Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information – Tuning the Photoreactivity of Z-Hexatriene Photoswitches by Substituents - A Non-Adiabatic Molecular Dynamics Study

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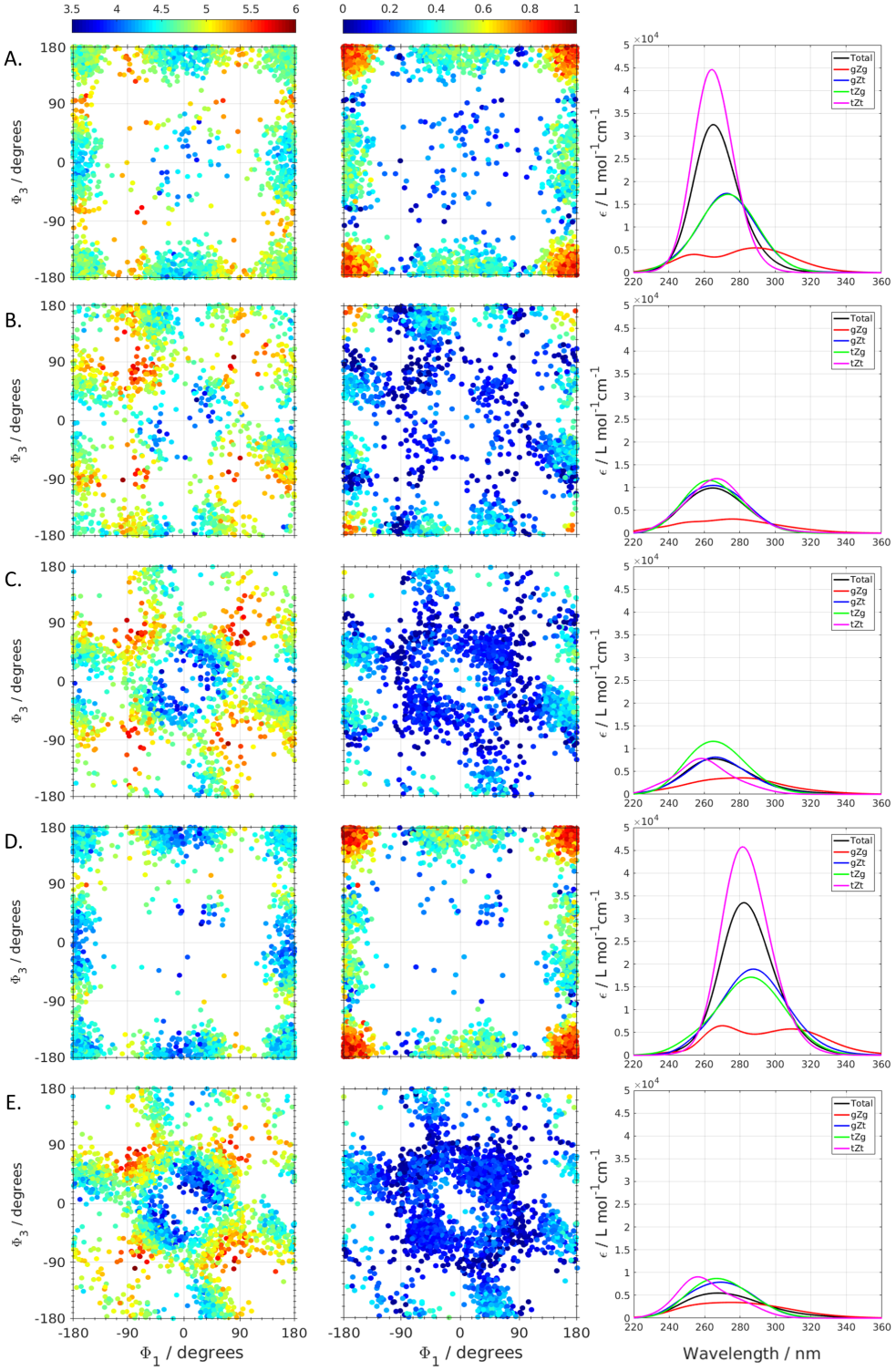

Figure 1: TDPBE0 $S_1 \leftarrow S_0$ excitation energy in eV (left column), oscillator strength (length gauge) in atomic units (middle column) as a function of dihedral angles ϕ_1 and ϕ_3. Right column: absorption spectra of the HT derivatives and their conformers. Molecules are listed by rows. A: HT, B: DMHT, C: 2,5-IMHT, D: 1,4-IMHT, E: DIHT.

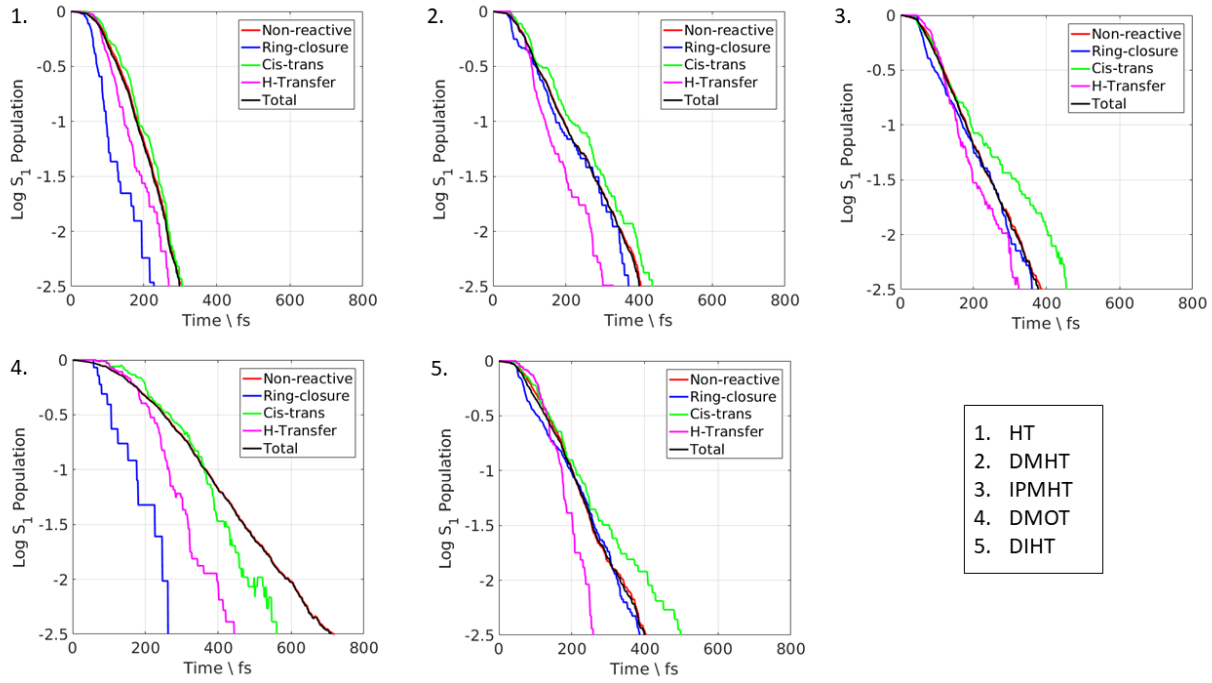

Figure 2: Logarithm of the excited state populations of the HT derivatives for the different reaction channels.