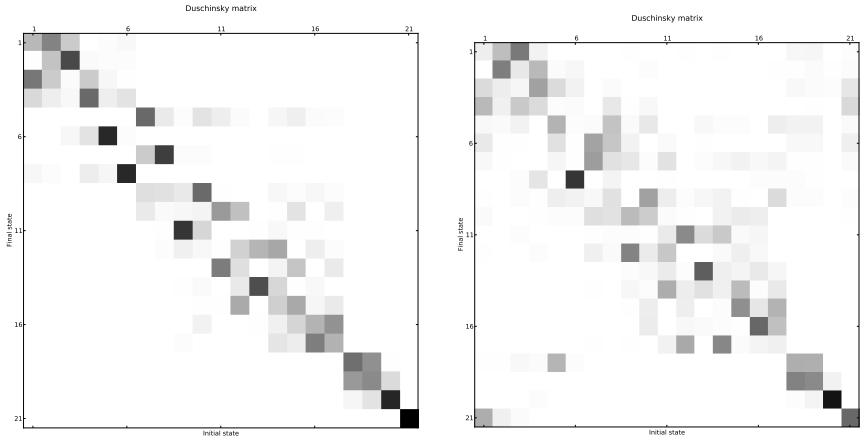


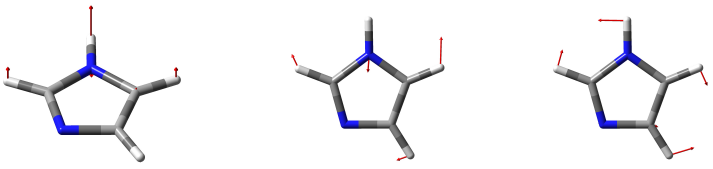
(a) ImH^+ D_0 **(b)** ImH T_0

Figure 1: Duschinsky matrices for the doublet cation (left) and neutral triplet (right). The figure shows two 21×21 matrices, where 21 is the number of normal modes. A darker shade denotes a higher absolute value of the matrix element.

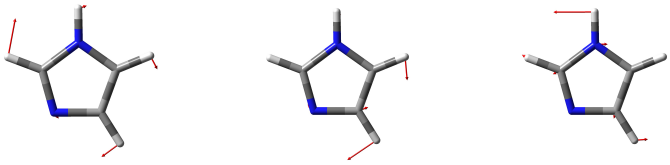
1 Supporting Information

Figure 1 shows the Duschinsky matrices which relate the normal modes of the Imidazole neutral triplet and doublet cation to the ones of the ground state neutral singlet, respectively. It can be noted that the Duschinsky matrix for the cation is much more diagonal than the one for the triplet, which is much more "dense" having several entries with a significant value for each row (or column). Such a matrix suggests that the Duschinsky approximation may not be suitable in the case of the triplet, therefore the anharmonic frequencies of the triplet state cannot be correctly estimated using the Duschinsky method. Figure 2 shows the normal modes of imidazole mentioned in the paper, where the red arrows denote the displacement of the atoms along the mode.

Figure 3 shows the effect of including overtones and combination bands in the spectrum of chlorophyll $a1$. The difference between the two spectra is negligible and they overlap almost perfectly, except for the 1600-1700 cm^{-1} zone, where they differ very slightly. Contributions from higher-excitation bands were therefore neglected in all calculations shown in the paper.



(a) Mode 1 **(b)** Mode 8 **(c)** Mode 11



(d) Mode 13 **(e)** Mode 14 **(f)** Mode 15

Figure 2: Normal modes of imidazole mentioned throughout the work.

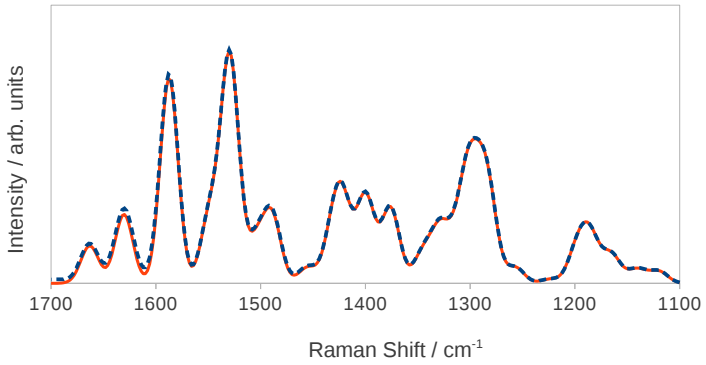


Figure 3: Calculated RR spectra of ChlA1 in methanol. The continuous orange spectrum only includes contributions from the fundamental bands, the dashed blue one includes all overtones and combination bands of two modes.