

Supporting Information For:

Emission quenching in tetraphenylfuran crystal:

Why this propeller-shaped molecule does not

emit in the condensed phase?

Ljiljana Stojanović, and Rachel Crespo-Otero*

*School of Physical and Chemical Sciences,
Queen Mary University of London, Mile End Road, London E1 4NS, UK*

E-mail: r.crespo-otero@qmul.ac.uk

Contents

S1 Geometries	3
S2 The CASSCF active space orbitals	3

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

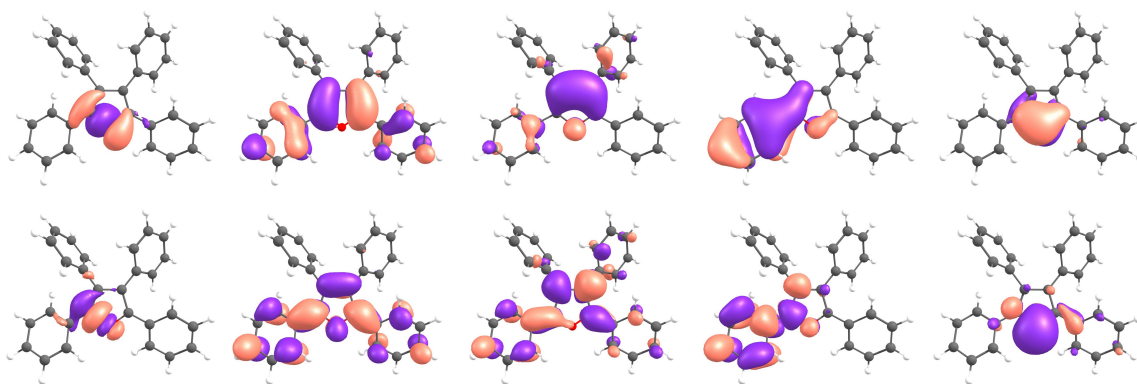


Figure S1: The CASSCF(10,10)/6-31G(d) orbitals used in the S_0/S_1 and S_0/T_1 minimum energy crossing point optimisations and MS-3-CASPT2/SA-3-CASSCF(10,10)/6-31G(d) single point computations along the optimised pathways in the vacuum and crystal.