

Magn. Reson. Discuss., community comment CC1
<https://doi.org/10.5194/mr-2022-20-CC1>, 2022
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Comment on mr-2022-20

Alexander G. Maryasov

Community comment on "The effect of the zero-field splitting interaction in light-induced pulsed dipolar EPR spectroscopy" by Andreas Scherer et al., Magn. Reson. Discuss., <https://doi.org/10.5194/mr-2022-20-CC1>, 2022

The authors pay attention on rather important issue, influence of ZFS on dipole interactions of paramagnetic centers with spin $S > 1$.

Here it is suitable to remind that influence of ZFS on dipole-dipole interactions of high-spin PCs was studied in our paper [1]. The system of weakly coupled doublet (spin 1/2) and triplet (spin 1) was studied in detail, analytic equations for the first order energy corrections and Pake patterns were derived in closed form. Dependences of Pake patterns on ZFS, geometry, and temperature were illustrated.

I think it is reasonable to cite the paper and to take some formulae from there using solution of cubic equation suggested long ago by G. Muha [2].

Cordially,

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[1] Maryasov A.G., Bowman M.K., Tsvetkov Yu.D. Dipole-Dipole Interactions of High-Spin Paramagnetic Centers in Disordered Systems. Applied Magn. Reson. 30: 683-702, 2006.

[2]. Muha G.M.: J. Chem. Phys. 73, 4139 (1980)

Please also note the supplement to this comment:

<https://mr.copernicus.org/preprints/mr-2022-20/mr-2022-20-CC1-supplement.pdf>