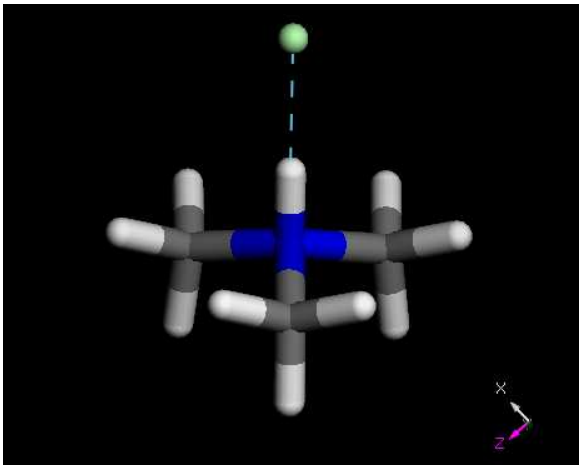
Supporting Information for "PAMAM Dendrimers Undergo pH Responsive Conformational Changes without Swelling" (Yi Liu, Vyacheslav S. Bryantsev, Mamadou S. Diallo, and William A. Goddard III*)

Figures S1-S3: New force field Dreiding III

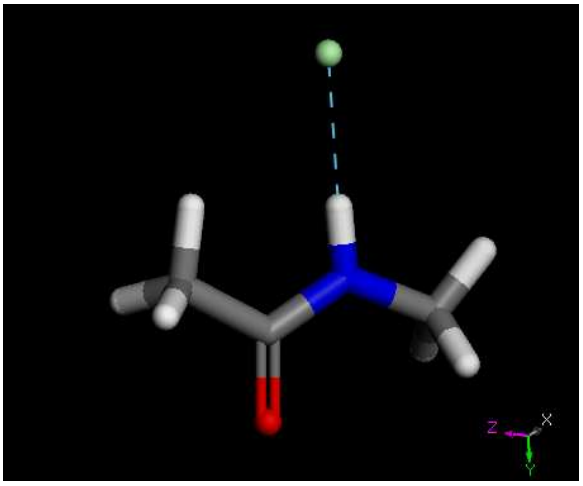
Figures S4-S5: Thermodynamics properties (energy, temperature and pressure etc.) from MD simulations

Figures S6-S10: SASA and SEV analyses

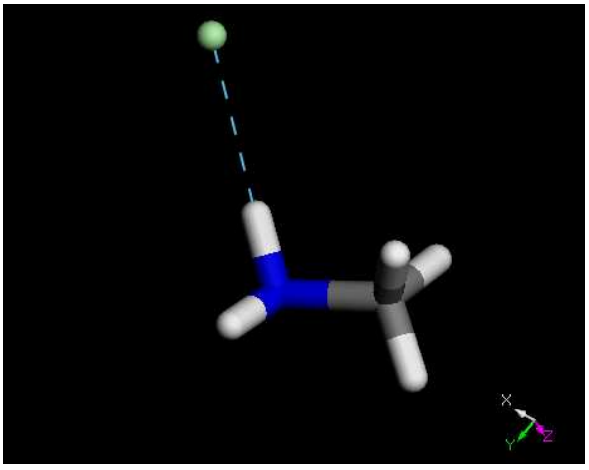
(a)



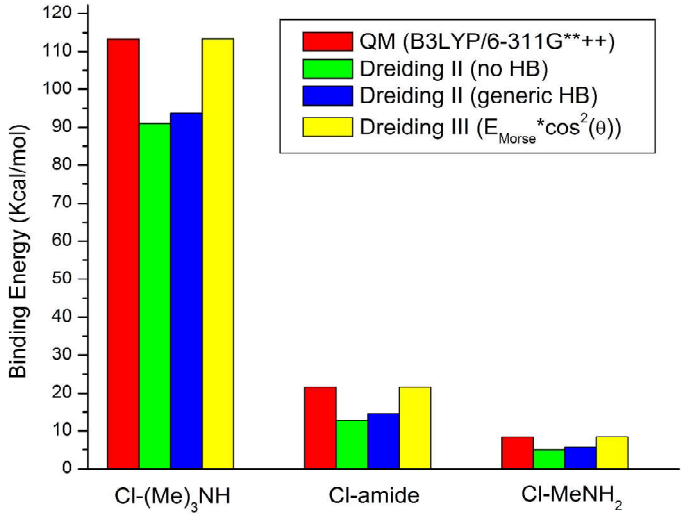
(b)



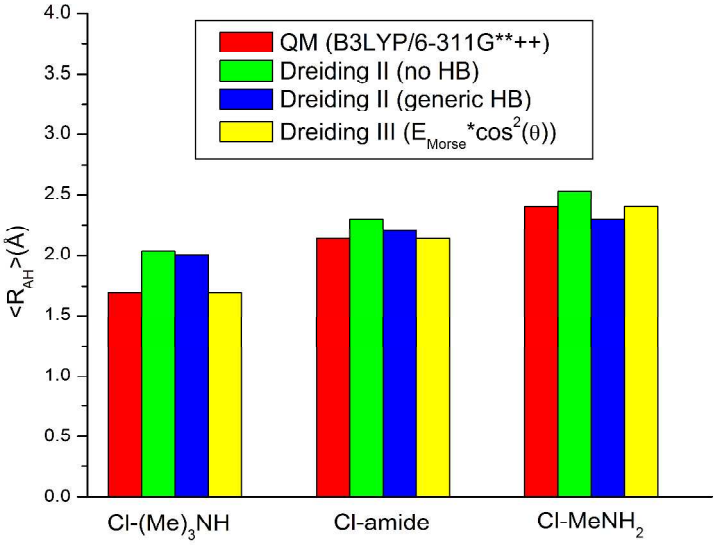
(c)



S1. Hydrogen bond complex of Cl^- with a (a) tertiary amine, (b) amide and (c) primary amine.



(a)



(b)

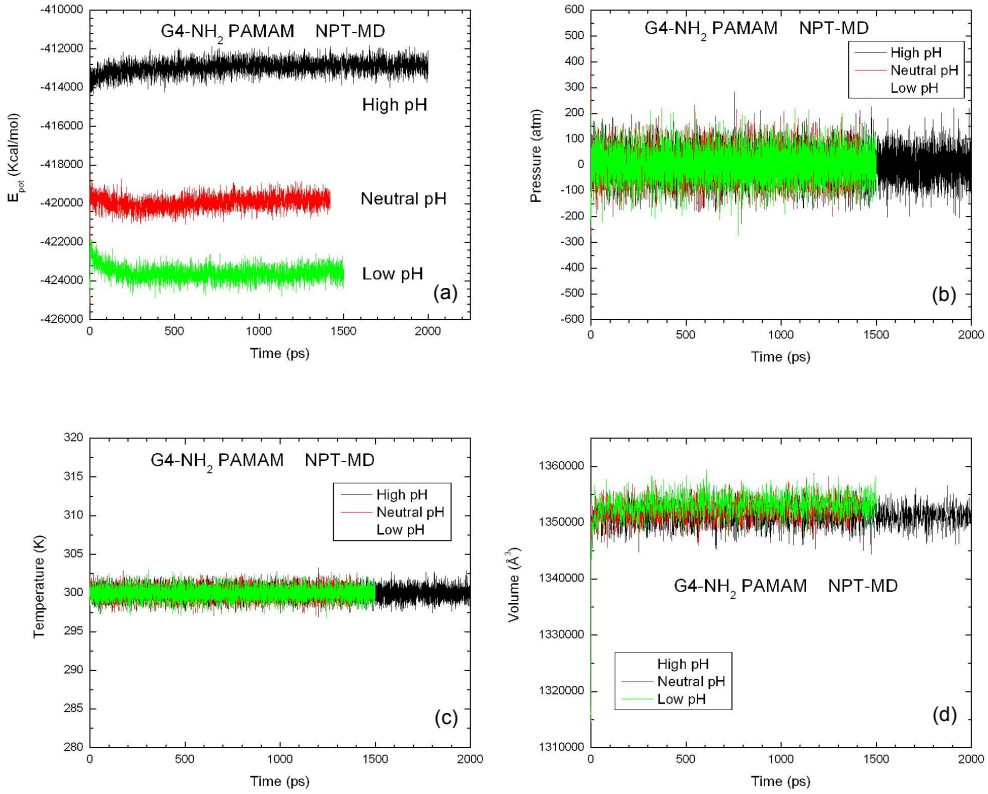
S2. (a) Binding energies and (b) distances between hydrogen bond acceptor Cl^- and donor H^+ of primary amine, tertiary amine and amide calculated using QM, old Dreiding II FF (with and without HB), and new Dreiding III FF.

S3. New hydrogen bond term in Drieding III force field:

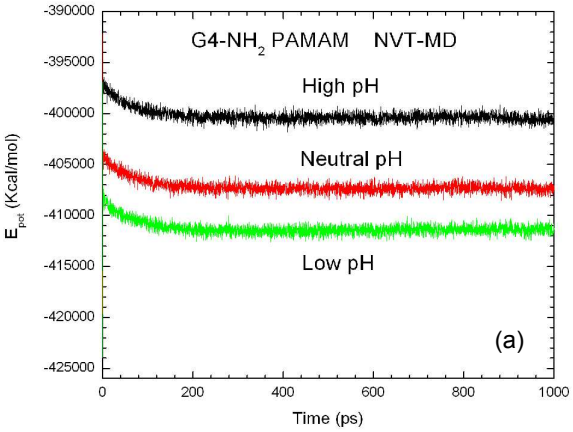
$$E_{HB}(R,\theta) = E_{Morse}(R)\cos^2(\theta) = D_0(\chi^2 - 2\chi)\cos^2(\theta)$$

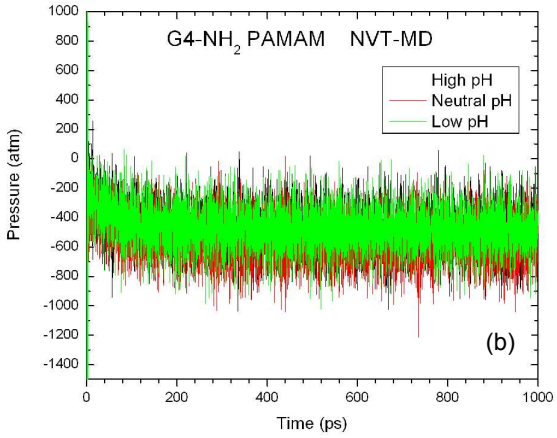
$$\text{where } \chi = \exp[\frac{\gamma}{2}(1-\frac{R}{R_0})],\ \gamma = 10$$

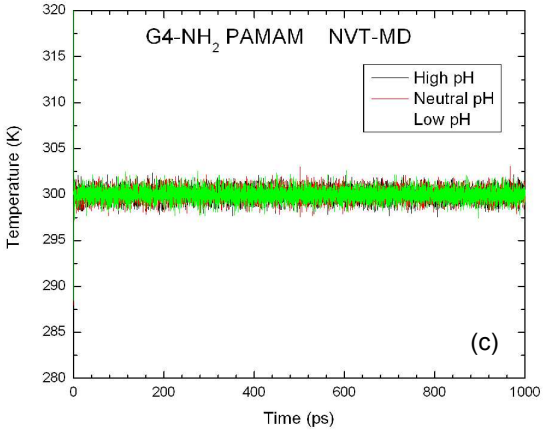
HB complex (Donor-H-Acceptor)	D_0 (Kcal/mol)	R_0 (Å)
N_3H -H___A-Cl	3.2300	3.5750
N_3P -H___A-Cl	10.0000	2.9795
N_3HP-H___A-Cl	7.6000	3.2750
N_R -H___A-Cl	5.6000	3.2650
N_3H -H___A-O_3F	1.3100	3.4100
N_3P -H___A-O_3F	2.2100	3.1200
N_3HP-H___A-O_3F	1.2200	3.2000
N_R -H___A-O_3F	1.3800	3.1700
O_3F -H_F -O_2	1.3300	3.1500
N_3H -H___A-O_2	1.2500	3.4050
N_3P -H___A-O_2	8.3800	2.7700
N_3HP-H___A-O_2	8.5600	2.6350
N_R -H___A-O_2	3.8800	2.9000
O_3F -H_F -N_3	1.2500	3.1500
N_3H -H___A-N_3	0.1870	3.9000
N_3P -H___A-N_3	5.0000	2.7650
N_3HP-H___A-N_3	0.8000	3.2200
N_R -H___A-N_3	0.4300	3.4000
O_3F -H_F -N_3H	1.9700	3.1200
N_3H -H___A-N_3H	0.9300	3.4700
N_3P -H___A-N_3H	8.4500	2.8400
N_3HP-H___A-N_3H	10.1400	2.6000
N_R -H___A-N_3H	2.4400	3.1500



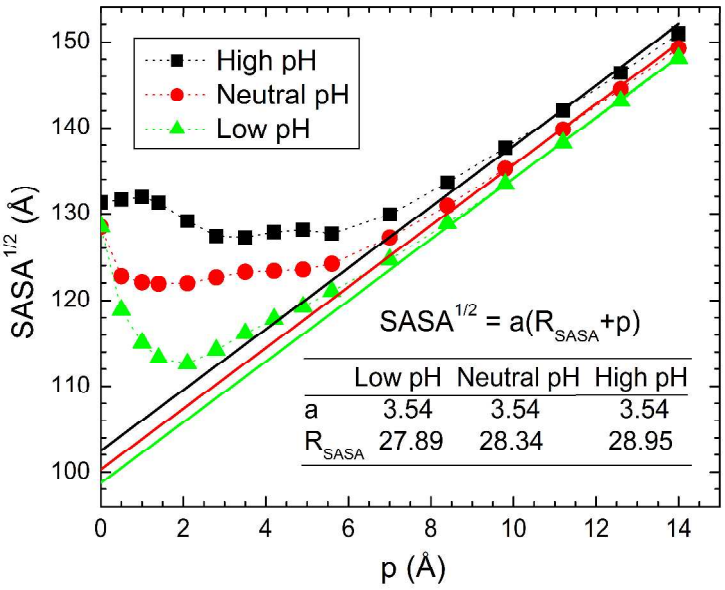
S4. Evolution of thermodynamics properties from constant particle, pressure and temperature (NPT) MD simulations: (a) potential energy; (b) pressure; (c) temperature; (d) volume.



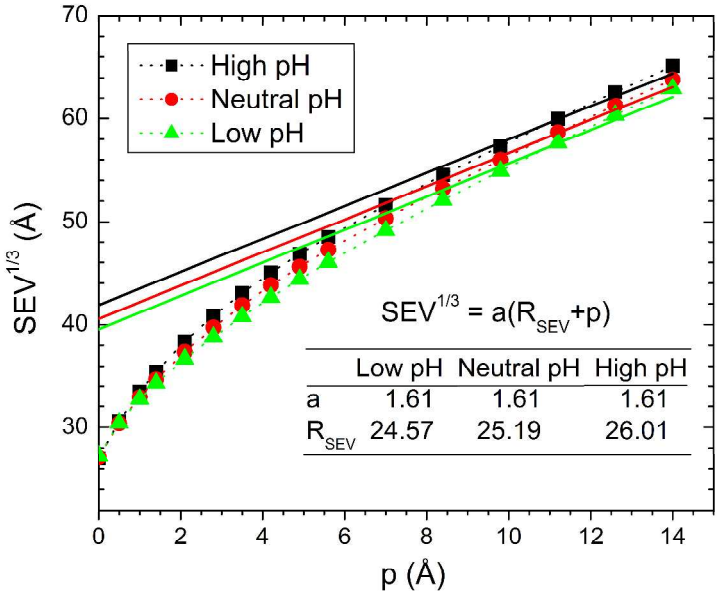




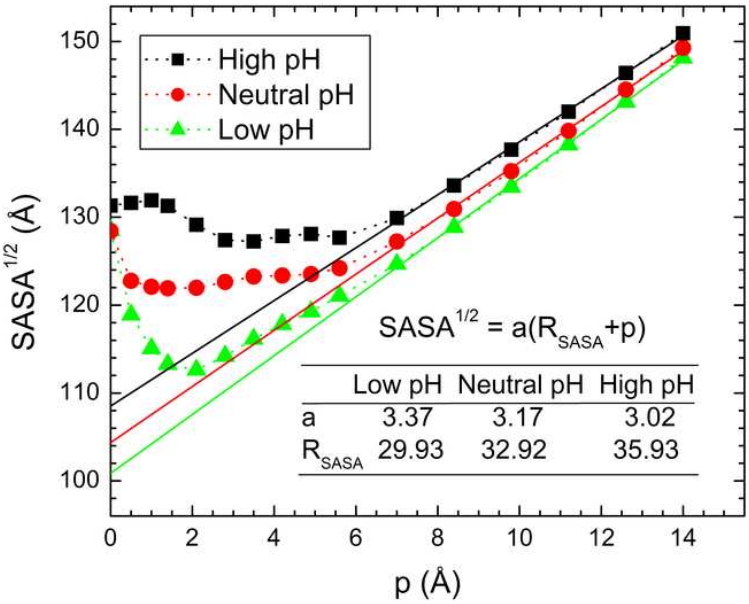
S5. Evolution of thermodynamics properties from constant particle, volume and temperature (NVT) MD simulations: (a) potential energy; (b) pressure; (c) temperature.



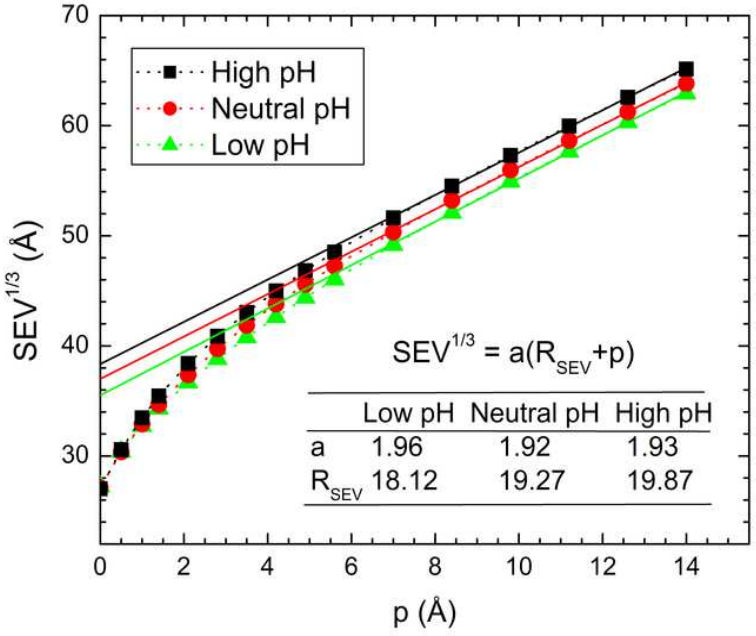
S6. Squared root of solvent accessible surface areas (SASA) as a function of probe radius at high, neutral, and low pH. The insert shows the equation and parameters used in linear regression fitting for p > 7 Å. The theoretical slope $\sqrt{4\pi}$ =3.54 was used.



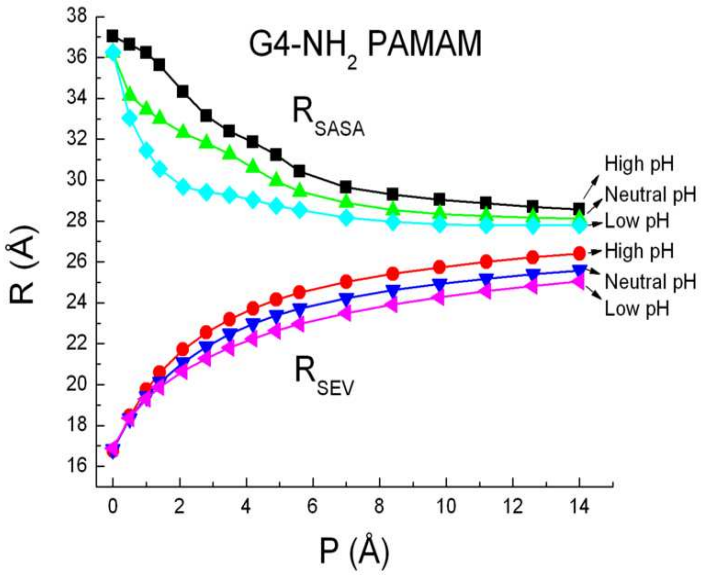
S7. Cubic root of solvent excluded volume (SEV) as a function of probe radius at high, neutral, and low pH. The insert shows the equation and parameters used in linear regression fitting for p > 7 Å. The theoretical slope $\sqrt[3]{\frac{4}{3}\pi}$ = 1.61 was used.



S8. Squared root of solvent accessible surface areas (SASA) as a function of probe radius at high, neutral, and low pH. The insert shows the equation and parameters used in linear regression fitting for p > 7 Å.



S9. Cubic root of solvent excluded volume (SEV) as a function of probe radius at high, neutral, and low pH. The insert shows the equation and parameters used in linear regression fitting for p > 7 Å.



S10. R_{SASA} and R_{SEV} as a function of probe radius at high, neutral, and low pH. The theoretical slopes $\sqrt{4\pi}$ =3.54 and $\sqrt[3]{\frac{4}{3}\pi}$ = 1.61 were used for deriving R_{SASA} and R_{SEV}, respectively.