

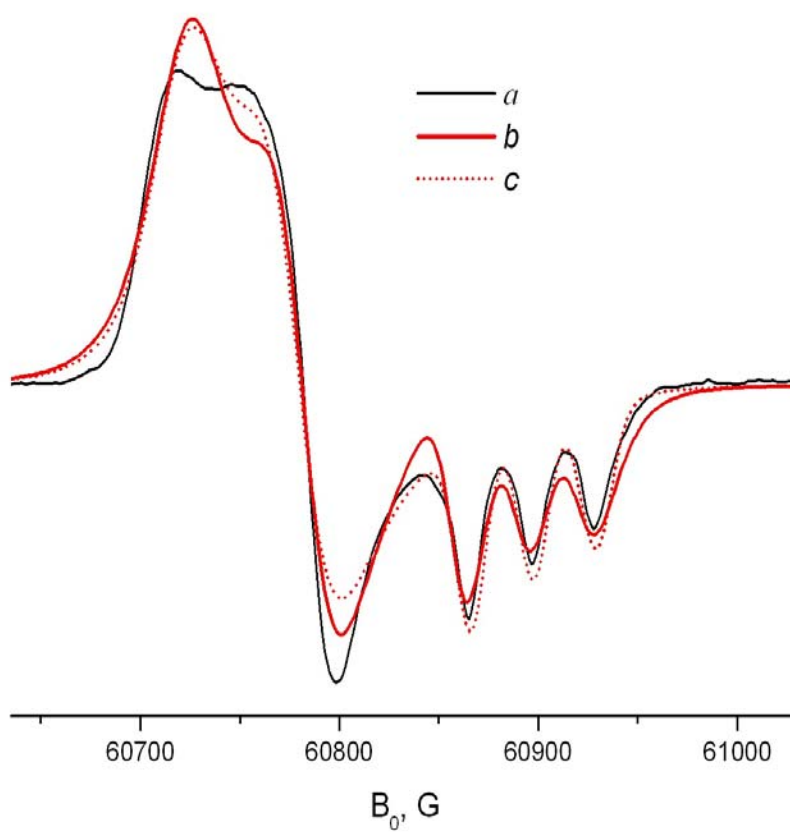
Supplemental material:

For Fig. 5. Simulations for 5-sasl in γ -CD at 293K (*a*) using different models. Simple anisotropic rotation (*b*) with $R_{\perp} = 2.5 \cdot 10^7 \text{s}^{-1}$; $R_{\parallel} = 1.7 \cdot 10^8 \text{s}^{-1}$ and MOMD (*c*) with $R_{\perp} = 1 \cdot 10^8 \text{s}^{-1}$; $R_{\parallel} = 1.7 \cdot 10^8 \text{s}^{-1}$, $C_{20} = 10$

For Fig. 10. Simulations for TEMPOyl- caprylate in β -CD at different temperatures (*a*, experiment) using models of simple anisotropic rotation (*b*) and MOMD (*c*). The simulation parameters are:

260K: $R_{\perp} = 2.5 \cdot 10^7 \text{s}^{-1}$; $R_{\parallel} = 1 \cdot 10^9 \text{s}^{-1}$ (simple model); $R_{\perp} = 1.6 \cdot 10^8 \text{s}^{-1}$; $R_{\parallel} = 1 \cdot 10^9 \text{s}^{-1}$, $C_{20} = 8$ (MOMD). 200K: $R_{\perp} = 1 \cdot 10^7 \text{s}^{-1}$; $R_{\parallel} = 5.6 \cdot 10^8 \text{s}^{-1}$ (simple model); $R_{\perp} = 1.4 \cdot 10^8 \text{s}^{-1}$; $R_{\parallel} = 5.6 \cdot 10^8 \text{s}^{-1}$, $C_{20} = 10$ (MOMD). 140K: $R_{\perp} = 4 \cdot 10^6 \text{s}^{-1}$; $R_{\parallel} = 1.7 \cdot 10^8 \text{s}^{-1}$ (simple model); $R_{\perp} = 1 \cdot 10^8 \text{s}^{-1}$; $R_{\parallel} = 1.7 \cdot 10^8 \text{s}^{-1}$, $C_{20} = 10$, $C_{20} = 5$ (MOMD).

Supplement – simulations for Fig. 5



Supplement - simulations for Fig . 10

