

Mg and Sr: Define the Substitution Basis

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Abstract. Define Mg or Sr substitution on a clear site and composition basis. This note converts a nominal substitution level into elemental mass fractions and sets out checks for composition and phase identity. A feed recipe does not establish crystallographic site occupancy.

Keywords: calcium phosphate; magnesium; strontium; substitution; site occupancy

1. Convert site fraction into a formula

For a simplified divalent substitution model, write $\text{Ca}_{10-x}\text{M}_x(\text{PO}_4)_6(\text{OH})_2$, where M is Mg or Sr. A target of 5 mol% replacement on the ten calcium sites gives $x = 0.5$, not $x = 5$. The nominal formula is therefore $\text{Ca}_{9.5}\text{M}_{0.5}(\text{PO}_4)_6(\text{OH})_2$.

Calculated from this ideal formula, the Sr mass fraction is approximately 4.26 wt%, whereas the Mg mass fraction is approximately 1.22 wt%. The same site percentage therefore gives very different elemental mass percentages. These calculations assume the target composition forms without vacancies or secondary phases.

Use bulk elemental analysis to assess the overall composition and diffraction to assess phases; neither alone proves site occupancy. Quantitative phase analysis also depends on the model and detection capability [1]. A small peak shift is supporting evidence only after calibration and alternative explanations have been assessed.

2. Separate chemistry from mixture effects

2.1 Use an explicit control set. Compare an unsubstituted reference, the candidate synthesized powder and a physical blend with comparable total added element where practical. Match size and thermal history as closely as possible. This helps test whether a response follows incorporation, a secondary phase or simply a changed particle population.

Table 1. Development comparison and interpretation controls.

Label in the recipe	Meaning	Required distinction
5 mol% on Ca sites	$x = 0.5$ in the ideal formula	Not 5 wt% of the total powder
5 wt% Sr element	Elemental mass fraction	Not 5 wt% Sr-containing salt
5 wt% additive	Physical blend fraction	May remain a separate phase
Measured substitution	Structural interpretation	Requires more than feed chemistry

Scope. The ideal-formula calculations are original examples, not measured incorporation efficiencies or evidence of a biological benefit.

References

1. León-Reina L, García-Maté M, Álvarez-Pinazo G, Santacruz I, Vallcorba O, De la Torre AG, et al. Accuracy in Rietveld quantitative phase analysis: a comparative study of strictly monochromatic Mo and Cu radiations. J Appl Crystallogr. 2016;49(3):722-735. doi:10.1107/s1600576716003873.

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