Supporting Information for "Chiroptical characterization tools for asymmetric small molecules – Experimental and computational approaches for electronic circular dichroism (ECD) and anisotropy spectroscopy"

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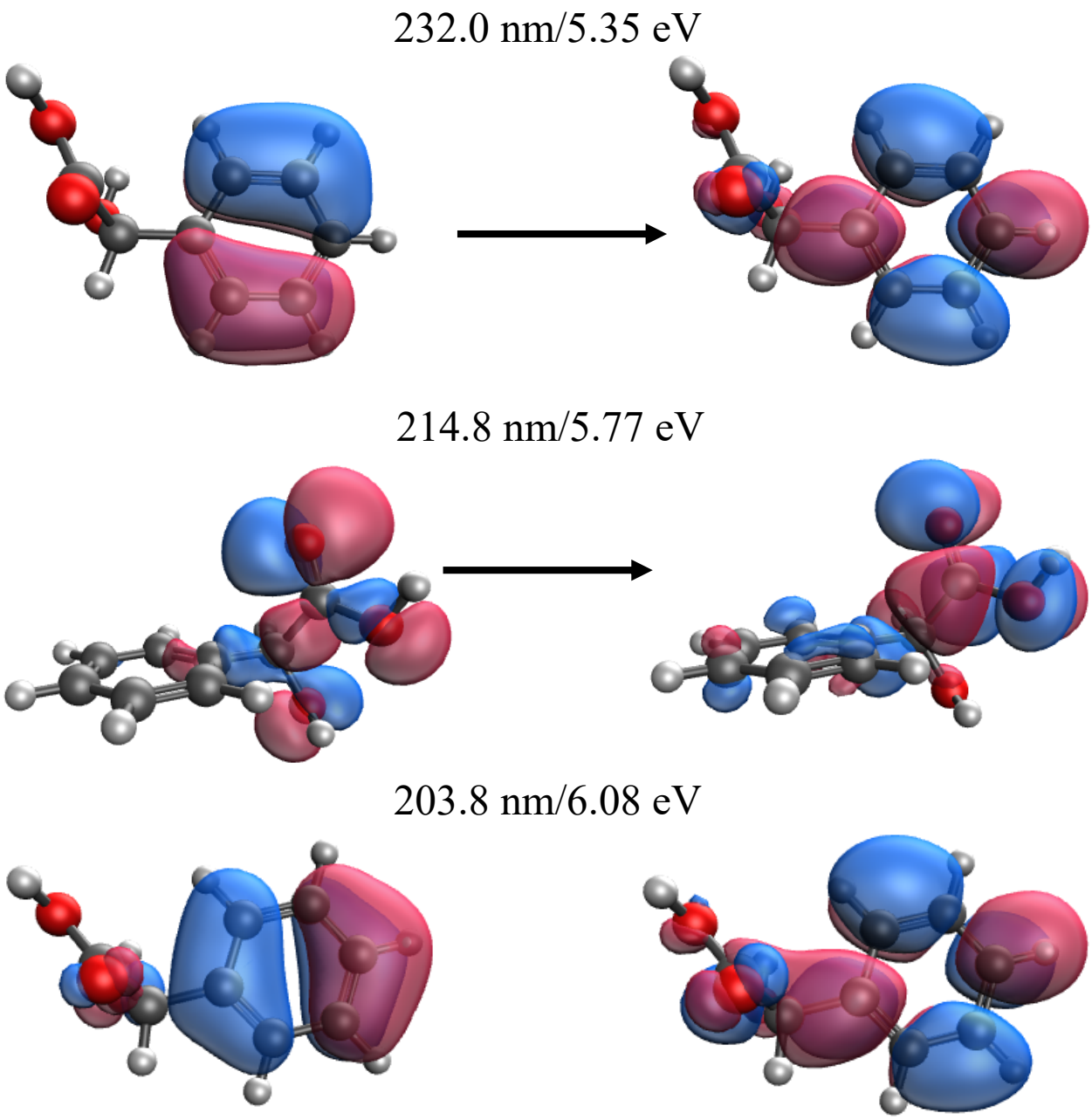


Figure S1: The Highest Occupied Natural Transition Orbitals (HONTOs) and Lowest Unoccupied Natural Transition Orbitals (LUNTOs) associated with the three lowest energy electronic transitions of mandelic acid. The natural transition orbitals were plotted with an isovalue of 0.06.

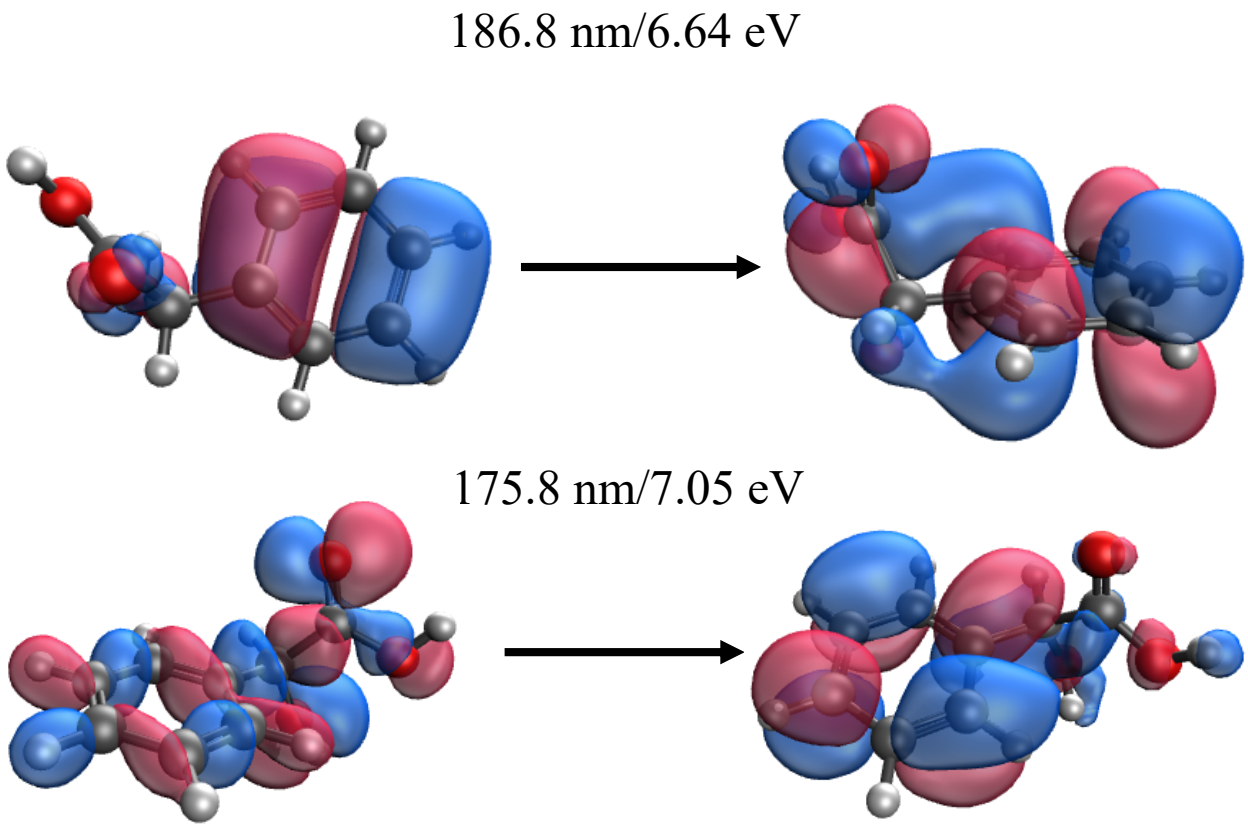


Figure S2: The Highest Occupied Natural Transition Orbitals (HONTOs) and Lowest Unoccupied Natural Transition Orbitals (LUNTOs) associated with the electronic transitions of mandelic acid at 186.8 nm and 175.8 nm. The natural transition orbitals were plotted with an isovalue of 0.06.

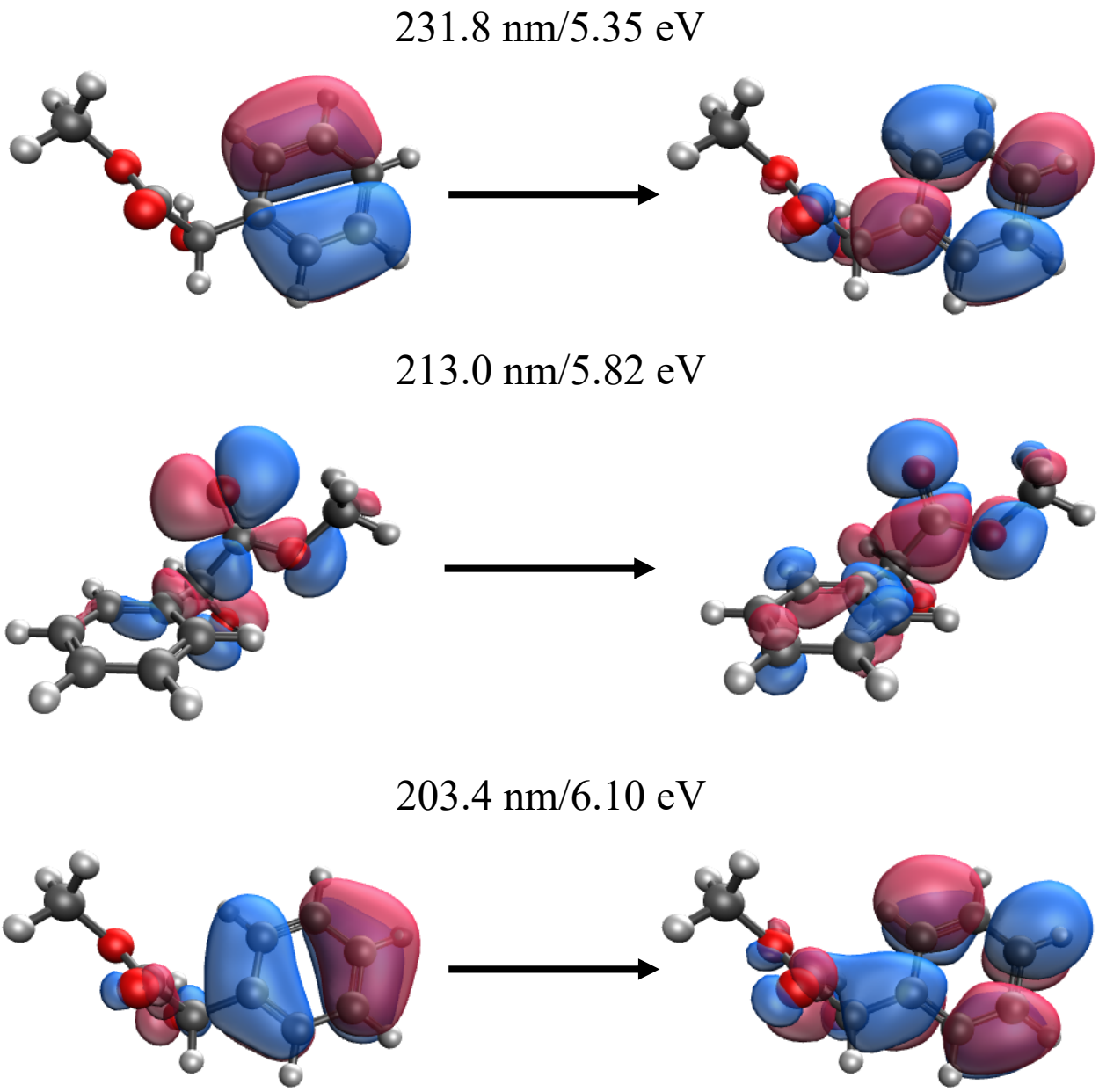


Figure S3: The Highest Occupied Natural Transition Orbitals (HONTOs) and Lowest Unoccupied Natural Transition Orbitals (LUNTOs) associated with the three lowest energy electronic transitions of methyl mandelate. The natural transition orbitals were plotted with an isovalue of 0.06.

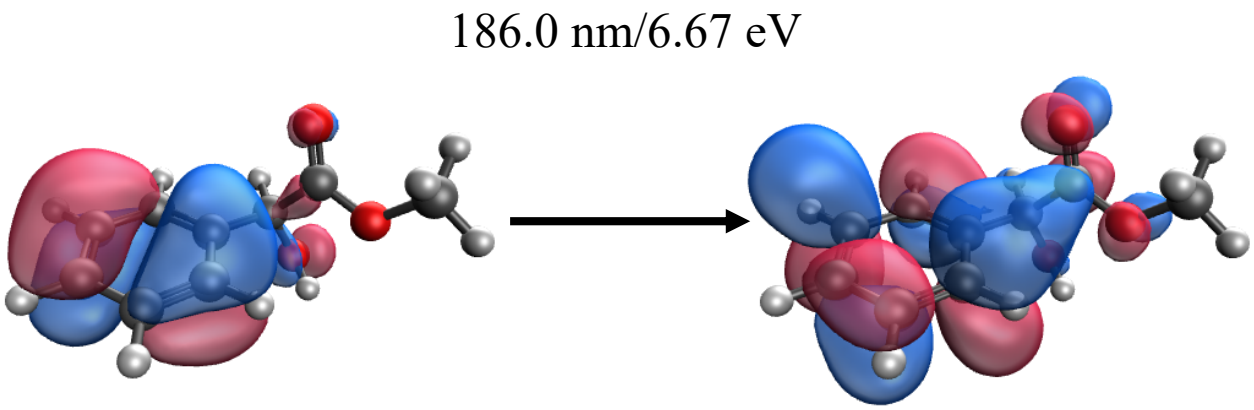


Figure S4: The Highest Occupied Natural Transition Orbitals (HONTOs) and Lowest Unoccupied Natural Transition Orbitals (LUNTOs) associated with electronic transition of methyl mandelate at 186.0 nm. The natural transition orbitals were plotted with an isovalue of 0.06.

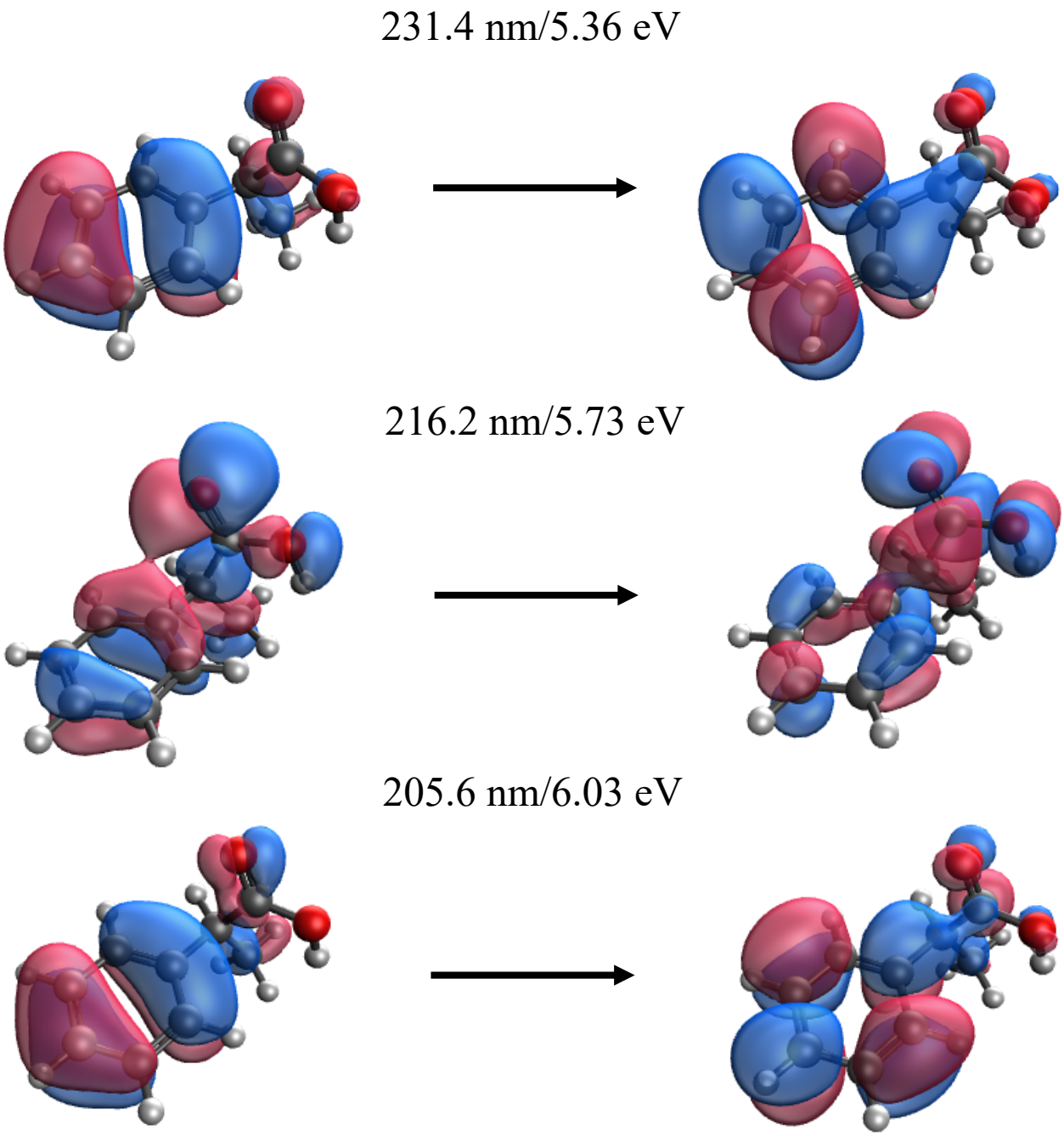


Figure S5: The Highest Occupied Natural Transition Orbitals (HONTOs) and Lowest Unoccupied Natural Transition Orbitals (LUNTOs) associated with the three lowest energy electronic transitions of 2-phenyl propionic acid. The natural transition orbitals were plotted with an isovalue of 0.06.

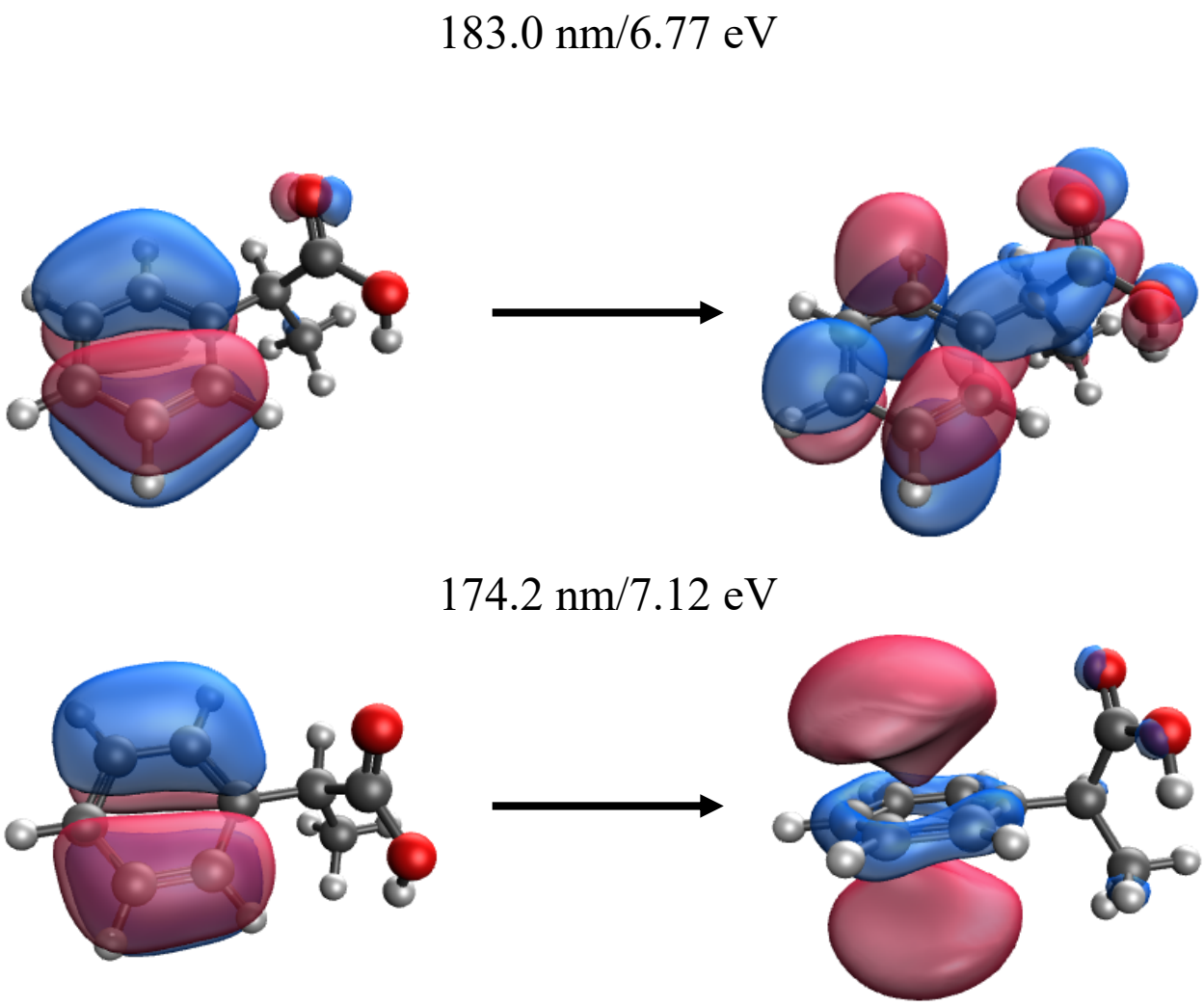


Figure S6: The Highest Occupied Natural Transition Orbitals (HONTOs) and Lowest Unoccupied Natural Transition Orbitals (LUNTOs) associated with the electronic transitions of 2-phenyl propionic acid at 183.0 nm and 174.2 nm. The natural transition orbitals were plotted with an isovalue of 0.06.

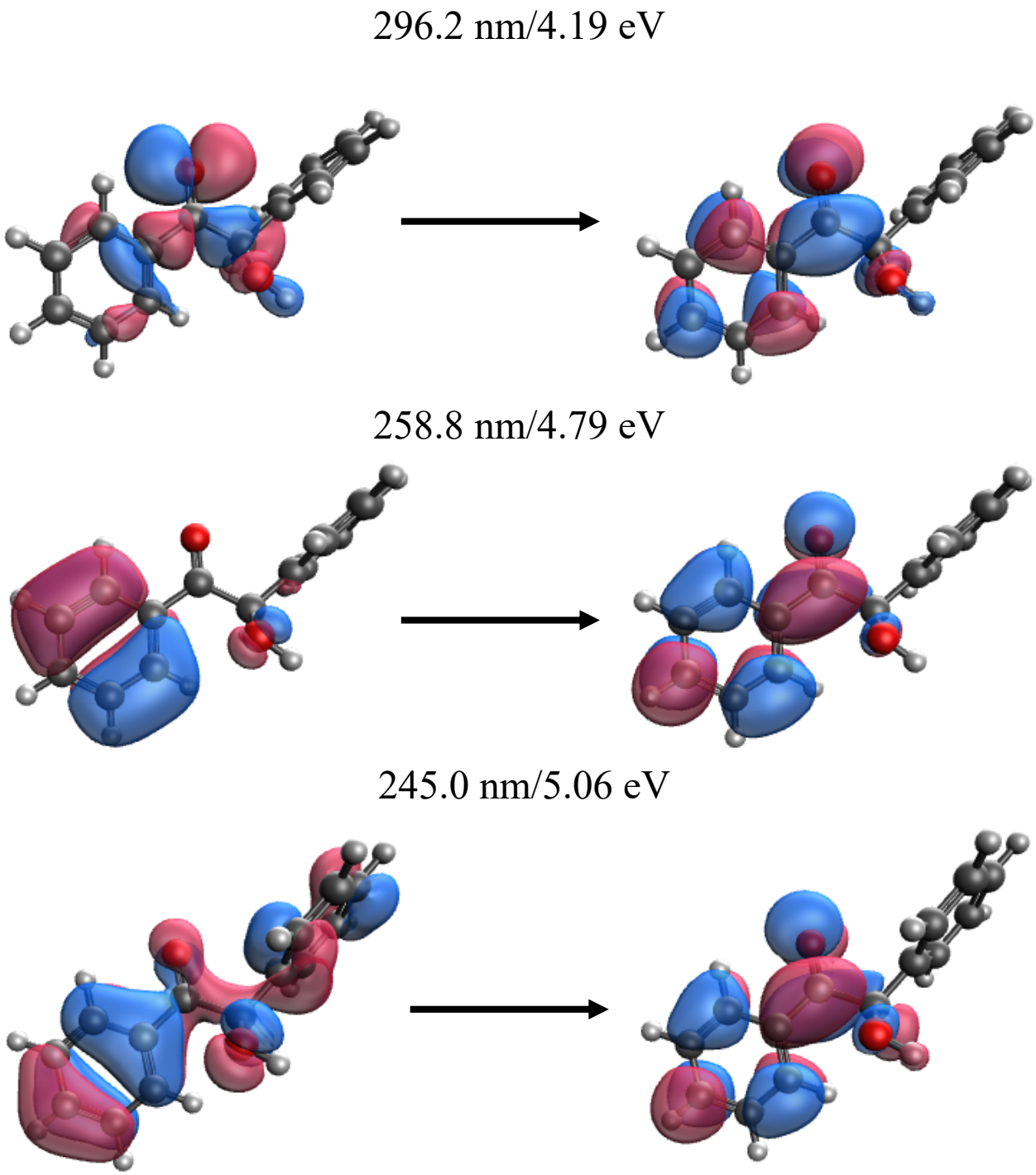


Figure S7: The Highest Occupied Natural Transition Orbitals (HONTOs) and Lowest Unoccupied Natural Transition Orbitals (LUNTOs) associated with the three lowest energy electronic transitions of benzoin. The natural transition orbitals were plotted with an isovalue of 0.06.

227.2 nm/5.46 eV
Both states contribute to this band in the spectrum

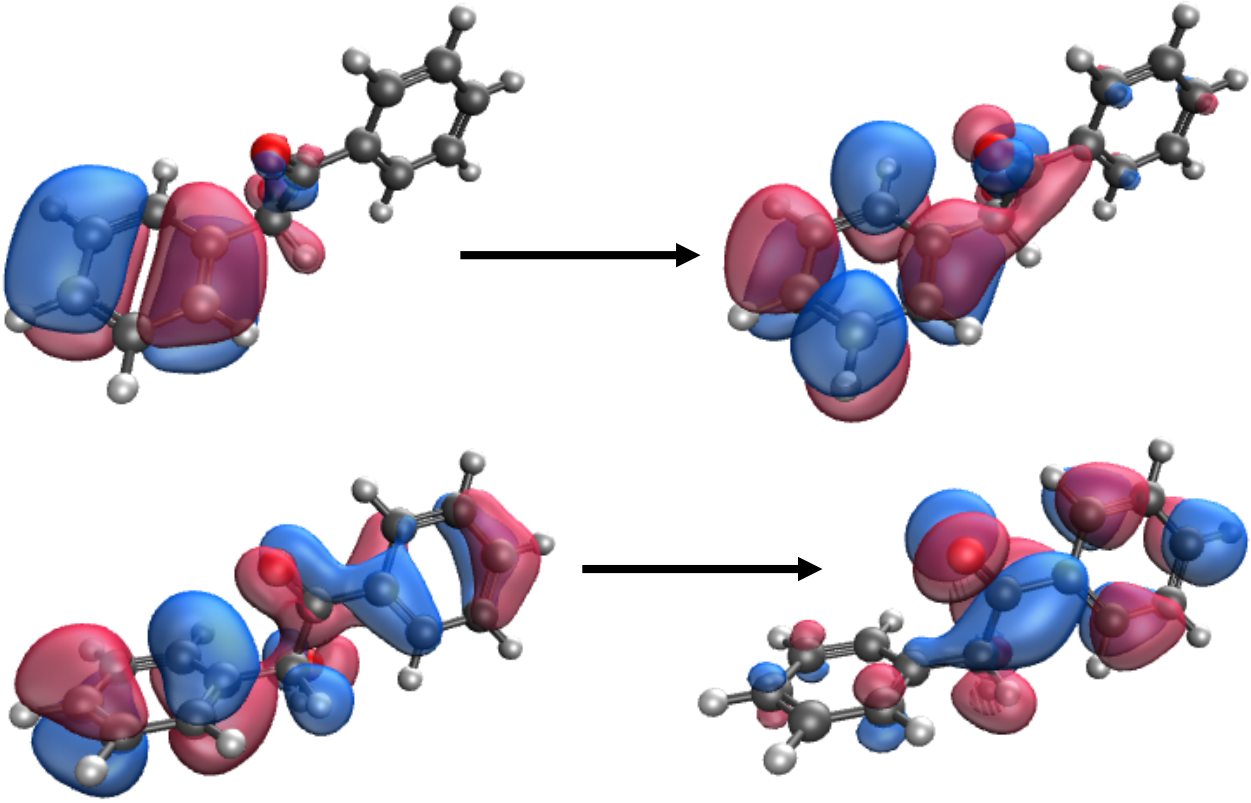
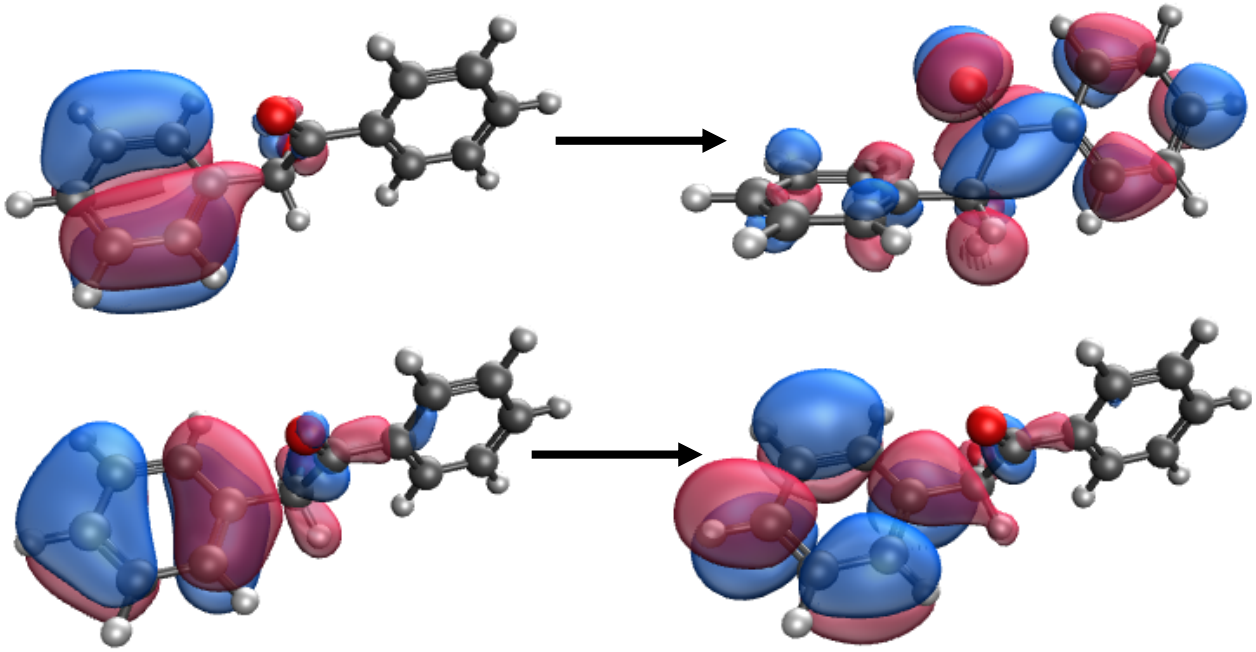


Figure S8: The Highest Occupied Natural Transition Orbitals (HONTOs) and Lowest Unoccupied Natural Transition Orbitals (LUNTOs) associated with the electronic transitions of benzoin that contribute to the band at 227.2 nm. The natural transition orbitals were plotted with an isovalue of 0.06.

206.2 nm/6.01 eV
Both states contribute to this band in the spectrum



195.2 nm/6.35 eV

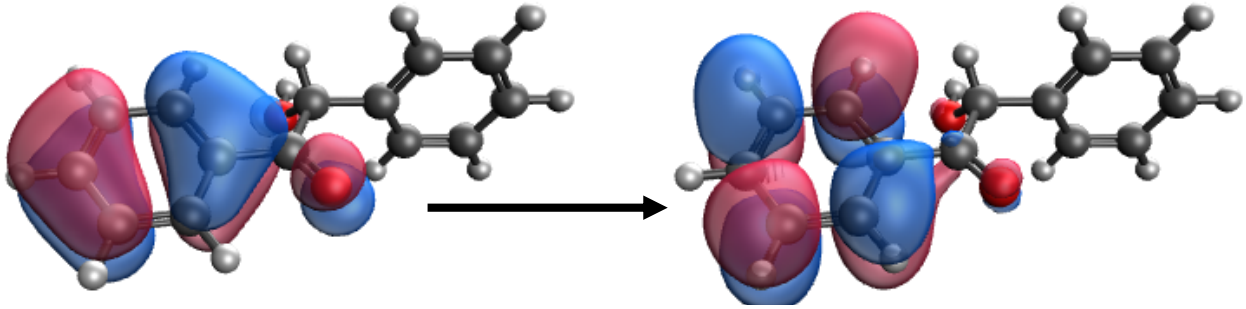


Figure S9: The Highest Occupied Natural Transition Orbitals (HONTOs) and Lowest Unoccupied Natural Transition Orbitals (LUNTOs) associated with the electronic transitions of benzoin that contribute to the bands at 206.2 nm and 195.2 nm. The natural transition orbitals were plotted with an isovalue of 0.06.

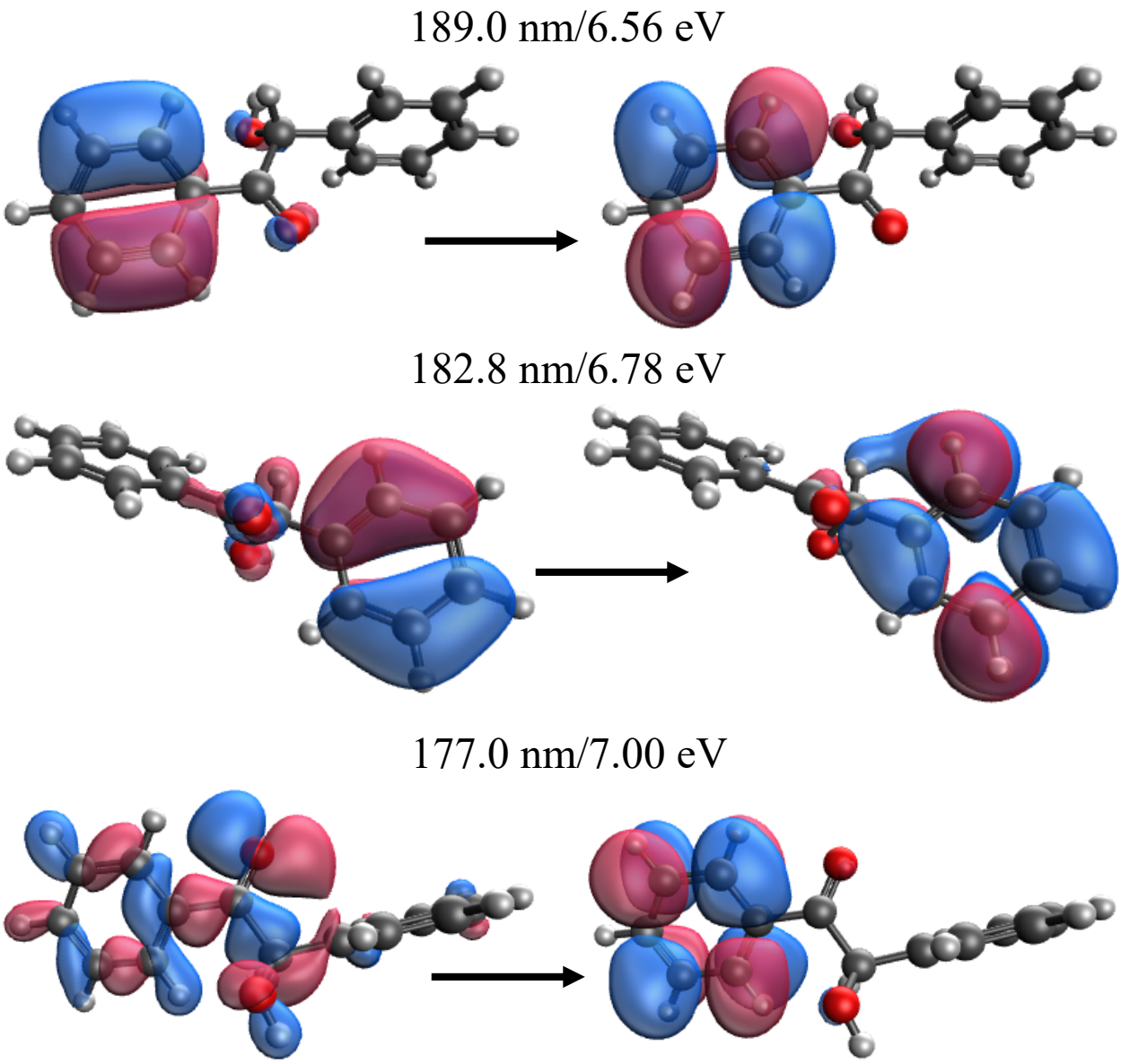


Figure S10: The Highest Occupied Natural Transition Orbitals (HONTOs) and Lowest Unoccupied Natural Transition Orbitals (LUNTOs) associated with the electronic transitions of benzoin that contribute to the bands at 189.0 nm, 182.8 nm, and 177.0 nm. The natural transition orbitals were plotted with an isovalue of 0.06.