table S1. Atomic coordinates and equivalent isotropic displacement parameters for Na₃Y (CO₃)₃

atom	x	Y	z	U _{eq} (Å ²)	BVS
Y1	-0.2500	0.72829 (6)	0.50003 (17)	0.010 (1)	2.81
O1	-0.2500	0.9120 (5)	0.6801 (8)	0.015 (1)	2.11
O2	-0.2500	0.6173 (5)	0.1931 (8)	0.015 (1)	2.06
O3	-0.4881 (3)	0.6923 (4)	0.4161 (5)	0.017 (1)	2.33
O4	-0.2500	0.5111 (4)	0.4587 (7)	0.013 (1)	2.10
O5	-0.3865 (4)	0.6674 (4)	0.7653 (5)	0.013 (1)	2.27
O6	-0.3899 (4)	0.8574 (3)	0.3034 (5)	0.014 (1)	2.19
C1	-0.2500	0.5119 (7)	0.2733 (11)	0.010 (2)	3.96
C2	-0.4986 (5)	0.7931 (5)	0.3254 (8)	0.011 (1)	4.04
Na1	-0.2500	0.0185 (3)	0.3863 (5)	0.015 (1)	0.95
Na2	-0.2500	-0.2051 (2)	0.0008 (9)	0.008 (1)	0.90
Na3	-0.5000	0.0000	0.0682 (5)	0.016 (1)	1.03

Table S2. Atomic coordinates and equivalent isotropic displacement parameters for Na₃Gd (CO₃)₃

atom	x	y	z	U _{eq} (Å ²)	BVS
Gd1	1.2500	0.77179 (2)	0.01265 (10)	0.006 (1)	3.17
O1	1.2500	0.8846 (4)	0.3199 (7)	0.013 (1)	2.09
O2	1.3869 (3)	0.8345 (3)	-0.2545 (5)	0.009 (1)	2.26
O3	1.3909 (3)	0.6416 (3)	0.2128 (4)	0.011 (1)	2.15
O4	1.2500	1.0875 (5)	0.3334 (8)	0.015 (1)	2.02
O5	1.4894 (3)	0.8045 (4)	0.0959 (6)	0.015 (1)	2.29
O6	1.2500	0.9907 (4)	0.0565 (6)	0.010 (1)	2.03
C1	1.2500	0.9877 (6)	0.2412 (10)	0.007 (1)	3.98
C2	1.5005 (4)	0.7957 (4)	-0.3123 (8)	0.007 (1)	3.94
Na1	1.2500	0.9819 (2)	0.6260 (4)	0.011 (1)	1.01
Na2	1.5000	1.0000	0.9448 (4)	0.013 (1)	1.16
Na3	1.2500	0.70621 (16)	0.5105 (10)	0.003 (1)	0.86

Table S3. Bond lengths (Å) for Na₃Y (CO₃)₃.

Y(1)-O(1)	2.367(6)	C(2)-O(5)#5	1.279(6)
Y(1)-O(4)	2.381(6)	C(2)-Na(3)#3	2.889 (9)
Y(1)-O(5)#1	2.392(4)	C(2)-Na(2)#4	2.922 (8)
Y(1)-O(5)	2.392(4)	Na(1)-O(5)#11	2.269 (7)
Y(1)-O(6)	2.404(4)	Na(1)-O(5)#9	2.269 (7)
Y(1)-O(6)#1	2.404(4)	Na(1)-O(6)#12	2.302 (7)
Y(1)-O(3)	2.443(5)	Na(1)-O(6)#13	2.302 (7)
Y(1)-O(3)#1	2.443(5)	Na(1)-O(1)#12	2.370 (9)
Y(1)-O(2)	2.475(6)	Na(1)-O(2)#13	2.412 (9)
Y(1)-C(2)	2.823(6)	Na(1)-C(1)#14	2.725 (12)
Y(1)-C(2)#1	2.823(6)	Na(1)-Na(2)#2	3.115 (7)
Y(1)-C(1)	2.845(8)	Na(1)-Y(1) #12	3.258 (6)
O(1)-C(1)#2	1.270(10)	Na(1)-Na(3)	3.329 (6)
O(1)-Na(1)#3	2.370 (9)	Na(1)-Na(3)#2	3.329 (6)
O(1)-Na(2)#4	2.592 (11)	Na(2)-O(2)#12	2.360 (10)
O(2)-C(1)	1.278(10)	Na(2)-O(4)#9	2.371 (8)
O(2)-Na(2)#3	2.360 (10)	Na(2)-O(5)#15	2.544 (8)
O(2)-Na(1)#5	2.412 (9)	Na(2)-O(5)#14	2.544 (8)
O(3)-C(2)	1.274(7)	Na(2)-O(1)#15	2.592 (11)
O(3)-Na(3)#2	2.354 (6)	Na(2)-O(6)#13	2.624 (10)
O(3)-Na(2)#6	2.644 (6)	Na(2)-O(6)#12	2.624 (10)
O(4)-C(1)	1.304(9)	Na(2)-O(3)#17	2.644 (6)
O(4)-Na(2)#2	2.371 (8)	Na(2)-O(3)#18	2.644 (6)
O(4)-Na(3)#7	2.576 (4)	Na(2)-C(1)#9	2.853 (13)
O(4)-Na(3)#2	2.576 (4)	Na(2)-C(2)#18	2.922 (8)
O(5)-C(2)#3	1.279(6)	Na(2)-C(2)#17	2.922 (8)
O(5)-Na(1)#2	2.269 (7)	Na(3)-O(3)#17	2.353 (6)
O(5)-Na(2)#4	2.544 (8)	Na(3)-O(3)#9	2.353 (6)
O(5)-Na(3)#2	2.546 (6)	Na(3)-O(6)#19	2.513 (6)
O(6)-C(2)	1.286(6)	Na(3)-O(6)#12	2.513 (6)

O(6)-Na(1)#3	2.302 (7)	Na(3)-O(5)#9	2.546 (6)
O(6)-Na(3)#3	2.513 (6)	Na(3)-O(5)#17	2.546 (6)
O(6)-Na(2)#3	2.624 (10)	Na(3)-O(4)#17	2.576 (4)
C(1)-O(1)#4	1.270(10)	Na(3)-O(4)#9	2.576 (4)
C(1)-Na(1)#5	2.725 (12)	Na(3)-C(2)#19	2.889 (9)
C(1)-Na(2)#2	2.853 (13)	Na(3)-C(2)#12	2.889 (9)

Symmetry transformations used to generate equivalent atoms:

#1 $-x-1/2, y, z$ #2 $x, y+1/2, z+1/2$ #3 $-x-1, -y+3/2, z+1/2$
 #4 $x, y-1/2, z-1/2$ #5 $-x-1, -y+3/2, z-1/2$

Table S4. Bond lengths (Å) for Na₃Gd (CO₃)₃.

Gd(1)-O(4)#1	2.394(5)	C(1)-Na(1)	2.740 (11)
Gd(1)-O(6)	2.426(4)	C(1)-Na(3)7#	2.910 (11)
Gd(1)-O(2)#2	2.437(3)	C(2)-O(5)#8	1.285(7)
Gd(1)-O(2)	2.437(3)	C(2)-O(3)#8	1.292(6)
Gd(1)-O(3)#2	2.456(3)	C(2)-Gd(1)#8	2.870(5)
Gd(1)-O(3)	2.456(3)	C(2)-Na(2)5#	2.897 (8)
Gd(1)-O(5)	2.475(3)	C(2)-Na(3)5#	2.957 (8)
Gd(1)-O(5)#2	2.475(3)	Na(1)-O(2)10#	2.279 (5)
Gd(1)-O(1)	2.515(5)	Na(1)-O(2)11#	2.279 (5)
Gd(1)-C(2)#4	2.870(5)	Na(1)-O(3)6#	2.328 (5)
Gd(1)-C(2)#3	2.870(5)	Na(1)-O(3)7#	2.328 (5)
Gd(1)-C(1)	2.878(7)	Na(1)-Na(3)	3.140 (5)
O(1)-C(1)	1.265(8)	Na(1)-Gd(1)6#	3.287 (4)
O(1)-Na(3)	2.385 (9)	Na(1)-Na(2)2#	3.369 (4)
O(1)-Na(1)	2.428 (8)	Na(1)-Na(2)	3.369 (4)
O(2)-C(2)	1.274(6)	Na(1)-Gd(1)11#	3.593 (4)
O(2)-Na(1)5#	2.279 (5)	Na(2)-O(5)13#	2.406 (6)

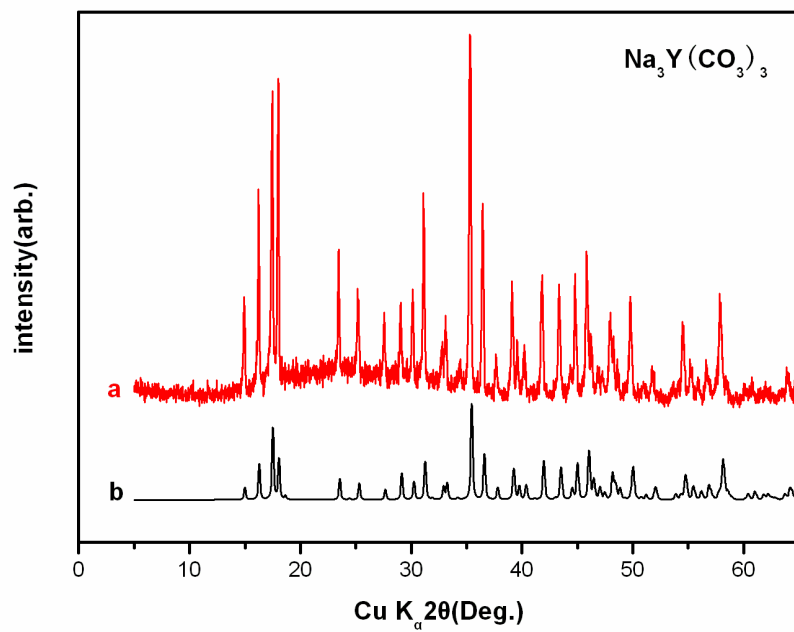
O(2)-Na(2)5#	2.566 (5)	Na(2)-O(5)11#	2.406 (6)
O(2)-Na(3)5#	2.576 (8)	Na(2)-O(3)3#	2.515 (5)
O(3)-C(2)#3	1.291(6)	Na(2)-O(3)6#	2.515 (5)
O(3)-Na(1)1#	2.328 (5)	Na(2)-O(2)11#	2.566 (5)
O(3)-Na(1)2#	2.515 (5)	Na(2)-O(2)13#	2.566 (5)
O(3)-Na(3)	2.637 (10)	Na(2)-O(6)13#	2.608 (2)
O(4)-C(1)	1.278(9)	Na(2)-O(6)11#	2.608 (2)
O(4)-Na(1)	2.385 (8)	Na(2)-C(2)11#	2.897 (8)
O(4)-Gd(1)#4	2.394 (7)	Na(2)-C(2)13#	2.897 (8)
O(4)-Na(3)7#	2.643 (11)	Na(3)-O(6)15#	2.391 (6)
O(5)-C(2)#3	1.284(7)	Na(3)-O(2)11#	2.576 (8)
O(5)-Na(2)5#	2.406 (6)	Na(3)-O(2)10#	2.576 (8)
O(5)-Na(3)8#	2.660 (5)	Na(3)-O(3)2#	2.637 (10)
O(6)-C(1)	1.315(8)	Na(3)-O(4)15#	2.643 (11)
O(6)-Na(3)7#	2.391 (6)	Na(3)-O(5)3#	2.660 (5)
O(6)-Na(2)4#	2.608 (2)	Na(3)-O(5)4#	2.660 (5)
O(6)-Na(2)5#	2.608 (2)		

Symmetry transformations used to generate equivalent atoms:

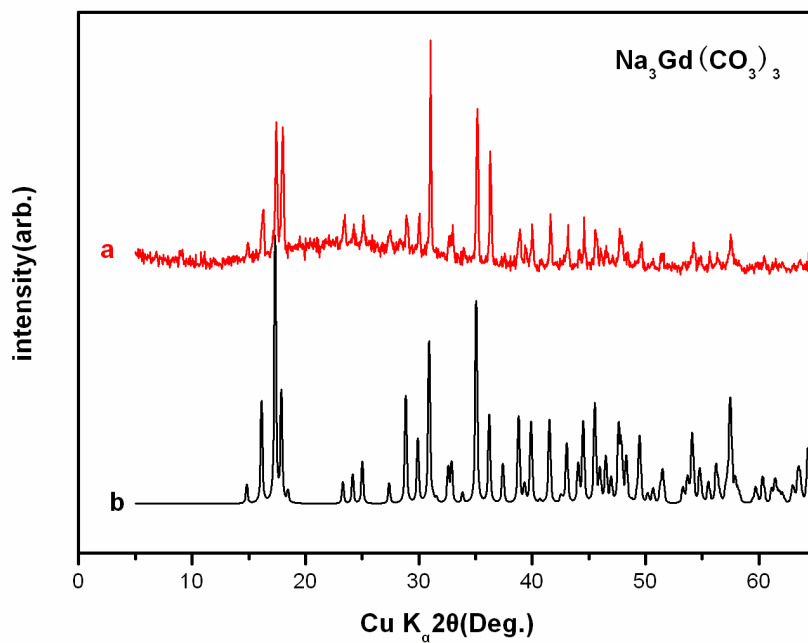
#1 $x, y-1/2, z-1/2$ #2 $-x+5/2, y, z$ #3 $-x+3, -y+3/2, z+1/2$

#4 $x-1/2, -y+3/2, z+1/2$ #5 $x, y+1/2, z+1/2$

#6 $-x+3, -y+3/2, z-1/2$



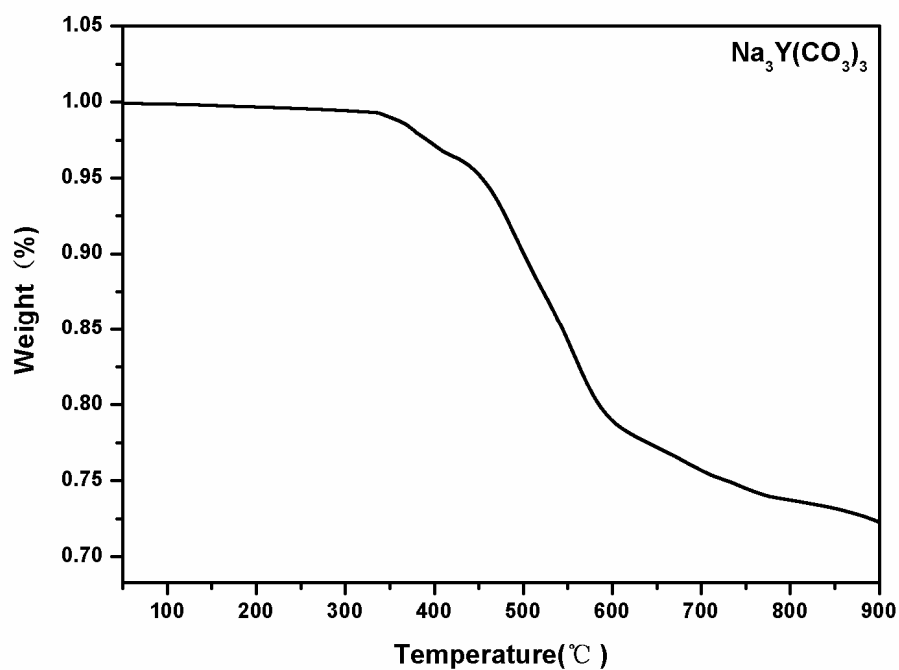
a. X-ray powder diffraction patterns of $\text{Na}_3\text{Y}(\text{CO}_3)_3$



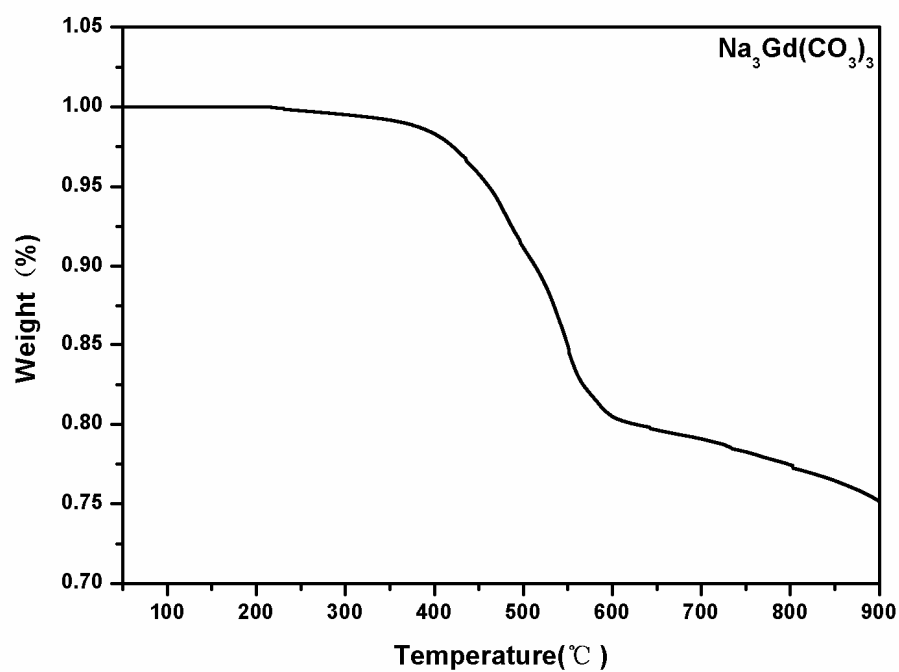
b. X-ray powder diffraction patterns of $\text{Na}_3\text{Gd}(\text{CO}_3)_3$

Figure S1. X-ray powder diffraction patterns of $\text{Na}_3\text{Y}(\text{CO}_3)_3$ and $\text{Na}_3\text{Gd}(\text{CO}_3)_3$.

(a) crystal sample and (b) simulation results

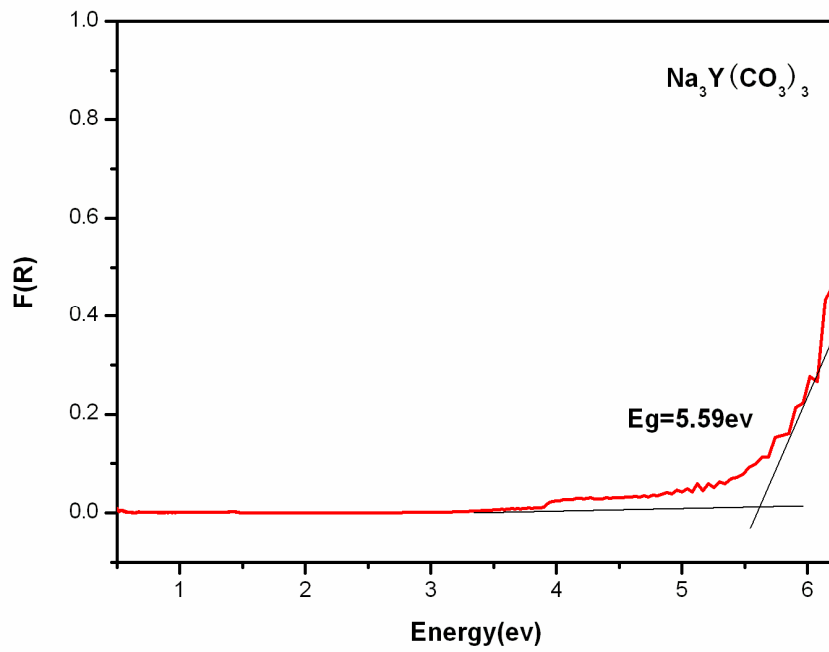


(a) TG diagrams for $\text{Na}_3\text{Y}(\text{CO}_3)_3$

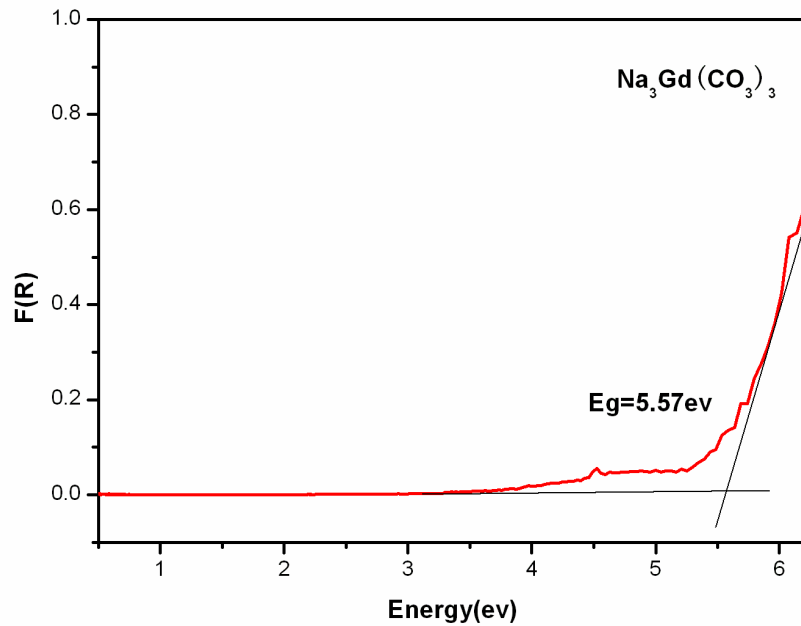


(b) TG diagrams for $\text{Na}_3\text{Gd}(\text{CO}_3)_3$

Figure S2. TG diagrams for $\text{Na}_3\text{Y}(\text{CO}_3)_3$ and $\text{Na}_3\text{Gd}(\text{CO}_3)_3$



a. Diffuse reflectance absorption curve of the powder sample of $\text{Na}_3\text{Y}(\text{CO}_3)_3$.



b. Diffuse reflectance absorption curve of the powder sample of $\text{Na}_3\text{Gd}(\text{CO}_3)_3$.

Figure S3. diffuse reflectance absorption curve of the powder sample of $\text{Na}_3\text{Y}(\text{CO}_3)_3$ and $\text{Na}_3\text{Gd}(\text{CO}_3)_3$.

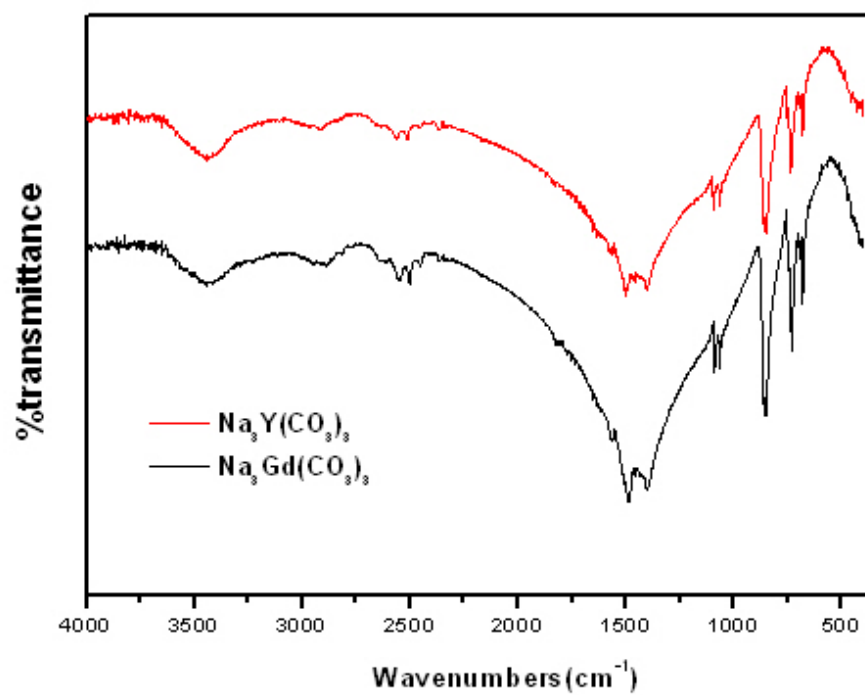
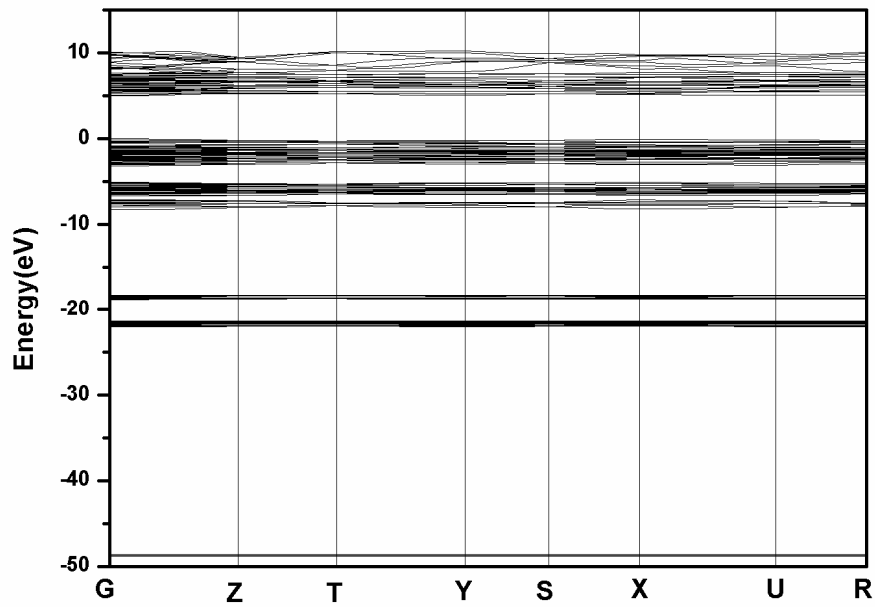
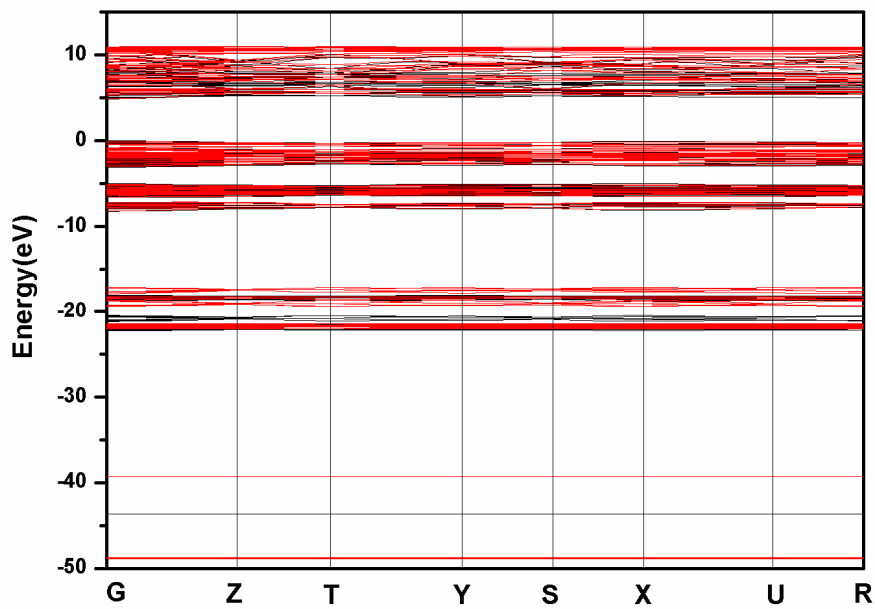


Figure S4. IR spectrum of $\text{Na}_3\text{Y}(\text{CO}_3)_3$ and $\text{Na}_3\text{Gd}(\text{CO}_3)_3$.



(a) Band structures for $\text{Na}_3\text{Y}(\text{CO}_3)_3$



(b) Band structures for $\text{Na}_3\text{Gd}(\text{CO}_3)_3$

Figure S5. Band structures for $\text{Na}_3\text{Y}(\text{CO}_3)_3$ and $\text{Na}_3\text{Gd}(\text{CO}_3)_3$.