

Electronic Supplementary Information

Photophysical properties of 5-substituted 2-thiopyrimidines

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Table S1. Total energies (in a.u.) for the optimised geometries of ground-state singlet (S_0) and lowest triplet (T_1) states of 2-thiopyrimidines TU, BTU and TT using different DFT functionals (B3LYP, CAM-B3LYP, ω B97XD, M062X and PBE0) and basis sets (6-31+G(d), cc-pVDZ, aug-cc-pVDZ and aug-cc-pVTZ) with solvent effects considered using PCM method. Note that only (U)B3LYP/aug-cc-pVDZ/PCM geometries and energies are discussed throughout the manuscript.

TU

S_0 Basis set / DFT functional	B3LYP	CAM-B3LYP	ωB97XD	M062X	PBE0
6-31+G(d)	-737.804185096	-737.640374854	-737.670177942	-737.627349352	-737.272251364
cc-pVDZ	-737.831460943	-737.666976242	-737.703236718	-737.675453511	-737.306565194
aug-cc-pVDZ	-737.862271802	-737.698826626	-737.729424804	-737.702437627	-737.333148505
aug-cc-pVTZ	-737.956269217	-737.698826626	-737.817267733	-737.791805939	-737.418253228
T_1 Basis set / DFT functional	UB3LYP	UCAM-B3LYP	UωB97XD	UM062X	UPBE0
6-31+G(d)	-737.692916563	-737.525859809	-737.553480929	-737.506787103	-737.161147680
cc-pVDZ	-737.719790530	-737.552333776	-737.586265375	-737.554012472	-737.194981776
aug-cc-pVDZ	-737.751892332	-737.584909651	-737.613157183	-737.582252437	-737.222763400
aug-cc-pVTZ	-737.844684484	-737.679663632	-737.699705595	-737.670567542	-737.306893073

TBU

S_0 Basis set / DFT functional	B3LYP	CAM-B3LYP	ωB97XD	M062X	PBE0
6-31+G(d)	-895.062698936	-894.800913459	-894.889464155	-894.808935272	-894.337651186
cc-pVDZ	-895.090510139	-894.827693163	-894.927022268	-894.863671545	-894.377760150
aug-cc-pVDZ	-895.130769355	-894.868800470	-894.960414224	-894.960414224	-894.411109048
aug-cc-pVTZ	-895.267179368	-895.008455768	-895.085882613	-895.028425878	-894.531642526
T_1 Basis set / DFT functional	UB3LYP	UCAM-B3LYP	UωB97XD	UM062X	UPBE0
6-31+G(d)	-894.954599820	-894.690161588	-894.777014449	-894.691889918	-894.229848257
cc-pVDZ	-894.981608757	-894.716262776	-894.813883305	-894.745593981	-894.269076275
aug-cc-pVDZ	-895.023218486	-894.758377650	-894.848093673	-894.783113868	-894.303778630
aug-cc-pVTZ	-895.158471229	-894.896616311	-894.972325689	-894.910836985	-894.423363946

TT

S_0 Basis set / DFT functional	B3LYP	CAM-B3LYP	ωB97XD	M062X	PBE0
6-31+G(d)	-777.124778774	-776.935940006	-776.979574313	-776.927164643	-776.544209555
cc-pVDZ	-777.151991624	-776.962475377	-777.013813894	-776.976993738	-776.580009269
aug-cc-pVDZ	-777.184914730	-776.996342210	-777.041496504	-777.005901358	-776.608023833
aug-cc-pVTZ	-777.289748630	-777.103750053	-777.138939798	-777.105396820	-776.702131850
T_1 Basis set / DFT functional	UB3LYP	UCAM-B3LYP	UωB97XD	UM062X	UPBE0
6-31+G(d)	-777.019418664	-776.828080123	-776.869575573	-776.812573948	-776.439370227
cc-pVDZ	-777.046450968	-776.854611148	-776.903713888	-776.861801355	-776.474908530
aug-cc-pVDZ	-777.080618142	-776.889406921	-776.932216885	-776.892071314	-776.504175476
aug-cc-pVTZ	-777.184348314	-776.995429449	-777.028501946	-776.990684269	-776.597445008

Table S2. Cartesian coordinates of the optimised geometries of the ground-state singlet (S_0) and lowest triplet (T_1) states of 2-thiopyrimidines TU, BTU and TT at (U)B3LYP/aug-cc-pVDZ/PCM level.

TU S_0

E(RB3LYP) = -737.862271802 a.u.

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.41072200
C	1.08540600	0.00000000	2.23981100
N	2.28765600	0.00002800	1.58954200
C	2.41233000	0.00003800	0.22131600
C	1.32465700	0.00002700	-0.58788500
S	0.96276600	0.00002400	3.92047500
O	-1.06976000	0.00001400	-0.60500900
H	3.43289600	0.00006100	-0.15434500
H	-0.91125900	0.00000100	1.85854900
H	3.11542900	0.00004500	2.17308300
H	1.42136400	0.00004200	-1.66930100

TU T_1

E(UB3LYP) = -737.751892332 a.u.

N	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.36719900
C	1.33207400	0.00000000	2.01057500
C	2.50693100	-0.22822000	1.23849300
N	2.28385100	-0.40865800	-0.15079500
C	1.07861900	-0.20085300	-0.79352500
O	3.66721700	-0.28503500	1.67388000
S	0.94180900	-0.22680800	-2.48309700
H	1.43188900	0.18805100	3.07606300
H	-0.92575800	0.23793000	1.87556700
H	3.10172600	-0.53507700	-0.73443200
H	-0.87720700	0.13203900	-0.49455900

BTU S_0

E(RB3LYP) = -895.130769355 a.u.

N	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.36234800
N	1.24732400	0.00000000	1.90337200
C	2.40606200	0.00000000	1.15851900
C	2.41924300	0.00000000	-0.20237000
C	1.11211300	0.00000000	-0.86819400
S	-1.40990700	0.00000000	2.29269700
C	3.71248000	0.00000000	-1.02454400
C	4.95244900	-0.00002200	-0.11131000
O	0.89672000	0.00000500	-2.07830100
C	3.76430300	-1.26720800	-1.91060200
C	3.76432100	1.26723300	-1.91056700
H	3.30980400	0.00000000	1.75870300
H	-0.90727800	0.00000000	-0.45530200
H	1.30397800	0.00000000	2.91441600
H	3.75071500	2.17491200	-1.29156200
H	4.69470100	1.26834200	-2.49506700
H	2.91956300	1.30555300	-2.60590600
H	5.85577900	-0.00002100	-0.73432800
H	4.99253500	0.89225700	0.52872700
H	4.99251800	-0.89231800	0.52870600

H	3.75066500	-2.17490600	-1.29162400
H	2.91955500	-1.30548900	-2.60595600
H	4.69469200	-1.26832300	-2.49508900

BTU T₁

E(UB3LYP) = -895.023218486 a.u.

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.43623000
N	1.28701800	0.00000000	2.05278700
C	2.46398300	0.33087700	1.42238200
N	2.42477400	0.27775100	0.06869100
C	1.33294000	-0.09917700	-0.67244500
O	-0.98915600	-0.00074500	2.18502000
S	3.87634400	0.72519300	2.26317200
C	-1.28520700	0.11028900	-0.80151600
C	-2.16147800	-1.14053400	-0.51048900
C	-2.05890000	1.39245200	-0.39905600
C	-1.01262500	0.16550700	-2.31820600
H	1.46377400	-0.10452000	-1.74495300
H	1.28133300	0.06274600	3.06381200
H	3.30213800	0.47624200	-0.40185100
H	-1.45963800	2.28866200	-0.60925000
H	-2.98414900	1.45570300	-0.98829700
H	-2.31935300	1.38374400	0.66367100
H	-1.96992200	0.24093500	-2.84936900
H	-0.40900300	1.04002400	-2.59455100
H	-0.50560400	-0.73926300	-2.67890400
H	-1.63552000	-2.06134800	-0.79616000
H	-2.42698400	-1.19950300	0.54943400
H	-3.08336100	-1.07508600	-1.10525100

TT S₀

E(RB3LYP) = -777.184914730 a.u.

C	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.40711100
C	1.08481100	0.00000000	2.23619100
N	2.27863600	0.00000900	1.58221100
C	2.40112000	0.00000800	0.20953100
C	1.32277300	-0.00000200	-0.61584100
S	0.95991800	0.00001200	3.92048800
C	1.42602000	-0.00000300	-2.11247000
O	-1.07135000	-0.00000500	-0.60349900
H	3.42433000	0.00001600	-0.15942200
H	2.47478500	0.00000500	-2.43052800
H	0.92920400	-0.88360900	-2.53731200
H	0.92919000	0.88359300	-2.53731600
H	-0.91205000	-0.00000400	1.85302300
H	3.11034300	0.00001600	2.15983000

TT T₁

E(UB3LYP) = -777.080618142 a.u.

N	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.37184800
C	1.33255800	0.00000000	2.03824200
C	2.49835700	-0.24819500	1.25067400
N	2.26952800	-0.44330000	-0.13862200
C	1.07740500	-0.23234600	-0.79159300
C	1.40207400	0.25084500	3.49400400

O	3.66468300	-0.31761000	1.67194400
S	0.94635100	-0.28075100	-2.47626300
H	-0.90710400	0.32330900	1.86987800
H	3.08889700	-0.59316800	-0.71425700
H	-0.87398500	0.14478100	-0.49521200
H	0.79210100	-0.49246300	4.03811200
H	2.43190900	0.21761600	3.86010400
H	0.95744500	1.23281900	3.73554300

Table S3A. Interatomic distances (in angstroms) of the optimised singlet ground-state (S_0) geometries of TU at different DFT levels (solvent effects considered using PCM method). See manuscript for atom numbering.

TU S_0				
	<i>B3LYP/</i> <i>6-31+G(d)</i>	<i>B3LYP/</i> <i>cc-pVDZ</i>	<i>B3LYP/</i> <i>aug-cc-pVDZ</i>	<i>B3LYP/</i> <i>aug-cc-pVTZ</i>
<i>C4=O</i>	1.23081	1.22296	1.22899	1.22205
<i>C4-N3</i>	1.41104	1.41534	1.41072	1.40676
<i>N3-C2</i>	1.36727	1.36559	1.36583	1.36019
<i>C2=S</i>	1.68020	1.68265	1.68513	1.67550
<i>C2-N1</i>	1.36809	1.36902	1.36684	1.36155
<i>N1-C6</i>	1.37427	1.37402	1.37389	1.36865
<i>C6=C5</i>	1.35510	1.35502	1.35567	1.34659
<i>C5-H</i>	1.08191	1.08762	1.08573	1.07684
<i>C5-C4</i>	1.44854	1.45339	1.44925	1.44418
	<i>CAM-B3LYP/</i> <i>6-31+G(d)</i>	<i>CAM-B3LYP/</i> <i>cc-pVDZ</i>	<i>CAM-B3LYP/</i> <i>aug-cc-pVDZ</i>	<i>CAM-B3LYP/</i> <i>aug-cc-pVTZ</i>
<i>C4=O</i>	1.22464	1.21675	1.22296	1.21612
<i>C4-N3</i>	1.40235	1.40644	1.40190	1.39794
<i>N3-C2</i>	1.36069	1.35902	1.35924	1.35370
<i>C2=S</i>	1.67341	1.67553	1.67837	1.66893
<i>C2-N1</i>	1.35898	1.36012	1.35782	1.35255
<i>N1-C6</i>	1.37246	1.37219	1.37206	1.36697
<i>C6=C5</i>	1.34678	1.34681	1.34747	1.33834
<i>C5-H</i>	1.08115	1.08687	1.08505	1.07628
<i>C5-C4</i>	1.44645	1.45134	1.44717	1.44226
	<i>ωB97XD/</i> <i>6-31+G(d)</i>	<i>ωB97XD/</i> <i>cc-pVDZ</i>	<i>ωB97XD/</i> <i>aug-cc-pVDZ</i>	<i>ωB97XD/</i> <i>aug-cc-pVTZ</i>
<i>C4=O</i>	1.22398	1.21692	1.22242	1.21545
<i>C4-N3</i>	1.40445	1.40842	1.40429	1.40059
<i>N3-C2</i>	1.36151	1.35972	1.35949	1.35427
<i>C2=S</i>	1.67486	1.67808	1.68104	1.67155
<i>C2-N1</i>	1.36023	1.36094	1.35857	1.35367
<i>N1-C6</i>	1.37252	1.37243	1.37238	1.36726
<i>C6=C5</i>	1.34844	1.34869	1.34934	1.34046
<i>C5-H</i>	1.08130	1.08688	1.08516	1.07659
<i>C5-C4</i>	1.44773	1.45257	1.44887	1.44429
	<i>M062X/</i> <i>6-31+G(d)</i>	<i>M062X/</i> <i>cc-pVDZ</i>	<i>M062X/</i> <i>aug-cc-pVDZ</i>	<i>M062X/</i> <i>aug-cc-pVTZ</i>
<i>C4=O</i>	1.22130	1.21491	1.22011	1.21487
<i>C4-N3</i>	1.40526	1.40820	1.40503	1.40099
<i>N3-C2</i>	1.36136	1.35995	1.35989	1.35631
<i>C2=S</i>	1.67314	1.67551	1.67846	1.66866
<i>C2-N1</i>	1.36031	1.36139	1.35936	1.35565
<i>N1-C6</i>	1.37314	1.37240	1.37261	1.36890
<i>C6=C5</i>	1.34871	1.34892	1.34951	1.34129
<i>C5-H</i>	1.08123	1.08613	1.08451	1.07675
<i>C5-C4</i>	1.45035	1.45398	1.45094	1.44624
	<i>PBE0/</i> <i>6-31+G(d)</i>	<i>PBE0/</i> <i>cc-pVDZ</i>	<i>PBE0/</i> <i>aug-cc-pVDZ</i>	<i>PBE0/</i> <i>aug-cc-pVTZ</i>
<i>C4=O</i>	1.22529	1.21864	1.22430	1.21864
<i>C4-N3</i>	1.40298	1.40651	1.40260	1.40651
<i>N3-C2</i>	1.36048	1.35873	1.35895	1.35873
<i>C2=S</i>	1.67027	1.67327	1.67576	1.67327
<i>C2-N1</i>	1.36136	1.36183	1.36006	1.36183
<i>N1-C6</i>	1.36728	1.36730	1.36732	1.36730
<i>C6=C5</i>	1.35182	1.35168	1.35248	1.35168
<i>C5-H</i>	1.08206	1.08727	1.08574	1.08727
<i>C5-C4</i>	1.44460	1.44838	1.44502	1.44838

Table S3B. Interatomic distances (in angstroms) of the optimised lowest triplet state (T_1) geometries of TU at different DFT levels (solvent effects considered using PCM method). See manuscript for atom numbering.

TU T_1				
	UB3LYP/ 6-31+G(d)	UB3LYP/ cc-pVDZ	UB3LYP/ aug-cc-pVDZ	UB3LYP/ aug-cc-pVTZ
C4=O	1.24216	1.23437	1.24059	1.23376
C4-N3	1.42097	1.42404	1.41861	1.41317
N3-C2	1.38226	1.37893	1.38162	1.37841
C2=S	1.68752	1.69177	1.69530	1.68773
C2-N1	1.35623	1.35681	1.35405	1.34776
N1-C6	1.37382	1.37466	1.36720	1.35646
C6=C5	1.48149	1.48530	1.47931	1.46994
C5-H	1.08257	1.08875	1.08655	1.07706
C5-C4	1.42305	1.42765	1.42425	1.41888
	UCAM-B3LYP/ 6-31+G(d)	UCAM-B3LYP/ cc-pVDZ	UCAM-B3LYP/ aug-cc-pVDZ	UCAM-B3LYP/ aug-cc-pVTZ
C4=O	1.23308	1.22589	1.23197	1.22560
C4-N3	1.40850	1.41202	1.40792	1.40404
N3-C2	1.37594	1.37306	1.37350	1.36881
C2=S	1.66840	1.67238	1.67370	1.66420
C2-N1	1.35614	1.35680	1.35491	1.34905
N1-C6	1.37683	1.37713	1.37498	1.36731
C6=C5	1.49000	1.49218	1.49049	1.48313
C5-H	1.08245	1.08883	1.08662	1.07738
C5-C4	1.42499	1.42899	1.42473	1.41848
	UwB97XD/ 6-31+G(d)	UwB97XD/ cc-pVDZ	UwB97XD/ aug-cc-pVDZ	UwB97XD/ aug-cc-pVTZ
C4=O	1.23204	1.22565	1.23096	1.22447
C4-N3	1.41082	1.41427	1.41080	1.40686
N3-C2	1.37745	1.37460	1.37456	1.37003
C2=S	1.66964	1.67440	1.67588	1.66643
C2-N1	1.35807	1.35843	1.35677	1.35132
N1-C6	1.37735	1.37772	1.37576	1.36815
C6=C5	1.49100	1.49306	1.49198	1.48523
C5-H	1.08277	1.08924	1.08701	1.07789
C5-C4	1.42727	1.43130	1.42746	1.42158
	UM062X/ 6-31+G(d)	UM062X/ cc-pVDZ	UM062X/ aug-cc-pVDZ	UM062X/ aug-cc-pVTZ
C4=O	1.22865	1.22232	1.22800	1.22271
C4-N3	1.41278	1.41515	1.41228	1.40788
N3-C2	1.37969	1.37790	1.37747	1.37440
C2=S	1.66785	1.67163	1.67333	1.66375
C2-N1	1.35762	1.35793	1.35677	1.35233
N1-C6	1.37568	1.37569	1.37329	1.36853
C6=C5	1.48997	1.49120	1.49037	1.48534
C5-H	1.08220	1.08838	1.08595	1.07777
C5-C4	1.43121	1.43544	1.43115	1.42611
	UPBE0/ 6-31+G(d)	UPBE0/ cc-pVDZ	UPBE0/ aug-cc-pVDZ	UPBE0/ aug-cc-pVTZ
C4=O	1.23406	1.22775	1.23354	1.22740
C4-N3	1.40911	1.41198	1.40871	1.40455
N3-C2	1.37619	1.37334	1.37375	1.36973
C2=S	1.67226	1.67658	1.67822	1.66985
C2-N1	1.35268	1.35298	1.35131	1.34575
N1-C6	1.37018	1.37109	1.36853	1.36064
C6=C5	1.48246	1.48472	1.48231	1.47594
C5-H	1.08304	1.08898	1.08709	1.07929
C5-C4	1.42496	1.42836	1.42475	1.41983

Table S3C. Interatomic distances (in angstroms) of the optimised singlet ground-state (S_0) geometries of BTU at different DFT levels (solvent effects considered using PCM method). See manuscript for atom numbering.

BTU S_0				
	B3LYP/ 6-31+G(d)	B3LYP/ cc-pVDZ	B3LYP/ aug-cc-pVDZ	B3LYP/ aug-cc-pVTZ
C4=O	1,23088	1,22654	1,22913	1,22214
C4-N3	1,41135	1,41174	1,41087	1,40693
N3-C2	1,36380	1,36405	1,36235	1,35675
C2=S	1,68411	1,68501	1,68920	1,67966
C2-N1	1,36103	1,36231	1,35960	1,35423
N1-C6	1,37763	1,37709	1,37749	1,37240
C6=C5	1,36056	1,36091	1,36095	1,35228
C5-C(CH₃)₃	1,53342	1,53346	1,53246	1,52855
C5-C4	1,46651	1,46940	1,46694	1,46273
	CAM-B3LYP/ 6-31+G(d)	CAM-B3LYP/ cc-pVDZ	CAM-B3LYP/ aug-cc-pVDZ	CAM-B3LYP/ aug-cc-pVTZ
C4=O	1,22473	1,2203	1,22305	1,21617
C4-N3	1,4026	1,40305	1,40209	1,39825
N3-C2	1,35743	1,35775	1,35601	1,35049
C2=S	1,67743	1,67789	1,68246	1,67314
C2-N1	1,35205	1,35357	1,35072	1,34538
N1-C6	1,37607	1,37546	1,37583	1,37092
C6=C5	1,35128	1,35176	1,35174	1,34304
C5-C(CH₃)₃	1,52665	1,52669	1,52569	1,52168
C5-C4	1,46316	1,46599	1,46356	1,45949
	ωB97XD/ 6-31+G(d)	ωB97XD/ cc-pVDZ	ωB97XD/ aug-cc-pVDZ	ωB97XD/ aug-cc-pVTZ
C4=O	1,22427	1,22016	1,22279	1,21592
C4-N3	1,40415	1,40501	1,40388	1,40009
N3-C2	1,35825	1,35808	1,35634	1,35116
C2=S	1,67888	1,68072	1,68501	1,67551
C2-N1	1,3532	1,35423	1,35152	1,34652
N1-C6	1,37586	1,37541	1,37571	1,3707
C6=C5	1,35305	1,35375	1,35374	1,34535
C5-C(CH₃)₃	1,52739	1,52783	1,5269	1,52287
C5-C4	1,46454	1,46754	1,46536	1,46153
	M062X/ 6-31+G(d)	M062X/ cc-pVDZ	M062X/ aug-cc-pVDZ	M062X/ aug-cc-pVTZ
C4=O	1,22193	1,21824	1,22279	1,21538
C4-N3	1,40475	1,40489	1,40388	1,40085
N3-C2	1,35883	1,35901	1,35634	1,35365
C2=S	1,67712	1,6782	1,68502	1,67258
C2-N1	1,35379	1,35508	1,35151	1,34894
N1-C6	1,3768	1,37577	1,37571	1,37276
C6=C5	1,35343	1,35408	1,35374	1,34635
C5-C(CH₃)₃	1,52322	1,52317	1,52691	1,51935
C5-C4	1,46603	1,46813	1,46537	1,4626
	PBE0/ 6-31+G(d)	PBE0/ cc-pVDZ	PBE0/ aug-cc-pVDZ	PBE0/ aug-cc-pVTZ
C4=O	1,22576	1,22205	1,22483	1,2183
C4-N3	1,40277	1,4031	1,40235	1,39875
N3-C2	1,35752	1,35739	1,35606	1,3511
C2=S	1,674	1,67561	1,67951	1,67054
C2-N1	1,35476	1,35561	1,35341	1,34863
N1-C6	1,37053	1,37013	1,37064	1,36591
C6=C5	1,35711	1,3574	1,35758	1,34983
C5-C(CH₃)₃	1,52288	1,52321	1,52236	1,51822
C5-C4	1,46113	1,46319	1,46121	1,45769

Table S3D. Interatomic distances (in angstroms) of the optimised lowest triplet state (T_1) geometries of BTU at different DFT levels (solvent effects considered using PCM method). See manuscript for atom numbering.

BTU T_1				
	UB3LYP/ 6-31+G(d)	UB3LYP/ cc-pVDZ	UB3LYP/ aug-cc-pVDZ	UB3LYP/ aug-cc-pVTZ
C4=O	1,24178	1,23729	1,24061	1,23381
C4-N3	1,42800	1,42778	1,42708	1,42325
N3-C2	1,37806	1,37783	1,37555	1,37084
C2=S	1,68445	1,68829	1,69032	1,68073
C2-N1	1,35694	1,35681	1,35530	1,34957
N1-C6	1,37525	1,37446	1,37239	1,36496
C6=C5	1,49678	1,49807	1,49624	1,48965
C5-C(CH₃)₃	1,51924	1,52103	1,51867	1,51388
C5-C4	1,43624	1,43949	1,43623	1,43071
	UCAM-B3LYP/ 6-31+G(d)	UCAM-B3LYP/ cc-pVDZ	UCAM-B3LYP/ aug-cc-pVDZ	UCAM-B3LYP/ aug-cc-pVTZ
C4=O	1,23301	1,22851	1,23190	1,22538
C4-N3	1,41550	1,41549	1,41526	1,41157
N3-C2	1,37197	1,37211	1,36951	1,36453
C2=S	1,67025	1,67282	1,67531	1,66572
C2-N1	1,35423	1,35459	1,35310	1,34752
N1-C6	1,37660	1,37613	1,37471	1,36766
C6=C5	1,50050	1,50101	1,50090	1,49470
C5-C(CH₃)₃	1,51239	1,51426	1,51170	1,50668
C5-C4	1,43578	1,43938	1,43538	1,42973
	UωB97XD/ 6-31+G(d)	UωB97XD/ cc-pVDZ	UωB97XD/ aug-cc-pVDZ	UωB97XD/ aug-cc-pVTZ
C4=O	1,23119	1,22691	1,23036	1,22379
C4-N3	1,41645	1,41689	1,41703	1,41307
N3-C2	1,37503	1,37470	1,37200	1,36720
C2=S	1,67164	1,67514	1,67773	1,66807
C2-N1	1,35586	1,35606	1,35459	1,34932
N1-C6	1,37719	1,37678	1,37537	1,36842
C6=C5	1,49900	1,49932	1,50018	1,49431
C5-C(CH₃)₃	1,51327	1,51523	1,51287	1,50795
C5-C4	1,44018	1,44415	1,43970	1,43440
	UM062X/ 6-31+G(d)	UM062X/ cc-pVDZ	UM062X/ aug-cc-pVDZ	UM062X/ aug-cc-pVTZ
C4=O	1,22974	1,22553	1,22933	1,22370
C4-N3	1,41933	1,41878	1,41989	1,41537
N3-C2	1,37629	1,37699	1,37373	1,37071
C2=S	1,66966	1,67245	1,67492	1,66532
C2-N1	1,35603	1,35613	1,35528	1,35090
N1-C6	1,37542	1,37470	1,37287	1,36866
C6=C5	1,49837	1,49825	1,49910	1,49454
C5-C(CH₃)₃	1,51062	1,51207	1,50954	1,50556
C5-C4	1,43982	1,44390	1,43924	1,43509
	UPBE0/ 6-31+G(d)	UPBE0/ cc-pVDZ	UPBE0/ aug-cc-pVDZ	UPBE0/ aug-cc-pVTZ
C4=O	1,23387	1,22997	1,23355	1,22728
C4-N3	1,41546	1,41530	1,41558	1,41165
N3-C2	1,37326	1,37306	1,37075	1,36616
C2=S	1,67179	1,67534	1,67737	1,66846
C2-N1	1,35222	1,35206	1,35106	1,34584
N1-C6	1,37069	1,37042	1,36915	1,36243
C6=C5	1,49338	1,49363	1,49345	1,48812
C5-C(CH₃)₃	1,51060	1,51253	1,51039	1,50553
C5-C4	1,43688	1,43989	1,43623	1,43155

Table S3E. Interatomic distances (in angstroms) of the optimised singlet ground-state (S_0) geometries of TT at different DFT levels (solvent effects considered using PCM method). See manuscript for atom numbering.

TT S_0				
	<i>B3LYP/</i> <i>6-31+G(d)</i>	<i>B3LYP/</i> <i>cc-pVDZ</i>	<i>B3LYP/</i> <i>aug-cc-pVDZ</i>	<i>B3LYP/</i> <i>aug-cc-pVTZ</i>
<i>C4=O</i>	1.23157	1.22468	1.22963	1.22273
<i>C4-N3</i>	1.40751	1.40972	1.40711	1.40302
<i>N3-C2</i>	1.36680	1.36621	1.36535	1.35980
<i>C2=S</i>	1.68380	1.68558	1.68892	1.67933
<i>C2-N1</i>	1.36269	1.36367	1.36122	1.35579
<i>N1-C6</i>	1.37822	1.37843	1.37813	1.37311
<i>C6=C5</i>	1.35752	1.35738	1.35797	1.34914
<i>C5-CH₃</i>	1.50107	1.49911	1.50019	1.49531
<i>C5-C4</i>	1.45850	1.46240	1.45911	1.45463
	<i>CAM-B3LYP/</i> <i>6-31+G(d)</i>	<i>CAM-B3LYP/</i> <i>cc-pVDZ</i>	<i>CAM-B3LYP/</i> <i>aug-cc-pVDZ</i>	<i>CAM-B3LYP/</i> <i>aug-cc-pVTZ</i>
<i>C4=O</i>	1.22528	1.21832	1.22343	1.21666
<i>C4-N3</i>	1.39901	1.40120	1.39856	1.39450
<i>N3-C2</i>	1.36032	1.35978	1.35889	1.35342
<i>C2=S</i>	1.67711	1.67857	1.68227	1.67290
<i>C2-N1</i>	1.35355	1.35470	1.35209	1.34669
<i>N1-C6</i>	1.37672	1.37700	1.37666	1.37179
<i>C6=C5</i>	1.34841	1.34836	1.34892	1.34003
<i>C5-CH₃</i>	1.49661	1.49483	1.49574	1.49079
<i>C5-C4</i>	1.45546	1.45933	1.45609	1.45173
	<i>ωB97XD/</i> <i>6-31+G(d)</i>	<i>ωB97XD/</i> <i>cc-pVDZ</i>	<i>ωB97XD/</i> <i>aug-cc-pVDZ</i>	<i>ωB97XD/</i> <i>aug-cc-pVTZ</i>
<i>C4=O</i>	1.22469	1.21842	1.22300	1.21615
<i>C4-N3</i>	1.40090	1.40324	1.40071	1.39683
<i>N3-C2</i>	1.36166	1.36028	1.35919	1.35407
<i>C2=S</i>	1.67850	1.68113	1.68480	1.67535
<i>C2-N1</i>	1.35479	1.35552	1.35294	1.34788
<i>N1-C6</i>	1.37669	1.37700	1.37680	1.37187
<i>C6=C5</i>	1.35020	1.35051	1.35094	1.34226
<i>C5-CH₃</i>	1.49782	1.49648	1.49718	1.49238
<i>C5-C4</i>	1.45682	1.46083	1.45788	1.45373
	<i>M062X/</i> <i>6-31+G(d)</i>	<i>M062X/</i> <i>cc-pVDZ</i>	<i>M062X/</i> <i>aug-cc-pVDZ</i>	<i>M062X/</i> <i>aug-cc-pVTZ</i>
<i>C4=O</i>	1.22214	1.21647	1.22076	1.21564
<i>C4-N3</i>	1.40140	1.40278	1.40122	1.39712
<i>N3-C2</i>	1.36147	1.36095	1.36005	1.35648
<i>C2=S</i>	1.67685	1.67869	1.68241	1.67259
<i>C2-N1</i>	1.35511	1.35610	1.35383	1.35000
<i>N1-C6</i>	1.37757	1.37726	1.37740	1.37385
<i>C6=C5</i>	1.35010	1.35031	1.35067	1.34264
<i>C5-CH₃</i>	1.49683	1.49507	1.49599	1.49202
<i>C5-C4</i>	1.45854	1.46146	1.45913	1.45479
	<i>PBE0/</i> <i>6-31+G(d)</i>	<i>PBE0/</i> <i>cc-pVDZ</i>	<i>PBE0/</i> <i>aug-cc-pVDZ</i>	<i>PBE0/</i> <i>aug-cc-pVTZ</i>
<i>C4=O</i>	1.22605	1.22020	1.22495	1.21852
<i>C4-N3</i>	1.39929	1.40111	1.39893	1.39515
<i>N3-C2</i>	1.36020	1.35937	1.35869	1.35379
<i>C2=S</i>	1.67370	1.67616	1.67936	1.67039
<i>C2-N1</i>	1.35622	1.35671	1.35471	1.34988
<i>N1-C6</i>	1.37115	1.37154	1.37144	1.36679
<i>C6=C5</i>	1.35425	1.35413	1.35476	1.34693
<i>C5-CH₃</i>	1.49287	1.49091	1.49192	1.48781
<i>C5-C4</i>	1.45402	1.45702	1.45434	1.45067

Table S3F. Interatomic distances (in angstroms) of the optimised lowest triplet state (T_1) geometries of TT at different DFT levels (solvent effects considered using PCM method). See manuscript for atom numbering.

TT T_1				
	UB3LYP/ 6-31+G(d)	UB3LYP/ cc-pVDZ	UB3LYP/ aug-cc-pVDZ	UB3LYP/ aug-cc-pVTZ
C4=O	1,24342	1,23690	1,24202	1,23528
C4-N3	1,42285	1,42407	1,42147	1,41761
N3-C2	1,37795	1,37593	1,37551	1,37107
C2=S	1,68478	1,68891	1,69045	1,68091
C2-N1	1,35826	1,35866	1,35698	1,35126
N1-C6	1,37470	1,37517	1,37185	1,36394
C6=C5	1,49109	1,49391	1,48990	1,48304
C5-CH₃	1,48051	1,47899	1,47885	1,47309
C5-C4	1,42813	1,43188	1,42862	1,42302
	UCAM-B3LYP/ 6-31+G(d)	UCAM-B3LYP/ cc-pVDZ	UCAM-B3LYP/ aug-cc-pVDZ	UCAM-B3LYP/ aug-cc-pVTZ
C4=O	1,23545	1,22928	1,23438	1,22790
C4-N3	1,41279	1,41426	1,41180	1,40816
N3-C2	1,37116	1,36918	1,36810	1,36341
C2=S	1,67062	1,67420	1,67602	1,66638
C2-N1	1,35550	1,35608	1,35446	1,34889
N1-C6	1,37571	1,37590	1,37363	1,36629
C6=C5	1,49588	1,49811	1,49540	1,48890
C5-CH₃	1,47493	1,47374	1,47286	1,46689
C5-C4	1,42563	1,42895	1,42548	1,41975
	UwB97XD/ 6-31+G(d)	UwB97XD/ cc-pVDZ	UwB97XD/ aug-cc-pVDZ	UwB97XD/ aug-cc-pVTZ
C4=O	1,23429	1,22873	1,23338	1,22682
C4-N3	1,41514	1,41684	1,41468	1,41083
N3-C2	1,37324	1,37114	1,36949	1,36486
C2=S	1,67179	1,67621	1,67836	1,66883
C2-N1	1,35725	1,35751	1,35599	1,35071
N1-C6	1,37606	1,37631	1,37426	1,36694
C6=C5	1,49681	1,49918	1,49713	1,49105
C5-CH₃	1,47650	1,47554	1,47468	1,46895
C5-C4	1,42792	1,43146	1,42798	1,42256
	UM062X/ 6-31+G(d)	UM062X/ cc-pVDZ	UM062X/ aug-cc-pVDZ	UM062X/ aug-cc-pVTZ
C4=O	1,23207	1,22655	1,23167	1,22641
C4-N3	1,41775	1,41868	1,41660	1,41246
N3-C2	1,37526	1,37431	1,37165	1,36843
C2=S	1,66976	1,67327	1,67538	1,66588
C2-N1	1,35729	1,35755	1,35670	1,35223
N1-C6	1,37449	1,37448	1,37208	1,36737
C6=C5	1,49439	1,49605	1,49412	1,48984
C5-CH₃	1,47681	1,47555	1,47458	1,46970
C5-C4	1,42912	1,43272	1,42904	1,42405
	UPBE0/ 6-31+G(d)	UPBE0/ cc-pVDZ	UPBE0/ aug-cc-pVDZ	UPBE0/ aug-cc-pVTZ
C4=O	1,23589	1,23062	1,23540	1,22914
C4-N3	1,41196	1,41302	1,41118	1,40724
N3-C2	1,37234	1,37023	1,36938	1,36516
C2=S	1,67236	1,67658	1,67805	1,66917
C2-N1	1,35322	1,35332	1,35223	1,34704
N1-C6	1,36970	1,37026	1,36819	1,36104
C6=C5	1,48931	1,49139	1,48864	1,48311
C5-CH₃	1,47293	1,47132	1,47115	1,46617
C5-C4	1,42766	1,43041	1,42754	1,42299

Table S4A. Singlet-singlet and singlet-triplet TD-DFT calculations from the S_0 optimised geometry of TU at the same computational level. Molecular orbitals involved, largest coefficients in the CI expansion, vertical excitation energies (in eV and nm) and oscillator strengths for each of the first six singlet and triplet excited states are reported. Note that singlet-triplet oscillator strengths of singlet-triplet excitations are set to zero due to the neglected spin-orbital coupling in the triplet TD-DFT calculation in Gaussian09.

TU TD-DFT					
B3LYP/6-31+G(d)/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	32→34	0.63960	3.7829	327.75	0.0000
S ₂	33→34	0.66405	4.2214	293.70	0.1204
S ₃	32→35	0.63170	4.3631	284.17	0.0001
S ₄	33→35	0.65621	4.7725	259.79	0.3793
S ₅	30→34	0.59560	5.0189	247.03	0.0001
S ₆	31→34	0.66889	5.3138	233.33	0.0039
T ₁	33→34	0.65598	3.1348	395.51	--
T ₂	33→34	0.65598	3.5794	346.38	--
T ₃	33→35	0.56225	3.6283	341.72	--
T ₄	32→35	0.56031	4.2556	291.34	--
T ₅	31→34	0.53963	4.3851	282.74	--
T ₆	30→34	0.49820	4.6956	264.04	--
B3LYP/cc-pVDZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	33→34	0.64743	3.8008	326.20	0.0000
S ₂	32→34	0.65810	4.3071	287.86	0.0940
S ₃	33→35	0.63249	4.4101	281.14	0.0000
S ₄	30→34	0.61187	4.9598	249.98	0.0000
S ₅	32→35	0.63775	5.0077	247.59	0.3496
S ₆	31→34	0.65021	5.3696	230.90	0.0116
T ₁	32→34	0.65207	3.1479	393.86	--
T ₂	33→34	0.60962	3.5747	346.83	--
T ₃	32→35	0.53416	3.6634	338.44	--
T ₄	33→35	0.51830	4.2464	291.97	--
T ₅	31→34	0.50437	4.4266	280.09	--
T ₆	30→34	0.47483	4.6556	266.31	--
B3LYP/aug-cc-pVDZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	32→34	0.63923	3.7392	331.58	0.0000
S ₂	33→34	0.67070	4.1559	298.33	0.1095
S ₃	32→35	0.63155	4.3072	287.86	0.0003
S ₄	33→35	0.66291	4.7310	262.07	0.3642
S ₅	30→34	0.60996	4.9509	250.43	0.0002
S ₆	31→34	0.67089	5.2577	235.82	0.0052
T ₁	33→34	0.65366	3.1085	398.85	--
T ₂	32→34	0.60291	3.5383	350.41	--
T ₃	33→35	0.56572	3.6040	344.02	--
T ₄	32→35	0.55903	4.1951	295.55	--
T ₅	31→34	0.54009	4.3515	284.92	--
T ₆	30→34	0.51604	4.6313	267.71	--
B3LYP/aug-cc-pVTZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	33→34	0.63913	3.7592	329.82	0.0000
S ₂	32→34	0.67054	4.1993	295.25	0.1147
S ₃	33→35	0.63166	4.3483	285.13	0.0004
S ₄	32→35	0.66324	4.7624	260.34	0.3573
S ₅	30→34	0.60691	5.0049	247.73	0.0002
S ₆	31→34	0.67343	5.3098	233.50	0.0051
T ₁	32→34	0.65437	3.1364	395.31	--
T ₂	33→34	0.60320	3.5466	349.59	--
T ₃	32→35	0.56204	3.6415	340.47	--
T ₄	33→35	0.56139	4.2377	292.57	--
T ₅	31→34	0.54290	4.4084	281.25	--
T ₆	30→34	0.51382	4.6815	264.84	--

Table S4B. Singlet-singlet and singlet-triplet TD-DFT calculations from the S_0 optimised geometry of TU at the same computational level. Molecular orbitals involved, largest coefficients in the CI expansion, vertical excitation energies (in eV and nm) and oscillator strengths for each of the first six singlet and triplet excited states are reported. Note that singlet-triplet oscillator strengths of singlet-triplet excitations are set to zero due to the neglected spin-orbital coupling in the triplet TD-DFT calculation in Gaussian09.

TU TD-DFT					
CAM-B3LYP/6-31+G(d)/PCM					
Excited state	Transition	CI coeff.	ΔE (eV)	ΔE (nm)	Oscillator strength
S ₁	32→34	0.56419	4.1133	301.42	0.0000
S ₂	33→34	0.68438	4.7009	263.74	0.4171
S ₃	33→35	0.67063	5.1498	240.75	0.1367
S ₄	30→35	0.41970	5.2099	237.98	0.0001
S ₅	32→35	0.45067	5.7427	215.90	0.0003
S ₆	33→36	0.66735	5.9547	208.21	0.0535
T ₁	33→34	0.63144	3.2105	386.18	--
T ₂	33→35	0.52816	3.6879	336.19	--
T ₃	32→34	0.55439	3.8839	319.23	--
T ₄	30→35	0.49564	4.8304	256.68	--
T ₅	31→35	0.58949	4.9567	250.14	--
T ₆	31→34	0.43419	5.1040	242.92	--
CAM-B3LYP/cc-pVDZ/PCM					
Excited state	Transition	CI coeff.	ΔE (eV)	ΔE (nm)	Oscillator strength
S ₁	32→34	0.54667	4.1600	298.04	0.0000
S ₂	33→34	0.68667	4.8625	254.98	0.3203
S ₃	30→35	0.40932	5.1713	239.75	0.0001
S ₄	33→35	0.67697	5.3662	231.05	0.1880
S ₅	32→35	0.45614	5.8016	213.71	0.0000
S ₆	31→34	0.66072	5.9388	208.77	0.0095
T ₁	33→34	0.62241	3.2207	384.96	--
T ₂	33→35	0.51951	3.7142	333.81	--
T ₃	32→34	0.53459	3.8946	318.35	--
T ₄	30→35	0.47265	4.7361	261.78	--
T ₅	31→35	0.62549	5.0062	247.66	--
T ₆	31→34	0.46246	5.1607	240.25	--
CAM-B3LYP/aug-cc-pVDZ/PCM					
Excited state	Transition	CI coeff.	ΔE (eV)	ΔE (nm)	Oscillator strength
S ₁	32→34	0.55108	4.0822	303.72	0.0000
S ₂	33→34	0.68436	4.6377	267.34	0.3733
S ₃	33→35	0.67093	5.0904	243.56	0.1478
S ₄	30→35	0.39544	5.1532	240.59	0.0001
S ₅	32→35	0.43324	5.6686	218.72	0.0007
S ₆	33→36	0.62600	5.8513	211.89	0.0488
T ₁	33→34	0.62781	3.1869	389.04	--
T ₂	33→35	0.53360	3.6653	338.26	--
T ₃	32→34	0.53974	3.8475	322.25	--
T ₄	30→35	0.47530	4.7802	259.37	--
T ₅	31→35	0.60601	4.9523	250.36	--
T ₆	31→34	0.45530	5.0607	244.99	--
CAM-B3LYP/aug-cc-pVTZ/PCM					
Excited state	Transition	CI coeff.	ΔE (eV)	ΔE (nm)	Oscillator strength
S ₁	32→34	0.55812	4.0878	303.30	0.0000
S ₂	33→34	0.68453	4.6695	265.52	0.3805
S ₃	33→35	0.67017	5.1280	241.78	0.1353
S ₄	30→35	0.39725	5.2033	238.28	0.0002
S ₅	32→35	0.43517	5.7115	217.08	0.0010
S ₆	33→36	0.61610	5.8444	212.14	0.0484
T ₁	33→34	0.63196	3.2182	385.25	--
T ₂	33→35	0.52342	3.7037	334.76	--
T ₃	32→34	0.54653	3.8415	322.75	--
T ₄	30→35	0.48019	4.8320	256.59	--
T ₅	31→35	0.59799	5.0223	246.87	--
T ₆	31→34	0.44919	5.1166	242.32	--

Table S4C. Singlet-singlet and singlet-triplet TD-DFT calculations from the S_0 optimised geometry of TU at the same computational level. Molecular orbitals involved, largest coefficients in the CI expansion, vertical excitation energies (in eV and nm) and oscillator strengths for each of the first six singlet and triplet excited states are reported. Note that singlet-triplet oscillator strengths of singlet-triplet excitations are set to zero due to the neglected spin-orbital coupling in the triplet TD-DFT calculation in Gaussian09.

TU TD-DFT					
ωB97XD/6-31+G(d)/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	32→34	0.56376	4.1327	300.01	0.0000
S ₂	33→34	0.68183	4.7334	261.94	0.4289
S ₃	33→35	0.66594	5.1836	239.18	0.1331
S ₄	30→35	0.42891	5.2126	237.86	0.0001
S ₅	32→35	0.46424	5.7965	213.90	0.0003
S ₆	31→34	0.66078	5.8940	210.36	0.0089
T ₁	33→34	0.63615	3.3141	374.11	--
T ₂	33→35	0.53059	3.7756	328.38	--
T ₃	32→34	0.55558	3.9261	315.79	--
T ₄	30→35	0.49274	4.8535	255.45	--
T ₅	31→35	0.56733	5.0146	247.25	--
T ₆	31→34	0.40605	5.1668	239.96	--
ωB97XD/cc-pVDZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	32→34	0.55241	4.1833	296.38	0.0000
S ₂	33→34	0.68460	4.8862	253.75	0.3329
S ₃	30→35	0.41638	5.1808	239.31	0.0001
S ₄	33→35	0.67252	5.3889	230.07	0.1799
S ₅	32→35	0.46881	5.8598	211.59	0.0000
S ₆	31→34	0.65619	5.9432	208.61	0.0084
T ₁	33→34	0.62909	3.3333	371.96	--
T ₂	33→35	0.52063	3.8127	325.18	--
T ₃	32→34	0.54216	3.9439	314.37	--
T ₄	30→35	0.47350	4.7758	259.61	--
T ₅	31→35	0.60550	5.0659	244.74	--
T ₆	31→34	0.42832	5.2226	237.40	--
ωB97XD/aug-cc-pVDZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	32→34	0.55366	4.1214	300.83	0.0000
S ₂	33→34	0.68175	4.6808	264.88	0.3882
S ₃	33→35	0.66550	5.1339	241.50	0.1405
S ₄	30→35	0.41238	5.1654	240.03	0.0001
S ₅	32→35	0.45453	5.7406	215.98	0.0009
S ₆	31→34	0.66027	5.8343	212.51	0.0119
T ₁	33→34	0.63267	3.3024	375.43	--
T ₂	33→35	0.53657	3.7642	329.37	--
T ₃	32→34	0.54440	3.9137	316.79	--
T ₄	30→35	0.47734	4.8095	257.79	--
T ₅	31→35	0.57437	5.0082	247.56	--
T ₆	31→34	0.41391	5.1384	241.29	--
ωB97XD/aug-cc-pVTZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	32→34	0.56084	4.1239	300.65	0.0000
S ₂	33→34	0.68177	4.7072	263.39	0.3974
S ₃	33→35	0.66409	5.1701	239.81	0.1278
S ₄	30→35	0.41600	5.2054	238.18	0.0001
S ₅	32→35	0.45953	5.7763	214.64	0.0015
S ₆	31→34	0.65869	5.8757	211.01	0.0139
T ₁	33→34	0.63615	3.3259	372.78	--
T ₂	33→35	0.52775	3.7955	326.66	--
T ₃	32→34	0.55140	3.9093	317.15	--
T ₄	30→35	0.48213	4.8507	255.60	--
T ₅	31→35	0.56220	5.0670	244.69	--
T ₆	31→34	0.40259	5.1867	239.04	--

Table S4D. Singlet-singlet and singlet-triplet TD-DFT calculations from the S_0 optimised geometry of TU at the same computational level. Molecular orbitals involved, largest coefficients in the CI expansion, vertical excitation energies (in eV and nm) and oscillator strengths for each of the first six singlet and triplet excited states are reported. Note that singlet-triplet oscillator strengths of singlet-triplet excitations are set to zero due to the neglected spin-orbital coupling in the triplet TD-DFT calculation in Gaussian09.

TU TD-DFT					
M062X/6-31+G(d)/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	32→34	0.57835	4.0327	307.45	0.0000
S ₂	33→34	0.68738	4.6729	265.32	0.4206
S ₃	30→35	0.48366	5.0910	243.54	0.0000
S ₄	33→35	0.67064	5.1482	240.83	0.1201
S ₅	32→35	0.49972	5.7294	216.40	0.0004
S ₆	33→36	0.66866	5.8311	212.63	0.0465
T ₁	33→34	0.64167	3.3904	365.69	--
T ₂	32→34	0.57141	3.8625	320.99	--
T ₃	33→35	0.49650	3.8647	320.81	--
T ₄	30→35	0.52330	4.7813	259.31	--
T ₅	31→35	0.59724	5.0852	243.82	--
T ₆	31→34	0.48952	5.1504	240.73	--
M062X/cc-pVDZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	32→34	0.56468	4.0564	305.65	0.0000
S ₂	33→34	0.69118	4.8207	257.19	0.3416
S ₃	30→35	0.47585	5.0589	245.08	0.0001
S ₄	33→35	0.67420	5.3337	232.45	0.1575
S ₅	32→35	0.49736	5.7899	214.14	0.0000
S ₆	31→34	0.66384	5.9643	207.88	0.0160
T ₁	33→34	0.63476	3.4096	363.64	--
T ₂	32→34	0.55724	3.8673	320.59	--
T ₃	31→34	-0.44259	3.9080	317.26	--
T ₄	30→35	0.50831	4.7185	262.76	--
T ₅	31→35	0.61488	5.1454	240.96	--
T ₆	31→34	0.48959	5.2116	237.90	--
M062X/aug-cc-pVDZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	32→34	0.56785	3.9924	310.55	0.0000
S ₂	33→34	0.68770	4.5999	269.54	0.3771
S ₃	30→35	0.46311	5.0423	245.89	0.0001
S ₄	33→35	0.67113	5.0764	244.24	0.1279
S ₅	32→35	0.48332	5.6454	219.62	0.0007
S ₆	33→36	0.64599	5.6934	217.77	0.0401
T ₁	33→34	0.63718	3.3591	369.10	--
T ₂	32→34	0.56030	3.8232	324.29	--
T ₃	33→35	0.50137	3.8387	322.98	--
T ₄	30→35	0.50683	4.7392	261.61	--
T ₅	31→35	0.60523	5.0723	244.44	--
T ₆	31→34	0.53951	5.1019	243.02	--
M062X/aug-cc-pVTZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	32→34	0.56932	4.0028	309.75	0.0000
S ₂	33→34	0.68706	4.6436	267.00	0.3848
S ₃	33→35	0.67132	5.1180	242.25	0.1200
S ₄	30→35	0.45729	5.1282	241.77	0.0002
S ₅	32→35	0.47622	5.7015	217.46	0.0008
S ₆	33→36	0.63643	5.7418	215.93	0.0428
T ₁	33→34	0.63684	3.3919	365.53	--
T ₂	32→34	0.56206	3.8340	323.38	--
T ₃	33→35	0.50125	3.8865	319.01	--
T ₄	30→35	0.50581	4.8381	256.27	--
T ₅	31→35	0.57484	5.1444	241.01	--
T ₆	31→34	0.54724	5.1802	239.34	--

Table S4E. Singlet-singlet and singlet-triplet TD-DFT calculations from the S_0 optimised geometry of TU at the same computational level. Molecular orbitals involved, largest coefficients in the CI expansion, vertical excitation energies (in eV and nm) and oscillator strengths for each of the first six singlet and triplet excited states are reported. Note that singlet-triplet oscillator strengths of singlet-triplet excitations are set to zero due to the neglected spin-orbital coupling in the triplet TD-DFT calculation in Gaussian09.

TU TD-DFT					
PBE0/6-31+G(d)/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	32→34	0.62593	3.9478	314.06	0.0000
S ₂	33→34	0.67528	4.4242	280.24	0.1700
S ₃	32→35	0.60456	4.6350	267.49	0.0002
S ₄	33→35	0.67072	4.9431	250.82	0.3533
S ₅	30→34	0.54414	5.1887	238.95	0.0001
S ₆	31→34	0.67974	5.4940	225.67	0.0033
T ₁	33→34	0.65159	3.1412	394.70	--
T ₂	33→35	0.54982	3.6659	338.21	--
T ₃	32→34	0.59772	3.7125	333.96	--
T ₄	32→35	0.47674	4.4609	277.93	--
T ₅	31→34	0.52599	4.5771	270.88	--
T ₆	31→35	0.65536	4.7725	259.79	--
PBE0/cc-pVDZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	32→34	0.63084	3.9791	311.59	0.0000
S ₂	33→34	0.66906	4.5196	274.32	0.1344
S ₃	32→35	0.59257	4.6772	265.08	0.0000
S ₄	30→34	0.55593	5.1574	240.40	0.0000
S ₅	33→35	0.65939	5.1730	239.68	0.3415
S ₆	31→34	0.66816	5.5482	223.47	0.0073
T ₁	33→34	0.64698	3.1595	392.42	--
T ₂	33→35	0.52937	3.7013	334.97	--
T ₃	32→34	0.59796	3.7205	333.25	--
T ₄	32→35	0.41979	4.4252	280.17	--
T ₅	31→34	0.49685	4.6357	267.45	--
T ₆	31→35	0.65470	4.8191	257.28	--
PBE0/aug-cc-pVDZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	32→34	0.62224	3.9162	316.59	0.0000
S ₂	33→34	0.68042	4.3592	284.42	0.1526
S ₃	32→35	0.60167	4.5793	270.75	0.0004
S ₄	33→35	0.67572	4.9002	253.02	0.3422
S ₅	30→34	0.56238	5.1240	241.97	0.0003
S ₆	31→34	0.68108	5.4393	227.94	0.0054
T ₁	33→34	0.64880	3.1190	397.51	--
T ₂	33→35	0.55558	3.6417	340.46	--
T ₃	32→34	0.59014	3.6804	336.88	--
T ₄	32→35	0.47522	4.4030	281.59	--
T ₅	31→34	0.52409	4.5476	272.63	--
T ₆	31→35	0.65792	4.7616	260.38	--
PBE0/aug-cc-pVTZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	32→34	0.62338	3.9267	315.75	0.0000
S ₂	33→34	0.68079	4.3957	282.06	0.1592
S ₃	32→35	0.60345	4.6154	268.63	0.0004
S ₄	33→35	0.67633	4.9288	251.55	0.3335
S ₅	30→34	0.55990	5.1684	239.89	0.0003
S ₆	31→34	0.68287	5.4854	226.03	0.0055
T ₁	33→34	0.65085	3.1359	395.37	--
T ₂	33→35	0.55066	3.6651	338.28	--
T ₃	32→34	0.59106	3.6745	337.41	--
T ₄	32→35	0.47916	4.4406	279.21	--
T ₅	31→34	0.52490	4.5962	269.76	--
T ₆	31→35	0.65735	4.8146	257.52	--

Table S5A. Singlet-singlet and singlet-triplet TD-DFT calculations from the S_0 optimised geometry of BTU at the same computational level. Molecular orbitals involved, largest coefficients in the CI expansion, vertical excitation energies (in eV and nm) and oscillator strengths for each of the first six singlet and triplet excited states are reported. Note that singlet-triplet oscillator strengths of singlet-triplet excitations are set to zero due to the neglected spin-orbital coupling in the triplet TD-DFT calculation in Gaussian09.

TU TD-DFT					
B3LYP/6-31+G(d)/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	<i>ΔE (eV)</i>	<i>ΔE (nm)</i>	<i>Oscillator strength</i>
S ₁	48→50	0.60837	3.8917	318.58	0.0000
S ₂	49→50	0.67450	4.2000	295.20	0.1558
S ₃	48→51	0.59723	4.3663	283.95	0.0001
S ₄	49→51	0.66716	4.6857	264.60	0.4712
S ₅	46→50	0.58886	4.9450	250.73	0.0001
S ₆	47→50	0.66570	5.3282	232.69	0.0053
T ₁	49→50	0.65502	3.1400	394.85	--
T ₂	49→51	0.61174	3.5763	346.69	--
T ₃	48→50	0.56762	3.6965	335.41	--
T ₄	48→51	0.50173	4.2442	292.13	--
T ₅	47→50	0.58450	4.3921	282.29	--
T ₆	46→50	0.48027	4.6489	266.69	--
B3LYP/cc-pVDZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	<i>ΔE (eV)</i>	<i>ΔE (nm)</i>	<i>Oscillator strength</i>
S ₁	48→50	0.61430	3.8961	318.23	0.0000
S ₂	49→50	0.66431	4.2714	290.27	0.1182
S ₃	48→51	0.60032	4.3795	283.10	0.0000
S ₄	49→51	0.65178	4.8893	253.58	0.4713
S ₅	46→50	0.60002	4.9279	251.59	0.0000
S ₆	46→51	0.61263	5.4664	226.81	0.0002
T ₁	49→50	0.65030	3.1496	393.66	--
T ₂	49→51	0.59498	3.6056	343.87	--
T ₃	48→50	0.56504	3.6709	337.74	--
T ₄	48→51	0.47928	4.2244	293.50	--
T ₅	47→50	0.56330	4.4247	280.21	--
T ₆	46→50	0.47004	4.6302	267.77	--
B3LYP/aug-cc-pVDZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	<i>ΔE (eV)</i>	<i>ΔE (nm)</i>	<i>Oscillator strength</i>
S ₁	48→50	0.60842	3.8521	321.86	0.0000
S ₂	49→50	0.67993	4.1385	299.59	0.1433
S ₃	48→51	0.59792	4.3137	287.42	0.0003
S ₄	49→51	0.67265	4.6483	266.73	0.4557
S ₅	46→50	0.60466	4.8852	253.80	0.0002
S ₆	49→52	0.67395	5.3808	230.42	0.0325
T ₁	49→50	0.65284	3.1141	398.14	--
T ₂	49→51	0.61375	3.5547	348.78	--
T ₃	48→50	0.56313	3.6592	338.83	--
T ₄	48→51	0.50193	4.1890	295.97	--
T ₅	47→50	0.58359	4.3638	284.12	--
T ₆	46→50	0.50022	4.5904	270.09	--
B3LYP/aug-cc-pVTZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	<i>ΔE (eV)</i>	<i>ΔE (nm)</i>	<i>Oscillator strength</i>
S ₁	48→50	0.60889	3.8728	320.14	0.0000
S ₂	49→50	0.67907	4.1845	296.29	0.1527
S ₃	48→51	0.59867	4.3590	284.43	0.0003
S ₄	49→51	0.67214	4.6783	265.02	0.4450
S ₅	46→50	0.59845	4.9439	250.78	0.0002
S ₆	49→52	0.67290	5.3754	230.65	0.0329
T ₁	49→50	0.65490	3.1478	393.88	--
T ₂	49→51	0.60913	3.5861	345.74	--
T ₃	48→50	0.56540	3.6678	338.03	--
T ₄	48→51	0.50631	4.2373	292.60	--
T ₅	47→50	0.58657	4.4228	280.33	--
T ₆	46→50	0.49558	4.6433	267.02	--

Table S5B. Singlet-singlet and singlet-triplet TD-DFT calculations from the S_0 optimised geometry of BTU at the same computational level. Molecular orbitals involved, largest coefficients in the CI expansion, vertical excitation energies (in eV and nm) and oscillator strengths for each of the first six singlet and triplet excited states are reported. Note that singlet-triplet oscillator strengths of singlet-triplet excitations are set to zero due to the neglected spin-orbital coupling in the triplet TD-DFT calculation in Gaussian09.

BTU TD-DFT					
CAM-B3LYP/6-31+G(d)/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	<i>ΔE (eV)</i>	<i>ΔE (nm)</i>	<i>Oscillator strength</i>
S ₁	48→50	0.52517	4.2193	293.85	0.0000
S ₂	49→50	0.68039	4.6764	265.13	0.5169
S ₃	49→51	0.66951	5.0772	244.20	0.1607
S ₄	46→51	0.42063	5.1256	241.89	0.0000
S ₅	48→51	0.44748	5.7447	215.82	0.0005
S ₆	49→52	0.64922	5.8329	212.56	0.0511
T ₁	49→50	0.62489	3.2151	385.63	--
T ₂	49→51	0.57696	3.6662	338.18	--
T ₃	48→50	0.51501	4.0011	309.88	--
T ₄	46→51	0.47069	4.7378	261.69	--
T ₅	47→51	0.58631	4.8858	253.76	--
T ₆	47→50	0.45946	5.1027	242.98	--
CAM-B3LYP/cc-pVDZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	<i>ΔE (eV)</i>	<i>ΔE (nm)</i>	<i>Oscillator strength</i>
S ₁	48→50	0.49946	4.2413	292.33	0.0000
S ₂	49→50	0.68781	4.8245	256.99	0.4070
S ₃	46→50	0.41935	5.1136	242.46	0.0001
S ₄	49→51	0.68594	5.2572	235.84	0.2482
S ₅	48→51	0.42808	5.7807	214.48	0.0000
S ₆	47→50	0.65964	5.9938	206.85	0.0085
T ₁	49→50	0.62152	3.2206	384.98	--
T ₂	49→51	0.57099	3.6834	336.60	--
T ₃	48→51	0.49855	3.9813	311.41	--
T ₄	46→51	0.45064	4.6889	264.42	--
T ₅	47→51	0.62354	4.9387	251.05	--
T ₆	47→50	0.49291	5.1406	241.19	--
CAM-B3LYP/aug-cc-pVDZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	<i>ΔE (eV)</i>	<i>ΔE (nm)</i>	<i>Oscillator strength</i>
S ₁	48→50	0.50632	4.1907	295.85	0.0000
S ₂	49→50	0.67962	4.6194	268.40	0.4694
S ₃	49→51	0.66886	5.0202	246.97	0.1740
S ₄	46→50	0.40581	5.0752	244.30	0.0000
S ₅	48→51	0.42723	5.6726	218.57	0.0008
S ₆	49→52	0.57623	5.7355	216.17	0.0464
T ₁	49→50	0.62200	3.1928	388.33	--
T ₂	49→51	0.58154	3.6444	340.20	--
T ₃	48→50	0.49460	3.9669	312.55	--
T ₄	46→51	0.44699	4.6925	264.21	--
T ₅	47→51	0.60162	4.8850	253.81	--
T ₆	47→50	0.47784	5.0648	244.80	--
CAM-B3LYP/aug-cc-pVTZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	<i>ΔE (eV)</i>	<i>ΔE (nm)</i>	<i>Oscillator strength</i>
S ₁	48→50	0.51972	4.1961	295.47	0.0000
S ₂	49→50	0.68000	4.6527	266.48	0.4840
S ₃	49→51	0.66811	5.0580	245.12	0.1546
S ₄	46→51	-0.40462	5.1313	241.62	0.0001
S ₅	48→51	0.43296	5.7183	216.82	0.0000
S ₆	49→52	0.55921	5.7282	216.44	0.0473
T ₁	49→50	0.62793	3.2337	383.42	--
T ₂	49→51	0.57232	3.6734	337.52	--
T ₃	48→50	0.50791	3.9608	313.03	--
T ₄	46→51	-0.45882	4.7482	261.12	--
T ₅	47→51	0.58816	4.9486	250.55	--
T ₆	47→50	0.46723	5.1261	241.87	--

Table S5C. Singlet-singlet and singlet-triplet TD-DFT calculations from the S_0 optimised geometry of BTU at the same computational level. Molecular orbitals involved, largest coefficients in the CI expansion, vertical excitation energies (in eV and nm) and oscillator strengths for each of the first six singlet and triplet excited states are reported. Note that singlet-triplet oscillator strengths of singlet-triplet excitations are set to zero due to the neglected spin-orbital coupling in the triplet TD-DFT calculation in Gaussian09.

BTU TD-DFT					
ωB97XD/6-31+G(d)/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	48→50	0.52829	4.2362	292.68	0.0000
S ₂	49→50	0.67875	4.7028	263.64	0.5350
S ₃	49→51	0.66651	5.1042	242.91	0.1565
S ₄	46→51	0.42727	5.1259	241.88	0.0000
S ₅	48→51	0.45717	5.8082	213.46	0.0004
S ₆	47→50	0.65554	5.9252	209.25	0.0101
T ₁	49→50	0.63176	3.3102	374.55	--
T ₂	49→51	0.58040	3.7424	331.30	--
T ₃	48→50	0.51988	4.0399	306.90	--
T ₄	46→51	0.47104	4.7616	260.38	--
T ₅	47→51	0.57041	4.9437	250.79	--
T ₆	47→50	0.44218	5.1676	239.93	--
ωB97XD/cc-pVDZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	48→50	0.51227	4.2683	290.47	0.0000
S ₂	49→50	0.68636	4.8454	255.88	0.4262
S ₃	46→50	0.42126	5.1231	242.01	0.0001
S ₄	49→51	0.68335	5.2808	234.78	0.2346
S ₅	48→51	0.44495	5.8507	211.91	0.0000
S ₆	47→50	0.65805	5.9991	206.67	0.0067
T ₁	49→50	0.62943	3.3235	373.05	--
T ₂	49→51	0.57371	3.7739	328.53	--
T ₃	48→50	0.50234	4.0346	307.30	--
T ₄	46→51	0.45651	4.7266	262.31	--
T ₅	47→51	0.60502	4.9972	248.11	--
T ₆	47→50	0.46802	5.2084	238.05	--
ωB97XD/aug-cc-pVDZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	48→50	0.51215	4.2260	293.38	0.0000
S ₂	49→50	0.67790	4.6569	266.24	0.4896
S ₃	49→51	0.66542	5.0567	245.19	0.1664
S ₄	46→50	0.41475	5.0821	243.96	0.0000
S ₅	48→51	0.44177	5.7543	215.46	0.0010
S ₆	49→52	0.51958	5.9669	207.79	0.0564
T ₁	49→50	0.62824	3.2963	376.13	--
T ₂	49→51	0.58521	3.7326	332.17	--
T ₃	48→50	0.50261	4.0281	307.80	--
T ₄	46→51	-0.45118	4.7211	262.62	--
T ₅	47→51	0.58215	4.9409	250.94	--
T ₆	47→50	0.45515	5.1424	241.10	--
ωB97XD/aug-cc-pVTZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	48→50	0.52510	4.2268	293.33	0.0000
S ₂	49→50	0.67806	4.6842	264.69	0.5058
S ₃	49→51	0.66381	5.0917	243.50	0.1478
S ₄	46→51	-0.41668	5.1298	241.69	0.0001
S ₅	48→51	0.45222	5.7920	214.06	0.0017
S ₆	49→52	0.47821	5.9329	208.98	0.0592
T ₁	49→50	0.63299	3.3288	372.46	--
T ₂	49→51	0.57646	3.7576	329.95	--
T ₃	48→50	0.51549	4.0219	308.28	--
T ₄	46→51	-0.46222	4.7691	259.98	--
T ₅	47→51	0.56787	4.9951	248.21	--
T ₆	47→50	0.44392	5.1947	238.67	--

Table S5D. Singlet-singlet and singlet-triplet TD-DFT calculations from the S_0 optimised geometry of BTU at the same computational level. Molecular orbitals involved, largest coefficients in the CI expansion, vertical excitation energies (in eV and nm) and oscillator strengths for each of the first six singlet and triplet excited states are reported. Note that singlet-triplet oscillator strengths of singlet-triplet excitations are set to zero due to the neglected spin-orbital coupling in the triplet TD-DFT calculation in Gaussian09.

BTU TD-DFT					
M062X/6-31+G(d)/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	<i>ΔE (eV)</i>	<i>ΔE (nm)</i>	<i>Oscillator strength</i>
S ₁	48→50	0.53842	4.1347	299.86	0.0000
S ₂	49→50	0.68342	4.6439	266.98	0.5197
S ₃	46→51	-0.45377	4.9911	248.41	0.0000
S ₄	49→51	0.67115	5.0659	244.74	0.1459
S ₅	49→52	0.65350	5.6951	217.70	0.0445
S ₆	48→51	0.47453	5.7137	216.99	0.0003
T ₁	49→50	0.63776	3.4283	361.65	--
T ₂	49→51	0.54687	3.8008	326.20	--
T ₃	48→50	0.53082	3.9728	312.08	--
T ₄	46→51	-0.47946	4.6814	264.85	--
T ₅	47→51	0.59475	5.0165	247.15	--
T ₆	47→50	0.49807	5.1309	241.64	--
M062X/cc-pVDZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	<i>ΔE (eV)</i>	<i>ΔE (nm)</i>	<i>Oscillator strength</i>
S ₁	48→50	0.52293	4.1380	299.62	0.0000
S ₂	49→50	0.69152	4.7813	259.31	0.4386
S ₃	46→51	0.44710	4.9826	248.83	0.0001
S ₄	49→51	0.68390	5.2219	237.43	0.2093
S ₅	48→51	0.46796	5.7551	215.43	0.0000
S ₆	47→50	0.66651	5.9981	206.71	0.0171
T ₁	49→50	0.63008	3.4368	360.76	--
T ₂	49→51	0.53009	3.8382	323.03	--
T ₃	48→50	0.51541	3.9539	313.57	--
T ₄	46→51	0.47156	4.6523	266.50	--
T ₅	47→51	0.61669	5.0739	244.36	--
T ₆	47→50	0.52387	5.1822	239.25	--
M062X/aug-cc-pVDZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	<i>ΔE (eV)</i>	<i>ΔE (nm)</i>	<i>Oscillator strength</i>
S ₁	48→50	0.51865	4.0949	302.78	0.0000
S ₂	49→50	0.68200	4.5766	270.91	0.4705
S ₃	46→51	0.42850	4.9360	251.19	0.0001
S ₄	49→51	0.66922	4.9941	248.26	0.1575
S ₅	49→52	0.61031	5.5643	222.82	0.0378
S ₆	48→51	0.45792	5.6173	220.72	0.0011
T ₁	49→50	0.62945	3.4012	364.53	--
T ₂	49→51	0.54648	3.7712	328.77	--
T ₃	48→50	0.51028	3.9347	315.10	--
T ₄	46→51	0.45660	4.6316	267.69	--
T ₅	47→51	0.61372	5.0010	247.92	--
T ₆	47→50	0.53605	5.0777	244.17	--
M062X/aug-cc-pVTZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	<i>ΔE (eV)</i>	<i>ΔE (nm)</i>	<i>Oscillator strength</i>
S ₁	48→50	0.52703	4.1068	301.90	0.0000
S ₂	49→50	0.68196	4.6227	268.21	0.4873
S ₃	46→51	-0.43235	5.0314	246.42	0.0001
S ₄	49→51	0.66953	5.0363	246.18	0.1424
S ₅	49→52	0.59809	5.6094	221.03	0.0401
S ₆	48→51	0.46245	5.6881	217.97	0.0016
T ₁	49→50	0.63248	3.4300	361.47	--
T ₂	49→51	0.54880	3.8143	325.05	--
T ₃	48→50	0.51922	3.9459	314.21	--
T ₄	46→51	-0.46227	4.7376	261.70	--
T ₅	47→51	0.60529	5.0793	244.10	--
T ₆	47→50	0.52452	5.1608	240.24	--

Table S5E. Singlet-singlet and singlet-triplet TD-DFT calculations from the S_0 optimised geometry of BTU at the same computational level. Molecular orbitals involved, largest coefficients in the CI expansion, vertical excitation energies (in eV and nm) and oscillator strengths for each of the first six singlet and triplet excited states are reported. Note that singlet-triplet oscillator strengths of singlet-triplet excitations are set to zero due to the neglected spin-orbital coupling in the triplet TD-DFT calculation in Gaussian09.

BTU TD-DFT					
PBE0/6-31+G(d)/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	48→50	0.59284	4.0553	305.73	0.0000
S ₂	49→50	0.68368	4.3921	282.29	0.2215
S ₃	48→51	0.56080	4.6266	267.98	0.0001
S ₄	49→51	0.67889	4.8504	255.62	0.4344
S ₅	46→50	0.53233	5.1132	242.48	0.0001
S ₆	47→50	0.67757	5.5131	224.89	0.0050
T ₁	49→50	0.65044	3.1356	395.41	--
T ₂	49→51	0.60244	3.6234	342.17	--
T ₃	48→50	0.56013	3.8288	323.82	--
T ₄	48→51	0.40839	4.4190	280.57	--
T ₅	47→50	0.56755	4.5686	271.38	--
T ₆	47→51	0.64115	4.7165	262.87	--
PBE0/cc-pVDZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	48→50	0.59442	4.0736	304.36	0.0000
S ₂	49→50	0.67401	4.4770	276.94	0.1719
S ₃	48→51	0.55471	4.6451	266.91	0.0000
S ₄	49→51	0.66801	5.0462	245.70	0.4533
S ₅	46→50	0.54092	5.1121	242.53	0.0000
S ₆	47→50	0.66824	5.5953	221.59	0.0057
T ₁	49→50	0.64761	3.1525	393.29	--
T ₂	49→51	0.59013	3.6551	339.21	--
T ₃	48→50	0.55512	3.8170	324.82	--
T ₄	46→50	0.38253	4.3949	282.11	--
T ₅	47→50	0.55463	4.6216	268.27	--
T ₆	47→51	0.65219	4.7563	260.68	--
PBE0/aug-cc-pVDZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	48→50	0.58676	4.0270	307.88	0.0000
S ₂	49→50	0.68775	4.3322	286.19	0.2005
S ₃	48→51	0.55631	4.5731	271.12	0.0003
S ₄	49→51	0.68288	4.8106	257.73	0.4253
S ₅	46→50	0.55174	5.0524	245.39	0.0003
S ₆	47→50	0.67886	5.4633	226.94	0.0081
T ₁	49→50	0.64799	3.1135	398.21	--
T ₂	49→51	0.60668	3.5999	344.41	--
T ₃	48→50	0.54892	3.7993	326.33	--
T ₄	48→51	0.40538	4.3653	284.02	--
T ₅	47→50	0.57000	4.5487	272.57	--
T ₆	47→51	0.65358	4.7022	263.68	--
PBE0/aug-cc-pVTZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	48→50	0.58965	4.0377	307.07	0.0000
S ₂	49→50	0.68760	4.3703	283.70	0.2118
S ₃	48→51	0.56046	4.6137	268.73	0.0004
S ₄	49→51	0.68287	4.8380	256.27	0.4125
S ₅	46→50	0.54684	5.1023	243.00	0.0004
S ₆	49→52	0.66282	5.6124	220.91	0.0363
T ₁	49→50	0.65104	3.1375	395.17	--
T ₂	49→51	0.60161	3.6182	342.67	--
T ₃	48→50	0.55248	3.7934	326.84	--
T ₄	48→51	0.41098	4.4090	281.21	--
T ₅	47→50	0.57164	4.5982	269.64	--
T ₆	46→50	0.39009	4.8327	256.55	--

Table S6A. Singlet-singlet and singlet-triplet TD-DFT calculations from the S_0 optimised geometry of TT at the same computational level. Molecular orbitals involved, largest coefficients in the CI expansion, vertical excitation energies (in eV and nm) and oscillator strengths for each of the first six singlet and triplet excited states are reported. Note that singlet-triplet oscillator strengths of singlet-triplet excitations are set to zero due to the neglected spin-orbital coupling in the triplet TD-DFT calculation in Gaussian09.

TT TD-DFT					
B3LYP/6-31+G(d)/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	<i>ΔE (eV)</i>	<i>ΔE (nm)</i>	<i>Oscillator strength</i>
S ₁	36→38	0.60651	3.8812	319.45	0.0000
S ₂	37→38	0.67265	4.1862	296.17	0.1343
S ₃	36→39	0.60022	4.3682	283.83	0.0001
S ₄	37→39	0.66616	4.6872	264.51	0.4323
S ₅	34→38	0.59002	5.0525	245.39	0.0001
S ₆	35→38	0.66461	5.3603	231.30	0.0070
T ₁	37→38	0.65548	3.1055	399.24	--
T ₂	37→39	0.61811	3.5526	349.00	--
T ₃	36→38	0.56504	3.6839	336.55	--
T ₄	36→39	0.52549	4.2691	290.42	--
T ₅	35→38	0.58950	4.3931	282.22	--
T ₆	35→39	0.67046	4.6328	267.62	--
B3LYP/cc-pVDZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	<i>ΔE (eV)</i>	<i>ΔE (nm)</i>	<i>Oscillator strength</i>
S ₁	36→38	0.62082	3.9000	317.91	0.0000
S ₂	37→38	0.66121	4.2868	289.22	0.1125
S ₃	36→39	0.61022	4.4199	280.51	0.0000
S ₄	37→39	0.65029	4.9034	252.85	0.4144
S ₅	34→38	0.59336	5.0273	246.62	0.0000
S ₆	35→38	0.65545	5.4358	228.09	0.0075
T ₁	37→38	0.65500	3.1233	396.97	--
T ₂	37→39	0.59797	3.5974	344.65	--
T ₃	36→38	0.57602	3.6739	337.47	--
T ₄	36→39	0.50190	4.2772	289.87	--
T ₅	35→38	0.56784	4.4398	279.26	--
T ₆	34→38	0.47271	4.6891	264.41	--
B3LYP/aug-cc-pVDZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	<i>ΔE (eV)</i>	<i>ΔE (nm)</i>	<i>Oscillator strength</i>
S ₁	36→38	0.60618	3.8415	322.75	0.0000
S ₂	37→38	0.67902	4.1191	301.00	0.1245
S ₃	36→39	0.60031	4.3132	287.46	0.0003
S ₄	37→39	0.67238	4.6447	266.94	0.4156
S ₅	34→38	0.60663	4.9903	248.45	0.0002
S ₆	37→40	0.68851	5.3789	230.50	0.0245
T ₁	37→38	0.65382	3.0754	403.15	--
T ₂	37→39	0.62161	3.5263	351.60	--
T ₃	36→38	0.55981	3.6470	339.96	--
T ₄	36→39	0.52325	4.2100	294.50	--
T ₅	35→38	0.59019	4.3629	284.18	--
T ₆	35→39	0.67319	4.6218	268.26	--
B3LYP/aug-cc-pVTZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	<i>ΔE (eV)</i>	<i>ΔE (nm)</i>	<i>Oscillator strength</i>
S ₁	36→38	0.60623	3.8613	321.10	0.0000
S ₂	37→38	0.67835	4.1630	297.83	0.1306
S ₃	36→39	0.60044	4.3550	284.69	0.0004
S ₄	37→39	0.67189	4.6746	265.23	0.4072
S ₅	34→38	0.60113	5.0446	245.78	0.0002
S ₆	37→40	0.68726	5.3725	230.78	0.0251
T ₁	37→38	0.65543	3.1093	398.75	--
T ₂	37→39	0.61709	3.5561	348.65	--
T ₃	36→38	0.56126	3.6549	339.22	--
T ₄	36→39	0.52590	4.2533	291.50	--
T ₅	35→38	0.59228	4.4199	280.52	--
T ₆	34→38	0.52119	4.7022	263.67	--

Table S6B. Singlet-singlet and singlet-triplet TD-DFT calculations from the S_0 optimised geometry of TT at the same computational level. Molecular orbitals involved, largest coefficients in the CI expansion, vertical excitation energies (in eV and nm) and oscillator strengths for each of the first six singlet and triplet excited states are reported. Note that singlet-triplet oscillator strengths of singlet-triplet excitations are set to zero due to the neglected spin-orbital coupling in the triplet TD-DFT calculation in Gaussian09.

TT TD-DFT					
CAM-B3LYP/6-31+G(d)/PCM					
Excited state	Transition	CI coeff.	ΔE (eV)	ΔE (nm)	Oscillator strength
S ₁	36→38	0.52009	4.2047	294.87	0.0000
S ₂	37→38	0.68139	4.6674	265.64	0.4649
S ₃	37→39	0.67159	5.0596	245.05	0.1605
S ₄	34→39	0.40784	5.2190	237.56	0.0000
S ₅	36→39	0.42386	5.7520	215.55	0.0005
S ₆	37→40	0.66628	5.8315	212.61	0.0457
T ₁	37→38	0.62423	3.1722	390.85	--
T ₂	37→39	0.58453	3.6375	340.85	--
T ₃	36→38	0.51013	3.9847	311.15	--
T ₄	34→39	0.47581	4.8320	256.59	--
T ₅	35→39	0.58278	4.8989	253.09	--
T ₆	35→38	0.45372	5.1073	242.76	--
CAM-B3LYP/cc-pVDZ/PCM					
Excited state	Transition	CI coeff.	ΔE (eV)	ΔE (nm)	Oscillator strength
S ₁	36→38	0.51774	4.2432	292.20	0.0000
S ₂	37→38	0.68966	4.8303	256.68	0.3797
S ₃	34→39	0.41788	5.2058	238.16	0.0001
S ₄	37→39	0.68486	5.2733	235.12	0.2148
S ₅	36→39	0.43788	5.8253	212.84	0.0000
S ₆	35→38	0.66120	6.0137	206.17	0.0070
T ₁	37→38	0.62572	3.1848	389.30	--
T ₂	37→39	0.57381	3.6711	337.73	--
T ₃	36→38	0.50681	3.9838	311.22	--
T ₄	34→39	0.47584	4.7630	260.31	--
T ₅	35→39	0.61111	4.9488	250.53	--
T ₆	35→38	0.47564	5.1632	240.13	--
CAM-B3LYP/aug-cc-pVDZ/PCM					
Excited state	Transition	CI coeff.	ΔE (eV)	ΔE (nm)	Oscillator strength
S ₁	36→38	0.50032	4.1772	296.81	0.0000
S ₂	37→38	0.68103	4.6026	269.38	0.4177
S ₃	37→39	0.67202	4.9985	248.04	0.1747
S ₄	34→38	0.39337	5.1659	240.00	0.0001
S ₅	36→39	0.40185	5.6807	218.25	0.0007
S ₆	37→40	0.60431	5.7178	216.84	0.0393
T ₁	37→38	0.62141	3.1456	394.16	--
T ₂	37→39	0.59142	3.6121	343.25	--
T ₃	36→39	0.49377	3.9519	313.73	--
T ₄	34→39	0.45117	4.7848	259.12	--
T ₅	35→39	0.59669	4.8952	253.28	--
T ₆	35→38	0.47034	5.0678	244.65	--
CAM-B3LYP/aug-cc-pVTZ/PCM					
Excited state	Transition	CI coeff.	ΔE (eV)	ΔE (nm)	Oscillator strength
S ₁	36→38	0.51089	4.1823	296.45	0.0000
S ₂	37→38	0.68075	4.6354	267.47	0.4283
S ₃	37→39	0.67109	5.0341	246.29	0.1586
S ₄	34→39	0.38542	5.2163	237.68	0.0001
S ₅	37→40	0.59101	5.7097	217.15	0.0374
S ₆	36→39	0.40595	5.7239	216.61	0.0029
T ₁	37→38	0.62612	3.1875	388.97	--
T ₂	37→39	0.58308	3.6388	340.73	--
T ₃	36→38	0.49912	3.9455	314.24	--
T ₄	34→39	0.45959	4.8358	256.39	--
T ₅	35→39	0.58453	4.9589	250.02	--
T ₆	35→38	0.46041	5.1263	241.86	--

Table S6C. Singlet-singlet and singlet-triplet TD-DFT calculations from the S_0 optimised geometry of TT at the same computational level. Molecular orbitals involved, largest coefficients in the CI expansion, vertical excitation energies (in eV and nm) and oscillator strengths for each of the first six singlet and triplet excited states are reported. Note that singlet-triplet oscillator strengths of singlet-triplet excitations are set to zero due to the neglected spin-orbital coupling in the triplet TD-DFT calculation in Gaussian09.

TT TD-DFT					
ω B97XD/6-31+G(d)/PCM					
Excited state	Transition	CI coeff.	ΔE (eV)	ΔE (nm)	Oscillator strength
S ₁	36→38	0.52587	4.2216	293.69	0.0000
S ₂	37→38	0.67997	4.6961	264.02	0.4820
S ₃	37→39	0.66879	5.0882	243.67	0.1554
S ₄	34→39	0.42267	5.2249	237.29	0.0000
S ₅	36→39	0.44143	5.8149	213.22	0.0004
S ₆	37→40	0.65352	6.0860	203.72	0.0598
T ₁	37→38	0.63151	3.2698	379.19	--
T ₂	37→39	0.58708	3.7142	333.81	--
T ₃	36→38	0.51779	4.0237	308.14	--
T ₄	34→39	0.47935	4.8584	255.19	--
T ₅	35→39	0.56332	4.9555	250.20	--
T ₆	35→38	0.43368	5.1770	239.49	--
ω B97XD/cc-pVDZ/PCM					
Excited state	Transition	CI coeff.	ΔE (eV)	ΔE (nm)	Oscillator strength
S ₁	36→38	0.52786	4.2667	290.59	0.0000
S ₂	37→38	0.68827	4.8481	255.74	0.3935
S ₃	34→39	0.42825	5.2156	237.72	0.0001
S ₄	37→39	0.68243	5.2930	234.24	0.2068
S ₅	36→39	0.45387	5.8886	210.55	0.0000
S ₆	35→38	0.65964	6.0167	206.07	0.0057
T ₁	37→38	0.63250	3.2879	377.10	--
T ₂	37→39	0.57608	3.7595	329.79	--
T ₃	36→38	0.51862	4.0329	307.43	--
T ₄	34→39	0.47992	4.8027	258.15	--
T ₅	35→39	0.58620	5.0036	247.79	--
T ₆	35→38	0.44586	5.2332	236.92	--
ω B97XD/aug-cc-pVDZ/PCM					
Excited state	Transition	CI coeff.	ΔE (eV)	ΔE (nm)	Oscillator strength
S ₁	36→38	0.50933	4.2134	294.26	0.0000
S ₂	37→38	0.67949	4.6436	267.00	0.4376
S ₃	37→39	0.66886	5.0366	246.17	0.1661
S ₄	34→38	0.40688	5.1799	239.36	0.0001
S ₅	36→39	0.42653	5.7617	215.19	0.0010
S ₆	37→40	0.53338	5.9540	208.24	0.0495
T ₁	37→38	0.62805	3.2528	381.16	--
T ₂	37→39	0.59381	3.7023	334.88	--
T ₃	36→38	0.50014	4.0141	308.87	--
T ₄	34→39	0.45961	4.8159	257.45	--
T ₅	35→39	0.57356	4.9500	250.47	--
T ₆	35→38	0.44499	5.1517	240.67	--
ω B97XD/aug-cc-pVTZ/PCM					
Excited state	Transition	CI coeff.	ΔE (eV)	ΔE (nm)	Oscillator strength
S ₁	36→38	0.52021	4.2151	294.14	0.0000
S ₂	37→38	0.67868	4.6710	265.43	0.4511
S ₃	37→39	0.66707	5.0718	244.46	0.1491
S ₄	34→39	0.40935	5.2217	237.44	0.0001
S ₅	36→39	0.43502	5.7986	213.82	0.0016
S ₆	37→40	0.48862	5.9189	209.47	0.0521
T ₁	37→38	0.63159	3.2857	377.35	--
T ₂	37→39	0.58615	3.7263	332.73	--
T ₃	36→38	0.51083	4.0090	309.26	--
T ₄	34→39	0.46769	4.8584	255.20	--
T ₅	35→39	0.56031	5.0036	247.79	--
T ₆	35→38	0.43335	5.2026	238.31	--

Table S6D. Singlet-singlet and singlet-triplet TD-DFT calculations from the S_0 optimised geometry of TT at the same computational level. Molecular orbitals involved, largest coefficients in the CI expansion, vertical excitation energies (in eV and nm) and oscillator strengths for each of the first six singlet and triplet excited states are reported. Note that singlet-triplet oscillator strengths of singlet-triplet excitations are set to zero due to the neglected spin-orbital coupling in the triplet TD-DFT calculation in Gaussian09.

TT TD-DFT					
M062X/6-31+G(d)/PCM					
Excited state	Transition	CI coeff.	ΔE (eV)	ΔE (nm)	Oscillator strength
S ₁	36→38	0.53986	4.1253	300.54	0.0000
S ₂	37→38	0.68408	4.6437	266.99	0.4713
S ₃	37→39	0.67236	5.0600	245.03	0.1399
S ₄	34→39	0.46864	5.0949	243.35	0.0001
S ₅	37→40	0.66710	5.7005	217.50	0.0394
S ₆	36→39	0.47122	5.7319	216.30	0.0000
T ₁	37→38	0.63891	3.4036	364.27	--
T ₂	37→39	0.55250	3.7854	327.54	--
T ₃	36→38	0.53252	3.9625	312.90	--
T ₄	34→39	0.50437	4.7815	259.30	--
T ₅	35→39	0.58421	5.0390	246.05	--
T ₆	35→38	0.47643	5.1493	240.78	--
M062X/cc-pVDZ/PCM					
Excited state	Transition	CI coeff.	ΔE (eV)	ΔE (nm)	Oscillator strength
S ₁	36→38	0.54350	4.1420	299.33	0.0000
S ₂	37→38	0.69308	4.7952	258.56	0.4089
S ₃	34→39	0.48268	5.0820	243.97	0.0001
S ₄	37→39	0.68263	5.2472	236.29	0.1771
S ₅	36→39	0.48486	5.8100	213.40	0.0000
S ₆	35→38	0.66696	6.0283	205.67	0.0133
T ₁	37→38	0.64148	3.4227	362.25	--
T ₂	37→39	0.53731	3.8381	323.04	--
T ₃	36→38	0.53667	3.9581	313.24	--
T ₄	34→39	0.51205	4.7378	261.69	--
T ₅	35→39	0.59472	5.0951	243.34	--
T ₆	35→38	0.47568	5.2169	237.66	--
M062X/aug-cc-pVDZ/PCM					
Excited state	Transition	CI coeff.	ΔE (eV)	ΔE (nm)	Oscillator strength
S ₁	36→38	0.52270	4.0902	303.13	0.0000
S ₂	37→38	0.68361	4.5726	271.15	0.4256
S ₃	37→39	0.67251	4.9868	248.62	0.1497
S ₄	34→39	-0.44478	5.0473	245.65	0.0001
S ₅	37→40	0.63040	5.5516	223.33	0.0310
S ₆	36→39	0.45166	5.6505	219.42	0.0010
T ₁	37→38	0.63324	3.3737	367.50	--
T ₂	37→39	0.55771	3.7544	330.24	--
T ₃	36→38	0.51465	3.9284	315.61	--
T ₄	34→39	-0.48380	4.7397	261.59	--
T ₅	35→39	0.60006	5.0309	246.45	--
T ₆	35→38	0.49362	5.1025	242.98	--
M062X/aug-cc-pVTZ/PCM					
Excited state	Transition	CI coeff.	ΔE (eV)	ΔE (nm)	Oscillator strength
S ₁	36→38	0.52712	4.0981	302.54	0.0000
S ₂	37→38	0.68255	4.6157	268.62	0.4358
S ₃	37→39	0.67210	5.0257	246.70	0.1388
S ₄	34→39	0.44306	5.1339	241.50	0.0002
S ₅	37→40	0.61933	5.5993	221.43	0.0331
S ₆	36→39	0.44948	5.7077	217.22	0.0015
T ₁	37→38	0.63299	3.4045	364.18	--
T ₂	37→39	0.55617	3.7963	326.59	--
T ₃	36→38	0.51945	3.9364	314.97	--
T ₄	34→39	0.48638	4.8382	256.26	--
T ₅	35→39	0.59651	5.1025	242.99	--
T ₆	35→38	0.49873	5.1753	239.57	--

Table S6E. Singlet-singlet and singlet-triplet TD-DFT calculations from the S_0 optimised geometry of TT at the same computational level. Molecular orbitals involved, largest coefficients in the CI expansion, vertical excitation energies (in eV and nm) and oscillator strengths for each of the first six singlet and triplet excited states are reported. Note that singlet-triplet oscillator strengths of singlet-triplet excitations are set to zero due to the neglected spin-orbital coupling in the triplet TD-DFT calculation in Gaussian09.

TT TD-DFT					
PBE0/6-31+G(d)/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	36→38	0.59193	4.0457	306.46	0.0000
S ₂	37→38	0.68186	4.3816	282.96	0.1935
S ₃	36→39	0.57393	4.6460	266.86	0.0001
S ₄	37→39	0.67732	4.8480	255.74	0.4009
S ₅	34→38	0.53950	5.2142	237.78	0.0001
S ₆	35→38	0.67683	5.5427	223.69	0.0064
T ₁	37→38	0.65103	3.0959	400.48	--
T ₂	37→39	0.60841	3.5999	344.41	--
T ₃	36→38	0.55937	3.8173	324.80	--
T ₄	36→39	0.44752	4.4797	276.77	--
T ₅	35→38	0.57111	4.5681	271.42	--
T ₆	35→39	0.64289	4.7349	261.85	--
PBE0/cc-pVDZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	36→38	0.60364	4.0766	304.13	0.0000
S ₂	37→38	0.67235	4.4896	276.16	0.1645
S ₃	36→39	0.57434	4.6984	263.89	0.0000
S ₄	37→39	0.66685	5.0592	245.07	0.3966
S ₅	34→38	0.53830	5.2091	238.01	0.0000
S ₆	35→38	0.67064	5.6178	220.70	0.0056
T ₁	37→38	0.65077	3.1175	397.70	--
T ₂	37→39	0.59179	3.6448	340.16	--
T ₃	36→38	0.56773	3.8196	324.60	--
T ₄	36→39	0.40464	4.4646	277.70	--
T ₅	35→38	0.55660	4.6299	267.79	--
T ₆	35→39	0.64193	4.7785	259.46	--
PBE0/aug-cc-pVDZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	36→38	0.58531	4.0185	308.53	0.0000
S ₂	37→38	0.68675	4.3150	287.34	0.1761
S ₃	36→39	0.56848	4.5906	270.08	0.0003
S ₄	37→39	0.68201	4.8045	258.06	0.3900
S ₅	34→38	0.56079	5.1533	240.59	0.0003
S ₆	35→38	0.67849	5.4869	225.96	0.0103
T ₁	37→38	0.64900	3.0700	403.86	--
T ₂	37→39	0.61413	3.5731	347.00	--
T ₃	36→38	0.54738	3.7893	327.20	--
T ₄	36→39	0.44313	4.4229	280.33	--
T ₅	35→38	0.57485	4.5467	272.69	--
T ₆	35→39	0.65386	4.7184	262.77	--
PBE0/aug-cc-pVTZ/PCM					
<i>Excited state</i>	<i>Transition</i>	<i>CI coeff.</i>	ΔE (eV)	ΔE (nm)	<i>Oscillator strength</i>
S ₁	36→38	0.58767	4.0284	307.77	0.0000
S ₂	37→38	0.68669	4.3513	284.94	0.1839
S ₃	36→39	0.57127	4.6270	267.96	0.0004
S ₄	37→39	0.68204	4.8313	256.63	0.3796
S ₅	34→38	0.55566	5.1984	238.50	0.0003
S ₆	37→40	0.67993	5.6078	221.09	0.0280
T ₁	37→38	0.65166	3.0930	400.85	--
T ₂	37→39	0.60952	3.5892	345.43	--
T ₃	36→38	0.55010	3.7829	327.75	--
T ₄	36→39	0.44776	4.4606	277.95	--
T ₅	35→38	0.57594	4.5942	269.87	--
T ₆	35→39	0.65467	4.7684	260.01	--