Errata

Erratum: Theoretical explanation of zero-field splitting and its pressure, stress, and temperature dependence in $\text{NiSiF}_6 \cdot 6\text{H}_2\text{O}$ [Phys. Rev. B 36, 8774 (1987)]

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The following changes should be made in our paper. There are two typographical errors. (1) The first two terms

$$\frac{\xi_d^2 v}{2W_1} - \frac{\xi_d^2 v}{2W_2}$$

on the right-hand side of Eq. (1) should read

$$\frac{\xi_d^2 v}{2W_1^2} - \frac{\xi_d^2 v}{2W_2^2}.$$

(2) On the right-hand side of Eq. (3), the coefficient of the second term is $5\sqrt{2}/42$, not $5\sqrt{2}/4$.

The values of certain parameters need modification. In Eq. (5), $\xi_{d0} = 650 \text{ cm}^{-1}$ should be replaced by $\xi_{d0} = 636 \text{ cm}^{-1}$ in accordance with a recent paper.¹ In the paragraph following Eq. (6), $\mu = 0.02 e \text{ \AA}$ should be $\mu = 0$, i.e., only the point-charge model is used in the calculations. Therefore, all the calculated results should be changed slightly. For example, $D_s = -0.784 \text{ cm}^{-1}$, $D_p = 0.267 \text{ cm}^{-1}$, $(\partial D/\partial P)_T = 0.834 \times 10^{-4} \text{ cm}^{-1}/(\text{kg/cm}^2)$.

It is noteworthy that for $(\partial D/\partial P)_T$, the calculated value decreases slightly with increasing pressure, whereas the experimental value is nearly a constant. One of the reasons is perhaps that the slight change of parameters N and q (effective charge of ligands) with pressure is not taken into account in the calculations. In addition, the second-order pressure effect of structural parameters is also an important factor. However, if we try to explain the linear D - P relation quantitatively, it may cause some uncertainty and randomness theoretically because of the multiple possibilities for the choice of parameters. For instance, even if only the second-order pressure effect, i.e.,

$$R(P) = R(1 + a_1 P + a_2 P^2), \quad \alpha(P) = \alpha(1 + b_1 P + b_2 P^2), \quad (1)$$

is taken into consideration, one can find that good agreement between calculated and experimental values of $(\partial D/\partial P)_T$ can be obtained by using several sets of the second-order parameters a_2 and b_2 . So, in our calculations, the slight change of $(\partial D/\partial P)_T$ with pressure is omitted, and the value of $(\partial D/\partial P)_T$ is an average value.

¹Zhao Min-Guang and Du Mao-Lu, J. Phys. C 20, 4467 (1987).

Erratum: Self-consistent full-potential linearized-augmented-plane-wave local-density electronic-structure studies of magnetism and superconductivity in C15 compounds: ZrZn_2 and ZrV_2 [Phys. Rev. B 37, 3489 (1988)]

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On page 3489, in the abstract, in lines 8 and 14, ZnZr_2 should read ZrZn_2 . In line 9, Zr should read Zn. On page 3490, left column, text lines 38 and 39, E'_i and atom-type n should read E'_i and atom-type t , respectively. On page 3494, in formulas (3a) to (3c), η_i should read $\eta_i n_i$. On page 3495, right column, in the first paragraph of the Conclusions section, text line 11, Zr should read Zn.