New Insights into the Influence of the $4f^5 5d^1$ State in the $4f^6$ Electronic Configuration of Sm^{2+} in Crystal Hosts

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Supporting Information

Effect of the temperature on the $^5D_0 - {}^7F_0$ peak position in $SrAlF_5:Sm^{2+}$

As can be seen on Figure S1, the four $^5D_0 - {}^7F_0$ peaks of Sm^{2+} in $SrAlF_5$ are displaced by less than 5 cm^{-1} from 282 to 5 K. A temperature issue within the data reported in the paper is then not expected.

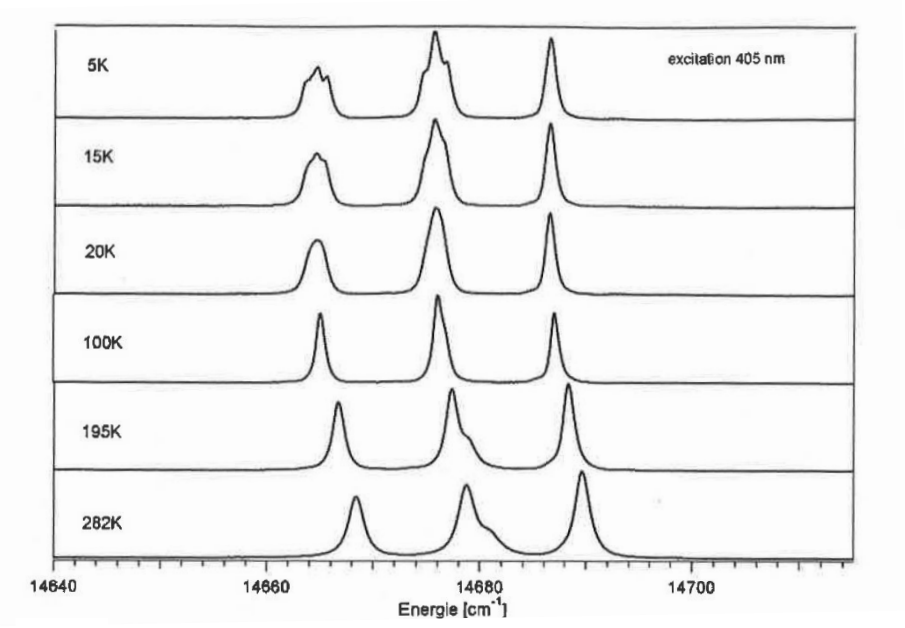

Figure S1: Variation of the $^5D_0 - {}^7F_0$ peak position of $SrAlF_5:Sm^{2+}$ between 5 and 282 K (reproduced from [S1]).

Superposition of the $4f^6$ and $4f^55d^1$ emissions and lifetime correlation in BaFI:Sm^{2+}

The $4f^6$ and $4f^55d^1$ emissions from Sm^{2+} in BaFI are superimposed, evidencing an interaction between these two configurations (Figure S2). Moreover, a study of the $^5D_0$ and $4f^55d^1$ lifetimes points out a strong correlation between these two levels (Figure S3).

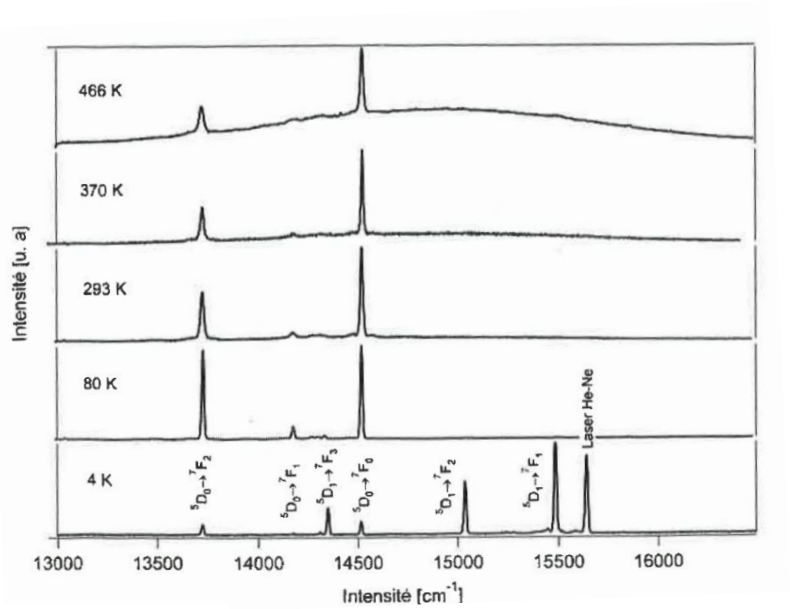

Figure S2: Emission spectra of BaFI:Sm^{2+} recorded at various temperatures (reproduced from [S1]).

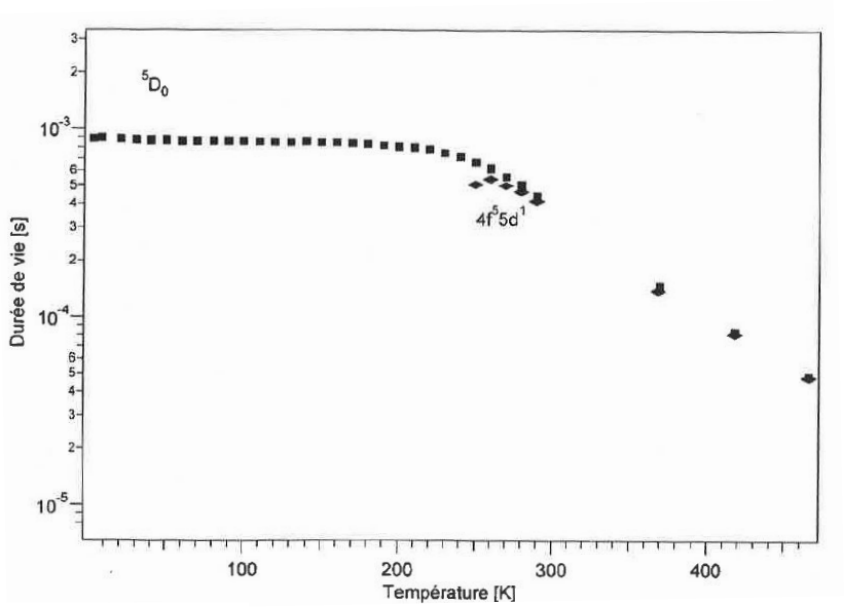

Figure S3: $^5D_0$ and $4f^55d^1$ lifetimes in BaFI:Sm^{2+} determined at various temperatures (reproduced from [S1]).

Effect of the crystal field on the $^7F_1$ splitting and the $^5D_0 - {}^7F_0$ energy for Eu^{3+}-doped crystals

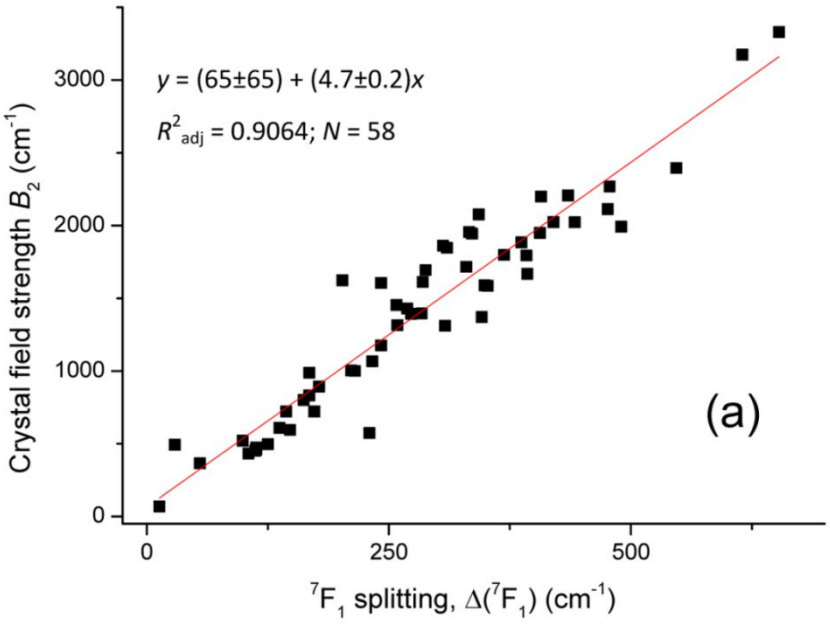

Figure S4: Axial scalar crystal field strength parameter N_v^2 (here called B_2) as a function of Δ^7F_1 for Eu^{3+}-doped crystals (reproduced from [S2]).

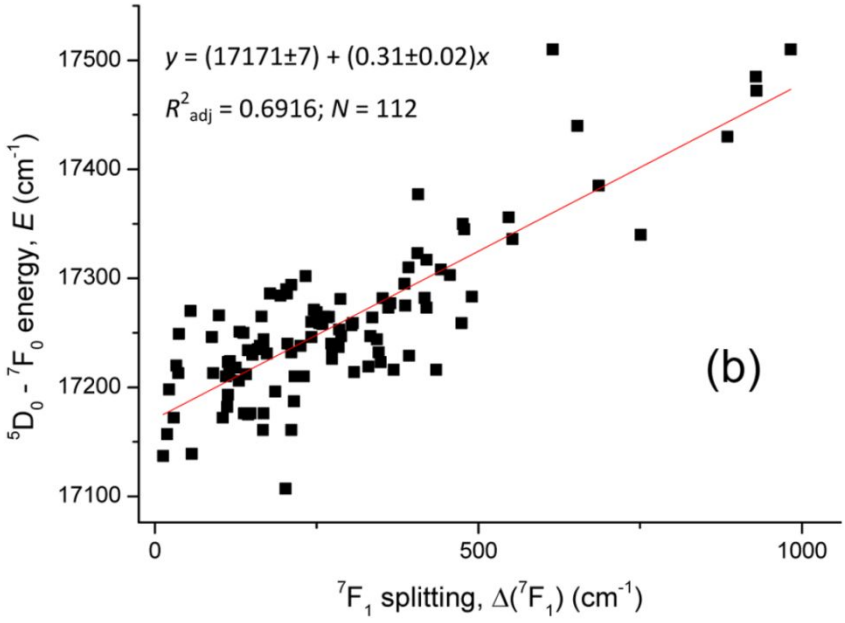

Figure S5: $^5D_0 - {}^7F_0$ energy E as a function of the $^7F_1$ state splitting Δ^7F_1 for Eu^{3+}-doped crystals (reproduced from [S2]).

Data of the $^5D_1$ state splitting in various Sm^{2+}-containing hosts

The $^5D_1$ states splitting (Δ^5D_1) was calculated as the difference between the highest and lowest energy levels, without any consideration for their symmetry.

Table S1: Δ^5D_1 of Sm^{2+}-doped hosts from the literature.

Host	Δ^5D_1 (cm^{-1})	Reference	Host	Δ^5D_1 (cm^{-1})	Reference
CaFCl	11.3	S3	BaFI	27.0	S1
SrFCl	6.9	S4	$BaCl_2$	16.7	S7
BaFCl	8.0	S5	$BaBr_2$	12.6	S7
SrFBr	14.6	S6	$BaMgF_4$	32.0	S1
BaFBr	9.7	S6	SrB_4O_7	32.4	S8

References

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