Data Article

Experimentally determined trace element partition coefficients between hibonite, melilite, spinel, and silicate melts

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A B S T R A C T

This article provides new data on mineral/melt partitioning in systems relevant to the evolution of chondrites, Calcium Aluminum-Rich Inclusions (CAI) in chondrites and related meteorites. The data set includes experimentally determined mineral/melt partition coefficients between hibonite (CaAl12O19), melilite (Ca2(Al,Mg)2SiO7), spinel (MgAl2O4) and silicate melts for a wide range of trace elements: Sc, Ti, V, Cr, Co, Ni, Cu, Zn, Ga, Ge, Rb, Sr, Y, Zr, Nb, Rh, Cs, Ba, La, Ce, r, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Hf, Ta, W, Pb, Th and U. The experiments were performed at high temperatures (1350 °C < T < 1550 °C) and ambient pressure. The experimental run products were analyzed using electron microprobe (EMPA) and laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS). The partition coefficients for 38 trace elements were calculated from the LA-ICP-MS data.

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Specifications table

| Subject area               | More specific subject area                    | Earth Sciences                          |
|----------------------------|-----------------------------------------------|-----------------------------------------|
|                            |                                               | Experimental petrology, Geochemistry, Planetology, Planetary sciences |

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Type of data | Table, figure
--- | ---
How data was acquired | High-temperature furnace: Gero GmbH, Germany (University of Münster)
Scanning electron microscope (SEM) JEOL JSM-6610 LV in high vacuum mode equipped with EDX system (University of Münster)
Electron microprobe analysis (EMPA): JEOL JXA-8530F Hyperprobe equipped with a field emission gun (University of Münster)
Laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS): Thermo element sector field – ICP-MS with Photon Machines Analyte G2 laser ablation system (University of Münster)

Data format | Major element data of minerals and quenched melts: data in .xlsx format
Trace element data of minerals and quenched melts: data in .xlsx format
Mineral/melt trace element partition coefficients: data in .xlsx format
Mineral/mineral trace element partition coefficients: data in .xlsx format

Experimental features | High temperature experiments were run at high temperatures to equilibrate hibonite, melilite, and spinel, with silicate melts. The experimental run products were mounted in epoxy resins and polished using a variety of diamond pastes. The mounts were carbon coated, and major elements were analyzed using EMPA techniques. Subsequently, trace element concentrations of minerals and glasses within the samples were determined using LA-ICP-MS techniques.

Data accessibility | Supplementary materials

**Value of the data**

- The new trace element partition coefficients supplement the existing database of mineral/melt partition coefficients of minerals that are frequently found in Ca- and Al-rich inclusions in chondritic meteorites.
- The new trace element partition coefficients between hibonite, melilite and spinel and silicate melts may be used to test whether these minerals crystallized from or equilibrated with a silicate melt or whether they condensed from a vapor phase.
- This partition coefficient data set is based on experiments under oxidizing conditions, since preliminary experiments under reducing conditions, which would have been more relevant to solar nebula processes, resulted in crystals which were too small to be analyzed.
- Our mineral/mineral partition coefficients may be used to test whether hibonite, melilite and spinel are in thermodynamic equilibrium or not.

**1. Data**

In this article, we report new experimentally determined trace element partition coefficients between hibonite (CaAl$_{12}$O$_{19}$), melilite (Ca$_2$(Al,Mg)$_2$SiO$_7$), spinel (MgAl$_2$O$_4$), and silicate melts at high temperatures (Tables 3 and 4). Data were generated using high temperature experiments, which were characterized using electron microprobe and LA-ICP-MS methods (Tables 1 and 2).
Table 1
Major element concentrations of minerals and quenched silicate melts determined by EMPA. All values are given in wt%.

| Sample          | MgO wt% | S.D. | Al₂O₃ wt% | S.D. | SiO₂ wt% | S.D. | CaO wt% | S.D. | TiO₂ wt% | S.D. |
|-----------------|---------|------|-----------|------|----------|------|---------|------|----------|------|
| H1-Ti2-R3       | 1.50 ± 0.14 | 86.8 ± 0.1 | 0.86 ± 0.14 | 8.33 ± 0.10 | 1.77 ± 0.21 |
| H1-Ti5-R4       | 2.01 ± 0.13 | 85.1 ± 0.7 | 0.64 ± 0.13 | 8.36 ± 0.08 | 3.16 ± 0.41 |
| H1-Ti5-R5       | 2.02 ± 0.47 | 84.9 ± 1.6 | 0.70 ± 0.17 | 8.39 ± 0.06 | 3.19 ± 0.97 |
| H2-Ti2-R2       | 1.87 ± 0.06 | 85.7 ± 0.3 | 1.22 ± 0.12 | 8.27 ± 0.09 | 1.84 ± 0.05 |
| H2-Ti2-R3       | 1.96 ± 0.28 | 85.5 ± 2.0 | 1.12 ± 0.25 | 8.29 ± 0.14 | 2.23 ± 0.62 |
| H2-Ti5-R4       | 2.41 ± 0.07 | 83.8 ± 0.3 | 0.90 ± 0.19 | 8.30 ± 0.09 | 3.61 ± 0.16 |
| H2-Ti5-R5       | 2.53 ± 0.18 | 83.6 ± 0.8 | 0.91 ± 0.15 | 8.34 ± 0.07 | 3.86 ± 0.57 |
| H3-Ti5-R4       | 2.37 ± 0.06 | 84.8 ± 0.4 | 0.81 ± 0.11 | 8.27 ± 0.09 | 3.57 ± 0.10 |
| H3-Ti5-R5       | 2.79 ± 0.11 | 82.7 ± 0.9 | 0.96 ± 0.39 | 8.39 ± 0.10 | 4.37 ± 0.41 |

Table 2
Trace element concentrations of minerals and quenched silicate melts determined with LA-ICP-MS. All values are given in µg/g.

| Sample          | Mg g/g | S.D. | Al g/g | S.D. | Si g/g | S.D. | Ca g/g | S.D. | Ti g/g | S.D. |
|-----------------|--------|------|--------|------|--------|------|--------|------|--------|------|
| H1-Ti2-R3       | 13.367 | ± 2518 | 15263 | ± 2195 | 14105 | ± 3235 | 14245 | ± 2822 | 17157 | ± 3259 |
| H1-Ti5-R4       | 7058 | ± 1008 | 3778 | ± 668 | 4712 | ± 780 | 5629 | ± 863 | 9282 | ± 1272 |
| H1-Ti5-R5       | 59563 | ± 2104 | 59749 | ± 2163 | 59697 | ± 2172 | 59707 | ± 2166 | 9234 | ± 2095 |
| H2-Ti2-R2       | 30.6 | ± 2.8 | 28.2 | ± 2.1 | 28.3 | ± 2.2 | 28.7 | ± 2.0 | 28.3 | ± 1.9 |
| H2-Ti2-R3       | 11302 | ± 1412 | 21355 | ± 1797 | 19485 | ± 2546 | 12899 | ± 1736 | 14804 | ± 1124 |
| H2-Ti5-R4       | 2099 | ± 28123 | 2099 | ± 28123 | 2099 | ± 28123 | 2099 | ± 28123 | 2099 | ± 28123 |
| H2-Ti5-R5       | 3082 | ± 3.3 | 358 | ± 0.8 | 358 | ± 0.8 | 358 | ± 0.8 | 358 | ± 0.8 |
| H2-Ti2-R2       | 52.9 | ± 841 | 4192 | ± 758 | 5382 | ± 9282 | 59349 | ± 2095 | 35977 | ± 2119 |
| H2-Ti2-R3       | 541 | ± 41 | 0.3 | ± 0.2 | 0.3 | ± 0.2 | 0.3 | ± 0.2 | 0.3 | ± 0.2 |
| H2-Ti5-R4       | 533 | ± 0.5 | 192 | ± 1.4 | 192 | ± 1.4 | 192 | ± 1.4 | 192 | ± 1.4 |
| H2-Ti5-R5       | 613 | ± 0.6 | 18.9 | ± 4.3 | 18.9 | ± 4.3 | 18.9 | ± 4.3 | 18.9 | ± 4.3 |
|         | H1-T2-R3 | H1-T2-R4 | H2-T2-R3 | H1-T5-R3 | H1-T5-R4 | H2-T5-R3 | H1-T5-R5 | H2-T5-R4 | H2-T5-R5 |
|---------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| S.      | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        |
| Nb.     | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        |
| Yb.     | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        |
| Eu.     | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        |
| Ce.     | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        |
| Lu.     | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        |
| Zr.     | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        |
| Y.      | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        |
| Sr.     | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        |
| Sr.     | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        |
| Ta.     | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        |
| Hf.     | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        |
| W.      | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        |
| H.      | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        |
| Cr.     | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        |
| Ni.     | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        |
| Cu.     | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        |
| Zn.     | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        |
| Ga.     | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        |
| Ge.     | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        |
| Pb.     | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        |
| Th.     | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        |
| U.      | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        | ±        |

### Table 2 (continued)

|         | H3-T3-R4 | H3-T3-R5 | H3-T5-R3 | H3-T5-R4 | H3-R8  | H3-R8  | Mel3-R9 |
|---------|----------|----------|----------|----------|--------|--------|---------|
| µg/g    | S.D.     | µg/g    | S.D.     | µg/g    | S.D.  | µg/g  | S.D.    |
| Mg.     | 16888 ± 2734 | 29955 ± 5971 | 55758 ± 10561 | 2525 ± 242 | 166434 ± 36418 | b.d.l | 124887 ± 9030 | 176044 ± 17334 |
| Si.     | 17111 ± 2303 | 7555 ± 1188 | 110371 ± 14987 | 104108 ± 13955 | b.d.l | b.d.l | b.d.l | b.d.l |
| Ca.     | 59120 ± 2034 | 59935 ± 2154 | 290740 ± 12078 | 292070 ± 9299 | 1627 ± 681 | 1872 ± 554 | 1044 ± 348 | b.d.l |
| Sc.     | 44.5 ± 2.7 | 52.8 ± 3.9 | 189 ± 14 | 3.23 ± 0.36 | 15.4 ± 2.2 | 33.6 ± 2.1 | 16.8 ± 1.3 | b.d.l |
| Ti.     | 21275 ± 1994 | 29299 ± 3489 | 57273 ± 4394 | 3.78 ± 1.35 | b.d.l | 16.2 ± 4.8 | 372 ± 34 | b.d.l |
| V.      | 16.3 ± 1.2 | 7.1 ± 0.74 | 109 ± 9 | 0.39 ± 0.09 | 1.04 ± 0.50 | 4.79 ± 0.39 | 0.62 ± 0.24 | b.d.l |
| Cr.     | 24.9 ± 6.3 | 23.7 ± 8.3 | b.d.l | b.d.l | 18.5 ± 9.8 | 25.5 ± 6.7 | b.d.l | b.d.l |
| Co.     | 142 ± 9 | 196 ± 11 | 686 ± 38 | 18.2 ± 1.1 | 3577 ± 467 | 1409 ± 94 | 413 ± 39 | b.d.l |
| Ni.     | 144 ± 25 | 207 ± 78 | 1206 ± 354 | 17.5 ± 5.9 | 12392 ± 5282 | 3732 ± 515 | 1098 ± 216 | b.d.l |
| Cu.     | 10.4 ± 10 | 5.93 ± 0.87 | 93.8 ± 9.9 | 2.42 ± 0.32 | 122 ± 17 | 73.3 ± 5.3 | 7.87 ± 1.01 | b.d.l |
| Zn.     | 8.41 ± 2.71 | 8.75 ± 3.25 | 73.0 ± 25.4 | 1.45 ± 0.70 | 137 ± 48 | 37.1 ± 9.2 | 9.32 ± 3.82 | b.d.l |
| Ga.     | 236 ± 12 | 244 ± 17 | 815 ± 47 | 112 ± 6.6 | 577 ± 69 | 258 ± 12 | 373 ± 21 | b.d.l |
| Ge.     | 6.28 ± 1.74 | 8.93 ± 2.46 | 2.73 ± 0.92 | 13.3 ± 5.5 | b.d.l | 5.03 ± 2.20 | b.d.l | b.d.l |
| Pb.     | b.d.l | b.d.l | b.d.l | 0.14 ± 0.06 | 0.82 ± 0.34 | b.d.l | 0.27 ± 0.15 | b.d.l |
| Sr.     | 86.3 ± 4.1 | 107 ± 5 | 422 ± 21 | 110 ± 5 | b.d.l | 5.02 ± 0.41 | b.d.l | b.d.l |
| Y.      | 28.7 ± 1.7 | 270 ± 2.2 | 189 ± 12 | 93.2 ± 4.1 | 4.59 ± 0.18 | 0.20 ± 0.08 | b.d.l | b.d.l |
| Zr.     | 23.0 ± 1.4 | 34.0 ± 2.7 | 169 ± 13 | b.d.l | b.d.l | 6.04 ± 1.75 | b.d.l | b.d.l |
| Nb.     | 12.6 ± 0.7 | 21.4 ± 1.4 | 117 ± 8 | 0.03 ± 0.02 | 0.14 ± 0.07 | 1.18 ± 0.09 | 0.03 ± 0.03 | b.d.l |
| Rh.     | 6.31 ± 0.81 | 8.78 ± 1.51 | 45.2 ± 5.4 | 0.05 ± 0.02 | b.d.l | 9.49 ± 0.81 | 14.4 ± 1.5 | b.d.l |
| Cs.     | b.d.l | b.d.l | 1.53 ± 1.00 | 0.08 ± 0.03 | b.d.l | b.d.l | b.d.l | b.d.l |
| Ba.     | 9.20 ± 1.06 | 4.85 ± 1.04 | 61.9 ± 10.5 | 1.15 ± 0.23 | 1.60 ± 0.79 | 3.65 ± 0.68 | 0.88 ± 0.35 | b.d.l |
| La.     | 319 ± 13 | 336 ± 19 | 1176 ± 53 | 51.2 ± 1.7 | 1.10 ± 0.11 | b.d.l | b.d.l | b.d.l |
| Ce.     | 359 ± 16 | 379 ± 20 | 1522 ± 69 | 74.1 ± 2.6 | 0.03 ± 0.06 | 0.19 ± 0.01 | 0.02 ± 0.03 | b.d.l |
Table 2 (continued)

|            | **Hibonite** | **Melilite** | **Spinel** | **Silicate Melt** |
|------------|--------------|--------------|------------|------------------|
|            | H3-Ti5-R4    | H3-Ti5-R5    | H1-Ti2-R3  | H3-R8            | H2-R8           | H3-R8           | Mel3-R9         |
|            | µg/g         | S.D.         | µg/g       | S.D.            | µg/g            | S.D.            | µg/g            | S.D.            |
| Pr         | 244 ± 12     | 269 ± 14     | 1258 ± 57  | 76.6 ± 2.7      | b.d.l           | 0.08 ± 0.01     | 0.03 ± 0.02     | 0.13 ± 0.09     |
| Nd         | 215 ± 11     | 237 ± 17     | 1082 ± 63  | 91.1 ± 3.9      | 0.15 ± 0.24     | 0.13 ± 0.02     | 0.13 ± 0.09     | 0.24 ± 0.05     |
| Sm         | 158 ± 9      | 182 ± 16     | 630 ± 61   | 129 ± 6.6       | 0.50 ± 0.30     | 0.24 ± 0.05     | 0.05 ± 0.05     | 0.05 ± 0.08     |
| Eu         | 87.6 ± 4.5   | 98.8 ± 16    | 555 ± 30   | 93.0 ± 3.6      | b.d.l           | 0.07 ± 0.01     | 0.03 ± 0.03     | 0.09 ± 0.14     |
| Gd         | 87.6 ± 6.4   | 104 ± 9      | 525 ± 38   | 124 ± 6.6       | b.d.l           | 0.25 ± 0.03     | 0.09 ± 0.14     | 0.09 ± 0.07     |
| Tb         | 56.4 ± 3.1   | 64.5 ± 5.1   | 392 ± 23   | 107 ± 4         | 0.06 ± 0.04     | 0.12 ± 0.01     | 0.03 ± 0.02     | 0.10 ± 0.02     |
| Dy         | 31.8 ± 2.2   | 34.7 ± 3.8   | 189 ± 17   | 78.2 ± 3.4      | 0.10 ± 0.19     | 0.12 ± 0.02     | 0.04 ± 0.04     | 0.04 ± 0.04     |
| Ho         | 31.6 ± 1.8   | 33.8 ± 3.3   | 222 ± 15   | 93.8 ± 3.9      | 0.05 ± 0.04     | 0.10 ± 0.01     | 0.05 ± 0.02     | 0.05 ± 0.02     |
| Er         | 13.2 ± 0.9   | 12.7 ± 1.5   | 101 ± 10   | 44.8 ± 2.0      | 0.14 ± 0.11     | 0.10 ± 0.01     | 0.08 ± 0.04     | 0.08 ± 0.03     |
| Tm         | 9.54 ± 0.57  | 8.28 ± 0.84  | 77.5 ± 5.9 | 36.5 ± 1.4      | 0.11 ± 0.05     | 0.06 ± 0.01     | 0.08 ± 0.03     | 0.08 ± 0.03     |
| Yb         | 14.0 ± 1.1   | 10.7 ± 1.2   | 109 ± 11   | 54.7 ± 2.3      | 0.17 ± 0.17     | 0.14 ± 0.02     | 0.16 ± 0.08     | 0.16 ± 0.08     |
| Lu         | 12.3 ± 0.7   | 8.70 ± 0.80  | 101 ± 7    | 46.7 ± 1.9      | 0.14 ± 0.06     | 0.12 ± 0.01     | 0.15 ± 0.03     | 0.15 ± 0.03     |
| Hf         | 32.4 ± 2.2   | 53.4 ± 4.8   | 200 ± 15   | 0.05 ± 0.02     | 0.29 ± 0.17     | 0.14 ± 0.02     | 0.16 ± 0.07     | 0.16 ± 0.07     |
| Ta         | 35.9 ± 2.0   | 70.5 ± 5.6   | 313 ± 18   | 0.02 ± 0.01     | 0.07 ± 0.04     | 0.20 ± 0.01     | 0.03 ± 0.02     | 0.03 ± 0.02     |
| W          | 1.62 ± 0.23  | 1.57 ± 0.29  | 6.59 ± 1.4 | 0.03 ± 0.03     | 0.27 ± 0.14     | 0.31 ± 0.02     | 0.07 ± 0.05     | 0.07 ± 0.05     |
| Pb         | b.d.l        | b.d.l        | b.d.l      | b.d.l           | b.d.l           | b.d.l           | b.d.l           | b.d.l           |
| Th         | 68.4 ± 3.5   | 74.2 ± 6.4   | 490 ± 29   | 9.05 ± 0.35     | 0.06 ± 0.03     | 0.95 ± 0.07     | 0.01 ± 0.01     | 0.01 ± 0.01     |
| U          | 0.05 ± 0.02  | 0.03 ± 0.01  | 0.13 ± 0.10 | 0.00 ± 0.00   | b.d.l           | b.d.l           | b.d.l           | b.d.l           |

|            | **Spinel**   | **Silicate Melt** |
|------------|--------------|--------------------|
|            | Mel3-R11     | Mel3-R12           |
|            | µg/g         | µg/g               |
| Mg         | 186262 ± 33494 | 181809 ± 31474     |
| Si         | 1293 ± 336   | 1010 ± 304         |
| Ca         | b.d.l        | 1190 ± 339         |
| Sc         | 13.1 ± 2.2   | 12.4 ± 1.7         |
| Ti         | 369 ± 57     | 333 ± 48           |
| V          | 0.54 ± 0.24  | 0.58 ± 0.23         |
| Cr         | 10.1 ± 4.65  | b.d.l              |
| Co         | 425 ± 70     | 425 ± 51           |
| Ni         | 1014 ± 251   | 1030 ± 223         |
| Cu         | 73.2 ± 10.6  | 26.3 ± 3.0         |
| Zn         | 23.5 ± 5.0   | 15.4 ± 4.0         |
| Ga         | 369 ± 60     | 413 ± 49           |
| Ge         | b.d.l        | b.d.l              |
| Rb         | 0.44 ± 0.18  | b.d.l              |
| Sr         | 0.72 ± 0.38  | b.d.l              |
| Y          | 0.10 ± 0.06  | 0.07 ± 0.05         |
| Zr         | 0.09 ± 0.07  | 138 ± 7            |
| Nb         | 0.03 ± 0.02  | 110 ± 5            |
| Rh         | 32.9 ± 6.4   | 61.6 ± 60          |
| Cs         | 0.24 ± 0.12  | b.d.l              |
| Ba         | 0.44 ± 0.05  | 106 ± 5            |
| La         | 50.3 ± 2.0   | 67.9 ± 2.5         |
| Ce         | 0.03 ± 0.03  | 0.04 ± 0.02         |
| Pr         | 0.06 ± 0.03  | 0.02 ± 0.02         |
| Nd         | 0.10 ± 0.09  | 0.09 ± 0.08         |
| Sm         | 0.16 ± 0.11  | 0.09 ± 0.07         |
| Eu         | 0.04 ± 0.05  | 106 ± 5            |
| Gd         | 0.12 ± 0.7   | 124 ± 8            |
| Tb         | 0.01 ± 0.02  | 0.04 ± 0.02         |
| Dy         | 0.08 ± 0.06  | 0.06 ± 0.05         |
| Ho         | 0.05 ± 0.02  | 0.02 ± 0.01         |
| Er         | 0.07 ± 0.05  | 0.10 ± 0.05         |
| Spinel | H3-Ti5-R4 | H3-Ti5-R5 | H3-R8 | Mel3-R9 | Mel3-R11 | Mel3-R12 |
|--------|-----------|-----------|-------|---------|----------|----------|
| µg/g   | µg/g      | µg/g      | µg/g  | µg/g    | µg/g     | µg/g     |
| S.D.   | S.D.      | S.D.      | S.D.  | S.D.    | S.D.     | S.D.     |
| Tm 0.05| 0.05      | 0.05      | 0.05  | 0.05    | 0.05     | 0.05     |
| Yb 0.07| 0.07      | 0.07      | 0.07  | 0.07    | 0.07     | 0.07     |
| Lu 0.10| 0.10      | 0.10      | 0.10  | 0.10    | 0.10     | 0.10     |
| Hf 0.04| 0.04      | 0.04      | 0.04  | 0.04    | 0.04     | 0.04     |
| Ta 0.01| 0.01      | 0.01      | 0.01  | 0.01    | 0.01     | 0.01     |
| W 0.03 | 0.03      | 0.03      | 0.03  | 0.03    | 0.03     | 0.03     |
| Pb b.d.| 0.07      | 0.07      | 0.07  | 0.07    | 0.07     | 0.07     |
| Th b.d.| 0.01      | 0.01      | 0.01  | 0.01    | 0.01     | 0.01     |
| U 0.01 | 0.01      | 0.01      | 0.01  | 0.01    | 0.01     | 0.01     |

| Silicate Melt |
|---------------|
| H3-Ti5-R4     | H3-Ti5-R5 | H3-R8 | Mel3-R9 | Mel3-R11 | Mel3-R12 |
| µg/g          | µg/g      | µg/g  | µg/g    | µg/g     | µg/g     |
| S.D.          | S.D.      | S.D.  | S.D.    | S.D.     | S.D.     |
| Tm 0.05       | 0.05      | 0.05  | 0.05    | 0.05     | 0.05     |
| Yb 0.07       | 0.07      | 0.07  | 0.07    | 0.07     | 0.07     |
| Lu 0.10       | 0.10      | 0.10  | 0.10    | 0.10     | 0.10     |
| Hf 0.04       | 0.04      | 0.04  | 0.04    | 0.04     | 0.04     |
| Ta 0.01       | 0.01      | 0.01  | 0.01    | 0.01     | 0.01     |
| W 0.03        | 0.03      | 0.03  | 0.03    | 0.03     | 0.03     |
| Pb b.d.       | 0.07      | 0.07  | 0.07    | 0.07     | 0.07     |
| Th b.d.       | 0.01      | 0.01  | 0.01    | 0.01     | 0.01     |
| U 0.01        | 0.01      | 0.01  | 0.01    | 0.01     | 0.01     |
Table 3
Mineral-melt partition coefficients including the available literature data. The 1e represents the mean absolute standard error on the average and “n” stands for the number of analyzes that had been incorporated in the calculations for the D-values in the form of “n” of the mineral vs. “n” of the silicate melt.

|     | H1-Ti2-R3 |     | H1-Ti5-R4 |     | H1-Ti5-R5 |     | H2-Ti2-R2 |     | H2-Ti2-R3 |     |
|-----|-----------|-----|-----------|-----|-----------|-----|-----------|-----|-----------|-----|
| D-Value | σ | n | D-Value | σ | n | D-Value | σ | n | D-Value | σ | n | D-Value | σ | n |
| Mg  | 1.86 ± 0.21 | 5/6 | 2.68 ± 0.22 | 6/6 | 2.98 ± 0.40 | 6/6 | 0.92 ± 0.11 | 6/6 | 1.12 ± 0.12 | 6/6 |
| Si  | 0.045 ± 0.004 | 5/6 | 0.027 ± 0.003 | 5/6 | 0.031 ± 0.003 | 5/6 | 0.033 ± 0.003 | 5/6 | 0.051 ± 0.004 | 5/6 |
| Ca  | 0.29 ± 0.01  | 5/6 | 0.31 ± 0.01  | 5/6 | 0.28 ± 0.01  | 6/6 | 0.34 ± 0.01  | 6/6 | 0.32 ± 0.01  | 6/6 |
| Sc  | 0.18 ± 0.01  | 5/6 | 0.19 ± 0.01  | 6/6 | 0.17 ± 0.01  | 6/6 | 0.20 ± 0.01  | 6/6 | 0.18 ± 0.01  | 6/6 |
| Ti  | 0.91 ± 0.06  | 5/6 | 0.68 ± 0.03  | 6/6 | 0.67 ± 0.05  | 6/6 | 1.08 ± 0.07  | 6/6 | 1.21 ± 0.05  | 6/6 |
| V   | 0.033 ± 0.002 | 5/6 | 0.020 ± 0.001 | 6/6 | 0.019 ± 0.001 | 6/6 | 0.044 ± 0.002 | 6/6 | 0.049 ± 0.002 | 6/6 |
| Cr  | 1.63 ± 0.05  | 5/6 | 2.40 ± 0.08  | 6/6 | 1.65 ± 0.23  | 6/6 | 0.62 ± 0.11  | 6/6 | 0.77 ± 0.12  | 6/6 |
| Ni  | 0.16 ± 0.01  | 5/6 | 0.18 ± 0.01  | 6/6 | 0.18 ± 0.01  | 6/6 | 0.069 ± 0.003 | 6/6 | 0.12 ± 0.01  | 6/6 |
| Cu  | 3.37 ± 0.05  | 4/5 | 3.53 ± 0.06  | 6/6 | 4.32 ± 1.07  | 2/5 | 2.21 ± 0.37  | 4/5 | 2.44 ± 0.35  | 5/6 |
| Zn  | 2.56 ± 0.08  | 6/6 | 1.81 ± 0.05  | 6/6 | 1.95 ± 0.07  | 6/6 | 1.66 ± 0.05  | 6/6 | 2.44 ± 0.07  | 6/6 |
| Ga  | 2.99 ± 0.74  | 3/1 | 3.80 ± 0.56  | 4/6 | 3.08 ± 0.83  | 3/4 | 3.76 ± 0.84  | 5/3 | 3.89 ± 0.92  | 6/3 |
| Nb  | 0.087 ± 0.003 | 5/6 | 0.083 ± 0.003 | 6/6 | 0.075 ± 0.003 | 6/6 | 0.20 ± 0.01  | 6/6 | 0.19 ± 0.01  | 6/6 |
| Rh  | 19.4 ± 1.5   | 5/6 | 13.6 ± 1.1   | 6/6 | 19.8 ± 2.5   | 6/6 | 1.97 ± 0.17  | 6/6 | –         | 0/6 |
| Cs  | 0.031 ± 0.003 | 4/6 | 0.027 ± 0.003 | 6/6 | 0.029 ± 0.003 | 6/6 | 0.025 ± 0.004 | 6/6 | 0.026 ± 0.003 | 6/6 |
| La  | 7.52 ± 0.19  | 5/6 | 4.29 ± 0.09  | 6/6 | 5.17 ± 0.15  | 6/6 | 7.07 ± 0.17  | 6/6 | 8.44 ± 0.20  | 6/6 |
| Ce  | 4.49 ± 0.11  | 5/6 | 2.89 ± 0.07  | 6/6 | 3.05 ± 0.10  | 6/6 | 5.18 ± 0.13  | 6/6 | 5.82 ± 0.14  | 6/6 |
| Pr  | 4.68 ± 0.12  | 5/6 | 2.94 ± 0.08  | 6/6 | 3.23 ± 0.12  | 6/6 | 5.29 ± 0.13  | 6/6 | 5.69 ± 0.14  | 6/6 |
| Nd  | 3.97 ± 0.12  | 5/6 | 2.52 ± 0.07  | 6/6 | 2.69 ± 0.10  | 6/6 | 4.60 ± 0.14  | 6/6 | 4.75 ± 0.14  | 6/6 |
| Sm  | 1.96 ± 0.07  | 5/6 | 1.36 ± 0.04  | 6/6 | 1.34 ± 0.06  | 6/6 | 2.56 ± 0.09  | 6/6 | 2.43 ± 0.08  | 6/6 |
| Eu  | 1.35 ± 0.04  | 5/6 | 0.95 ± 0.03  | 6/6 | 0.93 ± 0.04  | 6/6 | 1.83 ± 0.05  | 6/6 | 1.66 ± 0.05  | 6/6 |
| Gd  | 1.11 ± 0.04  | 5/6 | 0.84 ± 0.03  | 6/6 | 0.81 ± 0.05  | 6/6 | 1.58 ± 0.05  | 6/6 | 1.36 ± 0.04  | 6/6 |
| Tb  | 0.65 ± 0.02  | 5/6 | 0.50 ± 0.01  | 6/6 | 0.48 ± 0.02  | 6/6 | 1.00 ± 0.03  | 6/6 | 0.83 ± 0.03  | 6/6 |
| Dy  | 0.43 ± 0.02  | 5/6 | 0.32 ± 0.01  | 6/6 | 0.31 ± 0.02  | 6/6 | 0.67 ± 0.03  | 6/6 | 0.55 ± 0.02  | 6/6 |
| Ho  | 0.28 ± 0.01  | 5/6 | 0.21 ± 0.01  | 6/6 | 0.20 ± 0.01  | 6/6 | 0.45 ± 0.02  | 6/6 | 0.38 ± 0.01  | 6/6 |
| Er  | 0.18 ± 0.01  | 5/6 | 0.15 ± 0.01  | 6/6 | 0.13 ± 0.01  | 6/6 | 0.30 ± 0.01  | 6/6 | 0.25 ± 0.01  | 6/6 |
| Tm  | 0.11 ± 0.00  | 5/6 | 0.075 ± 0.002 | 6/6 | 0.077 ± 0.003 | 6/6 | 0.19 ± 0.01  | 6/6 | 0.15 ± 0.01  | 6/6 |
| Yb  | 0.069 ± 0.003 | 5/6 | 0.052 ± 0.002 | 6/6 | 0.050 ± 0.003 | 6/6 | 0.12 ± 0.01  | 6/6 | 0.098 ± 0.004 | 6/6 |
| Lu  | 0.053 ± 0.002 | 5/6 | 0.036 ± 0.001 | 6/6 | 0.035 ± 0.002 | 6/6 | 0.088 ± 0.003 | 6/6 | 0.072 ± 0.003 | 6/6 |
Table 3 (continued)

### Hibonite

|       | H1-Ti2-R3 | H1-Ti5-R4 | H1-Ti5-R5 | H2-Ti2-R2 | H2-Ti2-R3 |
|-------|-----------|-----------|-----------|-----------|-----------|
|       | D-Value   | σ         | n         | D-Value   | σ         | n         | D-Value   | σ         | n         | D-Value   | σ         | n         | D-Value   | σ         | n         |
| Hf    | 0.49 ± 0.2 | 5/6       | 0.47 ± 0.2 | 6/6       | 0.42 ± 0.2 | 6/6       | 0.66 ± 0.2 | 6/6       | 0.57 ± 0.2 | 6/6       |
| Ta    | 0.35 ± 0.1 | 5/6       | 0.35 ± 0.1 | 6/6       | 0.33 ± 0.1 | 6/6       | 0.74 ± 0.2 | 6/6       | 0.70 ± 0.2 | 6/6       |
| W     | 0.012 ± 0.004 | 5/6 | 0.007 ± 0.003 | 4/6 | 0.009 ± 0.002 | 4/6 | 0.053 ± 0.013 | 4/6 | 0.042 ± 0.008 | 6/6       |
| Pb    | –         | 0/4       | –         | 0/3       | –         | 1/0       | –         | 0/6       | –         | 0/2       |
| Th    | 1.56 ± 0.05 | 5/6 | 0.86 ± 0.02 | 6/6 | 0.81 ± 0.03 | 6/6 | 2.30 ± 0.08 | 6/6 | 2.01 ± 0.07 | 6/6       |
| U     | –         | 0/6       | 0.021 ± 0.015 | 1/6 | –         | 0/6       | 0.038 ± 0.010 | 3/6 | 0.047 ± 0.018 | 3/6       |

### Hibonite

|       | H2-Ti5-R4 | H2-Ti5-R5 | H3-Ti5-R4 | H3-Ti5-R5 | Ø Hibonite |
|-------|-----------|-----------|-----------|-----------|------------|
| Mg    | 1.47 ± 0.13 | 6/6 | 1.63 ± 0.26 | 6/6 | 1.04 ± 0.10 | 6/6 | 1.52 ± 0.25 | 6/6 | 1.69 ± 0.57 |
| Si    | 0.032 ± 0.003 | 6/6 | 0.028 ± 0.002 | 6/6 | 0.11 ± 0.01 | 6/6 | 0.050 ± 0.004 | 6/6 | 0.045 ± 0.011 |
| Ca    | 0.35 ± 0.01 | 6/6 | 0.33 ± 0.01 | 6/6 | 0.31 ± 0.01 | 6/6 | 0.29 ± 0.01 | 6/6 | 0.31 ± 0.02 |
| Sc    | 0.17 ± 0.01 | 6/6 | 0.17 ± 0.01 | 6/6 | 0.22 ± 0.01 | 6/6 | 0.23 ± 0.01 | 6/6 | 0.19 ± 0.02 |
| Ti    | 0.87 ± 0.04 | 6/6 | 0.91 ± 0.06 | 6/6 | 0.74 ± 0.04 | 6/6 | 1.01 ± 0.07 | 6/6 | 0.90 ± 0.15 |
| V     | 0.039 ± 0.002 | 6/6 | 0.028 ± 0.002 | 6/6 | 0.098 ± 0.004 | 6/6 | 0.040 ± 0.002 | 6/6 | 0.041 ± 0.006 |
| Cr    | –         | 1/0       | –         | 1/0       | 4.59 ± 2.21 | 5/1 | 4.15 ± 0.05 | 6/6 | 1.53 ± 0.14 |
| Co    | 1.46 ± 0.05 | 6/6 | 1.61 ± 0.05 | 6/6 | 0.90 ± 0.03 | 6/6 | 4.15 ± 0.05 | 6/6 | 1.53 ± 0.14 |
| Ni    | 1.26 ± 0.11 | 6/6 | 1.33 ± 0.27 | 6/6 | 0.73 ± 0.07 | 6/6 | 1.15 ± 0.25 | 6/6 | 1.18 ± 0.51 |
| Cu    | 0.13 ± 0.01 | 6/6 | 0.14 ± 0.01 | 6/6 | 0.15 ± 0.01 | 6/6 | 0.12 ± 0.01 | 6/6 | 0.14 ± 0.02 |
| Zn    | 3.73 ± 1.01 | 2/5 | 2.68 ± 0.41 | 5/6 | 1.49 ± 0.26 | 5/6 | 2.27 ± 0.45 | 5/5 | 2.89 ± 1.51 |
| Ga    | 2.18 ± 0.06 | 6/6 | 2.21 ± 0.09 | 6/6 | 1.72 ± 0.05 | 6/6 | 2.33 ± 0.09 | 6/6 | 2.10 ± 0.19 |
| Ge    | 3.57 ± 0.61 | 4/6 | 4.56 ± 1.00 | 3/4 | 2.00 ± 0.36 | 4/5 | 3.82 ± 0.78 | 3/5 | 3.39 ± 2.02 |
| Rb    | 0.86 ± 0.29 | 1/6 | 0.81 ± 0.25 | 1/6 | –         | 0/6       | –         | 0/6       | 0.83 ± 0.38 |
| Sr    | 0.57 ± 0.02 | 6/6 | 0.56 ± 0.02 | 6/6 | 0.48 ± 0.01 | 6/6 | 0.55 ± 0.02 | 6/6 | 0.53 ± 0.04 |
| Y     | 0.23 ± 0.01 | 6/6 | 0.19 ± 0.01 | 6/6 | 0.22 ± 0.01 | 6/6 | 0.17 ± 0.01 | 6/6 | 0.23 ± 0.02 |
| Zr    | 0.18 ± 0.01 | 6/6 | 0.19 ± 0.01 | 6/6 | 0.18 ± 0.01 | 6/6 | 0.27 ± 0.01 | 6/6 | 0.21 ± 0.02 |
| Nb    | 0.11 ± 0.00 | 6/6 | 0.10 ± 0.00 | 6/6 | 0.14 ± 0.00 | 6/6 | 0.22 ± 0.01 | 6/6 | 0.13 ± 0.01 |
| Rh    | 29.2 ± 2.7 | 6/6 | 21.2 ± 2.2 | 6/6 | 8.93 ± 0.73 | 6/6 | 30.0 ± 3.4 | 6/6 | 22.1 ± 5.5 |
| Cs    | –         | 0/0       | –         | 0/0       | –         | 0/0       | –         | 0/0       | –         |
| Ba    | 0.028 ± 0.003 | 5/6 | 0.028 ± 0.003 | 6/6 | 0.095 ± 0.005 | 6/6 | 0.043 ± 0.004 | 5/6 | 0.037 ± 0.012 |
| La    | 5.76 ± 0.13 | 6/6 | 6.91 ± 0.21 | 6/6 | 3.33 ± 0.08 | 6/6 | 4.83 ± 0.16 | 6/6 | 5.92 ± 0.43 |
| Ce    | 4.16 ± 0.10 | 6/6 | 4.47 ± 0.13 | 6/6 | 2.20 ± 0.06 | 6/6 | 2.90 ± 0.09 | 6/6 | 3.91 ± 0.29 |
| Pr    | 4.08 ± 0.11 | 6/6 | 4.49 ± 0.13 | 6/6 | 2.37 ± 0.07 | 6/6 | 3.12 ± 0.10 | 6/6 | 3.99 ± 0.31 |
| Element | D-Value | σ  | n  | D-Value | σ  | n  | D-Value | σ  |
|---------|---------|----|----|---------|----|----|---------|----|
| Mg      | 0.50    |    |    | 7.78    | ±0.12 | 2/6 | 0.21    | ±0.01 | 6/5 |
| Si      | 0.028   |    |    | 0.70    | ±0.08 | 2/6 | 0.68    | ±0.06 | 6/5 |
| Ca      | 0.30    |    |    | 1.42    | ±0.05 | 2/6 | 1.50    | ±0.03 | 6/5 |
| Sc      | 0.46    |    |    | 1.12    | ±0.07 | 2/6 | 0.012   | ±0.001 | 6/5 |
| Ti      | 1.29    |    |    | 4.60    | ±0.29 | 2/6 | 0.027   | ±0.010 | 1/5 |
| V       | 5.78    |    |    | 0.57    | ±0.04 | 2/6 | 0.002   | ±0.000 | 6/5 |
| Cr      | –       |    |    | –       |       | 0/0 | –       |       |     |
| Co      | –       |    |    | 6.07    | ±0.27 | 2/6 | 0.13    | ±0.00 | 6/5 |
| Ni      | –       |    |    | 4.25    | ±0.98 | 2/6 | 0.17    | ±0.03 | 4/5 |
| Cu      | –       |    |    | 1.32    | ±0.10 | 2/6 | 0.044   | ±0.003 | 6/5 |
| Zn      | –       |    |    | 17.9    | ±6.5  | 1/5 | 0.48    | ±0.18 | 2/5 |
| Ga      | –       |    |    | 8.47    | ±0.39 | 2/6 | 0.81    | ±0.03 | 6/5 |
| Ge      | 0.78    |    |    | –       |       | 0/3 | 1.21    | ±0.27 | 4/5 |
| Rb      | –       |    |    | –       |       | 0/6 | 0.36    | ±0.16 | 1/5 |
| Sr      | 0.62    |    |    | 2.24    | ±0.09 | 2/6 | 0.52    | ±0.01 | 6/5 |
| Y       | –       |    |    | 1.17    | ±0.06 | 2/6 | 0.58    | ±0.02 | 6/5 |
| Zr      | 0.35    |    |    | 1.22    | ±0.07 | 2/6 | –       |       |     |
| Nb      | 0.27    |    |    | 1.06    | ±0.05 | 2/6 | 0.0003  | ±0.0001 | 2/5 |
| Rh      | –       |    |    | 123    | ±13  | 2/6 | 0.32    | ±0.08 | 3/5 |
| Cs      | –       |    |    | 1.00    |       | 1/0 | –       |       |     |
| Ba      | 0.030   |    |    | 0.53    | ±0.06 | 2/6 | 0.009   | ±0.001 | 6/5 |

**Hibonite**

Kennedy et al. 1994

| Element | D-Value | σ  |
|---------|---------|----|
| Mg      | 0.50    |    |
| Si      | 0.028   |    |
| Ca      | 0.30    |    |
| Sc      | 0.46    |    |
| Ti      | 1.29    |    |
| V       | 5.78    |    |
| Cr      | –       |    |
| Co      | –       |    |
| Ni      | –       |    |
| Cu      | –       |    |
| Zn      | –       |    |
| Ga      | –       |    |
| Ge      | 0.78    |    |
| Rb      | –       |    |
| Sr      | 0.62    |    |
| Y       | –       |    |
| Zr      | 0.35    |    |
| Nb      | 0.27    |    |
| Rh      | –       |    |
| Cs      | –       |    |
| Ba      | 0.030   |    |

**Melilitel**

Beckett & Stolper 1994

| Element | D-Value | σ  |
|---------|---------|----|
| Mg      | 0.50    |    |
| Si      | 0.028   |    |
| Ca      | 0.30    |    |
| Sc      | 0.46    |    |
| Ti      | 1.29    |    |
| V       | 5.78    |    |
| Cr      | –       |    |
| Co      | –       |    |
| Ni      | –       |    |
| Cu      | –       |    |
| Zn      | –       |    |
| Ga      | –       |    |
| Ge      | 0.78    |    |
| Rb      | –       |    |
| Sr      | 0.62    |    |
| Y       | –       |    |
| Zr      | 0.35    |    |
| Nb      | 0.27    |    |
| Rh      | –       |    |
| Cs      | –       |    |
| Ba      | 0.030   |    |

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**Note:**

- D-Value and σ values are provided for each element in the table.
- The data includes information on the concentration of various elements in the Hibonite and Melilitel samples, with σ values indicating the precision or uncertainty of the measurements.
- The table format and structure are designed to facilitate comparison and analysis of the datasets.
| Element | D-Value | σ   | n   |
|---------|---------|-----|-----|
| La      | 5.50    |     |     |
| Ce      | 4.50    |     |     |
| Pr      | 3.80    |     |     |
| Nd      | 3.20    |     |     |
| Sm      | 1.65    |     |     |
| Eu      | 1.25    |     |     |
| Gd      | 1.03    |     |     |
| Tb      | 0.62    |     |     |
| Dy      | 0.36    |     |     |
| Ho      | 0.25    |     |     |
| Er      | 0.22    |     |     |
| Yb      | 0.21    |     |     |
| Lu      | 0.075   |     |     |
| Hf      | 0.73    |     |     |
| Ta      | 0.097   |     |     |
| W       | 0.093   |     |     |
| Pb      | –       | 0/4 | 0/5 |
| Th      | 0.080   |     |     |

**Melilite**

| Element | D-Value | σ   | n   |
|---------|---------|-----|-----|
| Mg      | –       |     |     |
| Si      | –       |     |     |
| Ca      | –       |     |     |
| Sc      | –       |     |     |
| Ti      | –       |     |     |
| V       | –       |     |     |
| Cr      | –       |     |     |
| Co      | –       |     |     |
| Ni      | –       |     |     |
| Cu      | –       |     |     |

**Spinel**

| Element | D-Value | σ   | n   |
|---------|---------|-----|-----|
| Mg      | –       |     |     |
| Si      | –       |     |     |
| Ca      | –       |     |     |
| Sc      | –       |     |     |
| Ti      | –       |     |     |
| V       | –       |     |     |
| Cr      | –       |     |     |
| Co      | –       |     |     |
| Ni      | –       |     |     |
| Cu      | –       |     |     |
| Element | Mel3-R11-Spinel | Mel3-R12-Spinel | Ø Spinel | Lundstrom et al. 2006 |
|---------|----------------|----------------|----------|---------------------|
|         | D-Value        | σ              | n        | D-Value             | σ               | n        | D-Value | σ               | n        |
| Zn      | –              | –              | 20.9 ± 7.9 | 4/6 | 12.2 ± 2.4 | 6/5 | 3.60 ± 0.90 | 8/5 |
| Ga      | –              | –              | 2.77 ± 0.40 | 4/7 | 1.85 ± 0.06 | 6/5 | 2.65 ± 0.09 | 8/5 |
| Ge      | –              | –              | 2.41 ± 1.20 | 1/2 | –            | –   | 0.5 ± 0.23  | 1/5 |
| Rb      | 0.013 ± 0.002  | 1.20 ± 0.52    | 6/5 | 0.51 ± 0.33 | 1/5 | 0.52 ± 0.23 | 1/5 |
| Sr      | 0.93 ± 0.00    | 0.68 ± 0.02    | 0.024 ± 0.002 | 1/5 | –            | –   | 0.5 ± 0.23  | 1/5 |
| Y       | 0.22 ± 0.00    | –              | 0.025 ± 0.001 | 1/5 | 0.0007 ± 0.0002 | 3/5 |
| Zr      | 0.002 ± 0.0000 | –              | 0.042 ± 0.012 | 1/5 | –            | –   | 0.5 ± 0.23  | 1/5 |
| Nb      | 0.003 ± 0.001  | 0.0009 ± 0.0003 | 2/7 | 0.011 ± 0.001 | 2/5 | 0.0001 ± 0.0001 | 1/5 |
| Rh      | –              | –              | 59.1 ± 5.4 | 6/5 | 52.1 ± 3.8  | 8/5 |           |     |
| Cs      | 0.003 ± 0.001  | –              | 0/1 | –            | 0/0 |           |     |
| Ba      | 0.018 ± 0.001  | 0.010 ± 0.005  | 1/7 | 0.029 ± 0.001 | 1/5 | 0.003 ± 0.001 | 1/5 |
| La      | 0.35 ± 0.00    | 0.056 ± 0.006  | –    | 0.0009 ± 0.0000 | 3/5 | –            | 0/5 |
| Ce      | 0.053 ± 0.002  | 0.0001 ± 0.0003 | 1/7 | 0.001 ± 0.0000 | 3/5 | 0.0001 ± 0.0001 | 1/5 |
| Pr      | –              | –              | 0.0007 ± 0.0000 | 4/5 | 0.0002 ± 0.0001 | 1/5 |
| Nd      | 0.066 ± 0.013  | 0.0008 ± 0.0013 | 1/7 | 0.001 ± 0.0000 | 4/5 | 0.0007 ± 0.0003 | 2/5 |
| Sm      | 0.38 ± 0.00    | 0.072 ± 0.003  | 0.002 ± 0.0000 | 4/5 | 0.0002 ± 0.0003 | 1/5 |
| Eu      | 0.067 ± 0.005  | –              | 0.0006 ± 0.0000 | 4/5 | 0.0002 ± 0.0002 | 1/5 |
| Gd      | –              | –              | 0.002 ± 0.0000 | 4/5 | 0.0004 ± 0.0004 | 2/5 |
| Tb      | –              | –              | 0.0003 ± 0.0001 | 2/7 | 0.0009 ± 0.0000 | 4/5 | 0.0001 ± 0.0000 | 5/5 |
| Dy      | –              | –              | 0.0006 ± 0.0001 | 1/7 | 0.0010 ± 0.0001 | 3/5 | 0.0003 ± 0.0002 | 3/5 |
| Ho      | –              | –              | 0.0002 ± 0.0000 | 4/5 | 0.0006 ± 0.0000 | 4/5 | 0.0002 ± 0.0000 | 6/5 |
| Er      | –              | –              | 0.001 ± 0.0000 | 4/5 | 0.0003 ± 0.0000 | 4/5 | 0.0003 ± 0.0000 | 8/5 |
| Tm      | –              | –              | 0.0008 ± 0.0000 | 4/5 | 0.0003 ± 0.0000 | 4/5 | 0.0003 ± 0.0000 | 8/5 |
| Yb      | 0.13 ± 0.00    | 0.019 ± 0.011  | 0.0008 ± 0.0000 | 2/7 | 0.0008 ± 0.0001 | 4/5 | 0.0007 ± 0.0001 | 6/5 |
| Lu      | –              | –              | 0.0006 ± 0.0001 | 4/5 | 0.0008 ± 0.0000 | 6/5 | 0.0006 ± 0.0001 | 8/5 |
| Hf      | –              | –              | 0.0001 ± 0.0001 | 2/7 | 0.001 ± 0.0000 | 5/5 | 0.0009 ± 0.0001 | 8/5 |
| Ta      | –              | –              | 0.0005 ± 0.0003 | 1/7 | 0.002 ± 0.0000 | 2/5 | 0.0002 ± 0.0001 | 2/5 |
| W       | 0.002 ± 0.001  | 0.002 ± 0.0000 | 1/7 | 0.002 ± 0.0000 | 2/5 | 0.0003 ± 0.0001 | 4/5 |
| Pb      | –              | –              | 0.004 ± 0.0002 | 1/7 | 0.009 ± 0.0000 | 4/5 | 0.0001 ± 0.0000 | 2/5 |
| Th      | –              | –              | 0.0004 ± 0.0000 | 4/5 | 0.0001 ± 0.0000 | 2/5 | 0.0001 ± 0.0000 | 2/5 |
| U       | –              | –              | 0.0002 ± 0.0000 | 1/7 | 0.029 ± 0.0029 | 1/5 | –            |   |

| Element | Mel3-R11-Spinel | Mel3-R12-Spinel | Ø Spinel | Lundstrom et al. 2006 |
|---------|----------------|----------------|----------|---------------------|
|         | D-Value        | σ              | n        | D-Value             | σ               | n        | D-Value | σ               | n        |
| Mg      | 3.99 ± 0.51    | –              | 6/6 | –            | –   | 6/6 | 4.97 ± 0.71 | 2/6 | 6/12 | 7.00 ± 2.20 | 8/6 |
| Si      | 0.008 ± 0.002  | 1/6 | 0.0005 ± 0.0001 | 2/12 | 0.014 ± 0.005 | 3/6 |
| Ca      | 0.063 ± 0.005  | 6/6 | 0.005 ± 0.0001 | 2/12 | 0.007 ± 0.003 | 3/6 |
| Sc      | 0.028 ± 0.002  | 6/6 | 0.025 ± 0.0002 | 6/12 | 0.048 ± 0.009 | 3/6 |
| Ti      | 0.002 ± 0.001  | 1/6 | 0.001 ± 0.0001 | 1/12 | 0.007 ± 0.006 | 3/6 |
| Cr      | –              | 6/0 | –            | –   | 6/0 | –   | –            | –   | –   | –            | –   |
| Element | Mel3-R11-Spinel | Mel3-R12-Spinel | Ø Spinel | Lundstrom et al. 2006 |
|---------|-----------------|-----------------|----------|----------------------|
| Co      | 3.70 ± 0.26     | 4.85 ± 0.26     | 6.74     ± 1.26       | –        |
| Ni      | 13.8 ± 2.3      | 12.6 ± 1.4      | 22.7     ± 9.5        | –        |
| Cu      | 0.42 ± 0.03     | 0.41 ± 0.02     | 0.85     ± 0.19       | –        |
| Zn      | 6.65 ± 0.91     | 4.80 ± 0.51     | 9.65     ± 5.04       | –        |
| Ga      | 2.77 ± 0.20     | 2.69 ± 0.13     | 2.55     ± 0.45       | –        |
| Ge      | –               | 0/6             | 1.47     ± 0.97       | –        |
| Rb      | 1.01 ± 0.42     | –               | 0.94     ± 0.76       | –        |
| Sr      | 0.0002 ± 0.0001 | –               | 0.013    ± 0.007      | –        |
| Y       | 0.0005 ± 0.0003 | 0.0006 ± 0.0003 | 0.003    ± 0.004      | 0.00004 ± 0.00001 |
| Zr      | –               | 0/6             | 0.008    ± 0.007      | –        |
| Nb      | –               | 0/6             | 0.001    ± 0.0001     | 0.00000  ± 0.00000 |
| Rh      | 69.3 ± 7.4      | 39.9 ± 11.8     | 55.1     ± 18.5       | –        |
| Cs      | –               | –               | 0.014    ± 0.009      | –        |
| Ba      | –               | 0/6             | 0.009    ± 0.000      | 0.000003 ± 0.000004 |
| La      | –               | 0/6             | 0.003    ± 0.000      | –        |
| Ce      | 0.0002 ± 0.0001 | 0.0001 ± 0.0001 | 0.001    ± 0.0005     | –        |
| Pr      | 0.0005 ± 0.0001 | 0.0001 ± 0.0001 | 0.0004   ± 0.0005     | –        |
| Nd      | 0.0007 ± 0.0006 | 0.0004 ± 0.0003 | 0.0007   ± 0.0015     | 0.0003 ± 0.0004 |
| Sm      | 0.0008 ± 0.0004 | 0.0003 ± 0.0001 | 0.001    ± 0.002      | –        |
| Eu      | –               | 0/6             | 0.003    ± 0.0005     | –        |
| Gd      | –               | 0/6             | 0.001    ± 0.001      | –        |
| Tb      | 0.0000 ± 0.0001 | 0.0002 ± 0.0000 | 0.0003   ± 0.0006     | –        |
| Dy      | 0.0007 ± 0.0006 | 0.0004 ± 0.0002 | 0.0006   ± 0.0013     | –        |
| Ho      | 0.0003 ± 0.0001 | 0.0001 ± 0.0000 | 0.0003   ± 0.0002     | –        |
| Er      | 0.0004 ± 0.0001 | 0.0004 ± 0.0001 | 0.0006   ± 0.0006     | 0.0003 ± 0.0001 |
| Tm      | 0.0003 ± 0.0001 | 0.0004 ± 0.0001 | 0.0005   ± 0.0003     | –        |
| Yb      | 0.0004 ± 0.0005 | 0.0005 ± 0.0002 | 0.0006   ± 0.0010     | –        |
| Lu      | 0.0006 ± 0.0001 | 0.0002 ± 0.0000 | 0.0006   ± 0.0002     | –        |
| Hf      | 0.0003 ± 0.0004 | 0.0007 ± 0.0003 | 0.001    ± 0.001      | 0.001 ± 0.000 |
| Ta      | 0.0001 ± 0.0003 | 0.0001 ± 0.0001 | 0.0005   ± 0.0019     | 0.0001 ± 0.0001 |
| W       | 0.0003 ± 0.0005 | 0.0002 ± 0.0000 | 0.0010   ± 0.0020     | –        |
| Pb      | –               | 0/2             | 3.47     ± 1.11       | 3.47 ± 1.11 |
| Th      | 0/6             | 0.0000 ± 0.0000 | 0.002    ± 0.003      | 0.0006 ± 0.0000 |
| U       | 0.001 ± 0.0001  | –               | 0.015    ± 0.021      | 0.0003 ± 0.0002 |

1 The D-values for melilite are directly influenced by the initial Ti concentration within the starting mixture. As far as two samples are appropriate enough to show, it could be that a higher Ti concentration is enhancing the incorporation possibilities for several elements.

2 The D-values for spinel are influenced by the very different starting compositions in respect to the aluminum and magnesium content between the starting mixtures H2, H3 and Mel3 (cf. Table 5)
Table 4
Mineral-mineral partition coefficients with corresponding 1σ error as the mean absolute standard error of the average.

|                | Hibonite/Melilite |       | Hibonite/Spinel |       | Melilite/Spinel |       |
|----------------|-------------------|-------|-----------------|-------|-----------------|-------|
|                | D-Value           | σ     | D-Value         | σ     | D-Value         | σ     |
| Mg             | 0.42              | ± 0.16| 0.24            | ± 0.11| 0.57            | ± 0.20|
| Si             | 0.066             | ± 0.018| 3.37            | ± 1.47| 51.3            | ± 20.2|
| Ca             | 0.21              | ± 0.01| 46.6            | ± 21.5| 217             | ± 100 |
| Sc             | 0.34              | ± 0.04| 2.54            | ± 0.58| 7.56            | ± 1.62|
| Ti             | 0.39              | ± 0.15| 18.8            | ± 4.7 | 48.6            | ± 20.0|
| V              | 0.14              | ± 0.03| 5.91            | ± 4.98| 41.0            | ± 34.3|
| Cr             | –                 | –     | –               | –     | –               | –     |
| Co             | 0.49              | ± 0.05| 0.23            | ± 0.05| 0.46            | ± 0.09|
| Ni             | 0.53              | ± 0.28| 0.052           | ± 0.031| 0.097           | ± 0.050|
| Cu             | 0.20              | ± 0.04| 0.16            | ± 0.04| 0.80            | ± 0.20|
| Zn             | 0.32              | ± 0.23| 0.30            | ± 0.22| 0.95            | ± 0.70|
| Ga             | 0.45              | ± 0.05| 0.82            | ± 0.16| 1.82            | ± 0.34|
| Ge             | 2.81              | ± 1.79| 2.31            | ± 2.06| 0.82            | ± 0.58|
| Rb             | 2.31              | ± 1.48| 0.89            | ± 0.83| 0.39            | ± 0.36|
| Sr             | 0.38              | ± 0.03| 40.1            | ± 21.6| 105             | ± 56  |
| Y              | 0.26              | ± 0.03| 29.9            | ± 26.1| 116             | ± 101 |
| Zr             | 0.17              | ± 0.02| 9.79            | ± 1.63| 56.6            | ± 8.1 |
| Nb             | 0.25              | ± 0.09| –               | –     | –               | –     |
| Rh             | 0.18              | ± 0.06| 0.40            | ± 0.17| 2.23            | ± 0.94|
| Cs             | –                 | –     | –               | –     | –               | –     |
| Ba             | 0.14              | ± 0.05| 2.60            | ± 1.85| 19.2            | ± 12.6|
| La             | 0.50              | ± 0.04| 64.20           | ± 522 | 12.915          | ± 706 |
| Ce             | 0.50              | ± 0.04| –               | –     | –               | –     |
| Pr             | 0.48              | ± 0.04| –               | –     | –               | –     |
| Nd             | 0.47              | ± 0.05| –               | –     | –               | –     |
| Sm             | 0.43              | ± 0.05| –               | –     | –               | –     |
| Eu             | 0.41              | ± 0.04| –               | –     | –               | –     |
| Gd             | 0.42              | ± 0.05| –               | –     | –               | –     |
| Tb             | 0.37              | ± 0.04| –               | –     | –               | –     |
| Dy             | 0.34              | ± 0.05| –               | –     | –               | –     |
| Ho             | 0.27              | ± 0.04| 997             | ± 848 | 3651            | ± 3086|
| Er             | 0.23              | ± 0.04| 287             | ± 273 | 1247            | ± 1178|
| Tm             | 0.18              | ± 0.02| 222             | ± 135 | 1238            | ± 740 |
| Yb             | 0.15              | ± 0.02| –               | –     | –               | –     |
| Lu             | 0.12              | ± 0.01| 103             | ± 37  | 876             | ± 303 |
| Hf             | 0.40              | ± 0.13| –               | –     | –               | –     |
| La             | 0.35              | ± 0.08| –               | –     | –               | –     |
| W              | 0.073             | ± 0.066| –              | –     | –               | –     |
| Pb             | –                 | –     | –               | –     | –               | –     |
| Th             | 0.45              | ± 0.05| –               | –     | –               | –     |
| U              | –                 | –     | –               | –     | –               | –     |

2. Experimental design, materials, and methods

2.1. Starting materials

The starting materials compositions are given in Table 5. Starting materials H1 and H2 are based on the starting materials Hib-1 and Hib-6 of Beckett and Stolper [1], our H3 is based on the HB-1 starting material of Kennedy et al. [2]; our starting materials Mel1, Mel2 and Mel3 are similar to the starting materials used by Kuehner et al. ([3], AK40), Beckett and Stolper ([1], AK80) and Lundstrom et al. (CAI-Glass, [4]). In total six different starting material mixtures were prepared from high purity oxides and carbonates. The resulting mixtures were homogenized in an agate mortar under acetone and were subsequently fused in a large Pt-crucible at 1500 °C for at least 3 h in a Linn VMK (Linn GmbH, Eschenfelden, Germany) high temperature box furnace. The resulting silicate glasses
were reground using the same agate mortar with acetone and the resulting powders were doped with 200 µg/g each of Sc, V, Cr, Co, Ni, Cu, Zn, Ga, Ge, Rb, Sr, Y, Zr, Nb, Rh, Cs, Ba, La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Hf, Ta, W, Pb, Th and U, using ICP-MS standard solutions (1000 µg/ml, Alfa Aesar, Germany). However, Ti was added to the hibonite starting mixtures (H1-Ti2, H1-Ti5, H2-Ti2, H2-Ti5 and H3-Ti2, H3-Ti5) using high purity TiO2 (Alfa Aesar, Germany).

### 2.2. Experimental techniques

Experiments were conducted in a vertical tube furnaces (Gero GmbH, Neuhausen, Germany) at atmospheric pressure. We used the so-called “wire-loop technique” [5–7] where small amounts of starting material powder are mixed with an organic glue (UHU Gmbh, Flinke Flasche, Germany) and suspended on a 0.1 mm thick Pt wire. The loops are about 3 mm in diameter each. Using a homemade platinum wire “chandelier”, several samples could be run simultaneously. The samples were placed in the hot zone of the furnace at 800 °C. The temperature paths were designed so that the samples were first heated to temperatures well above the liquidus (i.e. 1550 °C, T\text{max} in Table 6), the run was left at 1550 °C (T\text{max} in Table 6) for at least 8–10 h, and then slowly cooled down to the final run temperature (T\text{quench}) to equilibrate crystals with melts. Most experimental runs were performed with a single cooling ramp, whereas some experiments (H1-Ti5-R5, H2-Ti5, H3-Ti2, H2-Ti5 and H3-Ti2, H3-Ti5) using high purity TiO2 (Alfa Aesar, Germany).

Table 5

| Material | SiO2 [wt%] | MgO [wt%] | Al2O3 [wt%] | CaO [wt%] | TiO2 [wt%] | MnCO3 [wt%] | GeO2 [wt%] | K2CO3 [wt%] |
|----------|-----------|-----------|-------------|-----------|-----------|-------------|-----------|------------|
| H1       | 28.2      | 0.86      | 42.9        | 27.3      | –         | 0.17        | 0.42      | 0.15       |
| H1-Ti2   | 27.7      | 0.84      | 42.0        | 26.8      | 1.99      | 0.17        | 0.41      | 0.15       |
| H1-Ti5   | 26.8      | 0.82      | 40.7        | 25.9      | 4.99      | 0.16        | 0.40      | 0.14       |
| H2       | 31.9      | 1.89      | 41.3        | 25.1      | –         | 0.17        | 0.30      | 0.25       |
| H2-Ti2   | 31.3      | 1.85      | 40.5        | 24.6      | 1.95      | 0.17        | 0.29      | 0.25       |
| H2-Ti5   | 30.4      | 1.80      | 39.2        | 23.9      | 4.90      | 0.16        | 0.29      | 0.24       |
| H3       | 29.5      | 2.11      | 39.7        | 27.8      | –         | 0.25        | 0.40      | 0.30       |
| H3-Ti2   | 28.8      | 2.06      | 38.8        | 27.1      | 2.23      | 0.24        | 0.39      | 0.29       |
| H3-Ti5   | 28.0      | 2.01      | 37.8        | 26.4      | 4.87      | 0.24        | 0.38      | 0.29       |
| Mel1     | 29.9      | 6.30      | 21.9        | 40.8      | –         | 0.54        | 0.24      | 0.35       |
| Mel2     | 39.6      | 11.3      | 7.52        | 40.1      | –         | 0.72        | 0.46      | 0.35       |
| Mel3     | 32.9      | 8.88      | 26.4        | 29.1      | 1.62      | 0.33        | 0.47      | 0.29       |

were reground using the same agate mortar with acetone and the resulting powders were doped with 200 µg/g each of Sc, V, Cr, Co, Ni, Cu, Zn, Ga, Ge, Rb, Sr, Y, Zr, Nb, Rh, Cs, Ba, La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Hf, Ta, W, Pb, Th and U, using ICP-MS standard solutions (1000 µg/ml, Alfa Aesar, Germany). However, Ti was added to the hibonite starting mixtures (H1-Ti2, H1-Ti5, H2-Ti2, H2-Ti5 and H3-Ti2, H3-Ti5) using high purity TiO2 (Alfa Aesar, Germany).

### 2.3. Analytical techniques

Major elements analyses were performed with a JXA-8530F Hyperprobe field emission electron beam microprobe analyzer (EMPA) at the University of Münster. Operating at 15 kV acceleration voltage, a beam diameter of 3 µm and 5 nA beam current for the silicate melts and 15 nA for the
Table 6
Experimental run conditions. All samples were inserted into the furnace at 800 °C and heated to $T_{\text{max}}$ with the rate of 100 °C/h. For experiments with complex heating cycles the intermediate steps are given as well. The total duration of the experiments also includes the time for reaching $T_{\text{max}}$ and the time at $T_{\text{quench}}$.

| Sample   | Starting Mix | Run | Heating cycles | $T_{\text{max}}$ [°C] | Time [h] | Cooling rate [°C/h] | $T_1$ [°C] | Time [h] | Heating rate [°C/h] | $T_2$ [°C] | Time [h] | Cooling rate [°C/h] | $T_{\text{quench}}$ [°C] | Total Time [h] | Phases       |
|----------|--------------|-----|----------------|------------------------|----------|---------------------|------------|----------|---------------------|------------|----------|---------------------|------------------------|----------------|-------------|
| H2-Ti2-R2 | H2           | R2  |                | 1550                   | 8        | -                   | -          | -        | -                   | -          | -        | 5                   | 1450                    | 117.0         | hib, gl     |
| H1-Ti2-R3 | H1           | R3  |                | 1550                   | 8        | -                   | -          | -        | -                   | -          | -        | 1                   | 1350                    | 333.5         | hib, mel, gl |
| H2-Ti2-R3 | H2           | R3  |                | 1550                   | 8        | -                   | -          | -        | -                   | -          | -        | 1                   | 1350                    | 333.5         | hib, gl     |
| H1-Ti5-R4 | H1           | R4  |                | 1550                   | 8        | -                   | -          | -        | -                   | -          | -        | 5                   | 1450                    | 139.5         | hib, gl     |
| H2-Ti5-R4 | H2           | R4  |                | 1550                   | 8        | -                   | -          | -        | -                   | -          | -        | 5                   | 1450                    | 139.5         | hib, gl     |
| H3-Ti5-R5 | H3           | R4  |                | 1550                   | 8        | -                   | -          | -        | -                   | -          | -        | 5                   | 1450                    | 139.5         | hib, gl     |
| H1-Ti5-R5 | H1           | R5  |                | 1550                   | 8        | 5                   | 1350      | 40       | 50                  | 1437       | 24       | 2                   | 1350                    | 305.7         | hib, gl     |
| H2-Ti5-R5 | H2           | R5  |                | 1550                   | 8        | 5                   | 1350      | 40       | 50                  | 1437       | 24       | 2                   | 1350                    | 305.7         | hib, gl     |
| H3-Ti5-R5 | H3           | R5  |                | 1550                   | 8        | 5                   | 1350      | 40       | 50                  | 1437       | 24       | 2                   | 1350                    | 305.7         | hib, gl     |
| H2-R8     | H2           | R8  |                | 1550                   | 10       | 5                   | 1350      | 10       | 50                  | 1450       | 10       | 2                   | 1350                    | 140.0         | an, sp, gl  |
| H3-R8     | H3           | R8  |                | 1550                   | 10       | 5                   | 1350      | 10       | 50                  | 1450       | 10       | 2                   | 1350                    | 140.0         | mel, sp, gl |
| Mel3-R9   | Mel3         | R9  |                | 1550                   | 10       | 5                   | 1350      | 10       | 50                  | 1450       | 10       | 2                   | 1200                    | 142.5         | mel, sp, gl |
| Mel3-R11  | Mel3         | R11 |                | 1550                   | 8        | -                   | -          | -        | -                   | -          | -        | 3                   | 1200                    | 193.0         | sp, gl      |
| Mel3-R12  | Mel3         | R12 |                | 1550                   | 8        | -                   | -          | -        | -                   | -          | -        | 3                   | 1000                    | 211.0         | sp, gl      |

an = anorthite, gl = glass, hib = hibonite, mel = melilite, sp = spinel
minerals. We used a five WDX detector setup with two TAP crystals (Mg, Al), two PET (Ca, Si) and one LiF crystal (Ti). Natural and synthetic materials that were used for standardization are: jadeite (Na2O), kyanite (Al2O3), sanidine (K2O), Cr-diopside (Cr2O3), diopside (CaO), San Carlos olivine (MgO), fayalite (FeO), hypersthene (SiO2), rhodonite (MnO) and rutile (TiO2). A number of secondary standards (chromite, olivine, cr-diopside) were measured as unknowns to monitor external precision and accuracy.

Trace elements were measured by with a ThermoFisher Element II sector field ICP-MS coupled to a Photon Machines AnalyteG2 ArF Excimer laser at the University of Münster, operating with a 4 J/cm² laser fluency and a repetition rate of 5 Hz. A HelEx 2-volume sample cell was used which holds up to 8 one-inch diameter mounts, 6 thin sections and additional reference materials. Prior to sample analyses, the system was tuned with the NIST SRM 612 for high sensitivity, stability, and low oxide rates (232Th16O/232Th < 0.2%). Spot sizes for analysis were between 35 and 50 μm in diameter, while the 50 μm where mainly used for the silicate glasses. Total measurement time was 75 s with 40 s ablation time on the sample and 20 s on the background, the wash out delay was 15 s.

The NIST 612 standard glass [8] was used as an external standard and the BIR-1G [8] and BCR-2G [8] were analyzed as unknowns over the course of this study to monitor precision and accuracy. Twelve sample measurements were bracketed by three measurements of the NIST 612 glasses. For the hibonite and melilitic crystals, 43Ca was used as an internal standard, for spinel 26Mg and for the silicate melts 29Si was used internal standard element.

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Transparency document. Supplementary material

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Appendix A. Supplementary material

Supplementary data associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2018.10.100.

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