

Geometrical Constraints of Thermal Dehydration of β -Calcium Sulfate Hemihydrate Induced by Self-Generated Water Vapor

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S1. Sample Characterization

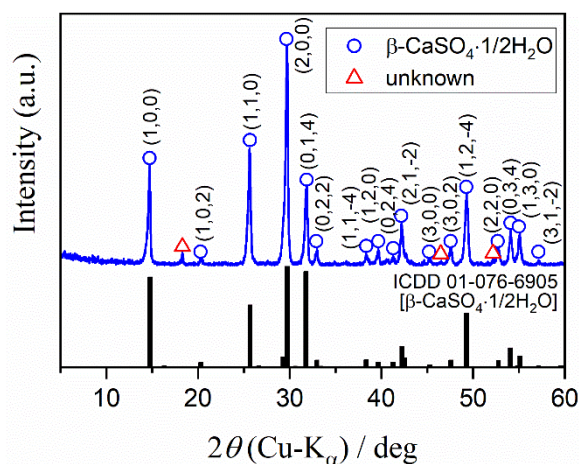


Figure S1. XRD pattern of the as-received calcium sulfate hemihydrate sample.

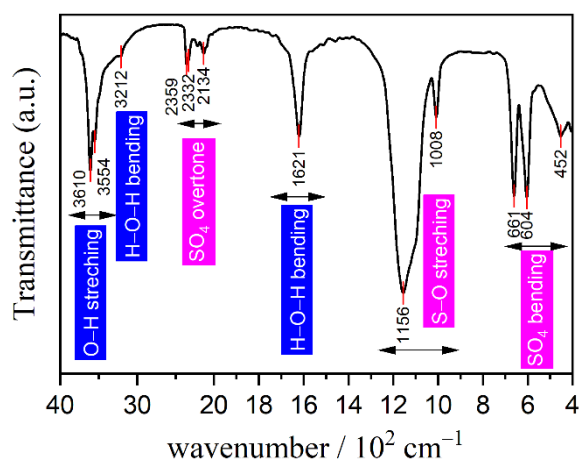


Figure S2. FT-IR spectrum of the as-received calcium sulfate hemihydrate sample.

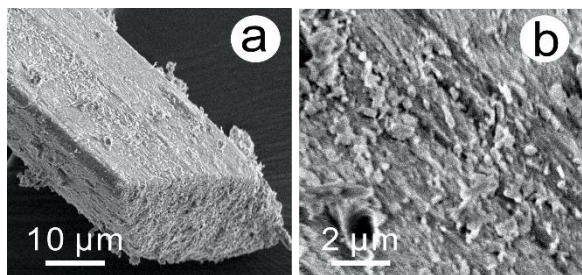


Figure S3. SEM images of the sample particle: (a) particle shape and (b) particle surface.

Supplementary Information

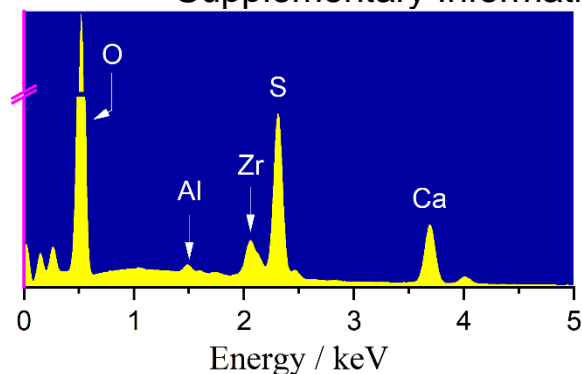


Figure S4. EDX spectrum of the calcium sulfate hemihydrate sample.

S2. Thermal Behavior

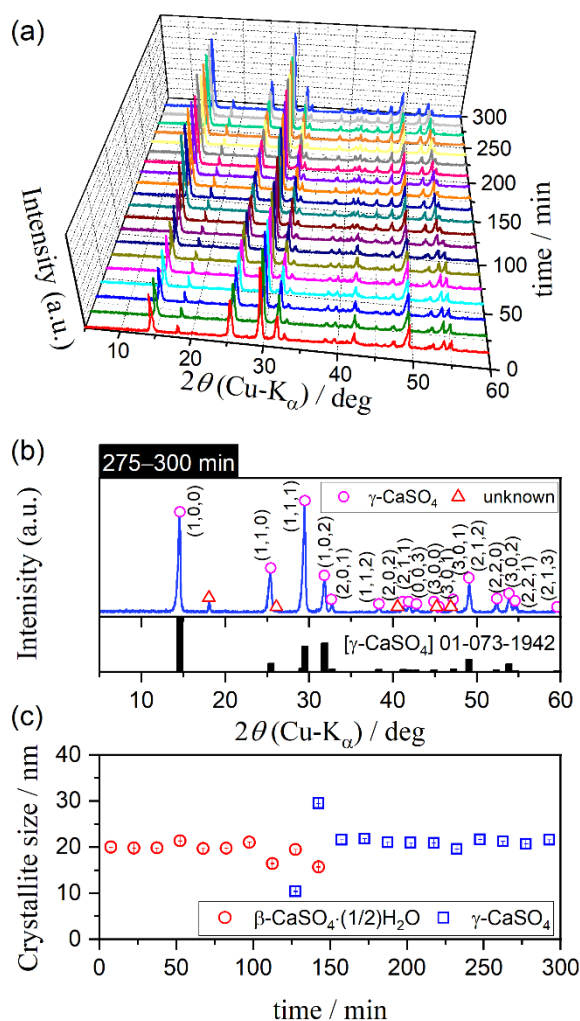


Figure S5. Results of the HT-XRD performed in the isothermal heating program mode at 383 K in a flow of dry N₂ gas: (a) changes in the XRD pattern with heating time, (b) XRD pattern recorded in the duration of 275–300 min, and (c) changes in the crystallite sizes of the reactant (β -CaSO₄·(1/2)H₂O) and product (γ -CaSO₄) during the thermal dehydration process.

S3. Formal Kinetic Analysis

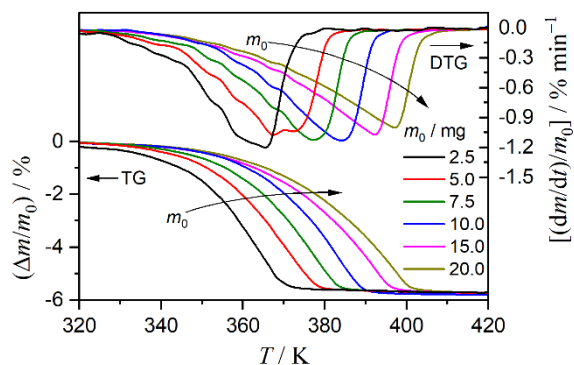


Figure S6. Influence of the sample mass (m_0) on the TG–DTG curves for the thermal dehydration of CS-HH in an open pan, recorded at a β of 5 K min⁻¹ in a flow of dry N₂ gas ($q_v = 80$ cm³ min⁻¹).

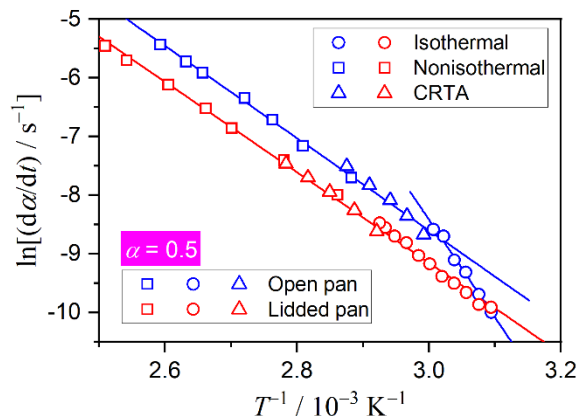


Figure S8. Comparison of the Friedman plots at $\alpha = 0.5$ for the thermal dehydration of CS-HH in open and lidded pans.

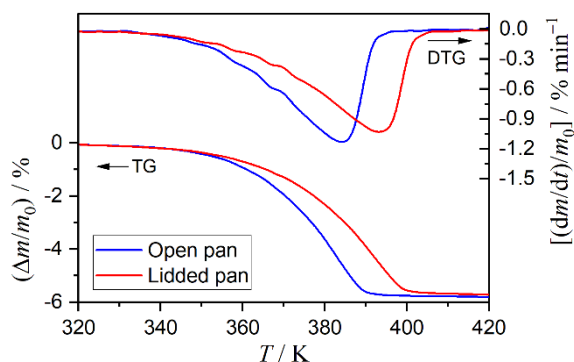


Figure S7. Comparison of TG–DTG curves for the thermal dehydration of CS-HH ($m_0 =$ approximately 10.0 mg) in open and lidded pans, recorded at a β of 5 K min⁻¹ in a flow of dry N₂ gas ($q_v = 80$ cm³ min⁻¹).

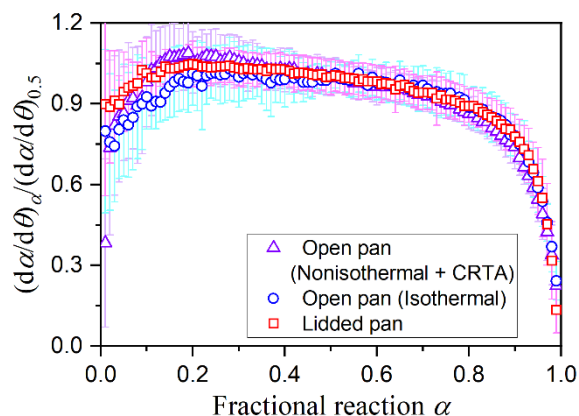


Figure S9. Comparison of the experimental master plots, normalized with reference to the $(d\alpha/d\theta)$ value at $\alpha = 0.5$, for the thermal dehydration of CS-HH in open and lidded pans.

S4. Physico-Geometrical Kinetic Modeling

Table S1. Optimized rate constants based on the SR–PBR(1) model for the thermal dehydration of CS–HH in open pan and lidded pans

Sampling	T / K	$k_{\text{SR}} / \text{s}^{-1}$	$k_{\text{PBR}(1)} / \text{s}^{-1}$	$R^2, ^a$	
				differential	Integral
Open pan	323.1	2.865×10^{-4}	4.461×10^{-5}	0.9882	0.9977
	325.0	7.395×10^{-4}	6.099×10^{-5}	0.9849	0.9987
	327.0	1.022×10^{-3}	8.158×10^{-5}	0.9793	0.9971
	329.0	2.294×10^{-3}	1.049×10^{-4}	0.9621	0.9984
	330.9	5.634×10^{-3}	1.568×10^{-4}	0.9628	0.9987
	333.0	9.940×10^{-3}	1.777×10^{-4}	0.9865	0.9990
Lidded pan	323.1	9.799×10^{-4}	4.854×10^{-5}	0.9769	0.9987
	325.1	1.066×10^{-3}	5.213×10^{-5}	0.9848	0.9989
	327.1	1.989×10^{-3}	6.105×10^{-5}	0.9795	0.9983
	329.0	2.502×10^{-3}	7.011×10^{-5}	0.9091	0.9976
	331.0	4.258×10^{-3}	8.335×10^{-5}	0.9583	0.9956
	333.1	5.500×10^{-3}	1.002×10^{-4}	0.9878	0.9992
	335.0	5.982×10^{-3}	1.154×10^{-4}	0.9773	0.9990
	337.0	9.936×10^{-3}	1.351×10^{-4}	0.9680	0.9992
	339.0	1.300×10^{-2}	1.564×10^{-4}	0.9835	0.9997
	340.9	1.599×10^{-2}	1.843×10^{-4}	0.9814	0.9997
	342.8	1.797×10^{-2}	2.092×10^{-4}	0.9724	0.9995

^aDetermination coefficient of the nonlinear least-squares analysis.