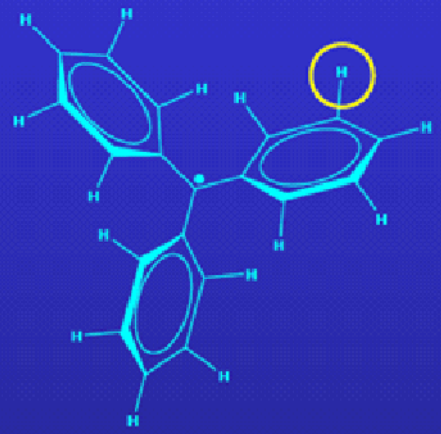
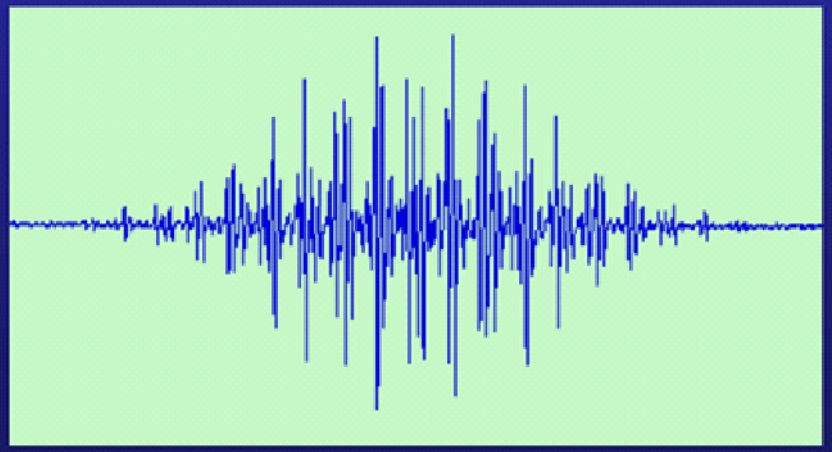
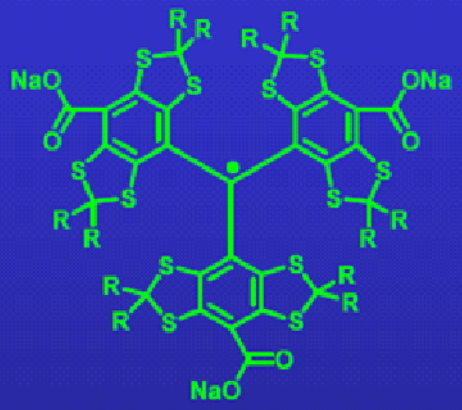
Trityl Radikale



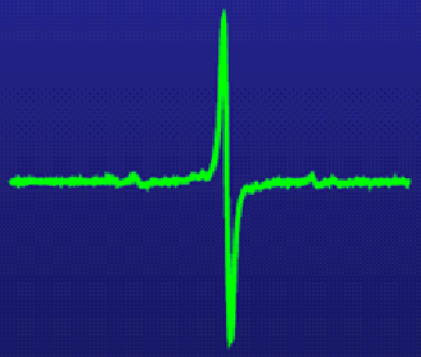
Triphenylmethyl radical



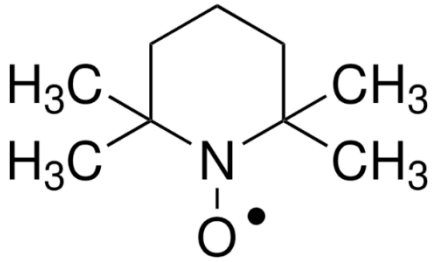
Gomberg, M. J. Am. Chem. Soc. 1900, 22, 757.

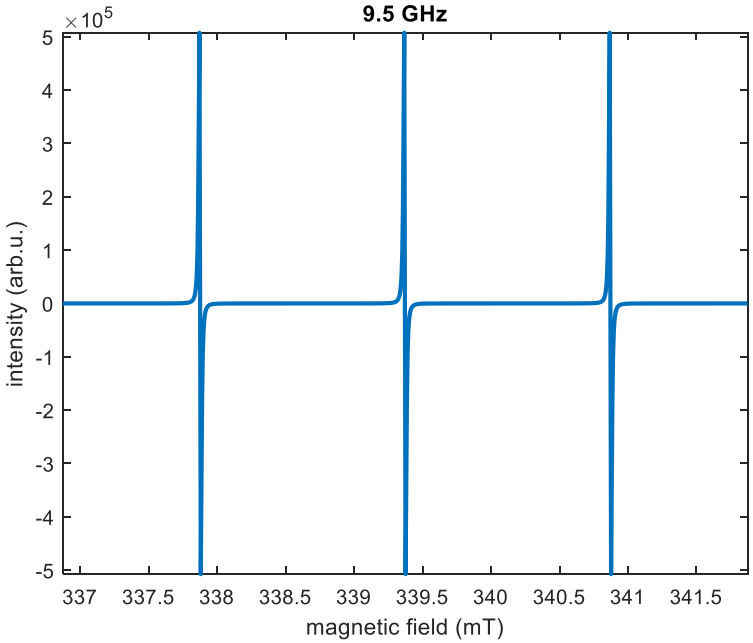


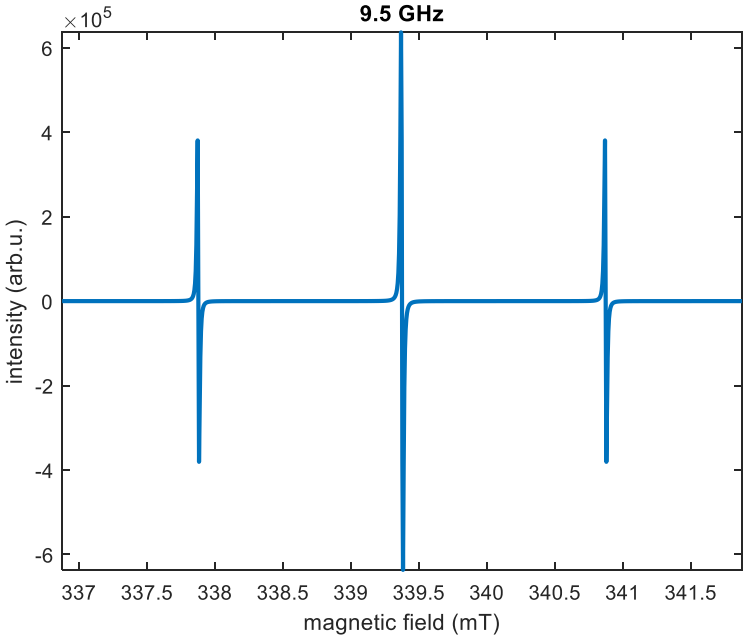
tetrathiatriarylmethyl radical (TAM)



1990's Nycomed

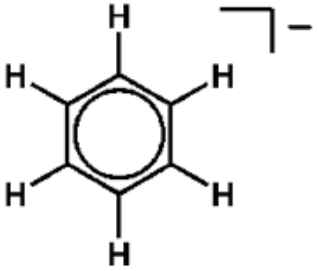




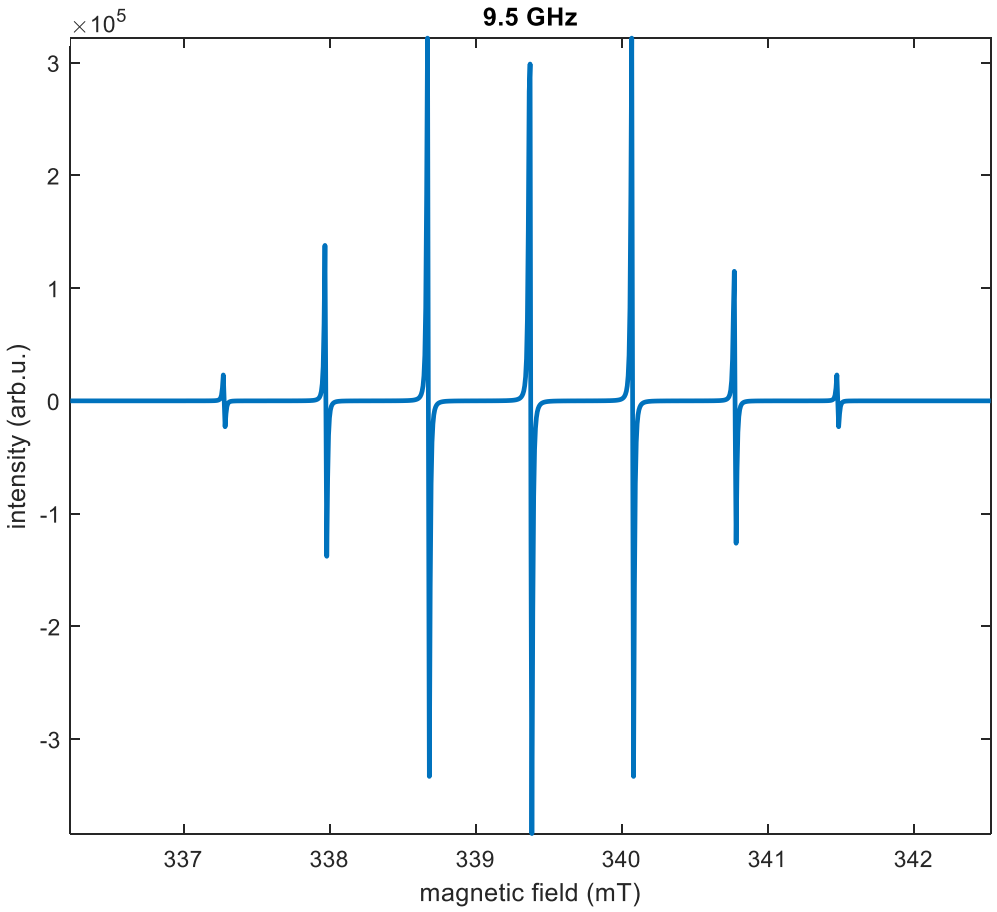


HF-Kopplung zu
1 ^{14}N Stickstoff Kern (I=1)

HF-Kopplung zu
2 äqivalente Protonen (I=1/2)

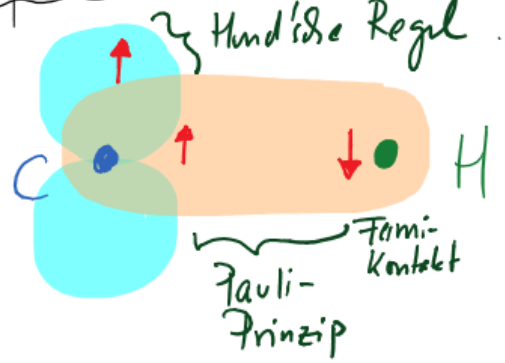


Benzol Anion Radikal



Spinpolarisation

Spinpolarisation bei π-Radikalen



Das ungepaarte e^--Spin im π-Orbital ist bevorzugt parallel zu dem nahen e^--Spin im σ-Orbital

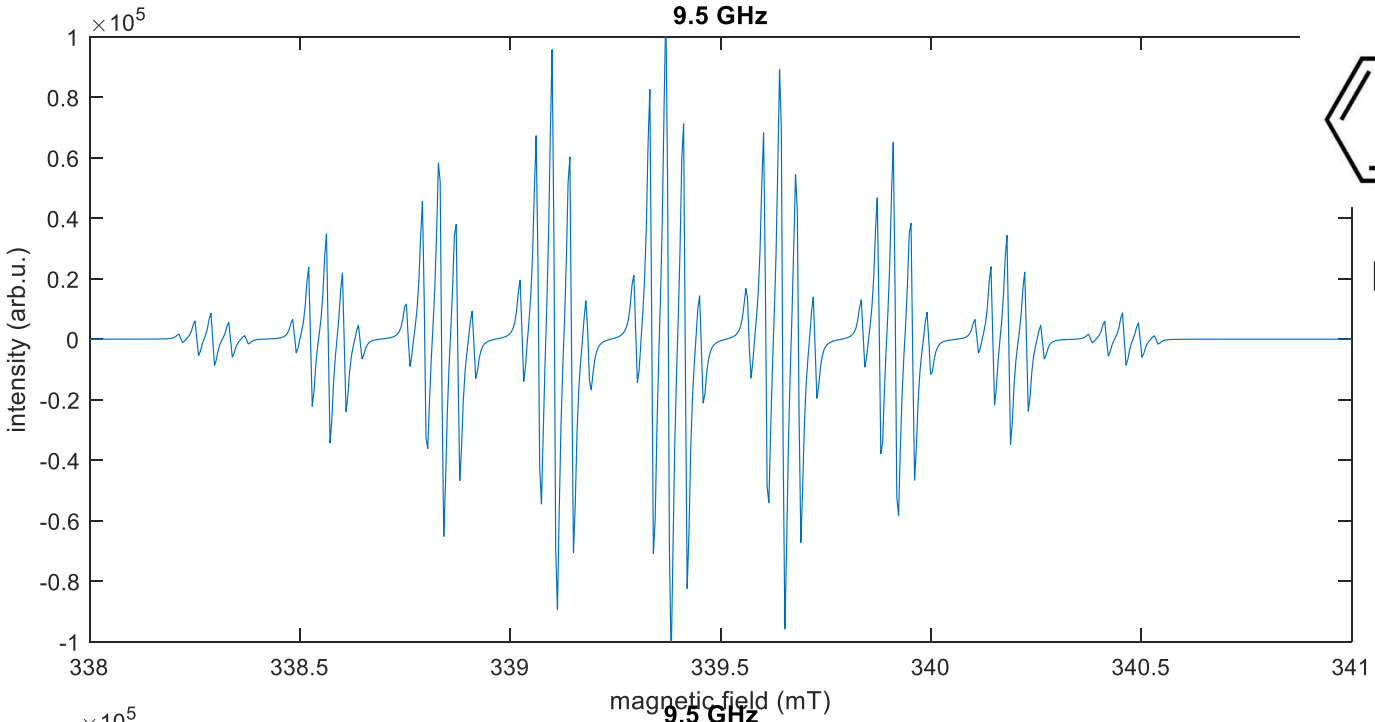
↳ $a_{iso}^{H} \neq 0$ {obwohl $\psi_\pi(H) = 0$}

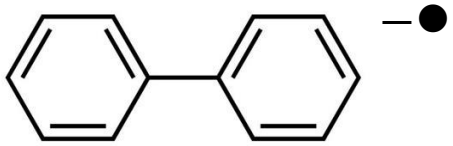
McConnell Beziehung

$$a_{iso}(H) = Q \cdot \underbrace{\rho(C)}_{\text{ungepaarte Elektronenspin-Dichte}}$$

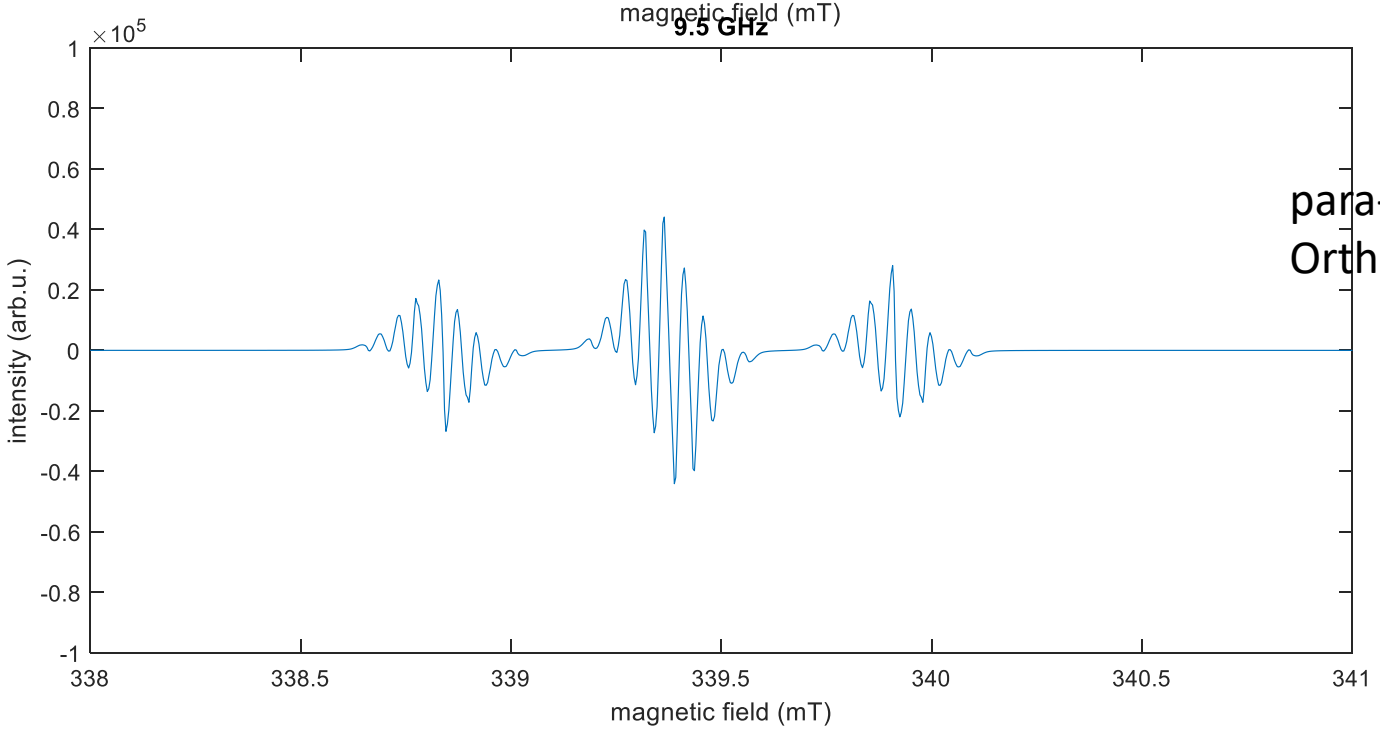
Q: McConnell-Faktor $\approx 2.3\ mT$

$\rho(C)$ z. Bsp. aus Hückel MO-Theorie
oder direkt aus QC-Berechnungen (Gaussian, ORCA)

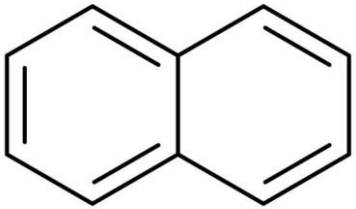




Biphenyl Anion Radikal



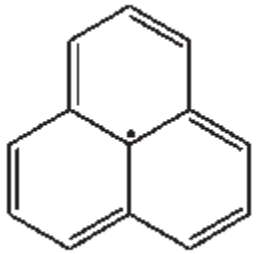
para-H
Ortho/meta-D

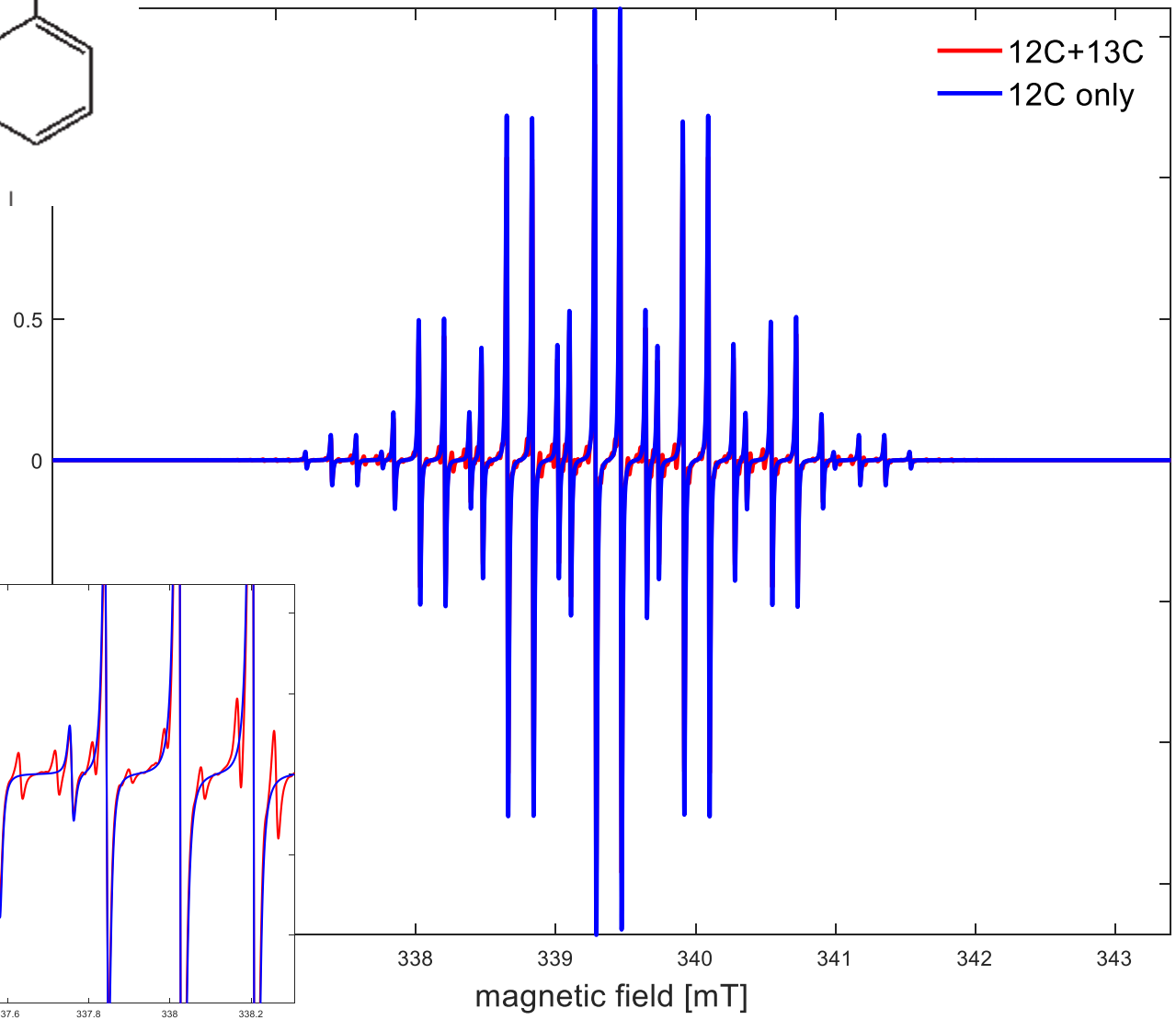


Napthalene

radical anion
radical cation
337
337.5
338
338.5
339
339.5
340
340.5
341
341.5
342
magnetic field [mT]

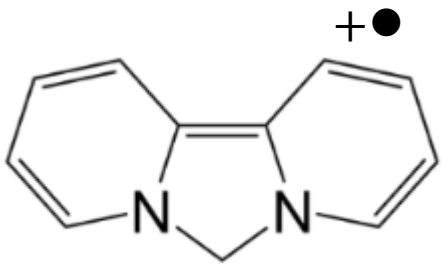
Phenalenyl Radikal

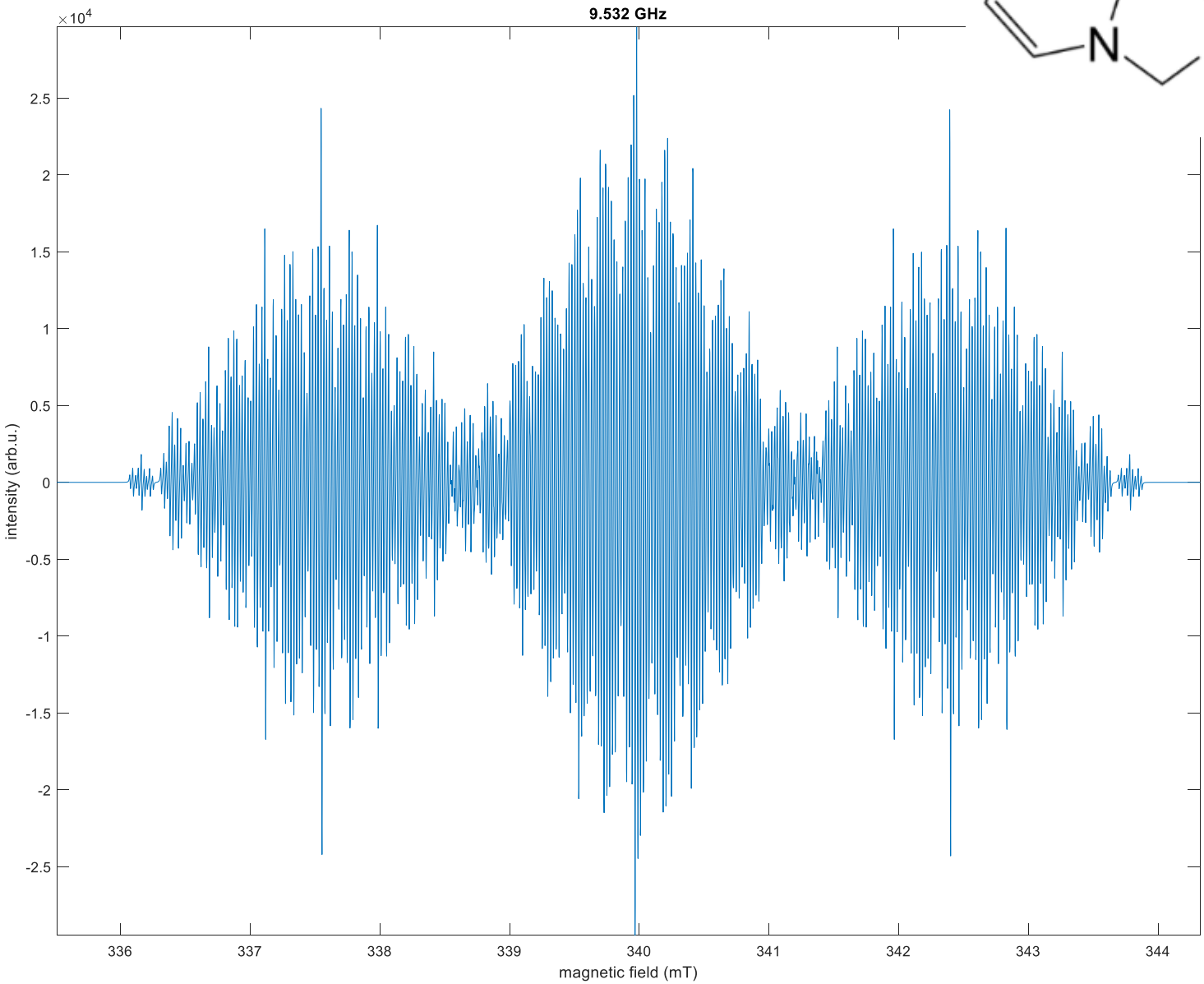




Biaryl cation radical (6-hydrodipyrido[1,2-c:2',1'-e]-imidazole)

$$N=\prod\left(2n_J \cdot I_J + 1\right) = 5 \cdot 3 \cdot 3 \cdot 3 \cdot 3 \cdot 3 = 972$$

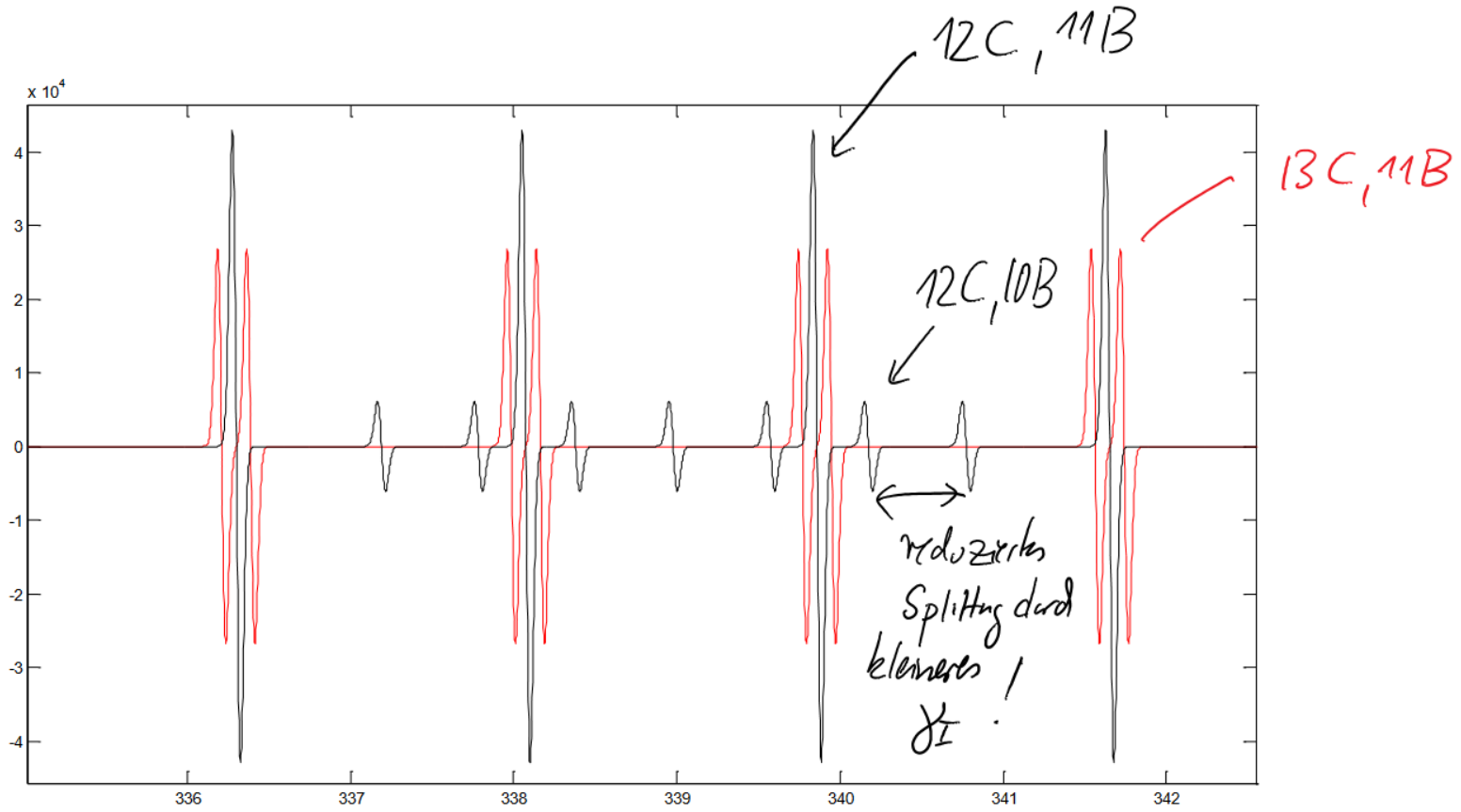




Isotopen-Signaturen

Beispiel: **B** 19.9% ^{10}B (I=3, $\frac{\gamma_I}{\gamma_S} = -1.6\ 10^{-4}$) 80.1% ^{11}B (I=3/2, $\frac{\gamma_I}{\gamma_S} = -4.9\ 10^{-4}$)

C 1.07% ^{13}C (I=1/2, $\frac{\gamma_I}{\gamma_S} = -3.8\ 10^{-4}$)



Easy-Spin

Free Simulation Software for EPR

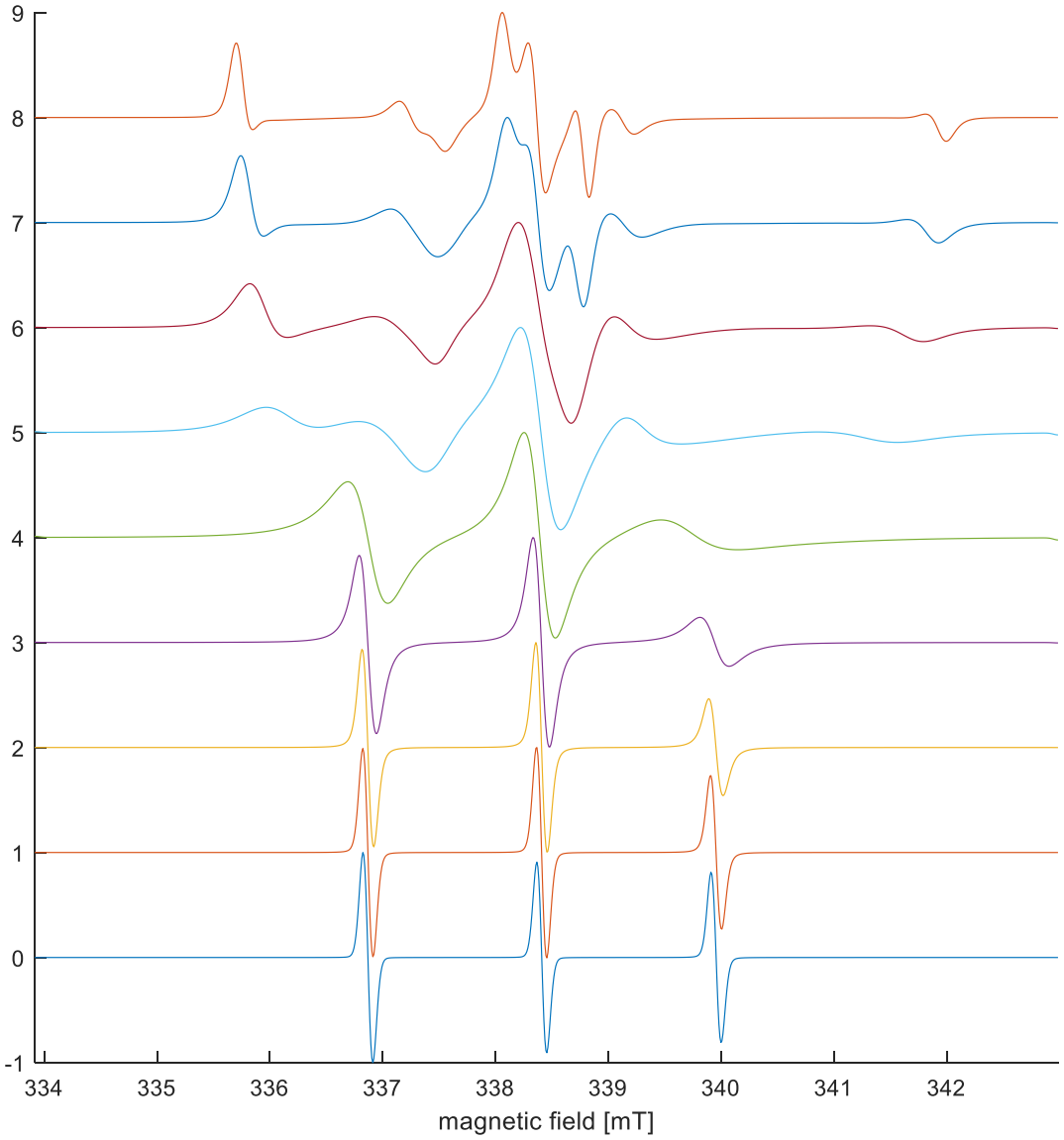
EasySpin - EPR spectrum simulation

https://easyspin.org

Auf Matlab basierend

Stefan Stoll
University of Washington
Seattle, USA

Nitroxide Radikal bei unterschiedlich viskosen Lösemitteln

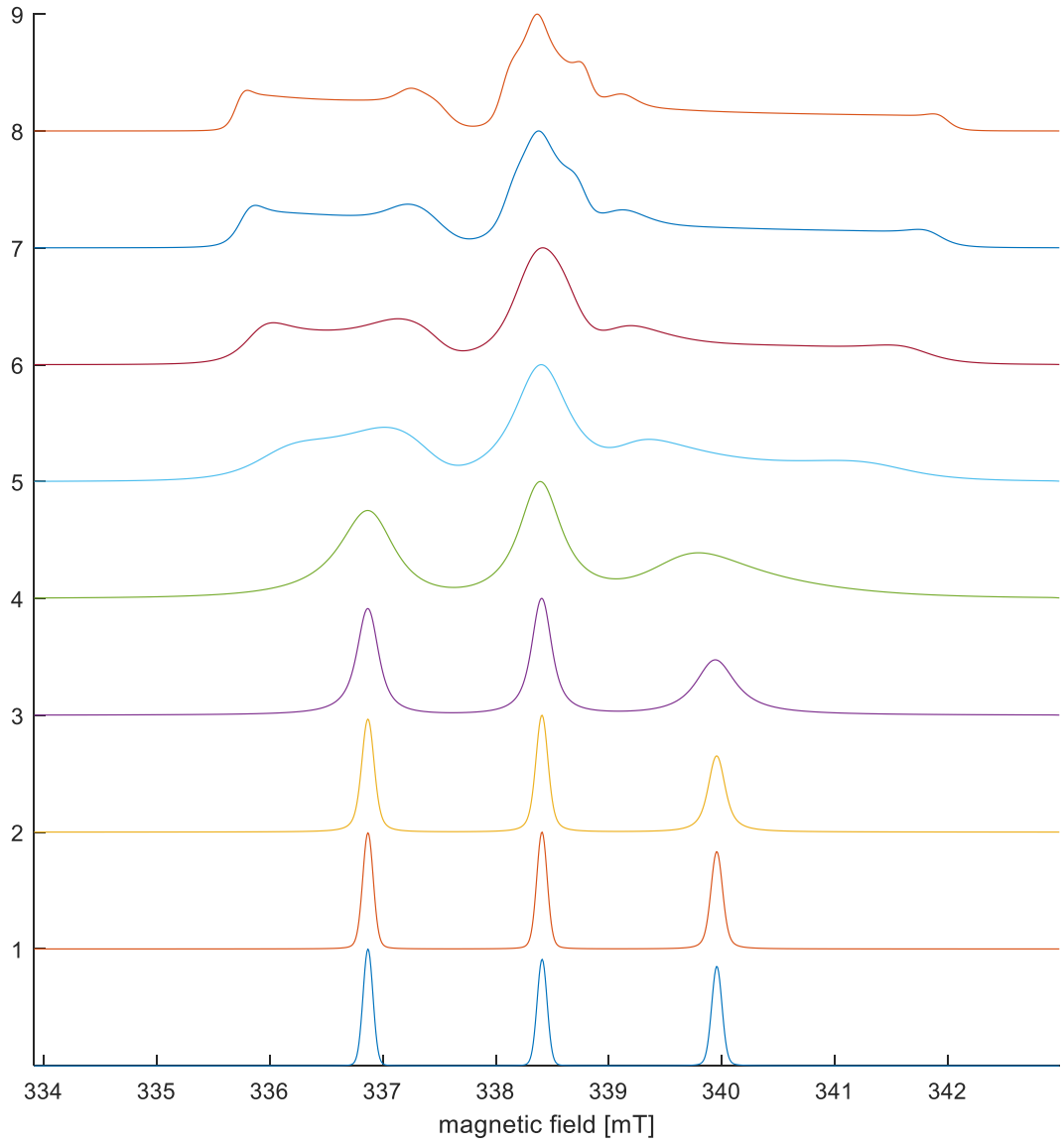


$\tau_R = 300\ ns$

$\tau_R = \frac{V\ \eta}{k_B T}$

$\tau_R = 30\ ps$

Nitroxide Radikal bei unterschiedlich viskosen Lösemitteln



$\tau_R = 300\ ns$

$\tau_R = \frac{V\ \eta}{k_B T}$

$\tau_R = 30\ ps$