Supplementary Material for

Influence of Amino Acids on Calcium Oxalate Precipitation in Systems of Different Chemical Complexity

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Content of listed material

Materials and Methods – ionic strength calculation

Table S1. Composition of artificial urine from literature sources.

Table S2. Thermogravimetric analyzes of the model system (MS) ($c(C_2O_4^{2-})$ = 6.0 mmol dm^{-3} and $c(Ca^{2+})$ = 7.5 mmol dm^{-3}) in a simple system, NaCl system and artificial urine at pH_i = 5 and pH_i = 9 (t_0 – initial temperature, t_{max} – maximum temperature, t_e – end temperature, Δm – mass loss expressed as a percentage, hydrate form that precipitates) [48, 52].

Figure S1. **A)** IR spectra of samples prepared in the model system at pH_i = 5 and pH_i = 9. **B)** Diffractograms of samples prepared in the model system at pH_i = 5 and pH_i = 9 (blue arrows indicate diffraction maxima from COD) [48].

Figure S2. Light microscope images a) and SEM images b) of calcium oxalate precipitated in the model systems (systems without AA) at pH_i = 5 and pH_i = 9. Note the difference in the SEM scale (×5.000, ×2.500) [48].

Figure S3. A) Morphology of COM crystals with characteristic Miller indices and crystal growth direction (black numbers correspond to Tazzoli notation (space group $P2_1/c$) [58] and red to Deganello notation (space group $I2/m$)) [59] B) The coordination of the oxalate ions with the calcium ions in the COM crystal, generated with the program MERCURY [51].

Figure S4. PXRD diffractograms of standards a) COM (black marked planes according to PDF card 75-1313, red marked planes according to PDF card 20-231) and b) COD (black marked planes according to PDF card 17-541 for COD)

Table S3. IR vibration bands (in cm^{-1}) of calcium oxalate standards COM and COD [17].

Materials and Methods – ionic strength calculation

Ionic strength was calculated according to the following equation:

$$I_c = \frac{1}{2}\sum_{i=1}^{n}(c_i\, z_i^2)$$

where z_i is the charge number of ion i (positive for cations, negative for anions), and c_i is the concentration of ion i.

Table S1.

COMPOUND	CONCENTRATION / mmol dm^{-3}						
	Isaacson [32]	Doremus [33]	Miller [34]	Barker [35]	Rose [36]	Brown [18]	Burns i Finlayson [31]
Na$_2$SO$_4$	14.9	16.5	23.4	16.5	14.9	16.95	16.95
KCl	92.6	25.0	111.5	52.0	92.6	63.70	63.70
NH$_4$Cl	65.1	20.0	59.5		65.1		27.60
NH$_4$OH				20.0		or HCl	17.90
MgSO$_4$·7H$_2$O	6.7	2.0	8.1	2.0	6.7	3.85	3.85
Na$_2$HPO$_4$	1.8		4.1	13.0	1.8	32.30	32.30
NaH$_2$PO$_4$·H$_2$O	39.6	16.5	29.9	3.5	39.6		
NaCl	213.9	170.0	158.3	170.0	213.9	105.50	105.50
C$_6$H$_5$Na$_3$O$_7$·2H$_2$O	2.7	1.6	2.7	1.6	2.7	3.21	3.21
Urea	291.4	500.0		500.0	291.4		
Creatinine		13.0		13.0			
Hippuric acid		3.0		3.0			
Uric acid				3.0			
pH	5.4	5.7		6.5	5.4	6.50	6.50

Table S2.

	MS	t_0 / °C	t_{max} / °C	t_e / °C	Δm / %	Phase
	simple system	89.96	152.49	193.45	12.12	COM
$pH_i = 5$	NaCl	89.00	148.96	184.74	12.23	COM
	artificial urine	89.24	147.60	188.72	11.54	COM
	simple system	71.51	147.02	181.09	11.23	COM
$pH_i = 9$	NaCl	89.12	145.70	177.86	11.59	COM
	artificial urine	86.47	143.49	184.35	12.45	COM/COD

Figure S1.

Simple System   **NaCl System**   **Artificial Urine System**

| pH$_i$ = 5 | pH$_i$ = 9 | pH$_i$ = 5 | pH$_i$ = 9 | pH$_i$ = 5 | pH$_i$ = 9 |

a)

b)

Figure S2.

(A)

(B)
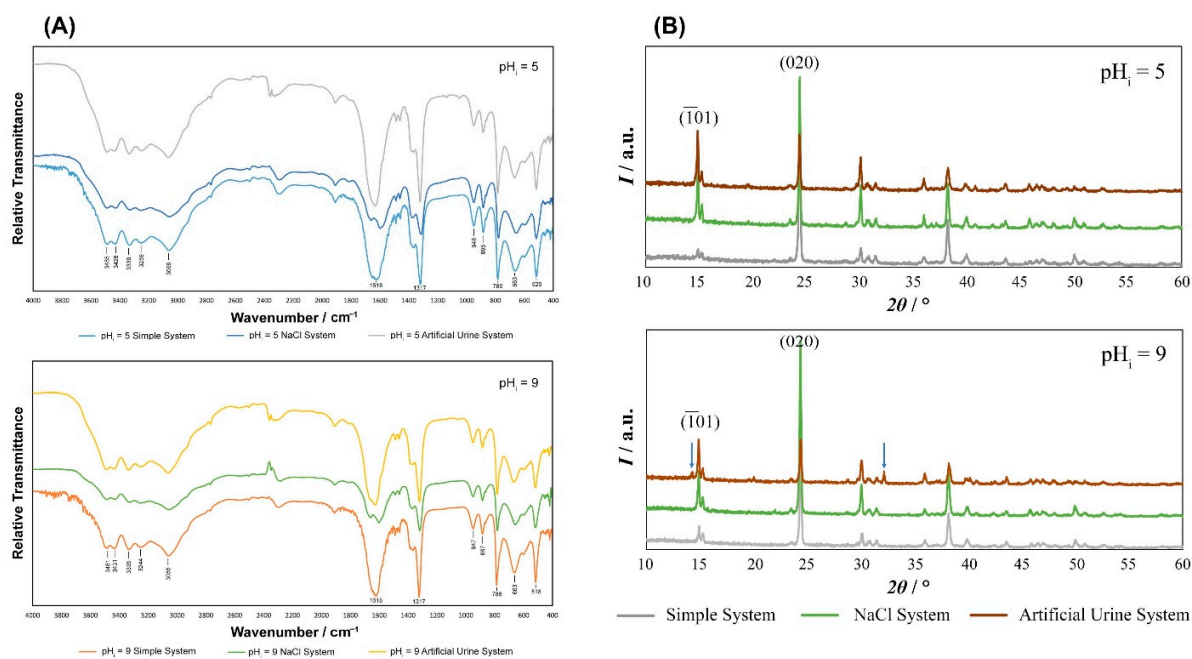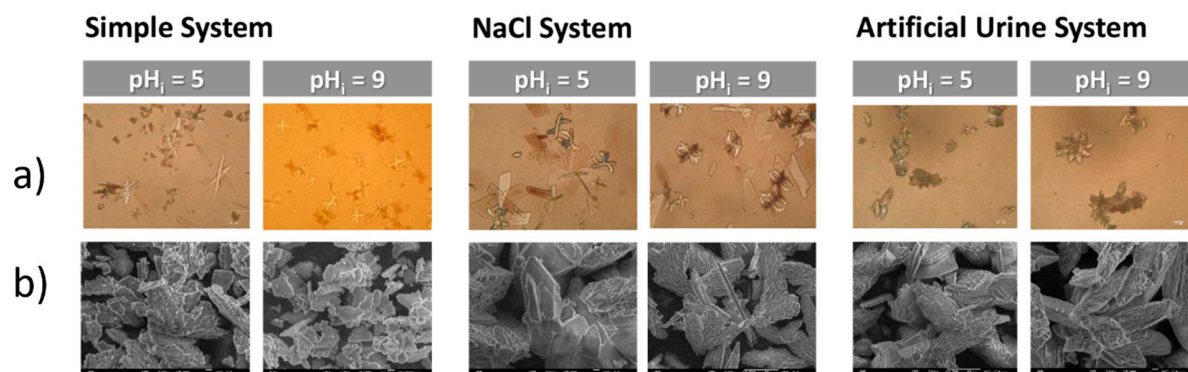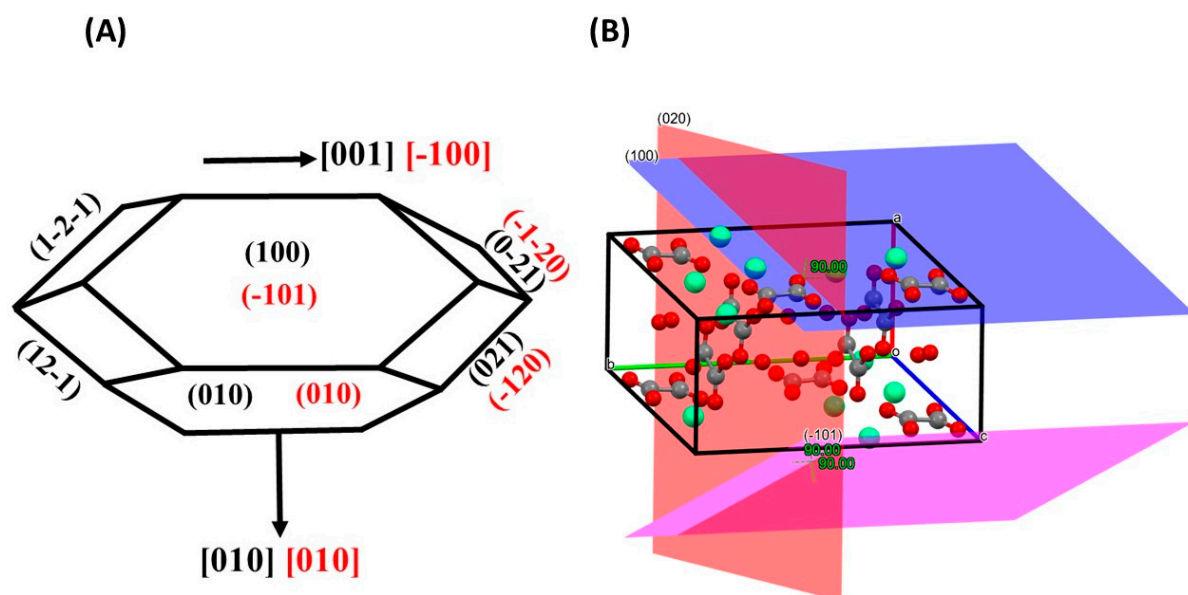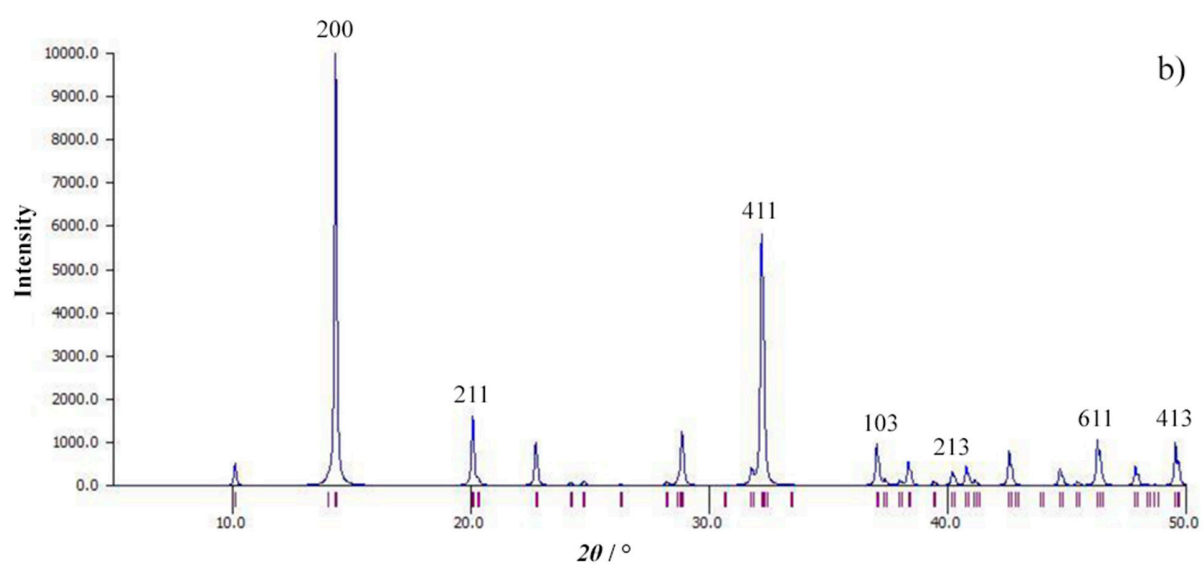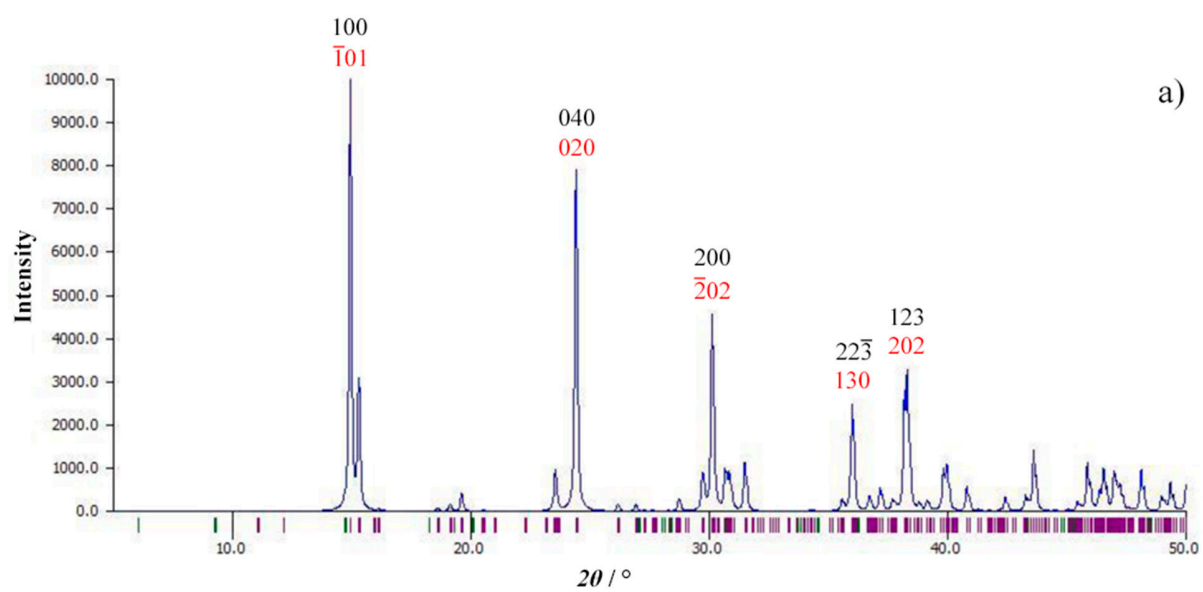
Figure S3.

Figure S4.

Table S3

COM	COD	Vibrational mode
3483	3469	v(OH)
3429		v(OH)
3336		v(OH)
3258		2δ(HOH)
3058		v(OH)
1624 - 1622	1640 - 1638	v_a(COO) - v_a(CO)
	1470	v(C − C) + v_s(COO)
1384		v_s(CO)
1368		
1320 - 1316	1324	v_s(COO)
958 - 889		L(H$_2$O)
	912	v_s(CO) + L(H$_2$O)
782	782	δ(OCO)
656	630	L(HOH)

v – stretching; δ – bending; a-antisymmetric; s – symmetric; L – libration.