Electronic Supplementary Material for PCCP

Supplementary materials to " Matrix Effects on Copper(II)phthalocyanine Complexes. A Combined Continuous Wave and Pulse EPR and ENDOR Study"

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A. UV/vis Data

Table S1 : Values of λ (nm) for CuPc, $CuPc^t$, and $CuPc^F$ in sulfuric acid and $CuPc^t$ in toluene.

	Soret	Q-band
$CuPc^t$ in toluene	429	802, 724
$CuPc^t$ in H_2SO_4	448	816, 721
CuPc in H_2SO_4	441	719, 701, 668, 636
$CuPc^F$ in H_2SO_4	452	772, 756, 712

B. cw EPR spectra

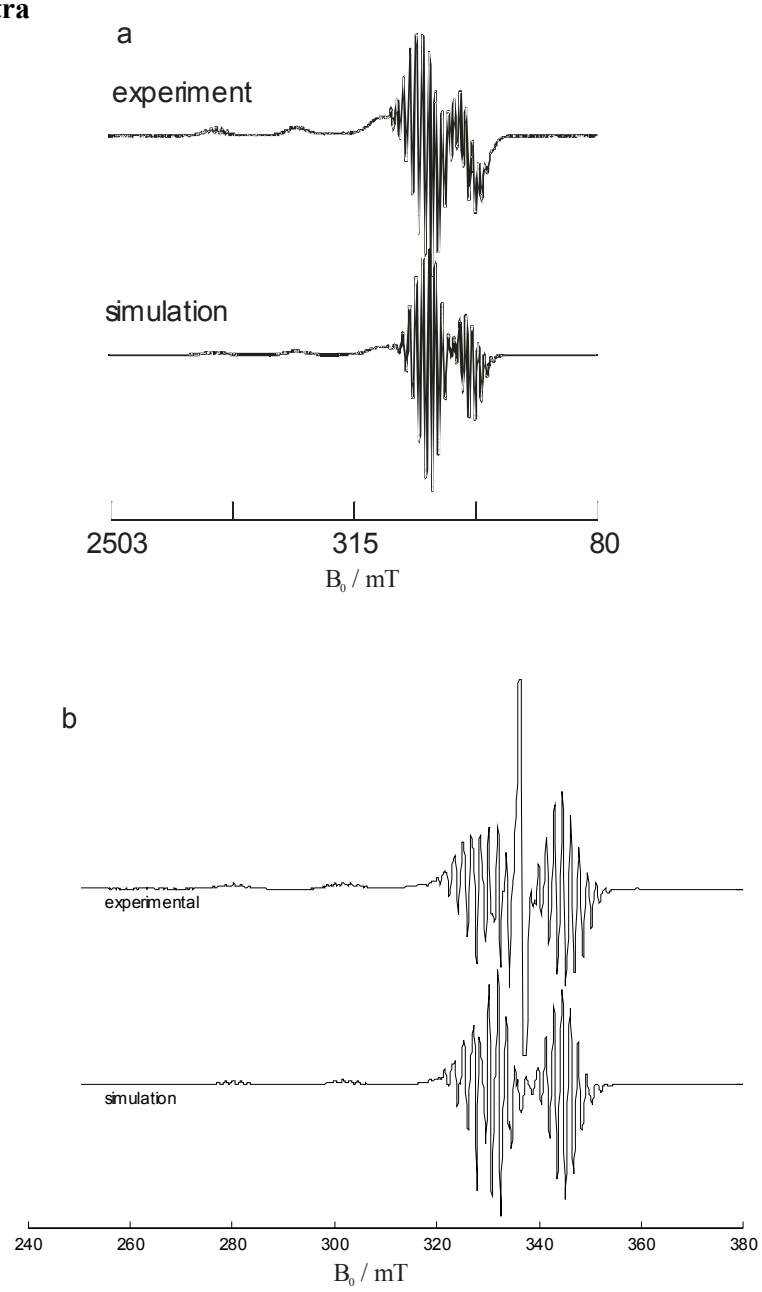


Figure S1: Experimental and simulated X-band cw-EPR spectra at 120 K. (a) $CuPc^t$ in sulfuric acid. (b) CuPc in H_2Pc.

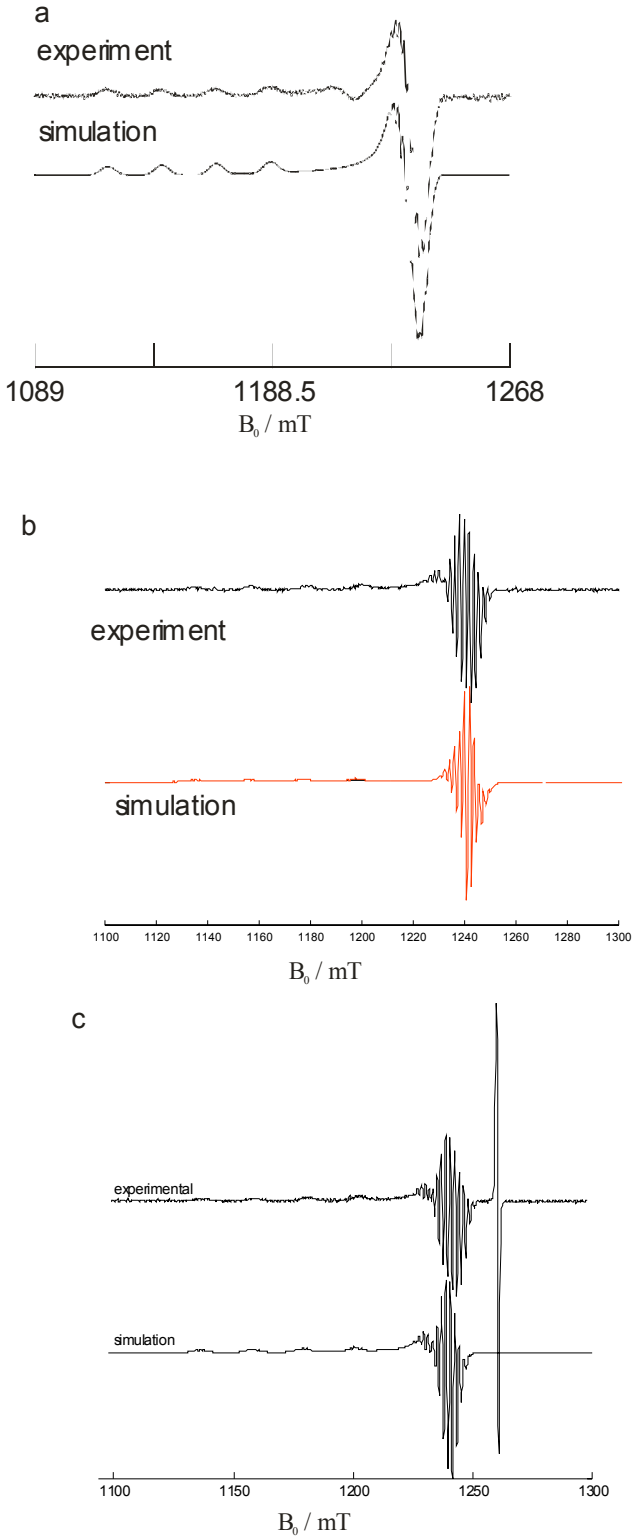
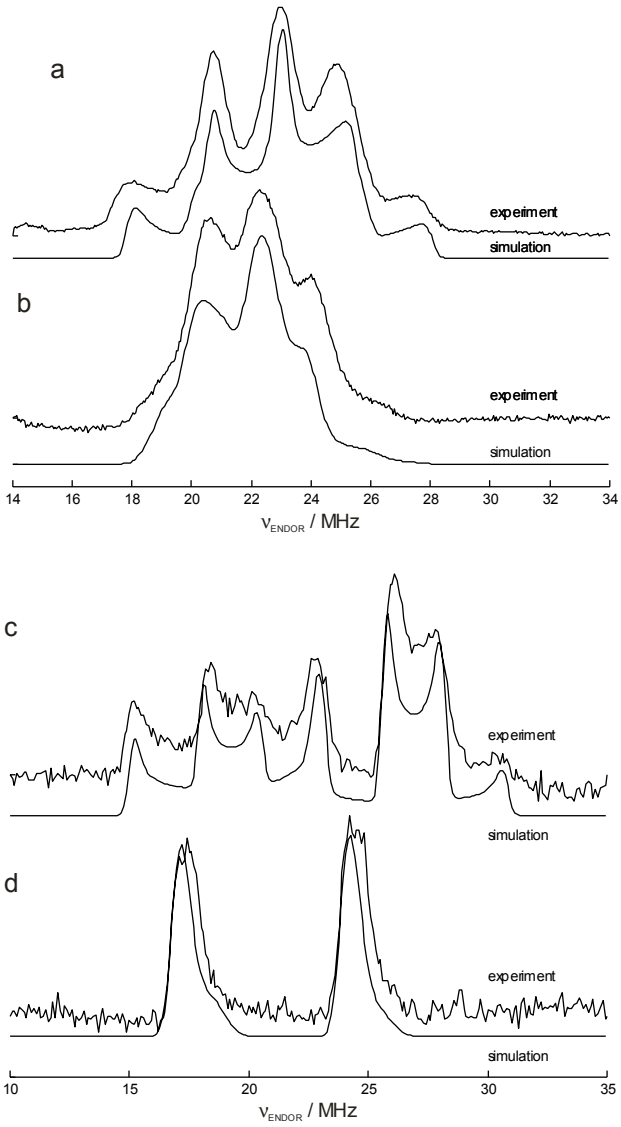
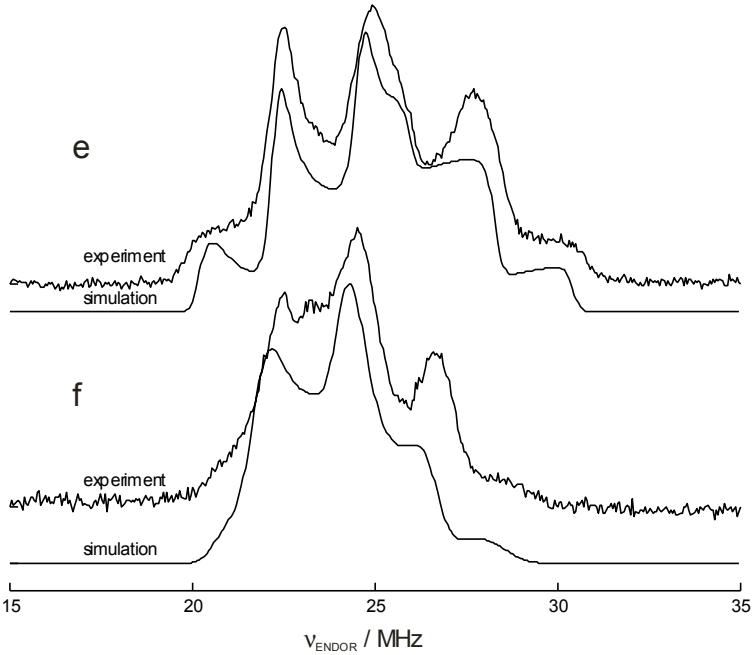


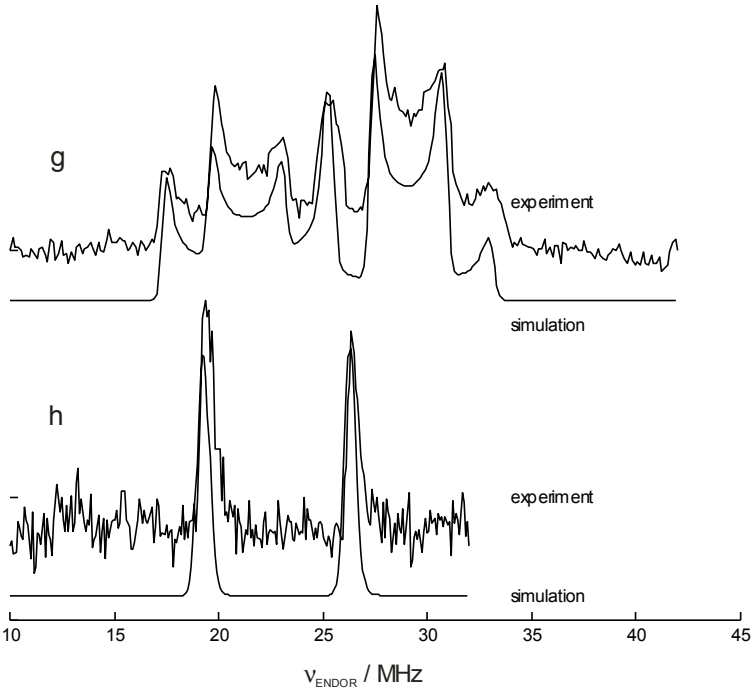
Figure S2: Experimental and simulated Q-band cw-EPR spectra at 120 K. (a) CuPc in sulfuric acid. (b) CuPc in H_2Pc. (c) $CuPc^t$ in toluene.

The fast and slow motion spectra were simulated using the Matlab-based toolbox EasySpin (http://www.easyspin.ethz.ch). The Cu-isotopes ratio has been taken into account. An residual line width of 0.1 mT has been assumed. The rotational correlation time was varied between 10^{-9} s (Figure 3a) and 10^{-6} s (Figure 3f) in order to simulate the experimental data.

C. **ENDOR experiments**







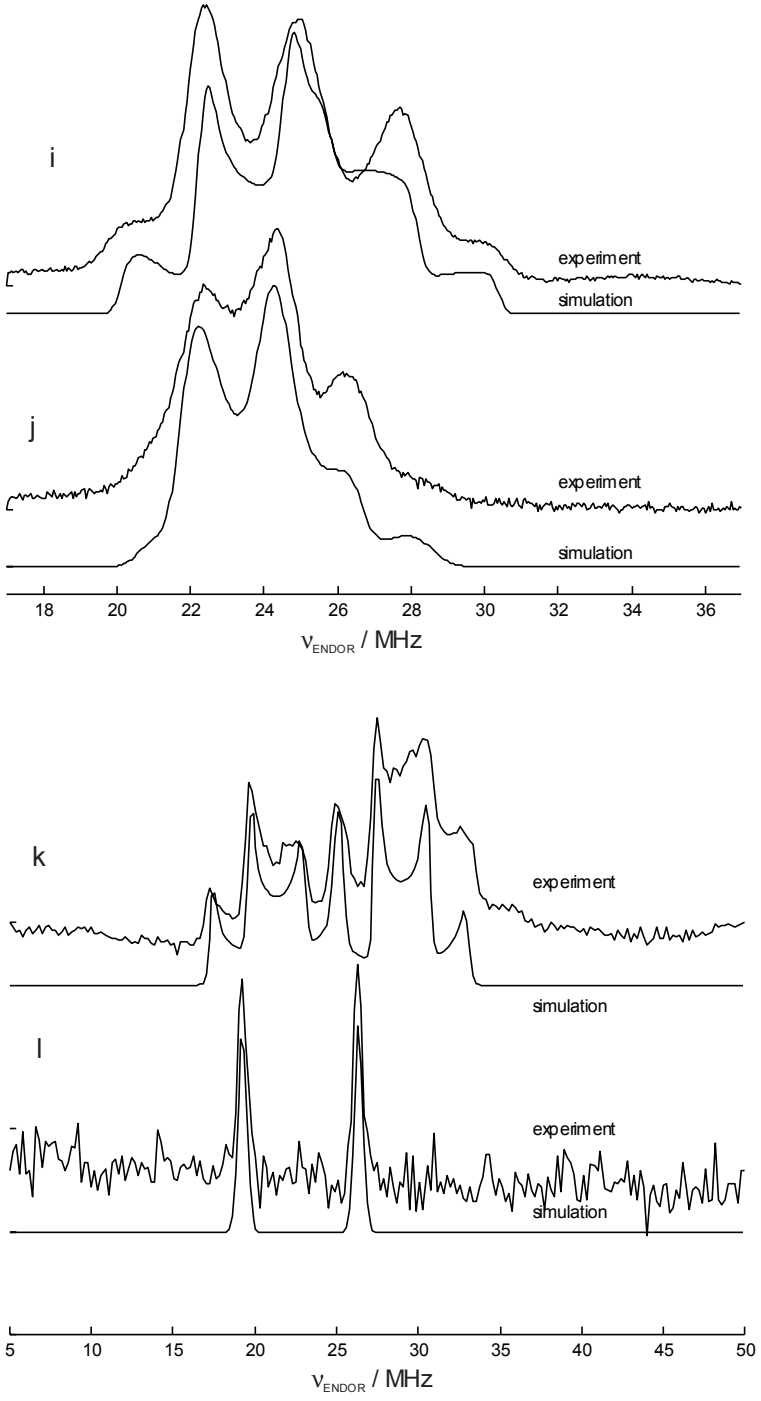


Figure S3: Experimental and simulated X- and Q-band Davies-ENDOR spectra of CuPc in H_2SO_4 (a-d), CuPc in H_2Pc (e-h), and $CuPc^t$ in toluene (i-l). (a,e,i) X-band, observer position $g_\perp$. (b,f,j) X-band, observer position $g_\parallel$. (c,g,k) Q-band, observer position $g_\perp$. (d,h,l) Q-band, observer position $g_\parallel$, m_I =- 3/2.

D. DFT data

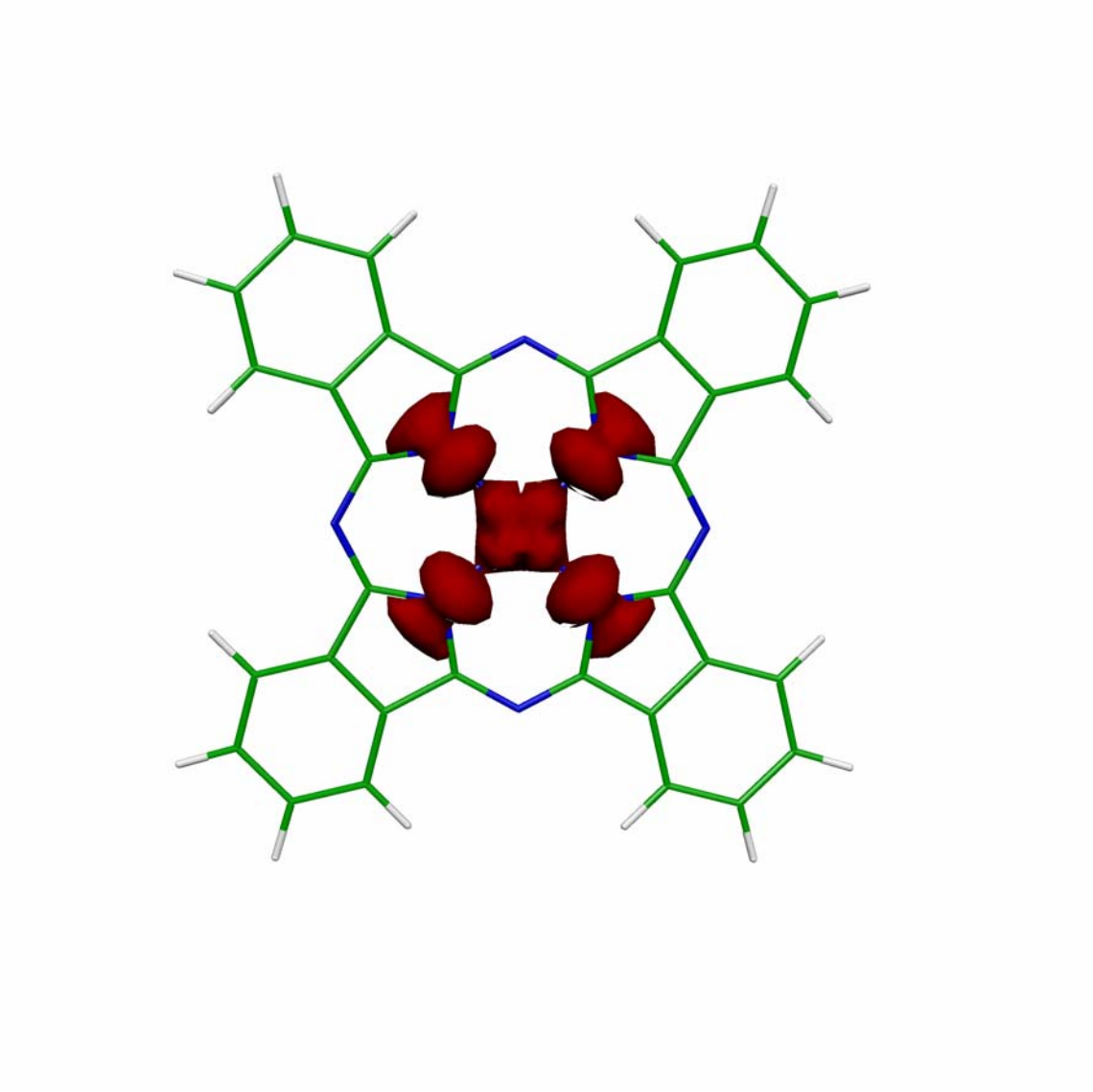


Figure S4: Spin density on the CuPc complex obtained from DFT calculations.