Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Table S3. 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 carbon tetrachloride solution (SCRF-PCM)

Conformer [a]	s_i	ΔE (kJ.mol^{-1})	ΔE_{zpve} [b] (kJ.mol^{-1})	$P_i(\Delta E_{zpve})$[c] (%)	ΔH (kJ.mol^{-1})	TΔS (kJ.mol^{-1})	ΔG (kJ.mol^{-1})	$P_i(\Delta G)$[d] (%)	μ[e] (D)
GGG'G	2	0.18	0.13	13.8	0.07	-0.37	0.44	8.8	2.09
TG'GG'	2	0.00	0.00	14.6	0.00	-0.20	0.20	9.7	3.54
TGGG'	2	2.71	1.94	6.5	2.43	2.00	0.43	8.8	3.16
TTTT	1	1.71	0.03	7.2	1.07	0.70	0.38	4.5	2.25
GGGG'	2	4.19	3.98	2.8	4.32	1.06	3.27	2.7	1.92
GG'G'G	2	5.21	3.54	3.4	4.28	1.75	2.54	3.7	1.07
TTGG'	2	3.97	2.03	6.3	2.98	2.53	0.45	8.7	3.18
TTTG	2	3.41	1.52	7.8	2.63	2.63	0.00	10.5	1.93
TGTT	2	3.12	1.58	7.6	2.42	2.12	0.30	9.3	1.78
GTGG'	2	5.07	3.30	3.7	4.17	2.17	2.01	4.6	1.57
TGTG	2	4.37	2.78	4.6	3.63	2.15	1.47	5.7	1.97
TGGT	2	3.47	3.01	4.2	3.37	-0.61	3.98	2.0	1.31
GTTG	2	5.35	3.42	3.5	4.56	0.98	3.58	2.4	1.62
GTG'G	2	6.27	4.37	2.4	5.39	2.77	2.62	3.6	1.79
TTGG	2	5.06	3.74	3.1	4.58	2.04	2.54	3.7	1.83
TGTG'	2	5.58	3.84	3.0	4.75	2.40	2.35	4.0	2.26
GTTG'	1	6.63	4.51	1.1	5.72	2.91	2.81	1.6	3.02
TGGG	2	6.93	5.16	1.7	5.99	2.36	3.63	2.3	2.12
GTG'G'	2	7.58	6.00	1.2	6.95	2.41	4.54	1.6	1.83
GGTG	2	8.19	6.44	1.0	7.41	2.45	4.96	1.4	2.96
GGGG	2	9.92	8.84	0.4	9.60	0.59	9.01	0.3	2.04
TGG'T	1	12.25	10.86	0.1	11.57	1.93	9.64	0.1	1.41
GGG'G'	1	11.59	11.03	0.1	11.40	0.58	10.82	0.1	3.12

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