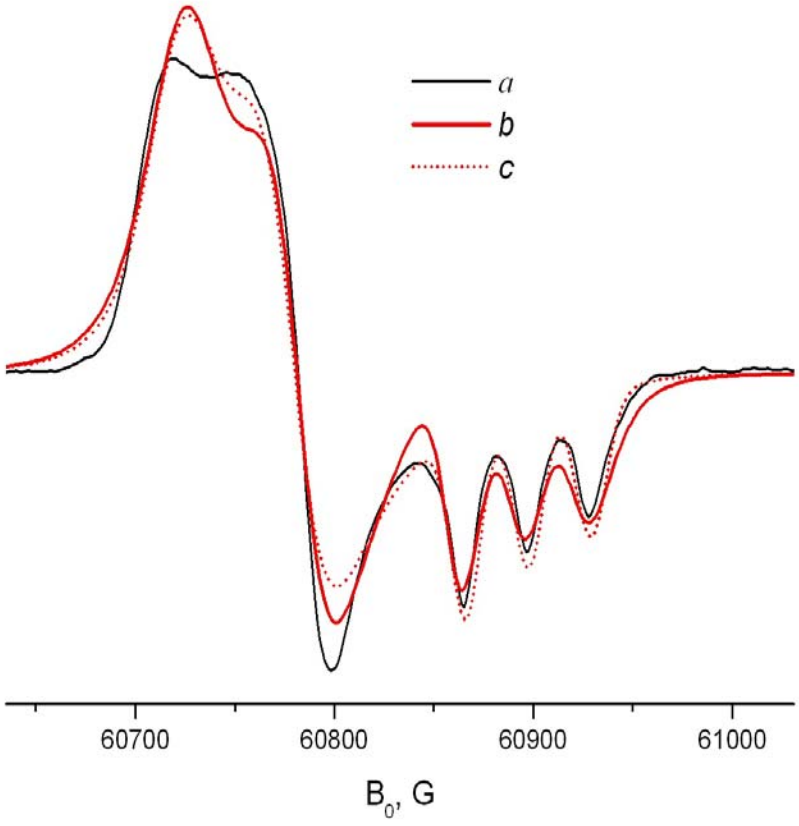
Supplemental material:

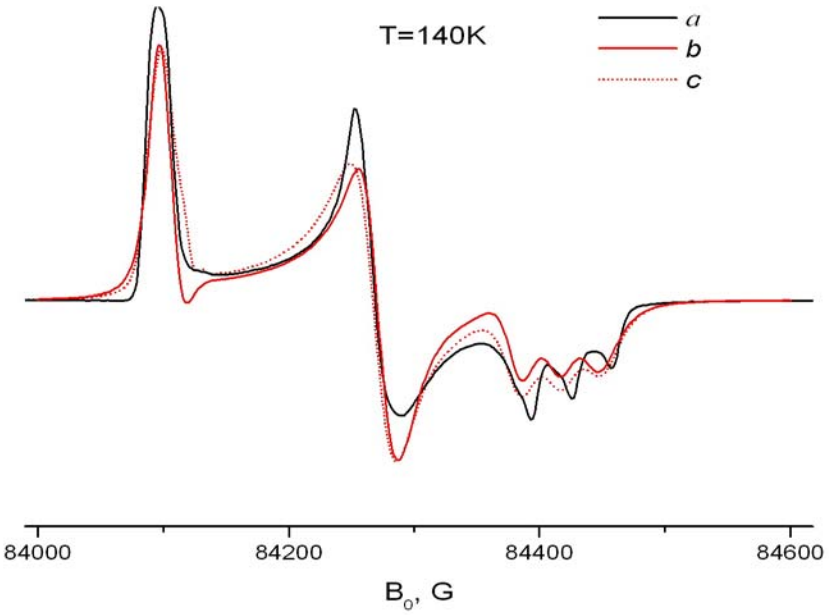
For Fig. 5. Simulations for 5-sasl in γ-CD at 293K (*a*) using different models. Simple anisotropic rotation (*b*) with $R_\perp = 2.5 \cdot 10^7 s^{-1}$; $R_\parallel = 1.7 \cdot 10^8 s^{-1}$ and MOMD (*c*) with $R_\perp = 1 \cdot 10^8 s^{-1}$; $R_\parallel = 1.7 \cdot 10^8 s^{-1}$, $C_{20}=10$

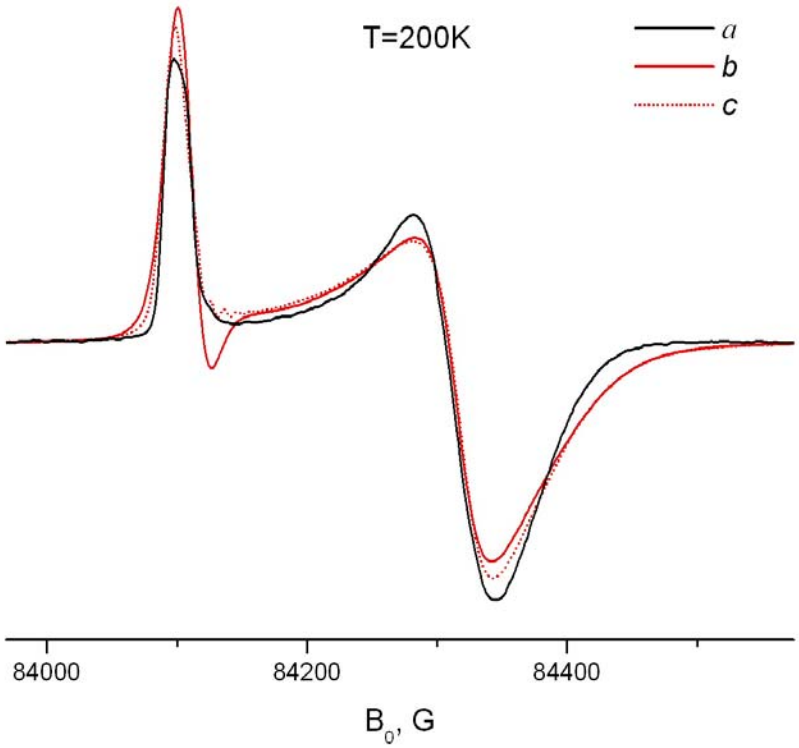
For Fig. 10. Simulations for TEMPOyl- caprylate in β-CD at different temperatures (*a*, experiment) using models of simple anisotropic rotation (*b*) and MOMD (*c*). The simulation parameters are:
260K: $R_\perp = 2.5 \cdot 10^7 s^{-1}$; $R_\parallel = 1 \cdot 10^9 s^{-1}$ (simple model); $R_\perp = 1.6 \cdot 10^8 s^{-1}$; $R_\parallel = 1 \cdot 10^9 s^{-1}$, $C_{20}=8$ (MOMD). 200K: $R_\perp = 1 \cdot 10^7 s^{-1}$; $R_\parallel = 5.6 \cdot 10^8 s^{-1}$ (simple model); $R_\perp = 1.4 \cdot 10^8 s^{-1}$; $R_\parallel = 5.6 \cdot 10^8 s^{-1}$, $C_{20}=10$ (MOMD). 140K: $R_\perp = 4 \cdot 10^6 s^{-1}$; $R_\parallel = 1.7 \cdot 10^8 s^{-1}$ (simple model); $R_\perp = 1 \cdot 10^8 s^{-1}$; $R_\parallel = 1.7 \cdot 10^8 s^{-1}$, $C_{20}=10$, $C_{20}=5$ (MOMD).

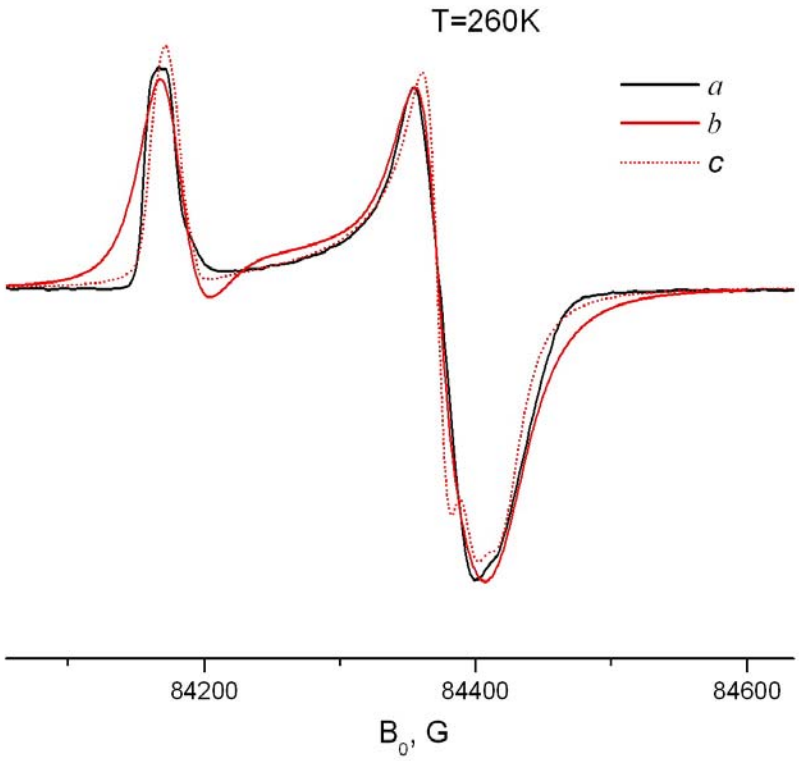
Supplement – simulations for Fig. 5



Supplement - simulations for Fig . 10






T=260K
a
b
c
84200
84400
84600
B0, G