Electronic Supplementary Material (ESI) for Analyst.

Support Information of the manuscript: "Discriminating the formation origin of calcium oxalate monohydrate in kidney stones via synchrotron microdiffraction"

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SI1: XRD fitting results

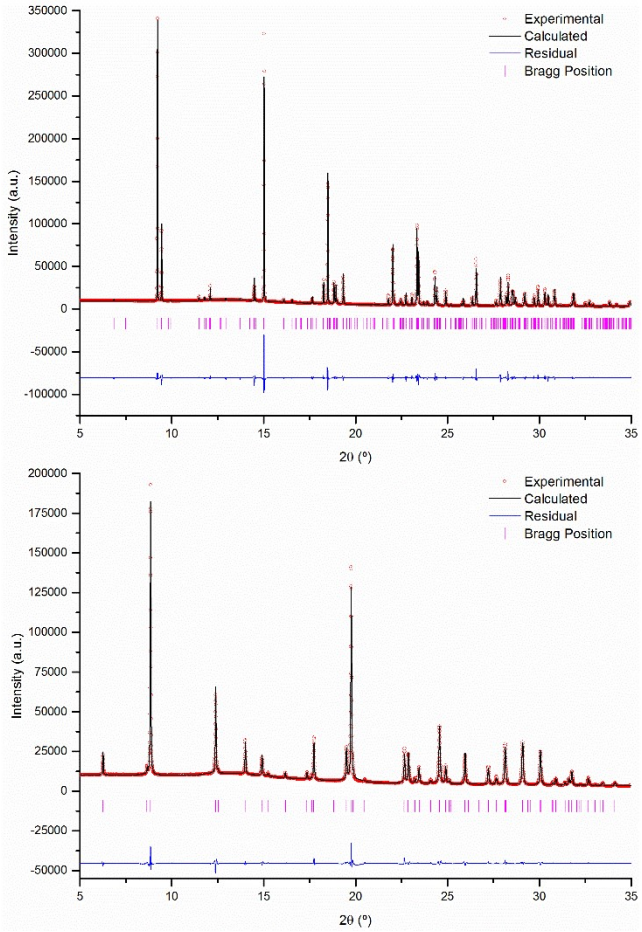

Figure 1. XRD pattern of the synthetized COM (top) and COD (bottom) after the profile matching

Table 2. XRD fitting results of the synthetized calcium oxalate hydrates reported in this work

	COD	**COM**
	Weddellite	Whewellite
Space group	*I4/m*, (No. 87)	*P21/c*, No. (14)
a (Å)	12.37906(7)	6.29504(4)
b (Å)	12.37906(7)	14.58911(8)
c (Å)	7.35282(4)	10.11829(5)
β (°)		109.459(5)
Vol (Å³)	1126.75(2)	876.2(3)
Wavelength (Å)	0.95349	
Refinement details:		
2θ range (°), 2θ step (°)	3.000 to 40.000, 0.006	
Profile function	Pseudo Voigt	
Loren. coef X	0.182064	0.105032
Loren. coef Y	0.015621	0.005174
Gauss coef W	0.000471	0.000523
Zero shift (°)	-0.01598(8)	-0.01547(9)
R_{Bragg}	0.0312	0.0698
R_{wp}	0.0268	0.0619
Chi (%)	2.37	5.45

Full-pattern matching performed with DAjust software, see [J. Appl. Cryst. (2012). 45, 844-848)] for details.

SI2: Examples of azimuthal plot

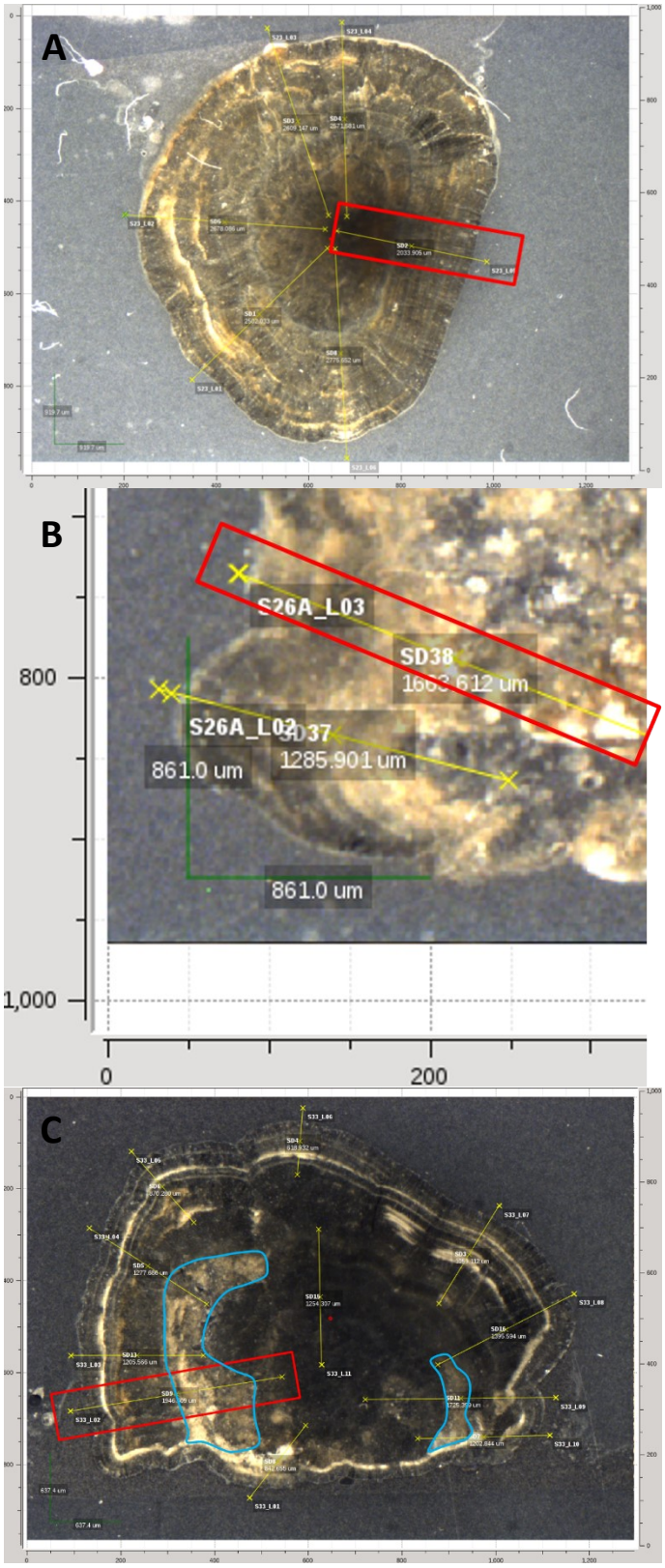

Figure 2. Images of the samples used as examples on the azimuthal Integration section of the manuscript, with the analyzed line highlighted in red. The kidney Stones are, S23 (top), S26A (middle) and S33 (bottom). In the S33, the regions marked in blue represent the ones suspected as TRA, by using the stereomicroscope, due to the differences in texture.

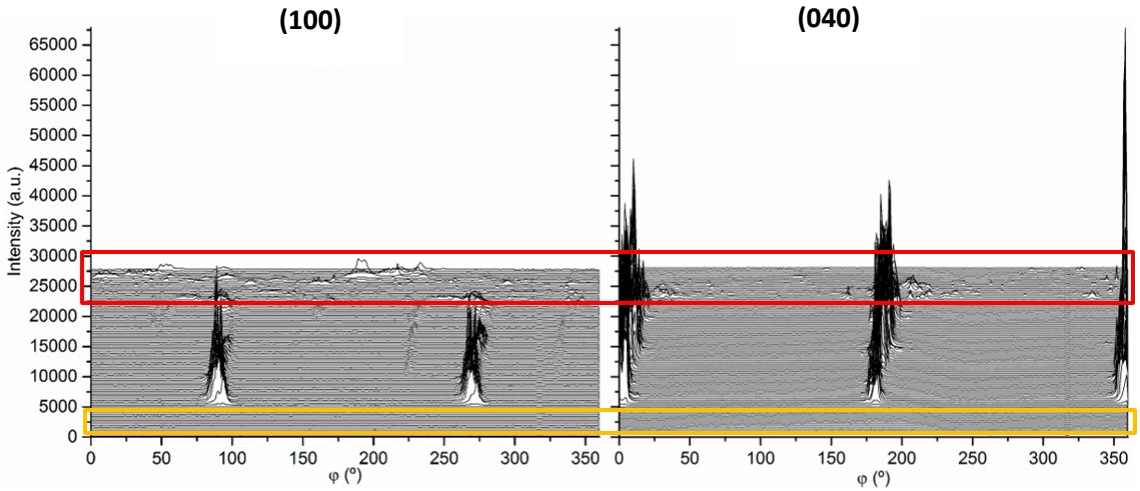

Figure 3. Representation of the azimuthal integration on the reflections (100) (Left) and (040) (Right) of a kidney classified as COM (S32). Orange square (bottom) mark the resin where the Stone is embedded, while red square represents the regions characterized as COM with organic matter. A clear orientation can be observed, since the pattern is repeated every 180º of the azimuthal angle.

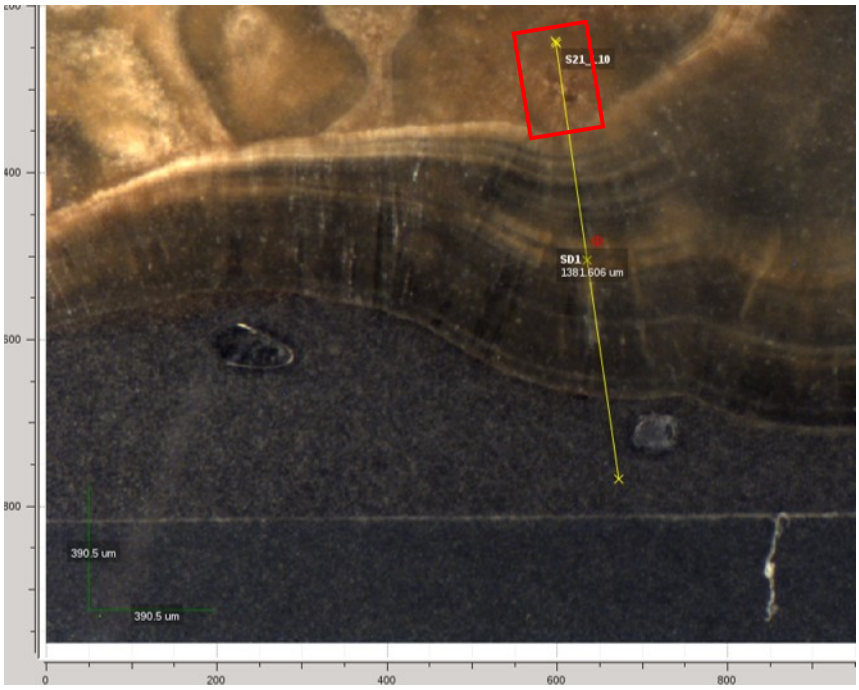

Figure 4. Image of the analyzed line from sample S32 represented in Figure 2. Highlighted in red is the region described as COM with organic matter.

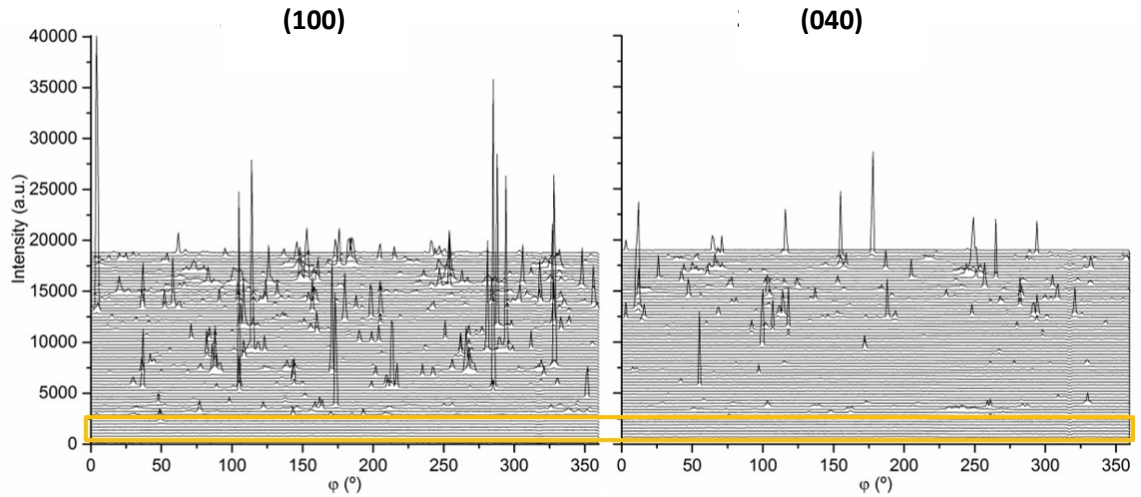

Figure 5. Representation of the azimuthal integration on the reflections (100) (Left) and (040) (Right) of a kidney classified as a transformed COD (S31). Orange square (bottom) mark the resin where the Stone is embedded.

Figure 6. Image of the analyzed line from sample S31 represented in Figure 4, with the analyzed line highlighted in red.

SI3: Multivariate Curve Resolution Analysis for the Transformation Monitoring

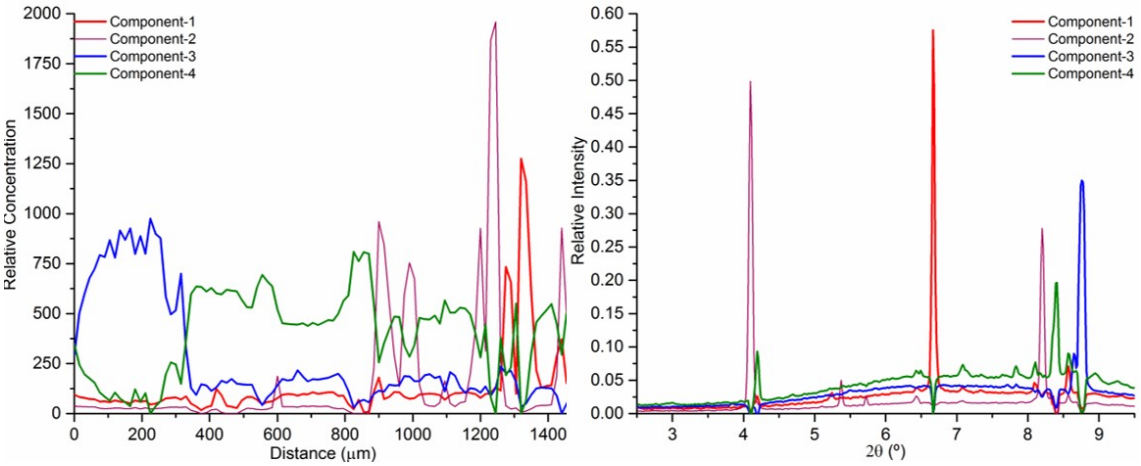

Figure 7. Example of MCR analysis of the diffractogram from a Correlated transformation from the superficial deposit of sample S24. In the left panel, the evolution of the four components along the diffraction analysis (from the surface to the inside of the stone) is represented, while on the right panel the simulated patterns for each component is shown.