

## Electronic Supplementary information

### Crystal growth of ternary metal sulfides from a melt:

#### Ba<sub>2</sub>MnS<sub>3</sub>

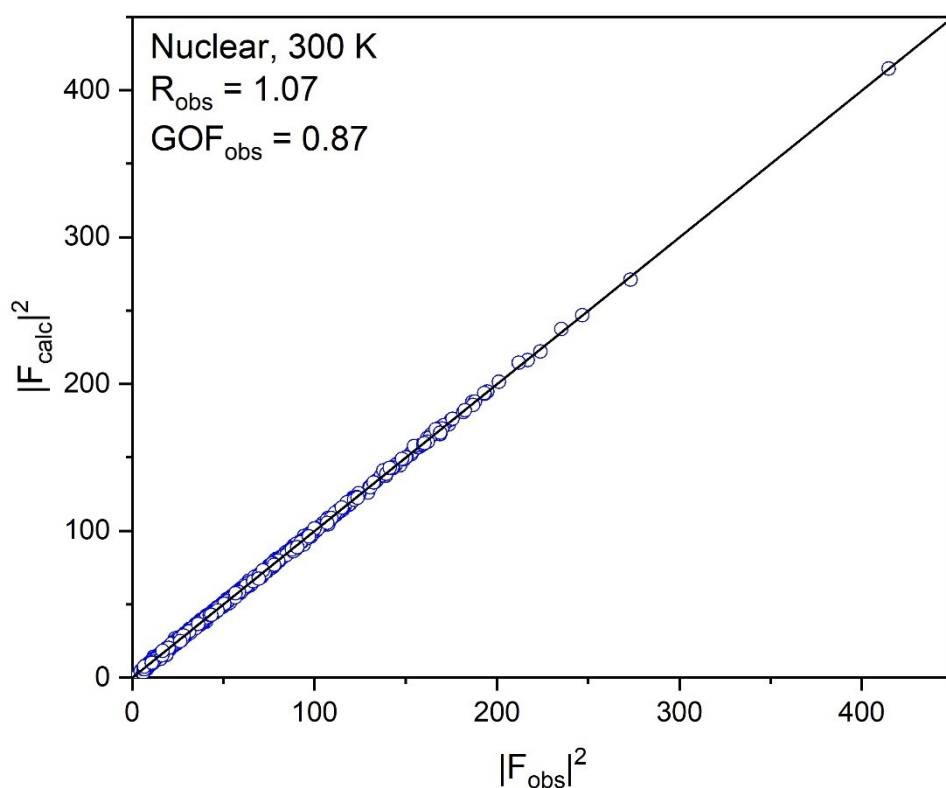
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**Figure S1.** Refinement of Ba<sub>2</sub>MnS<sub>3</sub> single crystal at 300 K from single crystal X-ray diffraction data

**Table S1.** Results of the Structure Refinement of Ba<sub>2</sub>MnS<sub>3</sub> derived from the single crystal X-ray diffraction data.

|                                |  |
|--------------------------------|--|
| Formula                        | Ba <sub>2</sub> MnS <sub>3</sub>       |
| Formula Weight                 | 425.79                                 |
| Radiation                      | Mo K $\alpha$ ( $\lambda$ = 0.71073 Å) |
| <i>T</i> (K)                   | 300                                    |
| Crystal System                 | Orthorhombic                           |
| Space Group                    | <i>Pnma</i> (No. 62)                   |
| <i>a</i> (Å)                   | 8.8409 (10)                            |
| <i>b</i> (Å)                   | 4.3182 (10)                            |
| <i>c</i> (Å)                   | 17.116 (2)                             |
| <i>V</i> (Å <sup>3</sup> )     | 653.45 (18)                            |
| <i>Z</i>                       | 4                                      |
| No. of measured reflections    | 1234                                   |
| <i>R</i> <sub>obs</sub> (%)    | 1.07                                   |
| <i>wR</i> 2 <sub>obs</sub> (%) | 2.65                                   |
| <i>GOF</i> <sub>obs</sub> (%)  | 0.87                                   |

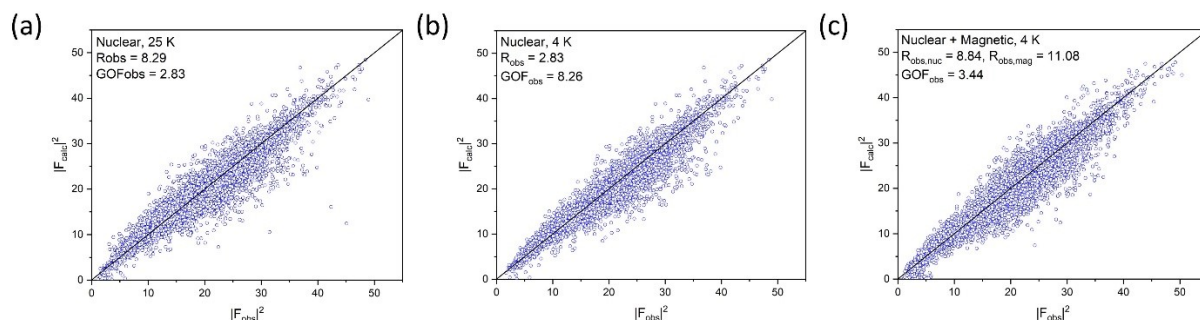
**Table S2.** Refined atomic positions and atomic displacement parameters derived from the single crystal X-ray diffraction data of Ba<sub>2</sub>MnS<sub>3</sub> collected at 300 K.

| Site | <i>x</i>     | <i>y</i> | <i>z</i>    | Occupation | U <sub>iso</sub> |
|------|--------------|----------|-------------|------------|------------------|
| Ba1  | 0.418436(15) | 0.25     | 0.286251(8) | 1.000      | 0.0110(4)        |
| Ba2  | 0.261490(16) | 0.25     | 0.544163(8) | 1.000      | 0.0120(4)        |
| Mn1  | 0.12508(4)   | 0.75     | 0.36819(2)  | 1.000      | 0.0110(9)        |
| S1   | -0.00088(7)  | 0.25     | 0.40045(3)  | 1.000      | 0.0120(15)       |
| S2   | 0.37279(7)   | 0.75     | 0.42764(3)  | 1.000      | 0.0110(14)       |
| S3   | 0.18017(7)   | 0.75     | 0.22877(3)  | 1.000      | 0.0120(14)       |

| Site | U <sub>11</sub> | U <sub>22</sub> | U <sub>33</sub> | U <sub>12</sub> | U <sub>13</sub> | U <sub>23</sub> |
|------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Ba1  | 0.01055(6)      | 0.00955(6)      | 0.01187(6)      | 0               | 0               | 0               |
| Ba2  | 0.01251(6)      | 0.01162(7)      | 0.01052(6)      | 0               | 0               | 0               |
| Mn1  | 0.01058(13)     | 0.01148(14)     | 0.01129(13)     | 0               | 0               | 0               |
| S1   | 0.0134(2)       | 0.0098(2)       | 0.0132(2)       | 0               | 0               | 0               |
| S2   | 0.01026(19)     | 0.0128(2)       | 0.0111(2)       | 0               | 0               | 0               |
| S3   | 0.0112(2)       | 0.0126(2)       | 0.01033(19)     | 0               | 0               | 0               |

**Figure S2.** (a) Nuclear refinement of 2<sup>nd</sup> Ba<sub>2</sub>MnS<sub>3</sub> crystal at 300 K. (b) Nuclear refinement of 2<sup>nd</sup> Ba<sub>2</sub>MnS<sub>3</sub> crystal at 4 K. (c) Nuclear and magnetic refinement of 2<sup>nd</sup> Ba<sub>2</sub>MnS<sub>3</sub> crystal at 4 K.



**Table S3.** Refined atomic positions and atomic displacement parameters of the 2<sup>nd</sup> Ba<sub>2</sub>MnS<sub>3</sub> crystal derived from the single crystal neutron diffraction data of Ba<sub>2</sub>MnS<sub>3</sub> collected at 25 K.

| Site | x            | y       | z           | Occupatio<br>n | Uiso       |
|------|--------------|---------|-------------|----------------|------------|
| Ba1  | 0.41872 (10) | 0.75000 | 0.28637(6)  | 1.000          | 0.00100(3) |
| Ba2  | 0.26129(10)  | 0.75000 | 0.54396(6)  | 1.000          | 0.00160(3) |
| Mn1  | 0.12494(15)  | 0.25000 | 0.36815(8)  | 1.000          | 0.00230(4) |
| S1   | -0.0004(2)   | 0.75000 | 0.40023(11) | 1.000          | 0.00240(5) |
| S2   | 0.3731(2)    | 0.25000 | 0.42752(11) | 1.000          | 0.00250(5) |
| S3   | 0.1805(2)    | 0.25000 | 0.22842(11) | 1.000          | 0.00240(6) |

| Site | U <sub>11</sub> | U <sub>22</sub> | U <sub>33</sub> | U <sub>12</sub> | U <sub>13</sub> | U <sub>23</sub> |
|------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Ba1  | 0.0014(5)       | 0.0000(5)       | 0.0017(4)       | 0               | 0               | 0               |
| Ba2  | 0.0011(5)       | 0.0015(5)       | 0.0022(4)       | 0               | 0               | 0               |
| Mn1  | 0.0018(7)       | 0.0025(7)       | 0.0026(6)       | 0               | 0               | 0               |
| S1   | 0.0033(9)       | 0.0011(10)      | 0.0030(9)       | 0               | 0               | 0               |
| S2   | 0.0031(9)       | 0.0023(10)      | 0.0020(8)       | 0               | 0               | 0               |
| S3   | 0.0028(9)       | 0.0015(10)      | 0.0028(10)      | 0               | 0               | 0               |