

Table 1: Lattice parameters of powder samples hematite (BF-26 and SYN-hem_{0.00-1.6}) and goethite (SYN-goe_{0.00-1.6}) compared to their respective W-concentrations. Additionally the table compares Fe₂O₃ and WO₃ chemistry determined by TXRF and EMPA (cf. Fig. 2). The Fe-loss per incorporated W, calculated by Eq. 1, is shown for the TXRF results of the synthetic samples. Table 2 shows the detailed chemistry of all natural samples.^{a, b}

| Sample | phase | Lattice parameters | | | | | | TXRF - Iron-loss | | | | | EMPA | | | |
|------------------------------|-------|--------------------|----------|----------|----------------|------|------|---|--------------------------|----------------|----------------|-----------|---|--------------------------|----------------|----------------|
| | | a [Å] | b [Å] | c [Å] | cryst. [nm] | Rwp | GOF | Fe ₂ O ₃ [wt%] | WO ₃ [wt%] | total [wt%] | N ^g | Fe – loss | Fe ₂ O ₃ [wt%] | WO ₃ [wt%] | total [wt%] | N ^g |
| BF-26 I | hem | 5.0357 | | 13.7569 | 61 | 4.26 | 1.13 | NM | bdl ^c | - | 3 | - | NM | NM | - | - |
| BF-26 II | hem | 5.0366 | | 13.7601 | 75 | 5.82 | 1.56 | NM | 0.23 ^c | - | 3 | - | NM | NM | - | - |
| BF-26 III | hem | 5.0362 | | 13.7599 | 79 | 6.66 | 1.79 | NM | 0.60 ^c | - | 3 | - | NM | NM | - | - |
| BF-26 IV | hem | 5.0362 | | 13.7577 | 77 | 5.92 | 1.57 | NM | 0.62 ^c | - | 3 | - | NM | NM | - | - |
| BF-26 V | hem | 5.0365 | | 13.7591 | 76 | 6.00 | 1.59 | NM | 0.76 ^c | - | 3 | - | NM | NM | - | - |
| BF-26 VI | hem | 5.0367 | | 13.7583 | 79 | 5.58 | 1.49 | NM | 1.19 ^c | - | 3 | - | 95.87 ^f | 1.05 ^f | 100.27 | 21 |
| BF-26 VII | hem | 5.0364 | | 13.7571 | 82 | 6.00 | 1.57 | NM | 1.53 ^c | - | 3 | - | 95.47 ^f | 1.37 ^f | 99.55 | 20 |
| SYN-hem _{0.00} | hem | 5.0391 | | 13.7613 | 22 | 6.38 | 1.30 | 99.6 ^d | bdl ^d | 99.6 | 2 | - | 67.88 ^e | bdl ^e | 68.26 | 10 |
| SYN-hem _{0.05} | hem | 5.0387 | | 13.7575 | 29 | 6.21 | 1.35 | 97.8 ^d | 0.2 ^d | 98.0 | 2 | 2.69 | 66.63 ^e | 0.24 ^e | 67.19 | 10 |
| SYN-hem _{0.1} | hem | 5.0392 | | 13.7578 | 25 | 6.43 | 1.38 | 100.4 ^d | 0.5 ^d | 100.9 | 2 | 2.81 | 63.84 ^e | 0.43 ^e | 64.56 | 10 |
| SYN-hem _{0.2} | hem | 5.0400 | | 13.7605 | 26 | 6.51 | 1.34 | 99.8 ^d | 1.2 ^d | 101.0 | 3 | 2.86 | 76.89 ^e | 1.11 ^e | 78.39 | 10 |
| SYN-hem _{0.4} | hem | 5.0400 | | 13.7652 | 22 | 6.37 | 1.27 | 94.4 ^d | 1.8 ^d | 96.2 | 3 | 2.88 | 75.51 ^e | 1.69 ^e | 77.64 | 10 |
| SYN-hem _{0.8} | hem | 5.0409 | | 13.7637 | 29 | 6.44 | 1.36 | 97.7 ^d | 2.2 ^d | 99.9 | 3 | 2.88 | 79.21 ^e | 1.99 ^e | 81.55 | 20 |
| SYN-hem _{1.6} | hem | 5.0398 | | 13.7620 | 38 | 6.50 | 1.36 | 101.2 ^d | 1.7 ^d | 103.0 | 3 | 2.87 | 80.45 ^e | 2.69 ^e | 83.40 | 10 |
| SYN-goe _{0.00;70°C} | goe | 9.9606 | 3.0240 | 4.6101 | 33 | 6.63 | 1.36 | 93.7 ^d | bdl ^d | 93.7 | 3 | - | 48.86 ^e | bdl ^e | 49.08 | 11 |
| SYN-goe _{0.05;25°C} | goe | 9.9653 | 3.0241 | 4.6122 | 31 | 6.98 | 1.47 | 83.5 ^d | 3.0 ^d | 86.5 | 3 | 2.90 | 48.30 ^e | 1.56 ^e | 50.08 | 28 |
| SYN-goe _{0.05;70°C} | goe | NM | NM | NM | NM | NM | NM | NM | NM | NM | - | - | 53.08 ^e | 1.86 ^e | 55.20 | 14 |
| SYN-goe _{0.1;70°C} | goe | 9.9644 | 3.0238 | 4.6145 | 47 | 6.36 | 1.38 | 83.6 ^d | 4.9 ^d | 88.5 | 3 | 2.90 | 45.46 ^e | 2.54 ^e | 48.22 | 10 |
| SYN-goe _{0.2;70°C} | goe | 9.9652 | 3.0238 | 4.6172 | 66 | 6.22 | 1.35 | 83.1 ^d | 5.0 ^d | 88.1 | 2 | 2.90 | 53.56 ^e | 3.96 ^e | 57.74 | 13 |
| SYN-goe _{0.4;70°C} | goe | 9.9665 | 3.0237 | 4.6210 | 102 | 5.92 | 1.33 | 78.8 ^d | 8.8 ^d | 87.6 | 3 | 2.90 | 60.50 ^e | 8.19 ^e | 68.94 | 10 |
| SYN-goe _{0.8;70°C} | goe | 9.9658 | 3.0232 | 4.6211 | 65 | 6.83 | 1.22 | 83.2 ^d | 7.7 ^d | 90.9 | 1 | 2.90 | 66.31 ^e | 6.65 ^e | 73.24 | 17 |
| SYN-goe _{1.6;70°C} | goe | 9.9630 | 3.0235 | 4.6243 | 45 | 7.08 | 1.21 | 68.8 ^d | 10.3 ^d | 79.0 | 2 | 2.90 | 61.47 ^e | 8.51 ^e | 70.33 | 21 |

^a bdl = signal detected but below detection limit; ^b NM = not measured; ^c TXRF bulk analysis of solid powder samples. Here a quantification of Fe₂O₃ is not possible due to self-absorption effects; ^d TXRF bulk analysis of solved powder samples; ^e EMPA data of resinated and polished powder samples; ^f EMPA data of polished thin sections. Deficit to total according to oxide components not presented (cf. Table 2); ^g Number of measurements.