

Supporting Information For:
Emission quenching in tetraphenylfuran crystal:
Why this propeller-shaped molecule does not
emit in the condensed phase?

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S1 Geometries

The optimised geometries of the ground, excited states, and the minimum energy crossing points between the ground state and S_1 state and the ground state and T_1 state discussed in the main paper are deposited at: https://github.com/Crespo-Otero-group/TPF_data

S2 The CASSCF active space orbitals

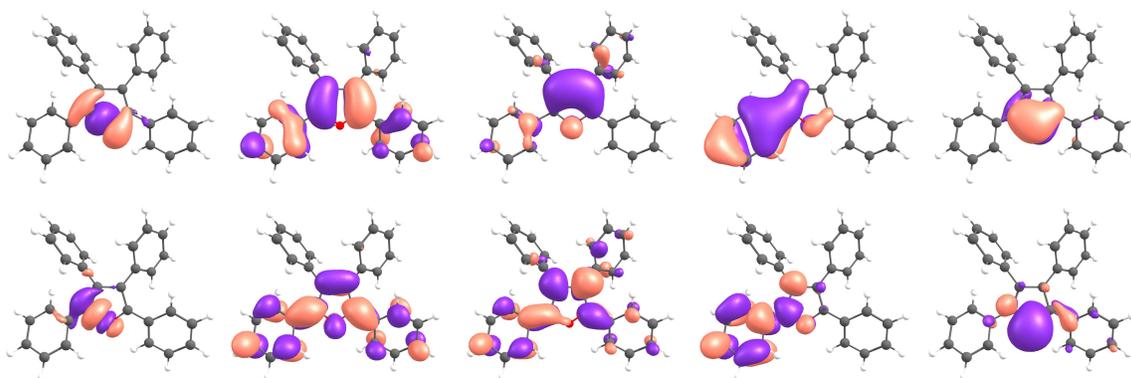


Figure S1: The CASSCF(10,10)/6-31G(d) orbitals used in the S_0/S_1 and S_0/T_1 minimum energy crossing point optimisations and MS-3-CASPT2/SA-3-CASSCF(10,10)/6-31G(d) single point computations along the optimised pathways in the vacuum and crystal.