Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information

The effect of temperature on internal dynamics of dansylated POPAM dendrimers

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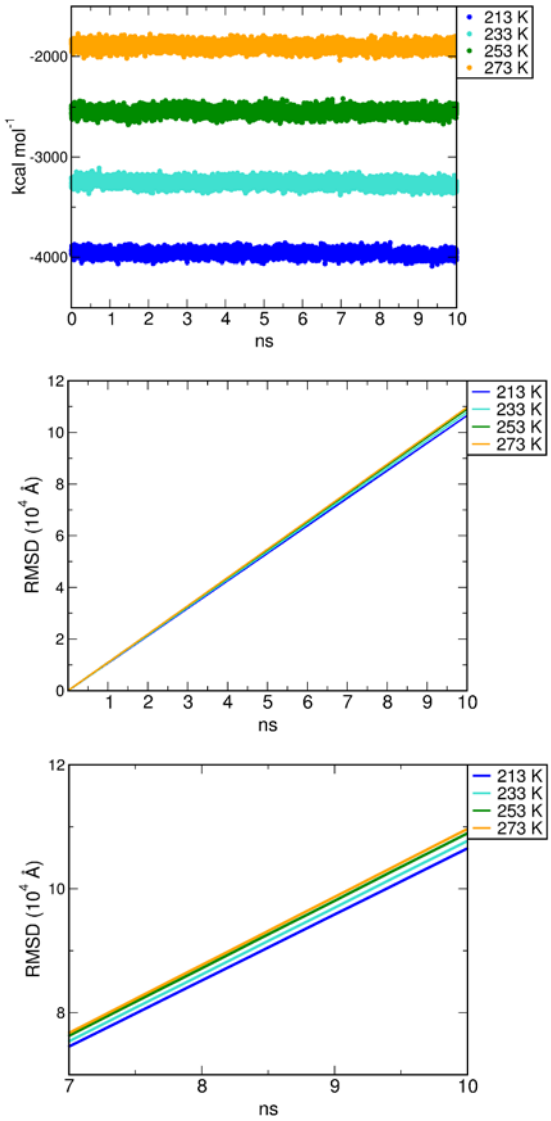

Figure S1. Time evolution of the potential energy (top) and of the Root Mean Square Displacement (RMSD, middle) of the simulated systems (G4+1728 $CHCl_3$) as a function of the considered temperature. The bottom panel reports a close up of the RMSD graph (middle) in the 7-10 ns window.

Table S1. The χ^2 values for all fits showed in Table 1.

		Emission		Anisotropy decay		
	T (K)	lifetime (ns)	χ^2	t_1 (ns)	t_2 (ns)	χ^2
G1	213	16.0	$2.54*10^{-5}$		1.58 (100 %)	1.10*10-^{4}
	233	15.3	$2.59*10^{-5}$		1.00 (100 %)	$6.65*10^{-5}$
	253	14.5	$2.93*10^{-5}$		0.63 (100 %)	$5.85*10^{-5}$
	273	13.9	$3.01*10^{-5}$		0.42 (100 %)	$5.34*10^{-5}$
	293	13.6	$2.69*10^{-5}$		0.30 (100 %)	$5.26*10^{-5}$
G2	213	15.8	$2.94*10^{-5}$	0.61 (24 %)	4.29 (76 %)	$1.02*10^{-4}$
	233	15.1	$3.13*10^{-5}$	0.45 (25 %)	2.47 (75 %)	$8.77*10^{-5}$
	253	14.5	$2.78*10^{-5}$	0.37 (31 %)	1.63 (69 %)	$7.39*10^{-5}$
	273	13.8	$3.92*10^{-5}$	0.36 (43 %)	1.21 (57 %)	$6.96*10^{-5}$
	293	13.6	$3.56*10^{-5}$	0.42 (72 %)	1.17 (28 %)	$5.02*10^{-5}$
G3	213	16.0	$2.34*10^{-5}$	0.85 (21 %)	9.24 (79 %)	$1.50*10^{-4}$
	233	15.3	$2.75*10^{-5}$	0.56 (23 %)	5.11 (77 %)	$1.05*10^{-4}$
	253	14.7	$3.30*10^{-5}$	0.46 (34 %)	3.17 (66 %)	$8.17*10^{-5}$
	273	14.0	$4.02*10^{-5}$	0.35 (33 %)	2.05 (67 %)	$7.26*10^{-5}$
	293	13.7	$4.14*10^{-5}$	0.34 (44 %)	1.48 (56 %)	$6.60*10^{-5}$
G4	213	15.9	$3.18*10^{-5}$	2.09 (23 %)	19.1 (77 %)	$8.13*10^{-4}$
	233	15.2	$3.70*10^{-5}$	1.46 (28 %)	11.1(72 %)	$2.96*10^{-4}$
	253	14.5	$4.51*10^{-5}$	0.94 (33 %)	6.54 (67 %)	$1.85*10^{-4}$
	273	13.7	$5.68*10^{-5}$	0.54 (36 %)	4.02 (64 %)	$1.33*10^{-4}$
	293	13.2	$6.24*10^{-5}$	0.40 (44 %)	2.61 (56 %)	$1.02*10^{-4}$

Table S2. The χ^2 values for all fits showed in Table 2.

		Emission lifetime (ns)			
	T (K)	Dansyl	χ^2	Eosin	χ^2
G2-eosin	213	15.0	$4.32*10^{-5}$	2.7	$3.00*10^{-5}$
	253	13.6	$5.37*10^{-5}$	2.5	$2.72*10^{-5}$
	293	13.1	$4.34*10^{-5}$	2.2	$3.05*10^{-5}$
G3-eosin	213	15.0	$9.86*10^{-5}$	1.5	$1.70*10^{-4}$
	253	13.9	$9.26*10^{-5}$	1.6	$2.08*10^{-4}$
	293	13.5	$6.88*10^{-5}$	1.4	$3.60*10^{-4}$
G4-eosin	213	15.3	$7.55*10^{-5}$	1.4	$3.04*10^{-4}$
	253	13.8	$7.94*10^{-5}$	1.3	$2.64*10^{-4}$
	293	13.3	$6.24*10^{-5}$	1.2	$2.33*10^{-4}$