240 GHz TR-EPR spectra calculated for different degrees of molecular biaxiality.

In Figure 1 we report calculated spectra at 240GHz, obtained considering the director ***n*** parallel to the Z_{ZFS} axis, ε=2 and increasing values of the biaxiality parameter λ. Spectra a-c correspond to the director parallel to the magnetic field, while for spectra d-f the director is perpendicular to the magnetic field. The spectra in Figure 1a,d refer to uniaxial distribution, λ =0.0; in Figure 1b,e to biaxial distribution with λ=0.7; in Figure 1c,f the same as before but with a negative value of the biaxiality parameter λ =-0.7. The biaxiality determines the relative intensity of the spectral features corresponding to the tensor components less aligned to the director, in this case X_{ZFS} and Y_{ZFS}. Changing the sign of λ is equivalent to exchanging the X and Y axes in the molecular frame.

Table 1: values of the Saupe tensor for the spectra in figure 1

Spectrum	ε	λ	S_{XX}^{ZFS}	S_{YY}^{ZFS}	S_{ZZ}^{ZFS}
a), d)	2.0	0.0	-0.22	-0.22	0.44
b), e)	2.0	0.7	-0.02	-0.33	0.35
c), f)	2.0	-0.7	-0.33	-0.02	0.35

Parameters for the simulation: *D = 554 MHz, E = 38 MHz,* g_{xx} *= 2.00105,* g_{yy} *= 2.00160,* g_{zz} *= 2.00215,* p_x *= 0.93,* p_y *= 0.07,* p_z *= 0.00,* $\Omega_g = \Omega_{ZFS} = (0°,0°,0°)$ [see Scheme 2 of the article].

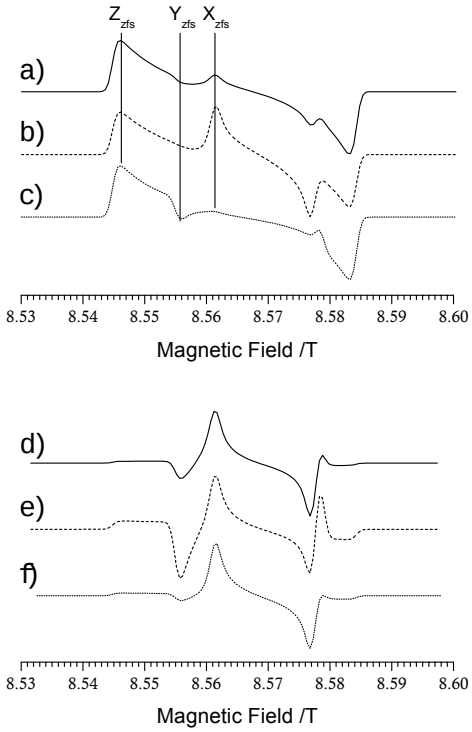

Fig.1. Calculated TR-EPR spectra at 240GHz, with ε= 2 and different values of λ, see table 1. Spectra a-c correspond to B_0 parallel to the director, spectra d-f to B_0 perpendicular to the director.