Theoretical investigation of the 7F1 level splitting in a series of Eu3+ doped oxides matrixes

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Résumé en anglais	The point charge electrostatic model (PCEM) and the simple overlap model (SOM) are applied to a series of oxide crystals (Gd2O3, Y2O3, Lu2O3, In2O3 and Sc2O3) and a silicate glass (Al2O3–SiO2) doped with the Eu3+ ion. The SOM factor ρ(2β)k+1 is input as the shielding factor for all B q k expressions, which enters in the calculations of the crystal-field strength parameter, NV. The maximum splitting ΔE of the 7F1 manifold of the Eu3+ ion is then obtained as a function of NV. It has been developed another way to calculate alpha, which is an expansion factor in the ΔE expression. For the glass, as the mean metal-ligating ions distances are larger than for the crystals, NV and ΔE are smaller, as expected. The prediction of the PCEM shows a linear dependence between ΔE and NV, even though the known mismatch in respect to the experimental splitting is kept. In the case of the SOM, two situations have been analyzed: firstly the charge factor varies in order to reproduce the experimental splitting (a phenomenological procedure); secondly the charge factor is the valence of the oxygen ions. The agreement between the experimental results and theoretical predictions for all investigated systems is very satisfactory in respect to both the linearity between ΔE and NV and the ΔE splitting.
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