

“Tracking Sodium Cobaltate Formation Pathways and its High Temperature CO₂ capture Dynamics in Real Time with Synchrotron X-ray Diffraction”

Tables S1

A:

Rp = 7.9, Rwp = 6.9, Chi² = 208

CoCO ₃				
a	4.6847 (0.0002)			
c	15.0215 (0.0006)			
Atom	x	y	z	Normalized Occ
Co	0	0	0	1
C	0	0	0.25	1
O	0.7233 (0.0002)	0.7233 (0.0002)	0.25	3
Na ₂ CO ₃ -m				
a	8.9148 (0.0006)			
b	5.2433 (0.0004)			
c	6.0506 (0.0004)			
beta	101.222 (0.007)			
Atom	x	y	z	Normalized Occ
Na1	0	0	0	1
Na2	0	0	0.5	1
Na3	0.1759 (0.0003)	0.5	0.7510 (0.0002)	2
C	0.1621 (0.0004)	0.5	0.2492 (0.0005)	2
O1	0.2890 (0.0003)	0.5	0.1763 (0.0006)	2
O2	0.1013 (0.0002)	0.2946 (0.0001)	0.2839 (0.0002)	4

B:

Rp = 6.8, Rwp = 7.4, Chi² = 176

CoCO ₃				
a	4.6875 (0.0002)			
c	15.0838 (0.0007)			
Atom	x	y	z	Normalized Occ
Co	0	0	0	1
C	0	0	0.25	1
O	0.7345 (0.0002)	0.7345 (0.0002)	0.25	3
Na ₂ CO ₃ -m				

a	8.9710 (0.0008)		
b	5.2612 (0.0004)		
c	6.1824 (0.0005)		
beta	101.222 (0.007)		

Atom	x	y	z	Normalized Occ
Na1	0	0	0	1
Na2	0	0	0.5	1
Na3	0.1762 (0.0003)	0.5	0.7493 (0.0003)	2
C	0.1626 (0.0002)	0.5	0.2508 (0.0004)	2
O1	0.2907 (0.0004)	0.5	0.1741 (0.0004)	2
O2	0.1015 (0.0003)	0.2946 (0.0001)	0.2926 (0.0002)	4

CoO

a	4.0546 (0.0004)			
Atom	x	y	z	Normalized Occ
Co	0	0	0	1
O	0.5	0.5	0.5	1

C:

Rp = 5.2, Rwp = 4.8, Chi² = 130

Co₃O₄

a	8.1141 (0.0005)			
Atom	x	y	z	Normalized Occ
Co1	0	0	0	2
Co2	0.625	0.625	0.625	1
O	0.3931 (0.0003)	0.3931 (0.0003)	0.3931 (0.0003)	4

Na₂CO₃-h

a	5.2127 (0.0003)			
b	6.5012 (0.0005)			
Atom	x	y	z	Normalized Occ
Na1	0.3333	0.6666	0.75	1
Na2	0	0	0	1
C	0.3333	0.6666	0.25	1
O	0.2016 (0.0004)	0.4032 (0.0008)	0.25	3

D:

Rp = 5.1, Rwp = 3.9, Chi² = 77

Co₃O₄

a				
				8.1175 (0.0003)
Atom	x	y	z	Normalized Occ
Co1	0	0	0	2
Co2	0.625	0.625	0.625	1
O	0.3942 (0.0005)	0.3942 (0.0005)	0.3942 (0.0005)	4

Na₂CO₃-h

a				
				5.2127 (0.0002)
b				
				6.5012 (0.0005)
Atom	x	y	z	Normalized Occ
Na1	0.3333	0.6666	0.75	1
Na2	0	0	0	1
C	0.3333	0.6666	0.25	1
O	0.2024 (0.0004)	0.4047 (0.0004)	0.25	3

E:

R_p = 8.3, R_{wp} = 6.1, Chi² = 118

Co₃O₄

a				
				8.1468 (0.0004)
Atom	x	y	z	Normalized Occ
Co1	0	0	0	2
Co2	0.625	0.625	0.625	1
O	0.3873 (0.0005)	0.3873 (0.0005)	0.3873 (0.0005)	4

Na₂CO₃-h

a				
				5.2206 (0.0002)
b				
				6.7633 (0.0005)
Atom	x	y	z	Normalized Occ
Na1	0.3333	0.6666	0.75	1
Na2	0	0	0	1
C	0.3333	0.6666	0.25	1
O	0.2021 (0.0003)	0.4042 (0.0005)	0.25	3

Na_{0.74}CO₂

a				
				2.8561 (0.0003)
b				
				11.0892 (0.0006)
Atom	x	y	z	Normalized Occ
Na1	0.3333	0.6666	0.25	0.51 (0.01)
Na2	0	0	0.25	0.22 (0.01)
Co	0	0	0	1
O	0.6666	0.3333	0.0908 (0.003)	2

F:

Rp = 9.1, Rwp = 6.6, Chi² = 210

Co ₃ O ₄				
a	8.1220 (0.0005)			
Atom	X	y	z	Normalized Occ
Co1	0	0	0	2
Co2	0.625	0.625	0.625	1
O	0.3792 (0.0004)	0.3792 (0.0004)	0.3792 (0.0004)	4
Na ₂ CO ₃ -h				
a	5.228 (0.002)			
b	6.782 (0.003)			
Atom	x	y	z	Normalized Occ
Na1	0.3333	0.6666	0.75	1
Na2	0	0	0	1
C	0.3333	0.6666	0.25	1
O	0.2012 (0.0003)	0.4024 (0.0006)	0.25	3
Na _{0.74} CO ₂				
a	2.8561 (0.0003)			
b	11.0892 (0.0006)			
Atom	x	y	z	Normalized Occ
Na1	0.3333	0.6666	0.25	0.47 (0.01)
Na2	0	0	0.25	0.27 (0.03)
Co	0	0	0	1
O	0.6666	0.3333	0.0911 (0.003)	2

Tables S2.

A:

Rp = 4.9, Rwp = 5.1, Chi² = 27

Co ₃ O ₄				
a	8.0582 (0.0004)			
Atom	x	y	z	Normalized Occ
Co1	0	0	0	2
Co2	0.625	0.625	0.625	1
O	0.3892 (0.0002)	0.3892 (0.0002)	0.3892 (0.0002)	3
Na ₂ CO ₃ -m				
a	8.9035 (0.0003)			
b	5.2304 (0.0003)			
c	6.0748 (0.0002)			
beta	100.771 (0.002)			
Atom	x	y	z	Normalized Occ
Na1	0	0	0	1
Na2	0	0	0.5	1
Na3	0.1760 (0.0004)	0.5	0.7478 (0.0002)	2
C	0.1635 (0.0004)	0.5	0.2487 (0.0002)	2
O1	0.2899 (0.0008)	0.5	0.1785 (0.0005)	2
O2	0.1021 (0.0003)	0.2956 (0.0003)	0.2857 (0.0003)	4

B:

Rp = 4.6, Rwp = 9.4, Chi² = 19

Co ₃ O ₄				
a	8.1053 (0.0002)			
Atom	x	y	z	Normalized Occ
Co1	0	0	0	2
Co2	0.625	0.625	0.625	1
O	0.3886 (0.0004)	0.3886 (0.0004)	0.3886 (0.0004)	3
Na ₂ CO ₃ -m				
a	9.0041 (0.0004)			
b	5.1499 (0.0006)			
c	6.0840 (0.0008)			
beta	102.638 (0.009)			
Atom	x	y	z	Normalized Occ
Na1	0	0	0	1

Na2	0	0	0.5	1
Na3	0.1803 (0.0003)	0.5	0.7399 (0.0005)	2
C	0.1726 (0.0007)	0.5	0.2496 (0.0003)	2
O1	0.2896 (0.0004)	0.5	0.1768 (0.0003)	2
O2	0.1036 (0.0006)	0.2953 (0.0003)	0.2895 (0.0004)	4

Co₂O₃

a	7.8979 (0.0004)			
Atom	x	y	z	Normalized Occ
Co1	0.125	0.125	0.125	1
Co2	0.5	0.5	0.5	0.83333
O	0.25	0.25	0.25	3

C:

Rp = 2.1, Rwp = 3.4, Chi² = 16

Co₃O₄

a	7.9097 (0.0006)			
Atom	x	y	z	Normalized Occ
Co1	0	0	0	2
Co2	0.625	0.625	0.625	1
O	0.3892 (0.0003)	0.3892 (0.0003)	0.3892 (0.0003)	3

Na₂CO₃-m

a	9.2719 (0.0004)			
b	5.1499 (0.0006)			
c	6.4162 (0.0008)			
beta	100.237 (0.009)			
Atom	x	y	z	Normalized Occ
Na1	0	0	0	1
Na2	0	0	0.5	1
Na3	0.1826 (0.0006)	0.5	0.7407 (0.0005)	2
C	0.1706 (0.0008)	0.5	0.2479 (0.0007)	2
O1	0.2877 (0.0004)	0.5	0.1766 (0.0007)	2
O2	0.1055 (0.0004)	0.2966 (0.0004)	0.2897 (0.0002)	4

Co₂O₃

a	7.9097 (0.0005)			
Atom	x	y	z	Normalized Occ
Co1	0.125	0.125	0.125	1
Co2	0.5	0.5	0.5	0.83333

O 0.25 0.25 0.25 3

D:

Rp = 8.2, Rwp = 5.5, Chi² = 181

Co ₃ O ₄				
a	8.1004 (0.0005)			
Atom	x	y	z	Normalized Occ
Co1	0	0	0	2
Co2	0.625	0.625	0.625	1
O	0.3872 (0.0005)	0.3872 (0.0005)	0.3872 (0.0005)	4

Na ₂ CO ₃ -h				
a	5.1988 (0.0003)			
b	6.6976 (0.0005)			
Atom	x	y	z	Normalized Occ
Na1	0.3333	0.6666	0.75	1
Na2	0	0	0	1
C	0.3333	0.6666	0.25	1
O	0.2018 (0.0004)	0.4036 (0.0008)	0.25	3

E:

Rp = 8.8, Rwp = 7.3, Chi² = 186

Co ₃ O ₄				
a	8.1468 (0.0004)			
Atom	x	y	z	Normalized Occ
Co1	0	0	0	2
Co2	0.625	0.625	0.625	1
O	0.3873 (0.0005)	0.3873 (0.0005)	0.3873 (0.0005)	4

Na ₂ CO ₃ -h				
a	5.197 (0.0002)			
b	6.6992 (0.0005)			
Atom	x	y	z	Normalized Occ
Na1	0.3333	0.6666	0.75	1
Na2	0	0	0	1
C	0.3333	0.6666	0.25	1
O	0.2014 (0.0003)	0.4028 (0.0005)	0.25	3
Na _{0.74} CO ₂				
a	2.8414 (0.0004)			

b		11.034 (0.002)		
Atom	x	y	z	Normalized Occ
Na1	0.3333	0.6666	0.25	0.51 (0.01)
Na2	0	0	0.25	0.23 (0.02)
Co	0	0	0	1
O	0.6666	0.3333	0.0903 (0.003)	2

F:

Rp = 6.5, Rwp = 7.4, Chi² = 106

Na ₂ CO ₃ -h				
a		5.226 (0.003)		
b		6.598 (0.007)		
Atom	x	y	z	Normalized Occ
Na1	0.3333	0.6666	0.75	1
Na2	0	0	0	1
C	0.3333	0.6666	0.25	1
O	0.2016 (0.0003)	0.4032 (0.0007)	0.25	3

Na _{0.74} CO ₂				
a		2.8438 (0.0002)		
b		11.012 (0.002)		
Atom	x	y	z	Normalized Occ
Na1	0.3333	0.6666	0.25	0.47 (0.01)
Na2	0	0	0.25	0.27 (0.03)
Co	0	0	0	1
O	0.6666	0.3333	0.0909 (0.003)	2

Tables S3**Beginning (50 °C):**Rp = 8.3, Rwp = 8.2, Chi² = 193

Na _{0.74} CO ₂				
a	2.8284 (0.0005)			
b	10.8894 (0.0003)			
Atom	x	y	z	Normalized Occ
Na1	0.3333	0.6666	0.25	0.47 (0.02)
Na2	0	0	0.25	0.26 (0.02)
Co	0	0	0	1
O	0.6666	0.3333	0.1073 (0.0006)	2

Halfway (500 °C):Rp = 9.8, Rwp = 8.4, Chi² = 167

Co ₃ O ₄				
a	8.0748 (0.0003)			
Atom	x	y	z	Normalized Occ
Co1	0	0	0	2
Co2	0.625	0.625	0.625	1
O	0.3896 (0.0005)	0.3896 (0.0005)	0.3896 (0.0005)	4

Na ₂ CO ₃ -h				
a	5.3658 (0.0005)			
b	6.7092 (0.0003)			
Atom	x	y	z	Normalized Occ
Na1	0.3333	0.6666	0.75	1
Na2	0	0	0	1
C	0.3333	0.6666	0.25	1
O	0.2554 (0.0003)	0.5108 (0.0006)	0.25	3

Na _{0.74} CO ₂				
a	2.8469 (0.0003)			
b	11.0965 (0.0006)			
Atom	x	y	z	Normalized Occ
Na1	0.3333	0.6666	0.25	0.53 (0.01)
Na2	0	0	0.25	0.22 (0.02)
Co	0	0	0	1
O	0.6666	0.3333	0.101 (0.003)	2

End (700 °C):

Rp = 8.8, Rwp = 7.3, Chi² = 45.2

Co ₃ O ₄				
a	8.1132 (0.0003)			
Atom	x	y	z	Normalized Occ
Co1	0	0	0	2
Co2	0.625	0.625	0.625	1
O	0.3862 (0.0003)	0.3862 (0.0003)	0.3862 (0.0003)	4
Na ₂ CO ₃ -h				
a	5.4036 (0.0005)			
b	6.6956 (0.0004)			
Atom	x	y	z	Normalized Occ
Na1	0.3333	0.6666	0.75	1
Na2	0	0	0	1
C	0.3333	0.6666	0.25	1
O	0.2613 (0.0002)	0.5226 (0.0004)	0.25	3