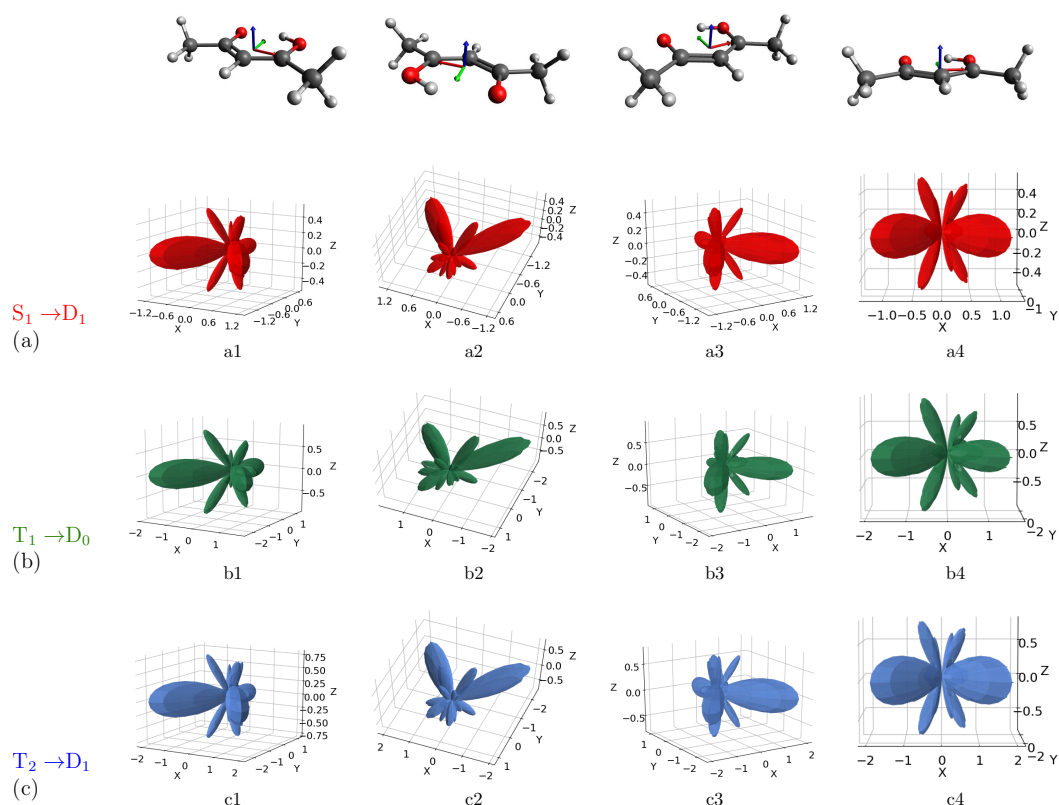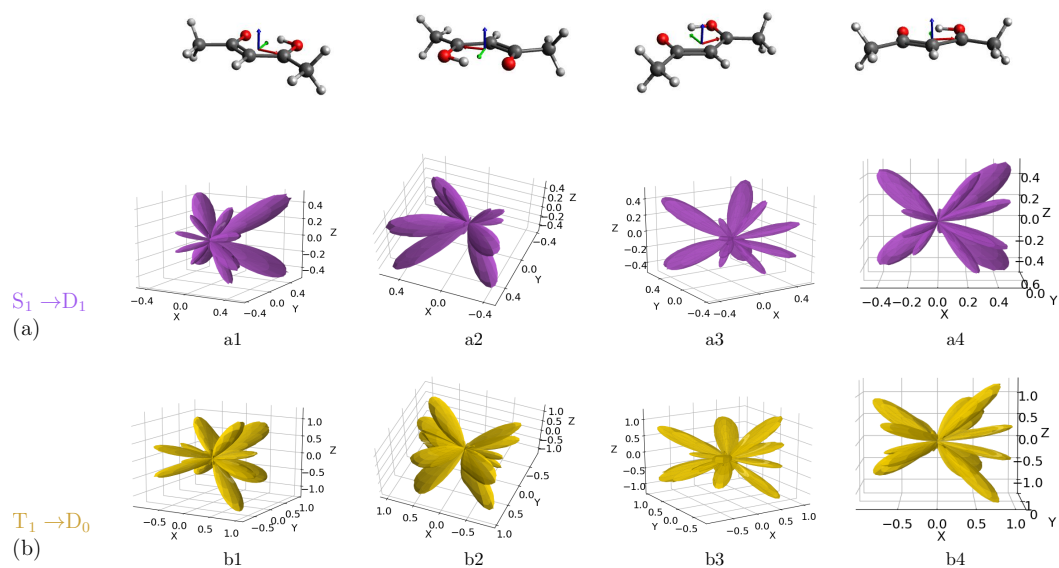# Supplementary Materials: DISCRIMINATION OF EXCITED STATES OF ACETYLACETONE THROUGH THEORETICAL MOLECULAR-FRAME PHOTOELECTRON ANGULAR DISTRIBUTIONS
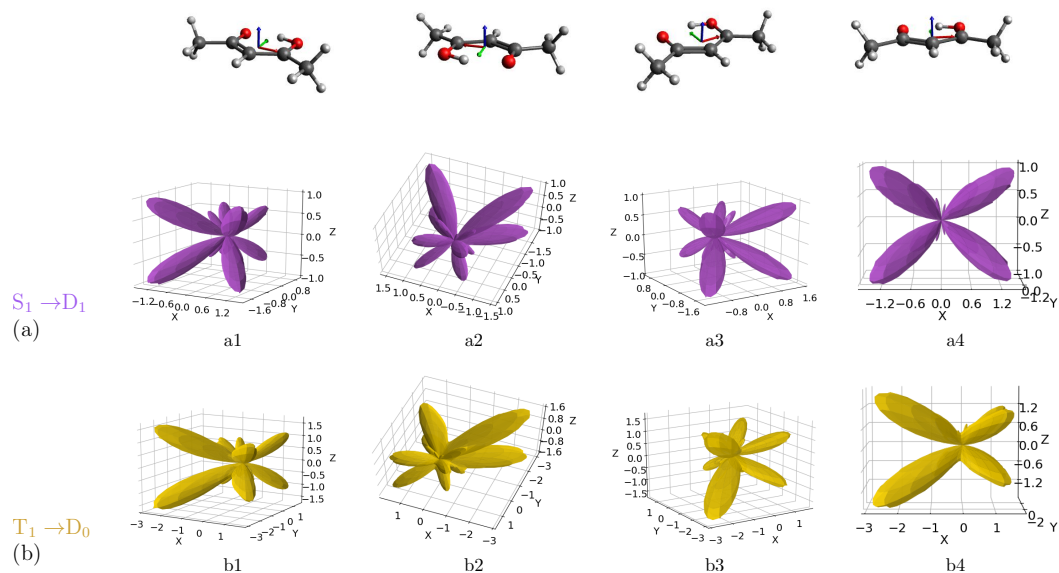
Aurora Ponzi [1]* , **Marin Sapunar** [1,a] , **Nađa Došlić**[1] and **Piero Decleva** [2]*
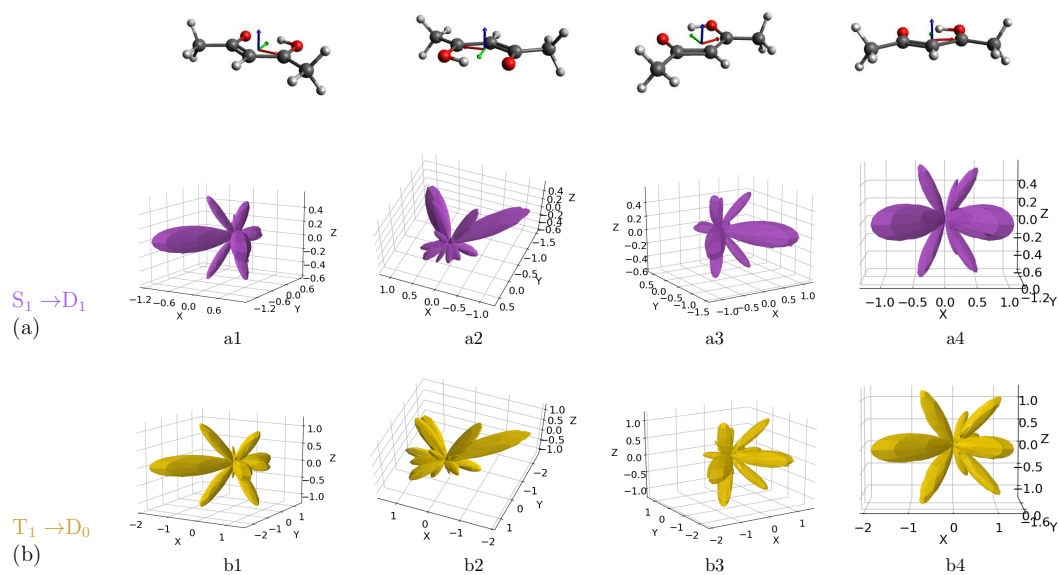
Figure S1. Computed MFPADs for the photoionization from the S_1 (a), T_1 (b), and T_2 (c) excited states of acetylacetone to the corresponding first ionic state, at the selected kinetic energy of 6.04 eV. The electric field is oriented along the z axis. Orientation of the molecule is also shown on top of figure (x, y, z axes are respectively identified by red, green and blue colours).

Figure S2. Computed MFPADs for the photoionization from the S_1 (a) and T_1 (b) excited states of acetylacetone to the corresponding first ionic state, at the selected kinetic energy of 7.14 eV. The electric field is oriented along the x axis. Orientation of the molecule is also shown on top of figure (x, y, z axes are respectively identified by red, green and blue colours).

Figure S3. Computed MFPADs for the photoionization from the S_1 (a) and T_1 (b) excited states of acetylacetone to the corresponding first ionic state, at the selected kinetic energy of 7.14 eV. The electric field is oriented along the y axis. Orientation of the molecule is also shown on top of figure (x, y, z axes are respectively identified by red, green and blue colours).

Figure S4. Computed MFPADs for the photoionization from the S_1 (a) and T_1 (b) excited states of acetylacetone to the corresponding first ionic state, at the selected kinetic energy of 7.14 eV. The electric field is oriented along the z axis. Orientation of the molecule is also shown on top of figure (x, y, z axes are respectively identified by red, green and blue colours).