# Towards controlled synthesis and better understanding of blue shift of the CaS crystals

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**Table SI-1.** Lattice parameters, Unit cell volume, R values obtained by Rietveld Refinement Data for the CaS crystals.

| **Calcium Sulfide (CaS); space group *Fm*-3*m* (225) ICSD-41956, cúbico; z = 1, a = b = c = 5.689 Å, α = β = γ = 90° - V = 184.12 Å³** | | | | | | |
|---|---|---|---|---|---|---|
| | **Parameters** | | | | | |
| **Sample** | a=b=c (Å) | V (Å³) | $\chi^2$ | R(F**2) (%) | wRp (%) | Rp (%) |
| **CaS – 4 min** | 5.647 | 180.0 | 2.480 | 0.03 | 0.07 | 0.05 |
| **CaS – 8 min** | 5.648 | 180.1 | 3.162 | 0.04 | 0.09 | 0.06 |
| **CaS – 16 min** | 5.647 | 180.0 | 2.434 | 0.02 | 0.07 | 0.05 |
| **CaS – 32 min** | 5.646 | 179.9 | 3.811 | 0.04 | 0.09 | 0.06 |
| **CaS – 64 min** | 5.645 | 179.9 | 3.299 | 0.03 | 0.08 | 0.06 |

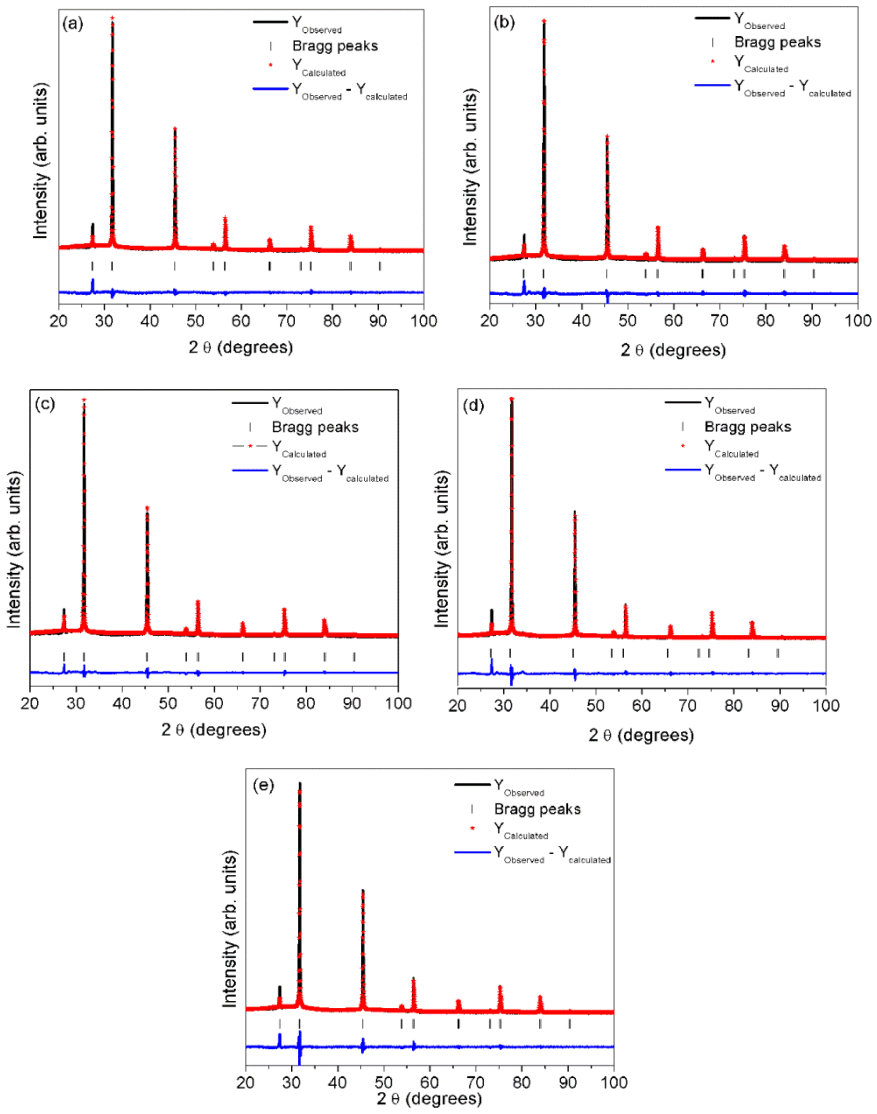


**Figure SI-1:** Rietveld refinement plot of CaS crystals prepared by MAS for (a) 4, (b) 8, (c) 16, (d) 32 and (e) 64 min.