

Supplementary material

Co nanoparticles supported on mixed magnesium–lanthanum oxides: Effect of calcium and barium addition on ammonia synthesis catalyst performance

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Table S1. The composition of the Co catalysts obtained by XRF.

Entry	Catalyst	Chemical composition (wt%)					
		Co	Mg	La	K	Ca	Ba
1	Co	44.4	15.7	16.1	0.16	–	–
2	0.5Ca–Co	42.9	16.7	15.9	0.19	0.7	–
3	1Ca–Co	42.6	15.7	15.6	0.18	1.2	–
4	3Ca–Co	41.7	14.9	15.4	0.25	3.3	–
5	5Ca–Co	42.7	15.7	15.1	0.19	5.5	–
6	7Ca–Co	36.9	14.2	13.7	0.22	6.9	–
7	9Ca–Co	37.2	14.2	13.5	0.21	9.9	–
8	0.5Ba–Co	41.0	14.8	14.7	0.11	–	0.4
9	1Ba–Co	41.7	15.6	15.3	0.12	–	0.8
10	3Ba–Co	41.6	15.5	14.4	0.08	–	2.4
11	5Ba–Co	40.9	14.7	13.9	0.06	–	4.5
12	7Ba–Co	39.2	15.9	13.0	0.05	–	6.3
13	9Ba–Co	39.3	16.3	12.8	0.05	–	8.3
14	(5Ca+5Ba)–Co	36.4	14.3	11.9	0.06	5.0	3.9

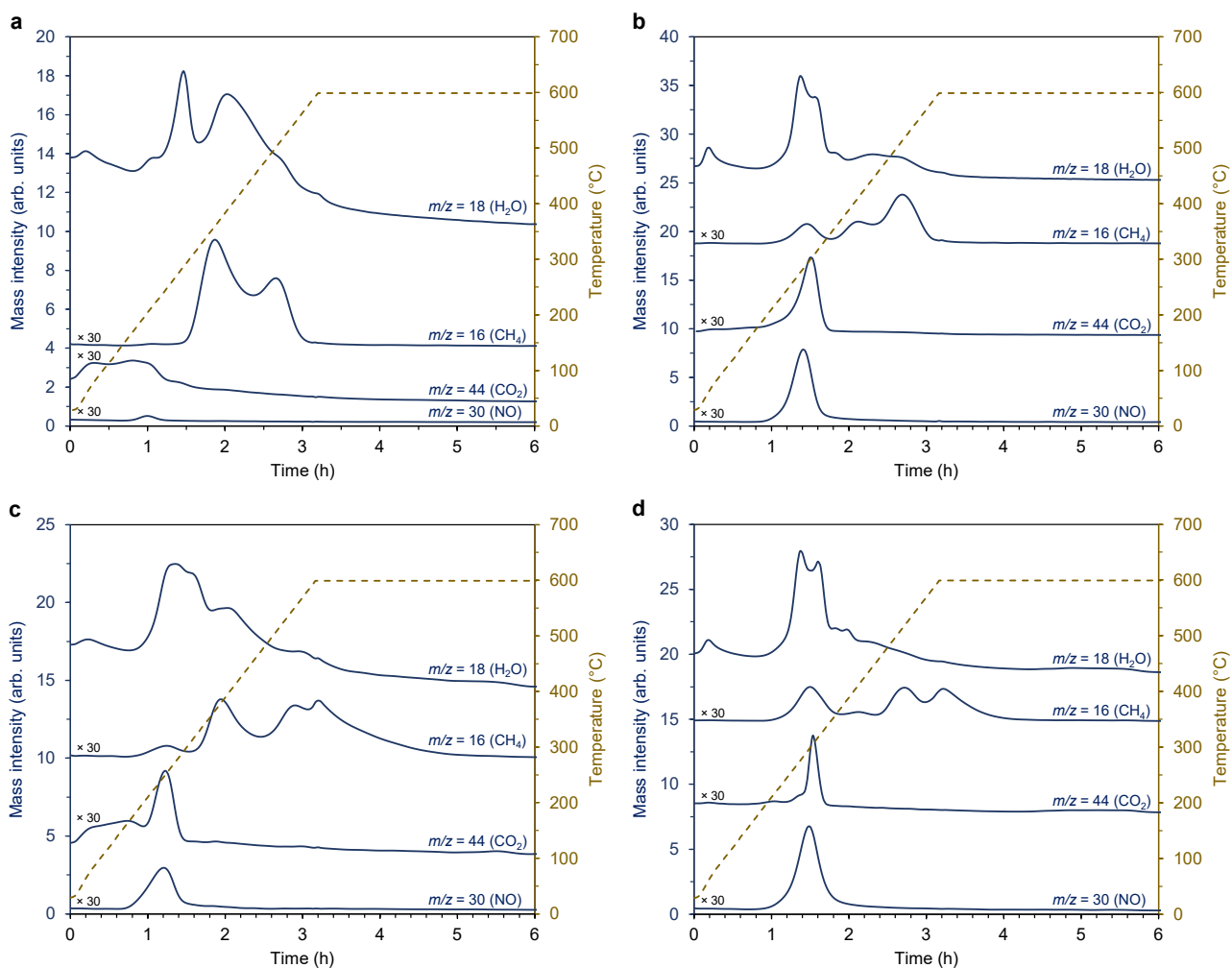


Figure S1. TPR-MS profiles of the as-prepared Co catalysts. **a** Co. **b** 5Ca-Co. **c** 5Ba-Co. **d** (5Ca+5Ba)-Co. The TPR-MS profiles of the as-prepared Co catalysts indicated that the H₂O, CH₄, CO₂, and NO formation was completed at about 600 °C.

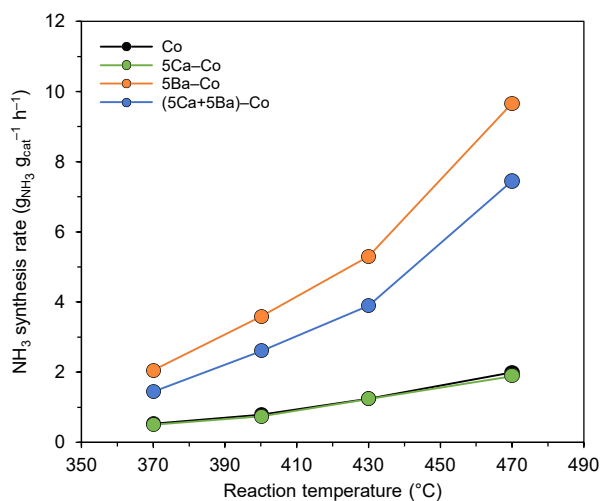


Figure S2. Temperature dependence of the ammonia synthesis rate of Co catalysts at 6.3 MPa. The rates were measured in the reaction mixture without ammonia.

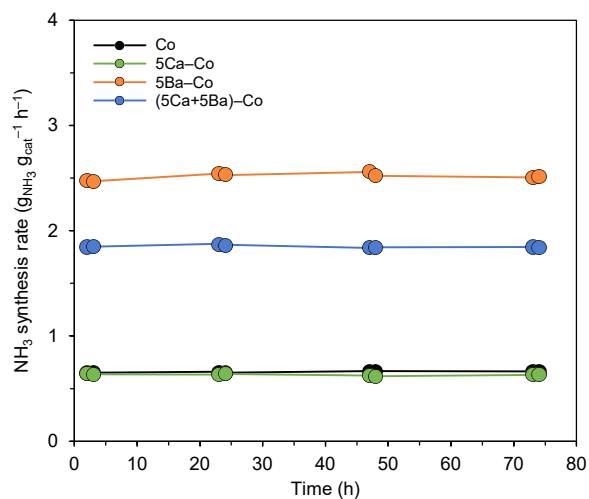


Figure S3. Time dependence of ammonia synthesis rate over Co catalysts at 370 °C and 9.0 MPa. The rates were measured in the reaction mixture without ammonia.

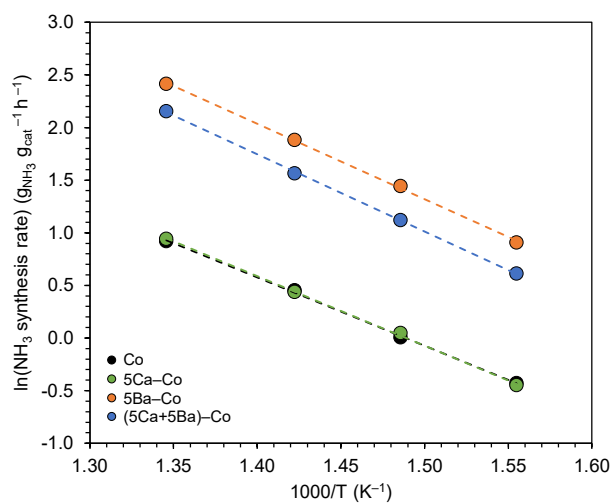


Figure S4. Arrhenius plots for NH₃ synthesis over the Co catalysts.

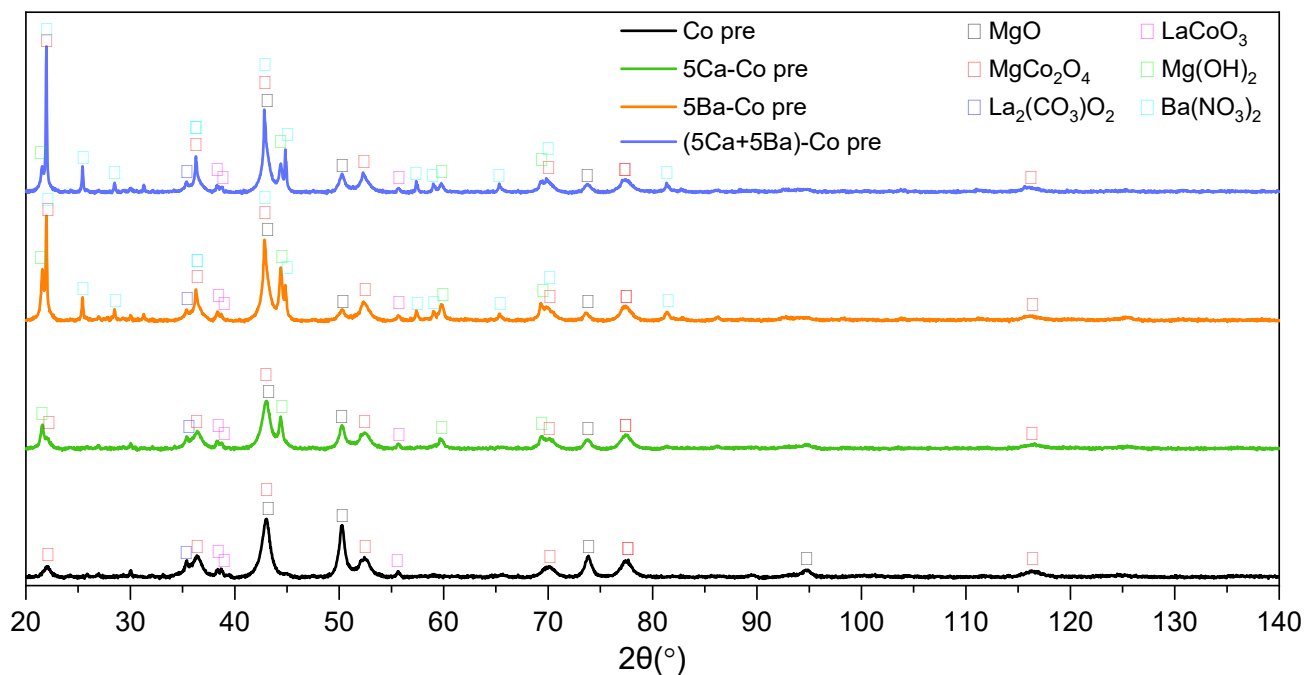


Figure S5. Diffractograms of the Co catalyst precursors collected under N₂ flow at 25 °C.

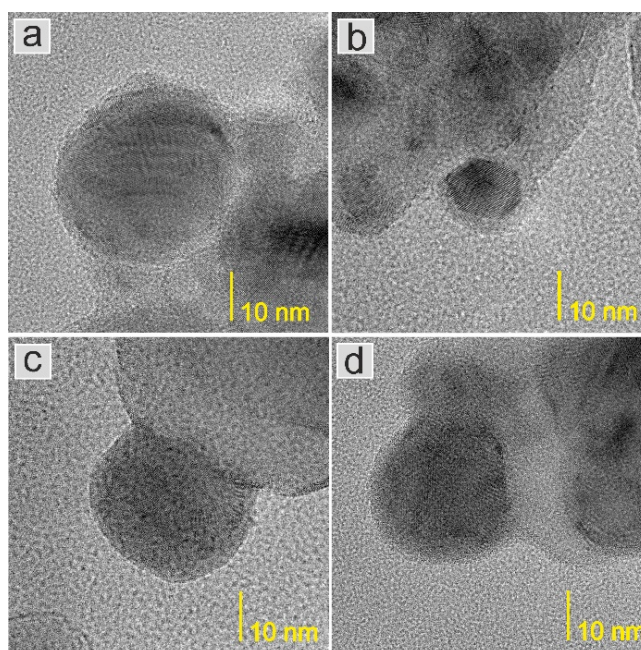


Figure S6. HR-TEM images of the Co catalysts. **a** Co. **b** 5Ca-Co. **c** 5Ba-Co. **d** (5Ca+5Ba)-Co. The crystal structure of the Co nanoparticles was identified as the face-centred-cubic (fcc).

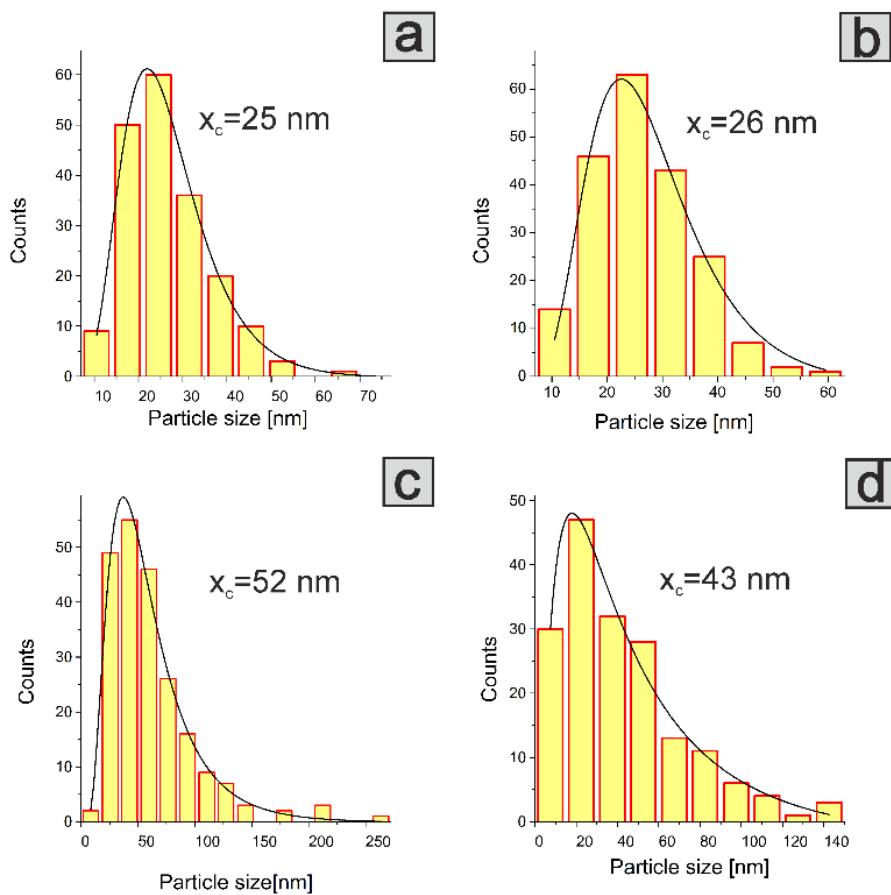


Figure S7. Co particle size distribution histograms for the Co catalysts. **a** Co. **b** 5Ca-Co. **c** 5Ba-Co. **d** (5Ca+5Ba)-Co.