Supporting Information:
ERRATUM: Harmonic models in Cartesian and internal coordinates to simulate the absorption spectra of carotenoids at finite temperatures
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Table 1: Largest normal mode displacements (atomic units) for low-frequency modes computed for *cis*-C_i conformer of β-carotene. Values for AH-int model reported in the original paper (orig) as well as the corrected ones (corr) are included along with those provided by the AH and VH models in Cartesian coordinates. Significant changes are observed between the original and the corrected values.

		Displacement			
Mode	Freq	VH	AH Cart	AH int (orig)	AH int (corr)
3[a]	13.89	**98.17**	**316.68**	**324.54**	**317.41**
5	24.31	-14.94	-17.54	60.55	-28.74
7	35.16	49.53	-54.80	34.52	-49.76
9[a]	45.56	**265.69**	**103.98**	**121.48**	**-109.35**
10	53.80	-43.87	-29.95	-14.15	-26.69
14	78.50	9.70	0.48	61.05	-11.22
15	90.81	6.87	14.98	-26.35	-20.17
19	119.50	30.21	26.65	38.63	-28.44
20	135.67	-13.10	-9.64	-3.96	8.91
23	144.82	-26.46	-9.14	-13.59	9.97

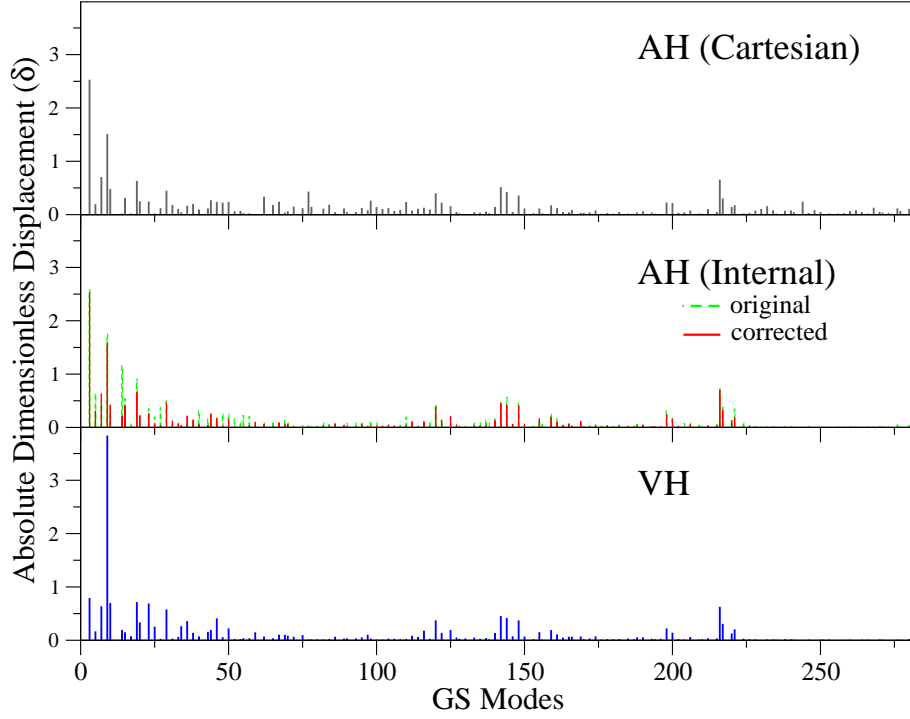[a]Significantly contributed by the dihedral connecting the ionone ring with the polyenic chain.

Figure 1: Absolute values of the dimensionless displacements, $\delta_i = (2\pi\nu_i^{GS}/\hbar)^{1/2}K_i$, computed with all the models for the cis-C_i conformer of β-carotene. In the center panel, both the original (dotted) and the corrected (straight line) values for AH-int model are included. Corrected values are generally smaller, maingly for torsional normal modes (low frequency), although a similar performance still holds when comparing AH-Cart, AH-int and VH models.
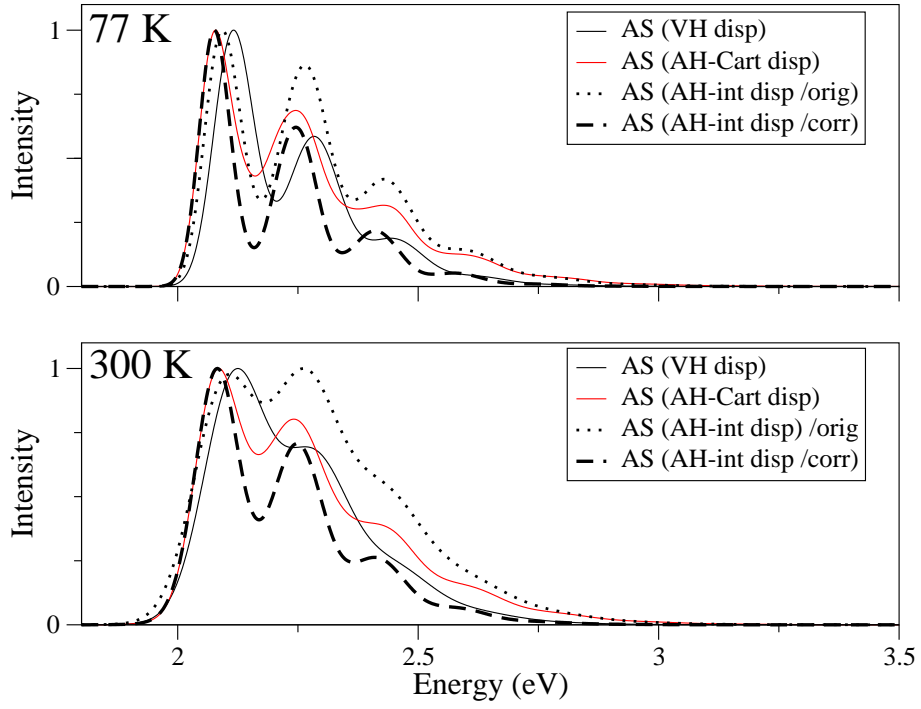
Figure 2: Adiabatic Shift (AS) spectra (i.e. setting Duschinsky matrix to the unit matrix) computed for the *cis-C_i* isomer of β-carotene using the normal mode displacements evaluated at VH, AH-Cart, AH-int models. Corrected AH-int calculations predict vibronic spectra sgnificantly different from the original ones, although a similar spectral width is observed in all the cases.
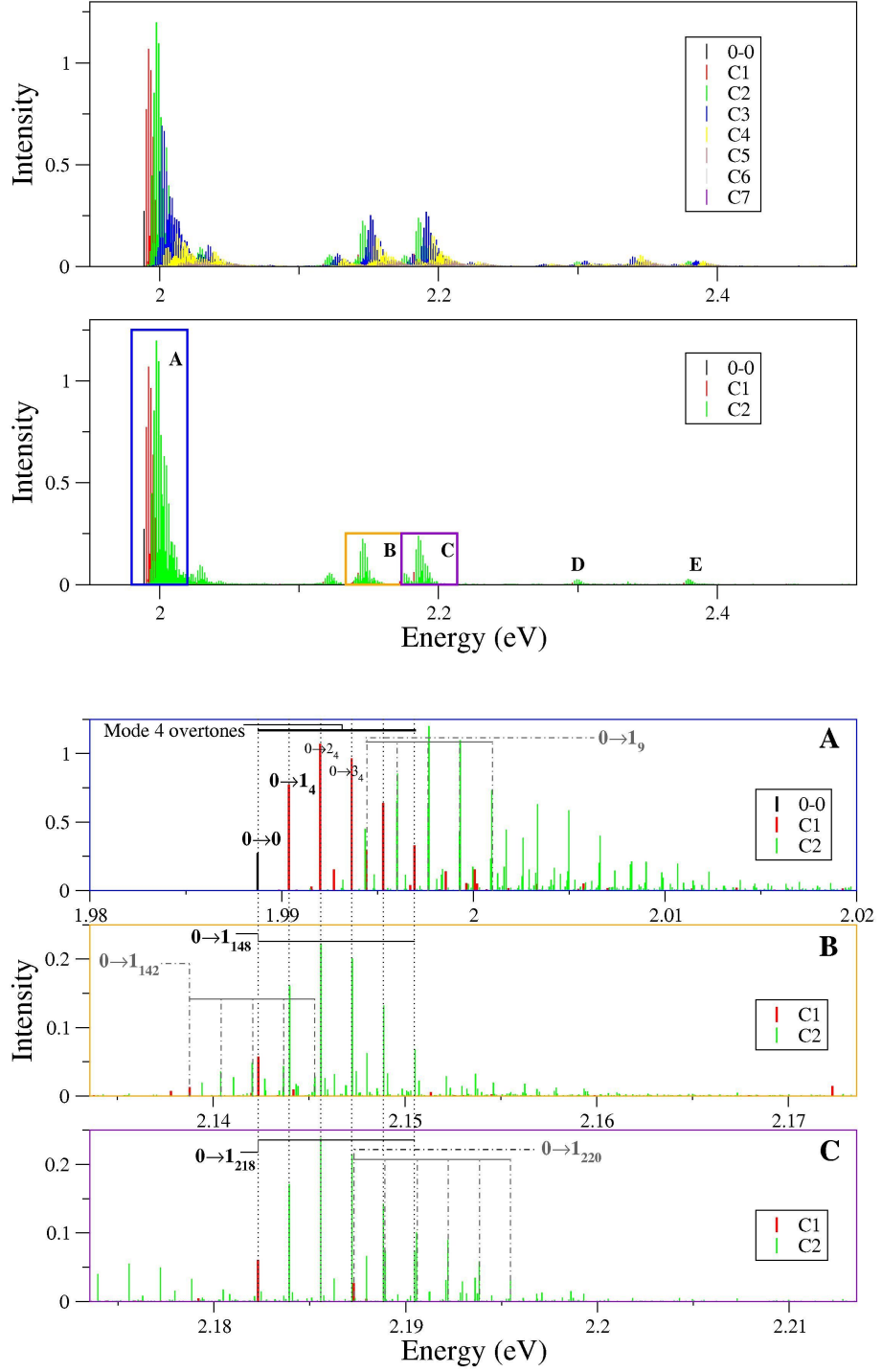
Figure 3: TI spectrum at 0 K (recovered fraction equal to 0.81), computed using internal coordinates with the corrected code. On the top, the contributions for all the computed *classes* are shown (up), and the selected regions with only C_0 (0-0) to C_2 *classes* transitions are indicated. A zoom on these regions is shown on the bottom panels. The same labels adopted in the original publication are used.