





Belo Horizonte, September 12 - 15th 2024

Study of Gadolinium Ion Matrices via EPR: Gd³⁺ as a Proximity Probe and Ligand Field Sensor

Marcelo C. Portes¹, Gustavo C. Portes¹ and Lucas C. V. Rodrigues¹

¹Departamento de Química Fundamental, Universidade de São Paulo, São Paulo, Brasil E-mail: Marcelo.portes@usp.br

Thematic Area: Rare-Earths

Keywords: epr, rare earth, gadolinium

Electron Paramagnetic Resonance (EPR) is a technique applied in various scientific fields, including dosimetry, structural determination of proteins, and studies on the generation of free radicals. It is also a highly efficient technique for studying paramagnetic species. In recent years, it has been possible to find reported studies primarily involving the Gd³⁺ ion, which provides information on the correlation of the signal from different glass composites with the crystal field where the Gd³⁺ ion is embedded [1]. Other investigations present information on the variation of the EPR signal from different Gd3+ complexes under a range of conditions. The Gd³⁺ ion (seven unpaired electrons) undergoes significant changes in its EPR signal, despite the spin-orbit interaction, responding to alterations in the ligand field, as reported by Miyamoto et al [2]. EPR spectra in CW X-Band were measured at room temperature (300K) to observe the Gd3+ signal under these conditions (Figure 1). In Figure 1, both pre- and postthermal treatment gadolinium oxide exhibits a broadened signal, indicating strong magnetic coupling between the Gd atoms, while in the complex, a splitting of signals can be observed, although they are also broadened. To dilute the Gd3+ signal, new materials were synthesized from Y2O3 doped with different amounts of Gd3+ to determine the concentration at which magnetic interaction between Gd3+ ions is observed and to compare to literature in order to determine the ligand field that the Gd ions are occupying. The materials were characterized by XRD and the variation in the Gd signal was recorded via EPR measurement.

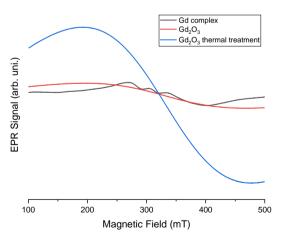


Figure 1. EPR spectra of the Gd³⁺ complex (black line), commercial Gadolinium oxide (red line), and commercial Gadolinium oxide after thermal treatment (blue line) recorded in the X-band (9.5 GHz) at room temperature (~300K).

Acknowledgments:





References

[1] R. G. Kunghatkar, V. L. Barai, and S. J. Dhoble, "Synthesis route dependent characterizations of CaMgP2O7: Gd3+ phosphor," Results Phys, vol. 13, p. 102295, Jun. 2019, doi: 10.1016/J.RINP.2019.102295.

[2] MiyamotoRyo and SudohSusumu, "EPR Spectra of Gadolinium(III)-β-diketonate Complexes," https://doi.org/10.1246/bcsj.68.3439, vol. 68, no. 12, pp. 3439–3443, Jul. 2006, doi: 10.1246/BCSJ.68.3439.