

# Supplementary Materials for

## In situ Identification of Hydrated Carbonates on Mars

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Data S1

SHERLOC Team Members

## Supplementary Text

### Arrhenius equation

The Arrhenius equation describes the temperature dependence of reaction rates:

$$k = Ae^{-E_a/RT}$$

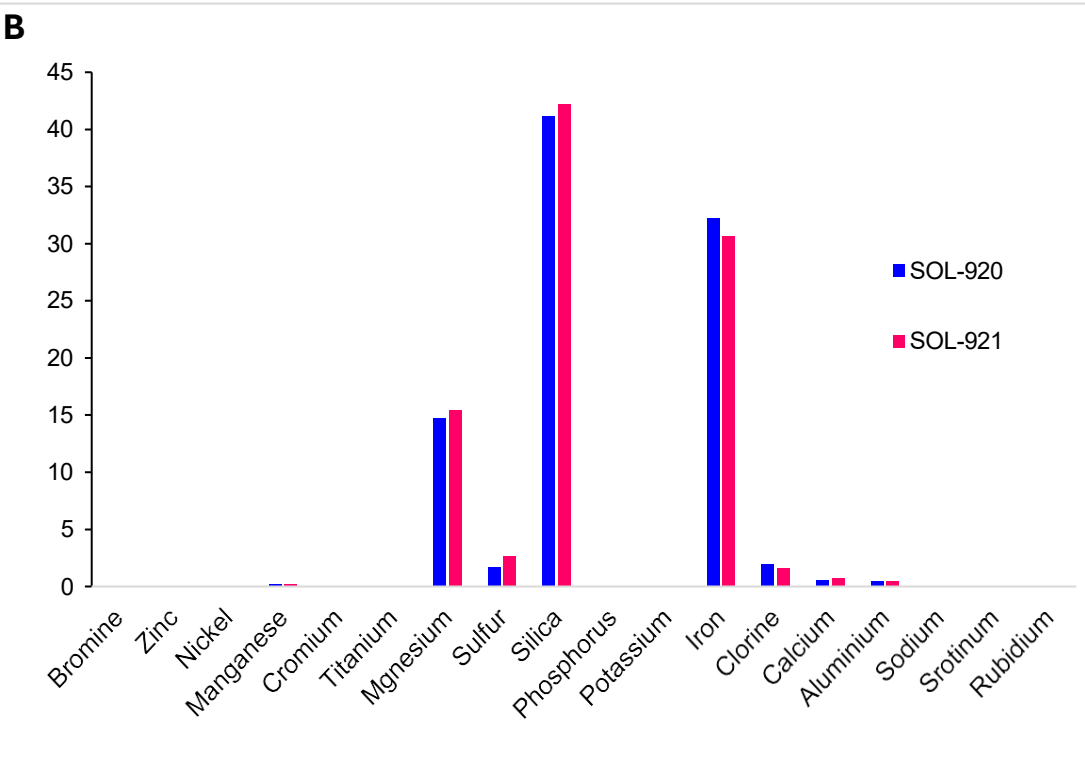
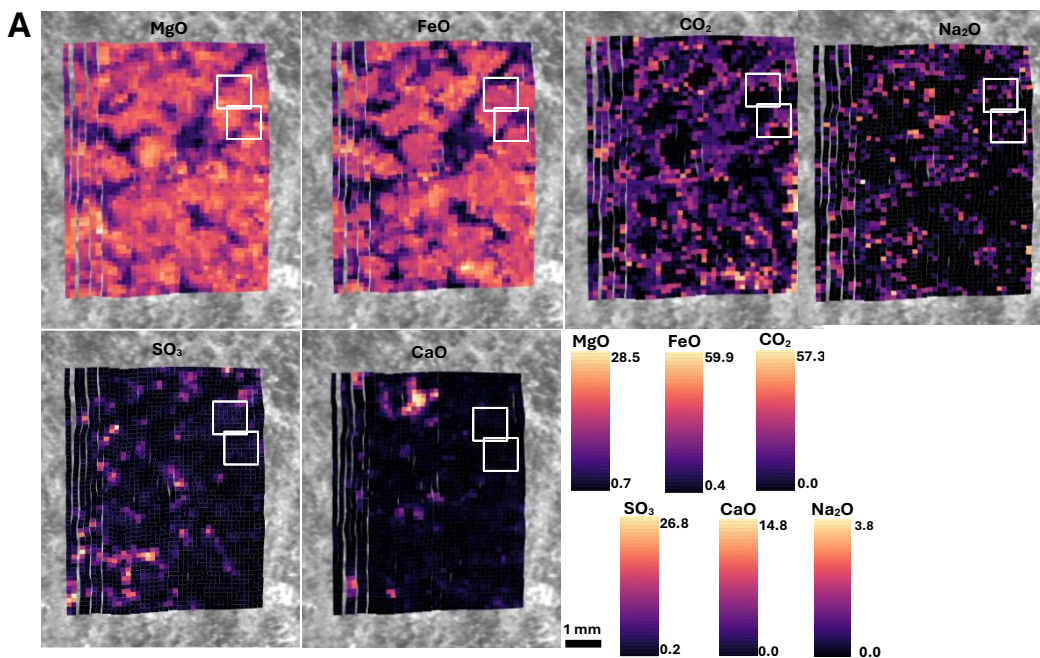
where:

- $k$  is the reaction rate constant,
- $A$  is the pre-exponential factor or Arrhenius factor,
- $E_a$  is the activation energy ( $\text{J mol}^{-1}$ )
- $R$  is the universal gas constant ( $8.314 \text{ J mol}^{-1} \text{ K}^{-1}$ )
- $T$  is the absolute temperature

Note: This expression shows that even modest decreases in temperature cause exponential decreases in reaction rates. For metastable carbonates like lansfordite and nesquehonite, this means that transformations/dehydration occurring on laboratory timescales at warm temperatures (31) should effectively stall under subzero Martian conditions.

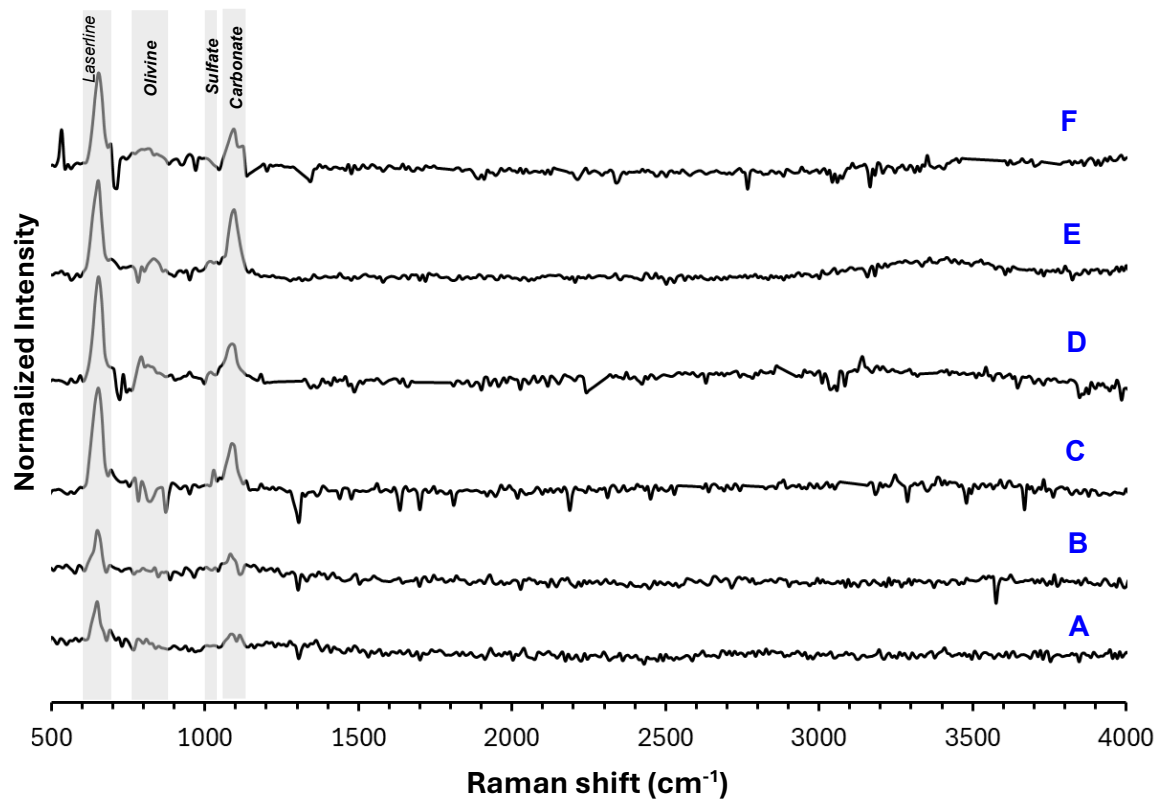
**Fig. S1.**

PIXL element abundance in the Amherst Point Sol 921 dataset. **A)** PIXL footprint on PIXL's Micro Context Camera (MCC), where the wt% distribution of MgO, FeO, CO<sub>2</sub>, Na<sub>2</sub>O, SO<sub>3</sub>, and CaO is shown. White boxes show the approximate position of the Sol 921 SHERLOC detail 1 (upper) and 2 (below). **B)** PIXL element oxide bulk chemistry across Sol 920 and 921 scans.



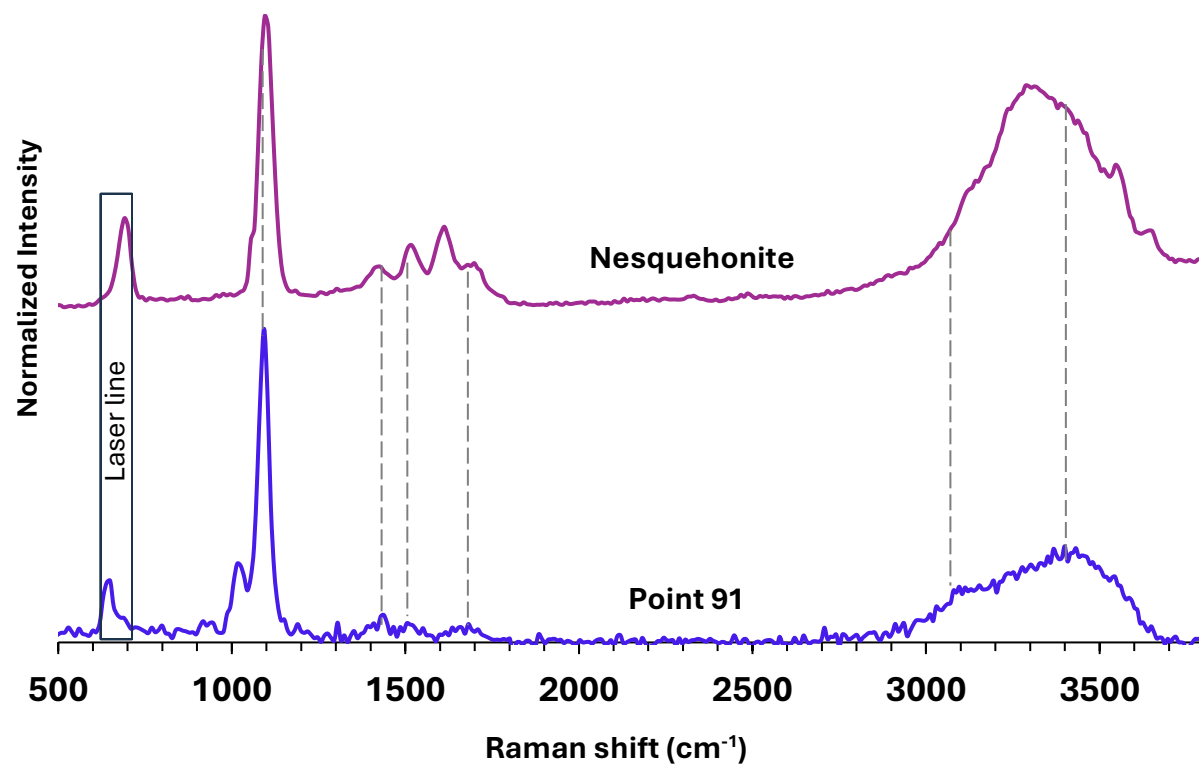
**Fig. S2.**

Total average background-subtracted SHERLOC Raman spectra of the Amherst Point detail and survey scans. A) sol 920 survey scan, B) sol 921 survey scan, C) sol 920 detail 1 scan, D) sol 920 detail 2 scan, E) sol 921 detail 1 scan, and F) sol 921 detail 2 scan.



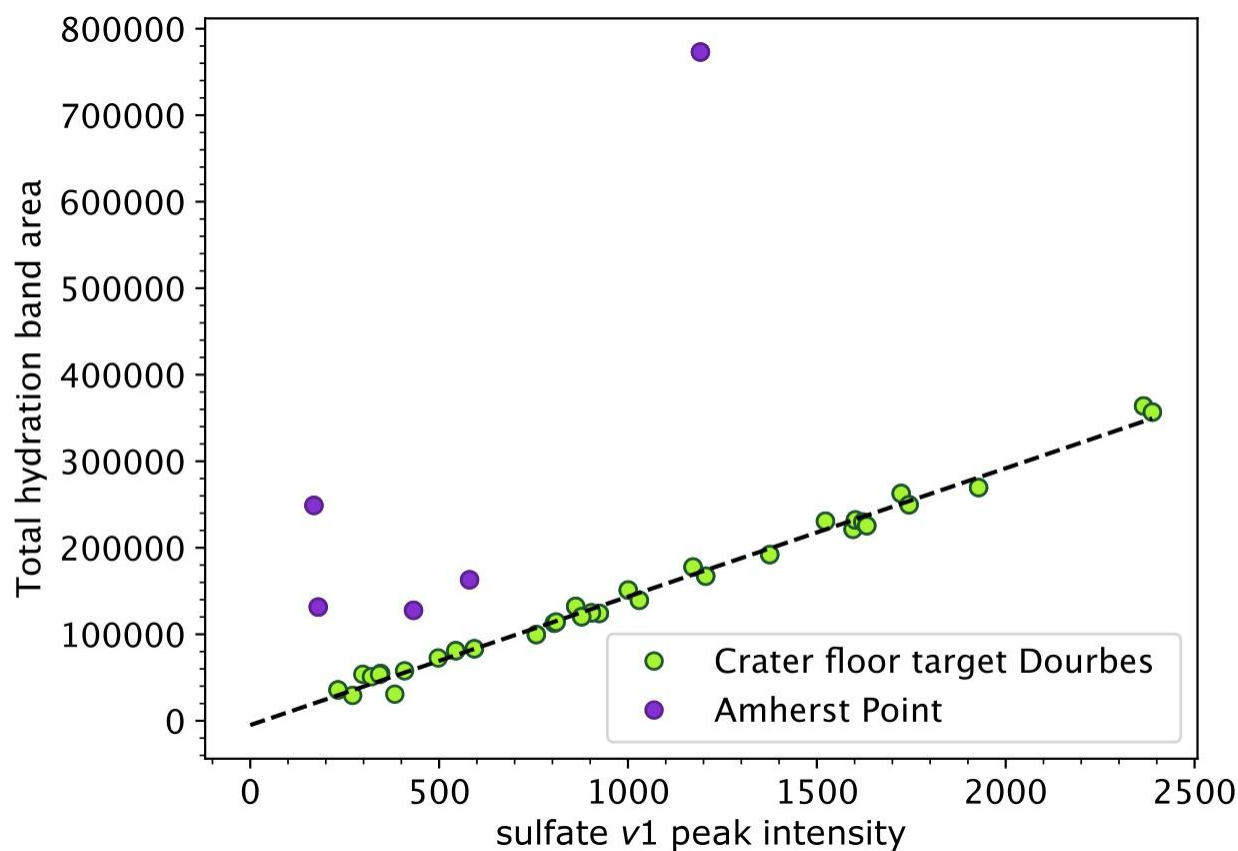
**Fig. S3.**

A comparison of SHERLOC Raman features at 1427 and 1517  $\text{cm}^{-1}$  ( $\nu_3$  carbonate antisymmetric stretching mode), and around 1670  $\text{cm}^{-1}$  (OH bending mode) in Point 91 in Amherst Point Sol 921 detail 1 with similar features in nesquehonite standard, measured with SHERLOC analog brassboard instrument (15).



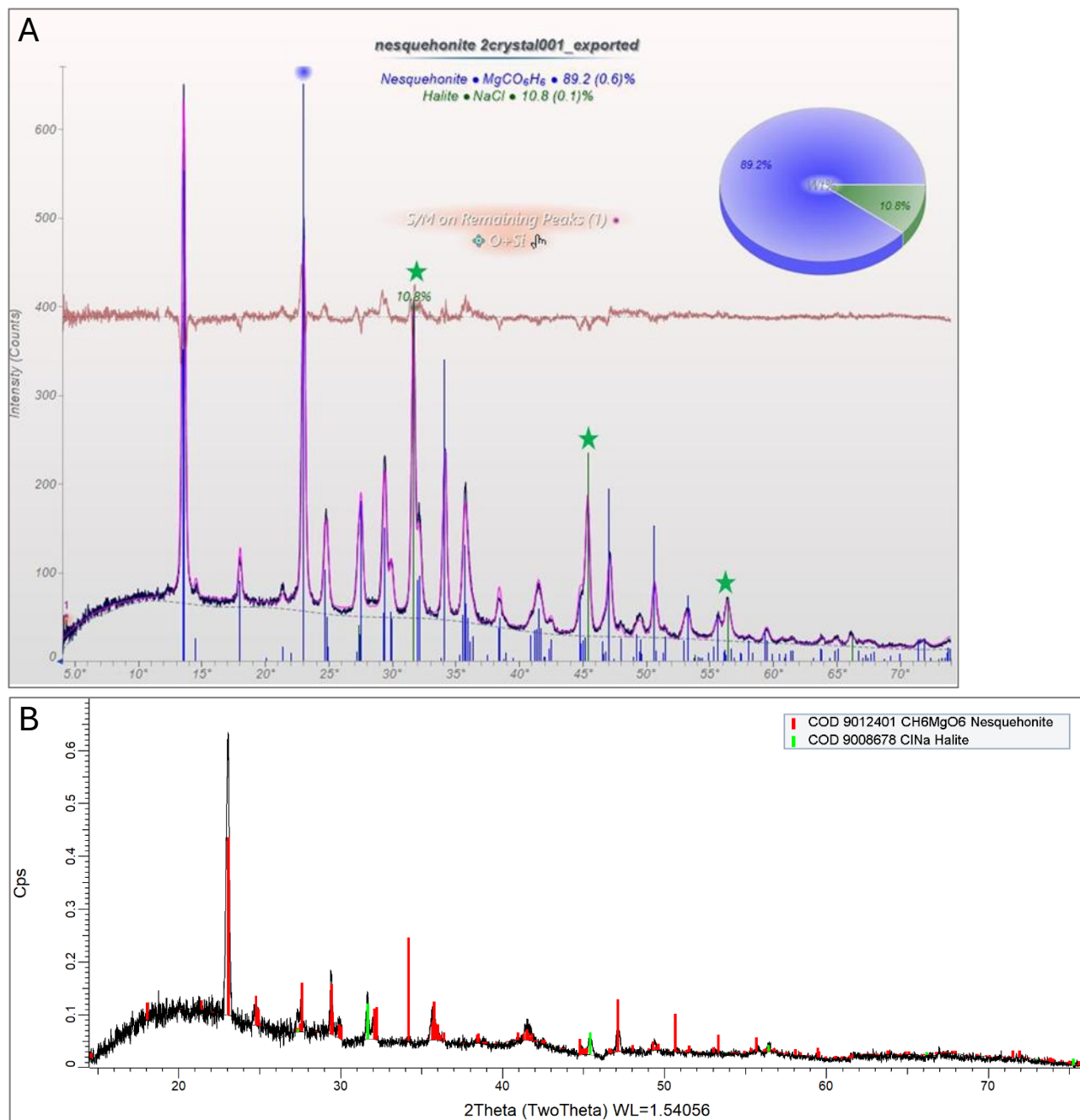
**Fig. S4.**

Total area of the hydration band at 2,800–3,900  $\text{cm}^{-1}$  as a function of sulfate  $\nu_1$  peak intensity at  $\sim 1,000 \text{ cm}^{-1}$  for the points in Amherst Point with observed sulfate and hydration signatures, as shown in Figure 3G. The Amherst Point values are compared to the points from a crater floor target called Dourbes taken by Phua et al (21), with the dashed line showing a linear trendline between the hydration band area and sulfate  $\nu_1$  peak intensity.



**Fig. S5.**

X-ray Diffraction analysis on lab-synthesized nesquehonite. **A)** Pre and **B)** Post-transportation diffractogram to assess potential phase changes (sample was transported to the Jet Propulsion Laboratory, California Institute of Technology, to obtain DUV spectra from the SHERLOC analog facility).



**Table S1.**

A summary of SHERLOC hydrated carbonate and hydrated sulfate detection points (68,71,87,88,90,91,92, and 95) their peak positions, FWHM, and signal-to-noise ratios (SNRs), and comparison with DUV spectra of mineral standards. The calibrated bandwidth has been calculated by Jakubek et al (81).

| Spectra                            | Band assignment                   | Band center / $\text{cm}^{-1}$ | SD   | Bandwidth / $\text{cm}^{-1}$ (cal.) | MP SNR | Comments                                                                                                                         |
|------------------------------------|-----------------------------------|--------------------------------|------|-------------------------------------|--------|----------------------------------------------------------------------------------------------------------------------------------|
| <b>Hydrated carbonate</b>          |                                   |                                |      |                                     |        |                                                                                                                                  |
| <b>Point 68</b>                    | $\nu 1$ carbonate                 | 1102                           | 2.6  | 31.6                                | 12.0   | Point 68: the lowest SNR detection                                                                                               |
|                                    | O-H stretching                    | 3382                           | 27.1 |                                     | 8.0    |                                                                                                                                  |
| <b>Point 71</b>                    | $\nu 1$ carbonate                 | 1092                           | 1.9  | 6.3                                 | 24.6   |                                                                                                                                  |
|                                    | O-H stretching                    | 3265                           | 10.9 |                                     | 14.8   |                                                                                                                                  |
|                                    | O-H stretching                    | 3475                           | 13.9 |                                     | 7.6    |                                                                                                                                  |
| <b>Point 87</b>                    | $\nu 1$ carbonate                 | 1095                           | 1.9  | 16.6                                | 43.3   |                                                                                                                                  |
|                                    | O-H stretching                    | 3087                           | 8.2  |                                     | 9.2    |                                                                                                                                  |
|                                    | O-H stretching                    | 3377                           | 5.2  |                                     | 33.4   |                                                                                                                                  |
| <b>Point 88</b>                    | $\nu 1$ carbonate                 | 1096                           | 2.0  | 8.4                                 | 22.2   |                                                                                                                                  |
|                                    | O-H stretching                    | 3243                           | 13.8 |                                     | 11.4   |                                                                                                                                  |
|                                    | O-H stretching                    | 3448                           | 6.6  |                                     | 16.5   |                                                                                                                                  |
| <b>Point 90</b>                    | $\nu 1$ carbonate                 | 1095                           | 2.2  |                                     | 14.6   |                                                                                                                                  |
|                                    | O-H stretching                    | 3183                           | 13.1 |                                     | 9.12   |                                                                                                                                  |
|                                    | O-H stretching                    | 3442                           | 7.2  |                                     | 16.0   |                                                                                                                                  |
| <b>Point 91</b>                    | $\nu 1$ carbonate                 | 1092                           | 1.8  | 12                                  | 109.9  | The highest SNR detection. $\nu 3$ carbonate spectral region is resolved. O-H stretching region clearly shows two resolved bands |
|                                    | $\nu 3$ carbonate                 | 1427                           | N/A  |                                     | N/A    |                                                                                                                                  |
|                                    | $\nu 3$ carbonate                 | 1517                           | N/A  |                                     | N/A    |                                                                                                                                  |
|                                    | O-H bending/carbonate combination | 1670                           | N/A  |                                     | N/A    |                                                                                                                                  |
|                                    | O-H stretching                    | 3217                           | 3.2  |                                     | 71.2   |                                                                                                                                  |
|                                    | O-H stretching                    | 3459                           | 2.6  |                                     | 64.1   |                                                                                                                                  |
| <b>Point 92</b>                    | $\nu 1$ carbonate                 | 1096                           | 1.9  | 17.2                                | 41.1   |                                                                                                                                  |
|                                    | O-H stretching                    | 3269                           | 6.6  |                                     | 29.0   |                                                                                                                                  |
|                                    | O-H stretching                    | 3499                           | 8.4  |                                     | 11.6   |                                                                                                                                  |
| <b>Point 95</b>                    | $\nu 1$ carbonate                 | 1104                           | 2.3  | 31.6                                | 10     |                                                                                                                                  |
|                                    | O-H stretching                    | 3319                           | 22.3 |                                     | 8.8    |                                                                                                                                  |
| <b>Magnesium carbonate hydrate</b> | $\nu 1$ carbonate                 | 1110                           | 1.8  |                                     | 70.5   | Sourced from Sigma Aldrich – has an unknown hydration state.                                                                     |
|                                    | O-H stretching                    | 3419                           | 2.0  |                                     | 39.6   |                                                                                                                                  |
|                                    | O-H stretching                    | 3496                           | 1.9  |                                     | 18.5   |                                                                                                                                  |
|                                    | O-H stretching                    | 3620                           | 1.8  |                                     | 36.3   |                                                                                                                                  |

|                       |                   |       |      |  |       |                                                                                                                                                                                                 |
|-----------------------|-------------------|-------|------|--|-------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                       |                   |       |      |  |       | DUV spectra obtained with Photon Systems RPL200 instrument located at INAF-Astrophysical Observatory of Arcetri                                                                                 |
| <b>Nesquehonite</b>   | $\nu$ 1 carbonate | 1098  | 1.9  |  | 45.9  | Laboratory synthesis (69) (fig S3), and DUV spectra obtained from Brassboard at JPL                                                                                                             |
|                       | O-H stretching    | 3327  | 2.33 |  | 104.9 |                                                                                                                                                                                                 |
|                       | O-H stretching    | 3555  | 2.2  |  | 14.5  |                                                                                                                                                                                                 |
|                       | O-H stretching    | 3648  | 2.5  |  | 7.3   |                                                                                                                                                                                                 |
| <b>Lansfordite</b>    | $\nu$ 1 carbonate | 1098  |      |  |       | Landsfordite could not be sourced and its DUV spectra could not be measured due to its rarity and high metastability; therefore, the data presented here is taken from (82) measured at 532 nm. |
|                       | O-H stretching    | ~3000 |      |  |       |                                                                                                                                                                                                 |
|                       | O-H stretching    | ~3500 |      |  |       |                                                                                                                                                                                                 |
| <b>Artinite</b>       | $\nu$ 1 carbonate | 1084  | 1.9  |  | 13.3  | Sourced from Smithsonian Institution's mineral and gem collection, and DUV spectra obtained from ACRONM at JSC.                                                                                 |
|                       | O-H stretching    | 3100  | 5.1  |  | 42    |                                                                                                                                                                                                 |
|                       | O-H stretching    | 3585  | 1.9  |  | 14    |                                                                                                                                                                                                 |
|                       | O-H stretching    | 3682  | 3.2  |  | 5.54  |                                                                                                                                                                                                 |
| <b>Dypingite</b>      | $\nu$ 1 carbonate | 1095  | 2.0  |  | 28    |                                                                                                                                                                                                 |
|                       | $\nu$ 1 carbonate | 1112  | 1.8  |  | 37.9  |                                                                                                                                                                                                 |
|                       | O-H stretching    | 3642  | 1.8  |  | 22.7  |                                                                                                                                                                                                 |
| <b>Hydromagnesite</b> | $\nu$ 1 carbonate | 1116  | 1.8  |  | 59.9  |                                                                                                                                                                                                 |
|                       | O-H stretching    | 3326  | 1.9  |  | 36.2  |                                                                                                                                                                                                 |
|                       | O-H stretching    | 3389  | 1.9  |  | 19.9  |                                                                                                                                                                                                 |
|                       | O-H stretching    | 3507  | 1.8  |  | 32.7  |                                                                                                                                                                                                 |
| <b>Trona</b>          | $\nu$ 1 carbonate | 1053  | 1.8  |  | 86.6  |                                                                                                                                                                                                 |
|                       | O-H stretching    | 3240  | 2.6  |  | 124.5 |                                                                                                                                                                                                 |
|                       | O-H stretching    | 3430  | 1.8  |  | 93.4  |                                                                                                                                                                                                 |
| <b>Brucite</b>        | $\nu$ 1 carbonate | 436   | 1.8  |  | 24.5  |                                                                                                                                                                                                 |
|                       | O-H stretching    | 3638  | 1.8  |  | 85    |                                                                                                                                                                                                 |

| Hydrated sulfate                      |                 |        |      |      |      |                                                                                    |
|---------------------------------------|-----------------|--------|------|------|------|------------------------------------------------------------------------------------|
| Point 71                              | $\nu_1$ sulfate | 1023   | 6.4  | 9.2  | 3.7  |                                                                                    |
|                                       | O-H stretching  | 3265   | 10.9 |      | 14.8 |                                                                                    |
|                                       | O-H stretching  | 3475   | 13.9 |      | 7.6  |                                                                                    |
| Point 88                              | $\nu_1$ sulfate | 1023.5 | 3.6  | 12.2 | 12.8 |                                                                                    |
|                                       | O-H stretching  | 3243   | 13.8 |      | 11.4 |                                                                                    |
|                                       | O-H stretching  | 3448   | 6.6  |      | 16.5 |                                                                                    |
| Point 90                              | $\nu_1$ sulfate | 1023   | 4.1  | 23   | 10.3 |                                                                                    |
|                                       | O-H stretching  | 3183   | 13.1 |      | 9.12 |                                                                                    |
|                                       | O-H stretching  | 3442   | 7.2  |      | 16.1 |                                                                                    |
| Point 91                              | $\nu_1$ sulfate | 1023   | 3.1  | 20.8 | 27.1 |                                                                                    |
|                                       | O-H stretching  | 3217   | 3.1  |      | 71.2 |                                                                                    |
|                                       | O-H stretching  | 3459   | 2.6  |      | 64.1 |                                                                                    |
| MgSO <sub>4</sub> ·4H <sub>2</sub> O* | $\nu_1$ sulfate | ~1000  | N/A  | N/A  | N/A  | DUV spectra could not be obtained and therefore VIS Raman data was taken from (83) |
|                                       | O-H stretching  | ~3430  | N/A  | N/A  | N/A  |                                                                                    |
| MgSO <sub>4</sub> ·3H <sub>2</sub> O* | $\nu_1$ sulfate | 1023   | N/A  | N/A  | N/A  |                                                                                    |
|                                       | O-H stretching  | ~3420  | N/A  | N/A  | N/A  |                                                                                    |
| MgSO <sub>4</sub> ·2H <sub>2</sub> O* | $\nu_1$ sulfate | 1033   | N/A  | N/A  | N/A  |                                                                                    |
|                                       | O-H stretching  | ~3450  | N/A  | N/A  | N/A  |                                                                                    |

**Table S2.**

The wt.% element oxide compositions of all SHERLOC hydrated Mg-carbonate detection points are taken from PIXL elemental chemistry data of Amherst Point sol 921.

| <b>SRLC point</b> | <b>MgO</b> | <b>CaO</b> | <b>FeO</b> | <b>SO<sub>3</sub></b> | <b>K<sub>2</sub>O</b> | <b>Na<sub>2</sub>O</b> | <b>Cl</b> | <b>SiO<sub>2</sub></b> | <b>CO<sub>2</sub></b> | <b>PIXL Point</b> | <b>Total</b> | <b>H<sub>2</sub>O (wt% by difference)</b> | <b>MgO:CO<sub>2</sub> wt% ratio</b> | <b>CO<sub>2</sub>:H<sub>2</sub>O wt% ratio</b> | <b>MgO in MgSO<sub>4</sub></b> | <b>MgO*</b> | <b>MgO*/CO<sub>2</sub> wt% ratio</b> |
|-------------------|------------|------------|------------|-----------------------|-----------------------|------------------------|-----------|------------------------|-----------------------|-------------------|--------------|-------------------------------------------|-------------------------------------|------------------------------------------------|--------------------------------|-------------|--------------------------------------|
| <b>92</b>         | 19.40      | 0.40       | 16.30      | 2.90                  | 0.50                  | 1.10                   | 2.10      | 27.90                  | 29.40                 | 280               | 100.0        | 0.00                                      | 0.66                                |                                                | 0.85                           | 18.55       | 0.63                                 |
|                   | 22.70      | 0.20       | 5.20       | 9.30                  | 0.00                  | 0.00                   | 2.60      | 13.70                  | 22.70                 | 281               | 76.4         | 23.60                                     | 1.00                                | 0.96                                           | 2.72                           | 19.98       | 0.88                                 |
|                   | 19.60      | 0.40       | 16.00      | 9.20                  | 0.00                  | 0.00                   | 2.70      | 21.20                  | 24.00                 | 298               | 93.1         | 6.90                                      | 0.82                                | 3.48                                           | 2.69                           | 16.91       | 0.70                                 |
|                   | 16.90      | 0.50       | 8.20       | 4.40                  | 0.00                  | 0.00                   | 2.40      | 31.00                  | 21.30                 | 299               | 84.7         | 15.30                                     | 0.79                                | 1.39                                           | 1.28                           | 15.62       | 0.73                                 |
| Average           | 19.65      | 0.38       | 11.43      | 6.45                  | 0.13                  | 0.28                   | 2.45      | 23.45                  | 24.35                 |                   |              | 11.45                                     | 0.82                                | 1.94                                           | 1.88                           | 17.77       | 0.74                                 |
| StDev             | 2.38       | 0.13       | 5.59       | 3.29                  | 0.25                  | 0.55                   | 0.26      | 7.68                   | 3.54                  |                   |              | 10.23                                     | 0.14                                | 1.35                                           | 0.96                           | 1.91        | 0.10                                 |
| <b>91</b>         | 19.40      | 0.40       | 16.30      | 2.90                  | 0.50                  | 1.10                   | 2.10      | 27.90                  | 29.40                 | 280               | 100.0        | 0.00                                      | 0.66                                |                                                | 0.85                           | 18.55       | 0.63                                 |
|                   | 19.60      | 0.40       | 16.00      | 9.20                  | 0.00                  | 0.00                   | 2.70      | 21.20                  | 24.00                 | 298               | 93.1         | 6.90                                      | 0.82                                | 3.48                                           | 2.69                           | 16.91       | 0.70                                 |
|                   | 22.70      | 0.20       | 5.20       | 9.30                  | 0.00                  | 0.00                   | 2.60      | 13.70                  | 22.70                 | 281               | 76.4         | 23.60                                     | 1.00                                | 0.96                                           | 2.72                           | 19.98       | 0.88                                 |
| Average           | 20.57      | 0.33       | 12.50      | 7.13                  | 0.17                  | 0.37                   | 2.47      | 20.93                  | 25.37                 |                   |              | 10.17                                     | 0.83                                | 2.22                                           | 2.08                           | 18.48       | 0.74                                 |
| StDev             | 1.85       | 0.12       | 6.32       | 3.67                  | 0.29                  | 0.64                   | 0.32      | 7.10                   | 3.55                  |                   |              | 12.13                                     | 0.17                                | 1.78                                           | 1.07                           | 1.54        | 0.13                                 |
| <b>90</b>         | 22.70      | 0.20       | 5.20       | 9.30                  | 0.00                  | 0.00                   | 2.60      | 13.70                  | 22.70                 | 282               | 76.4         | 23.60                                     | 1.00                                | 0.96                                           | 2.72                           | 19.98       | 0.88                                 |
|                   | 20.00      | 0.20       | 36.30      | 10.30                 | 0.00                  | 0.00                   | 4.00      | 17.50                  | 25.20                 | 282               | 113.5        | -13.50                                    | 0.79                                | -1.87                                          | 3.01                           | 16.99       | 0.67                                 |
|                   | 19.60      | 0.40       | 16.00      | 9.20                  | 0.00                  | 0.00                   | 2.70      | 21.20                  | 24.00                 | 298               | 93.1         | 6.90                                      | 0.82                                | 3.48                                           | 2.69                           | 16.91       | 0.70                                 |
| Average           | 20.77      | 0.27       | 19.17      | 9.60                  | 0.00                  | 0.00                   | 3.10      | 17.47                  | 23.97                 |                   |              | 15.25                                     | 0.91                                | 2.22                                           | 2.70                           | 18.45       | 0.79                                 |
| StDev             | 1.69       | 0.12       | 15.79      | 0.61                  | 0.00                  | 0.00                   | 0.78      | 3.75                   | 1.25                  |                   |              | 11.81                                     | 0.13                                | 1.78                                           | 0.02                           | 2.17        | 0.12                                 |
| <b>88</b>         | 16.00      | 0.30       | 41.10      | 3.20                  | 0.00                  | 0.00                   | 4.10      | 38.00                  | 3.70                  | 297               | 106.4        | -6.40                                     | 4.32                                | -0.58                                          | 0.93                           | 15.07       | 4.07                                 |
|                   | 19.60      | 0.40       | 16.00      | 9.20                  | 0.00                  | 0.00                   | 2.70      | 21.20                  | 24.00                 | 298               | 93.1         | 6.90                                      | 0.82                                | 3.48                                           | 2.69                           | 16.91       | 0.70                                 |
|                   | 15.90      | 0.80       | 7.90       | 4.30                  | 0.00                  | 0.50                   | 1.90      | 33.90                  | 21.10                 | 394               | 86.3         | 13.70                                     | 0.75                                | 1.54                                           | 1.26                           | 14.64       | 0.69                                 |
|                   | 12.40      | 0.60       | 10.70      | 3.50                  | 0.00                  | 0.00                   | 1.70      | 54.00                  | 17.00                 | 396               | 99.9         | 0.10                                      | 0.73                                | 170.00                                         | 1.02                           | 11.38       | 0.67                                 |
| Average           | 15.98      | 0.53       | 18.93      | 5.05                  | 0.00                  | 0.13                   | 2.60      | 36.78                  | 16.45                 |                   |              | 6.90                                      | 0.77                                | 58.34                                          | 1.65                           | 14.31       | 0.69                                 |
| StDev             | 2.94       | 0.22       | 15.16      | 2.81                  | 0.00                  | 0.25                   | 1.09      | 13.53                  | 8.97                  |                   |              | 6.80                                      | 0.05                                | 96.71                                          | 0.90                           | 2.78        | 0.02                                 |

|           |       |      |       |      |      |      |      |       |       |     |       |       |       |        |      |       |       |
|-----------|-------|------|-------|------|------|------|------|-------|-------|-----|-------|-------|-------|--------|------|-------|-------|
| <b>87</b> | 16.90 | 0.50 | 8.20  | 4.40 | 0.00 | 0.00 | 2.40 | 31.00 | 21.30 | 299 | 84.7  | 15.30 | 0.79  | 1.39   | 1.28 | 15.62 | 0.73  |
|           | 19.50 | 0.70 | 43.50 | 2.60 | 0.00 | 0.00 | 4.50 | 38.30 | 0.40  | 393 | 109.5 | -9.50 | 48.75 | -0.04  | 0.76 | 18.74 | 46.85 |
|           | 15.90 | 0.60 | 18.30 | 3.10 | 0.00 | 0.00 | 3.10 | 37.80 | 21.10 | 394 | 99.9  | 0.10  | 0.75  | 211.00 | 0.91 | 14.99 | 0.71  |
| Average   | 17.43 | 0.60 | 23.33 | 3.37 | 0.00 | 0.00 | 3.33 | 35.70 | 14.27 |     |       | 7.70  | 0.77  | 106.20 | 1.09 | 15.31 | 0.72  |
| StDev     | 1.86  | 0.10 | 18.18 | 0.93 | 0.00 | 0.00 | 1.07 | 4.08  | 12.01 |     |       | 10.75 | 0.03  | 148.22 | 0.27 | 0.44  | 0.02  |
| <b>71</b> | 15.90 | 0.60 | 18.30 | 3.10 | 0.00 | 0.00 | 3.10 | 37.80 | 21.10 | 394 | 99.9  | 0.10  | 0.75  | 211.00 | 0.91 | 14.99 | 0.71  |
|           | 16.40 | 0.80 | 7.90  | 4.30 | 0.00 | 0.50 | 1.90 | 33.90 | 10.50 | 395 | 76.2  | 23.80 | 1.56  | 0.44   | 1.26 | 15.14 | 1.44  |
|           | 8.80  | 0.30 | 5.30  | 3.70 | 0.10 | 0.00 | 1.50 | 61.00 | 10.70 | 412 | 91.4  | 8.60  | 0.82  | 1.24   | 1.08 | 7.72  | 0.72  |
|           | 12.90 | 0.50 | 13.70 | 2.80 | 0.10 | 0.00 | 2.70 | 42.10 | 20.70 | 413 | 95.5  | 4.50  | 0.62  | 4.60   | 0.82 | 12.08 | 0.58  |
| Average   | 13.50 | 0.55 | 11.30 | 3.48 | 0.05 | 0.13 | 2.30 | 43.70 | 15.75 |     |       | 9.25  | 0.94  | 54.32  | 1.01 | 12.49 | 0.86  |
| StDev     | 3.49  | 0.21 | 5.84  | 0.67 | 0.06 | 0.25 | 0.73 | 12.01 | 5.95  |     |       | 10.30 | 0.42  | 104.47 | 0.19 | 3.48  | 0.39  |
| <b>68</b> | 15.90 | 0.60 | 18.30 | 3.10 | 0.00 | 0.00 | 3.10 | 37.80 | 21.10 | 394 | 99.9  | 0.10  | 0.75  | 211.00 | 0.91 | 14.99 | 0.71  |
|           | 16.40 | 0.80 | 7.90  | 4.30 | 0.00 | 0.50 | 1.90 | 33.90 | 10.50 | 395 | 76.2  | 23.80 | 1.56  | 0.44   | 1.26 | 15.14 | 1.44  |
|           | 8.80  | 0.30 | 5.30  | 3.70 | 0.10 | 0.00 | 1.50 | 61.00 | 10.70 | 412 | 91.4  | 8.60  | 0.82  | 1.24   | 1.08 | 7.72  | 0.72  |
|           | 12.90 | 0.50 | 13.70 | 2.80 | 0.10 | 0.00 | 2.70 | 42.10 | 20.70 | 413 | 95.5  | 4.50  | 0.62  | 4.60   | 0.82 | 12.08 | 0.58  |
|           | 7.40  | 0.50 | 7.40  | 2.20 | 0.10 | 0.00 | 1.70 | 62.00 | 11.00 | 509 | 92.3  | 7.70  | 0.67  | 1.43   | 0.64 | 6.76  | 0.61  |
| Average   | 12.28 | 0.54 | 10.52 | 3.22 | 0.06 | 0.10 | 2.18 | 47.36 | 14.80 |     |       | 8.94  | 0.89  | 43.74  | 0.94 | 11.34 | 0.81  |
| StDev     | 4.07  | 0.18 | 5.35  | 0.81 | 0.05 | 0.22 | 0.69 | 13.23 | 5.57  |     |       | 8.95  | 0.39  | 93.51  | 0.24 | 3.95  | 0.36  |
| <b>95</b> | 20.20 | 0.40 | 24.40 | 5.50 | 0.00 | 2.00 | 3.60 | 30.00 | 19.00 | 42  | 105.1 | -5.10 | 1.06  | -3.73  | 1.61 | 18.59 | 0.98  |
|           | 22.90 | 0.10 | 17.10 | 3.90 | 0.00 | 0.70 | 3.20 | 27.70 | 33.70 | 80  | 109.3 | -9.30 | 0.68  | -3.62  | 1.14 | 21.76 | 0.65  |
|           | 24.70 | 0.20 | 23.50 | 2.80 | 0.00 | 0.40 | 3.40 | 24.30 | 17.60 | 81  | 96.90 | 3.10  | 1.40  | 5.68   | 0.82 | 23.88 | 1.36  |
|           | 16.70 | 1.20 | 29.10 | 4.70 | 0.00 | 2.00 | 3.00 | 36.20 | 31.40 | 82  | 124.3 | -24.3 | 0.53  | -1.29  | 1.37 | 15.33 | 0.49  |
|           | 18.20 | 0.70 | 41.10 | 2.40 | 0.00 | 0.00 | 2.80 | 30.00 | 0.00  | 155 | 95.20 | 4.80  | 0.00  | 0.00   | 0.70 | 17.50 | 0.00  |
|           | 18.90 | 0.40 | 33.20 | 1.90 | 0.00 | 0.00 | 3.80 | 29.50 | 40.00 | 156 | 127.7 | -27.7 | 0.47  | -1.44  | 0.55 | 18.35 | 0.46  |
|           | 24.40 | 0.10 | 16.40 | 3.00 | 0.00 | 0.00 | 3.40 | 29.00 | 19.60 | 157 | 95.90 | 4.10  | 1.24  | 4.78   | 0.88 | 23.52 | 1.20  |
| Average   | 20.85 | 0.44 | 26.4  | 3.46 | 0    | 0.73 | 3.31 | 29.52 | 23.04 |     |       | 4.00  | 0.77  | 5.23   | 1.01 | 19.85 | 0.9   |
| StDev     | 3.16  | 0.39 | 8.84  | 1.30 | 0    | 0.91 | 0.34 | 3.56  | 13.29 |     |       | 0.85  | 0.49  | 0.63   | 0.38 | 3.25  | 0.4   |

\* = MgO factor for sulfate is 0.58

StDev = Standard Deviation

**Table S3.**

The wt.% element oxide compositions of several relevant hydrous and anhydrous magnesium carbonate endmembers were computed based on stoichiometry using their ideal endmember mineral formulae. These compositions were used to determine MgO: CO<sub>2</sub> wt.% ratios compared to PIXL data.

| <u><b>Oxide</b></u>   | <u><b>Moles<br/>(pfu)</b></u> | <u><b>Mole wt.<br/>Oxide</b></u> | <u><b>Moles pfu *<br/>MwO</b></u> | <u><b>Wt.% Oxide</b></u> | <u><b>MgO:CO<sub>2</sub><br/>Wt% ratio</b></u> |
|-----------------------|-------------------------------|----------------------------------|-----------------------------------|--------------------------|------------------------------------------------|
| <b>Nesquehonite</b>   |                               |                                  |                                   |                          |                                                |
| MgO                   | 1                             | 40.3044                          | 40.3044                           | 29.13015                 | 0.9158114                                      |
| CO <sub>2</sub>       | 1                             | 44.0095                          | 44.0095                           | 31.80802                 |                                                |
| H <sub>2</sub> O      | 3                             | 18.01528                         | 54.04584                          | 39.06183                 |                                                |
| total                 |                               |                                  | 138.3597                          | 100                      |                                                |
| <b>Artinite</b>       |                               |                                  |                                   |                          |                                                |
| MgO                   | 2                             | 40.3044                          | 80.6088                           | 40.98487                 | 1.8316227                                      |
| CO <sub>2</sub>       | 1                             | 44.0095                          | 44.0095                           | 22.37626                 |                                                |
| H <sub>2</sub> O      | 4                             | 18.01528                         | 72.06112                          | 36.63887                 |                                                |
| total                 |                               |                                  | 196.6794                          | 100                      |                                                |
| <b>Hydromagnesite</b> |                               |                                  |                                   |                          |                                                |
| MgO                   | 5                             | 40.3044                          | 201.522                           | 43.09374                 | 1.1447642                                      |
| CO <sub>2</sub>       | 4                             | 44.0095                          | 176.038                           | 37.6442                  |                                                |
| H <sub>2</sub> O      | 5                             | 18.01528                         | 90.0764                           | 19.26205                 |                                                |
| total                 |                               |                                  | 467.6364                          | 100                      |                                                |
| <b>Dypingite</b>      |                               |                                  |                                   |                          |                                                |
| MgO                   | 5                             | 40.3044                          | 201.522                           | 41.49517                 | 1.1447642                                      |
| CO <sub>2</sub>       | 4                             | 44.0095                          | 176.038                           | 36.24779                 |                                                |
| H <sub>2</sub> O      | 6                             | 18.01528                         | 108.0917                          | 22.25704                 |                                                |
| total                 |                               |                                  | 485.6517                          | 100                      |                                                |
| <b>Lansfordite</b>    |                               |                                  |                                   |                          |                                                |

|                  |   |          |          |          |           |
|------------------|---|----------|----------|----------|-----------|
| MgO              | 1 | 40.3044  | 40.3044  | 23.11161 | 0.9158114 |
| CO <sub>2</sub>  | 1 | 44.0095  | 44.0095  | 25.23621 |           |
| H <sub>2</sub> O | 5 | 18.01528 | 90.0764  | 51.65218 |           |
|                  |   | total    | 174.3903 | 100      |           |
| <b>Magnesite</b> |   |          |          |          |           |
| MgO              | 1 | 40.3044  | 40.3044  | 47.80279 | 0.9158114 |
| CO <sub>2</sub>  | 1 | 44.0095  | 44.0095  | 52.19721 |           |
| H <sub>2</sub> O | 0 | 18.01528 | 0        | 0        |           |
|                  |   | total    | 84.3139  | 100      |           |

### Data S1. Data sources.

All SHERLOC spectra, WATSON, and ACI image data used for this study are available through the NASA PDS SHERLOC data bundle (84). Image data specifically can be found in the PDS Cartography and Imaging Sciences Node

<https://pds-imaging.jpl.nasa.gov/volumes/mars2020.html>

Reference Raman spectra used for hydrated magnesium carbonates used in Fig. 3 and Fig. S3, measured in the laboratory for this study, are archived (85). All other mineral laboratory spectra in Fig. 3 are already published and available in (86).

Below is additional information about the specific dataset used for each figure.

Fig. 1: HiRISE images are available in (87). Mastcam-Z images are available through the NASA PDS Mastcam-Z bundle (88). NavCam and Hazcam images are available through the NASA PDS ECAM bundle (89).

Fig. 2: SHERLOC WATSON and ACI observations used, and their metadata are available in (84) and described in the table below.

| Observation ID                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | Figures                                          | Instrument | Sol | Acquisition<br>standoff<br>distance (cm) | Pixel<br>resolution<br>( $\mu\text{m}/\text{pixel}$ ) | Illumination<br>condition                           |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------|------------|-----|------------------------------------------|-------------------------------------------------------|-----------------------------------------------------|
| SIF_0913_0748004503_000FDR_N0450000SRLC04001_0000LMJ01                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 1D                                               | WATSON     | 913 | $41.49 \pm 1.9$                          | $153.9 \pm 10.7$                                      | Daytime, direct<br>sunlight                         |
| SIF_0913_0748005255_042FDR_N0450000SRLC00701_0000LMJ01                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 1E                                               | WATSON     | 913 | $6.79 \pm 0.1$                           | $31.6 \pm 1.1$                                        | Daytime, direct<br>sunlight                         |
| SI1_0915_0748177135_062FDR_N0450000SRLC00003_000095J01                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 2A                                               | WATSON     | 915 | $7.64 \pm 0.1$                           | $34.7 \pm 1.4$                                        | Daytime, fully<br>shadowed/indir<br>ect daylight    |
| SIF_0915_0748197650_628FDR_N0450000SRLC08029_0000LMJ02                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 2B-2D,<br>used to<br>colorize<br>ACI in<br>2E-2F | WATSON     | 915 | $7.59 \pm 0.1$                           | $34.5 \pm 1.3$                                        | Nighttime,<br>both white-<br>light LED<br>groups on |
| Focus stack merge of:<br>SC3_0920_0748646442_730ECM_N0450000SRLC10402_0000LMJ01,<br>SC3_0920_0748646444_308ECM_N0450000SRLC10402_0000LMJ01,<br>SC3_0920_0748646445_886ECM_N0450000SRLC10402_0000LMJ01,<br>SC3_0920_0748646447_464ECM_N0450000SRLC10402_0000LMJ01,<br>SC3_0920_0748646449_042ECM_N0450000SRLC10402_0000LMJ01,<br>SC3_0920_0748646450_621ECM_N0450000SRLC10402_0000LMJ01,<br>SC3_0920_0748646452_199ECM_N0450000SRLC10402_0000LMJ01,<br>SC3_0920_0748646453_777ECM_N0450000SRLC10402_0000LMJ01,<br>SC3_0920_0748646455_355ECM_N0450000SRLC10402_0000LMJ01,<br>SC3_0920_0748646456_933ECM_N0450000SRLC10402_0000LMJ03,<br>SC3_0920_0748646458_511ECM_N0450000SRLC10402_0000LMJ01,<br>SC3_0920_0748646460_089ECM_N0450000SRLC10402_0000LMJ01,<br>SC3_0920_0748646461_667ECM_N0450000SRLC10402_0000LMJ01,<br>SC3_0920_0748646463_246ECM_N0450000SRLC10402_0000LMJ01,<br>SC3_0920_0748646464_824ECM_N0450000SRLC10402_0000LMJ01 | 2E                                               | ACI        | 920 | $\sim 4.8$                               | $\sim 10.1$                                           | Nighttime,<br>both white-<br>light LED<br>groups on |
| Focus stack merge of:<br>SC3_0921_0748734623_691ECM_N0450000SRLC10402_0000LMJ01,<br>SC3_0921_0748734625_253ECM_N0450000SRLC10402_0000LMJ01,<br>SC3_0921_0748734626_816ECM_N0450000SRLC10402_0000LMJ01,<br>SC3_0921_0748734628_378ECM_N0450000SRLC10402_0000LMJ01,<br>SC3_0921_0748734629_941ECM_N0450000SRLC10402_0000LMJ01,<br>SC3_0921_0748734633_066ECM_N0450000SRLC10402_0000LMJ01,<br>SC3_0921_0748734634_628ECM_N0450000SRLC10402_0000LMJ01,<br>SC3_0921_0748734636_191ECM_N0450000SRLC10402_0000LMJ01,<br>SC3_0921_0748734637_753ECM_N0450000SRLC10402_0000LMJ01,<br>SC3_0921_0748734639_316ECM_N0450000SRLC10402_0000LMJ01,                                                                                                                                                                                                                                                                                                       | 2F                                               | ACI        | 921 | $\sim 4.8$                               | $\sim 10.1$                                           | Nighttime,<br>both white-<br>light LED<br>groups on |

|                                                         |  |  |  |  |  |  |
|---------------------------------------------------------|--|--|--|--|--|--|
| SC3_0921_0748734640_878ECM_N0450000SRLC10402_0000LMJ01, |  |  |  |  |  |  |
| SC3_0921_0748734642_441ECM_N0450000SRLC10402_0000LMJ01, |  |  |  |  |  |  |
| SC3_0921_0748734644_003ECM_N0450000SRLC10402_0000LMJ01, |  |  |  |  |  |  |
| SC3_0921_0748734645_566ECM_N0450000SRLC10402_0000LMJ01, |  |  |  |  |  |  |
| SC3_0921_0748734647_128ECM_N0450000SRLC10402_0000LMJ01, |  |  |  |  |  |  |
| SC3_0921_0748734648_691ECM_N0450000SRLC10402_0000LMJ01, |  |  |  |  |  |  |
| SC3_0921_0748734650_253ECM_N0450000SRLC10402_0000LMJ01  |  |  |  |  |  |  |

Fig. 3, Fig. 4, Fig. S2, Fig. S3: Spectroscopic data from SHERLOC data bundle for sol 920 and 921. can be found in (84). Amherst Point abrasion patch data are listed under Processed data collection, sols 920 and 921, respectively. Colorized ACI imaging data from SHERLOC data bundle, Mars 2020 SHERLOC ACI Data Collection, sol 920 and 921.

Fig. 5, Fig. S1: PIXL data sets are available through the NASA PDS PIXL bundle (90).

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