Supplementary Materials

Twisting Aromaticity and Photoinduced Dynamics in Hexapole Helicenes

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Figure S1. Superposition of snapshots obtained from ground-state molecular dynamics indicating conformational flexibility of the molecules.
**Figure S2.** The twisting angles, indicated as red lines, are defined by the two carbon atoms and the two bond midpoints (black circles). The three nonfused C-C bonds for the benzene ring B are: C(1)-C(6), C(2)-C(3), and C(4)-C(5), the other three C-C bonds are fused bonds, equivalent definition corresponds to benzene rings C and D.
Figure S3. Evolution of twisting angles during non-adiabatic excited dynamics for different isomers of the hexapole [5]helicene.
Figure S4. Probability density function corresponding to the ensemble of initial conditions of the energy gap between a) $S_7$ and $S_6$ states and b) $S_3$ and $S_2$. 
Figure S5. Average fraction of transition density in the C₁ and C₂ isomers, δᵢ, in different [5]helicene units as a function of delay time (t-t_hop), relative to the moment of nonadiabatic transitions S₇→S₆ and S₃→S₂. Blue lines correspond to the [5]helicene unit with the largest twisting angle (~36°) and red lines correspond to the net contribution of the other two fragments.
Figure S6. Evolution in time of the fraction of transition density, $\delta^T_X$, localized over each type of atom depicted in the insets for a) $C_1$, b) $C_2$, and c) $D_3$ isomers.