

Correction to “Photogeneration of Spin Quintet Triplet–Triplet Excitations in DNA-Assembled Pentacene Stacks”

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Supporting Information

Pages 5436. In the analysis and discussion of the ESR experiments, the definition of the quintet zero-field-splitting Hamiltonian was mistakenly typed as

$$\frac{\hat{H}_{\text{zfs}}}{h} = \mathbf{S}^T \cdot \mathbf{D}_q \cdot \mathbf{S} = D_q(\hat{S}_z^2 - 2\hat{I}_3) + E_q(\hat{S}_z^2 - \hat{S}_z^2)$$

The equation and definition of its terms should read as follows:

$$\frac{\hat{H}_{\text{zfs}}}{h} = \mathbf{S}^T \cdot \mathbf{D}_q \cdot \mathbf{S} = D_q(\hat{S}_z^2 - 2\hat{I}) + E_q(\hat{S}_x^2 - \hat{S}_y^2)$$

where \mathbf{S} is the vector of quintet spin operators, \hat{I} is the 5×5 identity matrix, and \hat{S}_i is the spin operator defined along the principal axis $i \in (\hat{x}, \hat{y}, \hat{z})$ of the ZFS tensor \mathbf{D}_q , determined by the symmetry of the underlying spin–spin interactions.

This is also updated in Section K (“Theoretical quintet ($S=2$) zero-field splitting parameters”, page S22) of the [Supporting Information](#).

These corrections do not affect the conclusions presented in the published article.

■ ASSOCIATED CONTENT

SI Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/jacs.3c02230>.

Experimental methods, synthetic procedures, and additional spectroscopic data (updated) ([PDF](#))

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