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# Structural study of spinels in manganese doped zinc gallate ($ZnGa_2O_4:Mn^{2+}$) by electronic paramagnetic resonance (EPR)

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## Highlights

EPR analysis of manganese doped zinc gallate using X band Bruker EMX equipment at room temperature. The manganese sites were investigated using Easyspin toolkit in a MATLAB environment to determine the possible formation of inverted spinel in the structure.

## Resumo/Abstract

$ZnGa_2O_4$ (ZGO) matrix is a spinel-type compound. When we dope the matrix with $Mn^{2+}$ we expect manganese to substitute primarily in the tetrahedral site of zinc ($Zn^{2+}$), but with the smaller possibility of also substituting in the octahedral site of gallium ($Ga^{3+}$), forming the so-called inverted spinel. To address this possibility the manganese dopped matrix was studied by Electronic Paramagnetic Resonance (EPR) to help identify if there were more than one type of manganese present on the system.

The EPR spectrum was obtained using a Bruker EMX X-Band 9.4Ghz equipment, at room temperature in solid state. Then the recorded spectrum was treated using a Easyspin toolkit in a MATLAB environment to obtain the spectrum parameters. Simultispin toolkit was also used to help narrow down the possibilities and adjust the fitting of the simulation. The results can be seen at Figure 1 below.

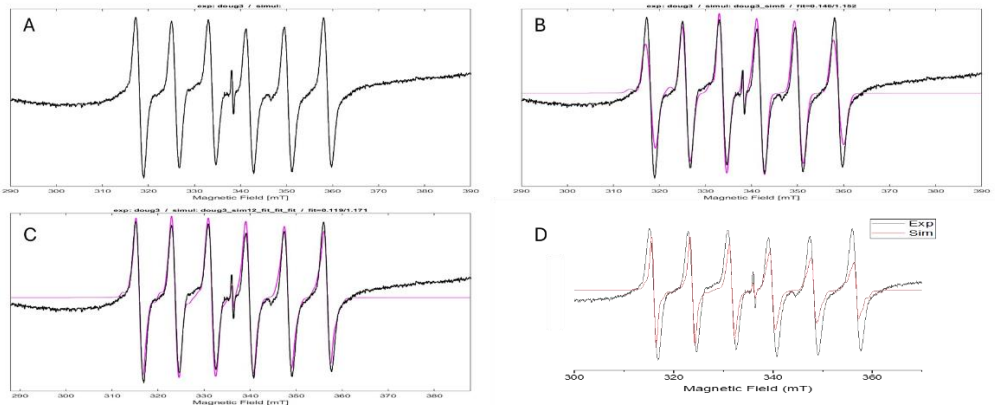


Figure 1. A) Raw spectrum of ZGO:$Mn^{2+}$, B) Simultispin simulation considering two Mn sites. C) Simultispin simulation considering one Mn site. D) Easyspin simulation considering one Mn site.

At first the inverted spinel hypothesis, with the $Mn^{2+}$ substituting both $Zn^{2+}$ and $Ga^{3+}$, showed a good fit, we can see on Figure 1B that peak correlation it is not the best for peak intensities. On Figure 1C the simulation was adjusted for one Mn site, considering a magnetic interaction between different electrons of the same Mn atom [1]. This adjustment was carried out to the Easyspin toolkit, Figure 1D, adding a zero-field tensor, D, that helped to field a better fitting for the simulation. Therefore, it was possible to attest that the inverted spinel did not form, with the Mn occupying only the Zn sites.

[1] J. Chem. Soc., Faraday Trans. 2, 1973,69, 1537-1541

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