Supporting information of publication: On the Role of Internal Degrees of Freedom in Structural Relaxation of Ring–Tail Structured Liquids Across Temperature Regimes

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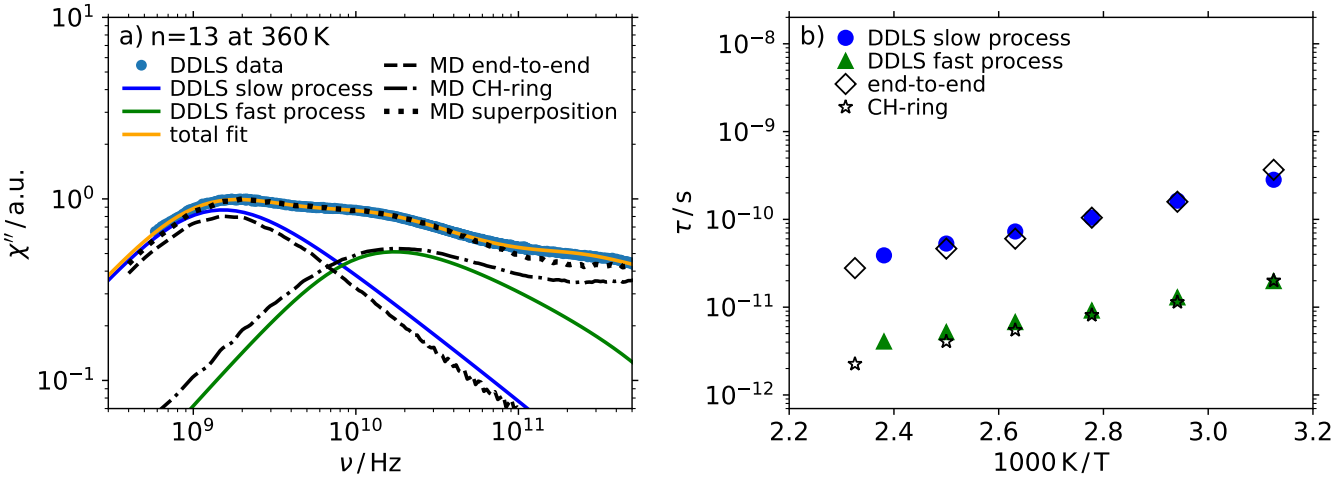

FIG. 1: a) DDLS spectrum of 1-phenyltridecane ($n = 13$) at 360 K. Solid blue and green curves are the model functions of the fitting procedure of ref. 1 and the solid orange curve is the total fit function. The dashed and dashed-dotted curves represent the susceptibilities obtained from Fourier-Laplace transformation of the second rank orientational correlation function from MD simulation of the end-to-end vector (MD end-to-end) as well as the averaged correlation function of the CH-vectors (MD CH-ring) in the phenyl ring. The dotted curve is the superposition of the MD susceptibilities scaled in amplitude and shifted along the frequency axis by the same factor. b) Relaxation times of the slow (solid blue dots) and the fast (solid green triangles) contribution to the DDLS relaxation peak and MD simulations (open symbols).

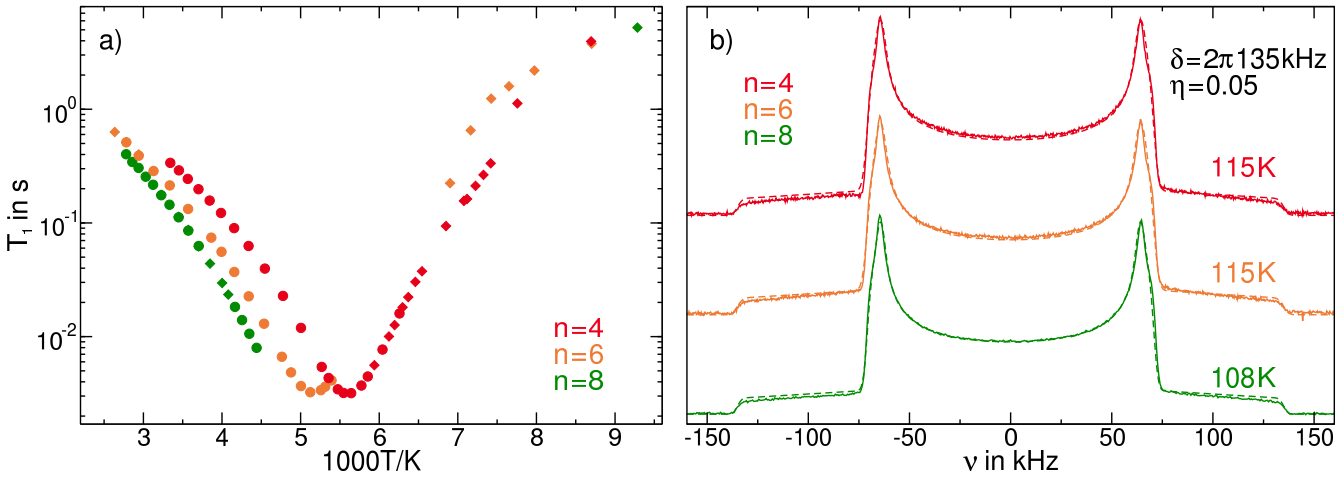

FIG. 2: ^{2}H NMR measurements of ring labeled 1-phenylalkanes with different chain length n. a) SLR times T_1 at different temperatures. Different symbols discriminate between inversion recovery (circles) and saturation recovery (diamonds) experiments. The $n = 4$ sample was measured at a Larmor frequency of 46.7 MHz while $n = 6, 8$ were measured at 46.1 MHz. b) ^{2}H NMR spectra recorded at temperatures below T_g. The indicated anisotropy parameters δ and asymmetry parameters η obtained from fits with Pake spectra (dashed lines) are in agreement with literature data of C—D bonds in phenyl rings [2] and were used to calculate $\tau(T)$ from $T_1(T)$.

[1] R. Zeißler, F. Pabst, T. Böhmer and T. Blochowicz, *Phys. Chem. Chem. Phys.*, 2023, **25**, 16380–16388.
[2] E. Rössler and H. Sillescu, *Chem. Phys. Lett.*, 1984, **112**, 94–98.