

CHEMPHYSICHEM

Supporting Information

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End-to-End Distance Determination in a Cucurbit[6]uril-Based Rotaxane by PELDOR Spectroscopy**

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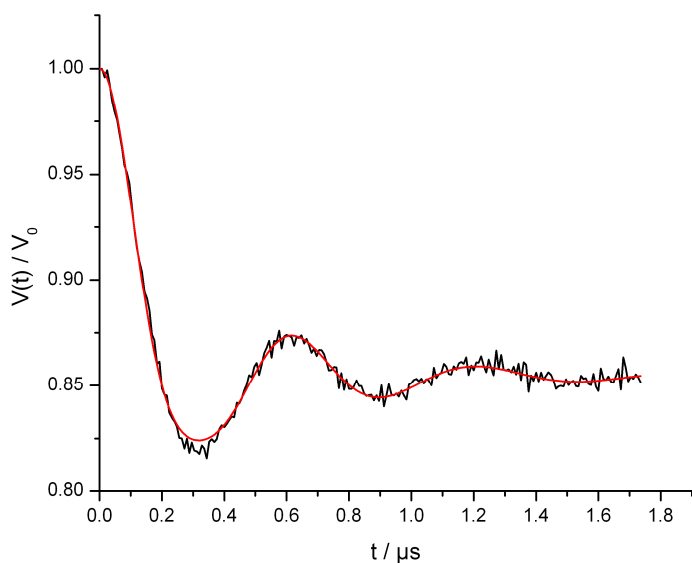


Figure S1 Background-corrected time-domain trace of **1** at 40K (black) and simulation (red)

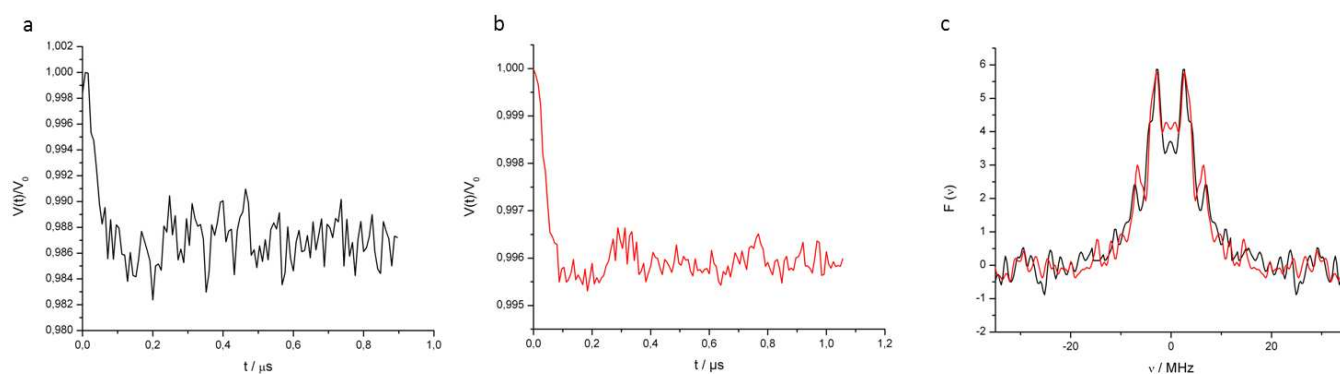


Figure S2. Background-corrected time-domain data for **2** carried out at (a) 9-GHz (black line) and (b) 34-GHz (red line). (c) Comparison of the Pake patterns obtained after Fourier transformation of the signal in (a) and (b) (in black and red, respectively).

PELDOR data collection at 34-GHz. The pulse EPR measurements of **2** at Q band (mw frequency 34 GHz) were performed with a Bruker Eleksys E580 X/Q-band spectrometer (with the 3 W output power upgrade for Q band) with a EN 5107D2 Q-band EPR/ENDOR probehead. The ELDOR pulse (ν_{pump} , 36 ns) was positioned at the maxima of the echo-detected nitroxide spectrum, whereas the frequency of the observer pulses (ν_{obs} , 16 and 32 ns) was decreased by 50 MHz. The amplitude of the observer pulses was adjusted to optimize refocused echo. The PELDOR trace was recorded with an experiment repetition time of 8 ms, a video amplifier bandwidth of 20 MHz and an amplifier gain of 27 dB. τ_1 was set to 300 ns and τ_2 to 1800 ns. The signal was accumulated with 245 data points giving an approximate measurement time of 17h. Traces were acquired using a two-step phase cycle for baseline correction. The PELDOR traces were processed and analyzed by using DeerAnalysis2010 software package.

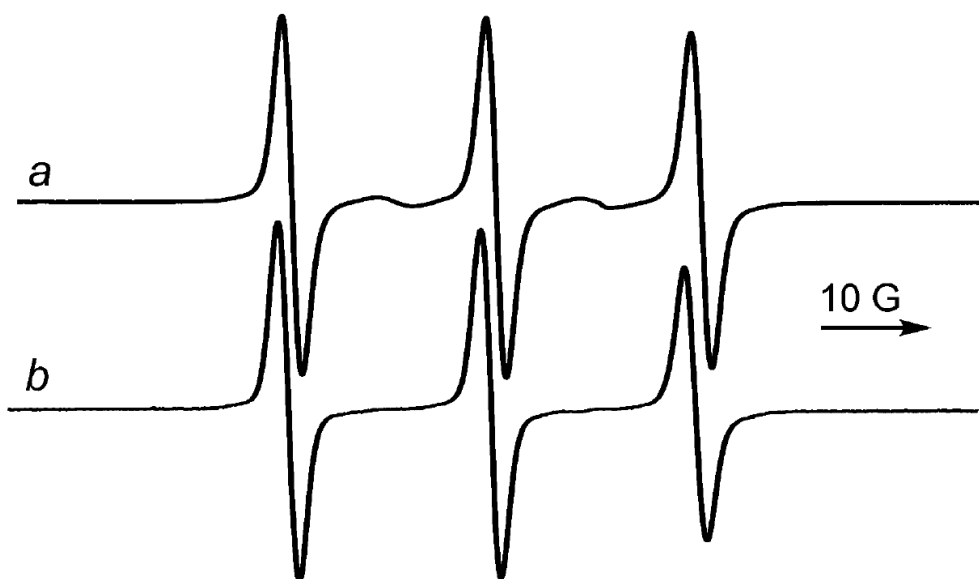


Figure S3. X-band CW-ESR spectra of free thread **2** (a) and rotaxane **1** (b) in water at 340 K (from Ref. 13).

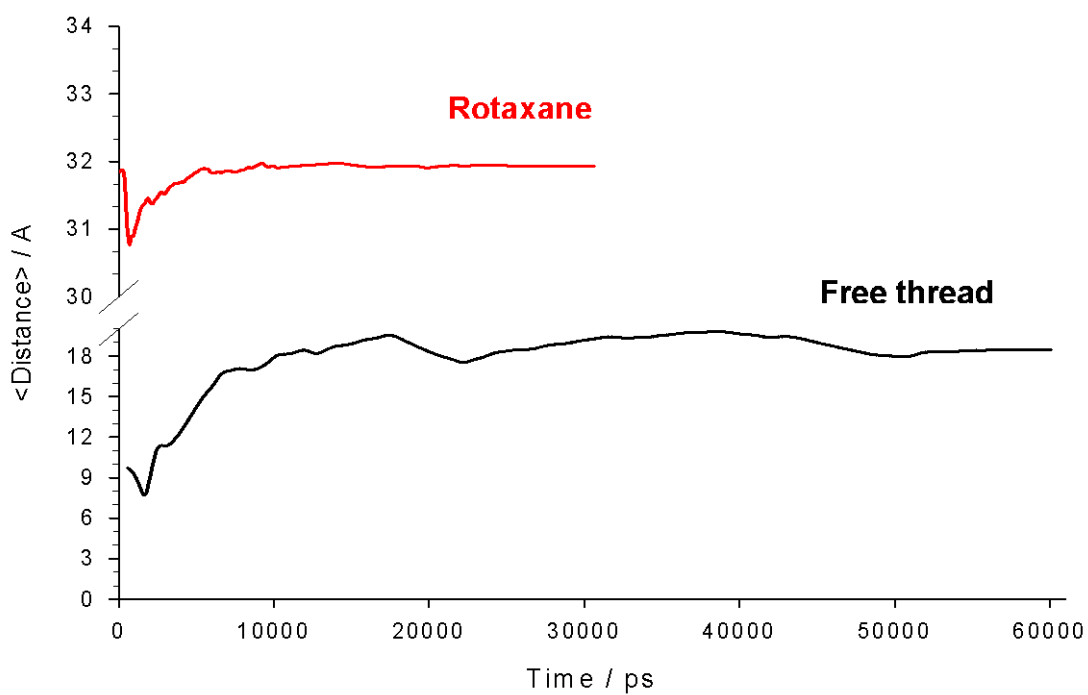


Figure S4. Variation of spin labels mean distance during MD simulation.