Terahertz EPR Spectroscopy in the High-Homogeneity 36T Series-Connected Hybrid Magnet

T. Dubroca[1], X. Wang[1,2], F. Mentink-Vigier[1], B. Trociewitz[1], M. Starck[3], D. Parker[3], S. Hill[1,4], J. Krzystek[1], M.S. Sherwin[5]
1. NHMFL FSU; 2. Cal State University East Bay Chemistry; 3. University of Durham Chemistry, UK; 4. FSU Physics; 5. UCSB Physics

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MagLab scientists have developed instrumentation for performing ultra-high-resolution Electron Paramagnetic Resonance (EPR) in the high-homogeneity 36 T series-connected hybrid (SCH) magnet. In order to demonstrate this unique new capability, experiments were carried out on a series of Gd^{III} molecular compounds that are of interest as so-called "spin-labels". Spin labels can be attached to large biomolecules so that EPR can then be used to report on structural and dynamical properties that cannot be determined by any other method. *The larger magnetic moments of electrons - compared to nuclei - enables distances between spin-labels to be determined that exceed those able to be measured by NMR by an order of magnitude, providing access to structural details of intrinsically disordered proteins that are unobtainable from NMR, X-ray, and cryo-electron microscopy techniques*. Meanwhile, the higher Larmor frequencies of electrons probe much faster dynamics, roughly three orders of magnitude faster than NMR probes.

In analogy to NMR of certain quadrupolar nuclei (nuclei with half-integer nuclear spin, $I > ½$), the EPR spectrum of Gd^{III} (with electronic spin, $S = {}^7/_2$) exhibits a sharp central component with a linewidth that decreases ($\propto 1/B$) with increasing magnetic field, B. It is this property that makes Gd^{III} labels ideal for high-resolution biological EPR studies at very high magnetic fields. However, this also requires a magnet with higher homogeneity, that is, the magnetic field variation across the sample must be less than the EPR linewidth. As such, these experiments require the SCH magnet.

The figure shows results for two Gd^{III} spin-labels. The expected $1/B$ narrowing of the linewidth is found in one case, whereas a weak increase is seen above ~15T for the other sample. In both cases, *the SCH spectrometer enables resolution of the exceptionally narrow EPR lines (~1mT width) at the highest magnetic fields, paving the way towards use of Gd^{III} spin-labels in ultra-high resolution biostructural studies*.

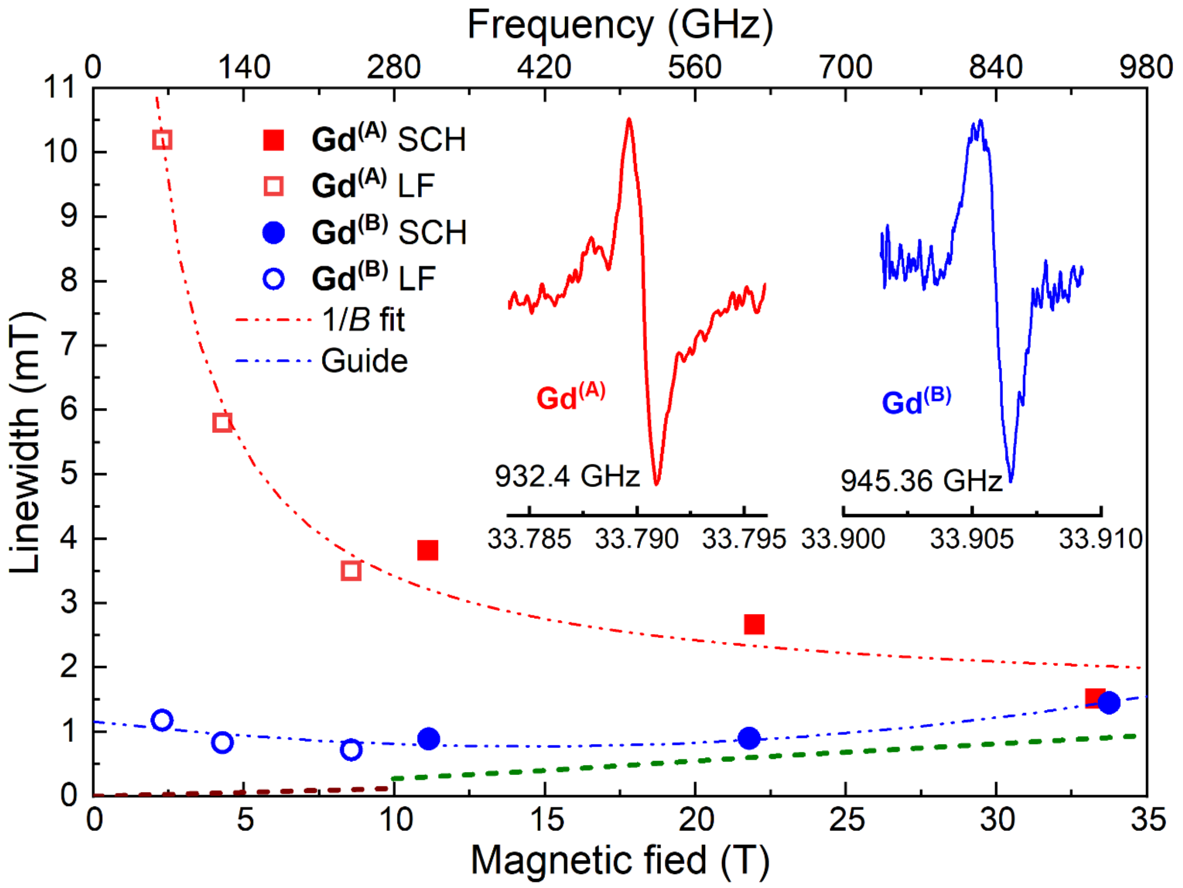

Figure. High field EPR linewidth variation with field/frequency, measured in the SCH and a lower-field (LF) spectrometer, for two Gd^{III} spin-labels on large biomolecules ($Gd^{(A)}$ = Gd[DTPA], $Gd^{(B)}$ = Gd[sTPATCN]-SL, see citation). Dashed lines at bottom represent the respective spectrometer resolutions. Representative ultra-high-resolution EPR spectra are shown in the inset.

Facilities and instrumentation used: EMR and DC Field Facilities, 15/17 Tesla Transmission Spectrometer and 36 Tesla Series Connected Hybrid Magnet.

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