

Supplementary data

Table 1S. Energies and oscillator strengths for $S_0 \rightarrow S_i$ transitions in 2M5M and 2B5M calculated by TD DFT/B3LYP// DFT/B3LYP/6-31G(d,p) and maxima observed in absorption spectra measured in hexane.

	2M5M			2B5M		
	cal		exp	cal		exp
S_i	ΔE [cm ⁻¹]	f	ΔE [cm ⁻¹]	ΔE [cm ⁻¹]	f	ΔE [cm ⁻¹]
S_1	24093	0.079	24510	23885	0.066	24096
S_2	29213	0.000		29184	0.000	
S_3	30018	0.000		29973	0.000	
S_4	31788	0.153	30488	31734	0.155	30030
S_5	34200	0.000	34843	34216	0.000	34602
S_6	37396	0.198	35971	37304	0.211	35587
S_7	41724	0.263	39841	41535	0.312	39526
S_8	44548	0.070		44128	0.100	
S_9	45397	0.000		45305	0.000	
S_{10}	46195	0.039		46156	0.035	
S_{11}	47617	0.196	47619	47440	0.187	47169
S_{12}	49089	0.000		48999	0.000	
S_{13}	49629	0.000		49670	0.000	
S_{14}	50606	0.952		50296	0.832	
S_{15}	52567	0.089		50873	0.280	