

SUPPLEMENTARY MATERIAL

Multiple sorption cycles evaluation of cadmium oxide/alkali metal halide mixtures for pre-combustion CO₂ capture

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1 Pore size distribution of SBA-15

The nitrogen physisorption experiment at 77 K on the SBA-15 sample used in this study was performed on a Coulter Omnisorp 360CX gas sorption analyser. The isotherm and the pore size distribution calculated by the BJH method are given in Figure A. The BET surface area, determined between 0.05 and 0.35 relative pressures, was determined to be 974.8 m²/g.

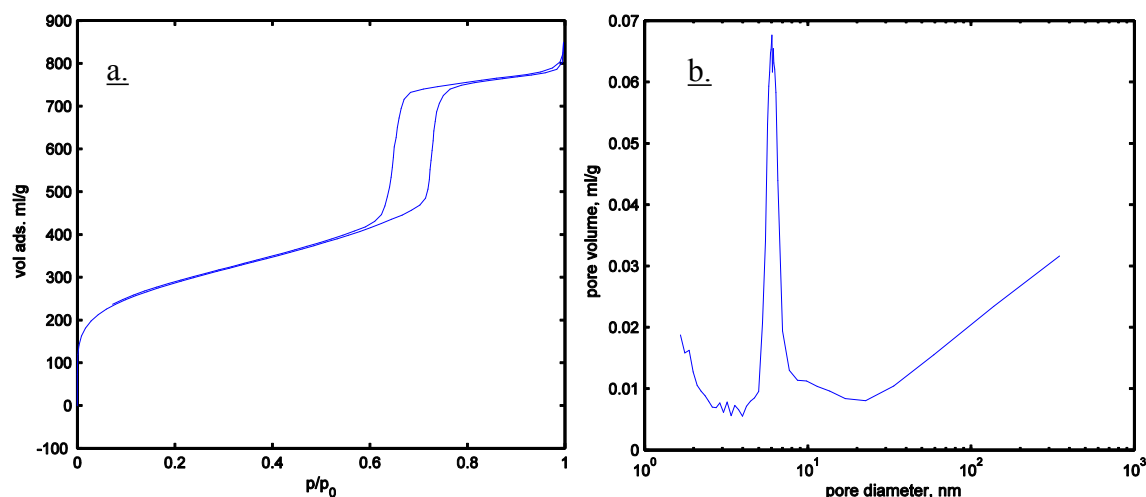
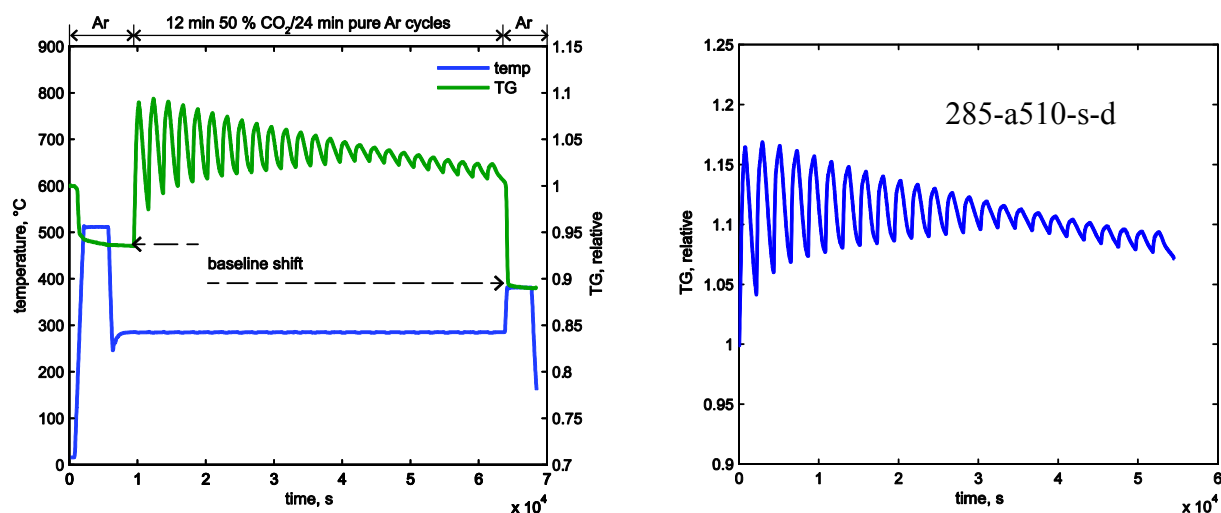
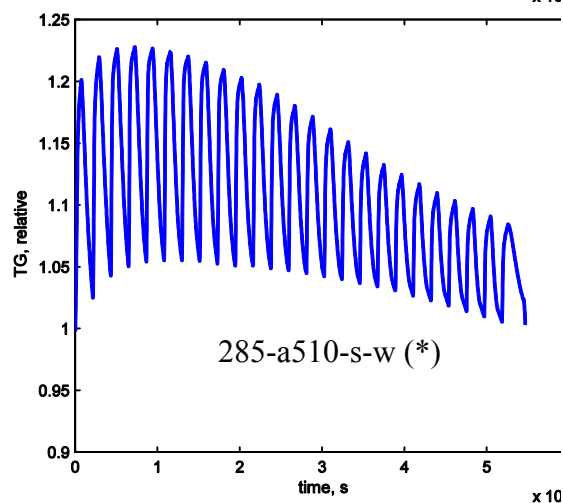
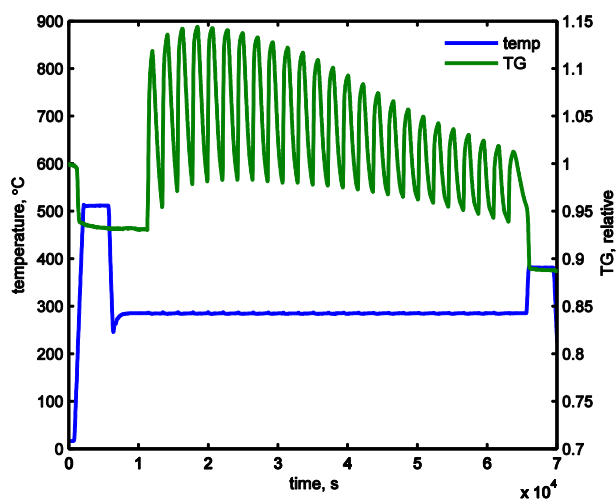
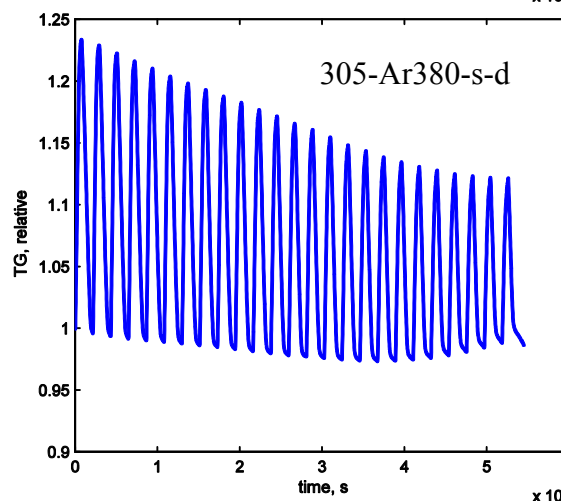
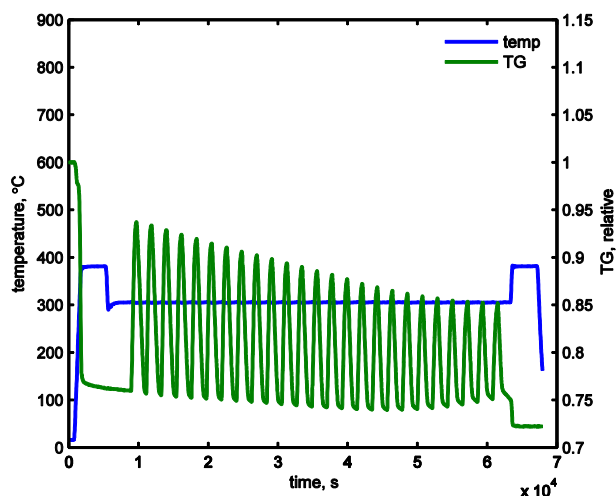
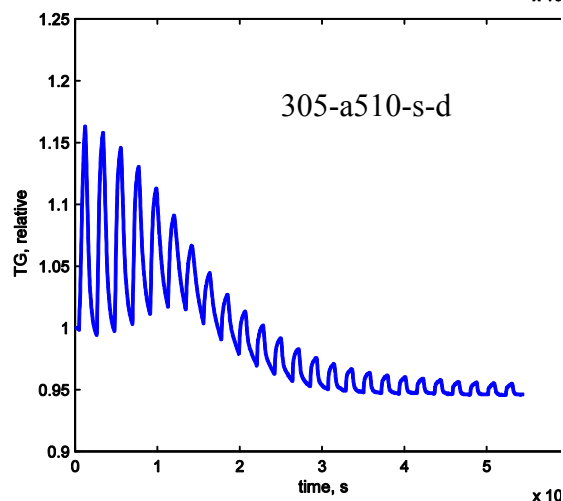
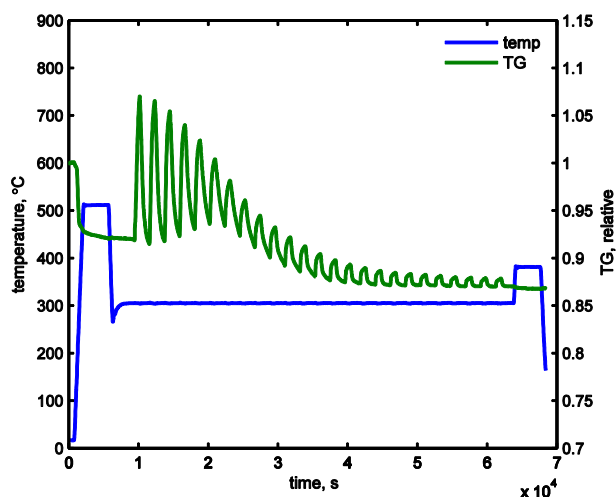
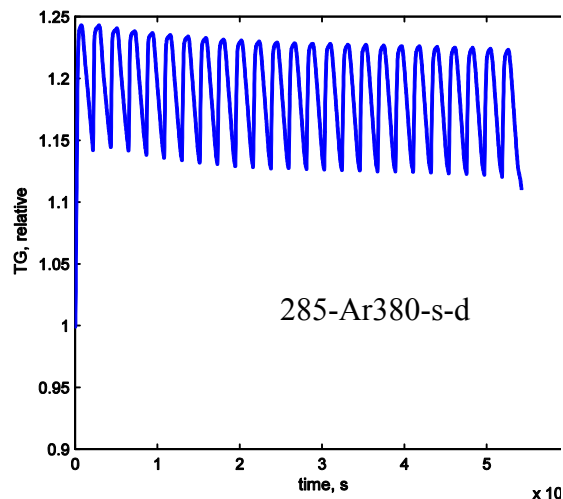
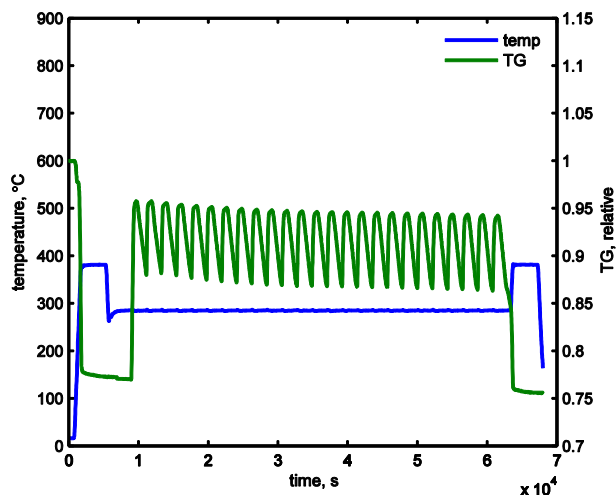


Figure A: a. N₂ adsorption isotherm, b. BJH pore volume for SBA-15.

2 TGA cyclic experiments plots





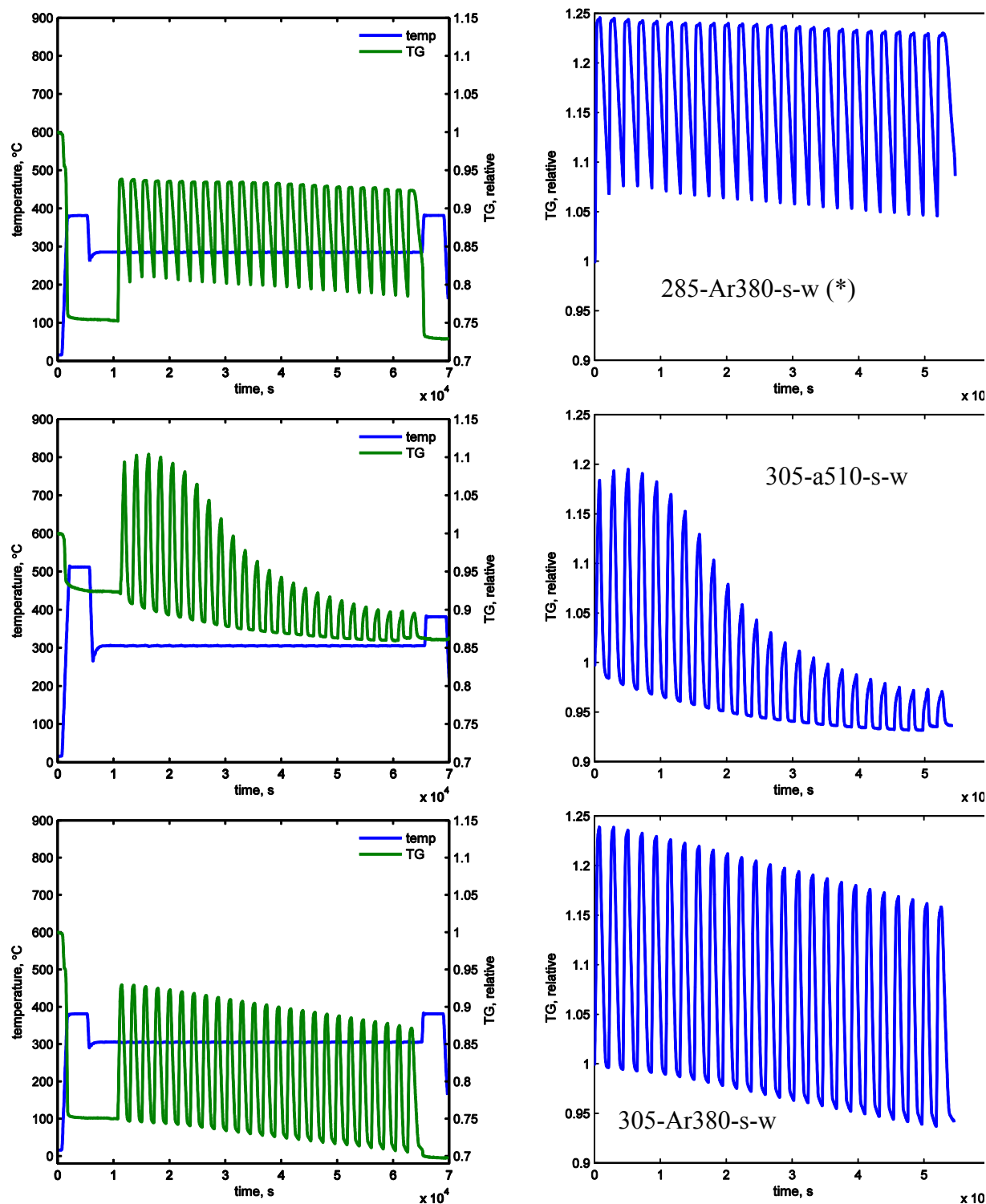


Figure B: Full thermograms (left) and normalised thermograms to 100 % active sorbent (right) of multicyclic sorption-desorption of Cd-NaI (17.5 %) sorbent at constant temperatures (275 and 295 °C) in dry and wet gas. Refer to Table 1 in the main article for sample labels. Starred (*) sample thermograms appear in full in main article as well.

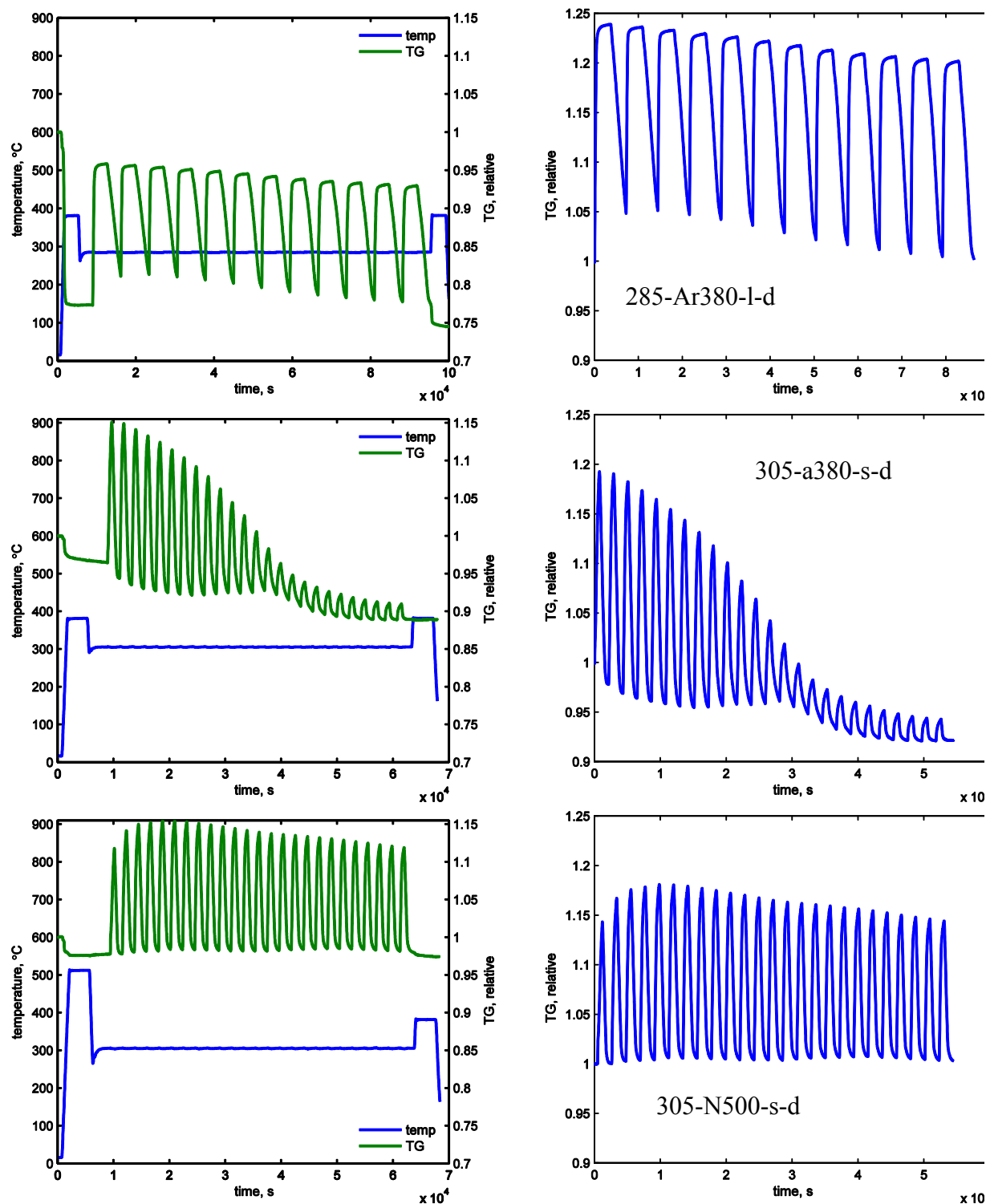
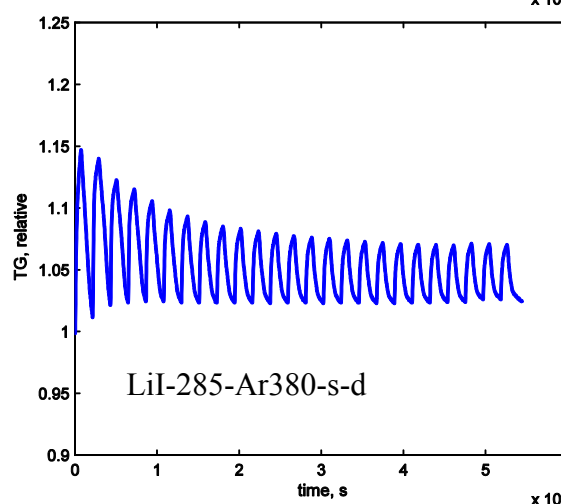
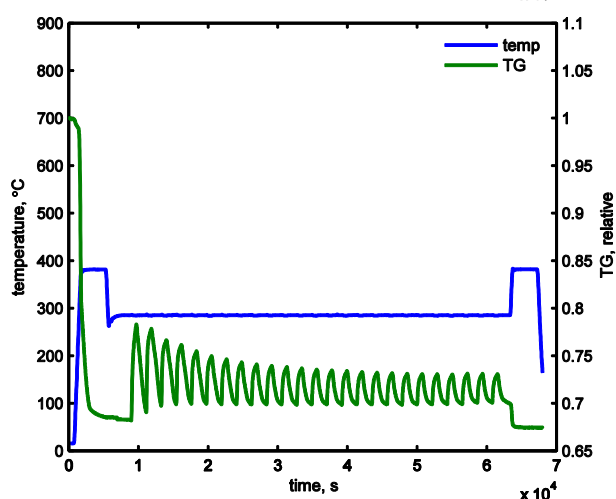
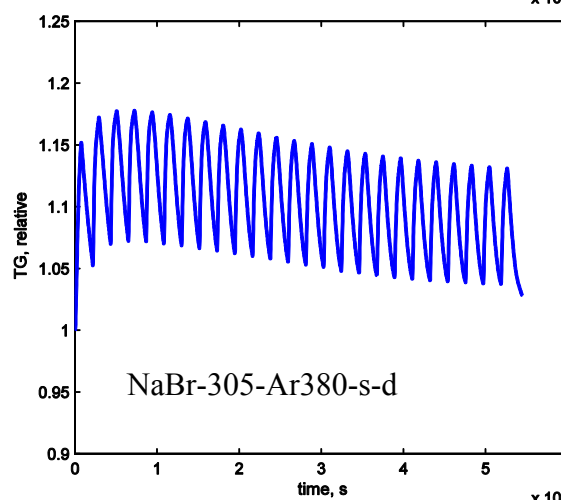
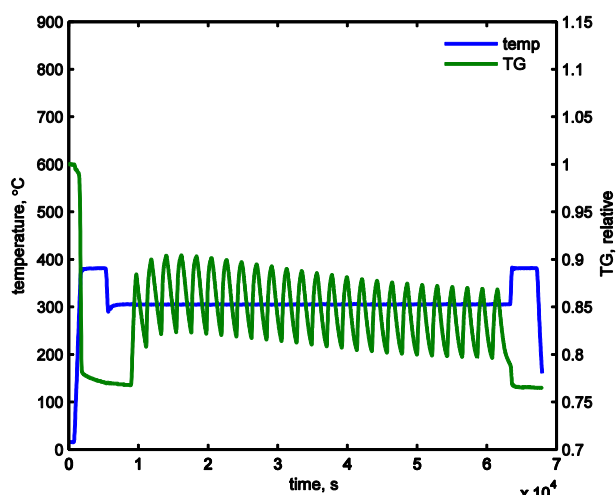
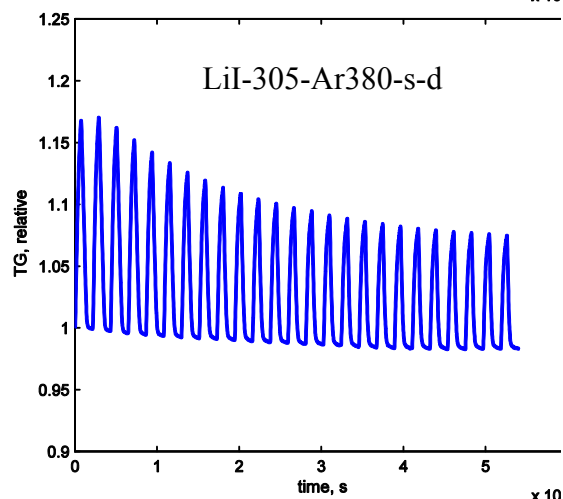
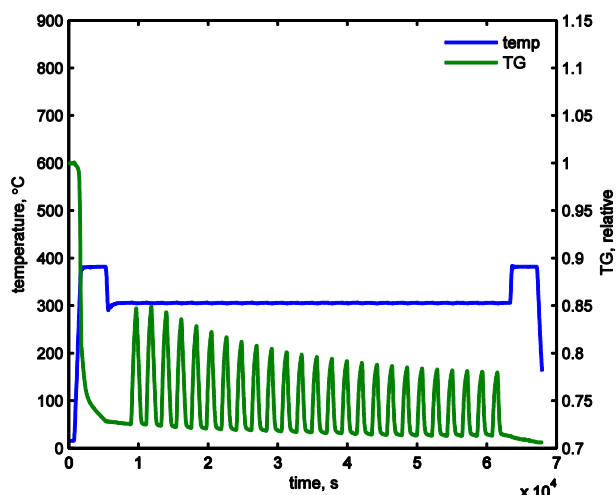
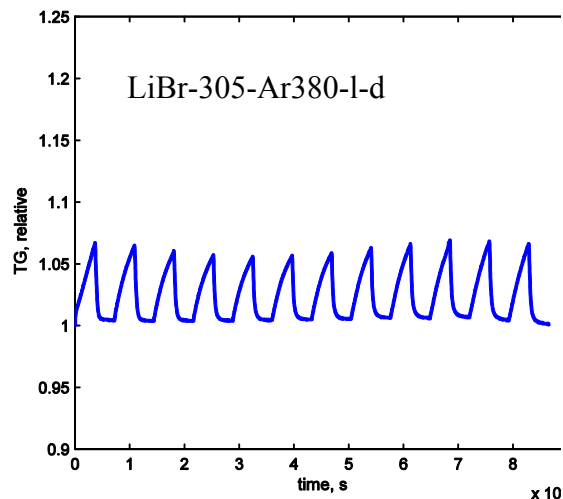
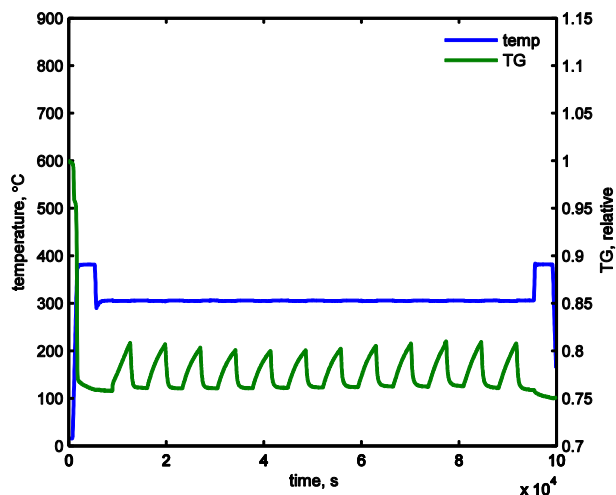


Figure C: Full thermograms (left) and normalised thermograms to 100 % active sorbent (right) of multicyclic sorption-desorption of Cd-NaI (17.5 %) sorbent at constant temperatures (275 and 295 °C) in dry gas, comparing different pre-treatments, as well as short and long cycles. Refer to Table 1 in the main article for sample labels.



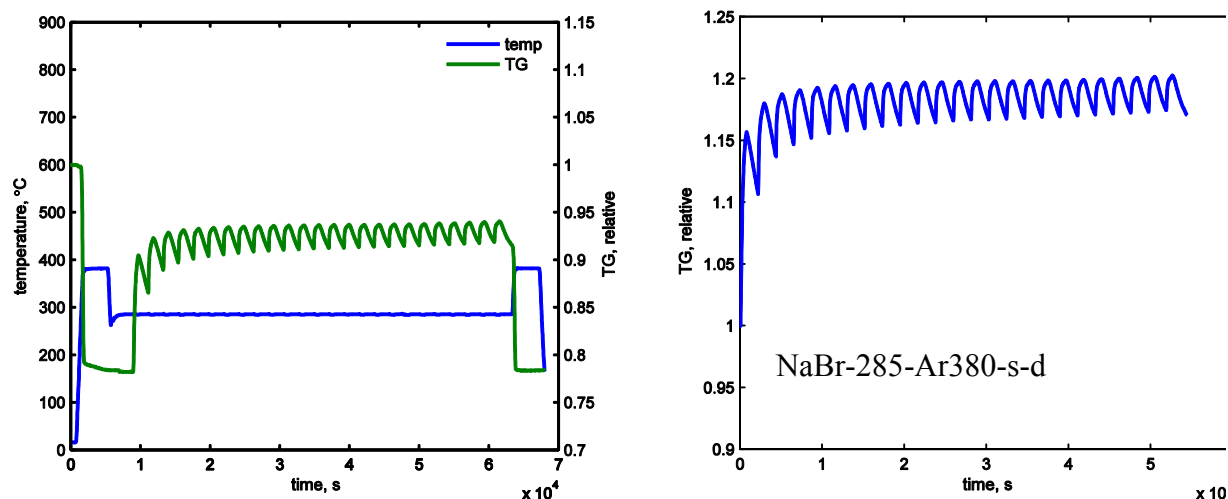
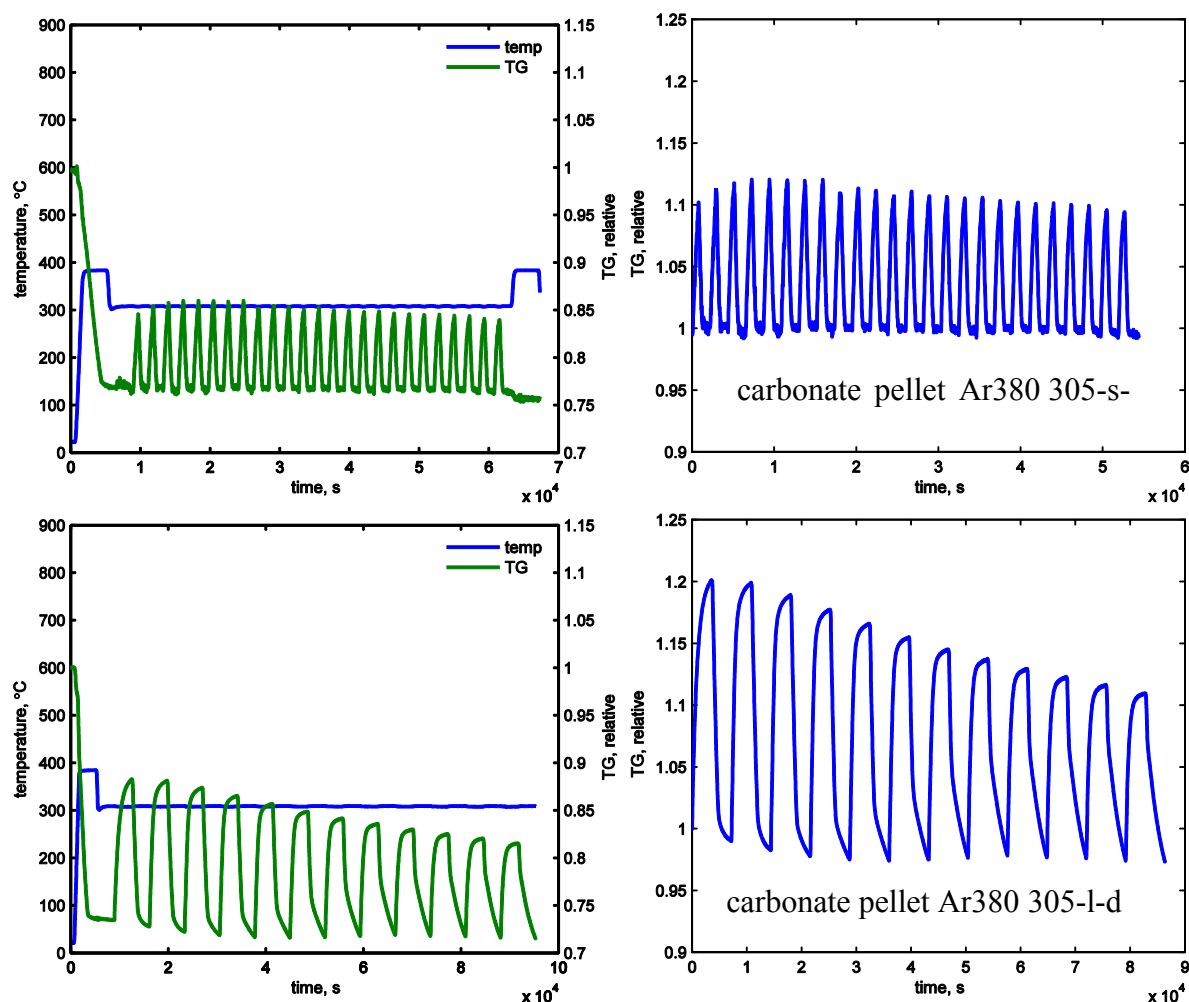
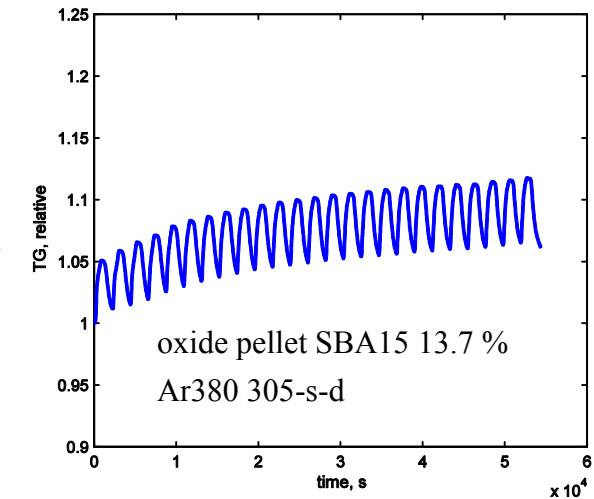
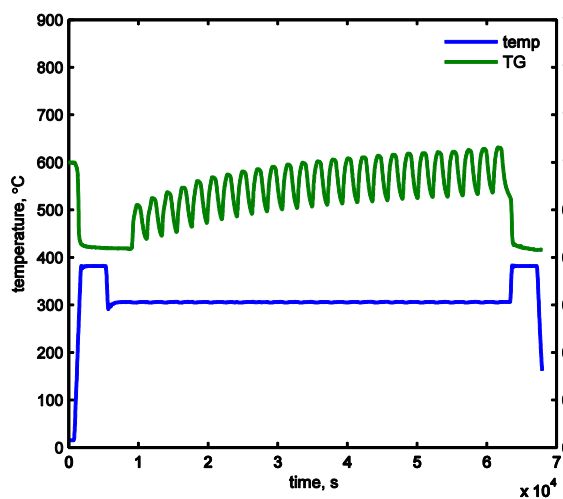
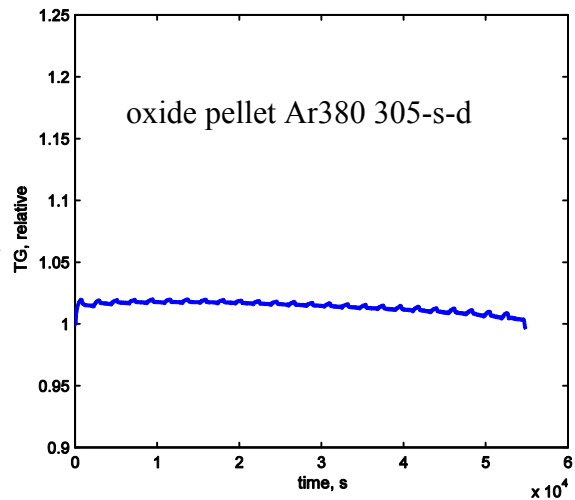
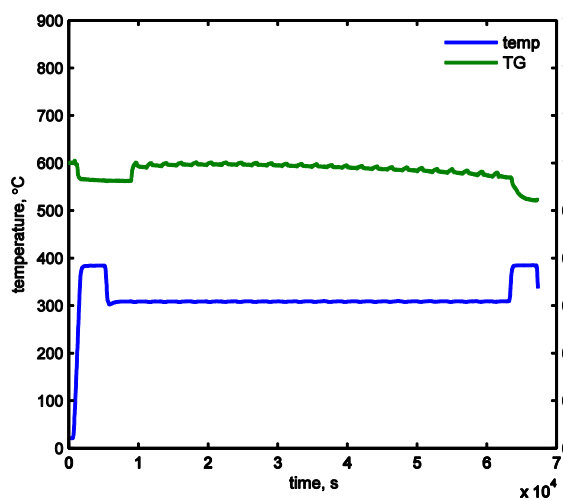
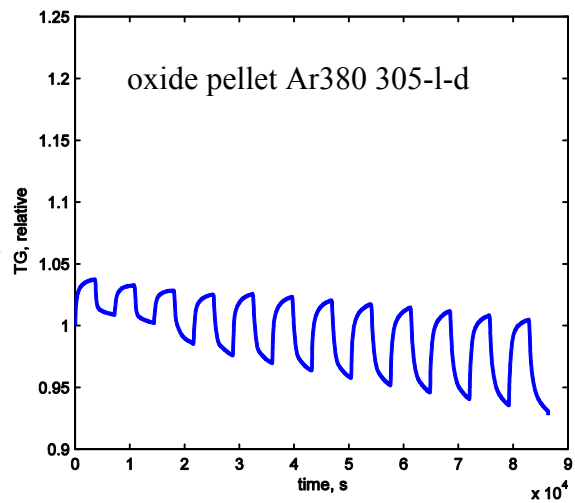
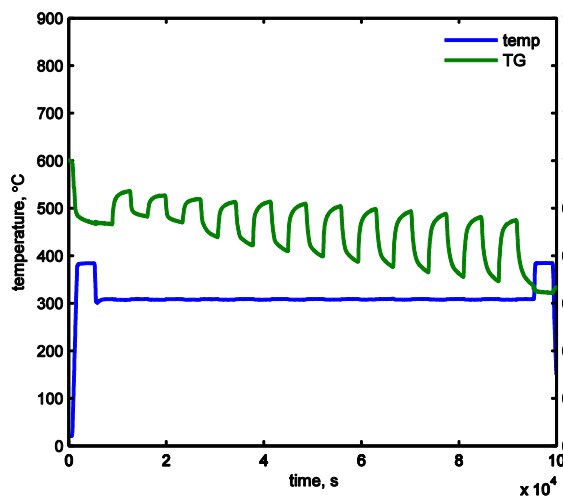


Figure D: Full thermograms (left) and normalised thermograms to 100 % active sorbent (right) of multicyclic sorption-desorption of Cd sorbent with different alkali promoters at constant temperatures (275 and 295 °C) in dry gas, comparing short and long cycles. Refer to Table 1 in the main article for sample labels.





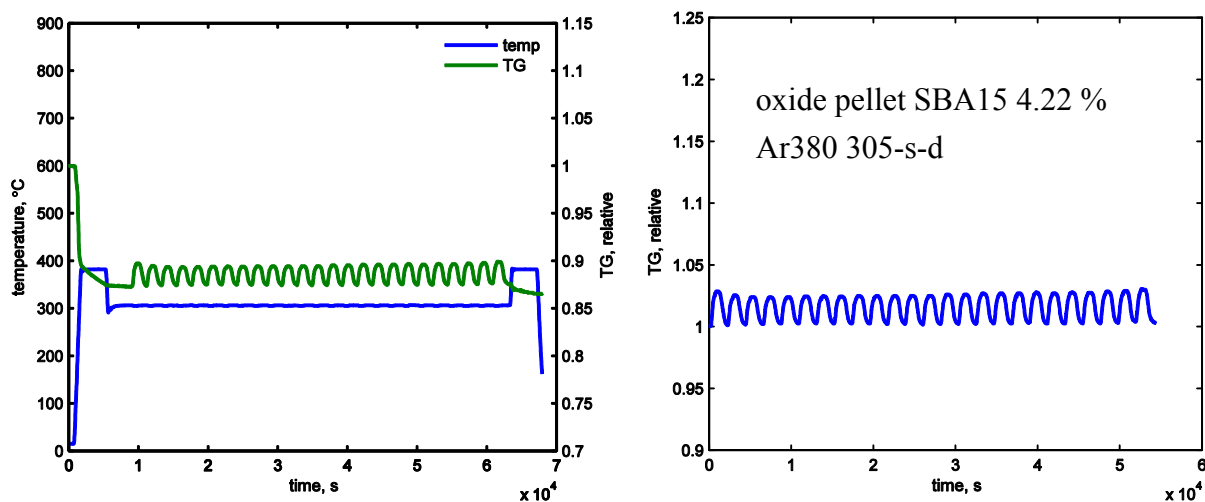


Figure E: Full thermograms (left) and normalised thermograms to 100 % active sorbent (right) of multicyclic sorption-desorption of pelletised Cd-17.5 % NaI sorbent at constant temperature (295 °C) in dry gas, comparing short and long cycles. Refer to Table 1 in the main article for sample labels.

3 Le Bail fit of the powder XRD data

3.1 Results

The unit cell sized obtained by Le Bail refinement are given in Table A.

Table A: Results of the Le Bail refinement of the synchrotron XRD data (refer Figure 6) for cadmium oxide and carbonate

sample	phase	unit cell lengths a = b	unit cell length c	space group
decarbonated cycle #3	CdO	4.7121 Å	= a	Fm-3m
carbonated cycle #3	CdO	4.7125 Å	= a	Fm-3m
PDF 4+ 2011 entry 04-001-3770	CdO	4.6951 Å	= a	Fm-3m
carbonated cycle #3	CdCO ₃	4.9207 Å	16.4269 Å	R-3c
PDF 4+ 2011 entry 04-014-4823	CdCO ₃	4.9207 Å	16.2968 Å	R-3c

3.2 Statistics

The statistical values of the Le Bail fits performed in the paper are given in Table B.

Table B: Statistics of the Le Bail fits

sample	reference	reference in supplement	wRp	Rp	χ^2
LaB ₆ standard	text/paper	Figure E	0.0396	0.0332	3.337
17.5 % NaI decarb.	Table A	Figure F	0.0882	0.0544	13.80
carbonated cycle #3	Table A	Figure G	0.1042	0.0608	21.14

3.3 Le Bail fit graphs

The graphs of the Le Bail refinements of the powder XRD data are given in the figures below. The black crosses denote the observed, the red line the refined data. The background is plotted green; blue denotes the difference between calculated and observed. The difference graph is offset below the other graphs.

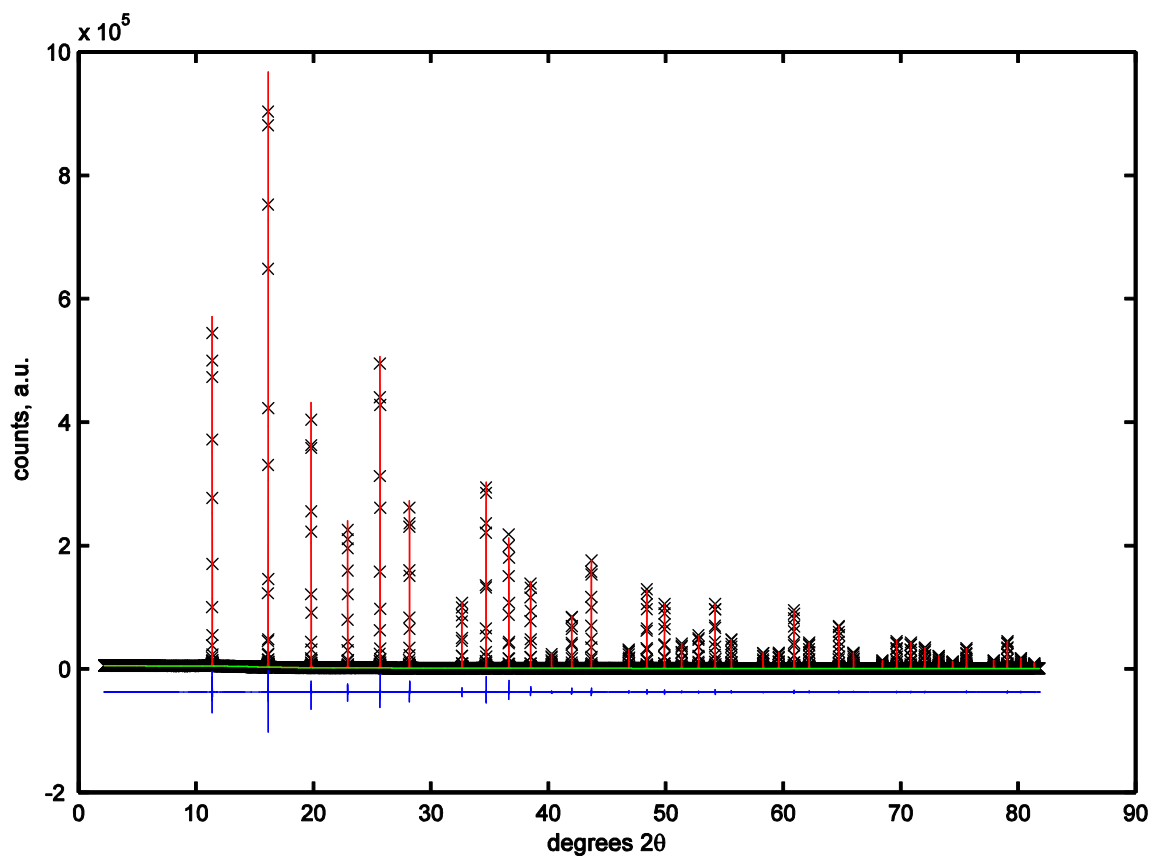


Figure F: Le Bail refinement plot of LaB₆ standard, synchrotron

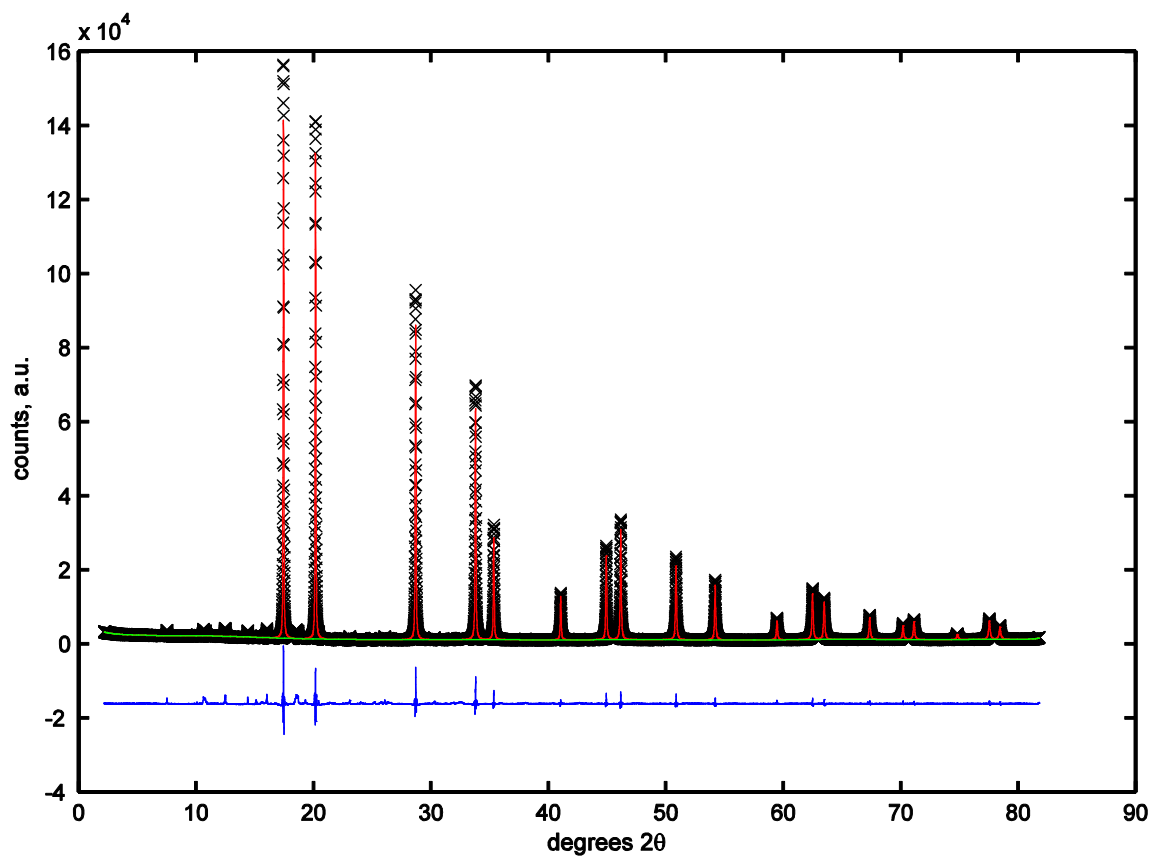


Figure G: Le Bail refinement plot of 17.5 % NaI sample, decarbonated in situ in 3rd cycle, synchrotron

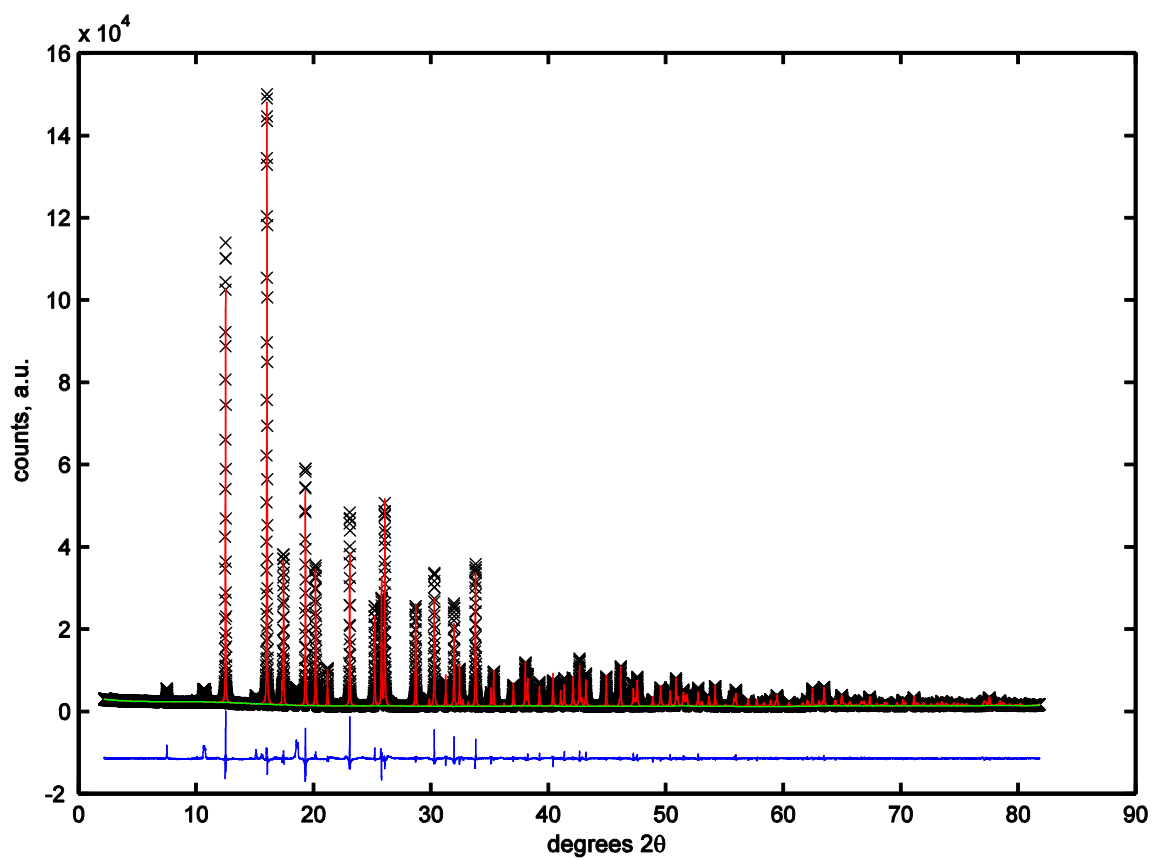


Figure H: Le Bail refinement plot of 17.5 % NaI sample, carbonated in situ in 3rd cycle, synchrotron