

FIG. 2. *a*, two-pulse ESEEM for $\text{VO}(\text{H}_2\text{O})_2$ obtained at 20K with a microwave frequency of 9.19 GHz and a magnetic field of 3250 G, which corresponds to a perpendicular line in the CW EPR spectrum. *b*, cosine Fourier transform of the data in *a*. *c*, simulated spectrum obtained with $r = 2.0 \text{ \AA}$, $a = 6.6 \text{ MHz}$, $eeqQ = 1.5 \text{ MHz}$, and $\eta = 0.5$. Proton modulation was not included in the simulation.

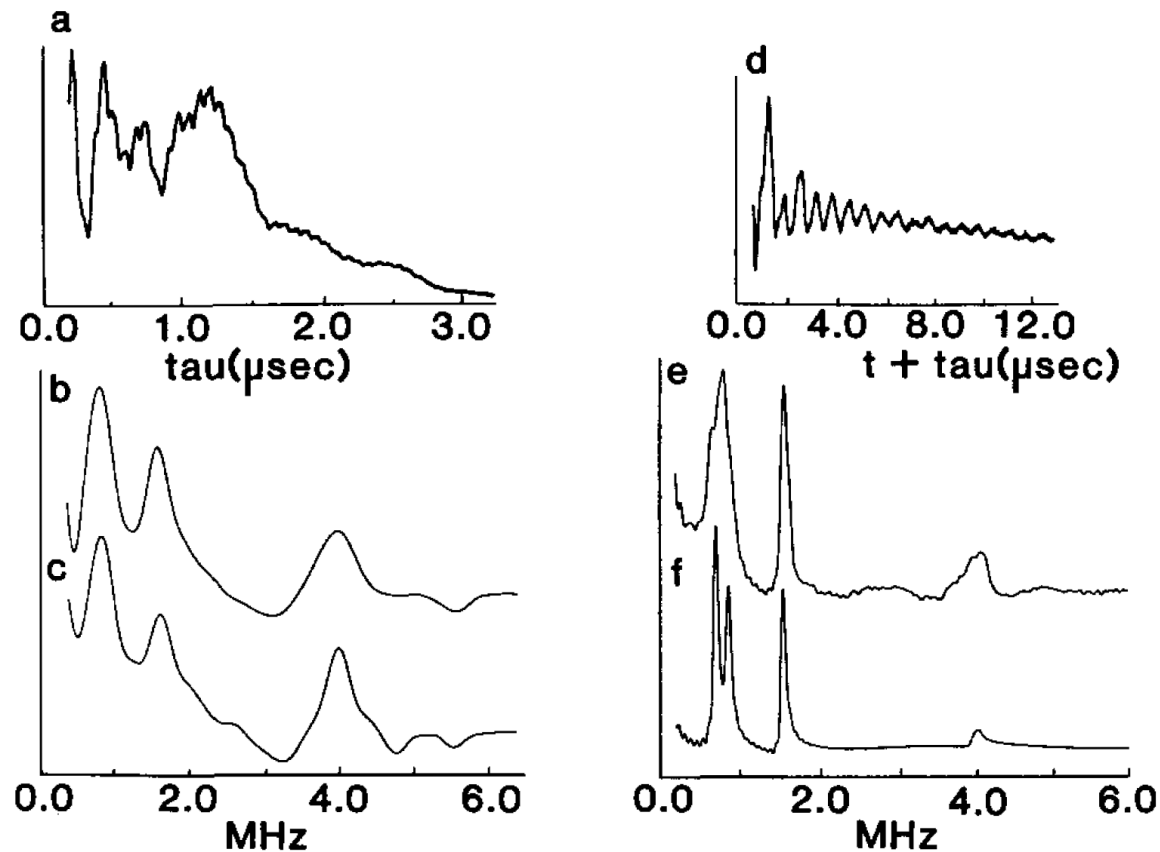
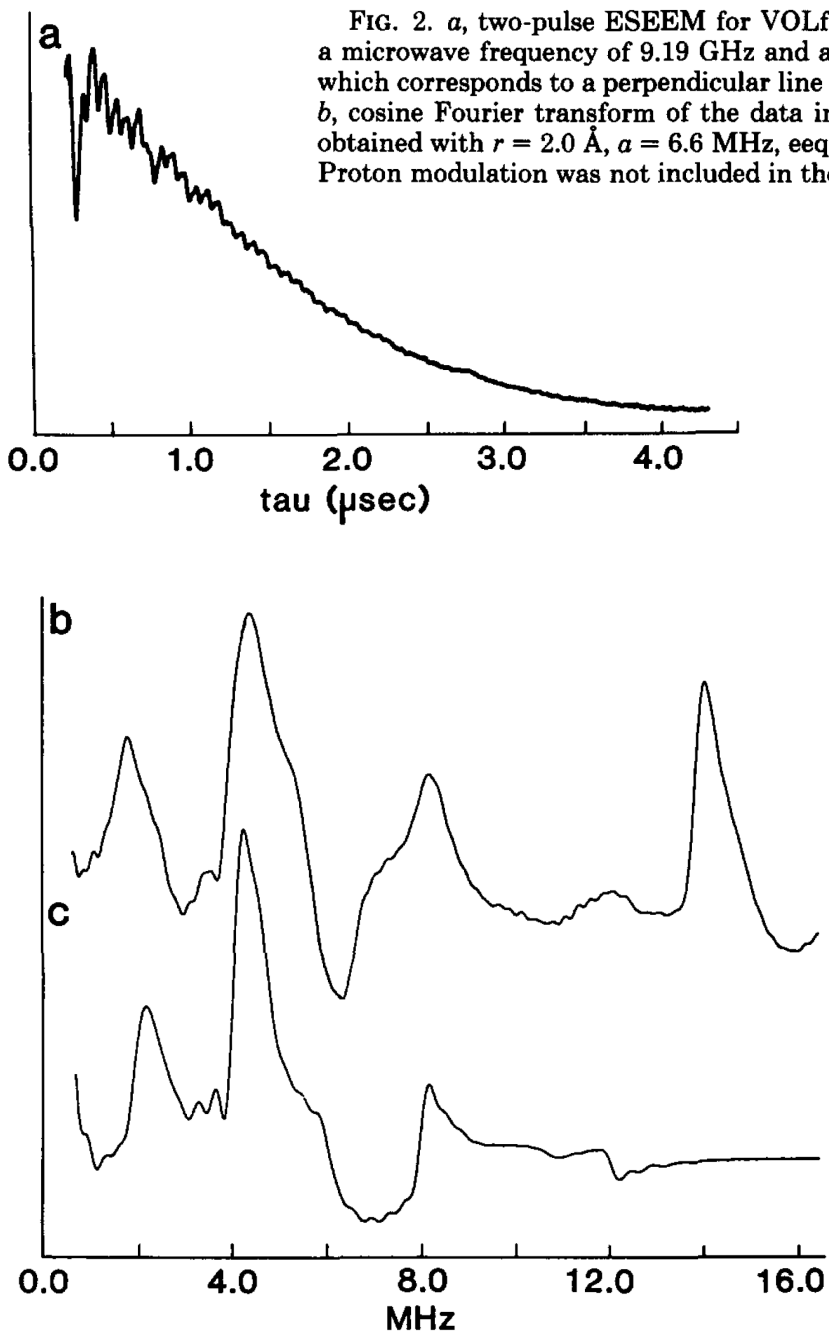
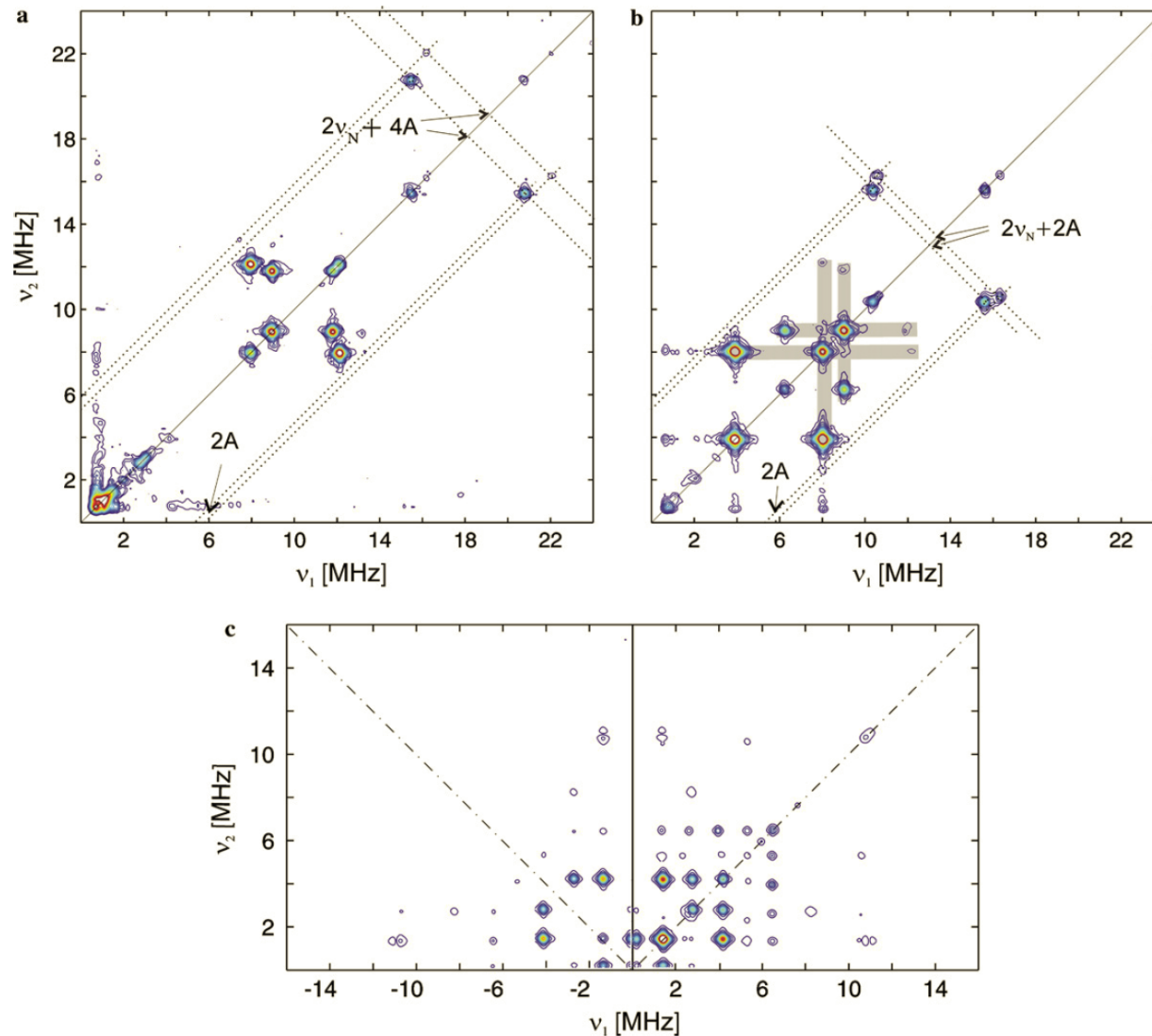


FIG. 1. ESEEM data for CuLfcO_3 obtained at approximately 5K with a microwave frequency of 9.19 GHz and a magnetic field of 3200 G which corresponds to a perpendicular line in the CW EPR spectrum. *a*, two-pulse ESEEM. *b*, cosine Fourier transform of the data in *a*. *c*, simulation of the two-pulse data obtained with $r = 4.2 \text{ \AA}$, $a = 1.7 \text{ MHz}$, $eeqQ = 1.6 \text{ MHz}$, and $\eta = 0.9$. *d*, three-pulse ESEEM. *e*, cosine Fourier transform of the data in *d*. *f*, simulation of the three-pulse data obtained with $r = 4.15 \text{ \AA}$, $a = 1.75 \text{ MHz}$, $eeqQ = 1.55 \text{ MHz}$, and $\eta = 0.90$.



Quelle: I. García-Rubio, A. Angerhofer, A. Schweiger, EPR and HYSORE investigation of the electronic structure of the model complex $\text{Mn}(\text{imidazole})_6$: Exploring $\text{Mn}(\text{II})$ –imidazole binding using single crystals, *J. Magn. Reson.*, 184 (2007) 130-142.

Fig. 5. Q -band HYSORE spectra of $\text{Mn}(\text{Im})_6$ recorded at one of the electron spin transitions: (a) $m_S : |-\frac{5}{2}\rangle \rightarrow |-\frac{3}{2}\rangle$, $B_0 = 1183$ mT, $\tau = 208$ ns; (b) $m_S : |-\frac{3}{2}\rangle \rightarrow |-\frac{1}{2}\rangle$, $B_0 = 1179$ mT, $\tau = 208$ ns; (c) $m_S : |-\frac{1}{2}\rangle \rightarrow |+\frac{1}{2}\rangle$, $B_0 = 1251$ mT, $\tau = 96$ ns. The magnetic field for all spectra is parallel to the z -axis of the D tensor (z_D). This orientation is labeled with an asterisk in the rotation patterns shown in Figs. 3, 4 and 8. The nuclear frequencies in correlation patterns a and b can be calculated in a first-order approximation. In this case the hyperfine coupling constant can be directly extracted from the spectrum tracing a line parallel to the diagonal from the dq peaks. The value where this line crosses the abscissa is $2A$. If a line perpendicular to the diagonal is drawn, it crosses the diagonal at $2\nu_N + 4A$ for the $|-\frac{5}{2}\rangle \rightarrow |-\frac{3}{2}\rangle$ transitions and at $2\nu_N + 2A$ for $|-\frac{3}{2}\rangle \rightarrow |-\frac{1}{2}\rangle$. In spectrum b the crosses formed by the dq peaks (see text) have been highlighted.

HYSCORE an Cu-tetrapyridin

Pöpl et al., *J. Phys. Chem. A* **1998**, *102*, 3599.

