

Thermodynamic insights into the Ba-S system for the formation of BaZrS₃ perovskites and other Ba sulfides

SUPPORTING INFORMATION

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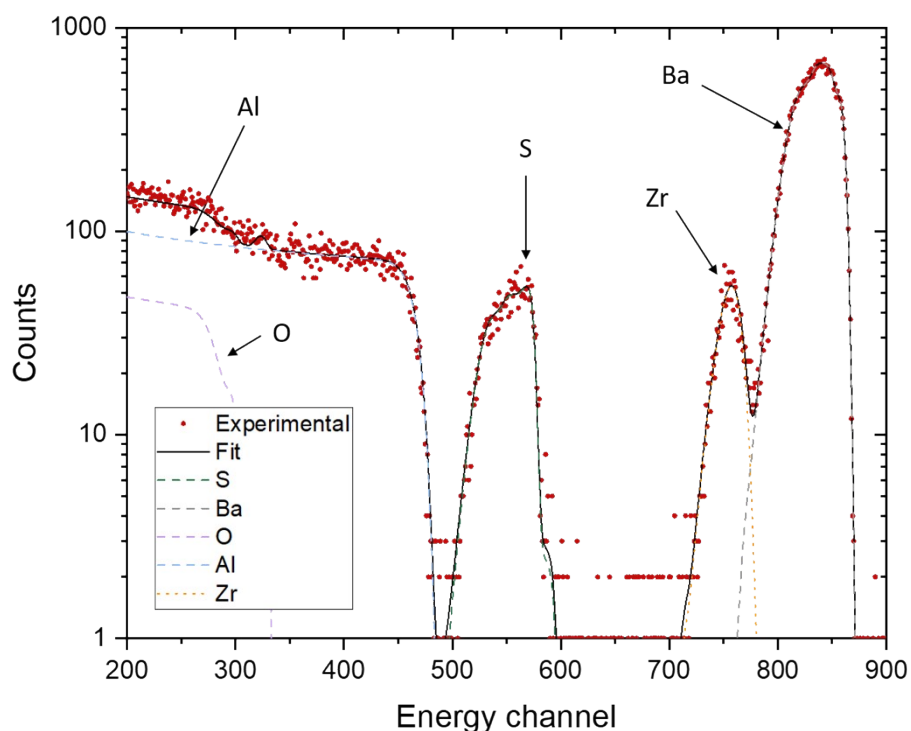


Figure S1: RBS analysis of a sample sulfurized with T_S and T_{sample} of 100 and 488 °C, respectively. The estimated total ratio of [Ba] to [S] is 1:1.

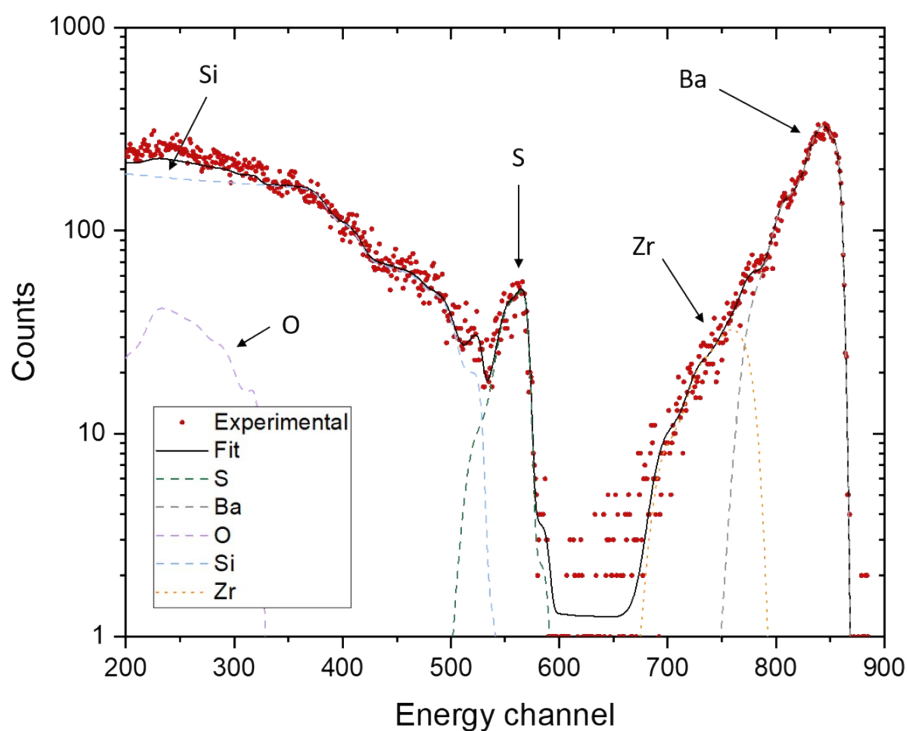


Figure S2: RBS analysis of a sample sulfurized with T_S and T_{sample} of 165 and 548 °C, respectively. The estimated total ratio of [Ba] to [S] is 1:1.5.

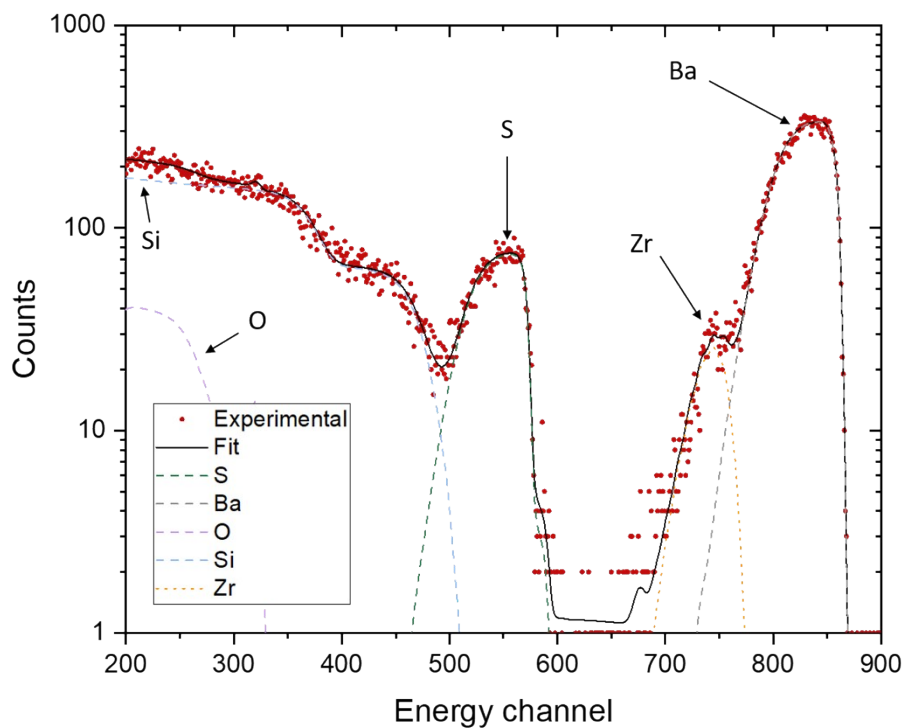


Figure S3: RBS analysis of a sample sulfurized with T_S and T_{sample} of 230 and 430 °C, respectively. The estimated total ratio of [Ba] to [S] is 1:2.7.

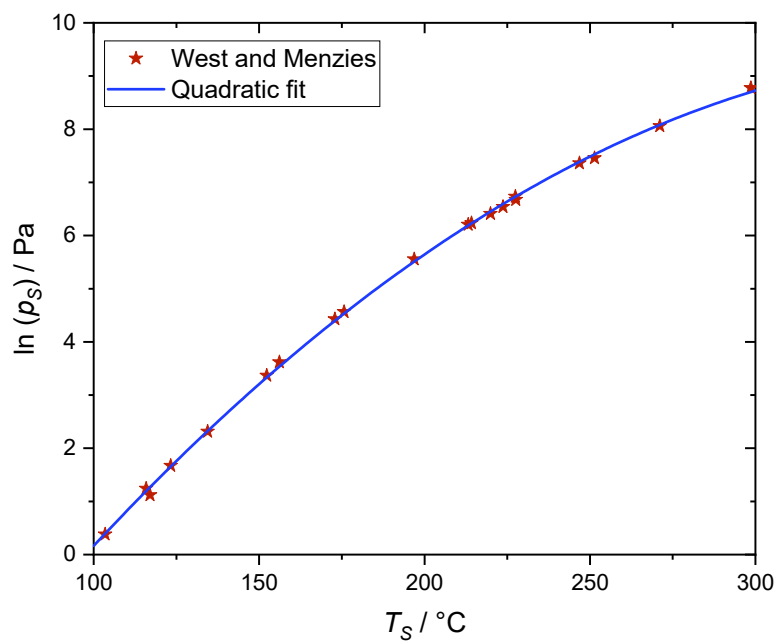


Figure S4: Relationship between T_S and p_S . Scatter points are taken from published experimental work.¹ The line is a least squares fit to the experimental data. The analytic form is given by $\ln(p_S) = -7.715 + 9.08 \cdot 10^{-2} T_S - 1.20 \cdot 10^{-4} T_S^2$.

REFERENCES

- (1) West, W. A.; Menzies, A. W. C. The Vapor Pressures of Sulphur between 100° and 550° with Related Thermal Data. *J. Phys. Chem.* **1929**, 33 (12), 1880–1892.
<https://doi.org/10.1021/j150306a002>.