Electronic Supplementary Information (ESI)

MicroED: Unveiling the Structural Chemistry of Plant Biomineralisation

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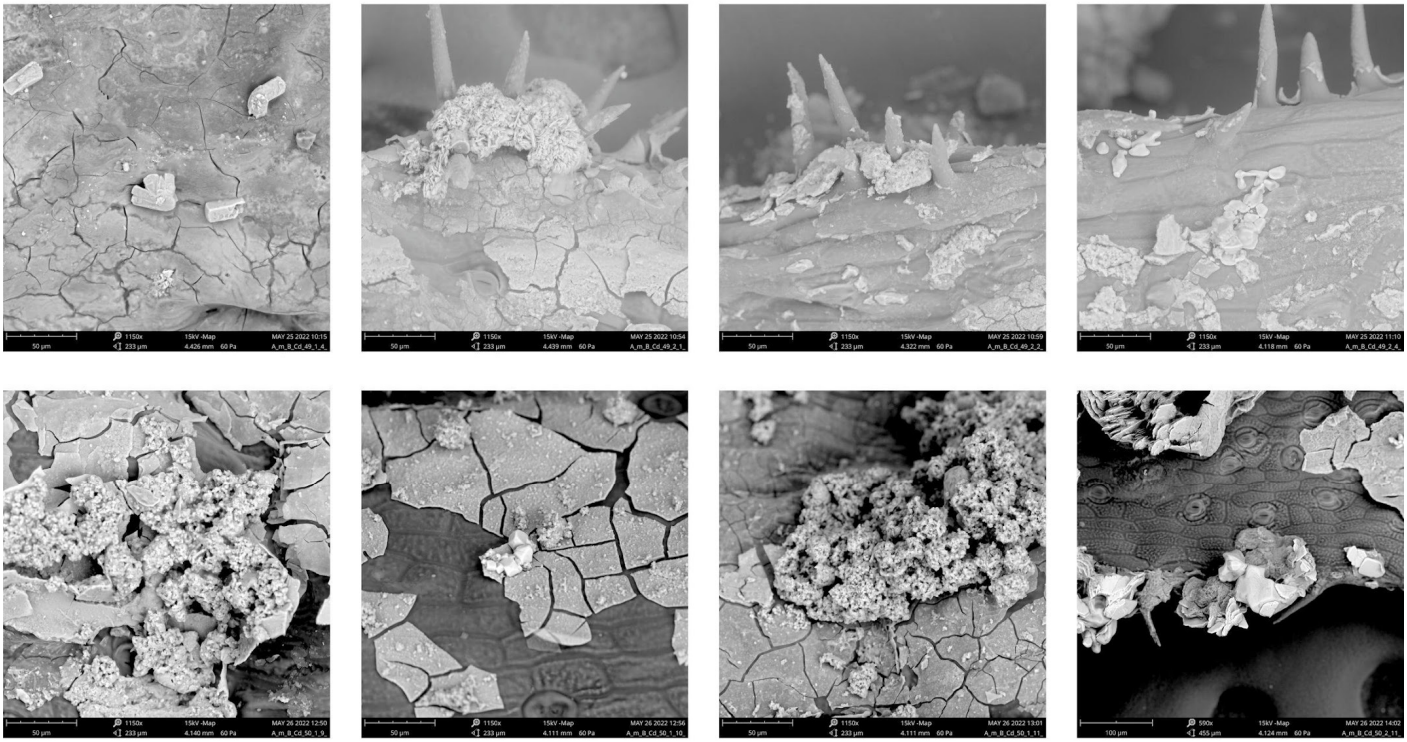
a)



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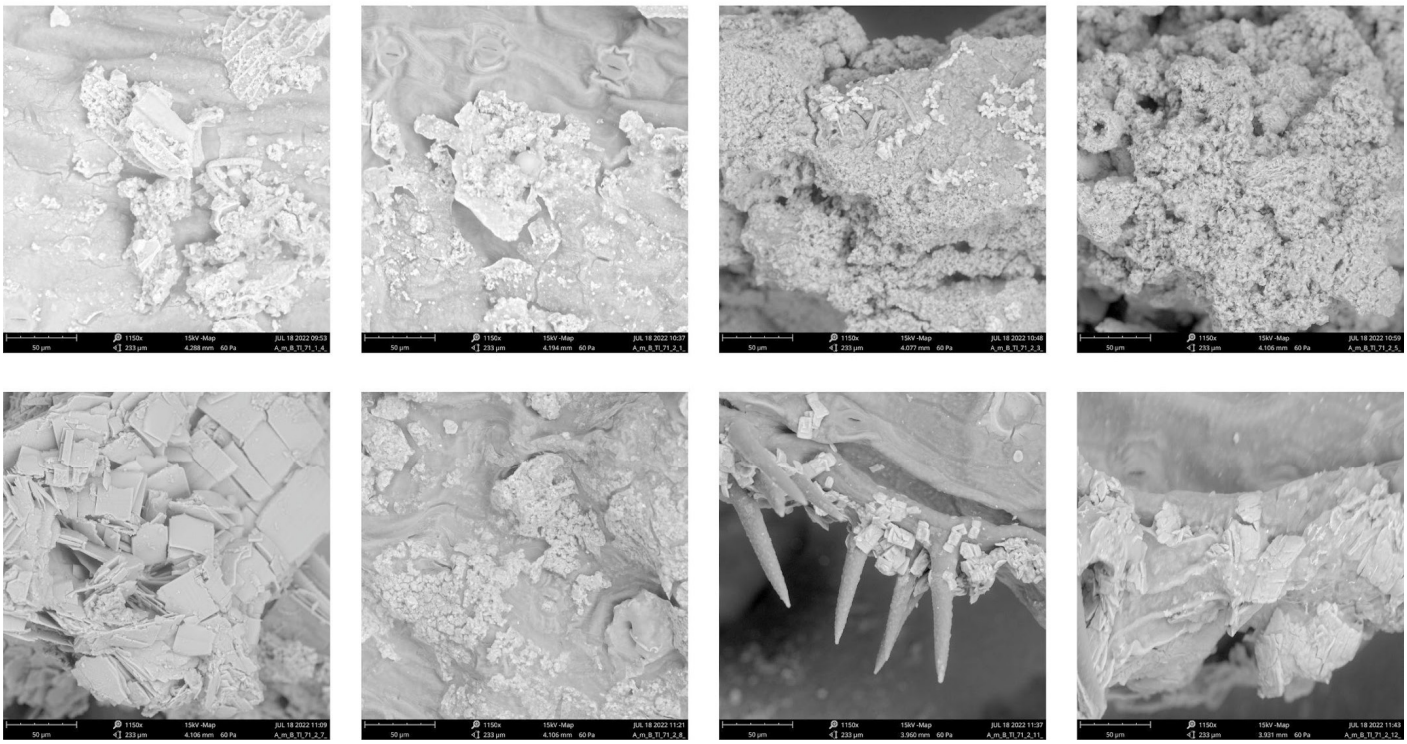

Figure S1. Examples of crystalline material formed on the surface of the leaves of *A. maritima* plants after exposure to cadmium (d) and thallium

Table S1. Bond lengths for investigated sodium chloride.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl01	Na02[1]	2.75(5)	Cl01	Na02[3]	2.75(5)
Cl01	Na02[2]	2.75(5)	Cl01	Na02[4]	2.75(5)
Cl01	Na02	2.75(5)	Cl01	Na02[5]	2.75(5)

[1]1/2+X,1/2+Y,+Z; [2]1/2+X,-1/2+Y,+Z; [3]1/2+X,+Y,1/2+Z; [4]1+X,+Y,+Z; [5]1/2+X,+Y,-1/2+Z

Table S2. Valence angles for investigated sodium chloride.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Na02[1]	Cl01	Na02	90.0	Cl01[6]	Na02	Cl01	90.0
Na02[2]	Cl01	Na02[3]	180.0	Cl01[7]	Na02	Cl01[8]	180.0
Na02[2]	Cl01	Na02[4]	90.0	Cl01[7]	Na02	Cl01[9]	90.0
Na02[5]	Cl01	Na02[3]	90.0	Cl01[10]	Na02	Cl01[8]	90.0
Na02	Cl01	Na02[4]	90.0	Cl01	Na02	Cl01[9]	90.0
Na02[5]	Cl01	Na02[4]	90.0	Cl01[10]	Na02	Cl01[9]	90.0
Na02[1]	Cl01	Na02[2]	90.0	Cl01	Na02	Cl01[8]	90.0
Na02[1]	Cl01	Na02[5]	90.0	Cl01[6]	Na02	Cl01[10]	90.0
Na02	Cl01	Na02[2]	90.0	Cl01	Na02	Cl01[7]	90.0
Na02[1]	Cl01	Na02[4]	180.0	Cl01[6]	Na02	Cl01[9]	180.0
Na02[5]	Cl01	Na02[2]	90.0	Cl01[10]	Na02	Cl01[7]	90.0
Na02	Cl01	Na02[5]	180.0	Cl01	Na02	Cl01[10]	180.0
Na02[1]	Cl01	Na02[3]	90.0	Cl01[6]	Na02	Cl01[8]	90.0
Na02	Cl01	Na02[3]	90.0	Cl01[8]	Na02	Cl01[9]	90.0
Na02[3]	Cl01	Na02[4]	90.0	Cl01[6]	Na02	Cl01[7]	90.0

[1]1/2+X,1/2+Y,+Z; [2]1/2+X,+Y,-1/2+Z; [3]1/2+X,+Y,1/2+Z; [4]1/2+X,-1/2+Y,+Z; [5]1+X,+Y,+Z; [6]-1/2+X,1/2+Y,+Z; [7]-1/2+X,+Y,-1/2+Z; [8]-1/2+X,+Y,1/2+Z; [9]-1/2+X,-1/2+Y,+Z; [10]-1+X,+Y,+Z

Table S3. Bond lengths for investigated sodium sulfate.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S2	O3	1.441(4)	Na1	O3[5]	2.329(5)
S2	O3[1]	1.441(4)	Na1	O3[6]	2.265(4)
S2	O3[2]	1.441(4)	Na1	O3[7]	2.474(6)
S2	O3[3]	1.441(4)	Na1	O3[8]	2.329(5)
Na1	Na1[3]	3.082(6)	Na1	O3[9]	2.474(6)
Na1	Na1[4]	3.082(6)	Na1	O3	2.265(4)

[1]1/4-X,+Y,5/4-Z; [2]+X,5/4-Y,5/4-Z; [3]1/4-X,5/4-Y,+Z; [4]5/4-X,5/4-Y,+Z; [5]1-X,3/2-Y,3/2-Z; [6]3/4-X,+Y,7/4-Z; [7]1/4+X,-1/4+Y,3/2-Z; [8]-1/4+X,3/2-Y,1/4+Z; [9]1/2-X,-1/4+Y,1/4+Z

Table S4. Valence angles for investigated sodium chloride.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O3	S2	O3[1]	111.1(3)	O3[8]	Na1	O3	169.2(3)
O3[1]	S2	O3[2]	110.4(3)	O3	Na1	O3[5]	108.53(19)
O3	S2	O3[2]	106.9(3)	O3	Na1	O3[7]	81.06(15)
O3	S2	O3[3]	110.4(3)	O3	Na1	O3[6]	81.31(12)
O3[3]	S2	O3[2]	111.1(3)	O3[8]	Na1	O3[9]	81.06(15)
O3[1]	S2	O3[3]	106.9(3)	O3[7]	Na1	O3[5]	137.63(17)
Na1[3]	Na1	Na1[4]	130.6(3)	O3	Na1	O3[9]	94.74(14)
O3	Na1	Na1[4]	105.92(10)	O3[8]	Na1	O3[7]	94.74(14)
O3[5]	Na1	Na1[4]	86.0(2)	O3[7]	Na1	O3[9]	134.7(3)
O3[6]	Na1	Na1[3]	86.0(2)	O3[7]	Na1	O3[6]	86.71(16)
O3[7]	Na1	Na1[4]	52.17(12)	O3[8]	Na1	O3[5]	81.31(12)
O3[5]	Na1	Na1[3]	48.04(14)	O3[9]	Na1	O3[5]	86.71(16)
O3	Na1	Na1[3]	78.73(9)	O3[8]	Na1	O3[6]	108.53(19)
O3[8]	Na1	Na1[4]	78.73(9)	O3[9]	Na1	O3[6]	137.63(17)

O3[7]	Na1	Na1[3]	159.32(11)	S2	O3	Na1	129.7(2)
O3[9]	Na1	Na1[3]	52.17(13)	S2	O3	Na1[7]	120.7(2)
O3[9]	Na1	Na1[4]	159.32(11)	S2	O3	Na1[10]	98.65(19)
O3[8]	Na1	Na1[3]	105.92(10)	Na1	O3	Na1[10]	119.2(2)
O3[6]	Na1	Na1[4]	48.04(14)	Na1[7]	O3	Na1[10]	79.79(14)
O3[5]	Na1	O3[6]	55.8(2)	Na1	O3	Na1[7]	98.94(15)

[1]+X,5/4-Y,5/4-Z; [2]1/4-X,+Y,5/4-Z; [3]1/4-X,5/4-Y,+Z; [4]5/4-X,5/4-Y,+Z; [5]1/2-X,-1/4+Y,1/4+Z; [6]1/4+X,-1/4+Y,3/2-Z; [7]1-X,3/2-Y,3/2-Z; [8]3/4-X,+Y,7/4-Z; [9]-1/4+X,3/2-Y,1/4+Z; [10]-1/4+X,1/4+Y,3/2-Z

Table S5. Torsion angles for investigated sodium sulfate.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O3[1]	S2	O3	Na1	-99.3(3)	O3[2]	S2	O3	Na1	140.2(3)
O3[2]	S2	O3	Na1[3]	0.000(1)	O3[4]	S2	O3	Na1[3]	-121.01(18)
O3[1]	S2	O3	Na1[3]	120.54(19)	O3[1]	S2	O3	Na1[5]	37.33(15)
O3[4]	S2	O3	Na1	19.15(16)	O3[4]	S2	O3	Na1[5]	155.8(3)
O3[2]	S2	O3	Na1[5]	-83.2(2)					

[1]+X,5/4-Y,5/4-Z; [2]1/4-X,+Y,5/4-Z; [3]-1/4+X,1/4+Y,3/2-Z; [4]1/4-X,5/4-Y,+Z; [5]1-X,3/2-Y,3/2-Z

Table S6. Bond lengths for investigated calcium sulfate dihydrate.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ca1	O5	2.31(2)	Ca1	O4[2]	2.46(3)
Ca1	O5[1]	2.31(2)	Ca1	O4[3]	2.46(3)
Ca1	O3[2]	2.46(4)	S2	O3	1.448(15)
Ca1	O3	2.32(3)	S2	O3[4]	1.448(15)
Ca1	O3[1]	2.32(3)	S2	O4[4]	1.448(15)
Ca1	O3[3]	2.46(4)	S2	O4	1.448(15)

[1]1-X,+Y,1/2-Z; [2]-1/2+X,3/2-Y,-1/2+Z; [3]3/2-X,3/2-Y,1-Z; [4]1-X,+Y,3/2-Z

Table S7. Valence angles for investigated calcium sulfate dihydrate.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O5	Ca1	O5[1]	99.3(9)	O3	Ca1	O4[2]	124.0(7)
O5[1]	Ca1	O3	84.1(11)	O3	Ca1	O4[3]	80.6(8)
O5	Ca1	O3[2]	131.8(3)	O3[1]	Ca1	O4[3]	124.0(7)
O5	Ca1	O3[1]	84.1(11)	O3[1]	Ca1	O4[2]	80.6(8)
O5	Ca1	O3[3]	77.7(6)	O4[3]	Ca1	O3[3]	55.9(9)
O5[1]	Ca1	O3[1]	160.0(4)	O4[3]	Ca1	O3[2]	140.9(8)
O5[1]	Ca1	O3[2]	77.7(6)	O4[2]	Ca1	O3[3]	140.9(8)
O5	Ca1	O3	160.0(4)	O4[2]	Ca1	O3[2]	55.9(9)
O5[1]	Ca1	O3[3]	131.8(3)	O4[3]	Ca1	O4[2]	144.3(6)
O5[1]	Ca1	O4[2]	81.1(11)	O3	S2	O3[4]	111.1(9)
O5[1]	Ca1	O4[3]	76.0(11)	O3	S2	O4	105.6(11)
O5	Ca1	O4[3]	81.1(11)	O3[4]	S2	O4[4]	105.6(11)
O5	Ca1	O4[2]	76.0(11)	O3[4]	S2	O4	110.8(11)
O3[1]	Ca1	O3[2]	85.3(4)	O3	S2	O4[4]	110.8(11)
O3[1]	Ca1	O3[3]	68.2(4)	O4[4]	S2	O4	113.1(9)
O3[1]	Ca1	O3	99.4(12)	Ca1	O3	Ca1[2]	111.8(4)
O3[2]	Ca1	O3[3]	139.0(7)	S2	O3	Ca1[2]	99.1(9)
O3	Ca1	O3[3]	85.3(4)	S2	O3	Ca1	148.6(7)
O3	Ca1	O3[2]	68.2(4)	S2	O4	Ca1[2]	99.4(12)

[1]1-X,+Y,1/2-Z; [2]3/2-X,3/2-Y,1-Z; [3]-1/2+X,3/2-Y,-1/2+Z; [4]1-X,+Y,3/2-Z

Table S8. Torsion angles for investigated calcium sulfate dihydrate.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O3[1]	S2	O3	Ca1	67.6(9)	O4	S2	O3	Ca1	-172.3(6)

O3[1]	S2	O3	Ca1[2]	-122.7(6)	O4	S2	O3	Ca1[2]	-2.5(3)
O3	S2	O4	Ca1[2]	2.6(3)	O4[1]	S2	O3	Ca1[2]	120.3(6)
O3[1]	S2	O4	Ca1[2]	123.0(7)	O4[1]	S2	O4	Ca1[2]	-118.7(8)
O4[1]	S2	O3	Ca1	-49.5(9)					

[1]1-X,+Y,3/2-Z; [2]3/2-X,3/2-Y,1-Z