

# The nephelauxetic function $he$ and the spectroscopy of $\text{Cr}^{3+}$ , $\text{Mn}^{4+}$ and $\text{Mn}^{5+}$ (and few others) in solids

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These last years, it was shown that the energy of the  $s^2 \rightarrow s^1p^1$  transitions of p-block cations like  $\text{Tl}^+$ ,  $\text{Sn}^{2+}$ ,  $\text{Pb}^{2+}$ ,  $\text{Sb}^{3+}$ ,  $\text{Bi}^{3+}$  and  $\text{Te}^{4+}$  can be reproduced using an equation of the form  $E = E_f[1 - Khe^\alpha]$ , where  $E_f$  is the energy of the free ion,  $he$  is the “nephelauxetic function” that is calculated at the crystal sites occupied by the cations in the considered host lattices, and  $(K, \alpha)$  are adjustable parameters [1-3].

Here, we show that the same model can be used to reproduce the energy of the zero-phonon line of  $\text{Cr}^{3+}$  and  $\text{Mn}^{4+}$  ions ( ${}^2E_g$  state) within  $\approx \pm 350 \text{ cm}^{-1}$  in fluorides and within  $\approx \pm 600 \text{ cm}^{-1}$  in oxides [4,5]. It also reproduces the emission energy of  $\text{Mn}^{5+}$ -doped oxides with an accuracy of  $\approx \pm 300 \text{ cm}^{-1}$  [6]. We will discuss these data and, if time allows, extend the discussion to the case of  $\text{Mn}^{4+}$ -doped oxyhalides [6].

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[2] P. Boutinaud, Nephelauxetic effect and metal-to-metal charge transfer in solids doped with  $\text{Tl}^+$ ,  $\text{Sn}^{2+}$ ,  $\text{Pb}^{2+}$  or  $\text{Sb}^{3+}$ , *J. Lumin.*, 272 (2024) 120645.

[3] P. Boutinaud, On the spectroscopy of  $\text{Te}^{4+}$  and other  $ns^2$  ions in solids, *J. Lumin.*, 277 (2025) 120952.

[4] P. Boutinaud, The nephelauxetic function  $he$ : A tool to locate the emission of  $\text{Mn}^{4+}$  in oxides and fluorides, *Opt. Mater. X* 22 (2024) 133310.

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[6] P. Boutinaud, The nephelauxetic fonction  $he$  applied to the luminescence of  $\text{Mn}^{4+}$  and  $\text{Mn}^{5+}$  ions in oxides and oxyhalides, *Opt. Mater.* 157 (2024) 116232.

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