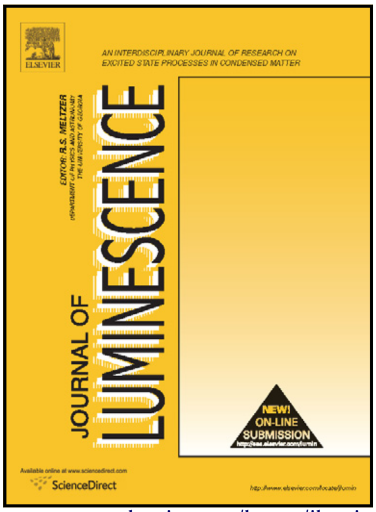

www.elsevier.com/locate/jlumin

Chemometric analysis of the luminescence quantum Yields in lanthanide ion complexes

Erico S. Teixeira, Benício B. Neto, Paulo M.C. de Oliveira, Ricardo L. Longo

PII: S0022-2313(14)00604-8
DOI: http://dx.doi.org/10.1016/j.jlumin.2014.10.033
Reference: LUMIN12963

To appear in: *Journal of Luminescence*

Received date: 10 June 2014
Revised date: 26 August 2014
Accepted date: 8 October 2014

Cite this article as: Erico S. Teixeira, Benício B. Neto, Paulo M.C. de Oliveira, Ricardo L. Longo, Chemometric analysis of the luminescence quantum Yields in lanthanide ion complexes, *Journal of Luminescence*, http://dx.doi.org/10.1016/j.jlumin.2014.10.033

Chemometric Analysis of the Luminescence Quantum Yields in Lanthanide Ion Complexes

Erico S. Teixeira,[a,*] Benício B. Neto,[a] Paulo M. C. de Oliveira [a] and Ricardo L. Longo [a]

[a] Departamento de Química Fundamental, Universidade Federal de Pernambuco, Recife, PE 50.740-560, Brazil
[*] Corresponding author. Tel. +55 81 21268459; fax +55 81 21268442
E-mail address: teixeira.erico@gmail.com

ABSTRACT

The photoluminescence of trivalent lanthanide complexes was modeled by five and eight energy states and analyzed by normal distribution plots and principal component analysis chemometric techniques that quantified the effects of the transition rates and their interactions on the quantum yield (ϕ). Numerical solutions of the rate equations with transition rates of known β-diketonate Eu^{3+} complexes (ϕ ≈ 40%) were used to calculate the quantum yields. Complete two-level factorial design was employed in generating the experiments from models with five- and eight-level systems. From them, others models with eight levels were devised in order to include the ligand-to-metal charge transfer (LMCT) state. These analyses demonstrated and quantified most of the empirical rules regarding the relationships between the photoluminescence quantum yields and the transition rates. In addition, revealed that some interactions are relevant and can, in some cases, cancel out the main effect leading to different conclusions from the empirical rules. For most models, the decaying rate of the lanthanide ion emitting state is the main (negative) effect on the quantum yield, suggesting that its optimization should improve the quantum yield of most lanthanide compounds. Furthermore, the analyses showed that the quantum yield could be improved by increasing, for instance, the singlet-to-triplet transition rate (intersystem crossing) in many complexes. The behavior of complexes containing LMCT state is quite different, because several transition rates and their interactions have significant effects on the quantum yield with similar absolute magnitudes. In addition, comparisons of specific examples showed that complexes with similar quantum yields could have very distinct luminescence emission intensities, whereas systems with very different quantum yields can have similar emission intensities. Thus, this chemometric study can lead to new and different conclusions if the response of interest is the photoluminescence emission intensity, instead of the quantum yield, with relevant implications on the design of new and more efficient luminescent compounds based on lanthanide ions.

Keywords: trivalent lanthanide complexes, photoluminescence quantum yield, chemometric technics