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Copper Line Shapes

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Copper Line Shapes

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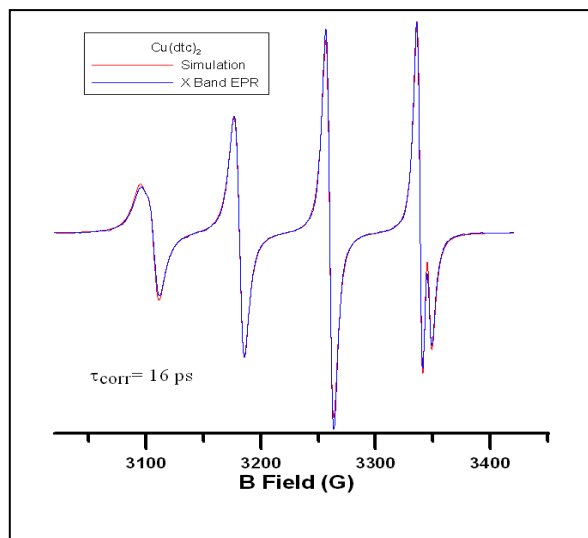
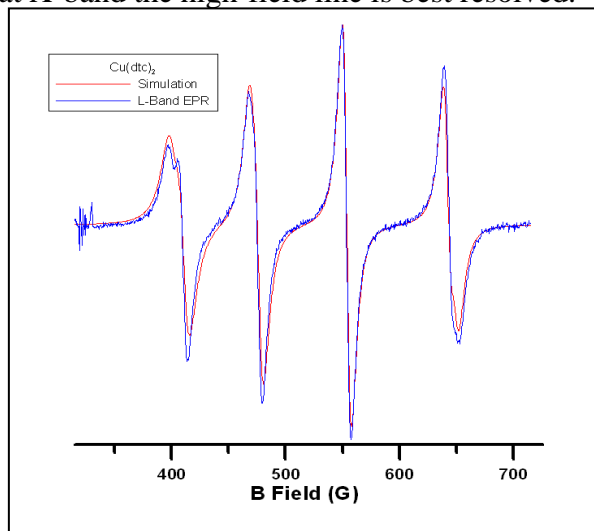
Copper line shapes

Gareth R. Eaton, University of Denver EPR Center, May 2019

CW EPR of Cu^{2+} Complexes

The spectrum of Cu^{2+} has 4 lines, since $I = 3/2$. Cu has two major isotopes, ^{63}Cu (69.2%) and ^{65}Cu (30.8%). The magnetic moment of ^{65}Cu is 7% larger than that for ^{63}Cu , so the hyperfine coupling is 7% larger. If the lines are narrow enough, one can observe superposition of spectra due to complexes of the two isotopes.

Spectra of $\text{Cu}(\text{diethyldithiocarbamate})_2$ in toluene solution were recorded by Michelle Collier, Deborah Mitchell, and Velavan at L-band and X-band. At L-band the low-field line exhibits the best resolution, and at X-band the high-field line is best resolved.



The 4 extrema marked as “z” in Figure 2A correspond to the four copper hyperfine lines for molecules aligned with the magnetic field along the magnetic z axis. For the low-field and high-field extrema, the ^{63}Cu and ^{65}Cu contributions are resolved. The 4 extrema marked as “ \perp ” correspond to the four copper hyperfine lines for molecules oriented with the magnetic field in the molecular plane. At X-band the g values for $\text{Cu}(\text{dte})_2$ along the x and y axes are so similar that the spectrum appears to be axial. It is important to remember that for each hyperfine line (each value of m_I), the spectrum actually extends from the parallel (z-axis) to the perpendicular extrema. Intermediate orientations of the molecule are at resonance at magnetic fields intermediate between the corresponding extrema, but the absorption spectrum changes relatively slowly with magnetic field in these intermediate regions, so the slope is small, and the first derivative signal is close to baseline. This orientation dependence is more clearly seen in the absorption display (Figure 2B) than in the first derivative display of the spectrum. The spectrum of $\text{Cu}(\text{dte})_2$ in glassy toluene solution at 100 K is very similar to that shown for the doped solid in Figure 2, because it too represents a random distribution of molecular orientations and the g and A values in toluene solution are similar to those in the doped solid.

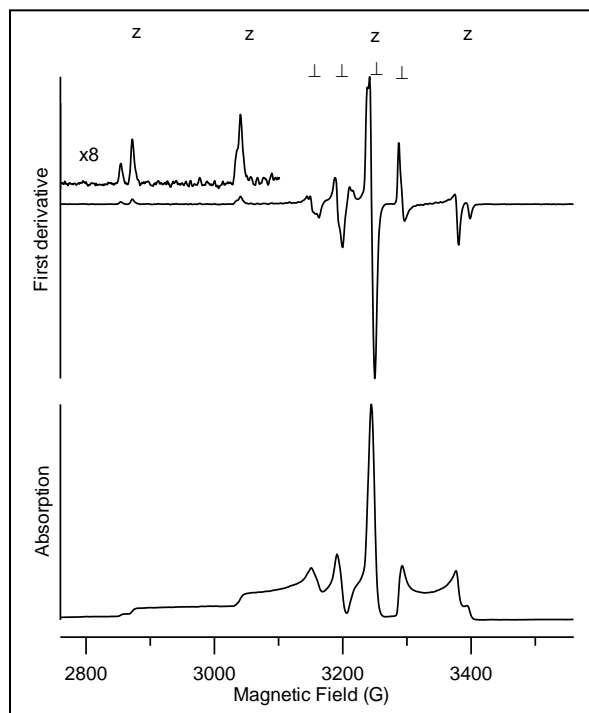


Figure 2. X-band (9.107 GHz) CW spectrum of a powdered sample of $\text{Ni}(\text{dte})_2$ doped 1:500 with $\text{Cu}(\text{dte})_2$ obtained at 150 K with 1.0 mW microwave power and 1.0 G modulation amplitude and displayed as the traditional first derivative (A). Computer integration of the spectrum in A gives the absorption spectrum (B). The turning points in the powder pattern that correspond to the four copper hyperfine lines for molecules aligned with the magnetic field along the magnetic z axis or in the perpendicular plane are marked as “z” or “ \perp ”, respectively.

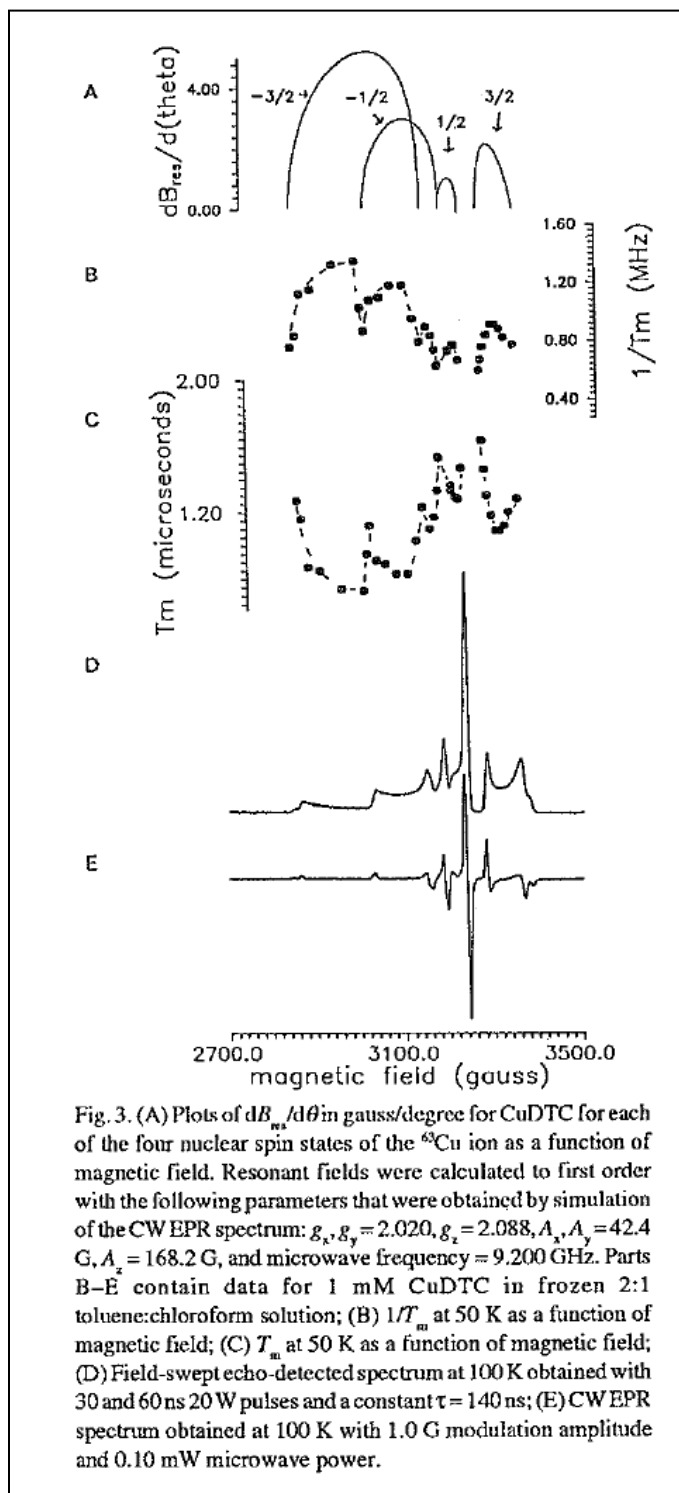


Figure from Du et al. (1992)

Orientation dependence of electron spin phase memory relaxation times in copper(II) and vanadyl complexes in frozen solution, J.-L. Du, K. M. More, S. S. Eaton, and G. R. Eaton, *Israel J. Chem.* **32**, 351-355 (1992).