ELECTRONIC SUPPLEMENTARY INFORMATION
ON THE ORIGIN OF THE INVERTED SINGLET-TRIPLET GAP OF THE 5TH GENERATION LIGHT-EMITTING MOLECULES

This directory contains optimized molecular geometries of molecules **1**-**6**. The subdirectories (below in **bold**) comprise geometries optimized at the following levels of theory denoted as follows:

MP2_ground_state

 - ground state molecular geometries optimized at the ab initio MP2 level employing the def2-TZVP basis set

B3LYP_ground_state

 - ground state molecular geometries optimized at the DFT level employing the B3LYP functional, D3-BJ dispersion correction, and the def2-TZVPD basis set ADC2_excited_states

ADC2_excited_states

 - excited states molecular geometries optimized at the ab initio ADC(2) level employing the def2-TZVP basis set
 - geometries of the first excited singlet state are denoted as *_s.xyz, whereas the first excited triplet state geometries are denoted as *_t.xyz

CASPT2_ground_state

 - ground state molecular geometries optimized at the XMC-QDPT2 (12 electrons in 9 orbitals) level employing the def2-TZVP basis set.