2002 Vol.37 No.1 pp.111-116 DOI:

# Pressure-Induced Shifts of Energy Spectra of $\alpha$-$Al_2O_3$:$Mn^{4+}$

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(Received: 2001-6-11; Revised: )

Abstract: By making use of the diagonalization of the complete $d^3$ energy matrix in a trigonally distorted cubic-field and the theory of pressure-induced shifts (PS) of energy spectra, the whole energy spectrum of $\alpha$-$Al_2O_3$:$Mn^{4+}$ and PS of levels have been calculated. All the calculated results are in excellent agreement with the experimental data. The comparison between the results of $\alpha$-$Al_2O_3$:$Mn^{4+}$ and ruby has been made. It is found that on one hand, $R_1$-line and $R_2$-line PS of $\alpha$-$Al_2O_3$:$Mn^{4+}$ and ruby are linear in pressure over 0～100 kbar, and their values of the principal parameter for PS are very close to each other. On the other hand, the sensitivities of $R_1$-line and $R_2$-line PS of $\alpha$-$Al_2O_3$:$Mn^{4+}$ are higher than those of ruby respectively, which comes mainly from the difference between the values of parameters at normal pressure of two crystals; moreover, the expansion of d-electron wavefunctions of $\alpha$-$Al_2O_3$:$Mn^{4+}$ with compression is slightly larger than the one of ruby, and the effective charge experienced by d-electrons of $\alpha$-$Al_2O_3$:$Mn^{4+}$ decreases with compression more rapidly than the one of ruby. In the final analysis, all these can be explained in terms of the facts that the two crystals are doped $\alpha$-$Al_2O_3$ with two isoelectronic ions; the strengths of the crystal field and covalency of $\alpha$-$Al_2O_3$:$Mn^{4+}$ are larger than those of ruby respectively, due to the charge of $Mn^{4+}$ to be larger than that of $Cr^{3+}$.

PACS: 78.20.Hp, 71.70.Ch, 76.30Fc
Key words: crystal fields, energy spectrum, optical properties, high-pressure effect, $\alpha$-$Al_2O_3$:$Mn^{4+}$

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