Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Manuscript title:

Ca-Tetrafluorophthalate and Sr-Isophthalate: Mechanochemical Synthesis and Characterization in Comparison with other Ca-and Sr-Coordination Polymers.

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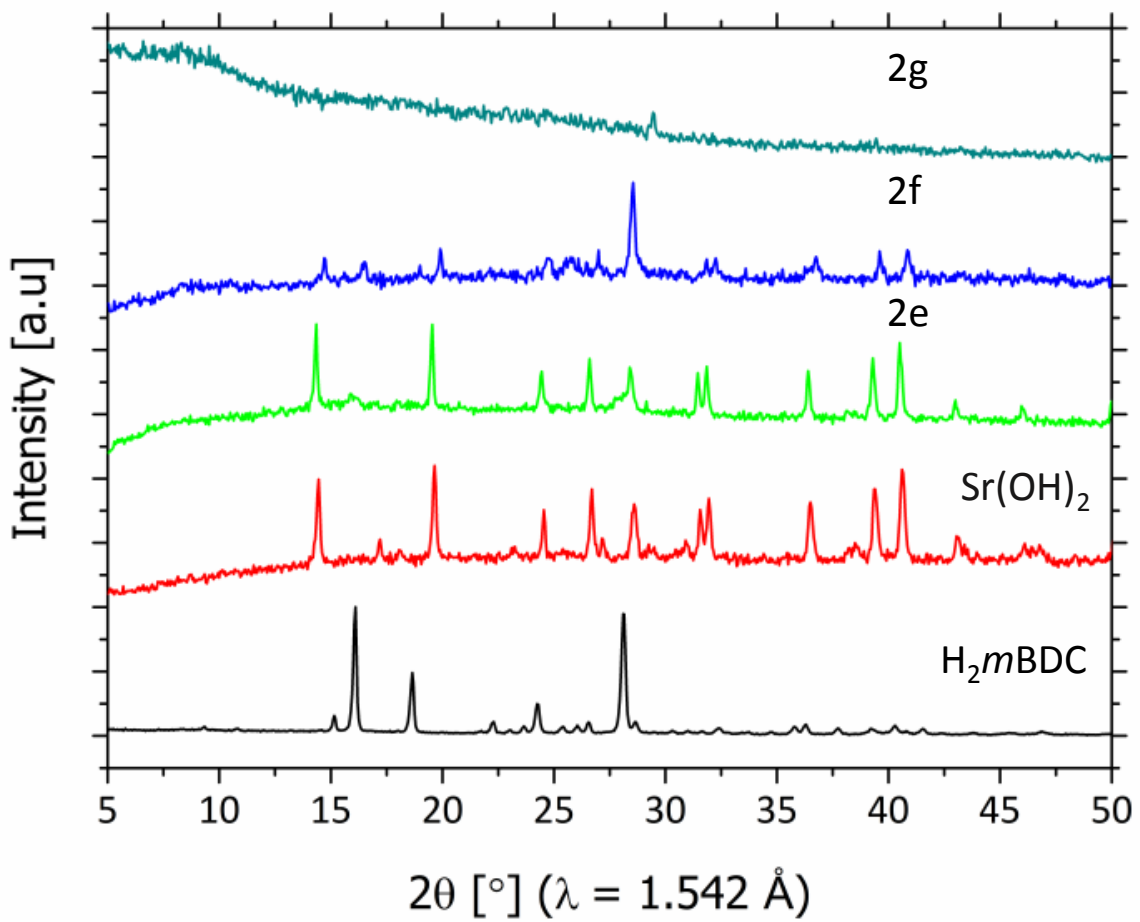
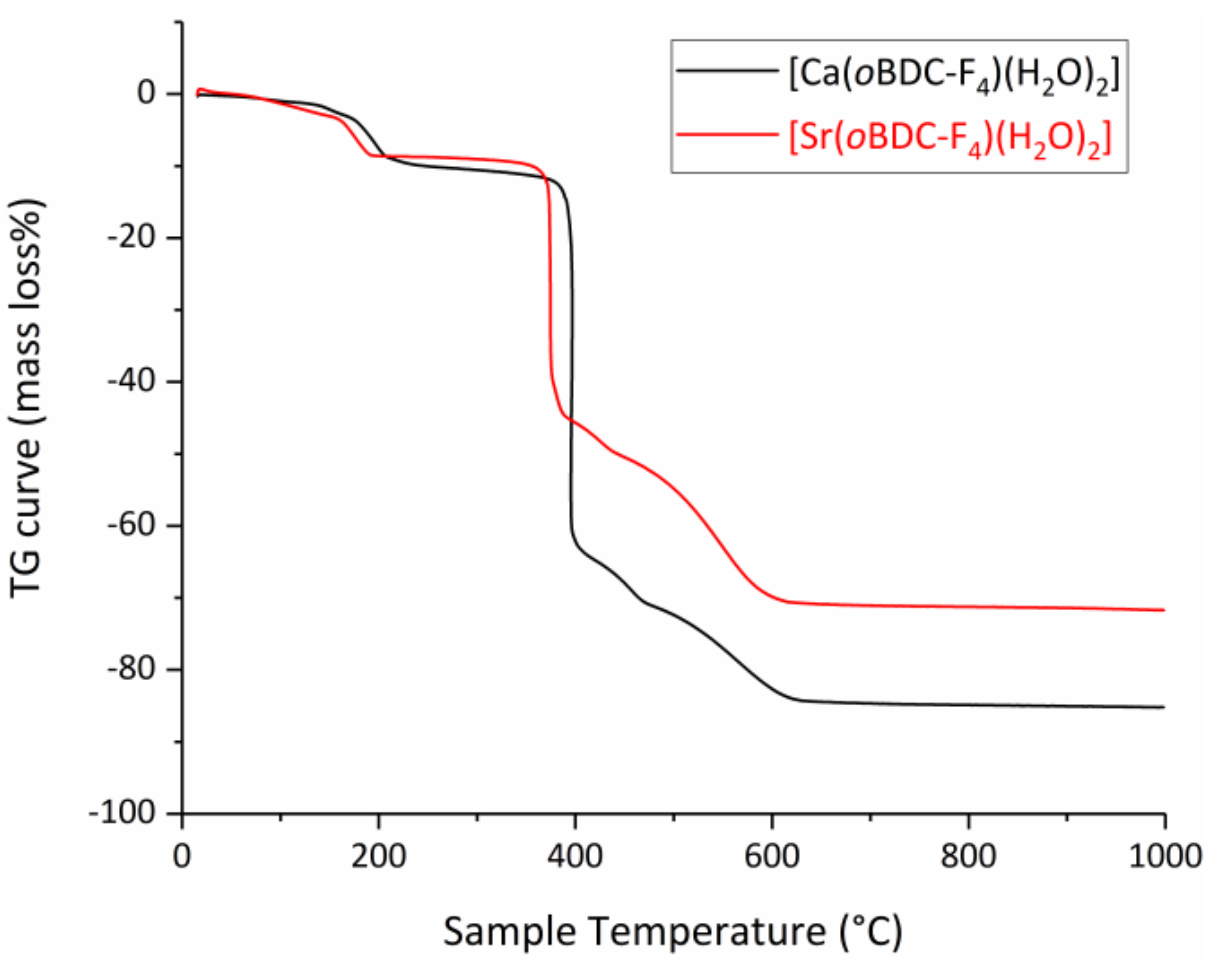
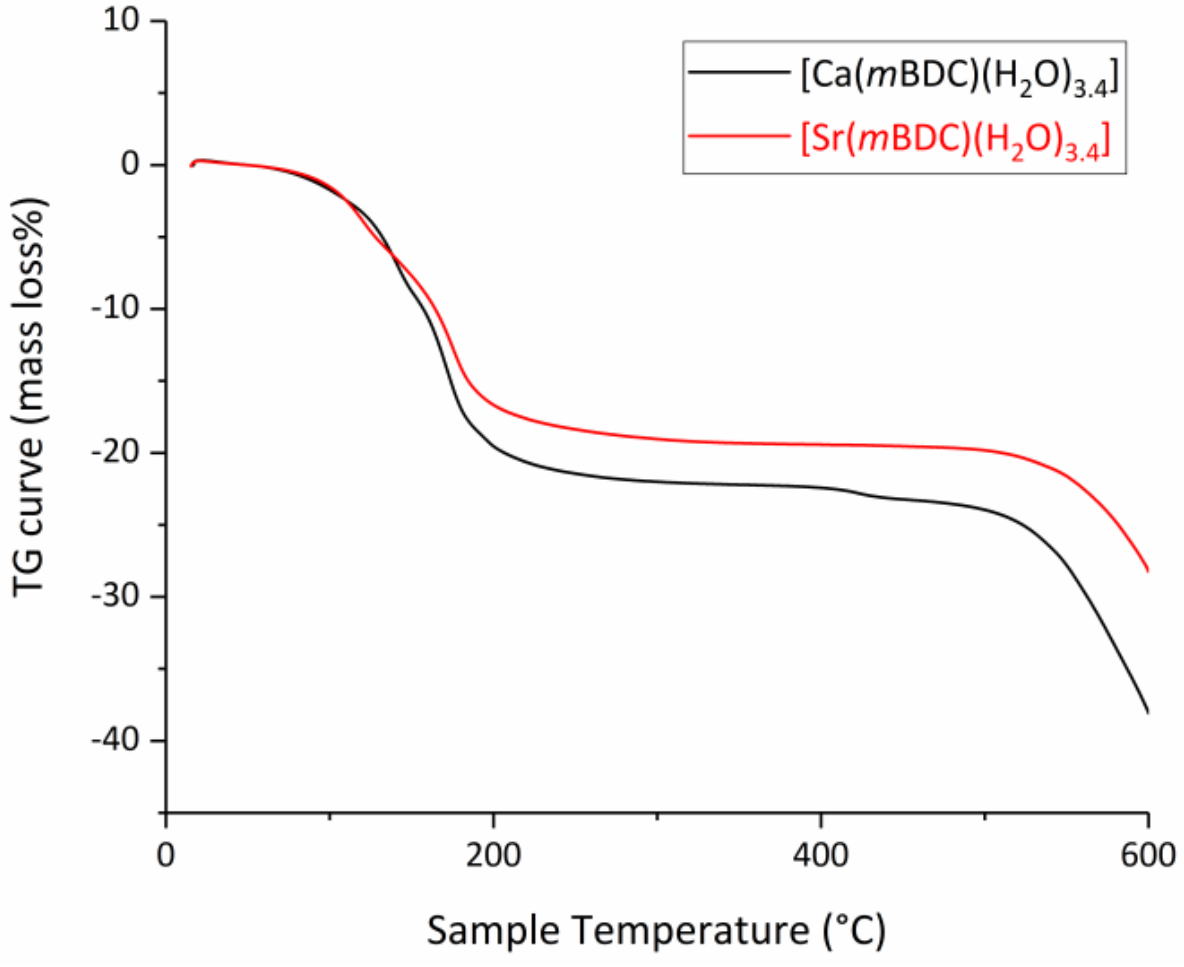


Figure S1. PXRD patterns of the reactants H_2*m*BDC (black PXRD pattern) and $Sr(OH)_2$ (red PXRD pattern). Product 2e (green PXRD pattern) obtained by milling $Sr(OH)_2$ + 130 µl H_2O and H_2*m*BDC for 15 min with an applied molar ratio 1:1. Product 2f (blue PXRD pattern) obtained by milling $Sr(OH)_2$ + 130 µl H_2O and H_2*m*BDC for 1h with an applied molar ratio 1:1. Product 2g (cyan PXRD pattern) obtained by milling $Sr(OH)_2$ and H_2*m*BDC for 4h with an applied molar ratio 1:1.

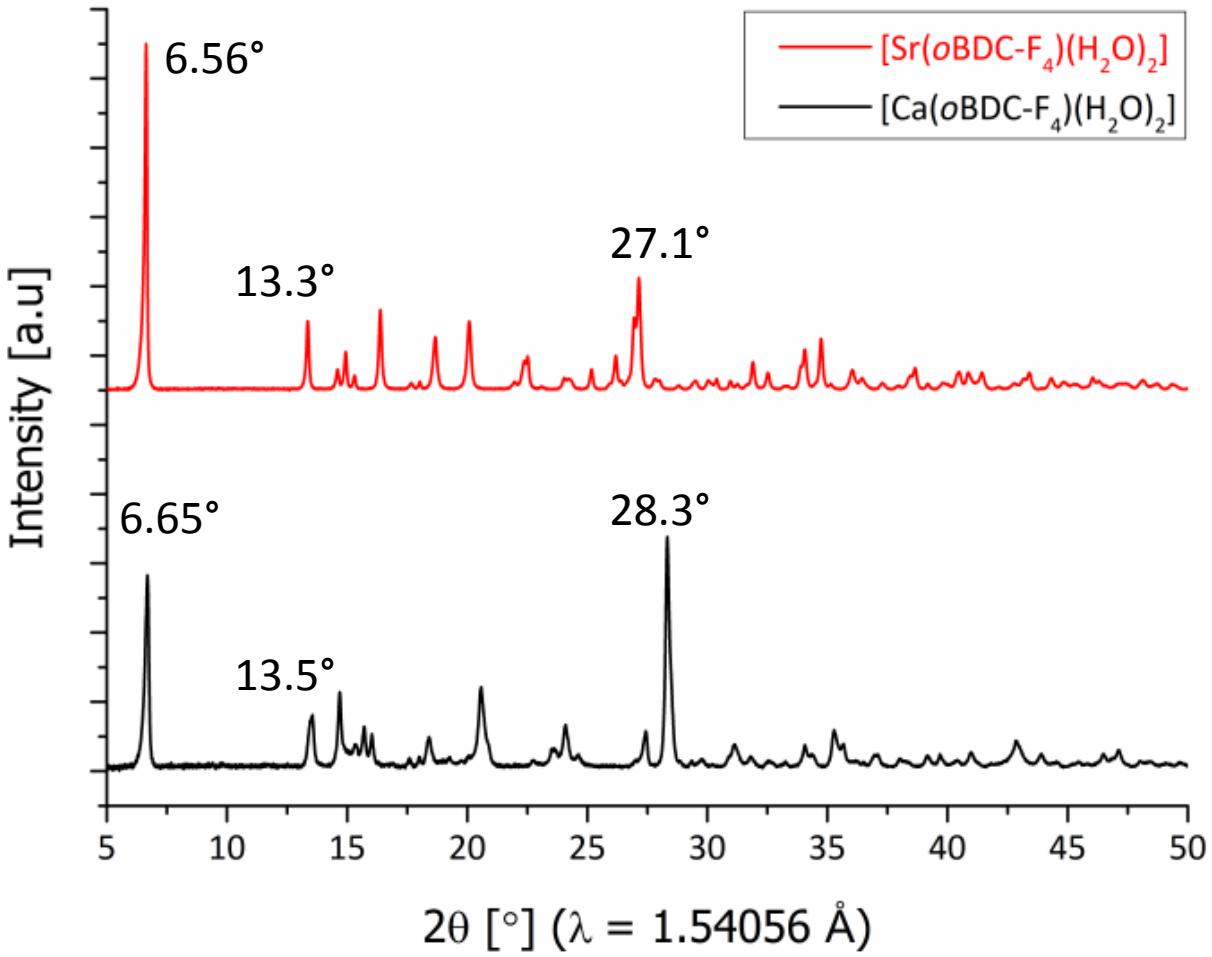


a



b

Figure S2. TG Curves for (a) [Ca(*o*BDC-F_4)(H_2O)$_2$] (**1**) (black curve) and [Sr(*o*BDC-F_4)(H_2O)$_2$] (red curve). (b) [Sr(*m*BDC)(H_2O)$_{3.4}$] (**2**) (red curve) and [Ca(*m*BDC)(H_2O)$_{3.4}$] (black curve).



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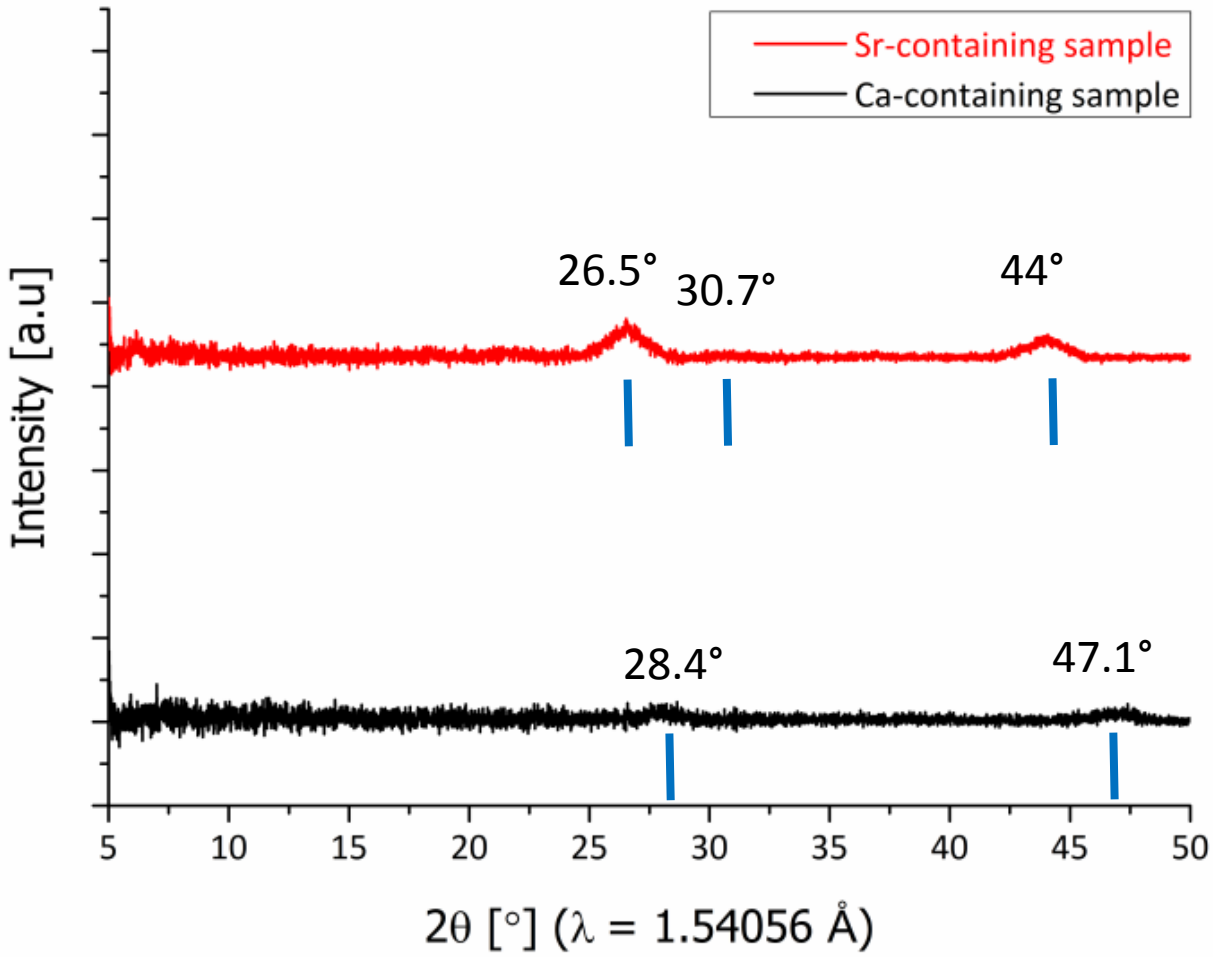
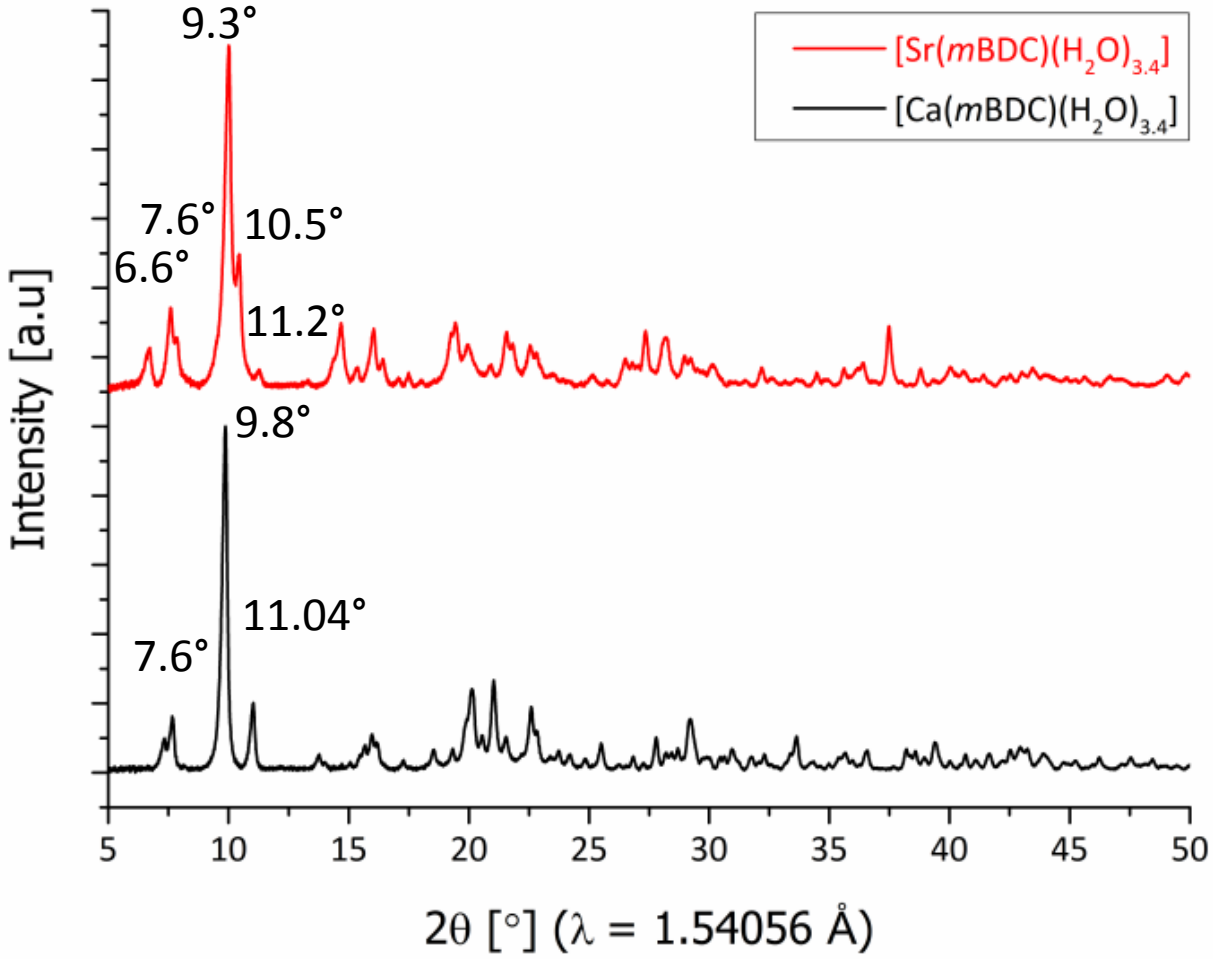
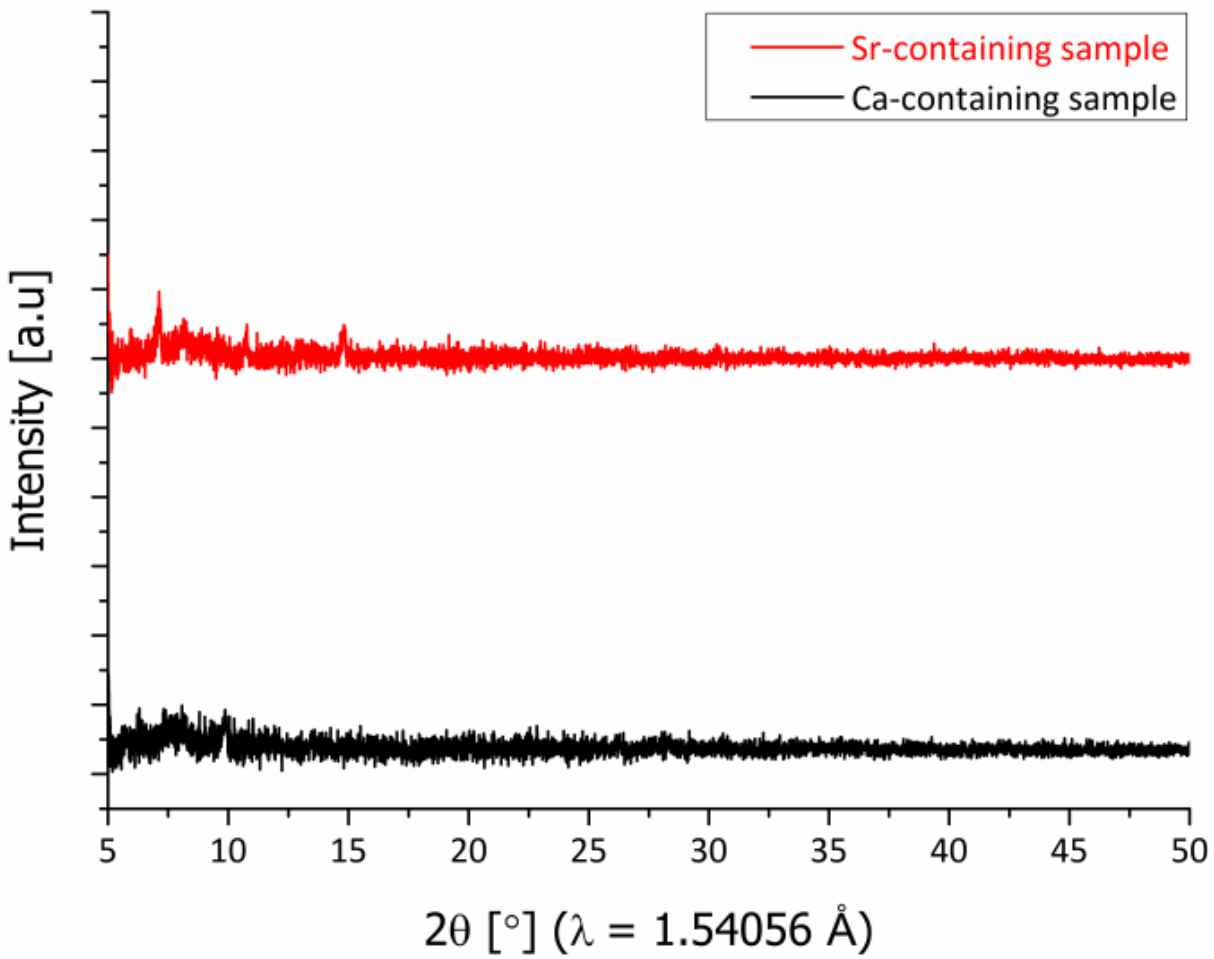


b

Figure S3. PXRD patterns of [Ca(*o*BDC-F_4)(H_2O)$_2$] (**1**) (black PXRD pattern) and [Sr(*o*BDC-F_4)(H_2O)$_2$] (red PXRD pattern). (a) samples as-synthesized. (b) Samples after decompositions compared to the standard X-ray lines for CaF_2 from the 00-075-0097 card and SrF_2 from the 00-001-0644 card (blue vertical lines).

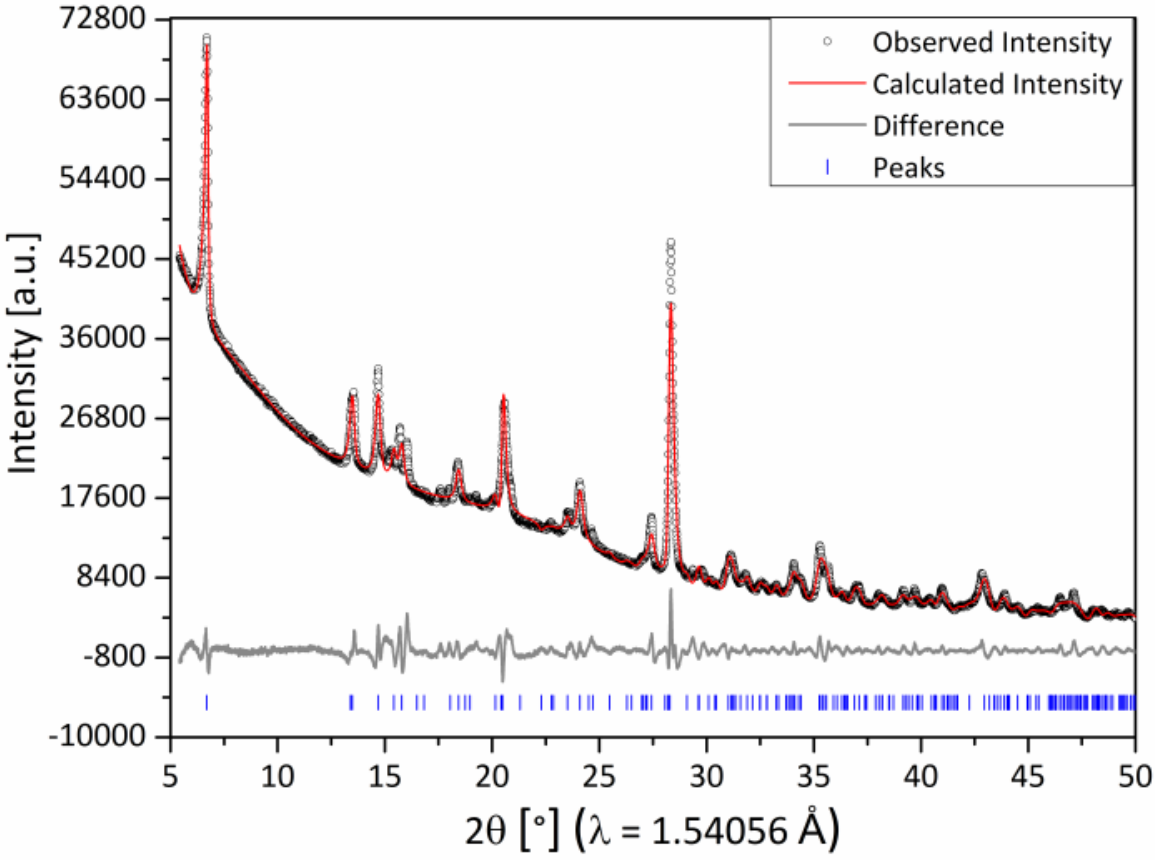


a



b

Figure S4. PXRD patterns for [Ca(*m*BDC)(H_2O)$_{3.4}$] (black PXRD pattern) and [Sr(*m*BDC)(H_2O)$_{3.4}$] (**2**) (red PXRD pattern). (a) samples as-synthesized. (b) samples after thermal post-treatments.



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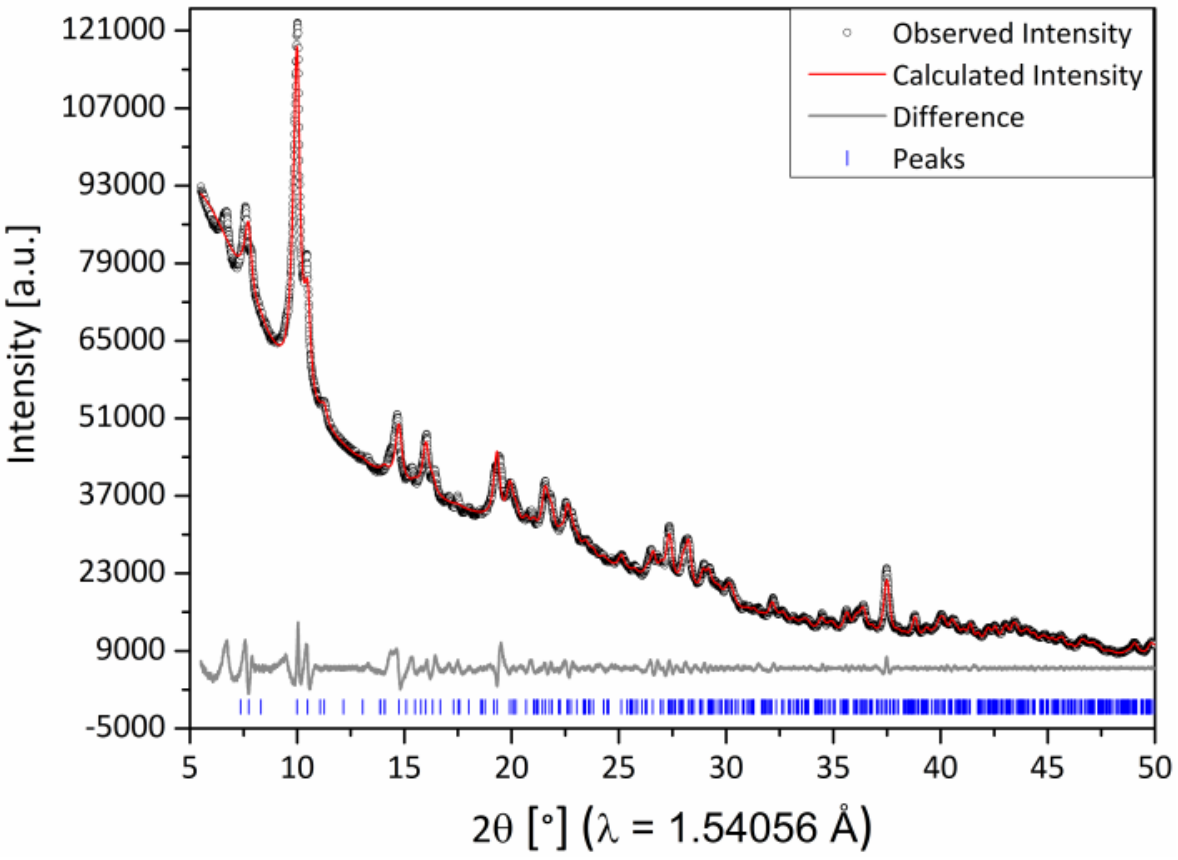
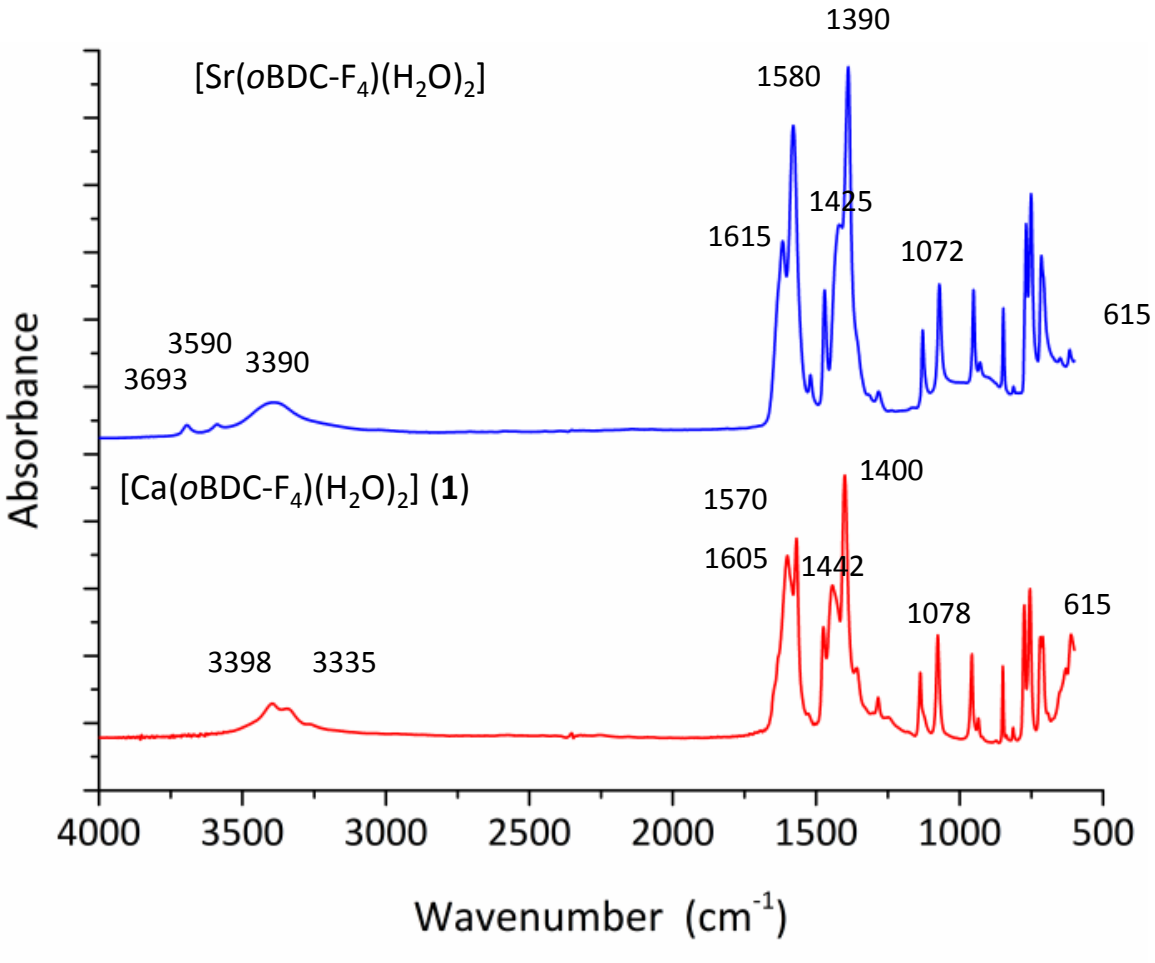


b

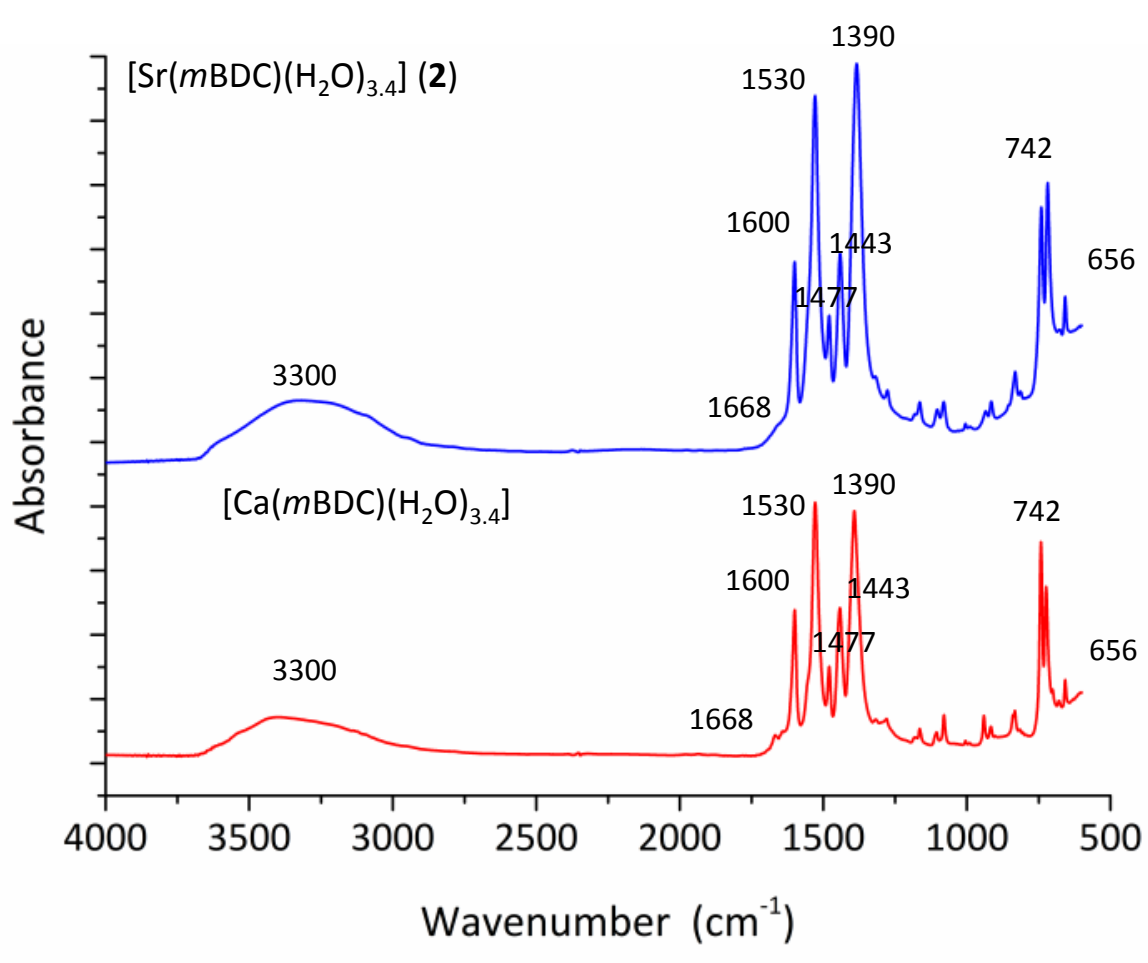
Figure S5. *LeBail* refinements for the PXRD patterns. (**a**) [Ca(*o*BDC-F_4)$(H_2O)_2$] (**1**)**.** (**b**) [Sr(*m*BDC)$(H_2O)_{3.4}$] (**2**). The refined parameters and R-values are given in Table S1.

Table S1. crystal lattice parameters and refinement data for [Ca(*o*BDC-F_4)(H_2O)$_2$] (**1**) compared to [Sr(*o*BDC-F_4)(H_2O)$_2$] and [Sr(*m*BDC)(H_2O)$_{3.4}$] (**2**) compared to [Ca(*m*BDC)(H_2O)$_{3.4}$]. The derived lattice parameters of compounds **1** and **2** are based on the Le Bail refinements of the corresponding PXRD patterns. The given crystal lattices of the analogs are derived from the crystal structures after the Rietveld refinements.

Lattice parameters	[Ca(*o*BDC-F_4)(H_2O)$_2$] (**1**)	[Sr(*o*BDC-F_4)(H_2O)$_2$] (**Ref. 39**)	[Ca(*m*BDC)(H_2O)$_{3.4}$] (**Ref. 40**)	[Sr(*m*BDC)(H_2O)$_{3.4}$] (**2**)
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	P 1 2_1 /c 1 (14)	P 1 2_1 /c 1 (14)	C 1 2/c 1 (15)	C 1 2/c 1 (15)
Cell volume (Å^3)	1056.9(6)	1089.58(12)	5334.1(5)	5316(5)
a (Å)	8.008(3)	8.101(5)	15.5899(7)	15.668(8)
b (Å)	26.410(8)	26.399(12)	21.4477(12)	21.256(14)
c (Å)	6.9712(15)	6.989(4)	17.1872(8)	17.191(7)
β (°)	134.209(15)	133.198(1)	111.848(3)	111.81(3)
λ (Å)	1.54056 (Cu-$K_{\alpha1}$)	1.54056 (Cu-$K_{\alpha1}$)	1.54056 (Cu-$K_{\alpha1}$)	1.54056 (Cu-$K_{\alpha1}$)
R_{wp}	3.96	2.99	2.13	2.33
R_p	2.68	2.08	1.60	1.66
R_{Bragg}	2.522	1.558	0.571	0.081
GOF	4.43	3.64	1.25	3.92

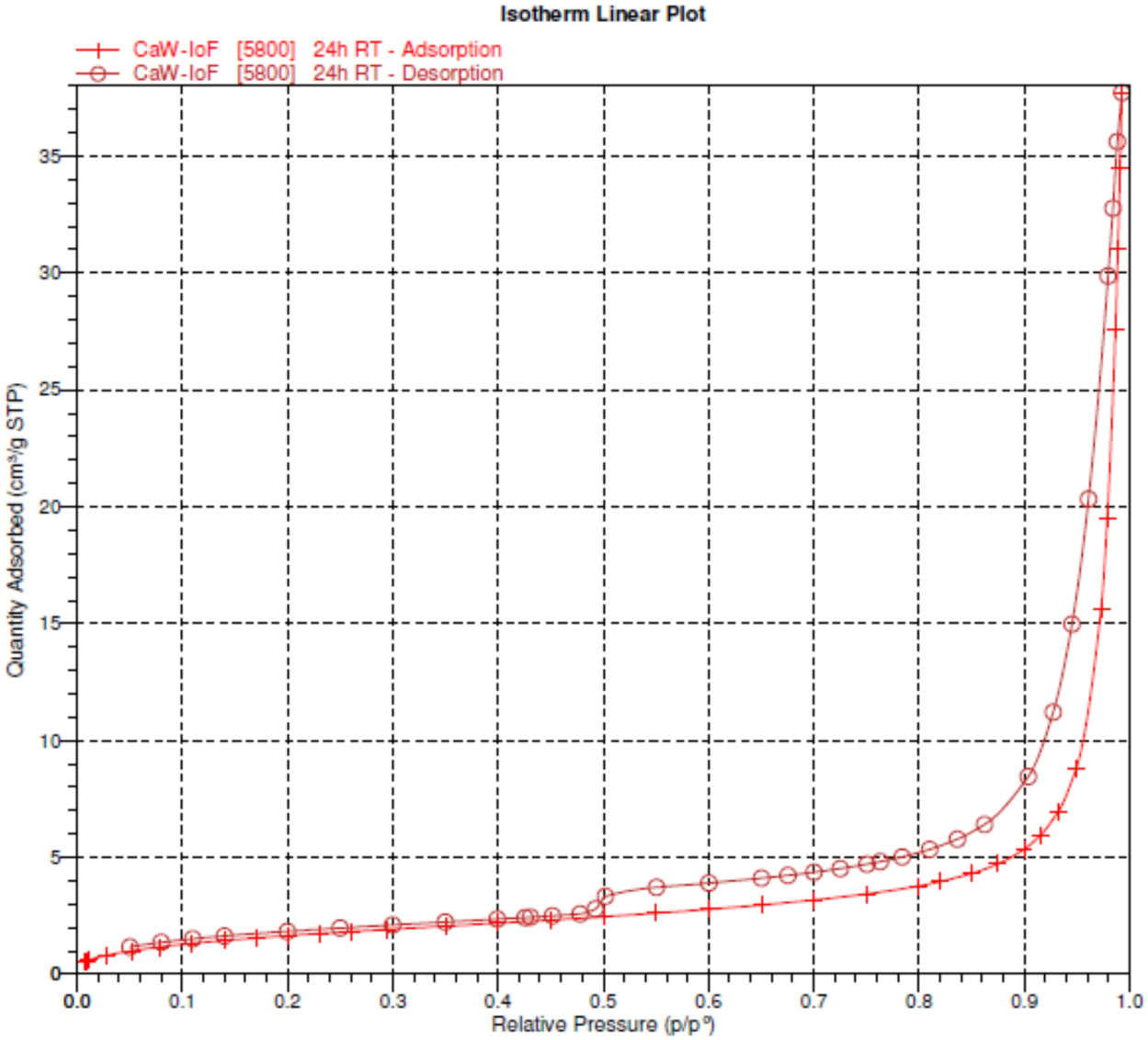


a

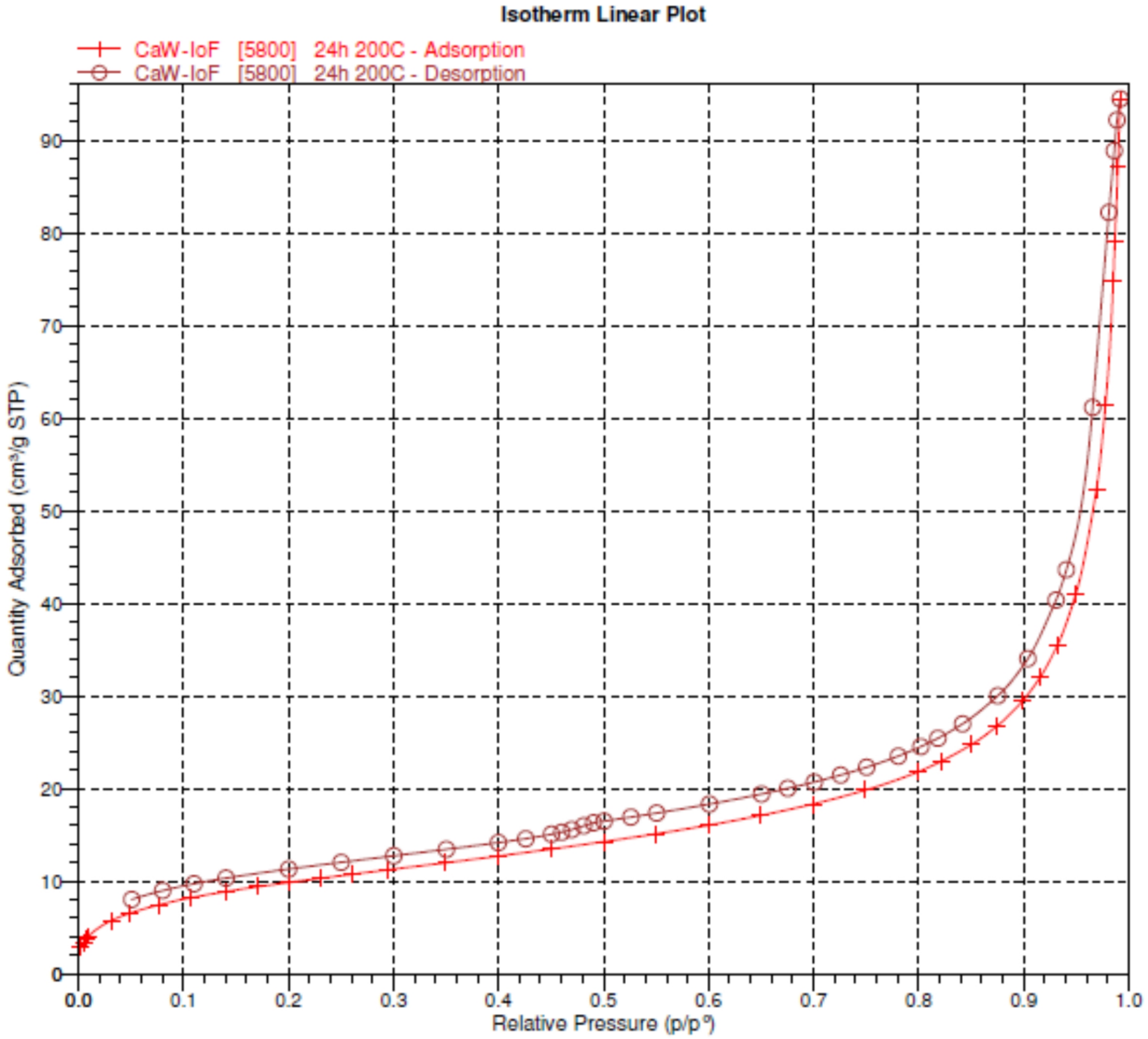


b

Figure S6. The ATR-IR spectra of (**a**) compound **1** (red spectrum) and Sr-containing sample (blue spectrum). (**b**) Ca-containing sample (red spectrum) and compound **2** (blue spectrum).

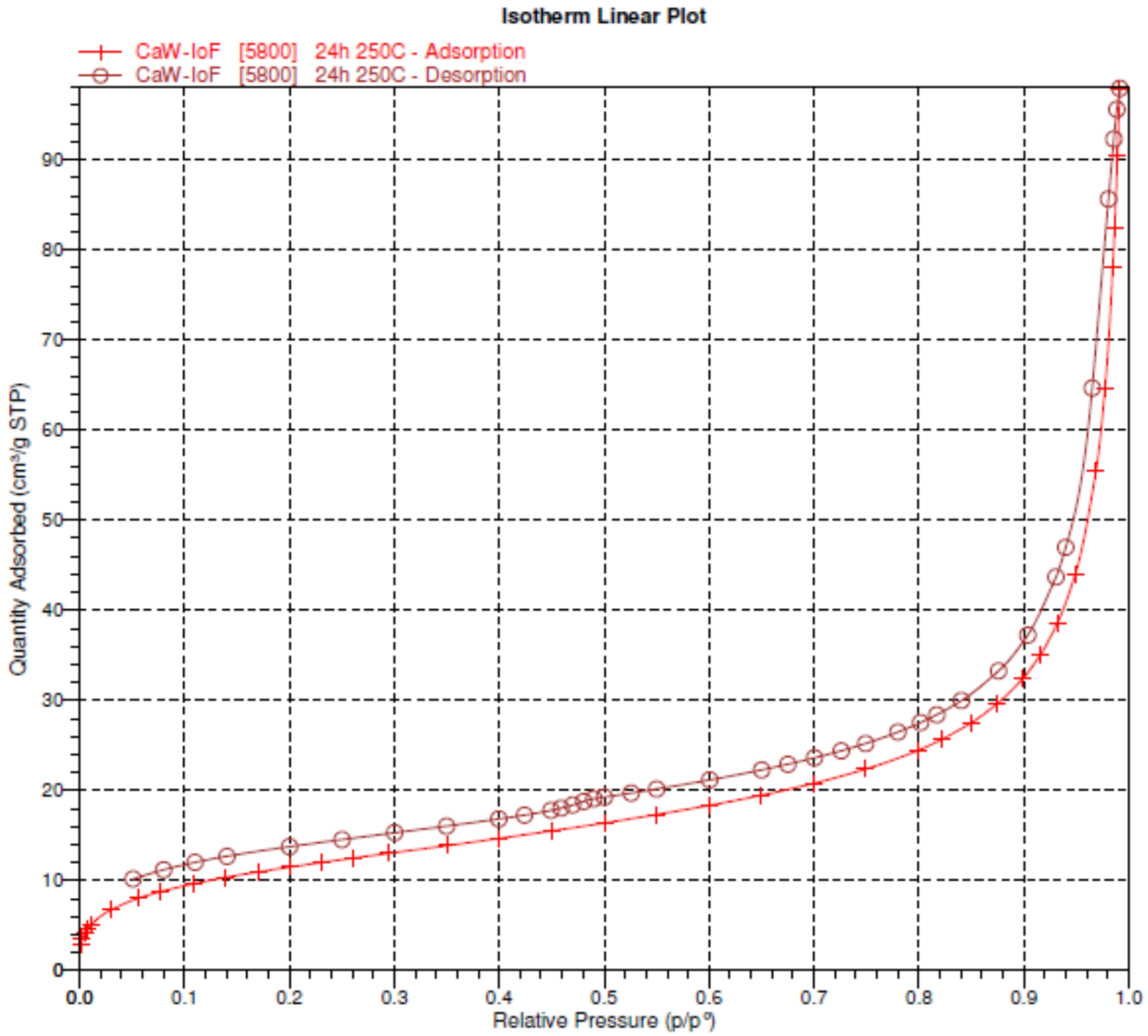


a



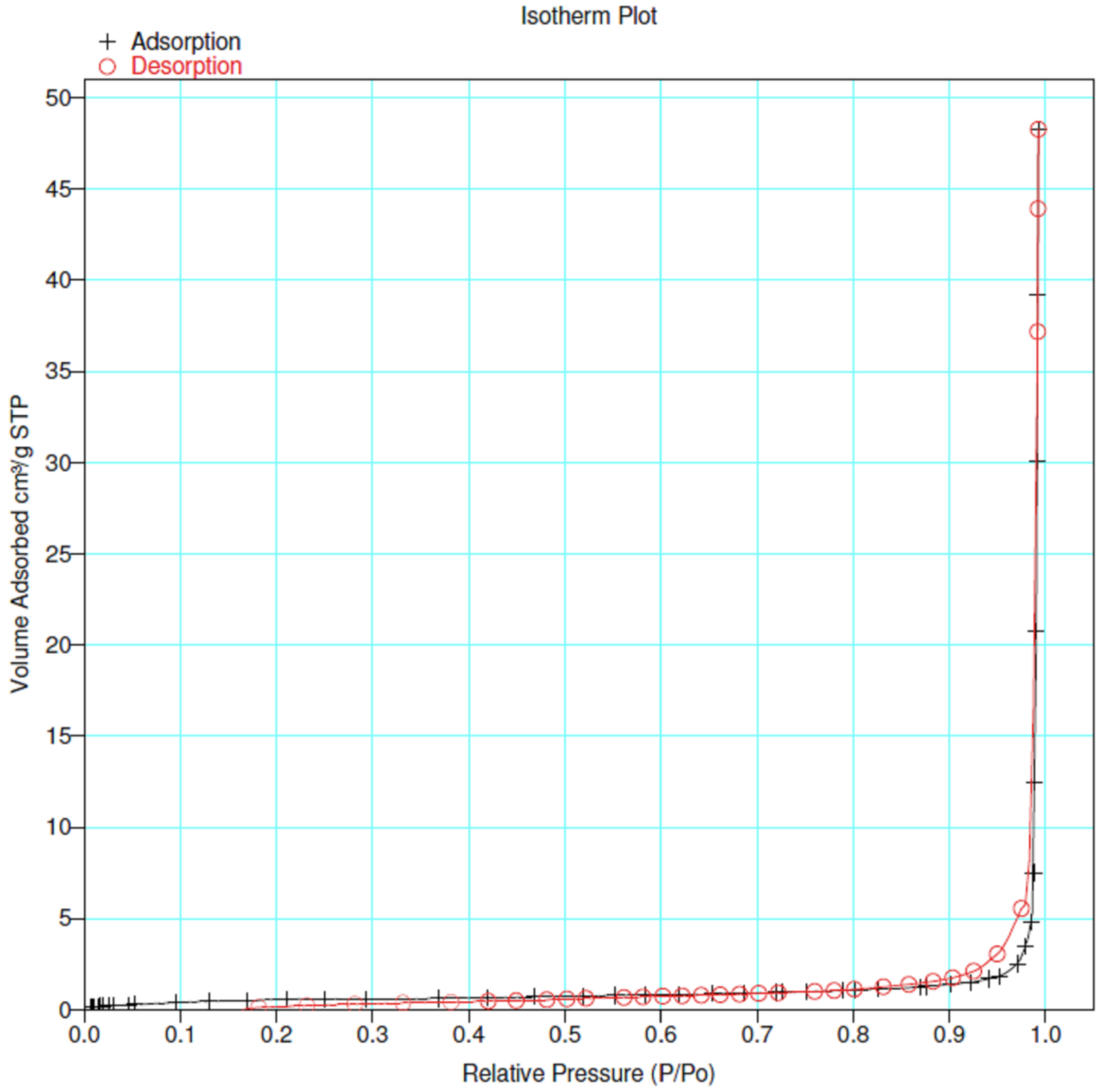
b

Figure S7. Isotherm curves of the compound **1**. Adsorption (crosses) and desorption pore volume (circles) isotherm for nitrogen at room temperature (a), at 200 °C (b), 250 (c).

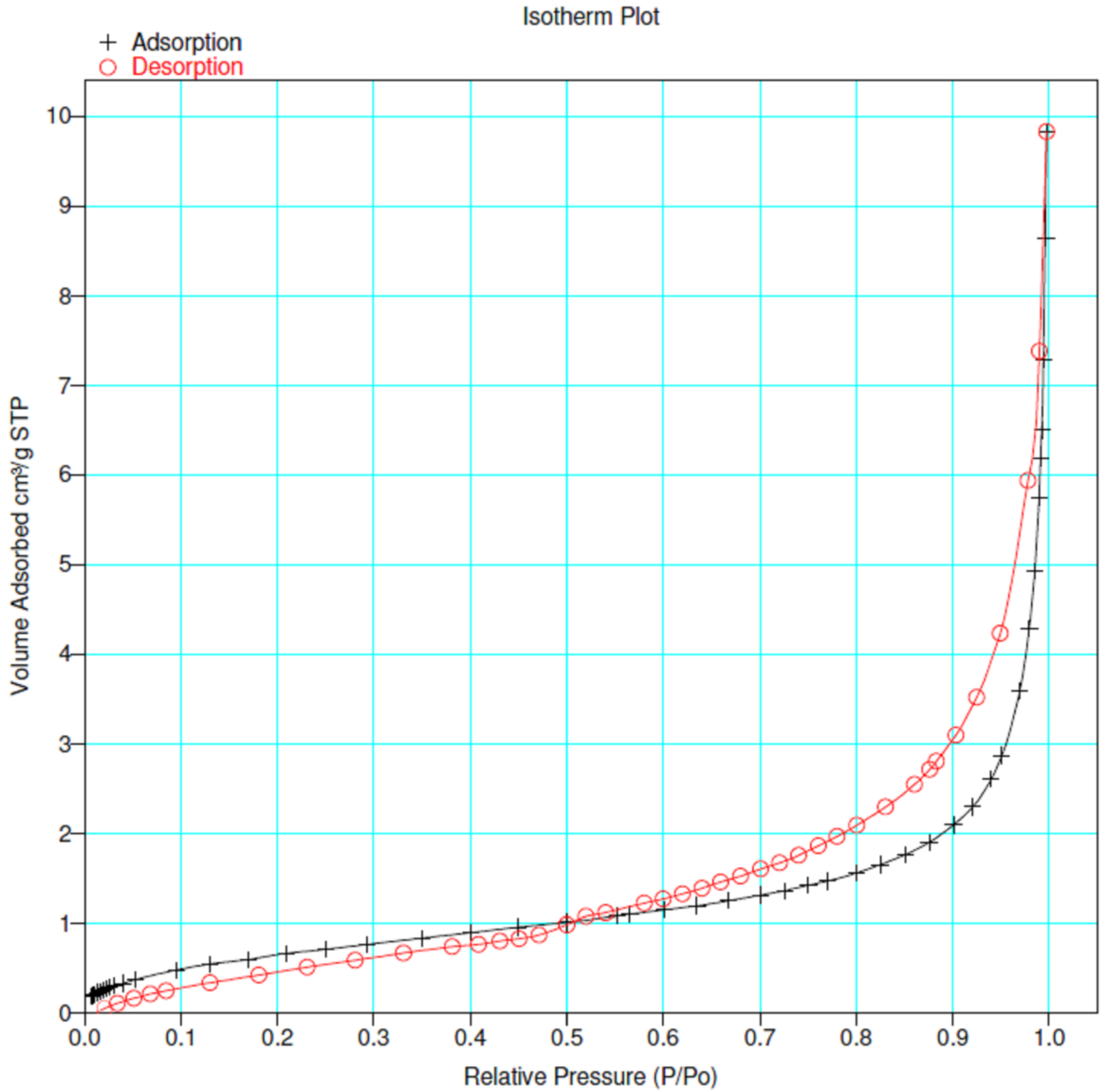


c

Figure S7. Isotherm curves of the compound **1**. Adsorption (crosses) and desorption pore volume (circles) isotherm for nitrogen at room temperature (a), at 200 °C (b), 250 (c).

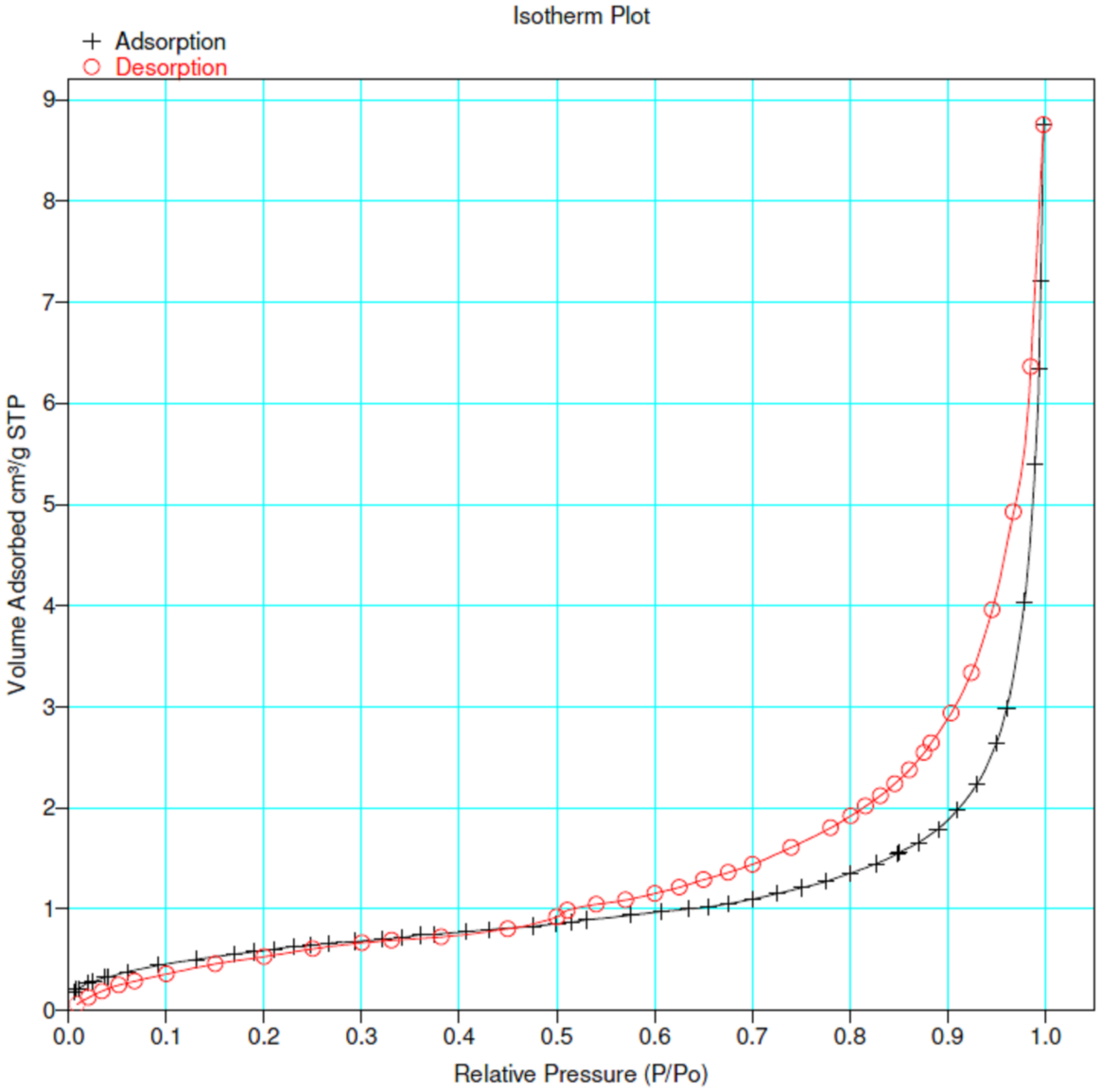


a



b

Figure S8. Isotherm curves of the compound **2**. Adsorption (crosses) and desorption pore volume (circles) isotherm for nitrogen at room temperature (a), at 200 °C (b), 240 (c), 290 °C (d).



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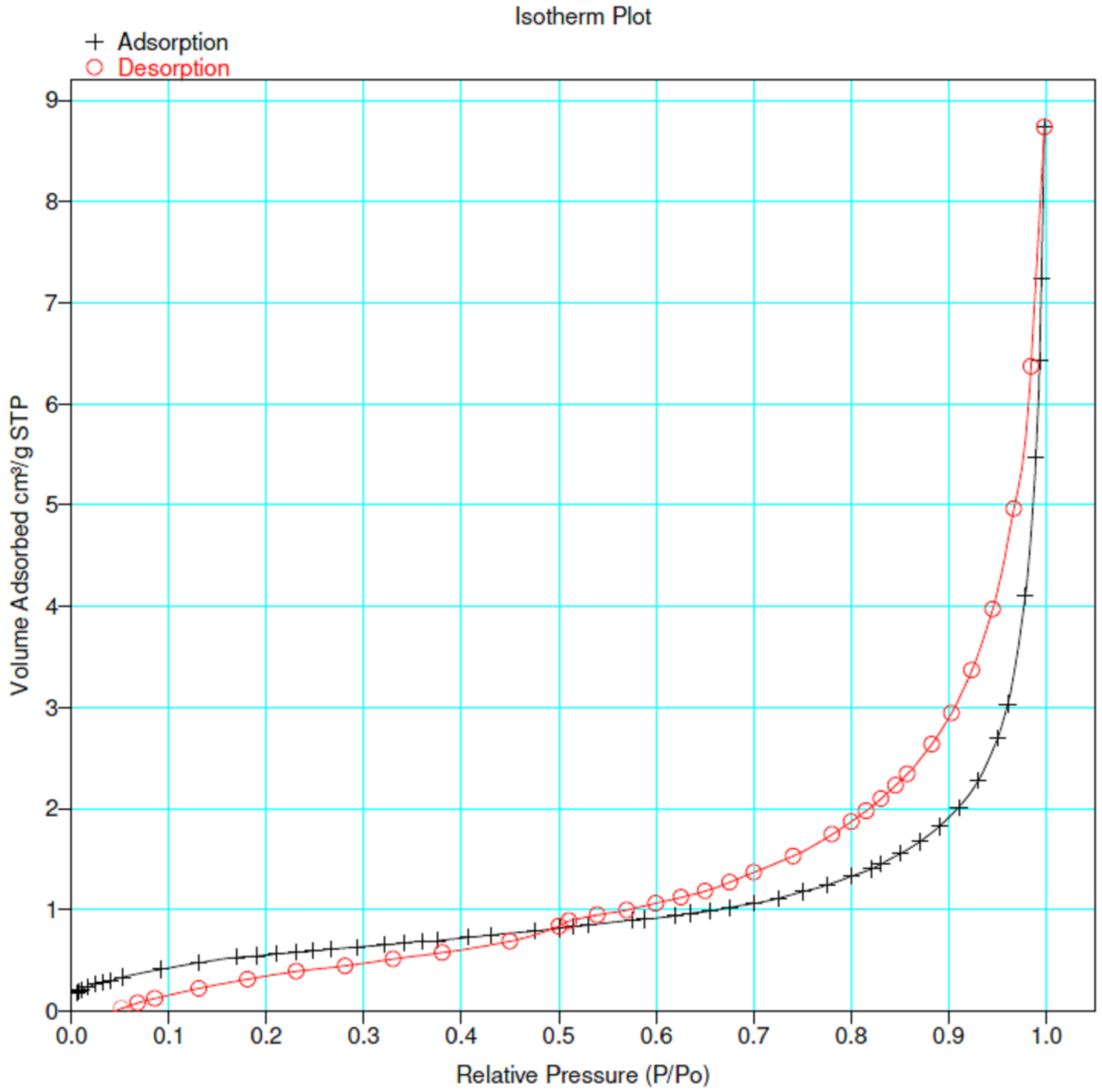

d

Figure S8. Isotherm curves of the compound **2**. Adsorption (crosses) and desorption pore volume (circles) isotherm for nitrogen at room temperature (a), at 200 °C (b), 240 (c), 290 °C (d).

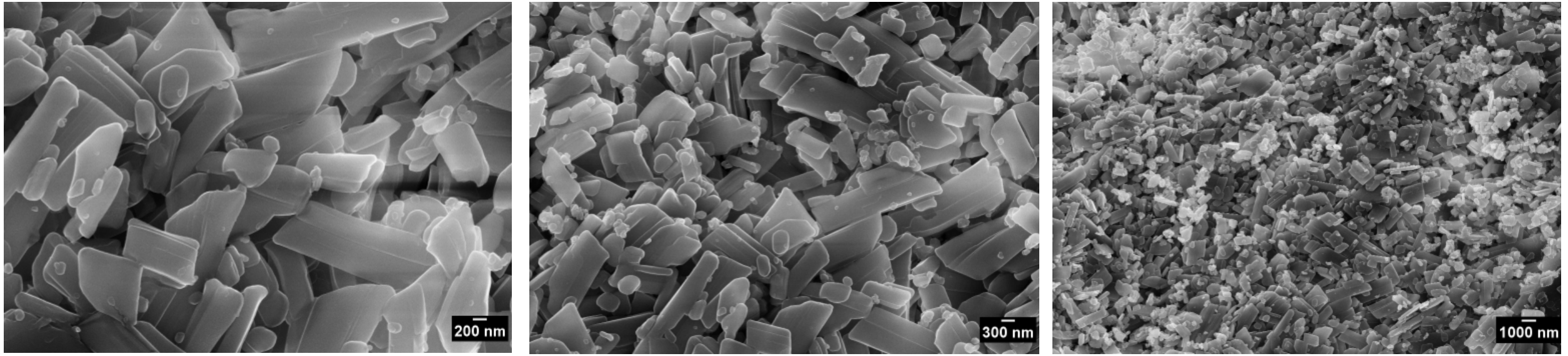

Figure S9. SEM images for [Ca(*o*BDC-F_4)(H_2O)$_2$] (**1**).

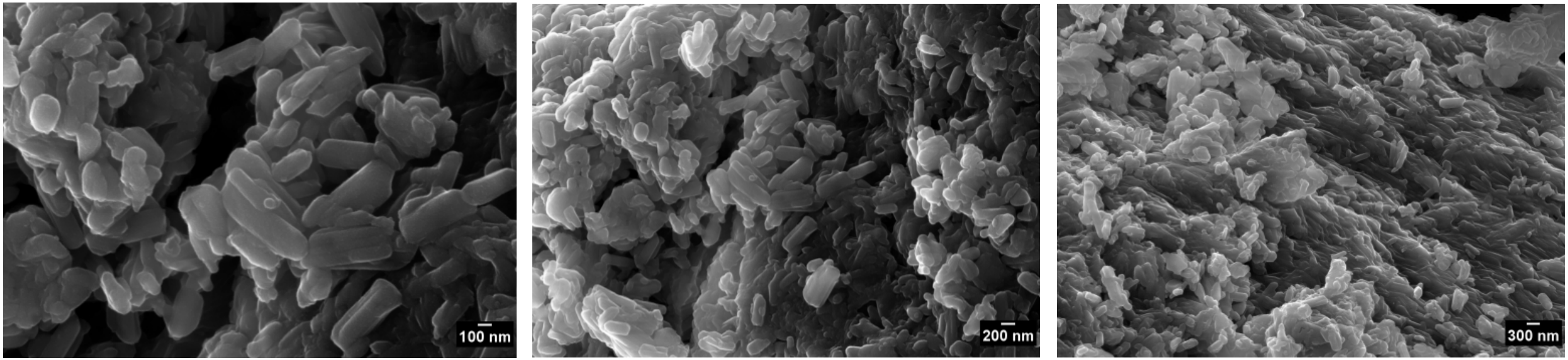

Figure S10. SEM images for [Sr(*m*BDC))$(H_2O)_{3.4}$] (**2**).