

**Room Temperature Mixed Spin-State of Co^{3+} in $\text{Sr}_2\text{Co}_{0.02}\text{Ga}_{0.98}\text{NbO}_6$ Double Perovskite:
Combined NMR and EPR Studies in a Potential Inorganic Pigment**

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Supporting Information

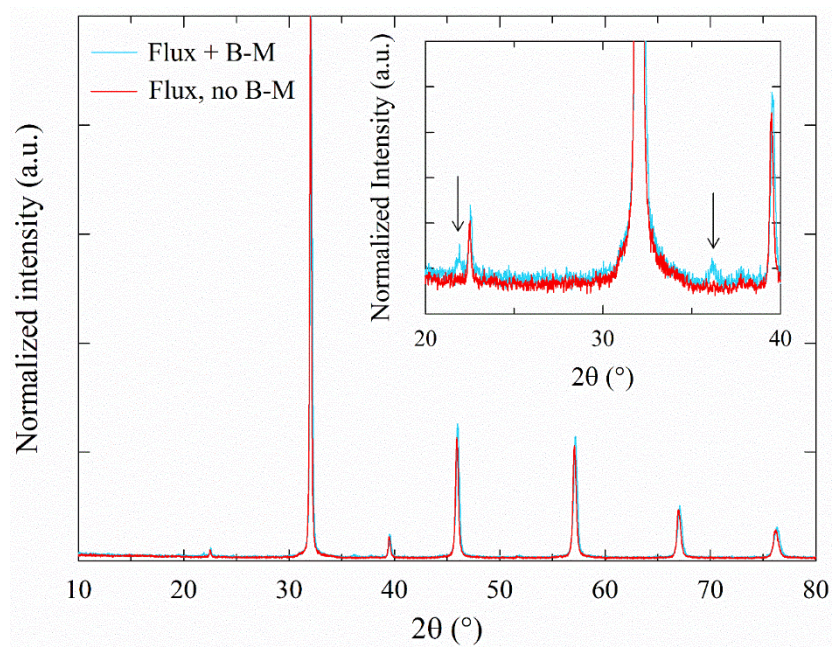
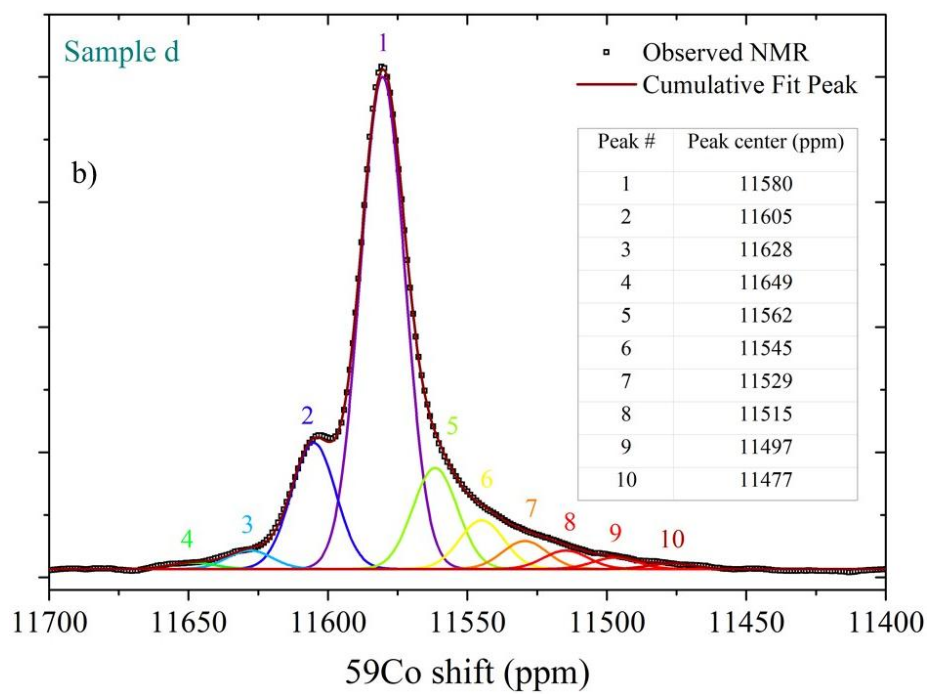
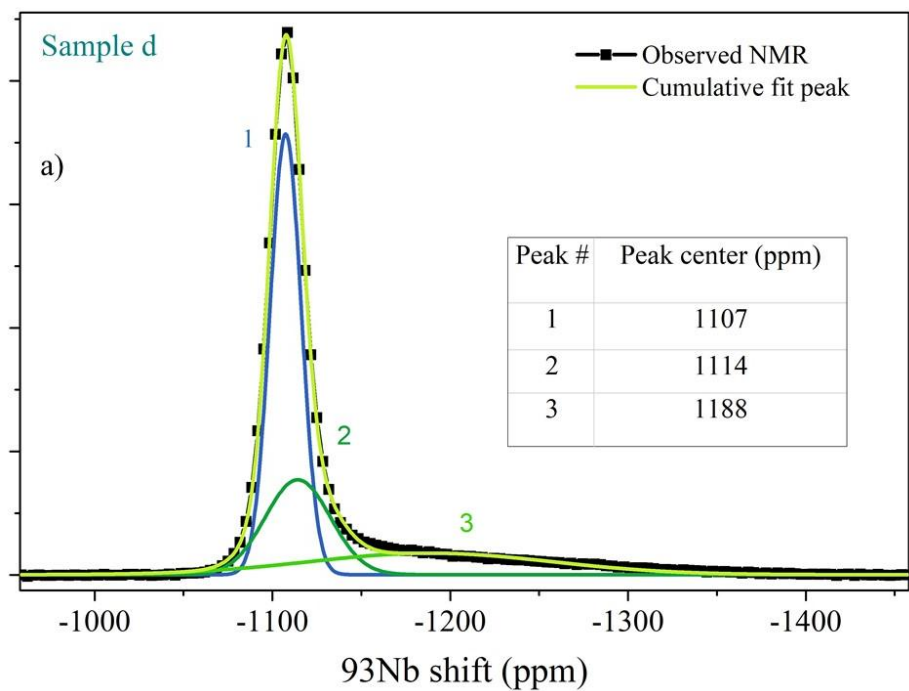
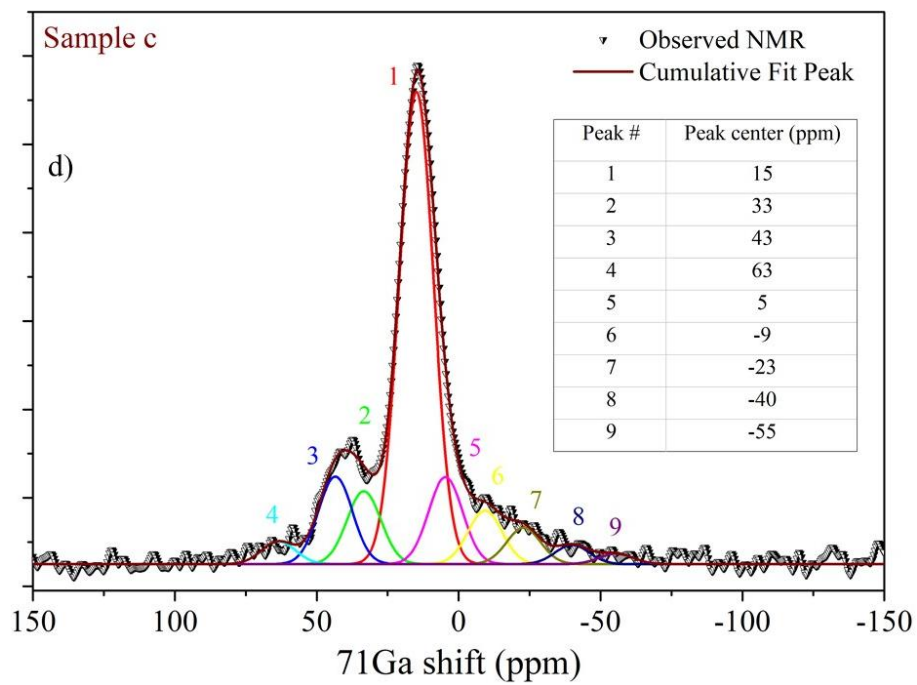
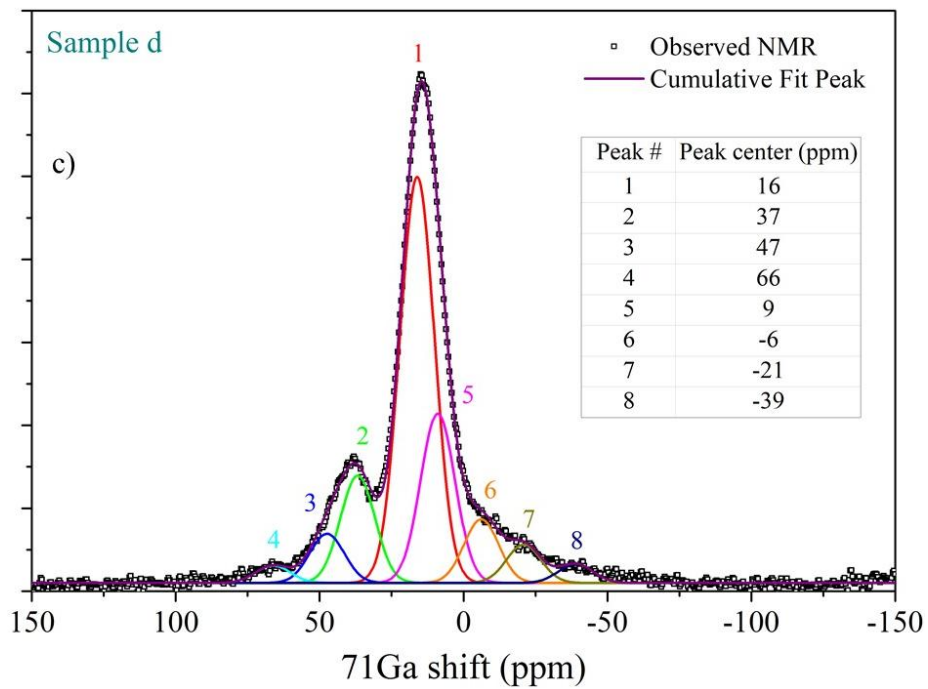


Figure S1. Comparison of the XRD patterns obtained for a sample synthesized by combining a precursory ball milling step with the flux method (Flux + B-M) and a sample synthesized with just the flux method (Flux, no B-M); the inset highlights the additional weak impurities observed.





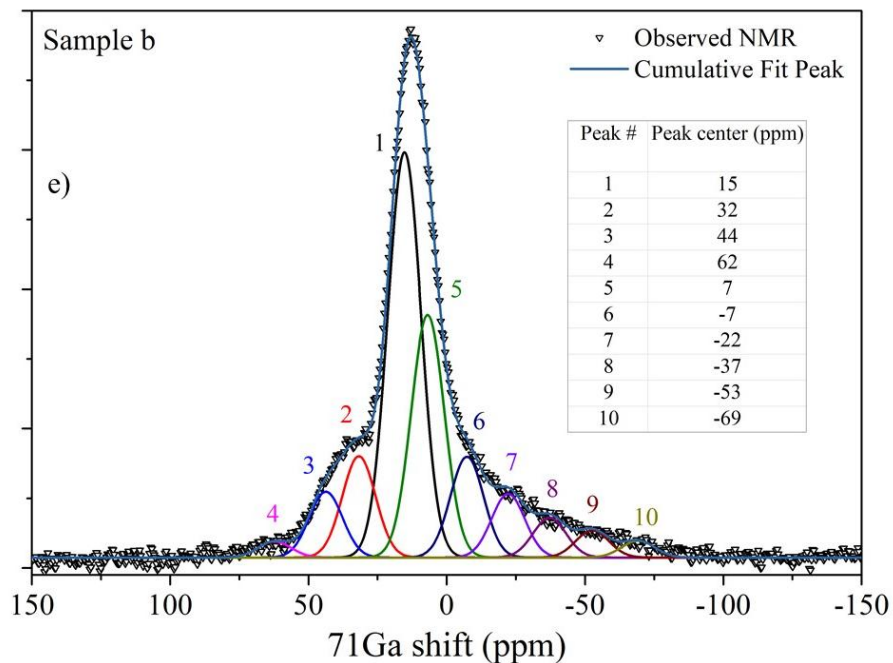


Figure S2. (a) deconvoluted Nb MAS NMR spectra of sample d, (b) deconvoluted ^{59}Co MAS NMR spectra of sample d, (c) deconvoluted ^{71}Ga MAS NMR spectra of sample d, (d) deconvoluted ^{71}Ga MAS NMR spectra of sample c, (e) deconvoluted ^{71}Ga MAS NMR spectra of sample b.

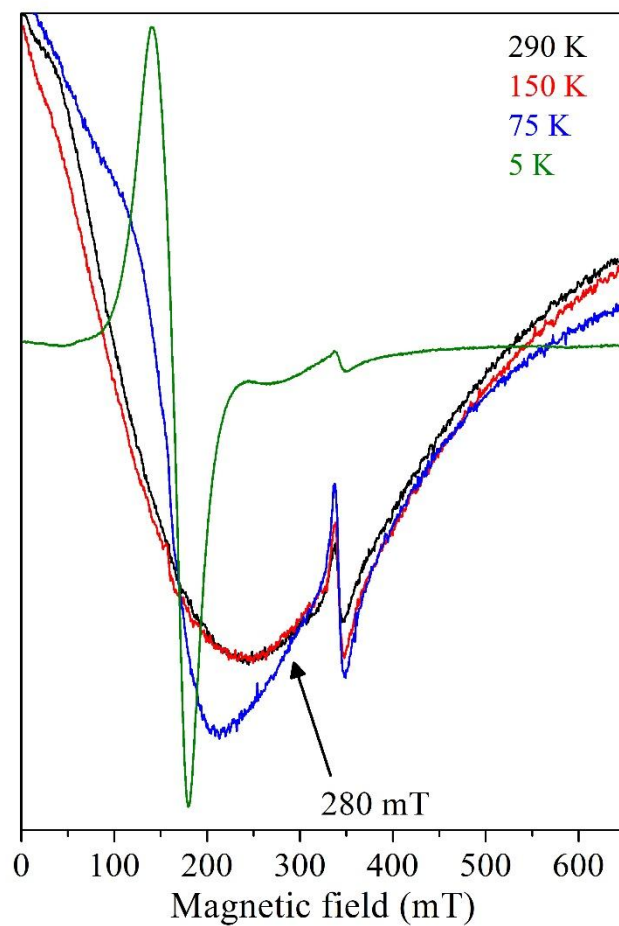


Figure S3. Exaggerated temperature dependent EPR spectra of sample b ($\text{Sr}_2(\text{Co}_{0.02}\text{Ga}_{0.98})\text{NbO}_6$, 900°C, 8h, 5°C/min, SrCl_2 (2:1)).

Wavelength (nm)	Wavenumber (cm ⁻¹)	Ratio to the lowest value	
430	23256	1.3	
490	20408	–	
547	18282	1	
d-d transition	E/B at $\Delta_o/B = 4$	Ratio to the lowest value	Co ³⁺ spin state (λ)
$^1A_{1g} \rightarrow ^1T_{2g}$	50	1.3	LS (430 nm)
$^1A_{1g} \rightarrow ^1T_{1g}$	38	1	LS (547 nm)

Table S1. Calculation of the d-d transitions corresponding to the LS, IS and HS Co³⁺ using Tanabe-Sugano diagram of d⁶ electronic configuration

As it was observed for Co doped LaGaO₃ and from the using Tanabe-Sugano diagram, the allowed d-d transitions corresponding to LS Co³⁺ are observed. As the forbidden d-d transition corresponding to HS Co³⁺ is expected in between the two LS Co³⁺ d-d transition features, we assume 490 nm corresponds to the HS Co³⁺. Further, the feature at ~645 nm might be from ³T₂ state (IS Co³⁺).