

66<sup>TH</sup> INTERNATIONAL



# OPEN READINGS

CONFERENCE FOR STUDENTS OF  
PHYSICS AND NATURAL SCIENCES

ANNUAL  
ABSTRACT BOOK

2023



Vilnius  
University

VILNIUS UNIVERSITY PRESS

Editors

Martynas Keršys  
Šarūnas Mickus

Cover and Interior design  
Milda Stancikaitė

Vilnius University Press  
9 Saulėtekio Av., III Building, LT-10222 Vilnius  
info@leidykla.vu.lt, www.leidykla.vu.lt/en/  
www.knygynas.vu.lt, www.journals.vu.lt

Bibliographic information is available  
on the Lithuanian Integral Library Information System (LIBIS) portal [ibiblioteka.lt](http://ibiblioteka.lt).  
ISBN 978-609-07-0883-5 (ePDF)  
DOI: <https://doi.org/10.15388/IOR2023>

Copyright © 2023 [Authors]. Published by Vilnius University Press  
This is an Open Access article distributed under the terms of the Creative Commons Attribution Licence, which permits  
unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

# NMR CHARACTERIZATION OF NOVEL $Y_{3-x}Na_xAl_{5-y}V_yO_{12}$ GARNETS

Carlos Martín Signes<sup>1,2</sup>, Diana Vištorskaja<sup>3</sup>, Aivaras Kareiva<sup>3</sup>, Vytautas Klimavičius<sup>1</sup>

<sup>1</sup> Institute of Chemical Physics, Vilnius University, Lithuania

<sup>2</sup> Faculty of Science, Physics, University of Granada, Spain

<sup>3</sup> Institute of Chemistry, Vilnius University, Lithuania

[carlosmsignes@correo.ugr.es](mailto:carlosmsignes@correo.ugr.es)

Yttrium Aluminum Garnets ( $Y_3Al_5O_{12}$ , **YAGs**) are materials with very suitable properties for lightning technologies. Their transparency, and high chemical and heat resistance make them a powerful basis for solid-state lightning applications. To do this, YAGs must be doped with optically-active ions of similar size to replace some of the Yttrium and Aluminum ions. The study of different doping elements and concentrations is of great importance to produce new materials with the desired optical profile, which allows the development of more powerful and precise devices for medicine, technological or lightning applications. Solid-state Nuclear Magnetic Resonance (**NMR**) is a very powerful experimental method for materials research. It provides information on the local structure at molecular level and defects of the material. This information allows to create structure-optical properties relations.

In this work, YAGs doped with different concentrations of  $^{23}Na$  and  $^{51}V$  were analyzed employing  $^{27}Al$ ,  $^{23}Na$  and  $^{51}V$  Magic Angle Spinning (**MAS**) NMR experiments. Multiple Quantum MAS technique was used to resolve overlapping signals from different chemical moieties. NMR was found to be very beneficial as crystalline and amorphous moieties formed during the synthesis of these novel garnets were detected. In contrary, XRD (X-ray diffraction) analysis which was performed provided information only on the crystalline phases.

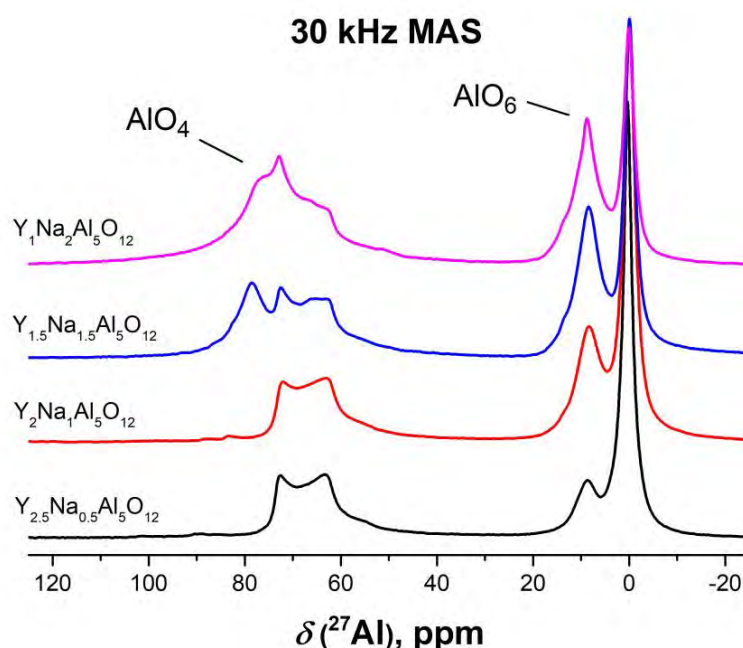


Fig. 1. 30kHz  $^{27}Al$  MAS NMR spectra obtained for studied garnets. More details in the figure.

In Fig. 1, we can observe the  $^{27}Al$  NMR spectra obtained for four YAG samples containing different doping levels of Na. It can be seen that the 4th-coordinated Aluminum peak changes with increasing concentrations of Na; mainly due to the apparition of other phases such as  $Al_2O_3$ , YAP and  $YAIO_3$ .

A better understanding of the structure and properties of the studied materials will allow for more methodic practical testing in applications; as oftentimes even slight variations in concentration can change the optical properties drastically. Through this research, we aim to produce an NMR characterization of these promising families of YAGs to facilitate the advancement of new technologies.

Funding by Vilnius University Science Promotion Foundation (MSF-JM-5/2022) is acknowledged.

[1] Levitt Malcolm H., Spin Dynamics: Basics of Nuclear Magnetic Resonance, John Wiley & Sons (2001)