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Crystallographic and Partitioning Constraints on Trace Element Incorporation in Willemite Zn_2SiO_4

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Willemite is an increasingly significant ore mineral as a green, non-sulfide source of zinc. Its trace element geochemistry has been explored as an ore provenance indicator. Analysis of natural willemites from deposits, including those in the USA, Belgium, Namibia, Brazil, and Zambia, frequently reveals high concentrations of trace elements. Specifically, Mondillo *et al.* [1] report Pb concentrations reaching up to 16,000 ppm and Fe concentrations exceeding 11,000 ppm in natural specimens. However, such high concentrations seem to contradict the theoretical partitioning behavior expected based on the willemite lattice. High-temperature XRD and ab-initio Density Functional Theory calculations provide a crystallographic framework for these observations. At elevated conditions, the two non-equivalent Zn sites in the willemite structure diverge significantly in size. This structural evolution potentially expands the range of elements that can be incorporated. This study investigates this apparent paradox by directly determining willemite partition coefficients (D values) through synthesis experiments in trace-element-doped melts at 1 atm. Our results show a distinct divide in element compatibility: Mg, Co, Ag, and Cd are compatible ($D \geq 1$), whereas Mn, Fe, Pb, and the REE are incompatible ($D < 1$). Specifically, experimental D values for Pb are as low as 2.8×10^{-5}, and Fe values hover around 0.5, incompatible with the high levels reported for these elements in the literature. To better understand these data, we applied Lattice Strain Theory modelling, which shows consistent radius-mismatch trends in D-values across the elements, including Pb and Fe. The incompatibility observed experimentally, and consistent with crystallo-chemistry, suggests that the high Pb and Fe concentrations reported in natural willemite likely stem from micro-inclusions or the occupation of interstitial sites without lattice control. By reconciling experimental partitioning data with crystallography, this research provides the understanding to interpret willemite composition and use it as a reliable probe of the geological environments that form these green zinc resources.

[1] Mondillo, N., Accardo, M., Boni, M., Boyce, A., Herrington, R., Rumsey, M., Wilkinson, C., & Santoro, L. (2020). New insights into the genesis of willemite (Zn_2SiO_4) from zinc nonsulfide deposits, through trace elements and oxygen isotope geochemistry. *Ore Geology Reviews*, *118*(103307)