**Supporting Information of**

# Mineral evolution and mineral niches of ammonium sulphates: the case of Pastora mine (Aliseda, Spain)

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## KEYWORDS

Ammoniojarosite, tschermigite, acid mine drainage, dissolution-precipitation, mineral evolution.

## 5.2. Chemistry of water mine

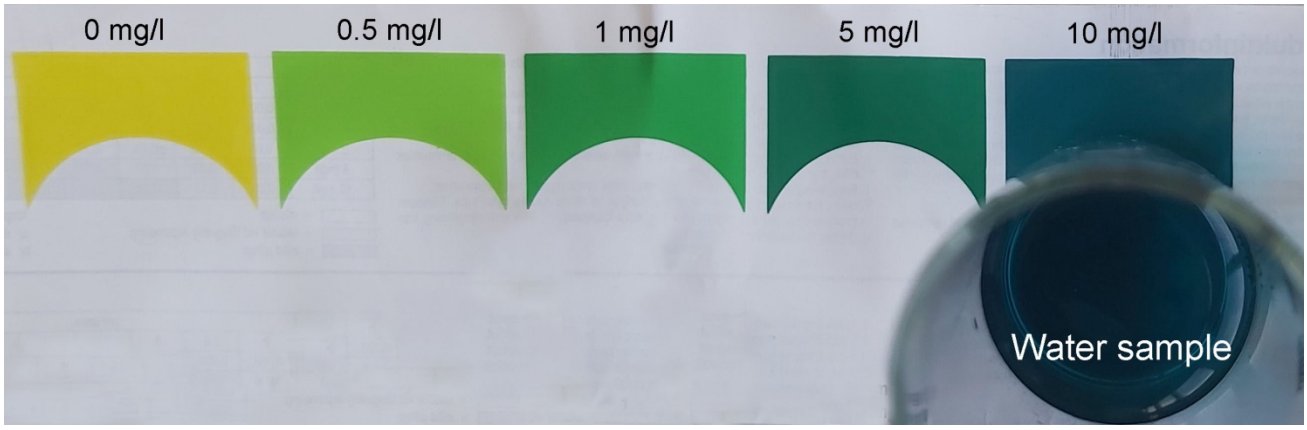


Figure SI1: Comparison with a colorimetric scale showed that the content of TAN in the water samples was at least 10 mg/L.

## 5.4. Ammonium sulphates in Pastora mine

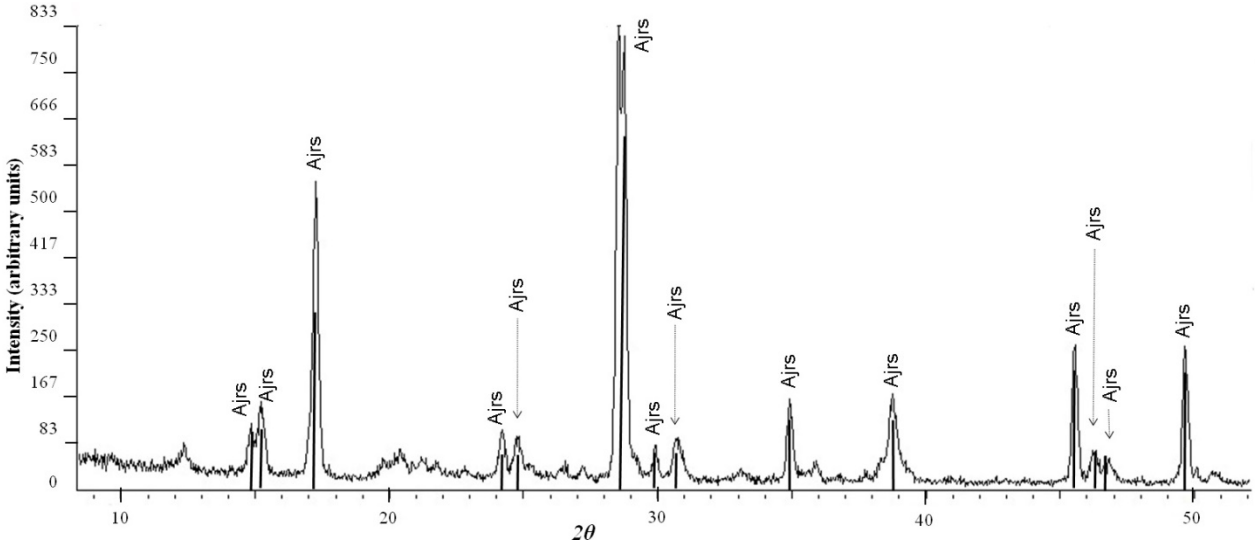


Figure SI2: Diffractogram of sample PA-42, collected at level 1. In this sample, ammoniojarosite is the main fase with accessory kaolinite. Vertical solid lines indicate the positions and relative intensities of ammoniojarosite (Ajrs) diffraction peaks (PDF number 26-1014). Unassigned peaks correspond to minority phase kaolinite (PDF number 14-0164).

### 5.4.1. Ammoniojarosite $(NH_4)Fe_3(SO_4)_2(OH)_6$

| PDF number 26-1014 | | | Ammoniojarosite from Pastora mine, sample PA42 | |
|---|---|---|---|---|
| d (Å) | % ($I/I_0$) | | d (Å) | % ($I/I_0$) |
| 5.945 | 9 | 1 0 1 | 5.9528 | 14.0 |
| 5.805 | 14 | 0 0 3 | 5.8129 | 19.2 |
| 5.116 | 60 | 0 1 2 | 5.1306 | 66.6 |
| 3.657 | 7 | 1 1 0 | 3.6748 | 12.7 |
| 3.587 | 4 | 1 0 4 | 3.5872 | 11.0 |
| 3.104 | 100 | 1 1 3 | 3.1144 | 81.1 |
| 2.976 | 7 | 2 0 2 | 2.9859 | 9.5 |
| 2.907 | 13 | 0 0 6 | 2.9090 | 10.8 |
| 2.564 | 14 | 0 2 4 | 2.5680 | 19.6 |
| 2.316 | 20 | 1 2 2 | 2.3219 | 20.8 |
| 1.987 | 30 | 3 0 3 | 1.9894 | 31.3 |
| 1.959 | 9 | 0 2 7 | 1.9602 | 8.0 |
| 1.831 | 30 | 2 2 0 | 1.8340 | 29.7 |
| 1.747 | 4 | 2 2 3 | 1.7494 | 9.4 |
| 1.725 | 8 | 3 1 2 | 1.7273 | 7.6 |
| 1.633 | 6 | 1 3 4 | 1.6327 | 6.9 |
| 1.549 | 13 | 2 2 6 | 1.5507 | 10.6 |
| 1.529 | 13 | 0 2 10 | 1.5297 | 9.1 |
| 1.491 | 4 | 4 0 4 | 1.4911 | 6.9 |
| 1.347 | 8 | 4 1 3 | 1.3484 | 6.6 |

Table SI1 shows XRD data, values of d-spacing and relative intensities of the sample PA42 main diffractograms peacks, data are in good agreement with synthetic compound PDF number 26-1014.

### 5.4.2. Tschemergite $(NH_4)Al(SO_4)_2 \cdot 12H_2O$

| PDF number 07-0022 | | | Tschermigite from Pastora mine, sample PA-107 | |
|---|---|---|---|---|
| d (Å) | % ($I/I_0$) | | d (Å) | % ($I/I_0$) |
| 7.07 | 55 | 1 1 1 | 7.04 | 34.61 |
| 6.13 | 12 | 2 0 0 | 6.10 | 11.87 |
| 5.48 | 55 | 2 1 0 | 5.46 | 44.85 |
| 5.00 | 35 | 2 1 1 | 5.12 | 40.44 |
| 4.33 | 100 | 2 2 0 | 4.32 | 98.01 |
| 4.08 | 80 | 2 2 1 | 4.08 | 84.29 |
| 3.69 | 35 | 3 1 1 | 3.69 | 43.07 |
| 3.40 | 6 | 2 3 0 | | |
| 3.27 | 75 | 3 2 1 | 3.27 | 100 |
| 3.06 | 30 | 4 0 0 | 3.11 | 45,34 |
| 2.97 | 20 | 4 1 0 | 2,97 | 28,22 |
| 2.88 | 14 | 4 1 1 | 2.88 | 19.90 |
| 2.81 | 35 | 3 3 1 | 2.81 | 35.82 |
| 2.74 | 18 | 4 2 0 | 2.74 | 26.79 |
| 2.67 | 14 | 4 2 1 | 2.67 | 17.41 |
| 2.61 | 12 | 3 3 2 | 2.61 | 14.85 |
| 2.50 | 10 | 4 2 2 | 2.56 | 9.24 |
| 2.36 | 12 | 5 1 1 | 2.35 | 15.14 |
| 2.28 | 8 | 2 5 0 | | |
| 2.24 | 12 | 5 2 1 | 2.23 | 11.09 |
| 2.13 | 8 | 4 4 1 | | |
| 2.07 | 8 | 5 3 1 | 2.07 | 12.22 |
| 2.04 | 10 | 6 0 0 | 2.04 | 15 |
| 2.01 | 10 | 6 1 0 | 2.01 | 13.15 |
| 1.99 | 10 | 6 1 1 | 1.99 | 22.89 |
| 1.94 | 16 | 6 2 0 | 1.93 | 20.82 |

Tabla SI2. The XRD data for tschermigite correspond to those for the ICDD-PDF 71-2203 compound which shows a good agreement with sample PA107.