The shape of the Electronic Circular Dichroism Spectrum of (2,6-dimethylphenyl)(phenyl)methanol. Interplay between Conformational equilibria and vibronic effects

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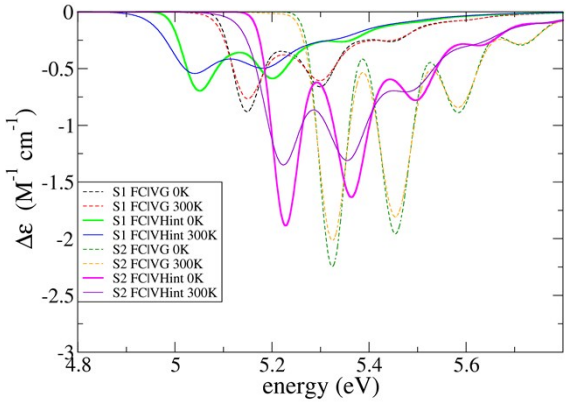
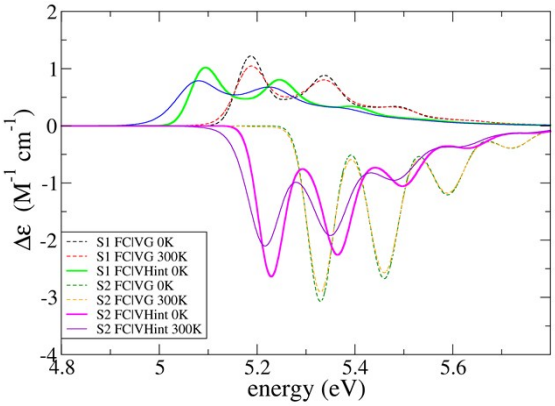
Electronic Supplementary Information

Table S1: Populations of the three conformers computed from free energy, and excitation energies (eV), oscillator strength (*f*) and rotatory strength (*R*, 10^{-40} erg-esu-cm/Gauss) for their first six excited states in ethanol.

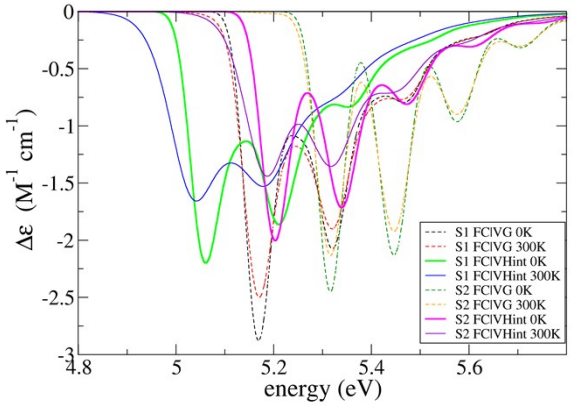
Conf.	TZVP					def2-TZVP				
	Pop		E_v	*f*	*R*	Pop		E_v	*f*	*R*
M0001	0.81	S1	5.29	0.03	-0.83	0.63	S1	5.27	0.03	-0.56
		S2	5.46	0.01	-1.81		S2	5.44	0.01	-1.34
		S3	5.86	0.12	-31.27		S3	5.82	0.13	-35.96
		S4	6.05	0.12	21.42		S4	6.01	0.12	23.50
		S5	6.34	1.44	173.36		S5	6.31	1.44	192.79
		S6	6.41	0.88	129.73		S6	6.39	0.85	117.59
M0002	0.08	S1	5.32	0.02	1.07	0.18	S1	5.30	0.02	1.84
		S2	5.46	0.00	-2.40		S2	5.45	0.01	-2.92
		S3	5.92	0.06	-26.80		S3	5.87	0.07	-30.99
		S4	6.08	0.09	3.04		S4	6.04	0.09	2.44
		S5	6.35	1.53	173.93		S5	6.32	1.52	201.00
		S6	6.42	0.91	174.33		S6	6.38	0.90	144.19
M0003	0.11	S1	5.30	0.03	-2.56	0.19	S1	5.29	0.03	-2.50
		S2	5.45	0.01	-1.97		S2	5.44	0.01	-1.60
		S3	5.88	0.14	-40.86		S3	5.84	0.14	-40.60
		S4	6.05	0.10	29.00		S4	6.01	0.10	28.90
		S5	6.34	1.39	190.26		S5	6.31	1.39	198.82
		S6	6.43	0.88	204.13		S6	6.40	0.88	201.95



M0001



M0002



M0003

Figure S1: Vibronic ECD spectra computed for the three conformers on the ground of ωB97X-D/TZVP calculations with different vibronic models. All computed spectra convolved with a Gaussian with HWHM=0.03 eV.

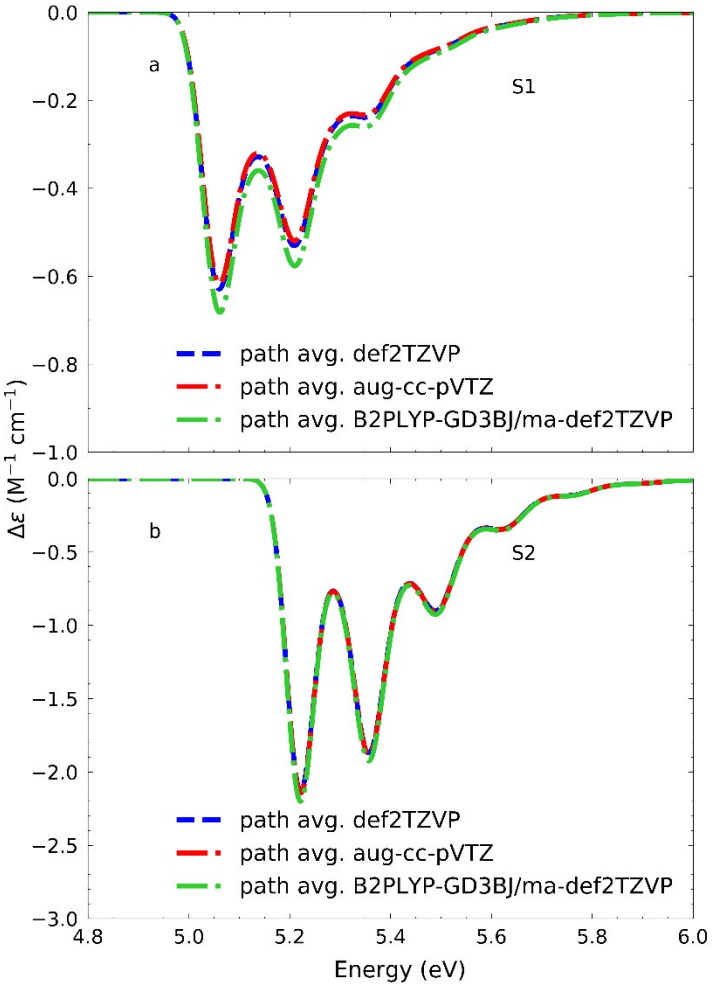


Figure S2: Path-averaged vibronic ECD spectra based on ωB97X-D/TZVP spectra. Boltzmann weights were obtained re-computing the electronic energy at different levels of theory, namely ωB97X-D/def2-TZVP, ωB97X-D/aug-cc-pVTZ and B2PLYP-GD3BJ/ma-def2-TZVP.

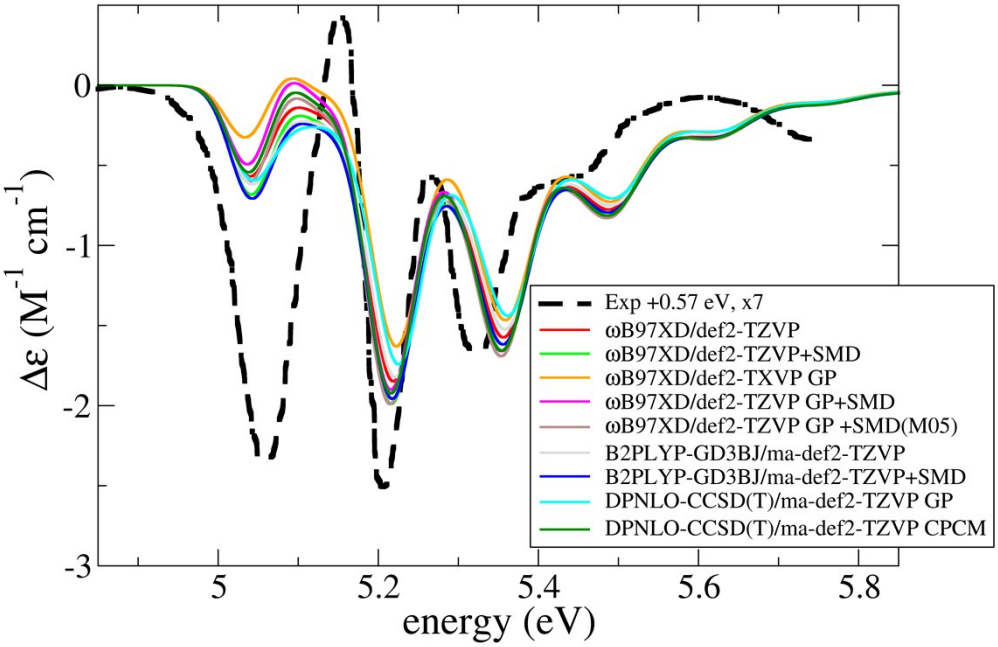


Figure S3: Average of vibronic ECD spectra computed for the three conformers, with Boltzmann populations estimated at different levels of theory. The experimental spectrum is also reported and for a better comparison it has been blue-shifted by 0.57 eV and its intensity multiplied by a factor 7. All computed spectra convolved with a Gaussian with HWHM=0.03 eV