

Table S2. Calculated (mPW1PW/6-31G*) conformational energies, populations (P_i), thermochemical data (at 298.15 K and 1 atm) and dipole moments (μ), for the 1,3-dap conformers in aqueous solution (SCRF-PCM)

Conformer ^a	s_i	ΔE (kJmol ⁻¹)	ΔE_{zpv} ^b (kJmol ⁻¹)	$P_i(\Delta E_{zpv})$ ^c (%)	ΔH (kJmol ⁻¹)	$T\Delta S$ (kJmol ⁻¹)	ΔG (kJmol ⁻¹)	$P_i(\Delta G)$ ^d (%)	μ ^e (D)
GGG'G	2	4.60	6.03	2.5	5.05	-0.75	5.80	1.5	2.53
TG'GG'	2	2.49	4.36	4.9	3.32	-0.94	4.26	2.9	4.03
TGGG'	2	3.96	4.21	5.3	3.99	2.62	1.37	9.4	3.58
TTTT	1	0.00	0.00	15.0	0.00	0.00	0.00	8.3	2.65
GGGG'	2	6.87	7.66	1.3	7.23	1.29	5.93	1.4	2.10
GG'G'G	2	6.74	6.57	2.0	6.32	1.25	5.06	2.0	1.60
TTGG'	2	3.64	3.31	7.6	3.26	1.95	1.32	9.6	3.66
TTTG	2	2.48	2.21	12.0	2.27	1.92	0.35	14.3	2.20
TGTT	2	1.99	2.18	12.2	2.00	1.56	0.43	13.8	2.04
GTGG'	2	5.77	5.45	3.2	5.37	1.74	3.63	3.7	1.88
TGTG	2	3.94	4.02	5.7	3.85	1.52	2.32	6.3	2.24
TGGT	2	2.56	4.17	5.3	3.40	-1.44	4.84	2.2	1.32
GTTG	2	4.85	4.44	4.8	4.58	0.36	4.22	2.9	1.91
GTG'G	2	6.81	6.38	2.1	6.40	2.17	4.23	2.9	2.05
TTGG	2	4.73	5.06	3.7	4.85	1.33	3.51	3.9	2.06
TGTG'	2	4.71	4.65	4.4	4.56	1.80	2.75	5.3	2.65
GTTG'	1	5.23	4.73	2.1	4.91	2.21	2.69	2.7	3.54
TGGG	2	6.23	6.28	2.2	6.06	1.69	4.37	2.7	2.56
GTG'G'	2	7.47	7.46	1.4	7.39	1.71	5.67	1.6	2.19
GGTG	2	6.91	6.95	1.7	6.81	1.53	5.28	1.9	3.49
GGGG	2	9.06	9.90	0.5	9.51	-0.51	10.02	0.3	2.42
TGGT	1	11.36	11.39	0.1	11.43	3.67	7.76	0.3	1.39
GGG'G'	1	13.23	14.38	0.0	13.80	0.13	13.67	0.0	3.62

^a See Figure 1; ^b ΔE_{zpv} , zero-point vibrational energy corrected relative energies; ^c population according to ΔE_{zpv} values; ^d population according to ΔG values; ^e 1 D = $1/3 \times 10^{-2}$ C m