Supplementary Information

Protic Processes in an Extended Pyrazinacene: The Case of Dihydrotetradecaazaheptacene

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Table S1. Bond length averages for optimised structures.

Average bond length (Å)				
Tautomer	Acene C-C	Outer Acene C-C	Ph C-C	C-N
T0	1.448	1.484	1.393	1.337
T1	1.449	1.484	1.393	1.337
T2	1.453	1.485	1.396	1.341
T3	1.452	1.480	1.393	1.339
T0-H0	1.450	1.472	1.393	1.343
T0-H1	1.449	1.474	1.393	1.338
T0-H2	1.449	1.474	1.394	1.337
T0-H3	1.449	1.475	1.393	1.337
T1-H0	1.449	1.474	1.393	1.338
T1-H1	1.449	1.474	1.394	1.336
T1-H2	1.449	1.474	1.393	1.336
T1-H3	1.449	1.475	1.393	1.336
T2-H0	1.450	1.474	1.393	1.337
T2-H2	1.453	1.485	1.396	1.341
T2-H3	1.451	1.475	1.393	1.337
Ox	1.472	1.478	1.393	1.332
MA	1.453	1.488	1.393	1.336
DA	1.459	1.489	1.393	1.336

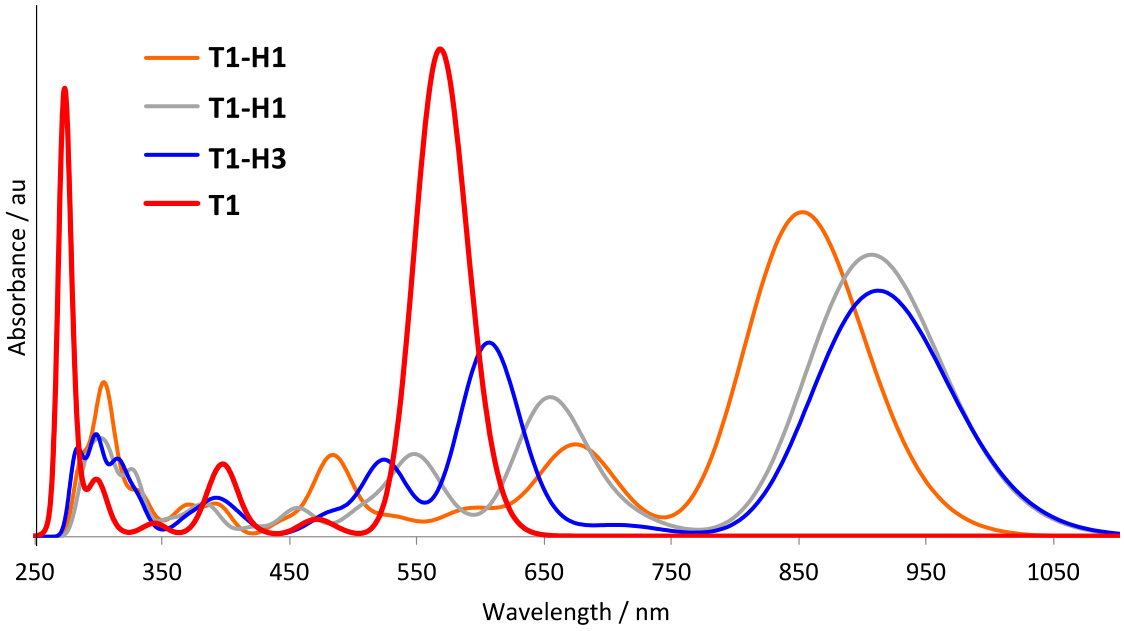

Figure S1. Calculated electronic absorption spectra for tautomer **T1** and the monoprotonated tautomers **T1-H1**, **T1-H2**, and **T1-H3**.

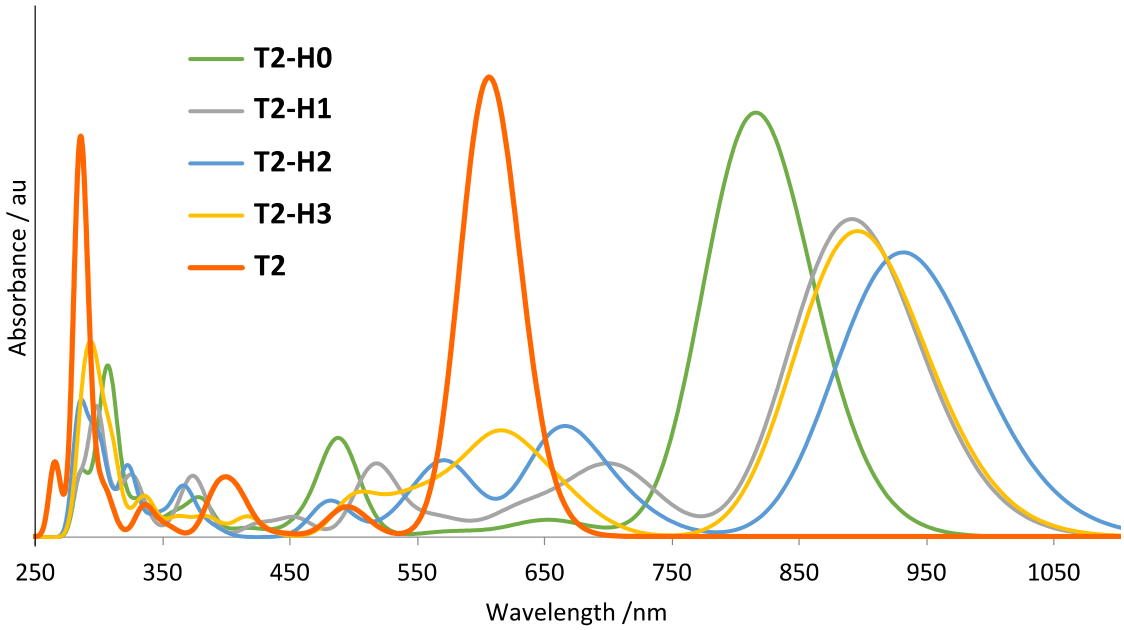

Figure S2. Calculated electronic absorption spectra for tautomer **T2** and the monoprotonated tautomers **T2-H0**, **T2-H1**, **T2-H2**, and **T2-H3**.