Endohedral fullerene Sc₂@C₈₀(CH₂Ph) as a standard sample for field calibration

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Endohedral fullerenes $Sc_2@C_{80}(CH_2Ph)$ have unique spectral characteristics due to the large hyperfine interaction (509 MHz) of a delocalized electron (S=1/2) with two equivalent ⁴⁵Sc nuclei (I=7/2) [1-2]. The EPR spectrum consists of 64 well-resolved lines, divided into 15 groups depending on the projection of the total spin of the scandium nuclei. The total EPR spectrum width of about 0.25 Tesla. In this regard, we show that this sample can be used as a standard for magnetic field calibration. In the EPR spectrum of endofullerene each group has a reference line with the maximum possible

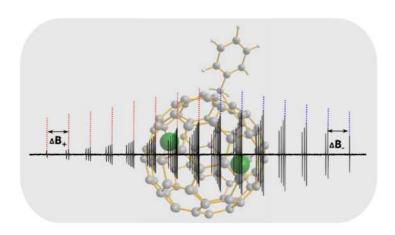


Fig. 1. Q-band EPR spectra recorded at liquid solution. The dotted lines show the reference lines. Also different splitting (ΔB_{\pm}) between these lines for the right and left parts of the spectrum are indicated.

total nuclear spin located on the right edge of the group. It is shown that these reference lines are equidistant in the regions of the spectrum with low and strong fields and, therefore, can serve as a reference for calibrating the magnetic field. The calibration procedure is tested by using the Q-band EPR. The results show the high accuracy of the procedure for correcting linear and nonlinear displacements of

the magnetic field.

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- [1] R.B. Zaripov, Yu.E. Kandrashkin, K.M. Salikhov, B. Büchner, F. Liu, M. Rosenkranz, A.A. Popov, V. Kataev: *Nanoscale* **2020**, *12*, p. 20513.
- [2] Yu.E. Kandrashkin, R.B. Zaripov, F. Liu, B. Büchner, V. Kataev, A.A. Popov: Physical Chemistry Chemical Physics **2021**, *2*3, p. 18206.