**Supplementary Information**

**Effect of transport agent boron triiodide on the synthesis and crystal quality of boron arsenide**

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**Calculation of the fraction of BAs**:

The reference intensity ratio (RIR) is a method used for quantitative analysis by powder diffraction. RIR values are measured with reference to the standard phase corundum, recorded in the powder diffraction files (PDF). The RIR method is applied to calculate the faction of BAs, according to references [1−2].

 $W\_{BAs}=\frac{I\_{BAs}}{I\_{BAs} + \frac{I\_{B}}{RIR\_{B}} ∙ RIR\_{BAs}}$ (S1)

where $W\_{BAs}$ is the faction of BAs; $I\_{BAs}$ and $I\_{B}$ are the intensities of X-rays diffracted by a selected reflection of components boron powders and BAs powders, and the selected refection for boron is (104) and for BAs is (111); $RIR\_{BAs}$ and $RIR\_{B}$ are RIR values of BAs and B, which are 9.14 and 0.22, derived from PDF 03-004-5090 and PDF 80-0324, respectively.

**Table S1. Calculated fraction of BAs\* in the products with agents I2 and BI3 under various reaction pressures at 820°C for 3 d**

|  |  |
| --- | --- |
| Addition of atomic iodine / at% | Fraction of BAs / wt% |
| 0.3 MPa | 0.7 MPa | 1.5 MPa |
| No addition | 0.0 | 4.5 ± 0.3 | 6.9 ± 0.4 | 12.1 ± 1.1 |
| I2 | 1.3 | 3.3 ± 0.5 | 40.4 ± 4.8 | >90\*\* |
| 2.5 | 8.4 ± 0.4 | 71.4 ± 13.8 | >90\*\* |
| BI3 | 1.3 | 9.9 ± 0.5 | 13.4 ± 0.9 | >90\*\* |
| 2.5 | 4.6 ± 0.4 | 79.6 ± 19.4 | >90\*\* |
| Note: \* Calculated from XRD in Fig. 2 with RIR method; \*\* Without obvious peaks of boron powders in XRD. |

[1] C.R. Hubbard and R.L. Snyder, RIR - Measurement and Use in Quantitative XRD, *Powder Diffr.*, 3(1988), No.2. p. 74.

[2] X. Zhou, D. Liu, H. Bu, L. Deng, H. Liu, P. Yuan, P. Du, and H. Song, XRD-based quantitative analysis of clay minerals using reference intensity ratios, mineral intensity factors, Rietveld, and full pattern summation methods: A critical review, *Solid Earth Sci.*, 3(2018), No.1. p. 16.