

Supporting Information

Orientational Relaxation of Poly(propylene
imine) Dendrimers at Different pH

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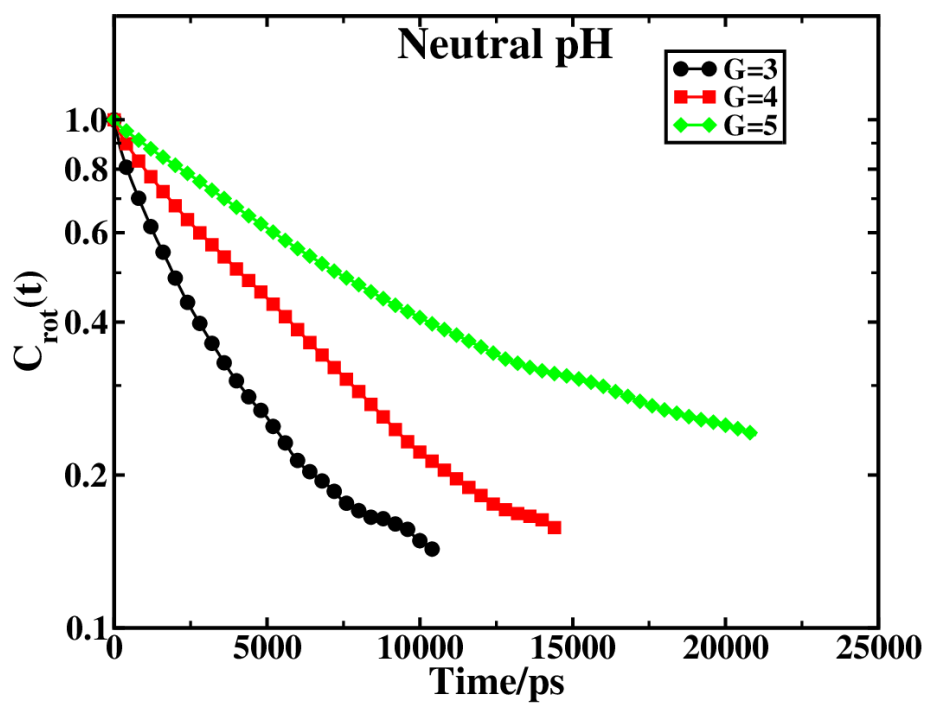


Figure S1: Semi-logarithmic plot of rotational autocorrelation function (ACF) as a function of time for DAB-dendr- $(NH_2)_x$ at neutral pH.

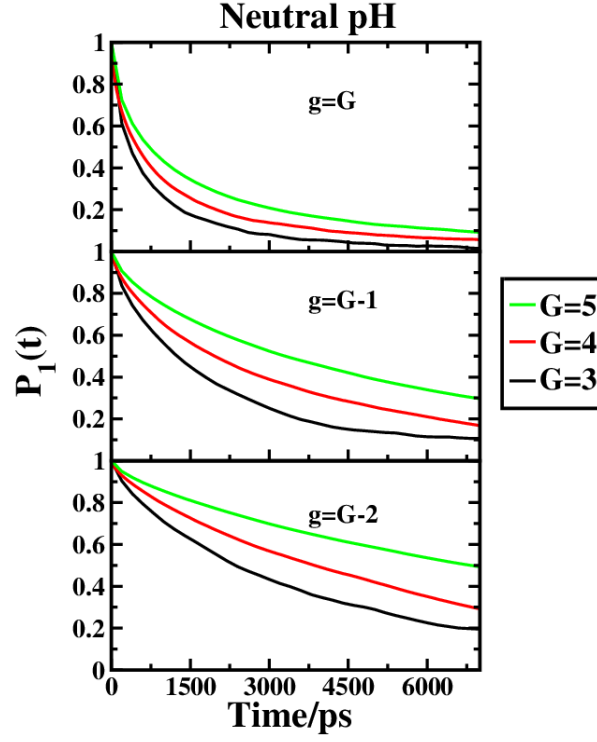


Figure S2: $P_1(t)$ as a function of time for the segments of the generations, $g = G$, $g = G - 1$, and $g = G - 2$ for $G = 3$ to $G = 5$ dendrimers at neutral pH.

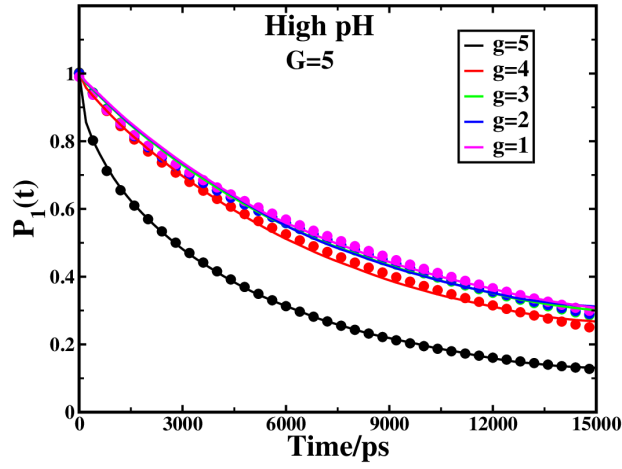


Figure S3: $P_1(t)$ as a function of time for $G = 5$ DAB-dendr- $(NH_2)_x$ at high pH.

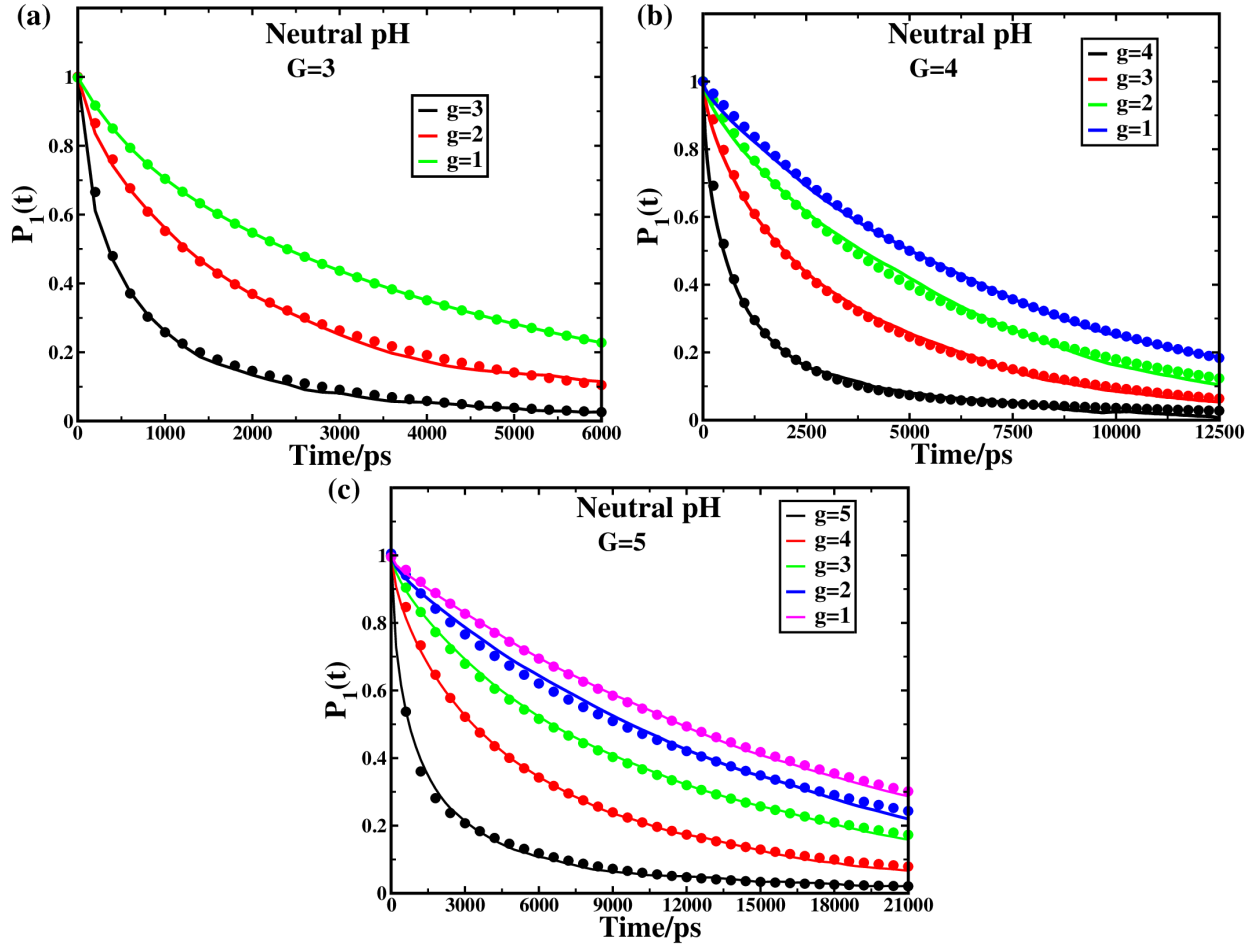


Figure S4: $P_1(t)$ as a function of time for (a) $G = 3$, (b) $G = 4$, and (c) $G = 5$ DAB-dendr- $(NH_2)_x$ at neutral pH condition.

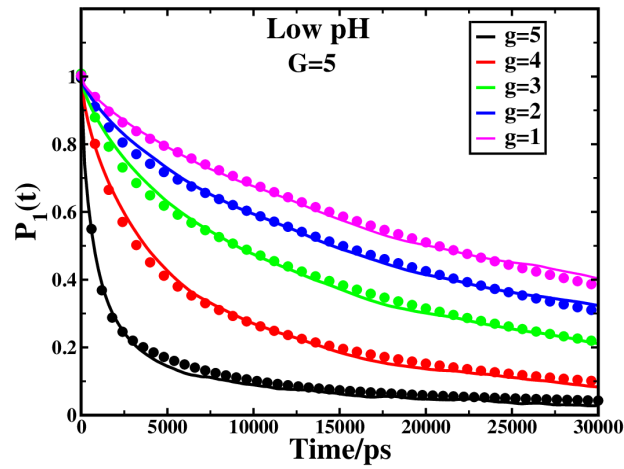


Figure S5: $P_1(t)$ as a function of time for $G = 5$ DAB-dendr- $(NH_2)_x$ at low pH condition.

Table S1: The approximation of $P_1(t)$ by a sum of three exponential terms at high pH. τ_r^G is the rotational time of the dendrimer as a whole, τ_{in} is the characteristic time corresponding to the local small-scale (segmental) mobility, and τ_{br} is the pulsation time for a dendrimer branch. C_r , C_{in} , and C_{br} are the relative amplitudes of the characteristic times τ_r^G , τ_{in} , and τ_{br} , respectively.

Generation	g	τ_r^G/ps	C_r	τ_{in}/ps	C_{in}	τ_{br}/ps	C_{br}
$G = 3$	3	2660	0.03	280	0.32	1755	0.65
	2		0.13	1100	0.11	1994	0.76
	1		0.10	1100	0.13	2000	0.77
$G = 4$	4	6597.6	0.045	300.4	0.275	3287.4	0.68
	3		0.09	1150	0.18	5191.5	0.73
	2		0.11	1150	0.13	5200	0.76
	1		0.10	1147	0.13	5715.9	0.77
$G = 5$	5	23094	0.13	410	0.25	5804	0.62
	4		0.16	1350	0.11	10000	0.73
	3		0.16	1350	0.11	11500	0.73
	2		0.15	1350	0.12	11914	0.73
	1		0.175	1300	0.105	12000	0.72

Table S2: The approximation of $P_1(t)$ by a sum of three exponential terms at neutral pH. τ_r^G is the rotational time of the dendrimer as a whole, τ_{in} is the characteristic time corresponding to the local small-scale (segmental) mobility, and τ_{br} is the pulsation time for a dendrimer branch. C_r , C_{in} , and C_{br} are the relative amplitudes of the characteristic times τ_r^G , τ_{in} , and τ_{br} , respectively.

Generation	g	τ_r^G/ps	C_r	τ_{in}/ps	C_{in}	τ_{br}/ps	C_{br}
$G = 3$	3	5780	0.035	300	0.61	1850	0.355
	2		0.10	580	0.31	2800	0.59
	1		0.18	600	0.16	4318	0.66
$G = 4$	4	9684	0.10	320	0.42	1420	0.48
	3		0.16	800	0.26	3700	0.58
	2		0.23	1000	0.08	5105.5	0.69
	1		0.27	1000	0.01	6631	0.72
$G = 5$	5	29053	0.03	547	0.63	4561	0.34
	4		0.11	1350	0.27	6596.5	0.62
	3		0.23	1350	0.13	8952	0.64
	2		0.25	1350	0.07	12234	0.68
	1		0.28	1250	0.01	14578	0.71

Table S3: The approximation of $P_1(t)$ by a sum of three exponential terms at low pH. τ_r^G is the rotational time of the dendrimer as a whole, τ_{in} is the characteristic time corresponding to the local small-scale (segmental) mobility, and τ_{br} is the pulsation time for a dendrimer branch. C_r , C_{in} , and C_{br} are the relative amplitudes of the characteristic times τ_r^G , τ_{in} , and τ_{br} , respectively.

Generation	g	τ_r^G/ps	C_r	τ_{in}/ps	C_{in}	τ_{br}/ps	C_{br}
$G = 3$	3	4630	0.03	300	0.59	1980	0.38
	2		0.04	661	0.35	3200	0.61
	1		0.21	600	0.10	3945	0.69
$G = 4$	4	13278	0.04	300	0.51	2234	0.45
	3		0.115	950	0.205	3590.7	0.68
	2		0.17	1250	0.10	5206.7	0.73
	1		0.225	1250	0.015	6807	0.76
$G = 5$	5	39793	0.09	608	0.67	4995	0.24
	4		0.18	1700	0.44	9100	0.38
	3		0.35	1500	0.24	14000	0.41
	2		0.40	1500	0.16	22835	0.44
	1		0.43	1250	0.09	30356	0.48

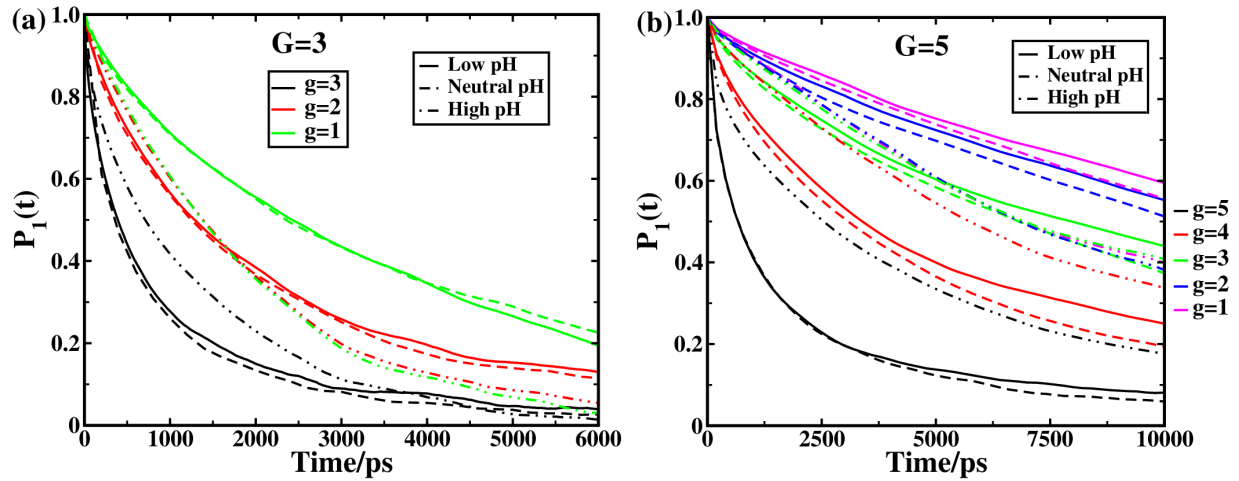


Figure S6: $P_1(t)$ as a function of time for generations (a) $G = 3$ and (b) $G = 5$ of PPI dendrimer at all three pH conditions.

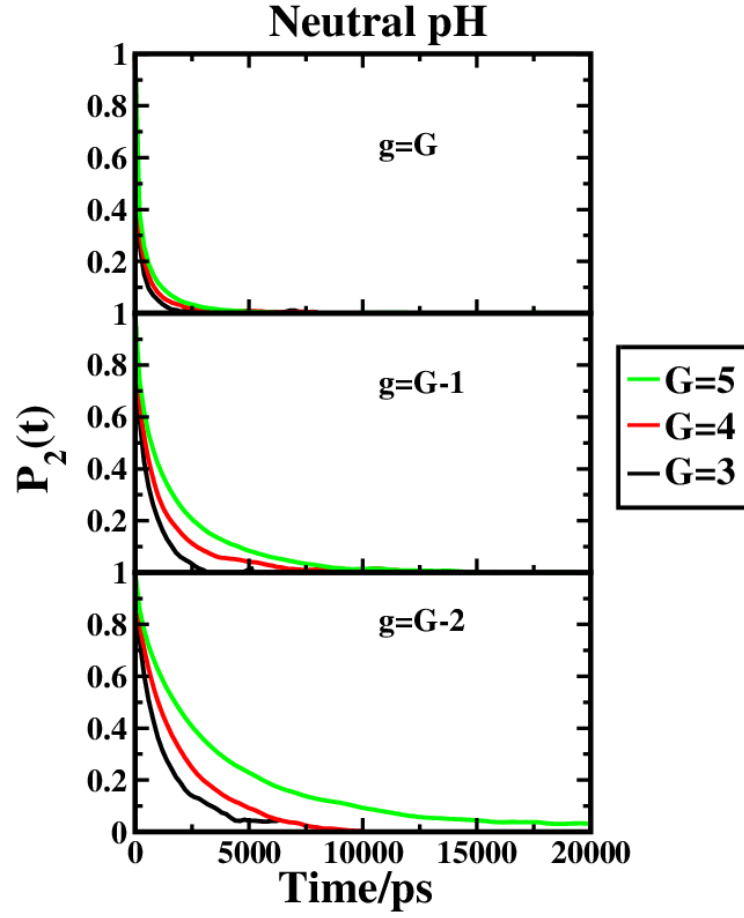


Figure S7: Second-order orientational ACF, $P_2(t)$ as a function of time for the terminal and various inner generations of DAB-dendr- $(NH_2)_x$ at neutral pH.

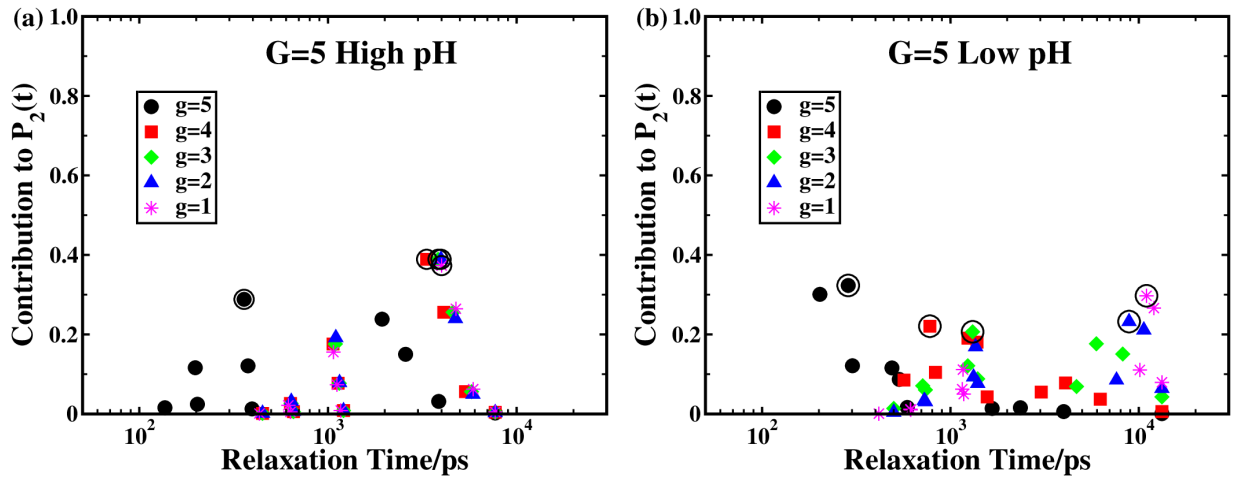


Figure S8: Contributions of the normal modes and their characteristic times to $P_2(t)$ for generation $G = 5$ at (a) high pH, and (b) low pH conditions.

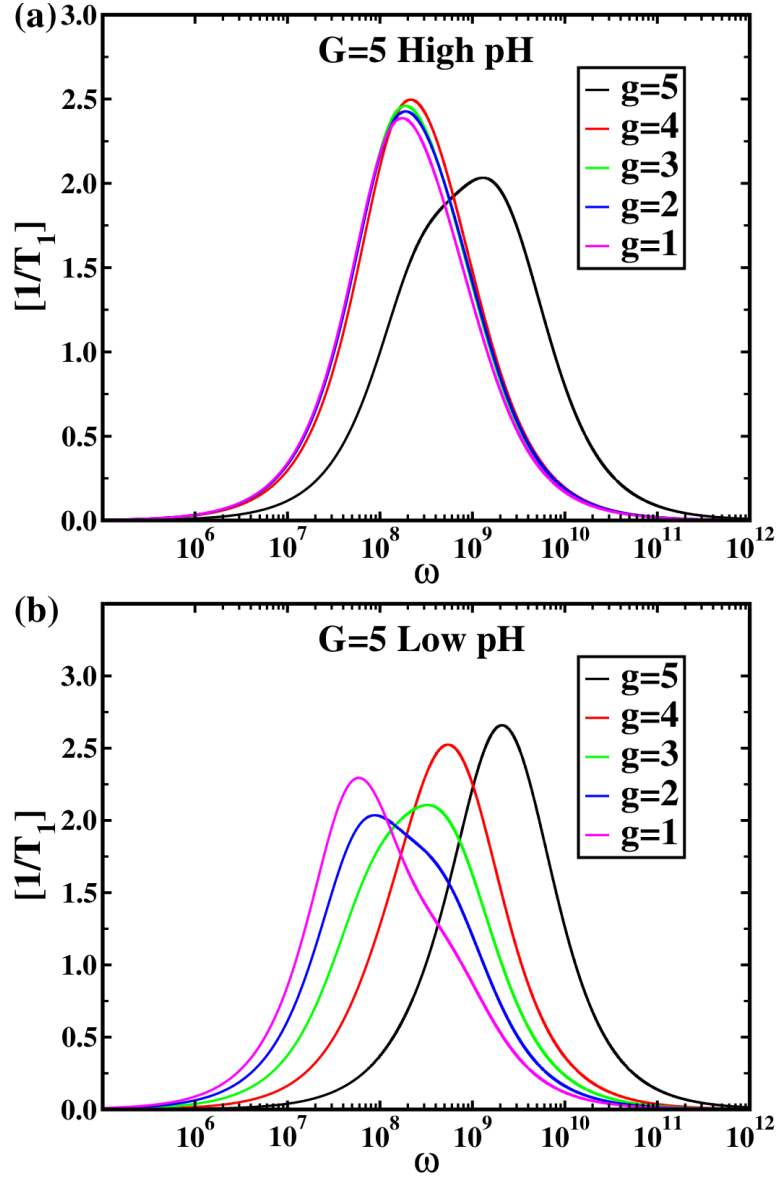


Figure S9: Semi-logarithmic plot of the spin-lattice relaxation rate, $1/T_1$, as a function of frequency, ω , for generation $G = 5$ at (a) high pH and at (b) low pH conditions. g indicates the inner generation for a particular generation G of the dendrimer.