Table 2. Computed VEE in aqueous solution for 9-methyl adenine PCM/TD-PBE0//PCM/PBE0/6-31G(d) calculations in aqueous solution

	Energy(Osc. Str.)	Orbitals	Description
	6-31G(d)		
S1	5.19(0.25)	H→L	π/π^*
S2	5.31(0.02)	H-1→L	n/π^*
S3	5.42(0.05)	H→L+1	π/π^*
S6	6.28(0.21)	H-2→L	π/π^*
	6-31+G(d,p)		
S1	5.05(0.31)	H→L	π/π^*
S2	5.31(0.01)	H-1→L	n/π^*
S3	5.33(0.04)	H→L+1	π/π^*
S6	6.11(0.28) H-2→L	π/π^*	
	6-311+G(2d,2p)		
S1	5.00(0.30)	H→L	π/π^*
S2	5.27(0.03)	H→L+1	π/π^*
S3	5.29(0.0)	H-1→L	n/π^*
S6	6.05(0.28)	H-2→L	π/π^*
	9MA·4 H_2O		
S1	5.09(0.24)	H→L	π/π^*
S2	5.37(0.12)	H→L+1	π/π^*
S3	5.61(0.00)	H-1→L	n/π^*
S6	6.30(0.18)	H-2→L	π/π^*

Experimental absorption maximum: 4.76 (1) Another strong feature at $\approx$ 6 eV (2)

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