Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information for: Interplay between Conformational and Solvent Effects in UV-visible Absorption Spectra: Curcumin Tautomers as Case Study

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M1

M2

M3

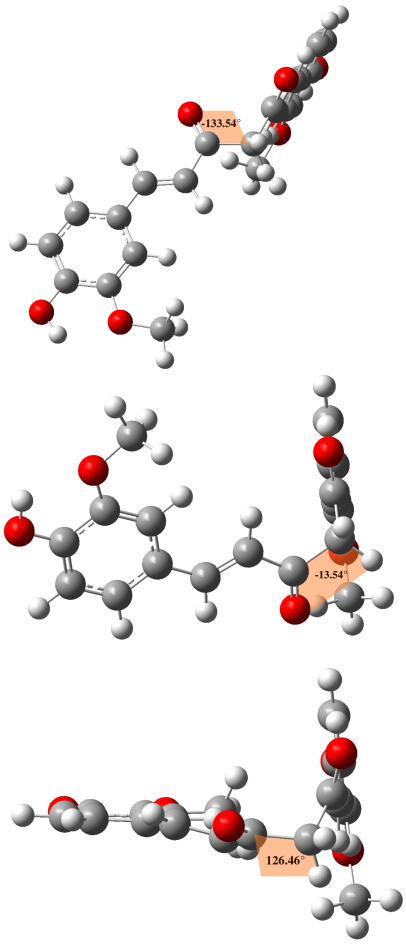

Figure 1: QM/PCMi Structure of the minima M1, M2 and M3 of the KK tautomer.

Table 1: KK tautomer QM/PCM Dihedral angles, maximum wavelength (λ_{max} in nm), molar absorptivity (ε in L mol^{-1} cm^{-1}) and charge transfer indexes (dCT in Å) for each point of the PES scan. For the located minima, Boltzmann weights are also reported.

	Dihedral angle (deg)	1st peak		dCT	weight
		λ_{max}	ϵ		
	-173.54	317.45	5.89E+04	1.053	
	-153.54	316.05	6.31E+04	0.97	
M1	-133.54	314.65	6.53E+04	1.32	0.47
	-113.54	315.25	6.71E+04	1.25	
	-93.54	317.85	6.80E+04	1.07	
	-73.54	320.71	6.82E+04	1.35	
	-53.54	321.53	6.64E+04	0.89	
	-33.54	322.57	6.23E+04	1.09	
M2	-13.54	325.72	5.74E+04	1.26	0.52
	6.46	325.93	5.28E+04	1.04	
	26.46	321.53	4.97E+04	0.33	
	46.46	317.25	5.08E+04	0.50	
	66.46	318.06	5.63E+04	1.32	
	86.46	308.06	5.23E+04	1.19	
	106.46	305.99	5.12E+04	1.04	
M3	126.46	305.99	4.72E+04	0.37	0.01
	146.46	306.55	4.33E+04	0.42	
	166.46	316.85	5.21E+04	1.07	

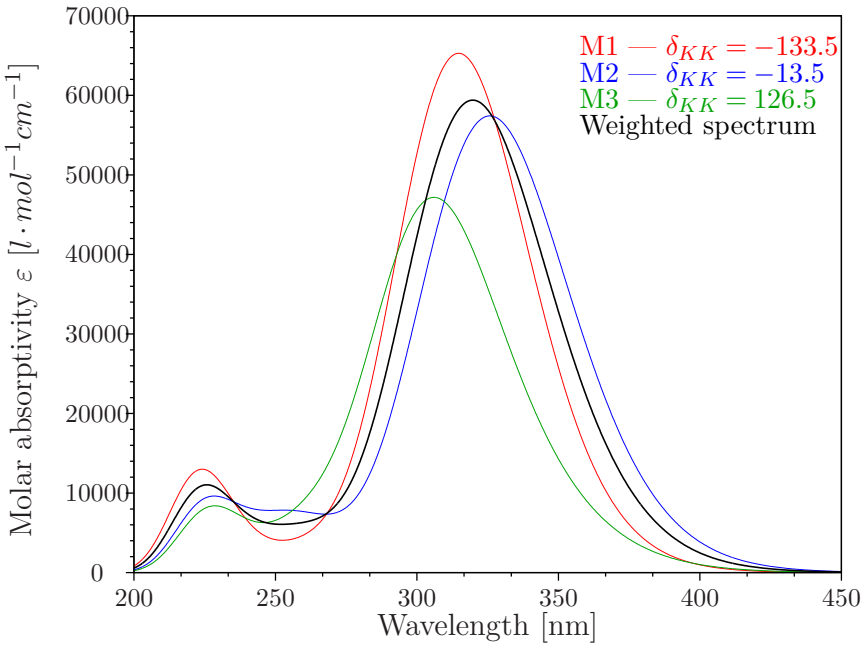

Figure 2: Computed QM/PCM absorption spectra for the three minima, M1, M2 and M3 of KK tautomer. The Boltzmann avergaed spectrum is also reported.

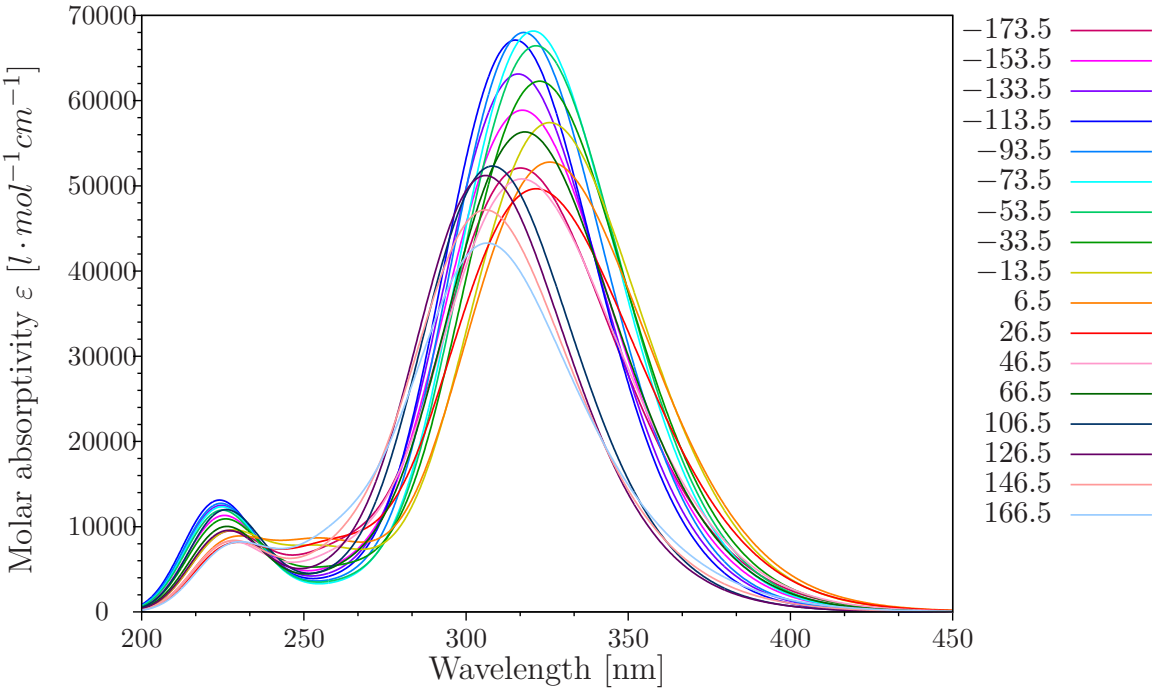

Figure 3: QM/PCM absorption spectra for selected δ_{KK} angle values.