


## Erratum: Spin Hamiltonian characterization and refinement for $\text{Pr}^{3+}:\text{YAlO}_3$ and $\text{Pr}^{3+}:\text{Y}_2\text{SiO}_5$ [Phys. Rev. B **85**, 014429 (2012)]

Marko Lovrić, Philipp Glasenapp, and Dieter Suter

 (Received 21 November 2022; published 26 January 2023)

DOI: [10.1103/PhysRevB.107.019903](https://doi.org/10.1103/PhysRevB.107.019903)

In Ref. [1] we provided data on the relevant parameters of the spin Hamiltonian (electronic and nuclear) of  $\text{Pr}^{3+}:\text{YAlO}_3$  and  $\text{Pr}^{3+}:\text{Y}_2\text{SiO}_5$  (YSO), which are often used for photonic applications, such as quantum memories. The relevant Hamiltonian is given by the (effective) nuclear quadrupole coupling,

$$\mathcal{H} = \vec{I} \cdot \mathbf{Q} \cdot \vec{I},$$

where  $\vec{I}$  is the nuclear spin operator and

$$Q = \begin{bmatrix} E - D/3 & & \\ & -E - D/3 & \\ & & 2D/3 \end{bmatrix},$$

the (effective) quadrupole tensor—written here in the principal axis system. The quadrupole tensor elements are given in Ref. [1] as  $D_g = -4.4435$ ,  $D_e = 1.35679$ ,  $E_g = -0.56253$ , and  $E_e = 0.42192$  MHz. To transform this into the common basis, we use the rotation matrix,

$$R(\alpha, \beta, \gamma) = \begin{pmatrix} c_3 c_2 c_1 - s_1 s_3 & c_3 c_2 s_1 + s_3 c_1 & -c_3 s_2 \\ -s_3 c_2 c_1 - c_3 s_1 & -s_3 s_1 c_2 + c_3 c_1 & s_3 s_2 \\ s_2 c_1 & s_2 s_1 & c_2 \end{pmatrix},$$

with the abbreviations,

$$\cos \alpha = c_1, \quad \sin \alpha = s_1,$$

$$\cos \beta = c_2, \quad \sin \beta = s_2,$$

$$\cos \gamma = c_3, \quad \sin \gamma = s_3.$$

Using the parameters from Ref. [1], and the above rotation matrix, we calculate the Hamiltonians for the ground and excited states, the corresponding eigenvalues and eigenstates. This allows one to calculate the transition strengths for all the possible transitions between the spin sublevels of the electronic ground state to all spin sublevels of the electronically excited state as the squares of the overlaps between the states,  $t_{ik} = |\langle g_i | e_k \rangle|^2$ , where  $g$  and  $e$  refer to the ground and excited states. Summing over degenerate transitions, we obtain

$D_g$ (MHz)	$E_g$ (MHz)	$D_e$ (MHz)	$E_e$ (MHz)
−4.4435	−0.56253	1.35679	0.42192
$ g, \pm 1/2\rangle$	$ e, \pm 1/2\rangle$	$ e, \pm 3/2\rangle$	$ e, \pm 5/2\rangle$
$ g, \pm 3/2\rangle$	0.067	0.373	0.560
$ g, \pm 5/2\rangle$	0.007	0.593	0.399
$ g, \pm 5/2\rangle$	0.926	0.033	0.041

comparing this to the experimental data from Ref. [1],

	$ e, \pm 1/2\rangle$	$ e, \pm 3/2\rangle$	$ e, \pm 5/2\rangle$
$\langle g, \pm 1/2 $	0.55	0.38	0.07
$\langle g, \pm 3/2 $	0.40	0.60	0.01
$\langle g, \pm 5/2 $	0.05	0.02	0.93

we find that the calculated transition strengths match the experimental ones quite well but two of the column headings are interchanged. They comply much better with the calculated ones if we take the excited-state quadrupole coupling parameters to be negative. To match the experimentally observed transition frequencies of 4.5776 and 4.8374 MHz, we use  $D_e = -1.31129$ ,  $E_e = -0.46743$  MHz. Then, the frequencies and transition strengths become

$D_g$ (MHz)	$E_g$ (MHz)	$D_e$ (MHz)	$E_e$ (MHz)
-4.4435	-0.56253	-1.31129	-0.46743
	$ e, \pm 1/2\rangle$	$ e, \pm 3/2\rangle$	$ e, \pm 5/2\rangle$
$\langle g, \pm 1/2 $	0.589	0.358	0.053
$\langle g, \pm 3/2 $	0.375	0.618	0.007
$\langle g, \pm 5/2 $	0.036	0.024	0.940

now in very good agreement with the experimental ones.

In conclusion, we would like to draw the readers' attention to this error and present a set of parameters that resolves the main discrepancies. A full optimization with a complete experimental dataset would be preferable but is beyond the scope of this Erratum; it will be published in the near future [2].

*Acknowledgments.* I am very grateful to Z. Levine for drawing our attention to this mistake and assisting in the search of a consistent solution.

[1] M. Lovric, P. Glasenapp, and D. Suter, *Phys. Rev. B* **85**, 014429 (2012).

[2] Z. H. Levine and D. Suter (to be published).