Supplementary Materials: Indications that Amorphous Calcium Carbonates Occur in Pathological Mineralisation—A Urinary Stone from a Guinea Pig

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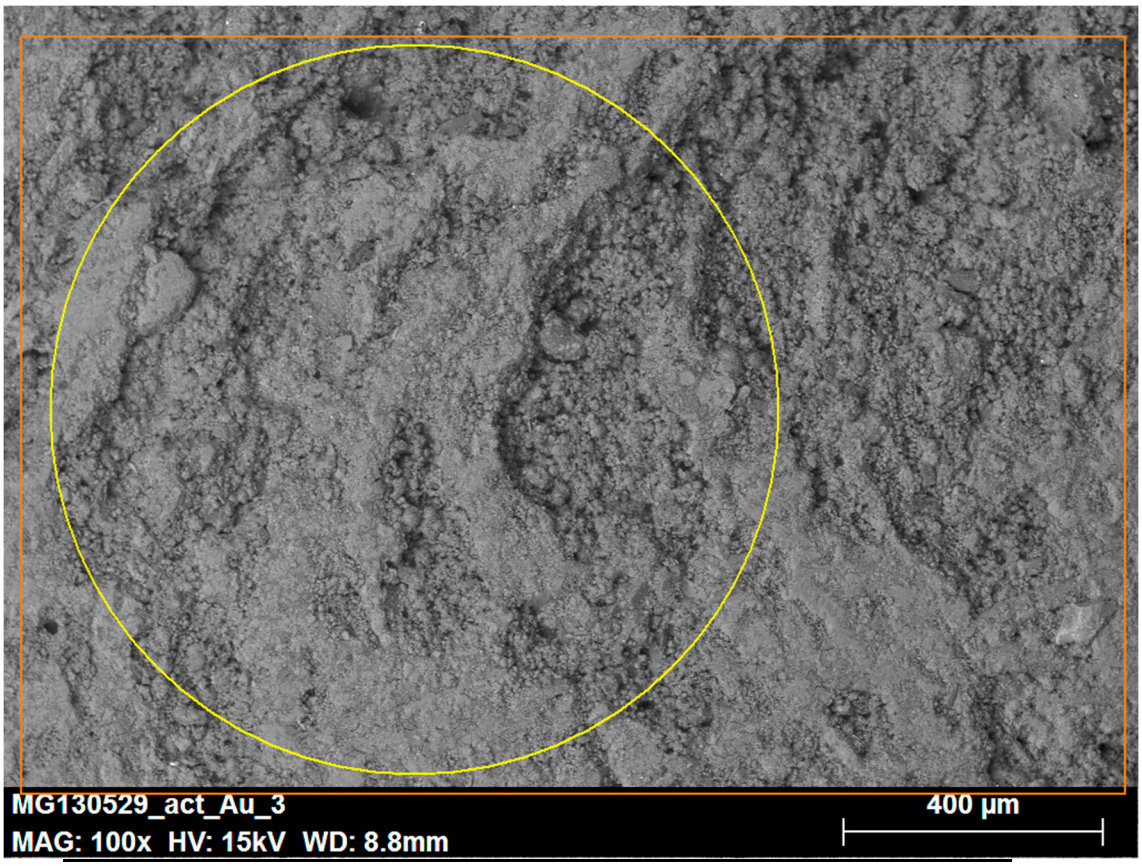
TGA

The onset of calcination of amorphous calcium carbonate (ACC) has been reported to occur at ca. 600 °C [1], which is consistent with the current analysis. Assuming that the weight loss occurring after 600 °C is due to the calcination of calcium carbonate alone, the theoretical weight loss in technical air may be expressed as follows: $CaCO_3$ (100u <=> 68%)→CaO + CO2↑ (56u + 44u↑ <=> 38% + **30%**↑). Italicised figures were calculated from the bold figure, which was determined experimentally based on the weight loss upon calcination.

Assuming that the 10% stable inorganics that remain after calcination and are not CaO are magnesium hydrogen phosphate, the decomposition of struvite occurring between ca. 50–250 °C in technical air can be written as [2]: $MgNH_4PO_4{\cdot}6H_2O$ (245u <=> 20.4%)→$MgHPO_4$ + NH_3↑ + $6H_2O$↑ (120u + 17u↑ + 108u↑ <=> **10%** + 1.4%↑ + 9%↑). Italicised figures were calculated from the bold figure, which was determined by comparing the calculated residual mass of CaO, see above, with the observed residual mass.

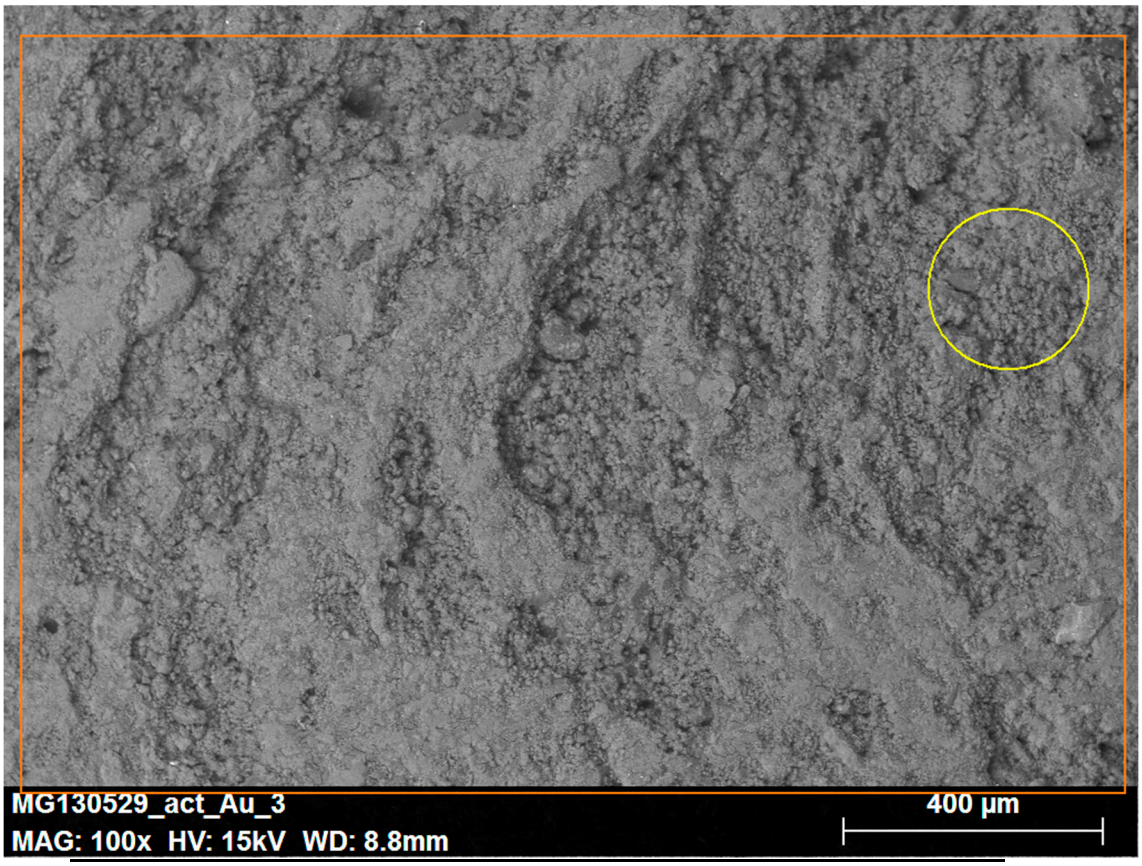


Spectrum: Point

Element	AN	Series	Net unn.	C norm.	C Atom.	C Error
			wt %	wt %	at %	%
Oxyge	8	K-series 38651	54.43	48.46	54.61	6.0
Carbon	6	K-series 15571	21.47	19.12	28.69	2.5
Calcium	20	K-series 71949	23.22	20.68	9.30	0.7

Magnesium	12	K-series 24133	5.72	5.09	3.78	0.3
Phosphorus	15	K-series 19346	3.48	3.10	1.81	0.2
Potassium	19	K-series 10062	2.50	2.23	1.03	0.1
Silicon	14	K-series 5241	0.95	0.85	0.54	0.1
Chlorine	17	K-series 2751	0.54	0.48	0.24	0.0
Total			112.30	100.00	100.00	

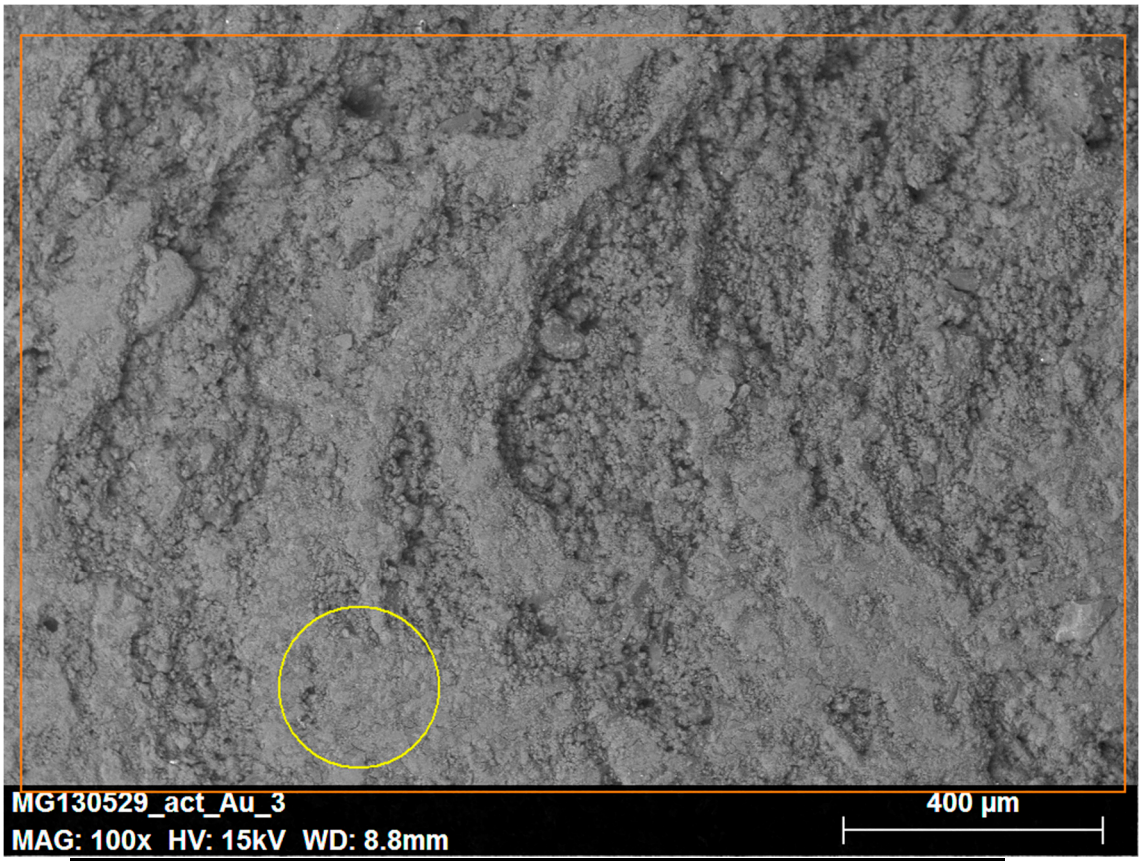
Figure S1. SEM micrograph with EDS mapping of a large area of the urinary stone of the Guinea Pig. The yellow circle in the SEM image marks the area of EDS mapping.



Spectrum: Point

Element	AN	Series	Net unn.	C norm.	C Atom.	C Error
			wt %	wt %	at %	%
Oxyge	8	K-series 1994	53.06	49.45	55.90	7.7
Carbon	6	K-series 708	18.97	17.68	26.62	3.3
Calcium	20	K-series 3574	19.96	18.60	8.39	0.6
Magnesium	12	K-series 1255	6.82	6.36	4.73	0.4
Phosphorus	15	K-series 846	3.57	3.33	1.94	0.2
Potassium	19	K-series 550	2.75	2.57	1.19	0.1
Silicon	14	K-series 381	1.61	1.50	0.97	0.1
Chlorine	17	K-series 155	0.55	0.52	0.26	0.0
Total			107.30	100.00	100.00	

Figure S2. SEM micrograph with EDS mapping of a smaller porous region of the urinary stone of the Guinea Pig. The yellow circle in the SEM image marks the area of EDS mapping.



Spectrum: Point

Element	AN	Series	Net unn.	C norm.	C Atom.	C Error
			wt %	wt %	at %	%
Oxyge	8	K-series 2601	51.32	50.21	57.19	7.2
Carbon	6	K-series 676	16.34	15.99	24.26	2.9
Calcium	20	K-series 3776	17.31	16.94	7.70	0.5
Magnesium	12	K-series 1816	7.38	7.22	5.42	0.4
Phosphorus	15	K-series 2069	6.56	6.42	3.78	0.3
Potassium	19	K-series 577	2.14	2.10	0.98	0.1
Silicon	14	K-series 231	0.74	0.72	0.47	0.1
Chlorine	17	K-series 115	0.41	0.40	0.21	0.0
Total			102.20	100.00	100.00	

Figure S3. SEM micrograph with EDS mapping of a smaller dense region of the urinary stone of the Guinea Pig. The yellow circle in the SEM image marks the area of EDS mapping.

References

1. Gebauer, D.; Gunawidjaja, P.N.; Ko, J.Y.P.; Bacsik, Z.; Aziz, B.; Liu, L.J.; Hu, Y.F.; Bergström, L.; Tai, C.W.; Sham, T.K.; Edén, M.; Hedin, N. Proto-calcite and proto-vaterite in amorphous calcium carbonates. *Angew. Chem. Int. Ed.* **2010**, *49*, 8889–8891, doi:10.1002/anie.201003220.
2. Bhuiyan, M.I.H.; Mavinic, D.S.; Koch, F.A. Thermal decomposition of struvite and its phase transition. *Chemosphere* **2008**, *70*, 1347–1356, doi:10.1016/j.chemosphere.2007.09.056.