Revisiting the Raman Spectra of Carbonate Minerals

SUPPLEMENTARY MATERIAL

Table Caption

Table S1: Sample information

Figure Captions

Figure S1: Results of EDS analysis for calcite A

Figure S2: Results of EDS analysis for calcite B

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Figure S5: Results of EDS analysis for calcite E

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Figure S7: Results of EDS analysis for aragonite B

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Figure S16: Results of EDS analysis for rhodochrosite B

Figure S17: Results of EDS analysis for witherite

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Figure S26: Results of EDS analysis for witherite sample

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Figure S30: Raman spectra normalized by the B_{1g}, B_{2g} and B_{3g} symmetries for aragonite samples

Figure S31: Raman spectra normalized by the E_g symmetry for dolomite samples

Figure S32: Raman spectra normalized by the E_g symmetry for dolomite samples showing the bands at 1078 cm^{-1} and 882 cm^{-1}

Figure S33: Raman spectra normalized by the E_g symmetry for Magnesite samples samples

Figure S34: Raman spectra normalized by the B_{1g}, B_{2g} and B_{3g} symmetries for a comparison between aragonite and witherite samples

Figure S35: Mineral samples photographs

Table S1

Structure	Sample	Characteristics	Origin Source
		Calcites	
Rhombohedral	A	Optical calcite; transparent; euhedral	Minas Gerais
	B	Gray; sulphur and graphite traces	Minas Gerais
	C	Orange, pink and white	Bahia
	D	White	Minas Gerais
	E	Orange	Minas Gerais
		Magnesites	
Rhombohedral	A	White	Bahia
	B	Purple and white	Bahia
		Dolomites	
Rhombohedral	A	Pale purple	Minas Gerais
	B	Gray; powder sample	São Paulo
	C	White	Bahia
	D	White and yellow	Minas Gerais
		Aragonites	
Orthorhombic	A	White	Minas Gerais
	B	White, yellow, and brown	Spain
	C	White	Minas Gerais
		Rhodochrosites	
Rhombohedral	A	Pink	Argentina
	B	Pink	Argentina
		Witherite	
Orthorhombic	A	White with black dots	Prague
		Siderite	
Rhombohedral	B	Brown	Prague
		Azurite	
Monoclinic	A	Blue	South Africa
		Malachite	
Monoclinic	A	Green	South Africa

Figure S1 (calcite A)

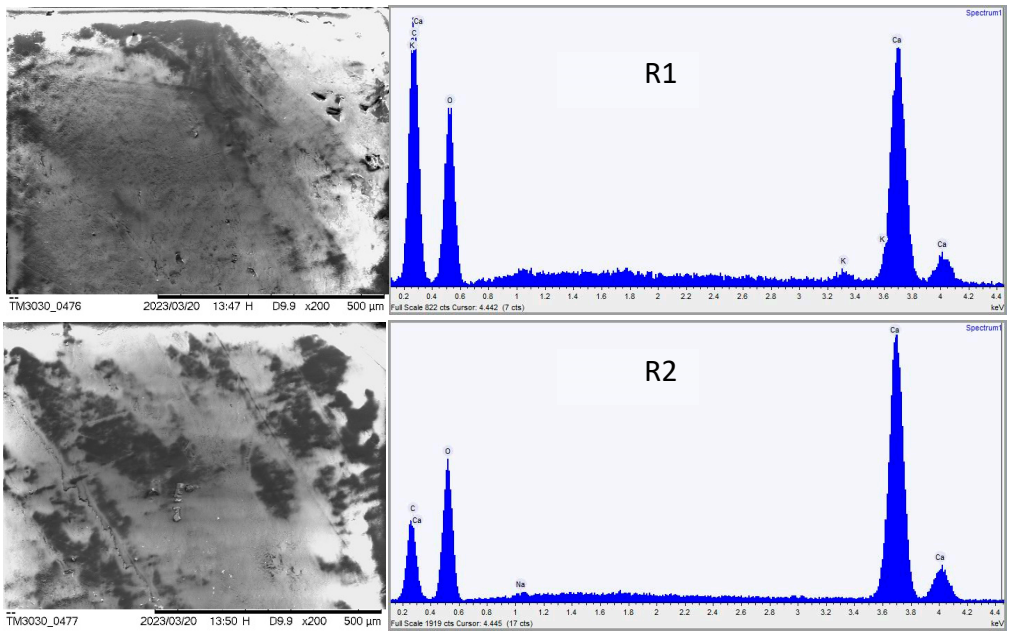


Figure S2 (calcite B)

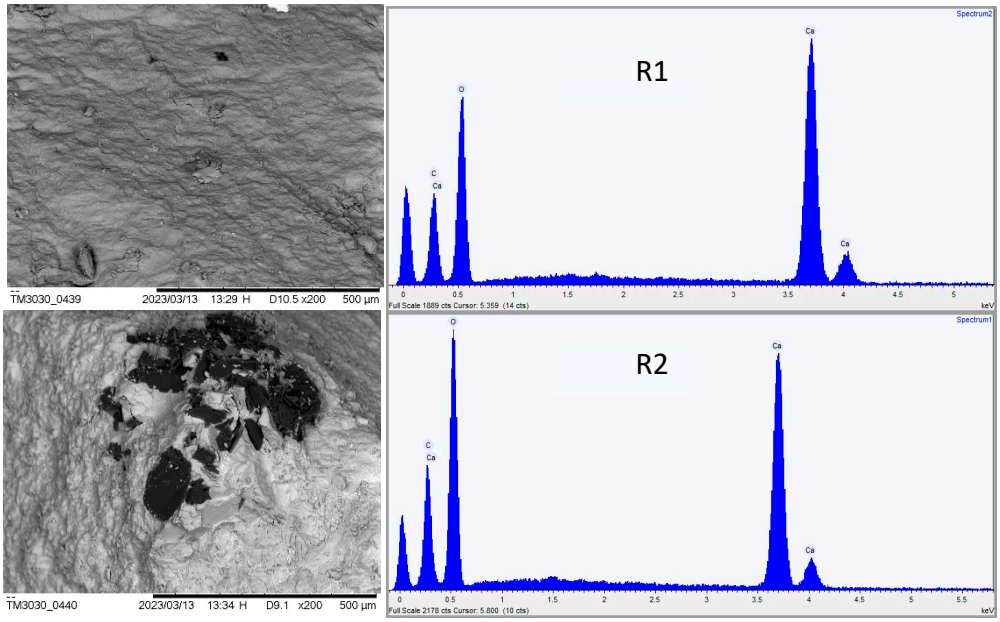


Figure S3 (calcite C)

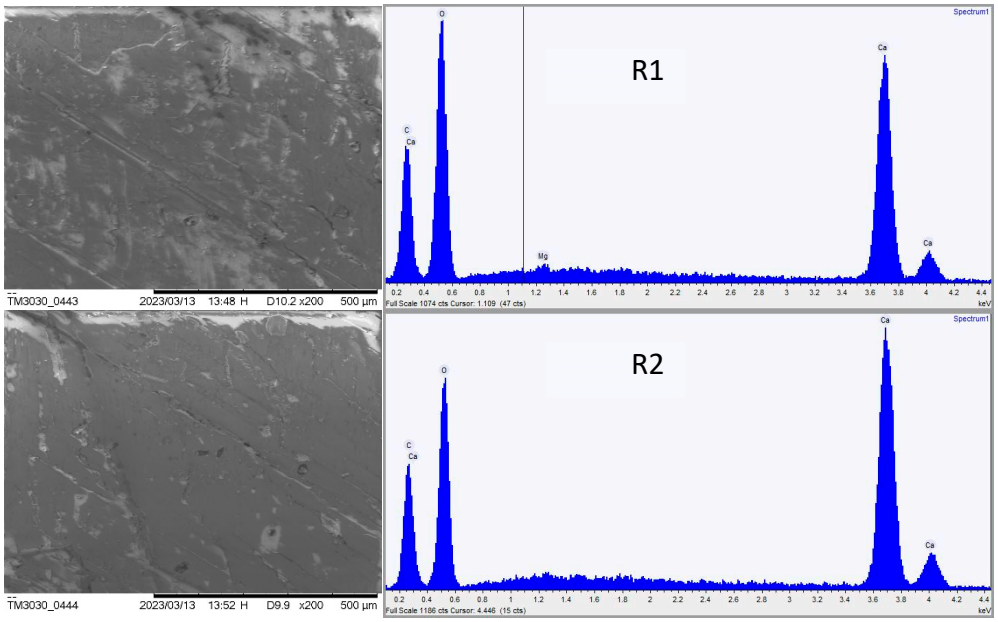


Figure S4 (calcite D)

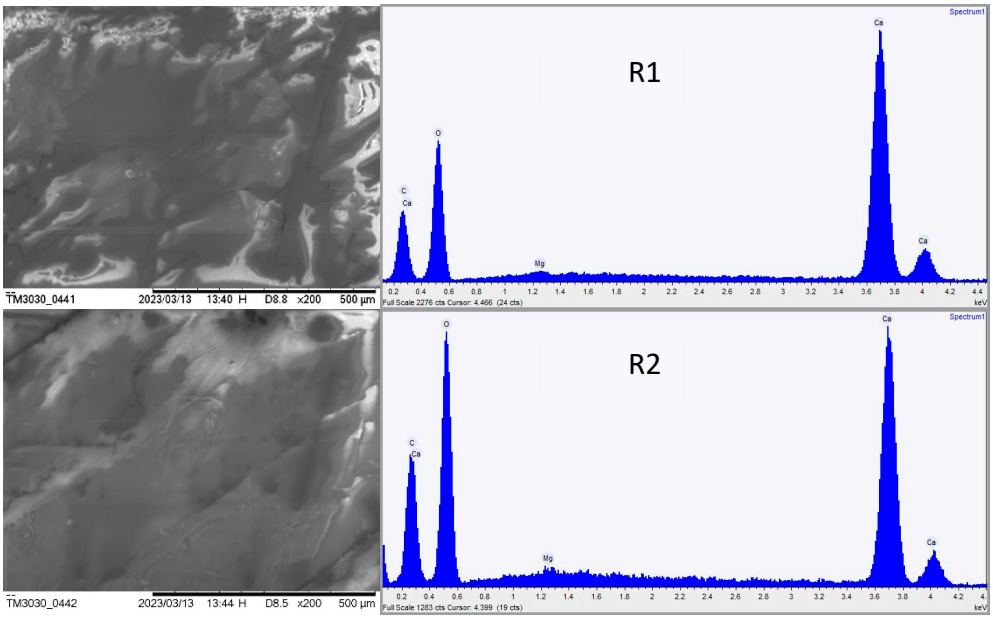


Figure S5 (calcite E)

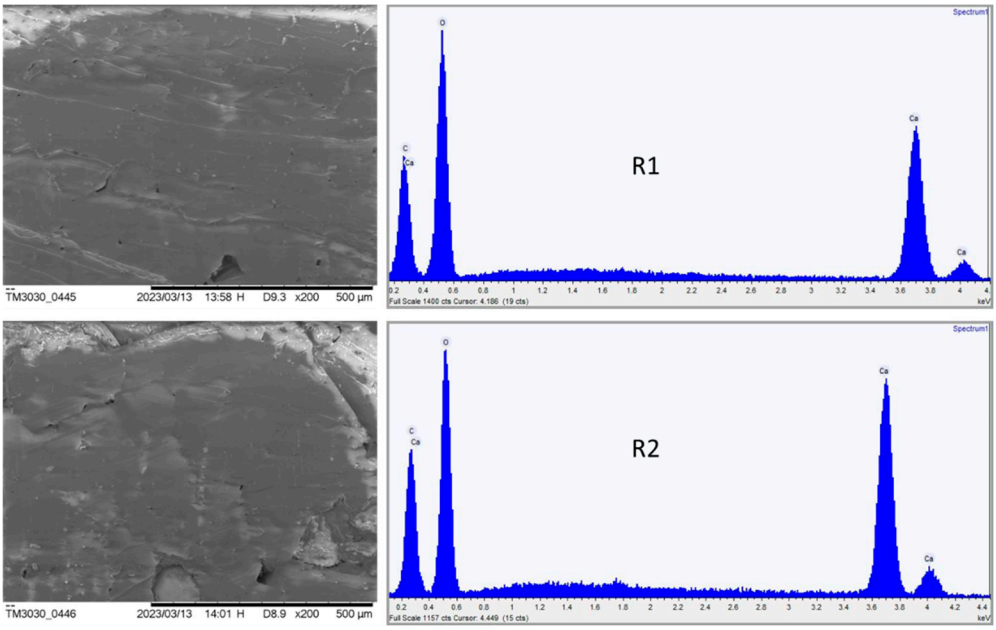


Figure S6 (aragonite A)

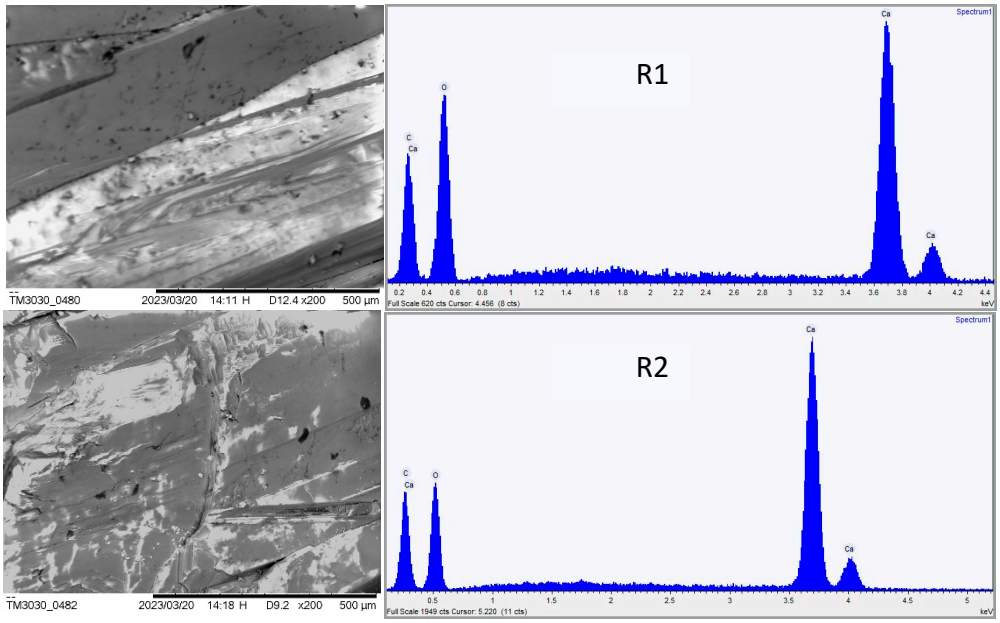


Figure S7 (aragonite B)

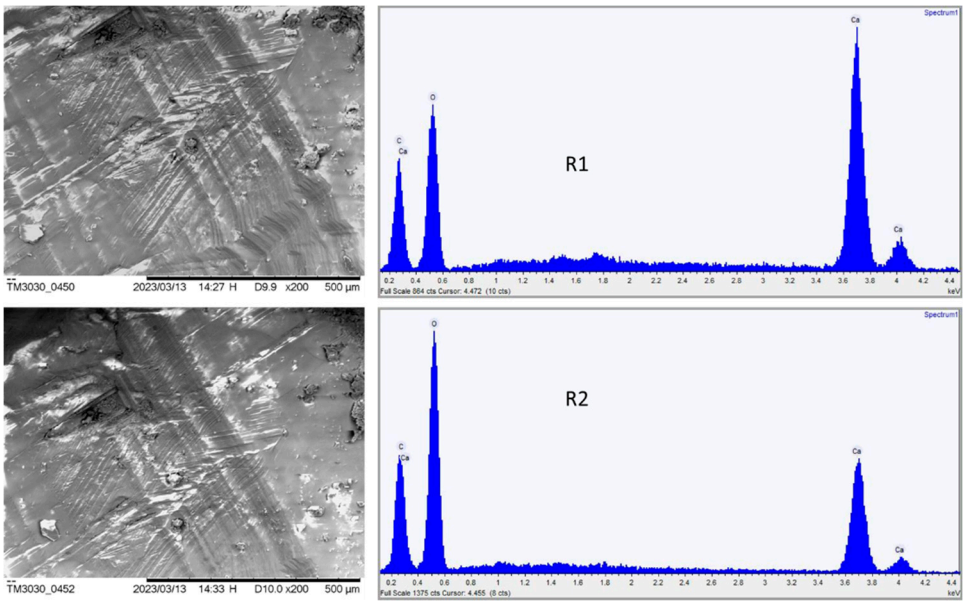


Figure S8 (aragonite C)

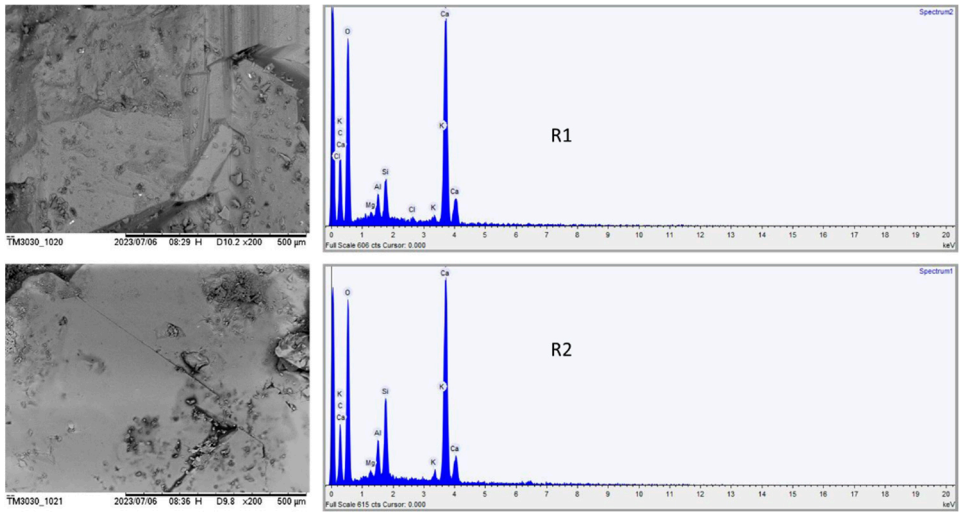


Figure S9 (dolomite A)

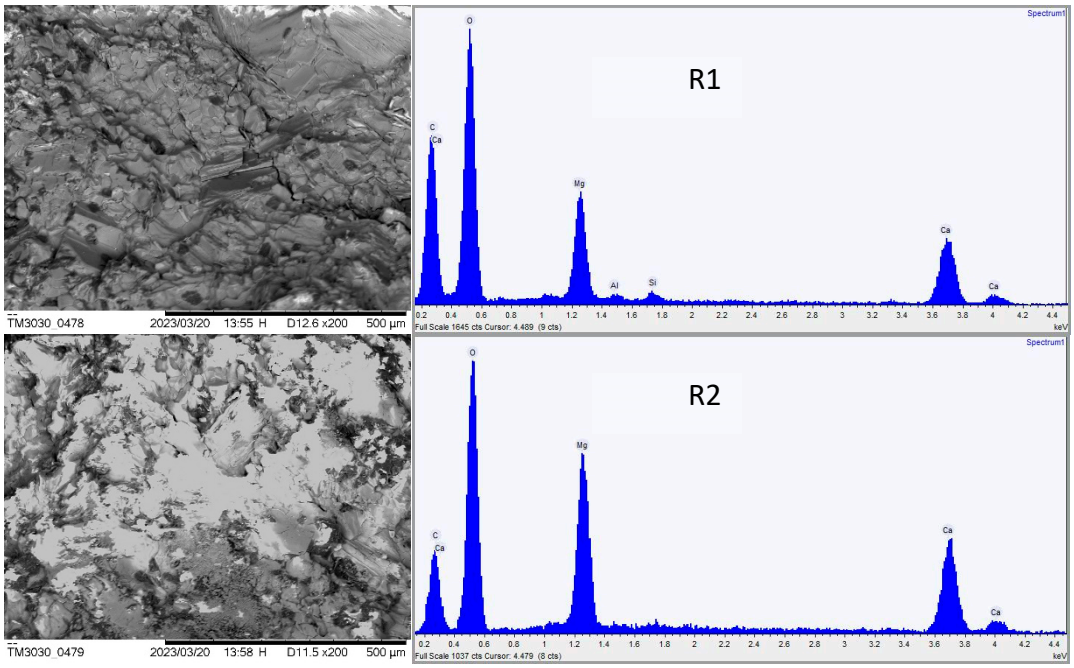


Figure S10 (dolomite B)

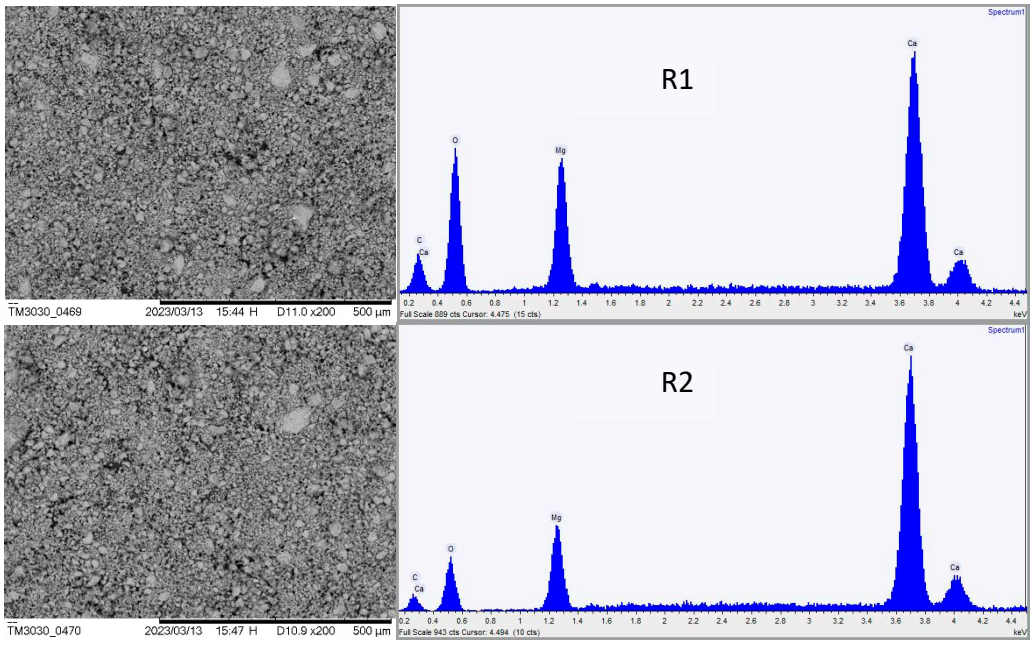


Figure S11 (dolomite C)

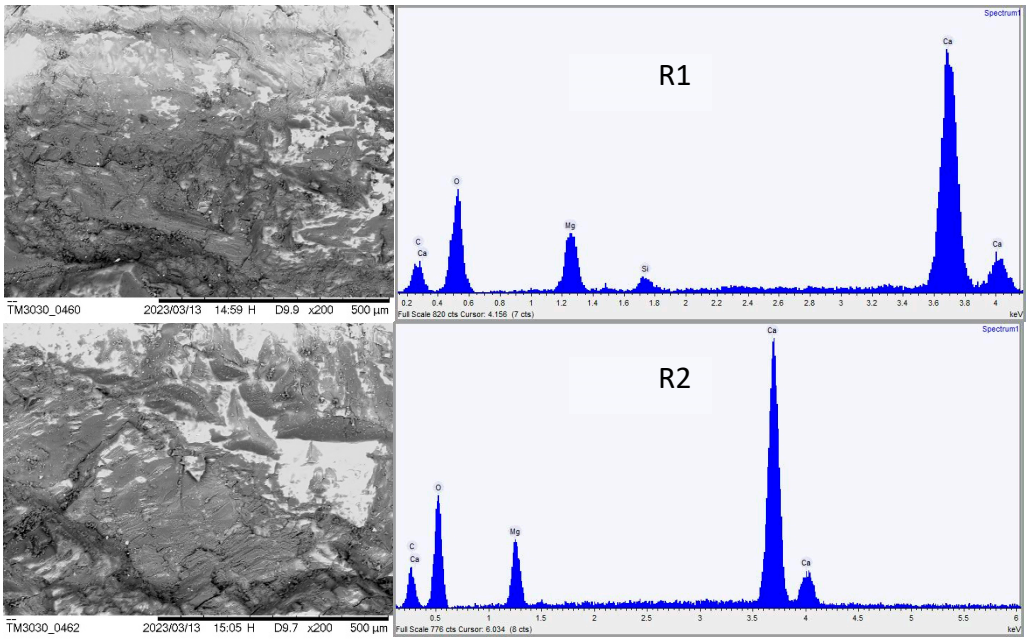


Figure S12 (dolomite D)

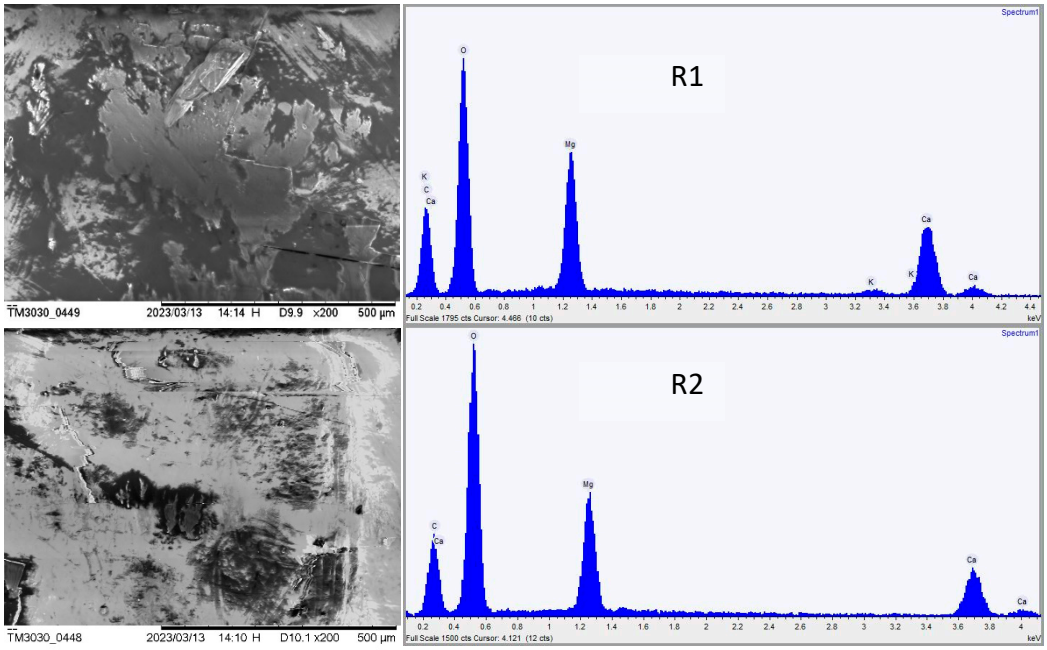


Figure S13 (magnesite A)

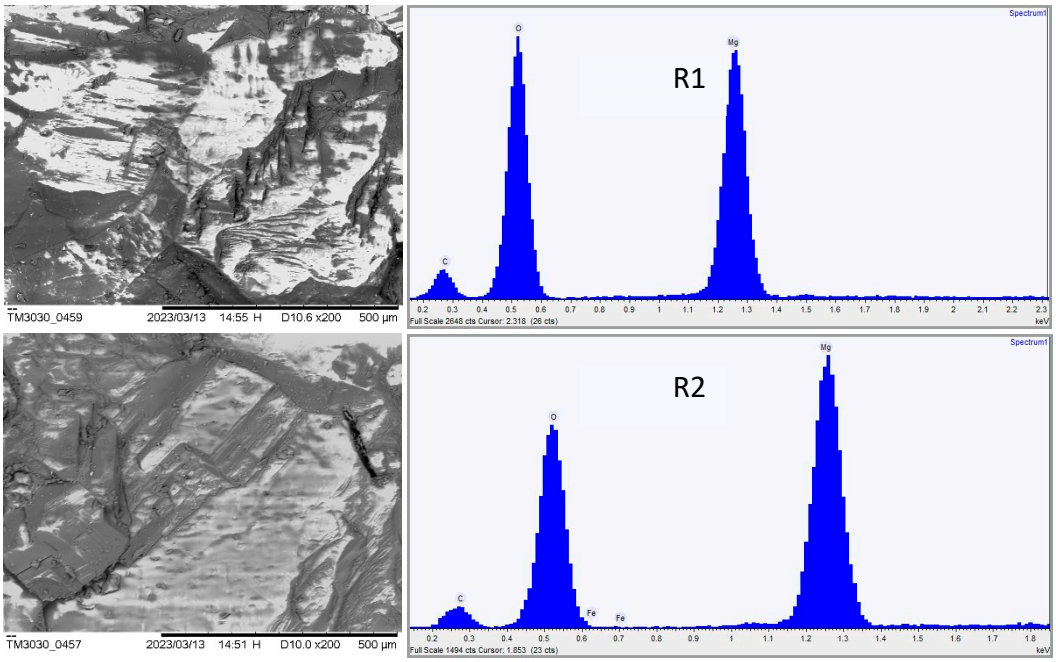


Figure S14 (magnesite B)

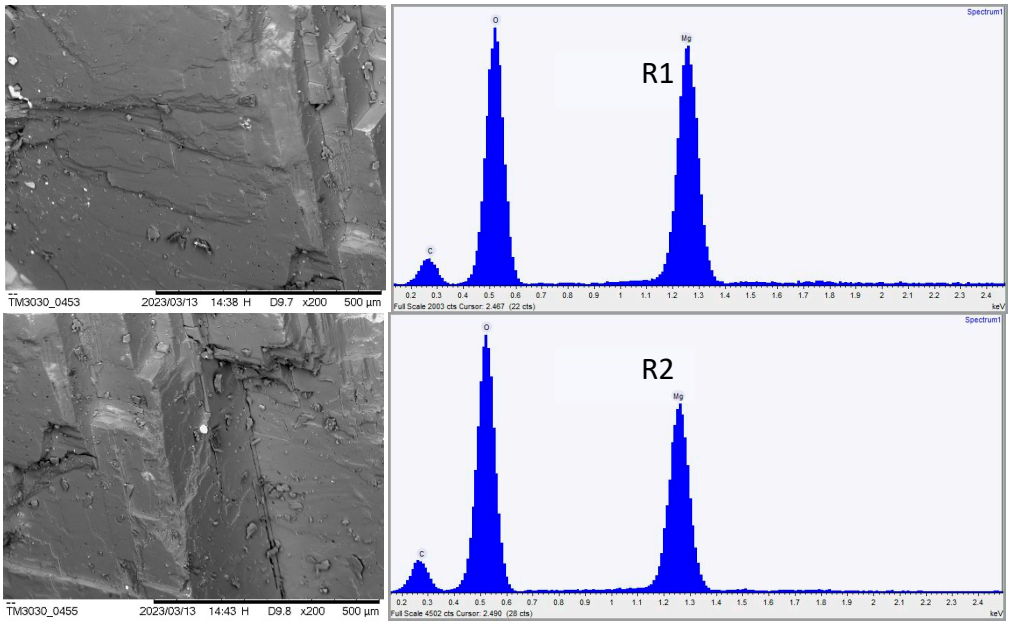


Figure S15 (rhodochrosite A)

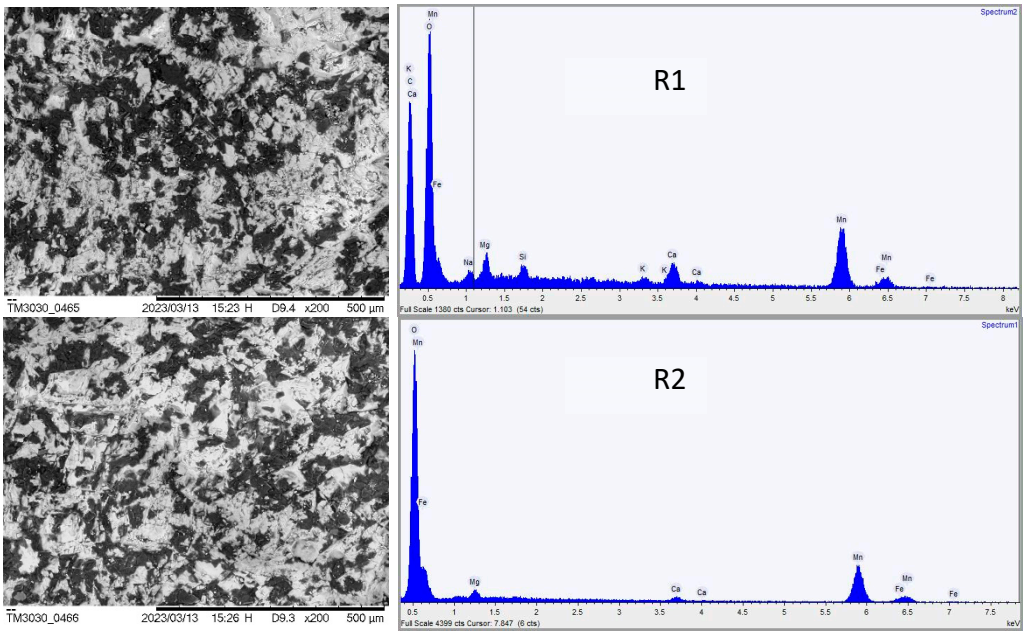


Figure S16 (rhodochrosite B)

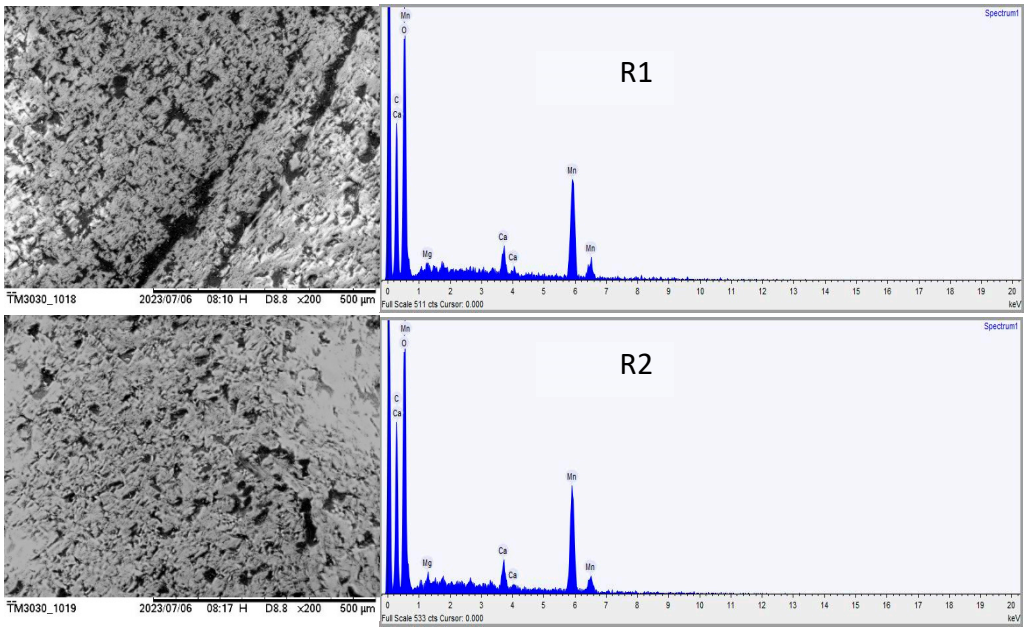


Figure S17 (witherite)

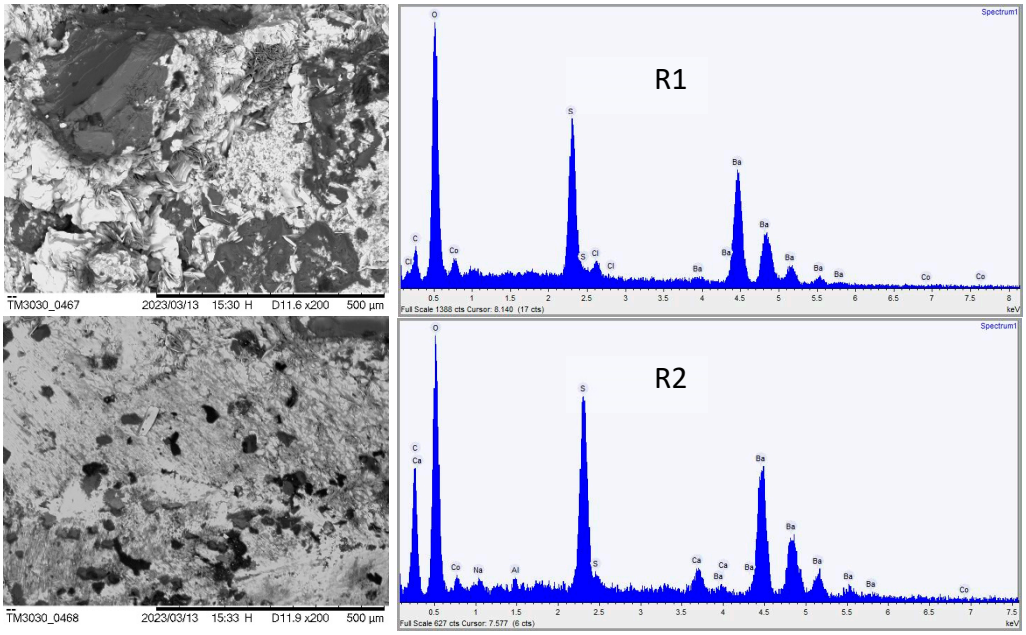


Figure S18 (siderite)

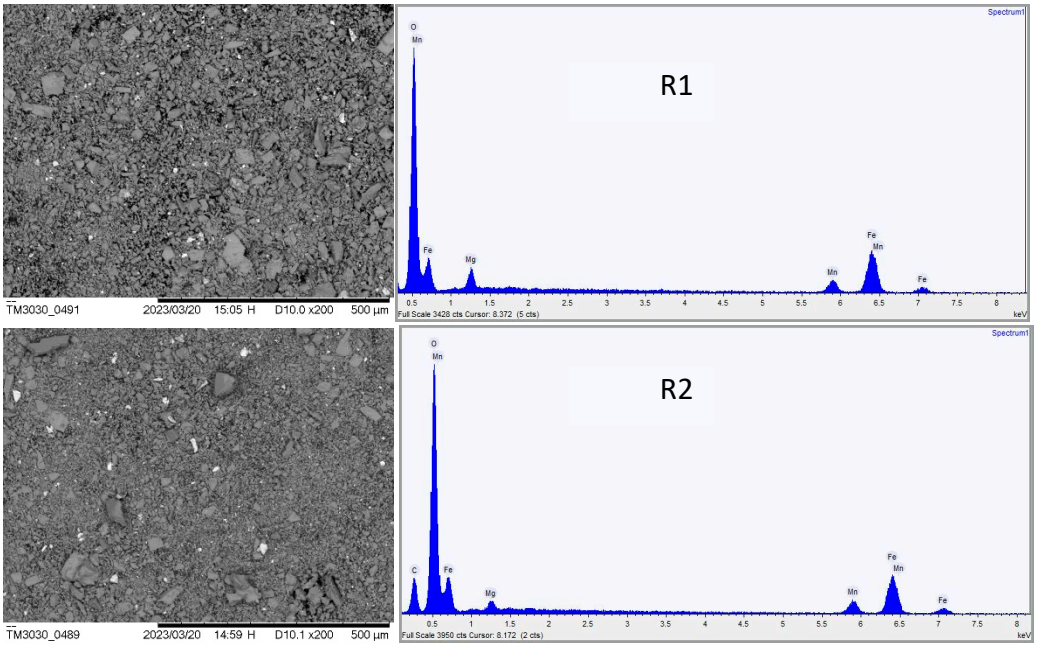


Figure S19 (azurite)

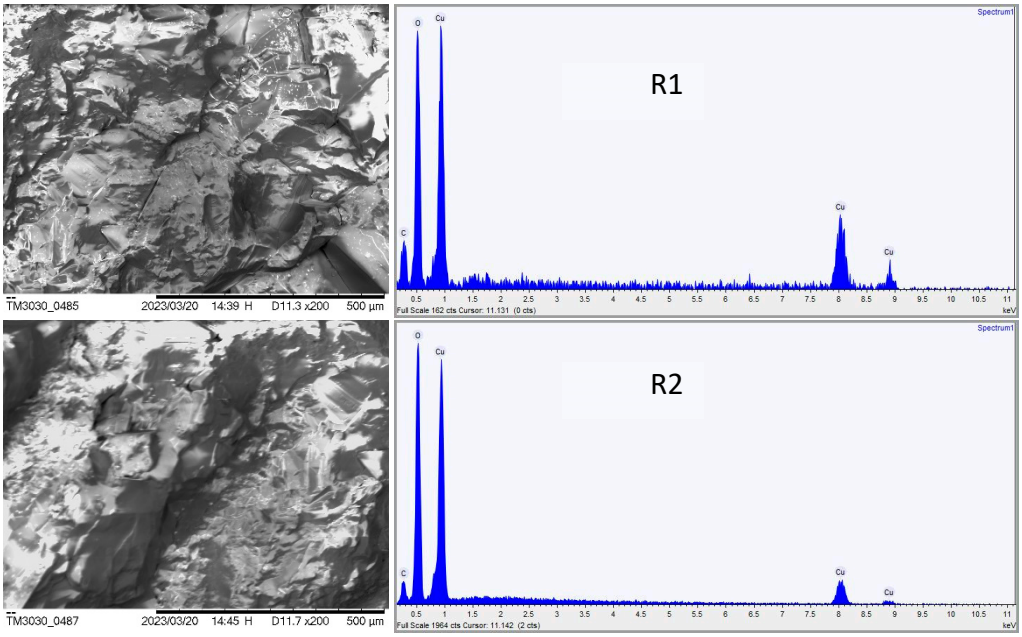


Figure S20 (malachite)

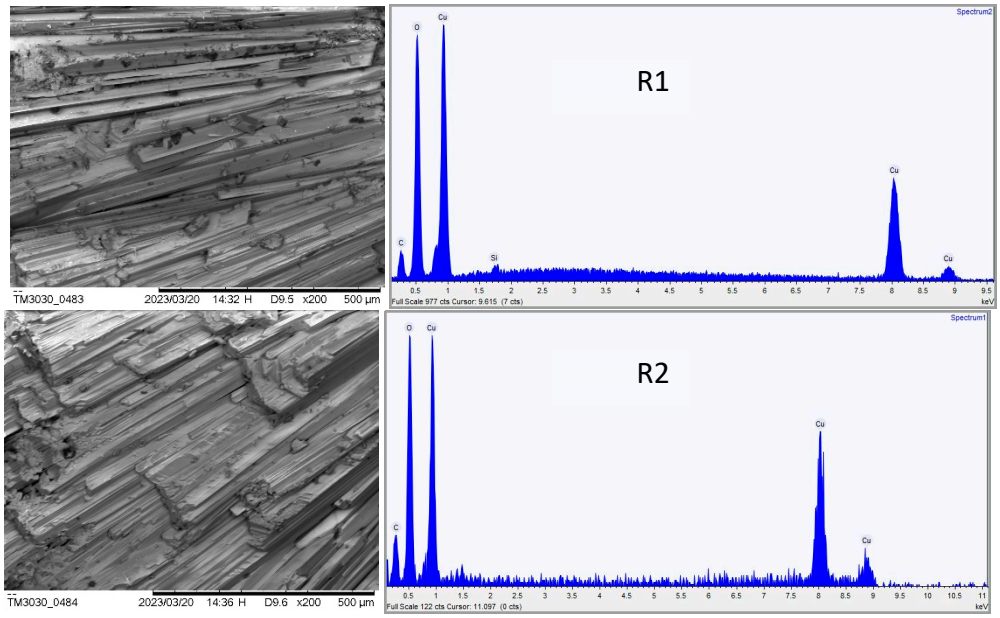


Figure S21 (calcites)

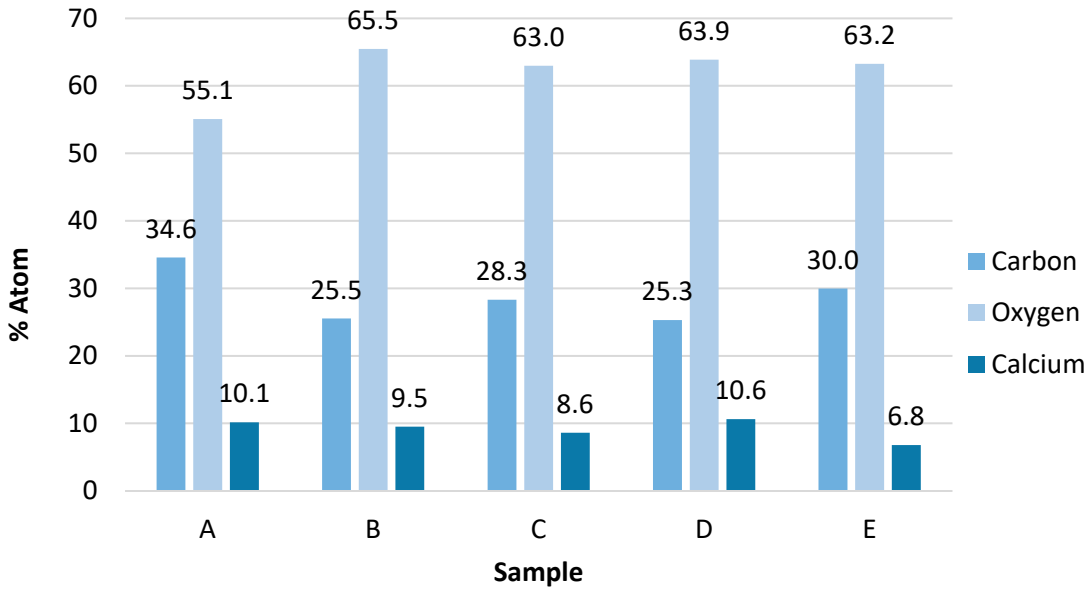


Figure S22 (aragonites)

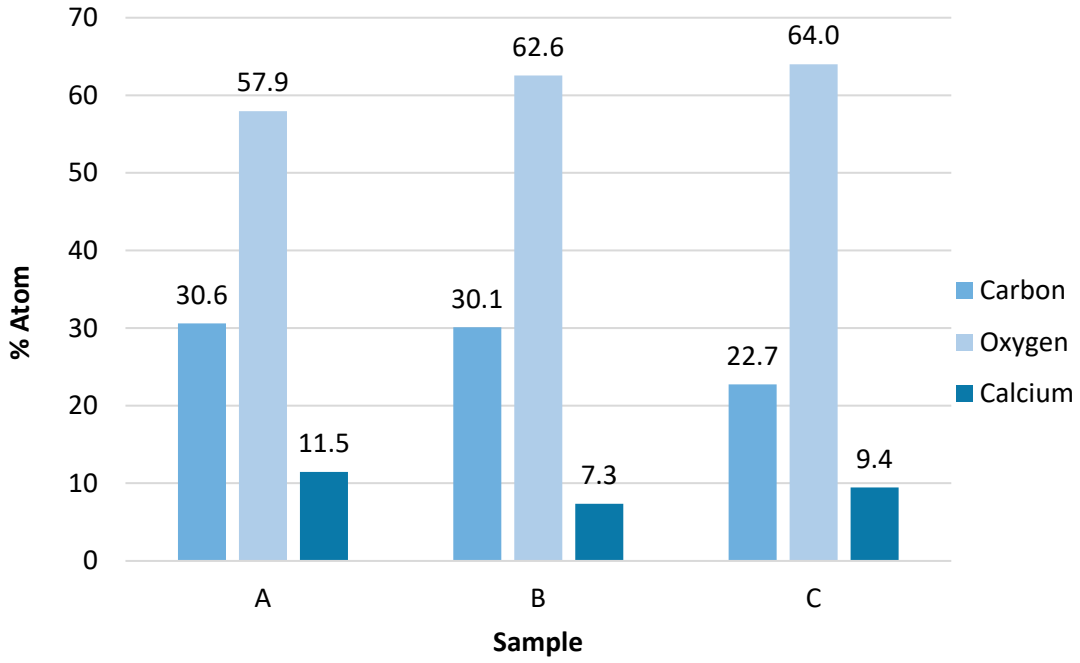


Figure S23 (dolomites)

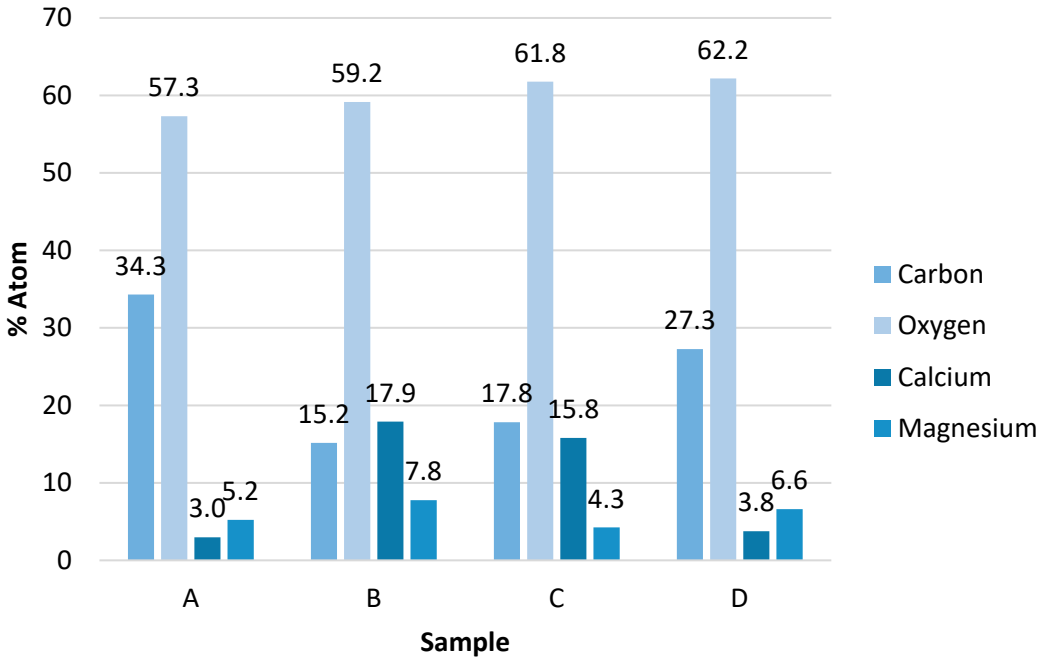


Figure S24 (magnesites)

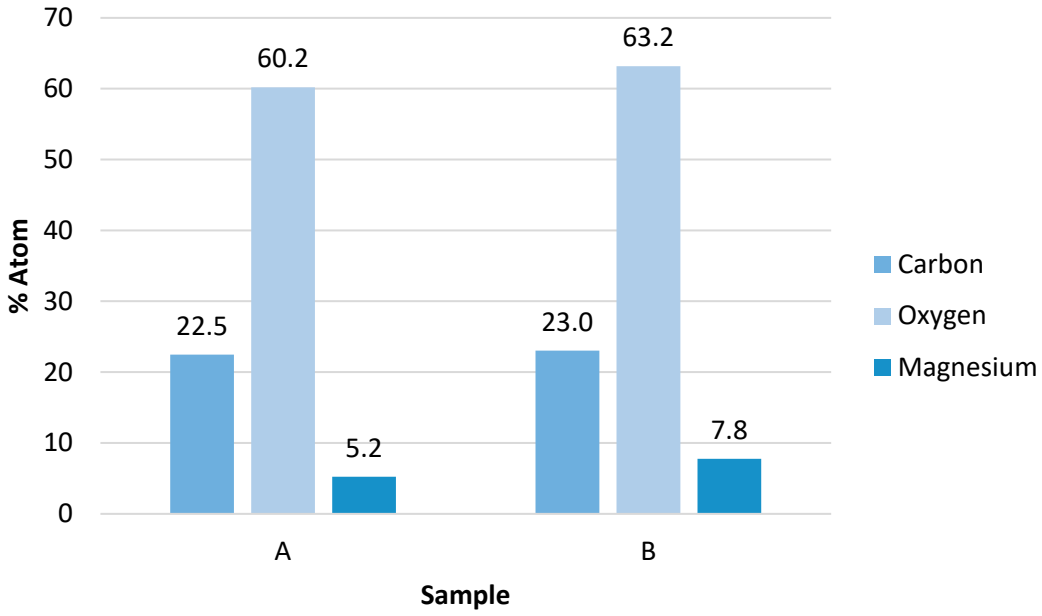


Figure S25 (rhodochrosites)

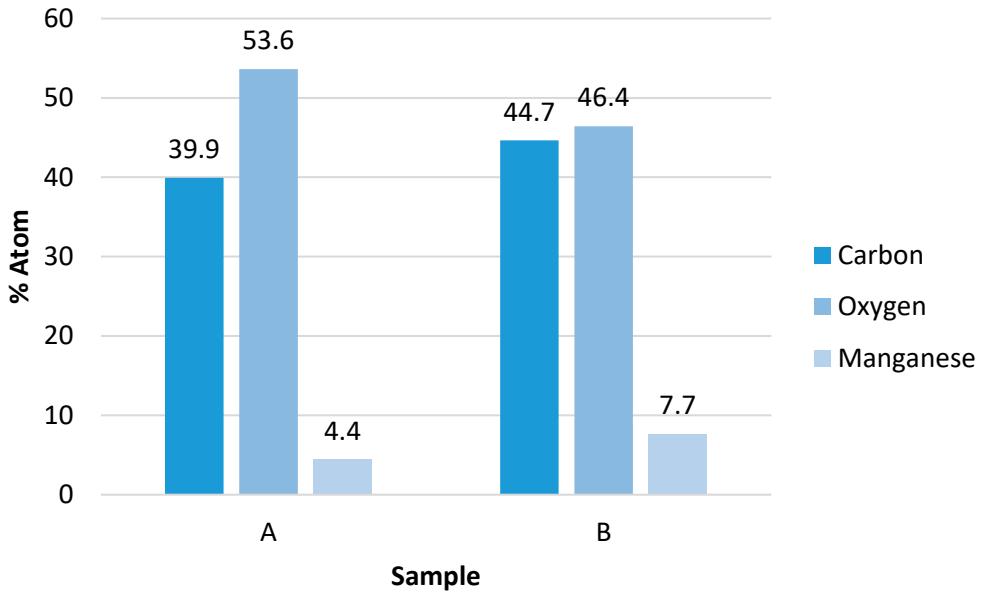


Figure S26 (witherite)

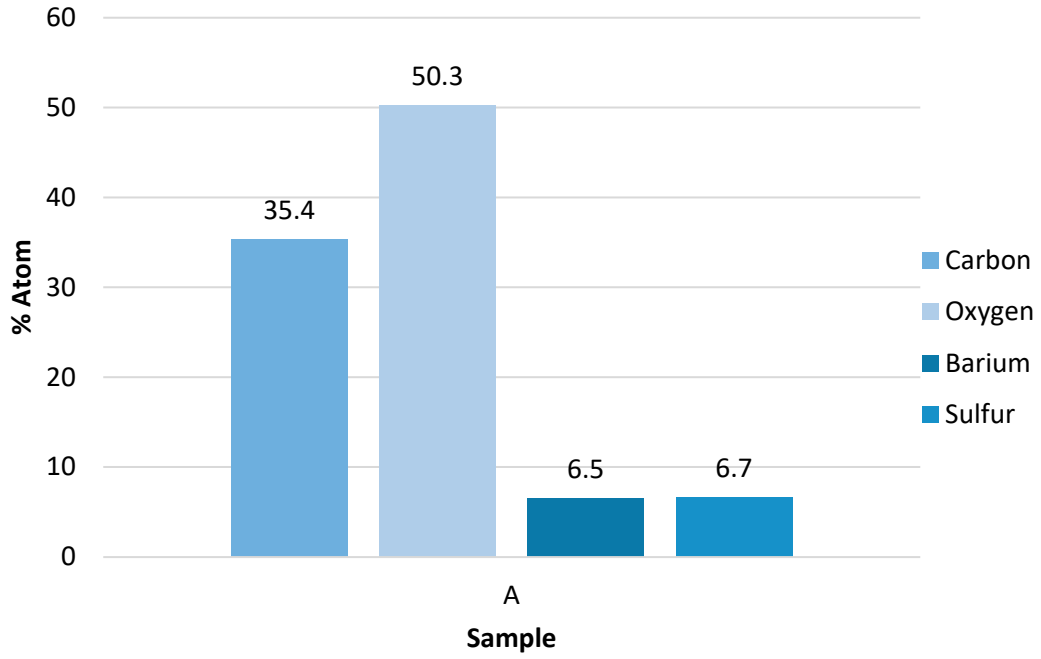


Figure S27 (siderite)

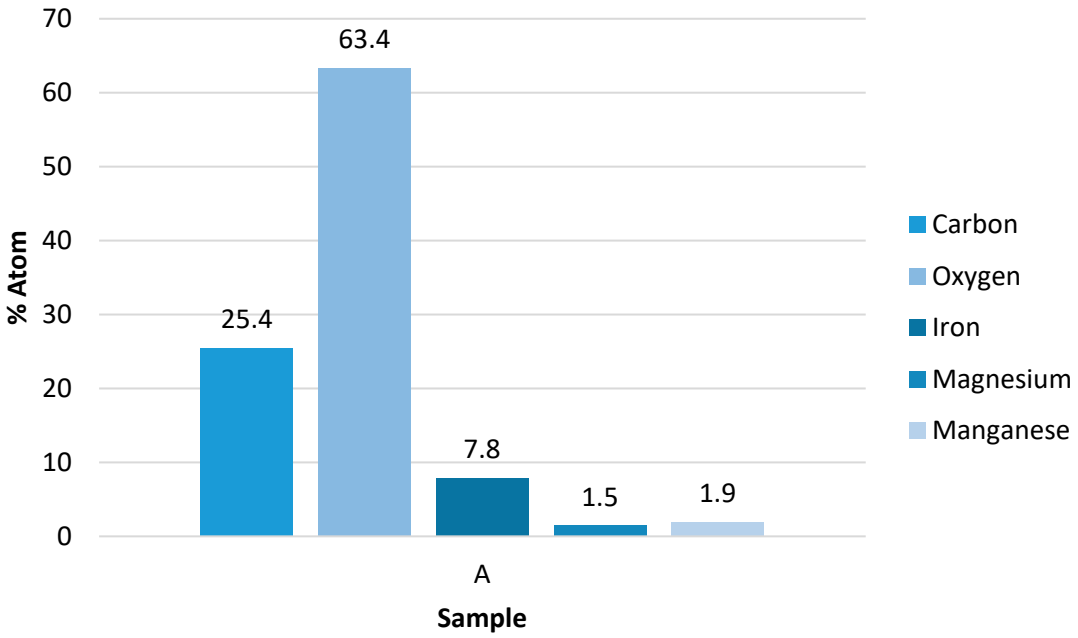


Figure S28 (azurite)

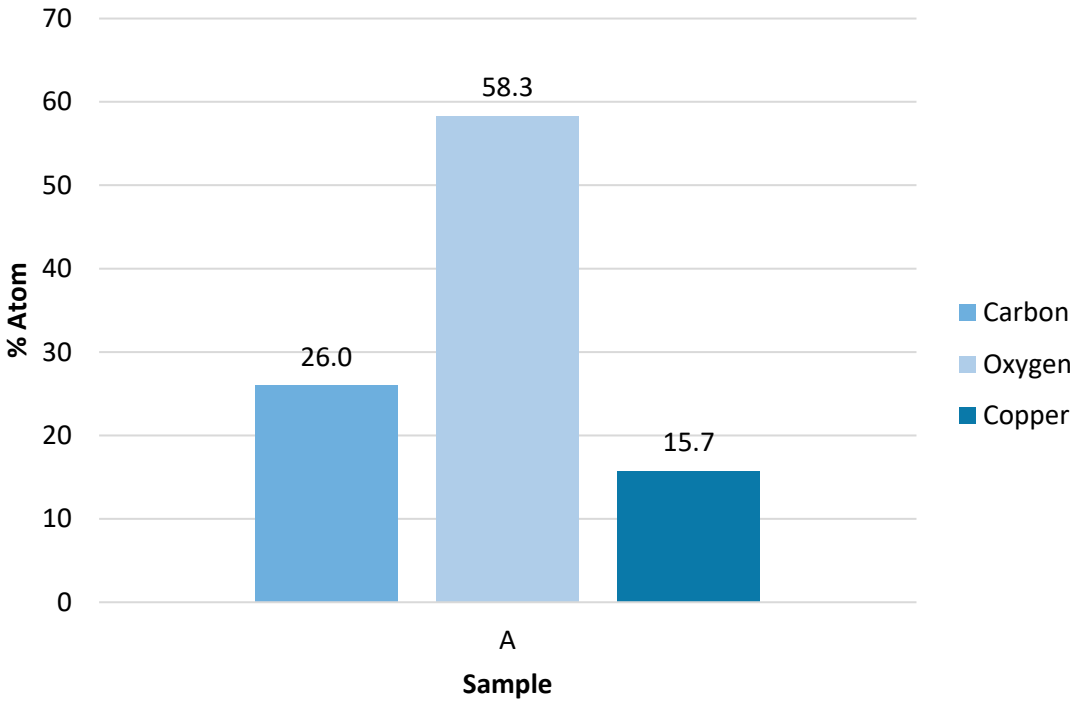


Figure S29 (malachite)

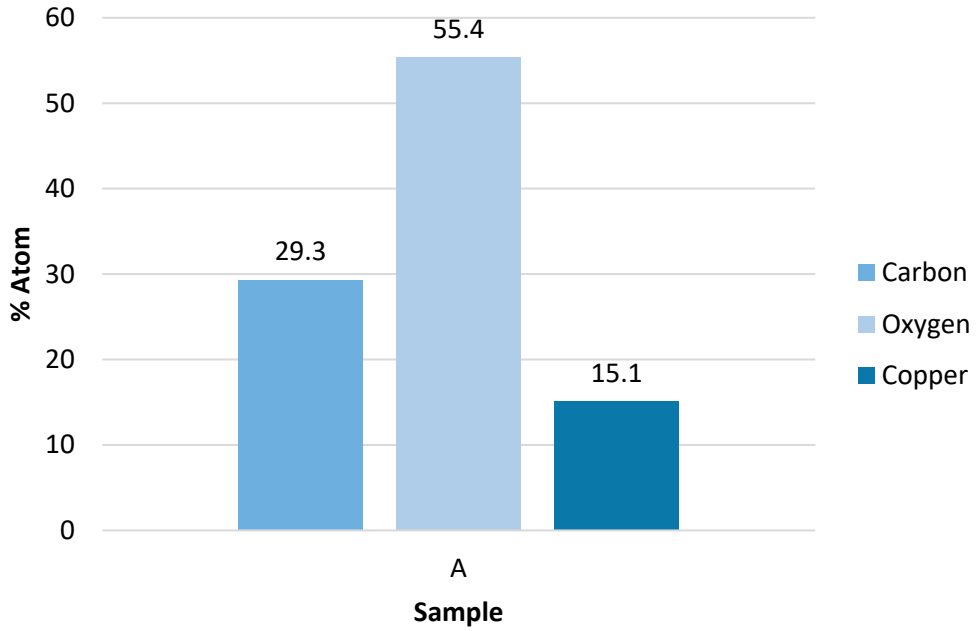
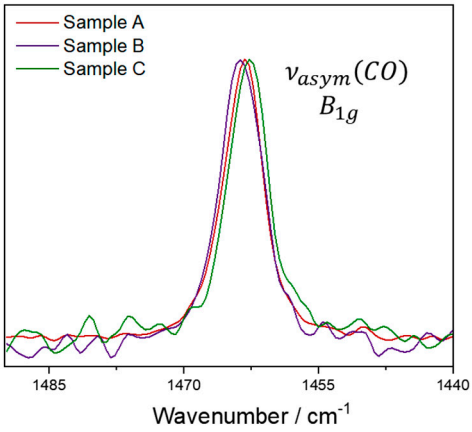
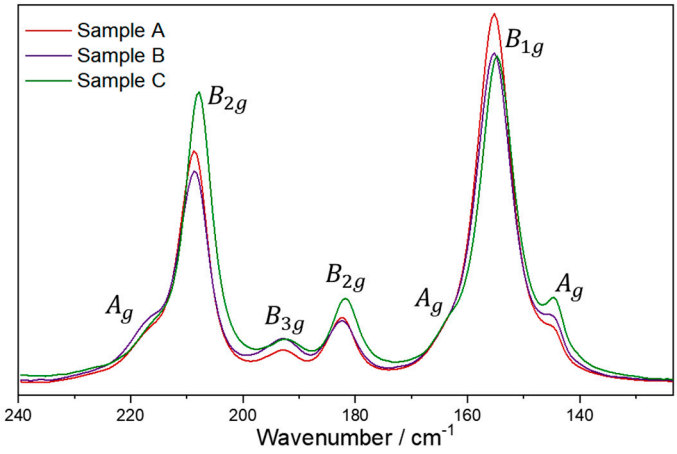
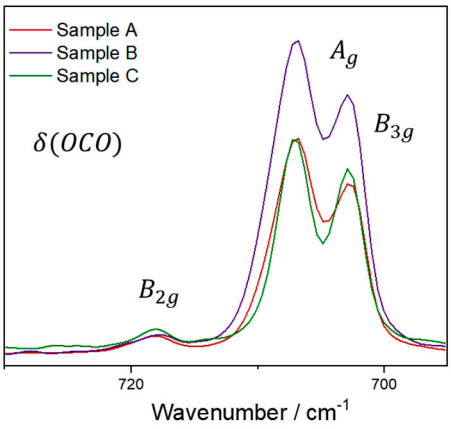
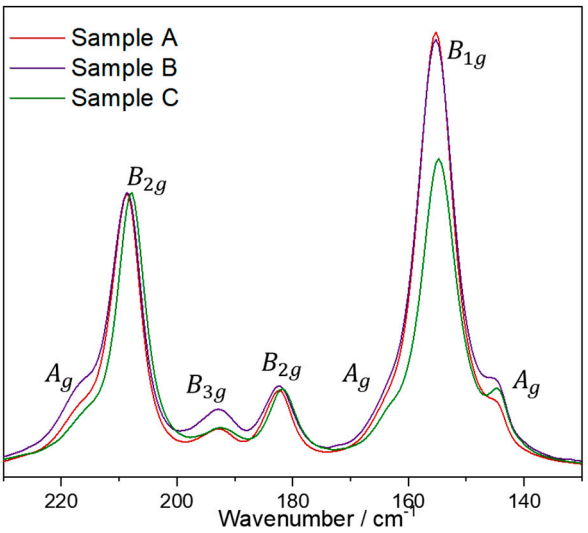


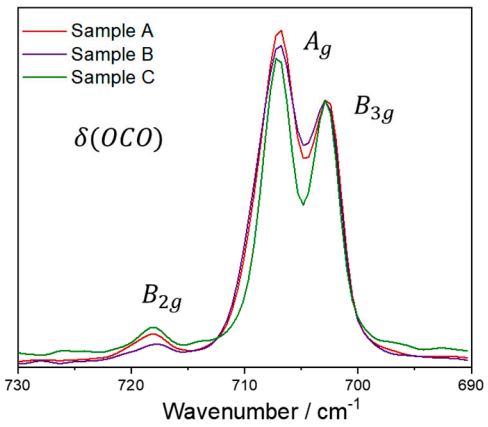
Figure S30


Sample A
Sample B
Sample C
$\nu_{asym}(CO)$
B_{1g}
1485
1470
1455
1440
Wavenumber / cm^{-1}


Sample A
Sample B
Sample C
B_{1g}
B_{2g}
A_g
B_{3g}
B_{2g}
A_g
A_g
240
220
200
180
160
140
Wavenumber / cm^{-1}


Sample A
Sample B
Sample C
$\delta(OCO)$
A_g
B_{3g}
B_{2g}
720
700
Wavenumber / cm^{-1}


Sample A
Sample B
Sample C
B_{1g}
B_{2g}
A_g
B_{3g}
B_{2g}
A_g
A_g
220
200
180
160
140
Wavenumber / cm^{-1}


Sample A
Sample B
Sample C
$\delta(OCO)$
A_g
B_{3g}
B_{2g}
730
720
710
700
690
Wavenumber / cm^{-1}

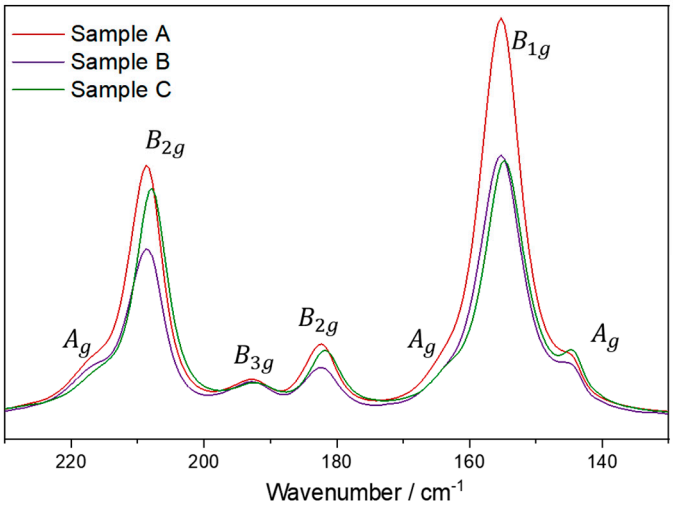

Sample A
Sample B
Sample C
B_{1g}
B_{2g}
A_g
B_{3g}
B_{2g}
A_g
A_g
220
200
180
160
140
Wavenumber / cm^{-1}

Figure S31

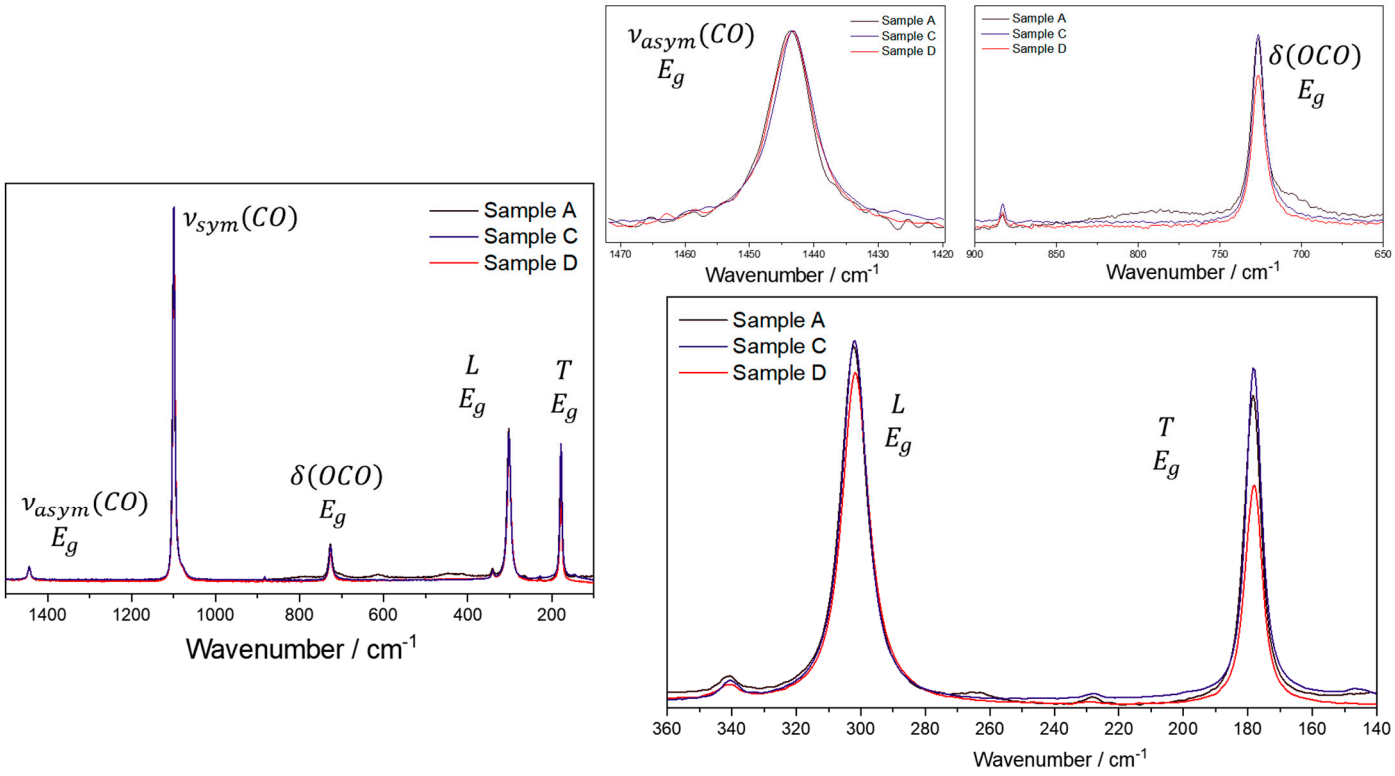


Figure S32

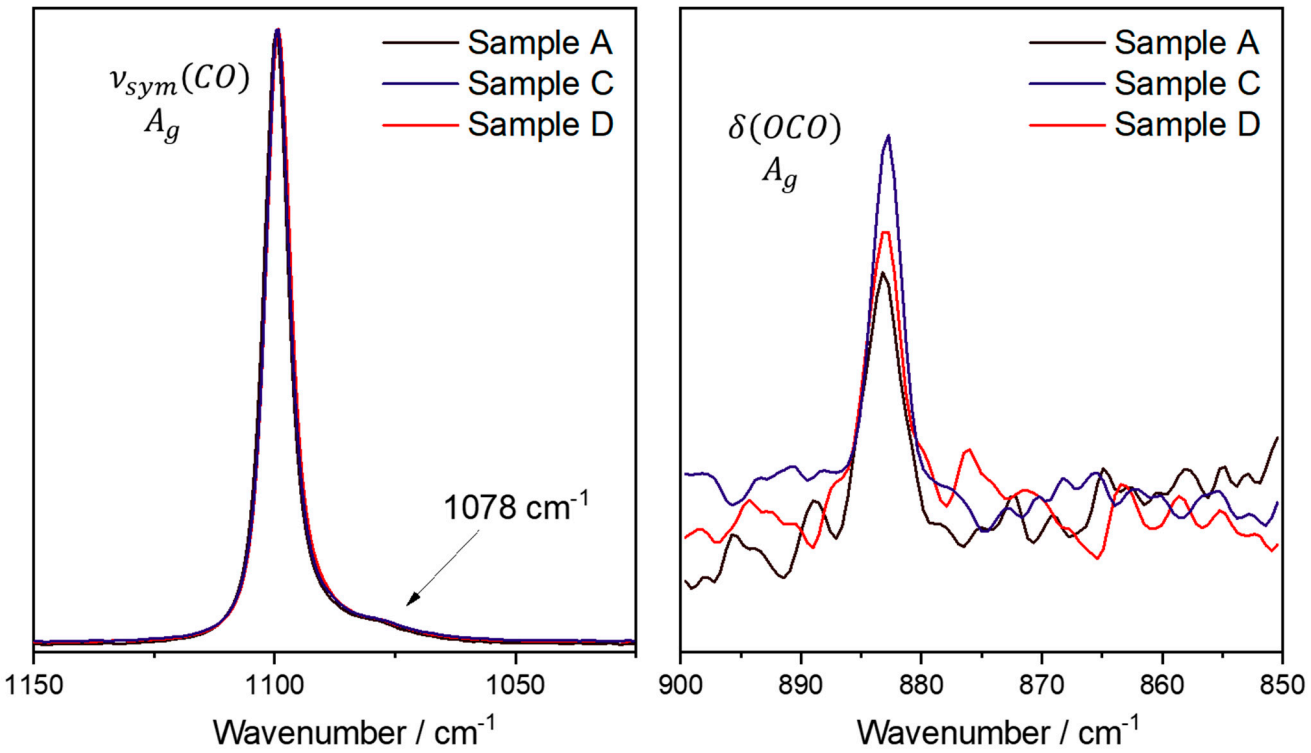


Figure S33

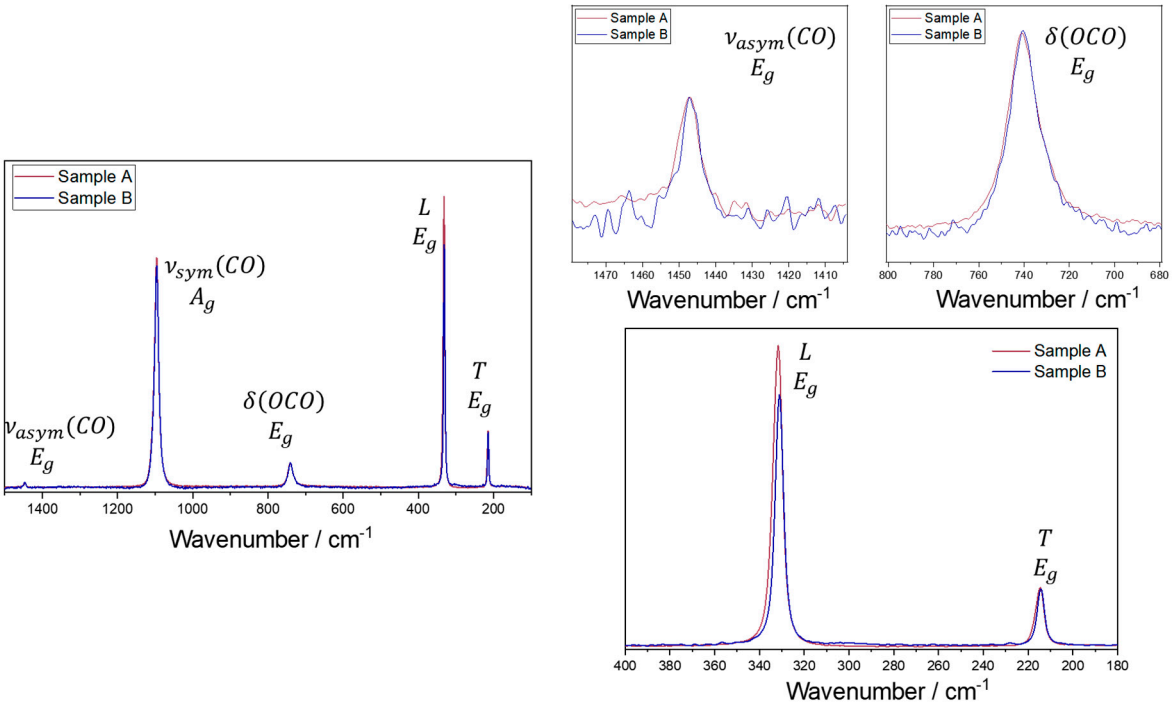
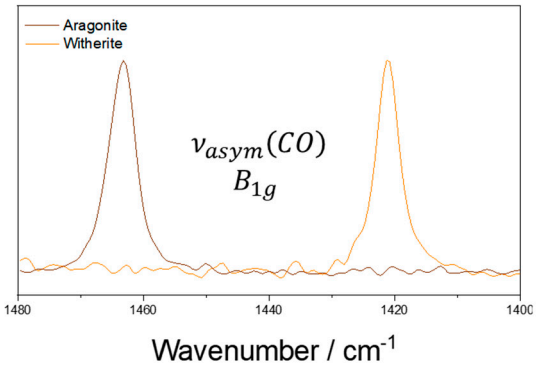
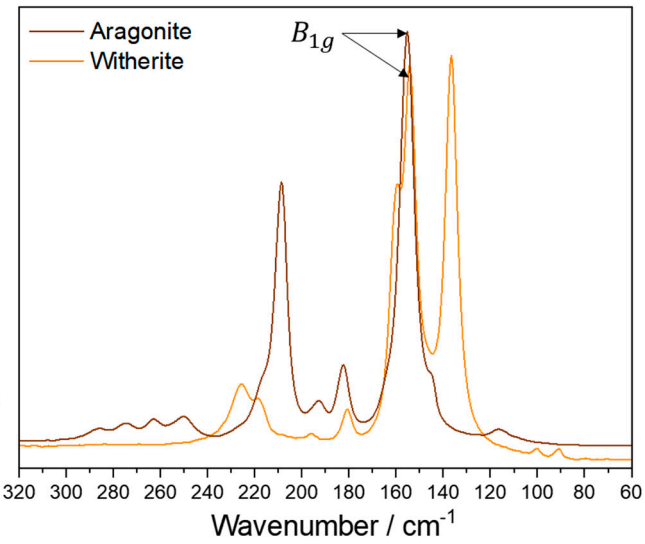
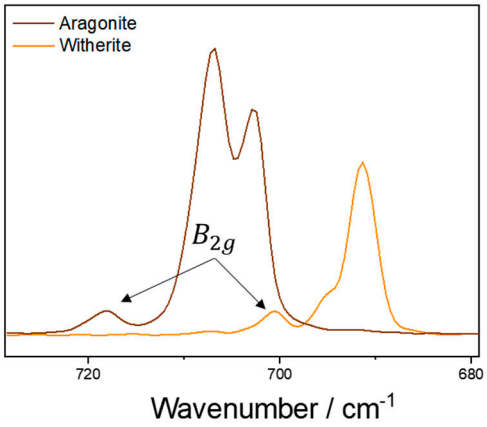
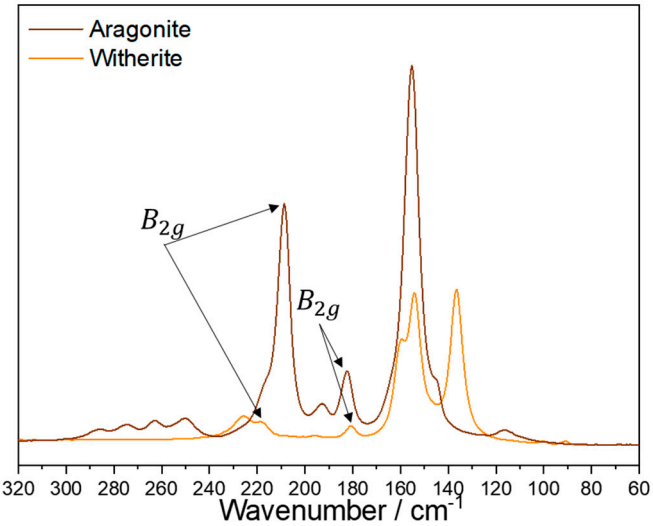

Sample A
Sample B
$\nu_{asym}(CO)$
E_g
$\nu_{sym}(CO)$
A_g
$\delta(OCO)$
E_g
L
E_g
T
E_g
1400 1200 1000 800 600 400 200
Wavenumber / cm-1
1470 1460 1450 1440 1430 1420 1410
800 780 760 740 720 700 680
400 380 360 340 320 300 280 260 240 220 200 180

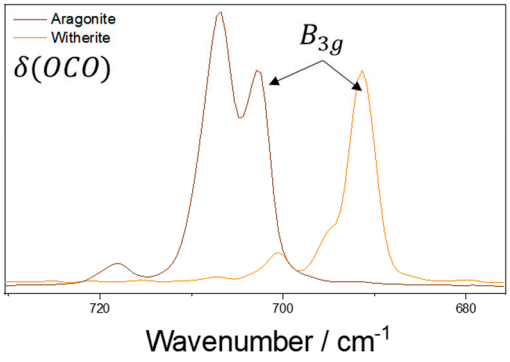
Figure S34


Aragonite
Witherite
$\nu_{asym}(CO)$
B_{1g}
1480
1460
1440
1420
1400
Wavenumber / cm^{-1}


Aragonite
Witherite
B_{1g}
320 300 280 260 240 220 200 180 160 140 120 100 80 60
Wavenumber / cm^{-1}


Aragonite
Witherite
B_{2g}
720
700
680
Wavenumber / cm^{-1}


Aragonite
Witherite
B_{2g}
B_{2g}
320 300 280 260 240 220 200 180 160 140 120 100 80 60
Wavenumber / cm^{-1}


Aragonite
Witherite
$\delta(OCO)$
B_{3g}
720
700
680
Wavenumber / cm^{-1}

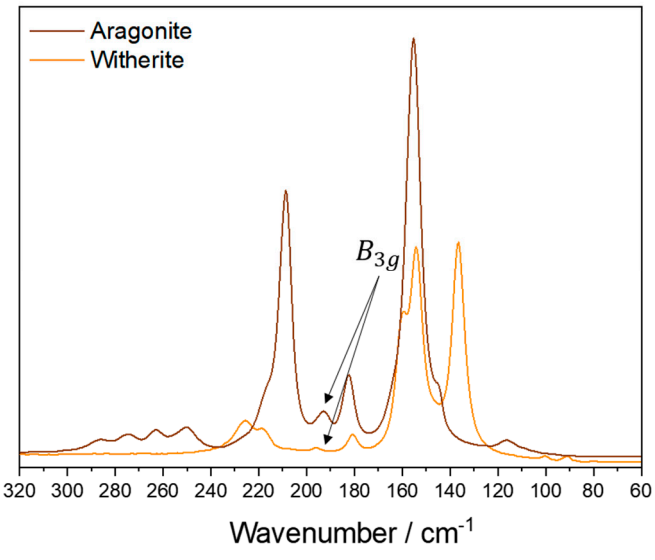

Aragonite
Witherite
B_{3g}
320 300 280 260 240 220 200 180 160 140 120 100 80 60
Wavenumber / cm^{-1}

Figure S35

Calcite A

Calcite B

Calcite C

Calcite D

Calcite E

Magnesite A

Magnesite B

Dolomite A

Dolomite B

Dolomite C

Dolomite D

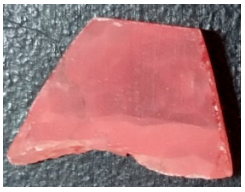
Aragonite A

Aragonite B

Aragonite C

Rhodochrosite A

Rhodochrosite B



Witherite

Siderite

Malachite

Azurite