

3-Ethynyltriimidazo[1,2-*a*:1',2'-*c*:1'',2''-*e*][1,3,5]triazine Dual Short- and Long-Lived Emissions with Crystallization-Enhanced Feature: Role of Hydrogen Bonds and π - π Interactions

Daniele Malpicci^{1,2}, Daniele Maver^{1,2}, Elisabetta Rosadoni³, Alessia Colombo^{1,4}, Elena Lucenti^{2,4},
Daniele Marinotto^{2,4}, Chiara Botta⁵, Fabio Bellina³, Elena Cariatì^{1,2,4,*} and Alessandra Forni^{2,4,*}

Supplementary information

Table of Contents

1. NMR and GC-MS Spectra	2
2. Photophysical Data	10
3. Crystal data	17
4. Theoretical Studies.....	18

1. NMR and GC-MS Spectra

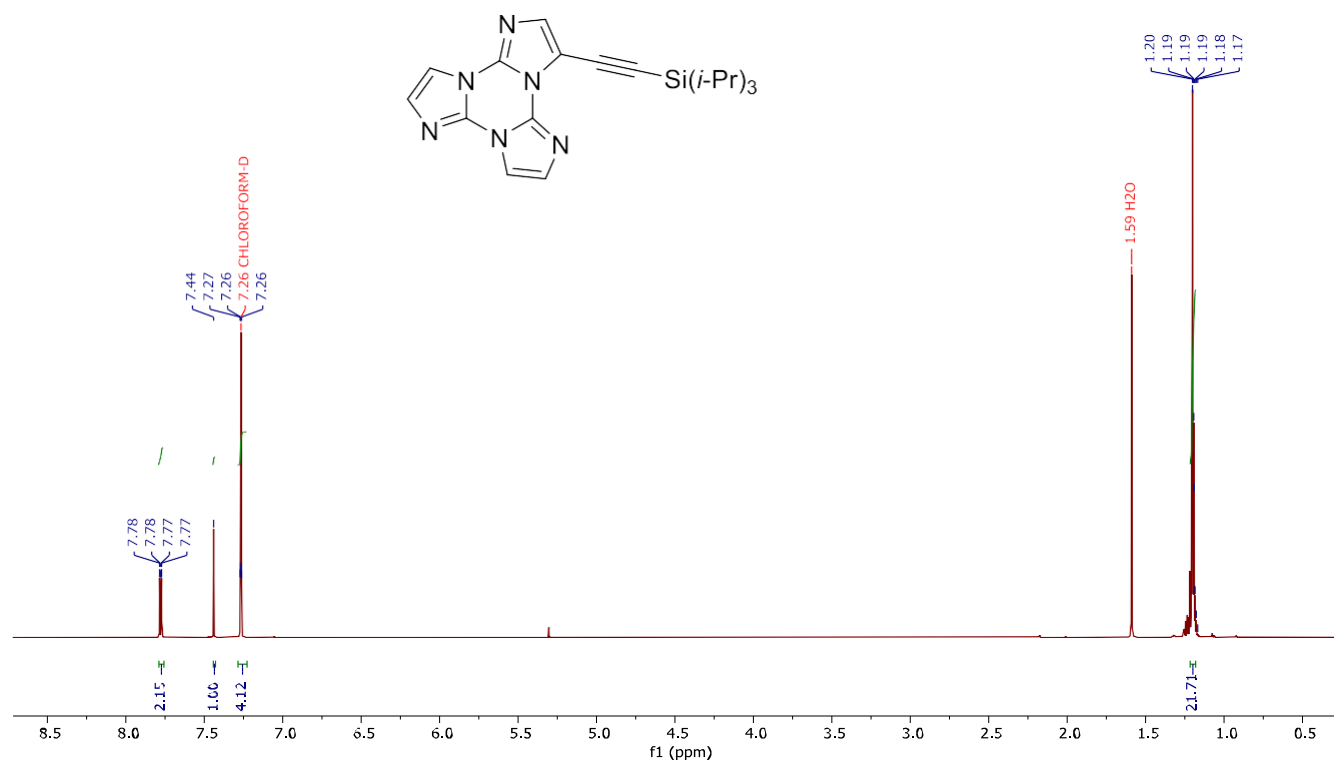


Figure S1. ¹H-NMR (CDCl₃, 500 MHz) of TT-CC-TIPS.

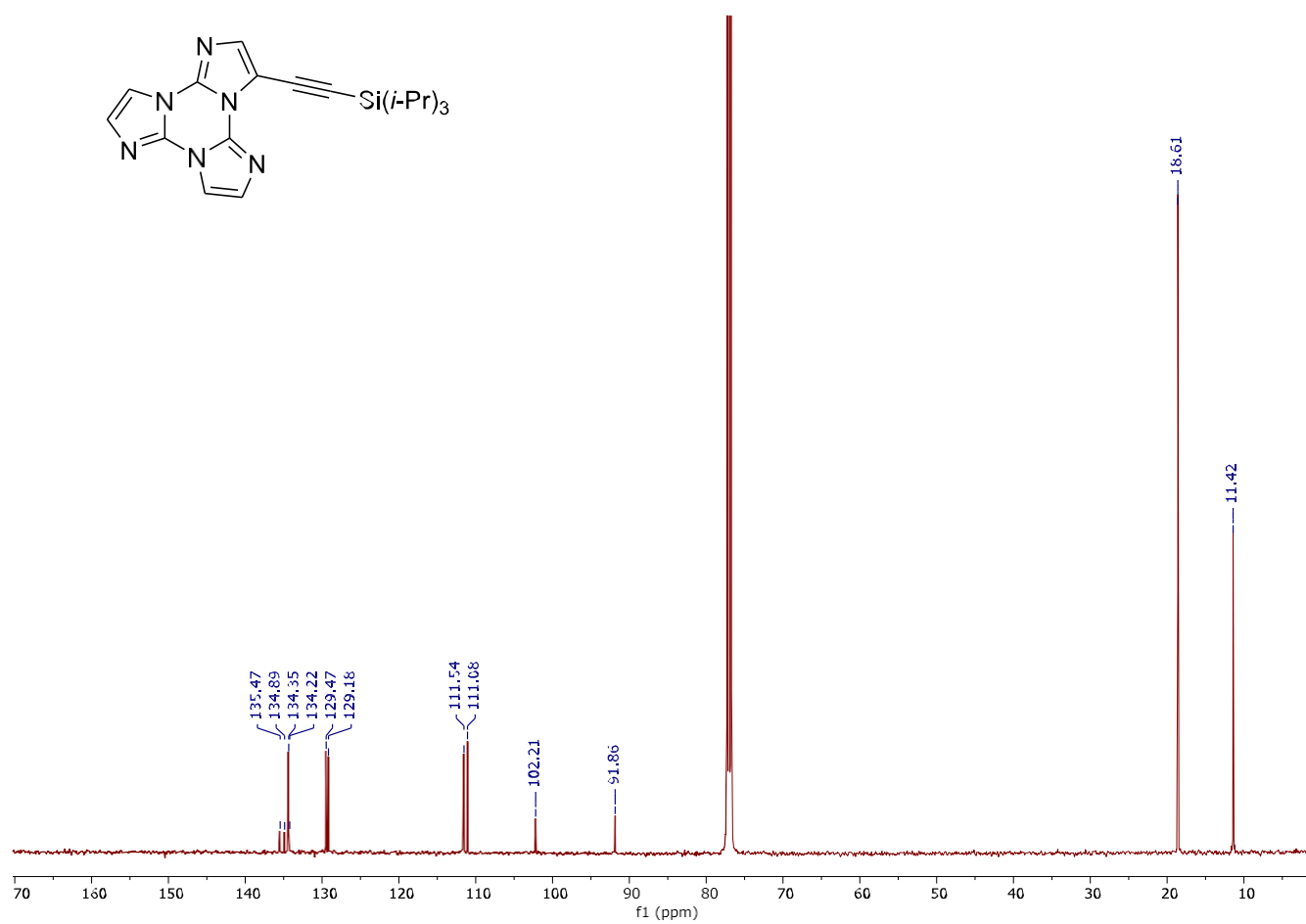


Figure S2. ¹³C-NMR (CDCl₃, 125 MHz) of TT-CC-TIPS.

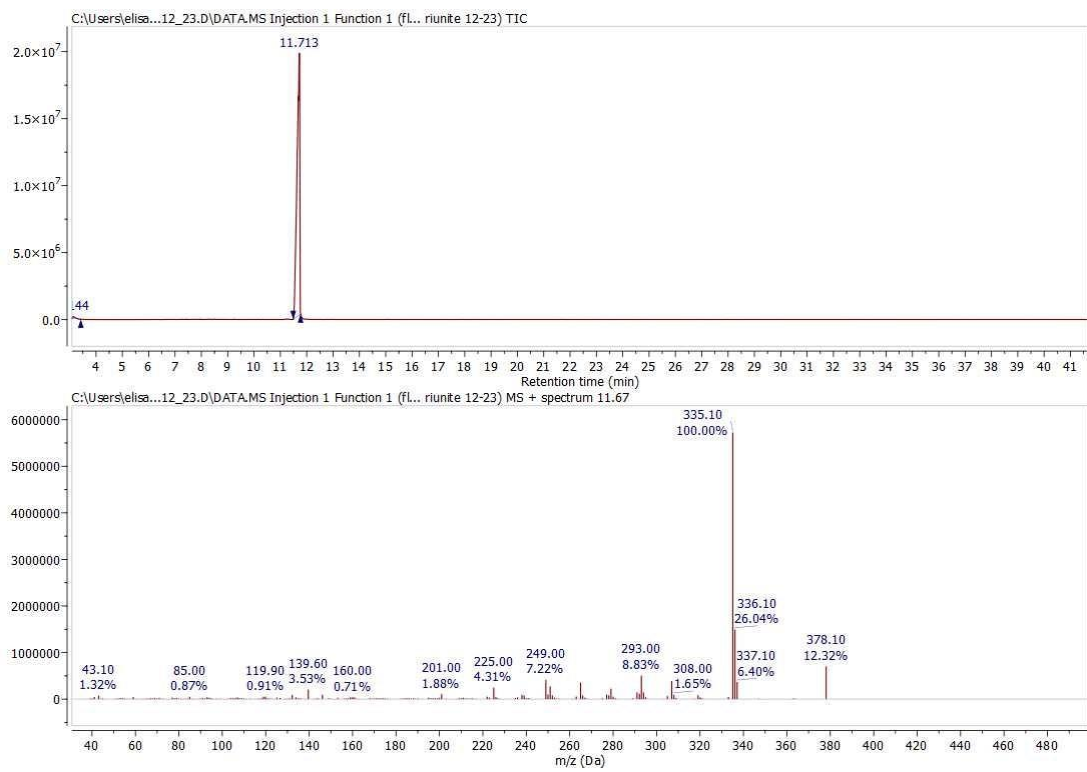


Figure S3. GC-MS(EI) profile of TT-CCH

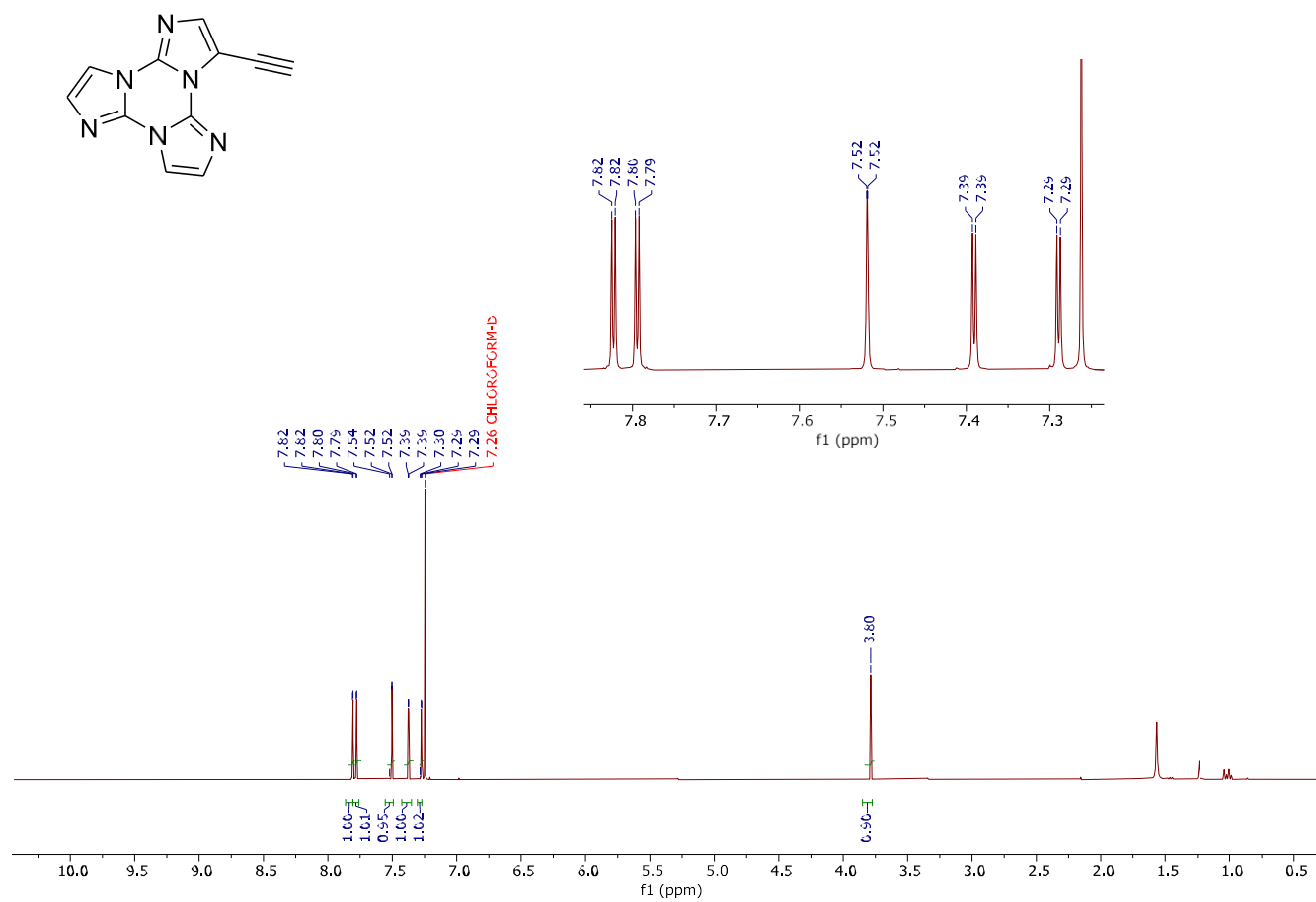


Figure S4. ¹H-NMR (CDCl₃, 500 MHz) of TT-CCH

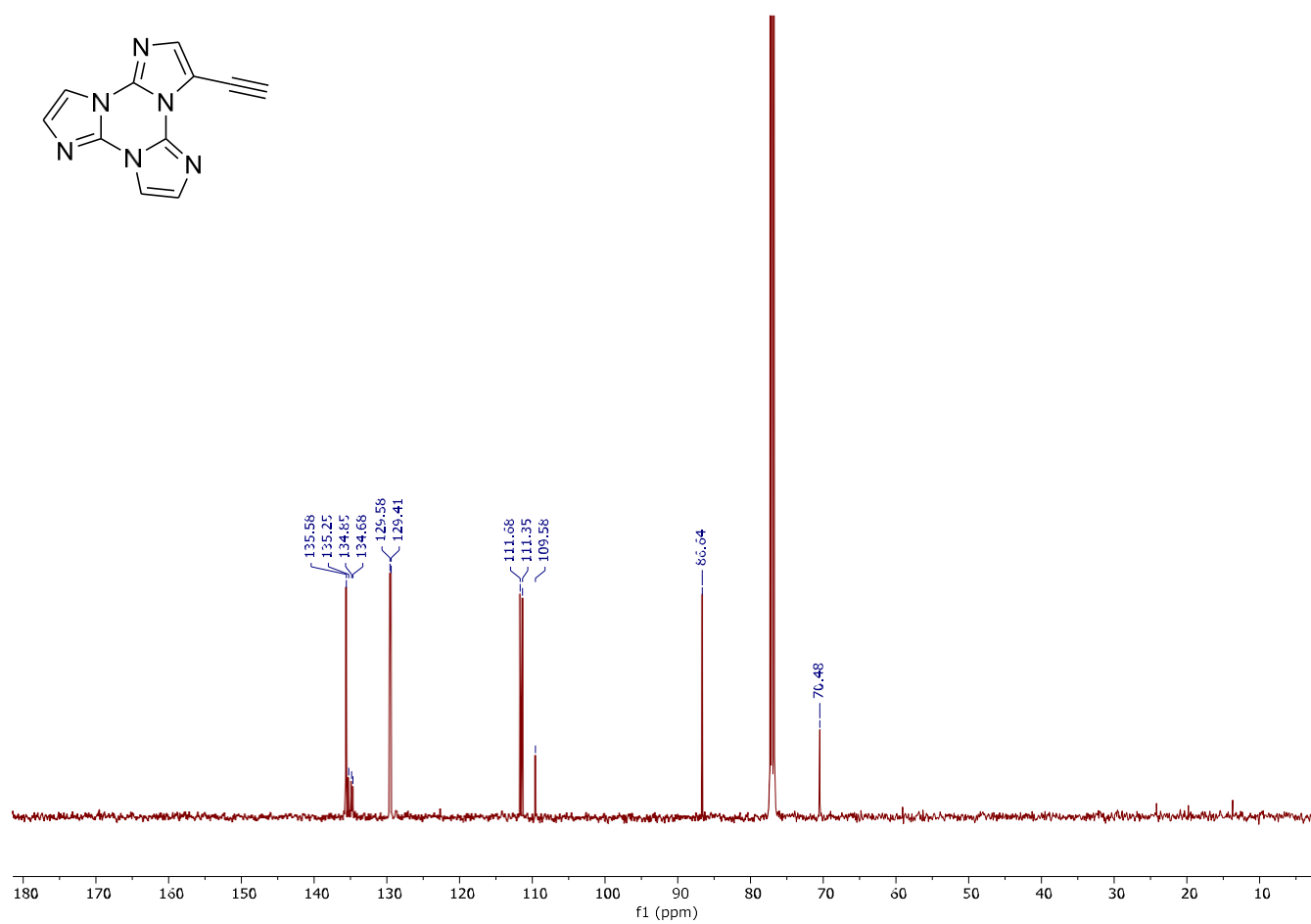


Figure S5. ¹³C-NMR spectra (CDCl₃, 125 MHz) of **TT-CCH**

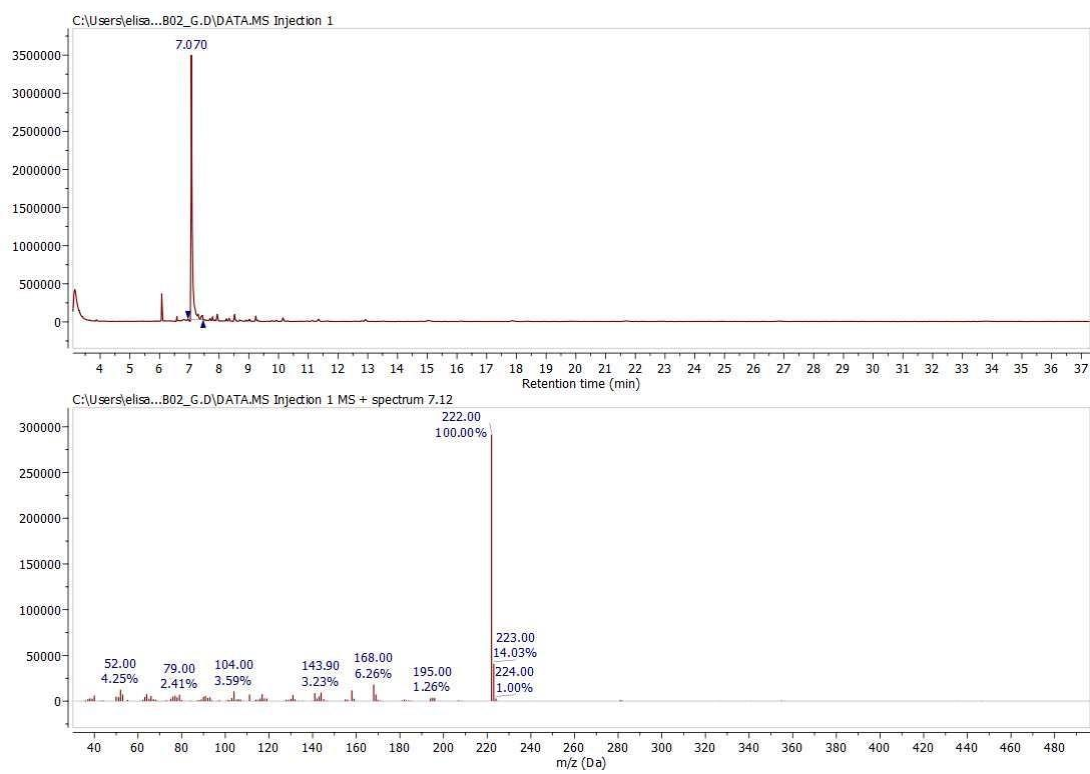


Figure S6. GC-MS(EI) profile of TT-CCH

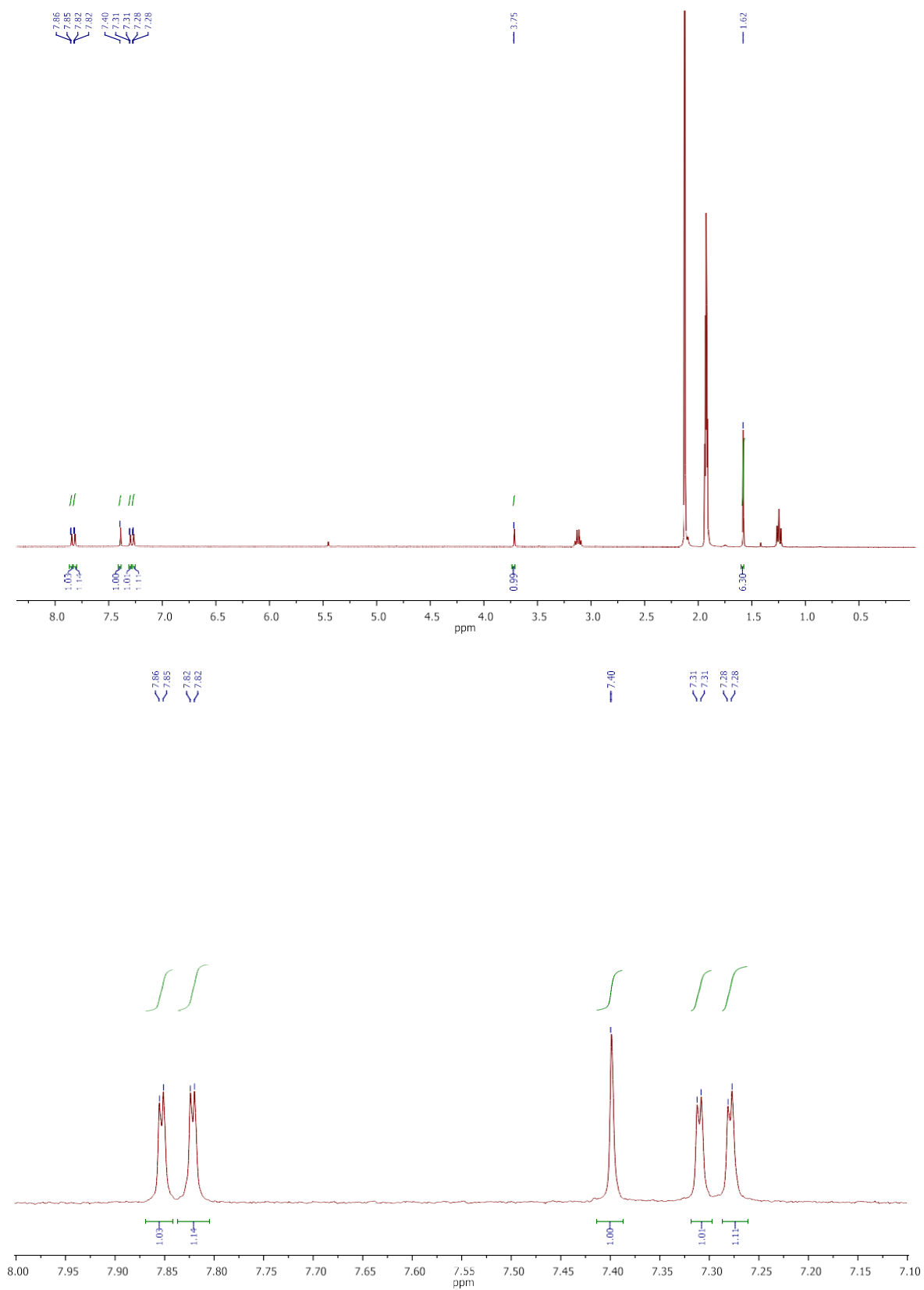


Figure S7. ^1H -NMR (CD_3CN , 400 MHz) of **TT-CC-*i*PrOH** (top) with expansion of aromatic region (below).

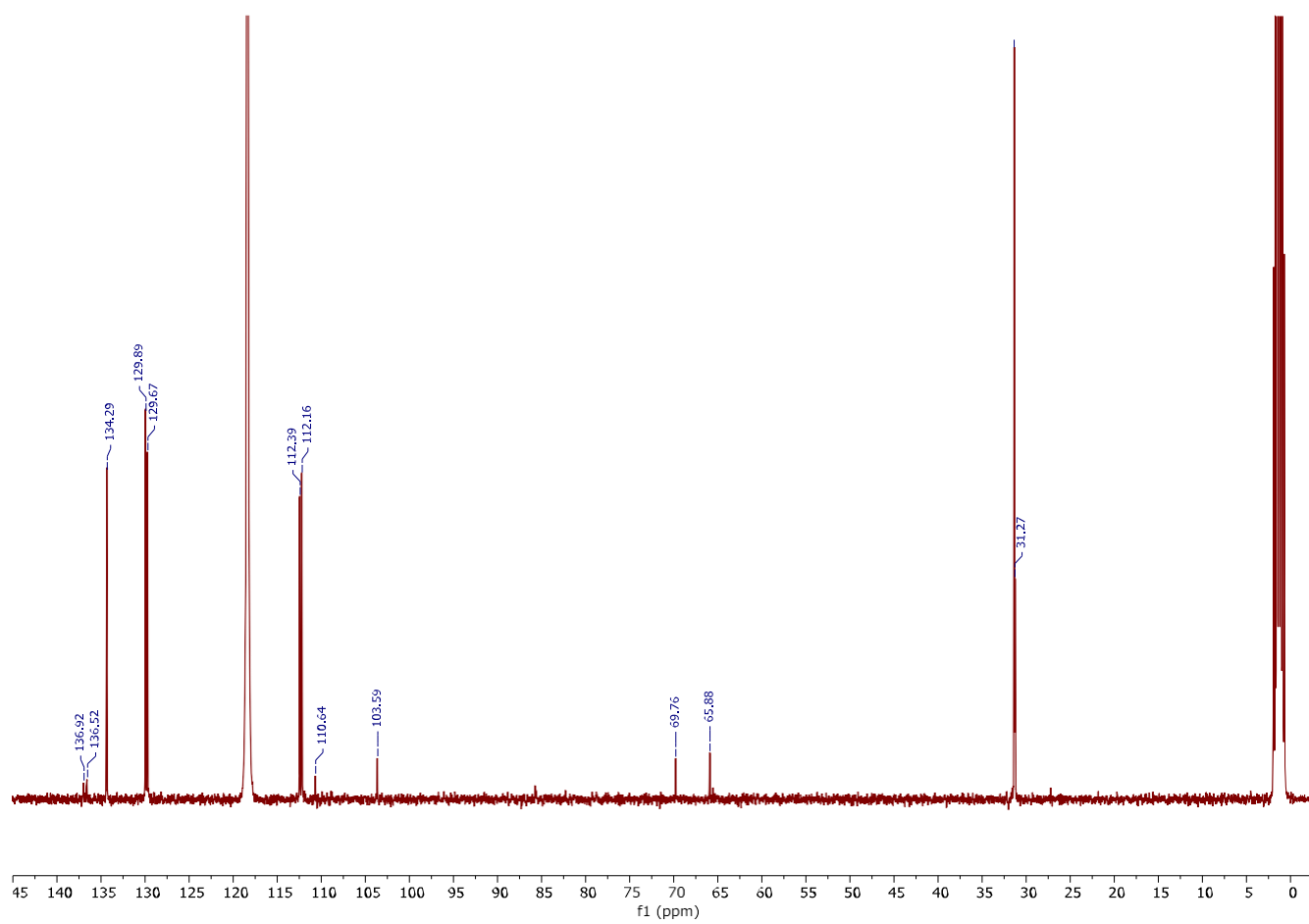


Figure S8. ^{13}C -NMR (CD_3CN , 101 MHz) of TT-CC-*i*PrOH.

2. Photophysical Data

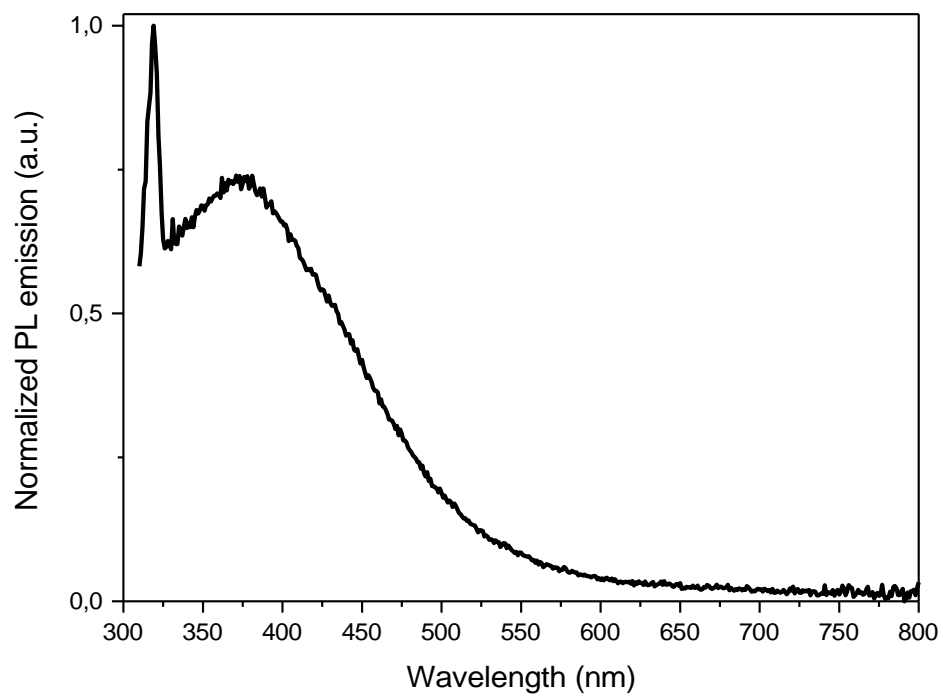


Figure S9. Normalized emission ($\lambda_{\text{exc}} = 290$ nm) of **TT-CCH** in DCM solution (1×10^{-5} M) at 298 K.

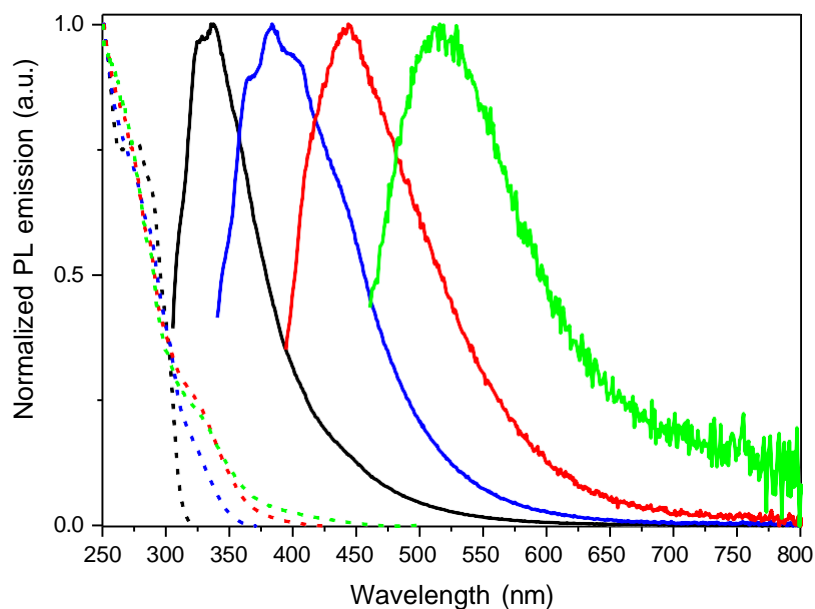


Figure S10. Normalized excitation (dashed lines: $\lambda_{\text{exc}} = 336$ nm (black), 382 nm (blue), 442 nm (red) and 516 nm (green)) and normalized emission (continuous lines: $\lambda_{\text{em}} = 290$ nm (black), 330 nm (blue), 380 nm (red) and 445 nm (green)) of **TT-CCH** in PMMA film (1.5 wt%) at 298 K.

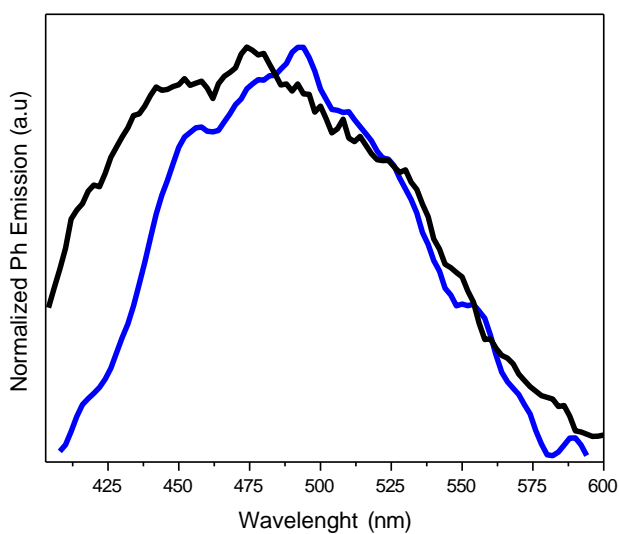


Figure S11. Normalized delayed spectra of **TT-CCH** in PMMA matrix (0.1 w/w%), at short (40 μ s delay, 200 μ s window; black line) and long (4 ms delay, 20 ms window; blue line) delay times.

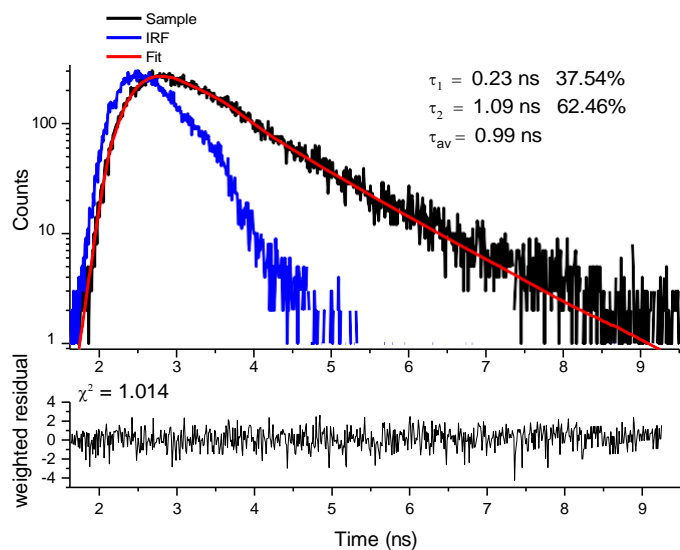


Figure S12. Lifetime measurement ($\lambda_{exc} = 300 \text{ nm}$, $\lambda_{em} = 336 \text{ nm}$) of TT-CCH in in PMMA film (5 wt%) at 298 K.

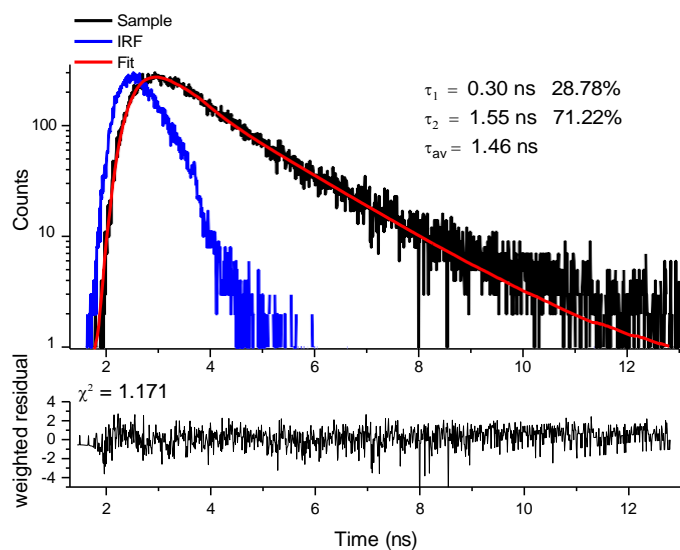


Figure S13. Lifetime measurement ($\lambda_{exc} = 300 \text{ nm}$, $\lambda_{em} = 383 \text{ nm}$) of TT-CCH in in PMMA film (5 wt%) at 298 K.

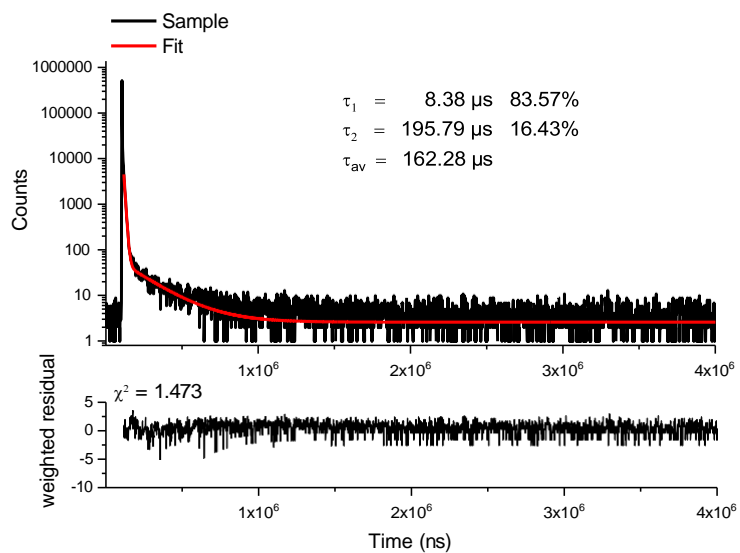


Figure S14. Lifetime measurement ($\lambda_{\text{exc}} = 300 \text{ nm}$, $\lambda_{\text{em}} = 445 \text{ nm}$) of TT-CCH in in PMMA film (5 wt%) at 298 K.

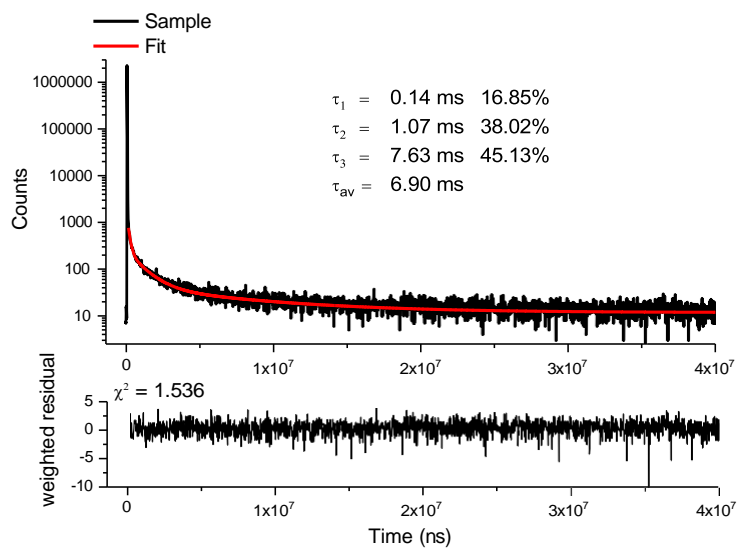


Figure S15. Lifetime measurement ($\lambda_{\text{exc}} = 300 \text{ nm}$, $\lambda_{\text{em}} = 516 \text{ nm}$) of TT-CCH in in PMMA film (5 wt%) at 298 K.

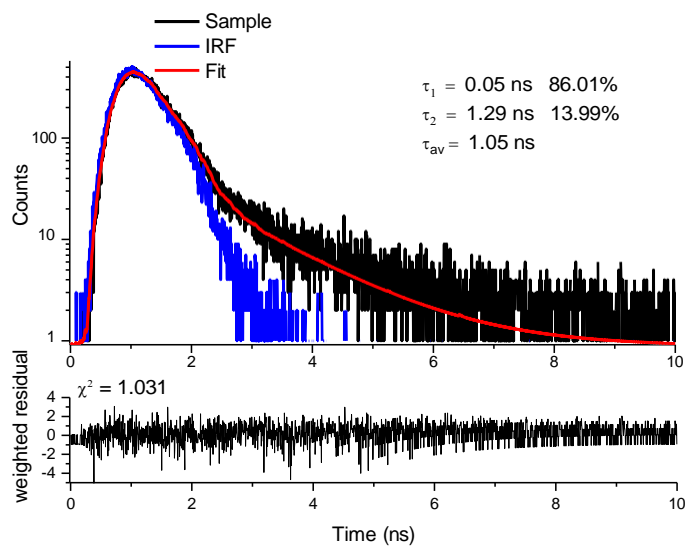


Figure S16. Lifetime measurement ($\lambda_{exc} = 300 \text{ nm}$, $\lambda_{em} = 370 \text{ nm}$) of **TT-CCH** crystals at 298 K.

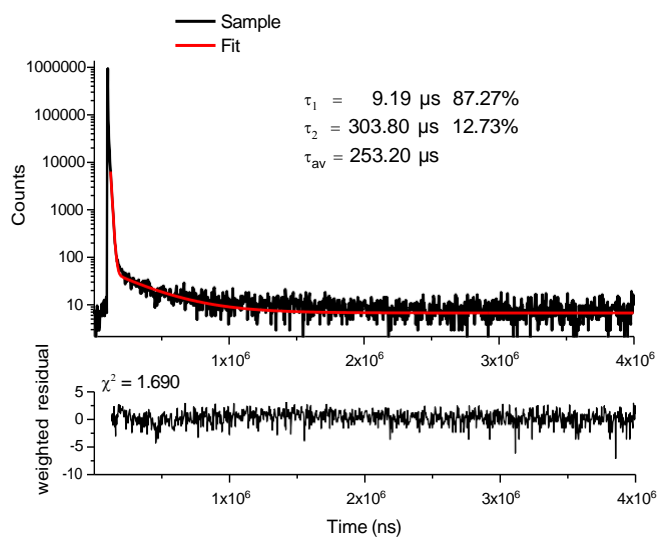


Figure S17. Lifetime measurement ($\lambda_{exc} = 300 \text{ nm}$, $\lambda_{em} = 418 \text{ nm}$) of **TT-CCH** crystals at 298 K.

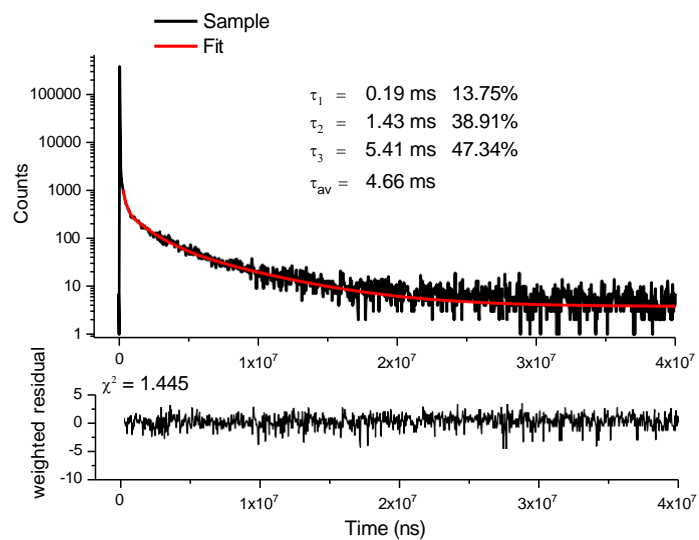


Figure S18. Lifetime measurement ($\lambda_{exc} = 300 \text{ nm}$, $\lambda_{em} = 520 \text{ nm}$) of TT-CCH crystals at 298 K.

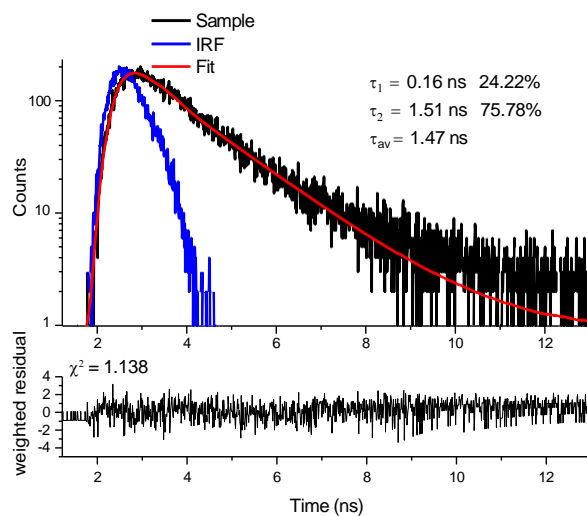


Figure S19. Lifetime measurement ($\lambda_{exc} = 300 \text{ nm}$, $\lambda_{em} = 379 \text{ nm}$) of TT-CCH crystals at 77 K.

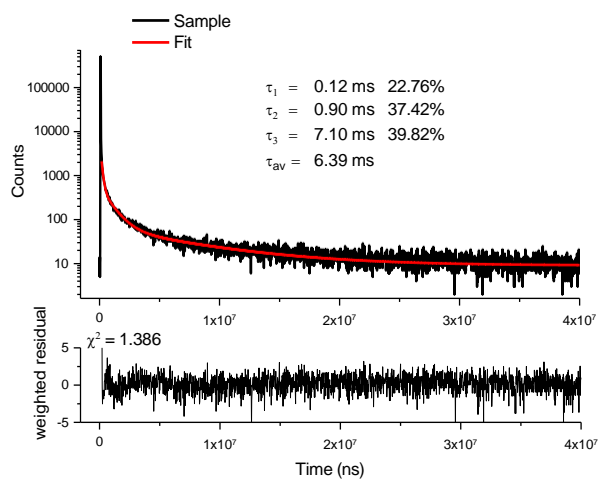


Figure S20. Lifetime measurement ($\lambda_{exc} = 300 \text{ nm}$, $\lambda_{em} = 419 \text{ nm}$) of TT-CCH crystals at 77 K.

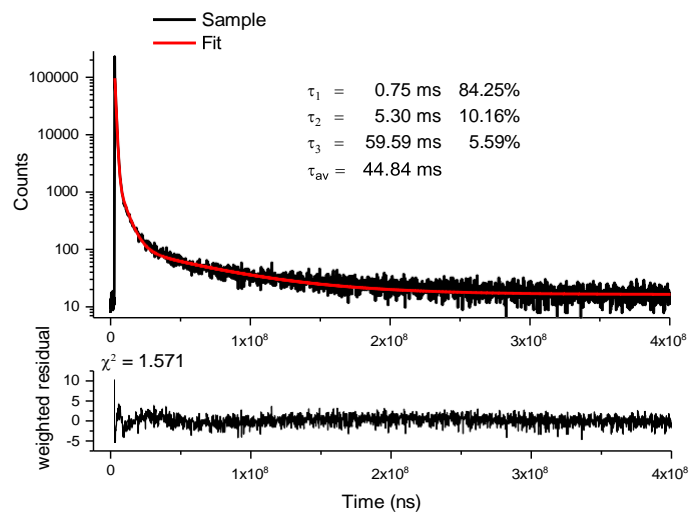


Figure S21. Lifetime measurement ($\lambda_{exc} = 300 \text{ nm}$, $\lambda_{em} = 525 \text{ nm}$) of TT-CCH crystals at 77 K.

3. Crystal data

Table S1 Crystal data, data collection and refinement details for **TT-CCH**

	TT-CCH
<i>Crystal data</i>	
Chemical formula	C ₁₁ H ₆ N ₆
M _r	222.22
Crystal system	monoclinic
Space group	P 21/1 (No. 14)
Temperature [K]	296(2)
a [Å]	13.35072(15)
b [Å]	4.63511(4)
c [Å]	16.41198(19)
α [°]	90
β [°]	96.7803(11)
γ [°]	90
V [Å ³]	1008.504(19)
Z	4
μ(CuKα) [mm ⁻¹]	0.805
Crystal size [mm]	0.32 × 0.17 × 0.10
<i>Data collection</i>	
No. of measured reflections	20327
No. of independent reflections	2177
No. of observed reflections, I > 2σ(I)	2010
R _{int}	0.044
R _σ	0.026
(sin θ/λ) _{max} [Å ⁻¹]	0.82
<i>Refinement</i>	
R[F ² > 2σ(F ²)]	0.0440
wR(F ²)	0.1164
S	1.050
No. of reflections	2177
No. of parameters	154
No. of restraints	0
ΔQ _{max} , ΔQ _{min} (e Å ⁻³)	0.162, -0.235

4. Theoretical studies

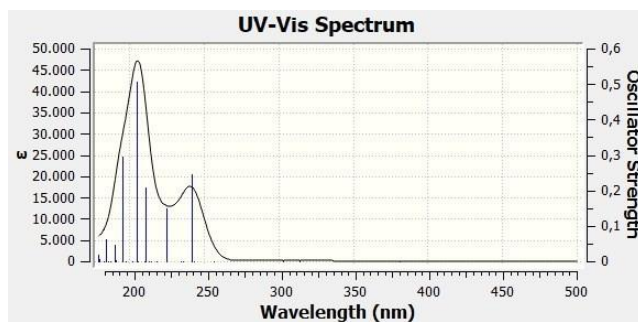


Figure S22. TD- ω B97X/6-311++G(d,p) absorption spectra of **TT-CCH** at the optimized geometry, obtained by convolution of the blue sticks with 0.2 eV of half-bandwidth.

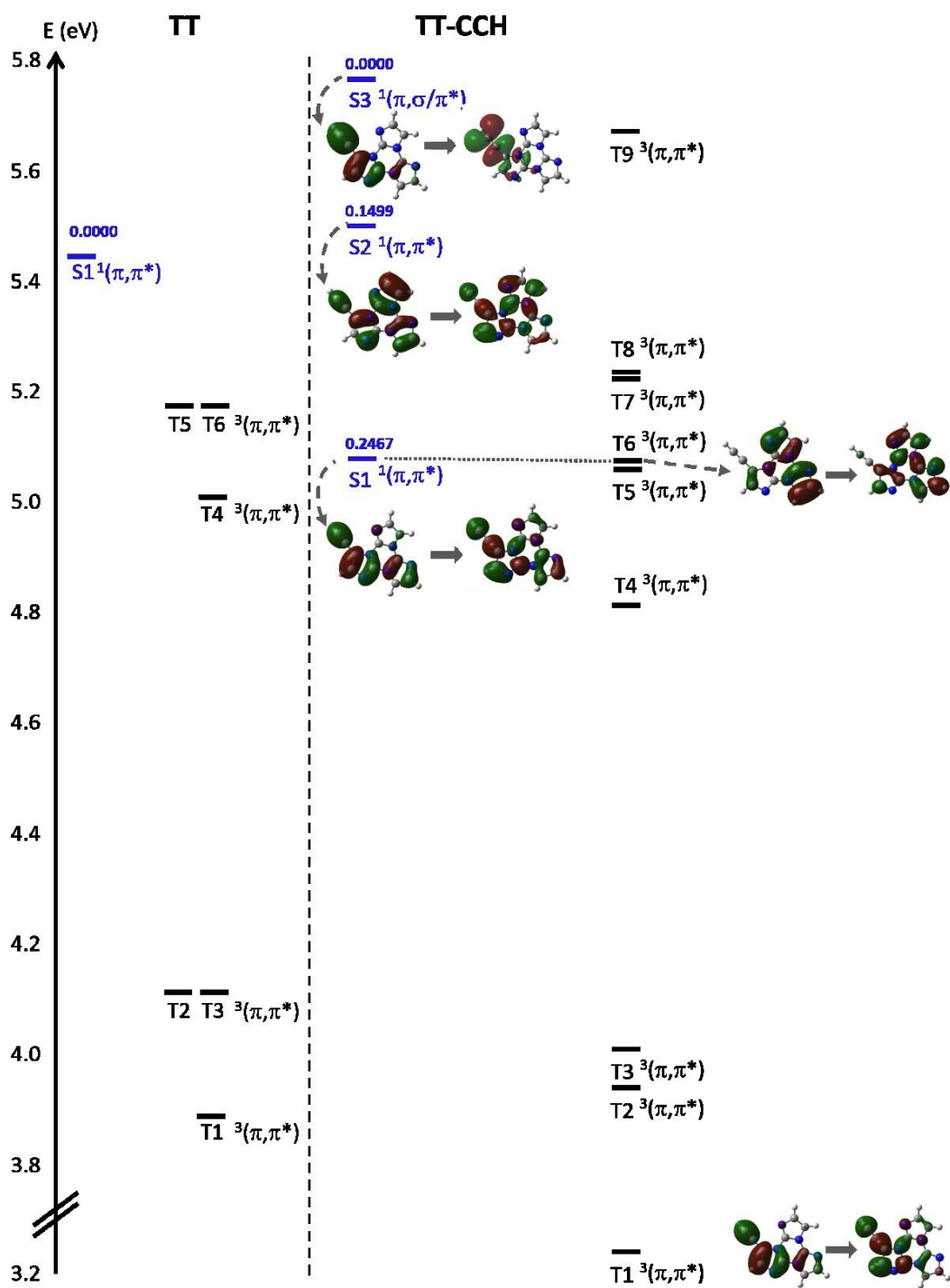


Figure S23. TD- ω B97X/6-311++G(d,p) electronic levels for **TT-CCH** at molecular level, compared with those of unsubstituted **TT**. In blue are reported the singlet levels with the corresponding values of oscillator strength f . Natural Transition Orbitals are included for selected transitions.

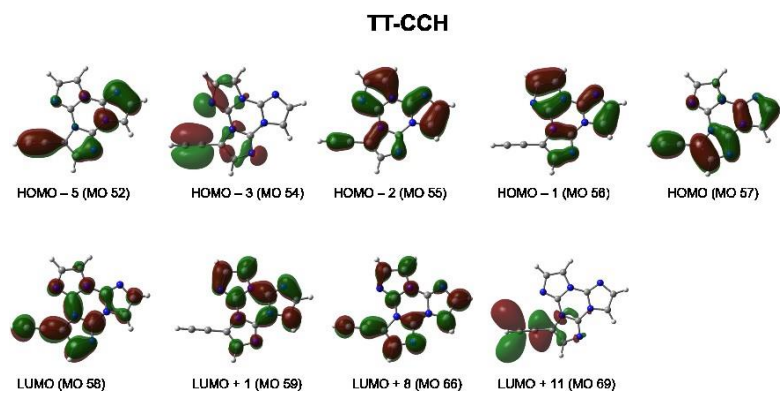


Figure S24. Plots of the ω B97X/6-311++G(d,p) MOs mainly involved in the lowest energy transitions of **TT-CCH** at the optimized ground state geometry (isosurfaces value 0.02).

Table S2 First TD- ω B97X/6-311++G(d,p) triplet and singlet electronic transitions computed for **TT-CCH** at the optimized ground state geometry.

Excitation energies and oscillator strengths:

Excited State	1:	Triplet-A	3.2486 eV	381.65 nm	f=n.d.	<S**2>=2.000
55 -> 58		0.12658				
57 -> 58		0.62532				
57 -> 66		-0.14362				
57 -> 58		0.10608				
Excited State	2:	Triplet-A	3.9434 eV	314.41 nm	f=n.d.	<S**2>=2.000
55 -> 58		0.24487				
55 -> 66		0.17562				
56 -> 59		0.53846				
57 -> 59		0.11600				
57 -> 66		-0.14104				
Excited State	3:	Triplet-A	4.0891 eV	303.20 nm	f=n.d.	<S**2>=2.000
50 -> 59		0.10554				
55 -> 59		0.42801				
56 -> 58		0.29856				
56 -> 66		0.26870				
57 -> 59		-0.20746				
Excited State	4:	Triplet-A	4.8239 eV	257.02 nm	f=n.d.	<S**2>=2.000
50 -> 58		0.11664				
52 -> 58		0.18287				
52 -> 59		-0.10998				
54 -> 69		-0.16366				
55 -> 58		-0.12945				
55 -> 66		0.11151				
56 -> 58		-0.23700				
56 -> 59		0.14448				
57 -> 58		0.14648				
57 -> 59		-0.24663				
57 -> 66		0.31145				
57 -> 70		-0.13974				
57 -> 77		0.13786				
Excited State	5:	Triplet-A	5.0893 eV	243.62 nm	f=n.d.	<S**2>=2.000
48 -> 58		-0.12214				
55 -> 58		0.10793				
55 -> 59		-0.28606				
55 -> 70		-0.15779				
56 -> 58		0.39989				
56 -> 70		-0.11775				
56 -> 72		0.14046				
57 -> 66		0.20520				
Excited State	6:	Triplet-A	5.1252 eV	241.91 nm	f=n.d.	<S**2>=2.000
50 -> 59		0.12441				
55 -> 58		-0.31590				
55 -> 66		-0.19073				
55 -> 72		-0.11210				
56 -> 59		0.13224				
56 -> 66		0.21350				
56 -> 70		0.17978				
57 -> 59		0.31860				
57 -> 77		-0.11562				
Excited State	7:	Singlet-A	5.1257 eV	241.89 nm	f=0.2467	<S**2>=0.000
56 -> 59		-0.19348				
57 -> 58		0.63615				
Excited State	8:	Triplet-A	5.2473 eV	236.28 nm	f=n.d.	<S**2>=2.000
47 -> 58		-0.12308				
49 -> 69		-0.19306				

52 -> 59	-0.11295				
54 -> 69	0.41961				
54 -> 75	0.10820				
54 -> 79	-0.12099				
55 -> 58	-0.10282				
55 -> 59	-0.13182				
56 -> 59	0.11404				
57 -> 59	-0.15741				
57 -> 66	0.13619				
Excited State 9:	Triplet-A	5.2837 eV	234.66 nm	f=n.d.	<S**2>=2.000
52 -> 69	-0.21578				
54 -> 58	0.29832				
54 -> 66	-0.14310				
55 -> 69	0.16518				
57 -> 65	0.11325				
57 -> 69	0.41306				
57 -> 75	0.10163				
57 -> 79	-0.10644				
Excited State 10:	Singlet-A	5.5093 eV	225.04 nm	f=0.1499	<S**2>=0.000
55 -> 58	0.27310				
56 -> 58	0.39090				
56 -> 59	0.27620				
56 -> 66	0.12738				
57 -> 58	0.13036				
57 -> 59	0.29348				
57 -> 66	-0.14448				
Excited State 11:	Triplet-A	5.6867 eV	218.02 nm	f=n.d.	<S**2>=2.000
47 -> 58	0.10962				
47 -> 59	-0.13982				
48 -> 58	-0.11166				
52 -> 59	0.18109				
54 -> 69	0.18107				
55 -> 66	0.16159				
55 -> 70	0.12960				
56 -> 58	0.13205				
56 -> 72	-0.14933				
56 -> 77	0.15553				
57 -> 59	0.26760				
57 -> 66	0.15159				
57 -> 70	-0.19197				
Excited State 12:	Singlet-A	5.7799 eV	214.51 nm	f=0.0000	<S**2>=0.000
52 -> 69	-0.21387				
54 -> 58	-0.19256				
55 -> 69	0.18331				
57 -> 65	0.14784				
57 -> 69	0.49033				
57 -> 75	0.10982				
57 -> 79	-0.11410				
Excited State 13:	Triplet-A	5.8169 eV	213.15 nm	f=n.d.	<S**2>=2.000
52 -> 69	0.11637				
54 -> 58	0.49806				
54 -> 66	-0.18848				
55 -> 69	-0.10429				
57 -> 69	-0.28791				
Excited State 14:	Singlet-A	5.8782 eV	210.92 nm	f=0.2084	<S**2>=0.000
55 -> 58	0.22377				
55 -> 66	0.14455				
56 -> 58	-0.36812				
56 -> 59	0.47550				
57 -> 59	-0.17946				
Excited State 15:	Triplet-A	5.9071 eV	209.89 nm	f=n.d.	<S**2>=2.000
47 -> 58	0.15576				
48 -> 58	0.18283				
50 -> 58	0.11910				

50 -> 66	-0.13462					
52 -> 58	0.19788					
54 -> 69	0.18537					
55 -> 59	0.14990					
55 -> 70	-0.21757					
55 -> 72	0.11767					
56 -> 58	-0.15760					
56 -> 72	0.17110					
56 -> 77	-0.11789					
56 -> 87	0.10047					
57 -> 59	0.13401					
57 -> 106	0.11428					
Excited State 16:	Singlet-A	6.0348 eV	205.45 nm	f=0.0003	<S**2>=0.000	
53 -> 58	0.11737					
54 -> 58	0.56379					
54 -> 66	-0.21685					
57 -> 69	0.17835					
Excited State 17:	Singlet-A	6.0392 eV	205.30 nm	f=0.5076	<S**2>=0.000	
55 -> 59	-0.38732					
56 -> 58	-0.29737					
57 -> 59	0.45048					
Excited State 18:	Triplet-A	6.1286 eV	202.30 nm	f=n.d.	<S**2>=2.000	
50 -> 58	-0.20930					
55 -> 58	0.33109					
55 -> 70	-0.10523					
55 -> 72	-0.11191					
55 -> 77	0.17012					
56 -> 58	-0.15760					
56 -> 59	-0.15644					
56 -> 70	0.24664					
57 -> 59	0.14654					
57 -> 66	0.13199					

Table S3 First TD- ω B97X/6-311++G(d,p) triplet and singlet electronic transitions computed for the hydrogen bonded dimer of TT-CCH (Figure 6a) at the optimized ground state geometry.

Excitation energies and oscillator strengths:

Excited State 1:	Triplet-A	3.2218 eV	384.83 nm	f=n.d.	<S**2>=2.000	
113 -> 115	-0.43313					
113 -> 129	0.11947					
114 -> 116	0.44973					
114 -> 127	-0.12338					
Excited State 2:	Triplet-A	3.2248 eV	384.47 nm	f=n.d.	<S**2>=2.000	
113 -> 116	-0.43783					
113 -> 127	0.11530					
114 -> 115	0.44586					
114 -> 129	-0.12603					
Excited State 3:	Triplet-A	3.9616 eV	312.97 nm	f=n.d.	<S**2>=2.000	
109 -> 116	0.16929					
109 -> 127	0.12687					
110 -> 115	-0.16744					
110 -> 129	-0.12004					
111 -> 117	-0.35547					
112 -> 117	-0.13365					
112 -> 118	0.38450					
113 -> 127	-0.10132					
Excited State 4:	Triplet-A	3.9616 eV	312.97 nm	f=n.d.	<S**2>=2.000	
109 -> 115	-0.16511					
109 -> 129	-0.11553					

110	->116	0.17117							
110	->127	0.13167							
111	->117	0.14107							
111	->118	0.37960							
112	->117	-0.35663							
Excited State	5:	Triplet-A	4.1119 eV	301.53 nm	f=n.d.	<S**2>=2.000			
109	->117	0.30927							
110	->118	-0.30736							
111	->116	-0.20158							
111	->127	-0.17999							
112	->115	0.22186							
112	->129	0.17324							
113	->117	-0.13228							
114	->118	0.12405							
Excited State	6:	Triplet-A	4.1120 eV	301.52 nm	f=n.d.	<S**2>=2.000			
109	->118	-0.29929							
110	->117	0.31733							
111	->115	0.22236							
111	->129	0.17263							
112	->116	-0.20273							
112	->127	-0.18121							
113	->118	0.14450							
114	->117	-0.11187							
Excited State	7:	Triplet-A	4.8011 eV	258.24 nm	f=n.d.	<S**2>=2.000			
105	->115	0.12447							
105	->118	0.10115							
106	->116	-0.15836							
108	->135	-0.14251							
111	->115	-0.11862							
111	->118	-0.11192							
112	->116	0.13526							
113	->118	0.21427							
113	->129	0.19310							
114	->116	-0.11655							
114	->117	-0.15175							
114	->127	-0.26244							
114	->139	0.11498							
Excited State	8:	Triplet-A	4.8114 eV	257.69 nm	f=n.d.	<S**2>=2.000			
105	->116	-0.14756							
106	->115	0.13178							
106	->118	0.10842							
111	->116	0.14246							
112	->115	-0.11777							
112	->118	-0.10977							
113	->116	-0.12721							
113	->117	-0.15549							
113	->127	-0.25672							
113	->139	0.11203							
114	->118	0.22983							
114	->129	0.20745							
114	->147	0.10093							
114	->150	-0.10132							
Excited State	9:	Singlet-A	5.0702 eV	244.54 nm	f=0.7426	<S**2>=0.000			
112	->117	0.10438							
113	->115	-0.44113							
113	->118	-0.11037							
114	->116	0.47680							
Excited State	10:	Triplet-A	5.0710 eV	244.49 nm	f=n.d.	<S**2>=2.000			
109	->118	0.19797							
110	->117	-0.18563							
110	->139	0.13657							
111	->115	0.30164							
111	->142	-0.10577							
112	->116	-0.27009							
112	->139	0.13492							

113	->129	0.11202					
114	->127	-0.11753					
Excited State	11:	Triplet-A	5.0716 eV	244.47 nm	f=n.d.	<S**2>=2.000	
109	->116	-0.10445					
109	->117	-0.18188					
109	->139	0.13761					
110	->118	0.20231					
110	->129	-0.10205					
111	->116	-0.26875					
111	->139	0.13890					
112	->115	0.30081					
112	->142	-0.10593					
113	->127	-0.12868					
114	->129	0.11104					
Excited State	12:	Singlet-A	5.1017 eV	243.03 nm	f=0.0000	<S**2>=0.000	
111	->117	0.14068					
112	->118	-0.13484					
113	->116	0.44890					
114	->115	-0.44126					
114	->118	-0.12170					
Excited State	13:	Triplet-A	5.1109 eV	242.59 nm	f=n.d.	<S**2>=2.000	
108	->135	-0.13801					
109	->115	-0.22307					
110	->116	0.21059					
111	->129	0.15491					
112	->127	-0.13567					
112	->139	-0.12489					
113	->118	-0.22341					
114	->117	0.22355					
Excited State	14:	Triplet-A	5.1175 eV	242.27 nm	f=n.d.	<S**2>=2.000	
109	->116	0.21500					
109	->127	0.11236					
110	->115	-0.25036					
111	->117	0.10823					
111	->127	-0.14091					
111	->139	-0.13078					
112	->118	-0.10478					
112	->129	0.16296					
113	->117	0.22444					
114	->118	-0.20220					
Excited State	15:	Triplet-A	5.2252 eV	237.28 nm	f=n.d.	<S**2>=2.000	
107	->138	0.13270					
107	->144	-0.18881					
108	->131	-0.10717					
108	->135	-0.34396					
108	->136	0.12979					
109	->115	0.13518					
110	->117	0.11116					
Excited State	16:	Triplet-A	5.2683 eV	235.34 nm	f=n.d.	<S**2>=2.000	
105	->144	-0.10193					
106	->135	-0.15879					
107	->115	0.20870					
107	->129	-0.10382					
108	->116	-0.26029					
108	->127	0.14173					
110	->135	0.10181					
113	->138	-0.13751					
113	->144	0.18481					
114	->131	0.10234					
114	->135	0.32266					
114	->136	-0.11529					
Excited State	17:	Triplet-A	5.2962 eV	234.10 nm	f=n.d.	<S**2>=2.000	
97	->135	-0.12698					
107	->135	0.29470					

107	->136	-0.11365				
108	->138	-0.16523				
108	->144	0.23116				
109	->117	-0.10314				
113	->117	-0.12255				
114	->118	0.12901				
Excited State	18:	Triplet-A	5.3048 eV	233.72 nm	f=n.d.	<S**2>=2.000
105	->135	-0.15345				
106	->144	-0.10306				
107	->116	-0.22082				
107	->127	0.11807				
108	->115	0.26278				
108	->129	-0.12793				
109	->135	0.10482				
113	->135	0.29771				
113	->136	-0.10761				
114	->138	-0.14927				
114	->144	0.19895				
Excited State	19:	Singlet-A	5.4935 eV	225.69 nm	f=0.3116	<S**2>=0.000
109	->115	0.17072				
110	->116	-0.18558				
111	->115	0.28406				
111	->118	-0.18494				
112	->116	-0.20783				
112	->117	0.26150				
113	->115	0.10250				
113	->118	-0.22809				
114	->117	0.21563				
114	->127	0.12594				
Excited State	20:	Singlet-A	5.5081 eV	225.09 nm	f=0.0000	<S**2>=0.000
109	->116	-0.18648				
110	->115	0.18875				
111	->116	-0.23282				
111	->117	0.22717				
112	->115	0.29800				
112	->118	-0.15557				
113	->117	0.21401				
113	->127	0.11995				
114	->115	0.13541				
114	->118	-0.20969				
Excited State	21:	Triplet-A	5.6408 eV	219.80 nm	f=n.d.	<S**2>=2.000
105	->118	0.12826				
106	->117	-0.14304				
108	->135	-0.17718				
109	->129	-0.11237				
110	->127	0.10873				
113	->118	0.18764				
113	->137	0.12369				
114	->117	-0.23637				
114	->127	0.13078				
114	->139	-0.14240				
Excited State	22:	Triplet-A	5.6641 eV	218.90 nm	f=n.d.	<S**2>=2.000
105	->117	-0.12950				
106	->118	0.12893				
107	->135	-0.16687				
108	->144	-0.12890				
109	->127	0.10631				
110	->129	-0.10565				
111	->140	-0.10220				
111	->151	-0.10010				
112	->142	-0.10835				
113	->117	-0.21779				
113	->127	0.12198				
113	->139	-0.14154				
114	->118	0.17587				
114	->129	-0.10750				

114 ->137	0.11991					
Excited State	23:	Triplet-A	5.7778 eV	214.59 nm	f=n.d.	<S**2>=2.000
107 ->115	-0.29946					
107 ->129	0.12500					
108 ->116	0.37077					
108 ->127	-0.17271					
113 ->138	-0.11359					
113 ->144	0.13947					
114 ->135	0.25671					
Excited State	24:	Singlet-A	5.7782 eV	214.57 nm	f=0.0000	<S**2>=0.000
106 ->135	-0.15028					
107 ->115	-0.17439					
108 ->116	0.21935					
108 ->127	-0.10788					
110 ->135	0.10621					
113 ->138	-0.16352					
113 ->144	0.20058					
114 ->131	0.11968					
114 ->135	0.37042					
114 ->136	-0.12939					
Excited State	25:	Triplet-A	5.7982 eV	213.83 nm	f=n.d.	<S**2>=2.000
107 ->116	-0.30242					
107 ->127	0.13541					
108 ->115	0.36502					
108 ->129	-0.15041					
113 ->135	-0.24658					
114 ->138	0.12661					
114 ->144	-0.15351					

Table S4 First TD- ω B97X/6-311++G(d,p) triplet and singlet electronic transitions computed for the hydrogen bonded tetramer of TT-CCH (Figure 6b) at the optimized ground state geometry.

Excitation energies and oscillator strengths:

Excited State	1:	Triplet-A	3.2221 eV	384.79 nm	f=n.d.	<S**2>=2.000
225 -> 231	-0.11473					
225 -> 232	-0.11715					
226 -> 231	0.14606					
226 -> 232	0.11314					
227 -> 230	-0.11359					
227 -> 231	0.24693					
227 -> 232	0.27163					
228 -> 231	0.29221					
228 -> 232	0.24174					
Excited State	2:	Triplet-A	3.2221 eV	384.79 nm	f=n.d.	<S**2>=2.000
225 -> 231	-0.13252					
225 -> 232	0.10144					
226 -> 231	-0.12662					
226 -> 232	0.13026					
227 -> 230	0.10245					
227 -> 231	0.29894					
227 -> 232	-0.24644					
228 -> 230	-0.10889					
228 -> 231	-0.24135					
228 -> 232	0.26527					
Excited State	3:	Triplet-A	3.2375 eV	382.96 nm	f=n.d.	<S**2>=2.000
225 -> 230	0.33500					
225 -> 232	0.19204					
226 -> 229	0.34829					
226 -> 231	-0.11406					
226 -> 249	-0.10107					
227 -> 230	0.19767					

228 -> 229	-0.21761					
Excited State 4:	Triplet-A	3.2377 eV	382.94 nm	f=n.d.	<S**2>=2.000	
225 -> 229	0.36273					
225 -> 231	-0.11526					
225 -> 249	-0.10666					
226 -> 230	0.32057					
226 -> 232	0.18681					
227 -> 229	0.20219					
228 -> 230	-0.21139					
Excited State 5:	Triplet-A	3.9432 eV	314.42 nm	f=n.d.	<S**2>=2.000	
219 -> 229	-0.14342					
220 -> 230	-0.12444					
223 -> 238	0.36631					
224 -> 233	-0.12932					
224 -> 235	-0.33946					
226 -> 235	0.10931					
Excited State 6:	Triplet-A	3.9444 eV	314.33 nm	f=n.d.	<S**2>=2.000	
219 -> 230	0.11588					
220 -> 229	0.15625					
220 -> 249	0.10038					
223 -> 233	-0.13037					
223 -> 235	-0.34268					
224 -> 238	0.36549					
226 -> 238	-0.10543					
Excited State 7:	Triplet-A	3.9617 eV	312.95 nm	f=n.d.	<S**2>=2.000	
217 -> 231	-0.10116					
218 -> 231	0.11136					
218 -> 232	-0.10284					
222 -> 233	0.34583					
222 -> 234	0.36550					
222 -> 235	-0.12057					
Excited State 8:	Triplet-A	3.9617 eV	312.95 nm	f=n.d.	<S**2>=2.000	
217 -> 231	-0.10278					
218 -> 231	-0.10941					
218 -> 232	-0.10458					
221 -> 233	-0.34852					
221 -> 234	0.36287					
221 -> 235	0.12052					
Excited State 9:	Triplet-A	4.1112 eV	301.58 nm	f=n.d.	<S**2>=2.000	
217 -> 235	0.14092					
219 -> 235	-0.25884					
220 -> 230	-0.11706					
220 -> 238	-0.27557					
223 -> 230	0.19146					
223 -> 257	0.15024					
224 -> 229	-0.20211					
224 -> 235	-0.10171					
224 -> 249	-0.16486					
225 -> 238	-0.10700					
Excited State 10:	Triplet-A	4.1123 eV	301.49 nm	f=n.d.	<S**2>=2.000	
217 -> 238	-0.11895					
218 -> 235	0.11274					
219 -> 230	0.10894					
219 -> 238	0.25194					
220 -> 233	0.11114					
220 -> 235	0.26338					
223 -> 229	-0.19427					
223 -> 249	-0.15811					
224 -> 230	0.18705					
224 -> 257	0.14511					
225 -> 235	0.10314					
Excited State 11:	Triplet-A	4.1125 eV	301.48 nm	f=n.d.	<S**2>=2.000	
217 -> 233	-0.24987					

218 -> 234	0.28328				
219 -> 233	-0.13643				
220 -> 234	-0.10119				
221 -> 232	-0.14628				
221 -> 253	-0.12433				
222 -> 231	0.19431				
222 -> 232	-0.12073				
222 -> 253	-0.10277				
222 -> 256	-0.15416				
227 -> 234	-0.10640				
Excited State 12:	Triplet-A	4.1125 eV	301.48 nm	f=n.d.	<S**2>=2.000
217 -> 234	-0.24460				
218 -> 233	0.26717				
219 -> 234	-0.15699				
220 -> 235	0.10748				
221 -> 231	0.18847				
221 -> 232	0.11891				
221 -> 253	0.10103				
221 -> 256	-0.15017				
222 -> 232	-0.13963				
222 -> 253	-0.11880				
228 -> 234	0.10084				
Excited State 13:	Triplet-A	4.7784 eV	259.47 nm	f=n.d.	<S**2>=2.000
211 -> 229	0.10386				
223 -> 229	0.12547				
224 -> 238	0.12420				
225 -> 229	-0.11613				
225 -> 235	0.14780				
225 -> 249	-0.18668				
226 -> 238	0.14382				
226 -> 253	-0.10057				
226 -> 257	-0.18894				
227 -> 249	-0.12030				
228 -> 253	0.10066				
Excited State 14:	Triplet-A	4.7788 eV	259.45 nm	f=n.d.	<S**2>=2.000
210 -> 229	-0.10331				
223 -> 238	0.11732				
224 -> 229	0.13082				
225 -> 238	-0.15278				
225 -> 253	0.10648				
225 -> 257	0.19487				
226 -> 229	0.10713				
226 -> 235	-0.13812				
226 -> 249	0.17952				
228 -> 249	-0.12878				
Excited State 15:	Triplet-A	4.8076 eV	257.89 nm	f=n.d.	<S**2>=2.000
221 -> 231	0.12539				
226 -> 253	-0.11529				
227 -> 233	0.16313				
227 -> 256	0.16954				
228 -> 234	-0.14676				
228 -> 253	-0.16793				
Excited State 16:	Triplet-A	4.8076 eV	257.89 nm	f=n.d.	<S**2>=2.000
209 -> 231	0.10085				
222 -> 231	0.12537				
225 -> 253	-0.10778				
227 -> 234	0.15075				
227 -> 253	0.17290				
228 -> 233	-0.15954				
228 -> 256	-0.16599				
Excited State 17:	Triplet-A	5.0381 eV	246.09 nm	f=n.d.	<S**2>=2.000
219 -> 235	0.15170				
220 -> 238	0.19039				
223 -> 230	0.25432				
223 -> 232	0.10506				

223 -> 295	-0.10143				
224 -> 229	-0.26096				
224 -> 235	-0.11258				
225 -> 238	0.10847				
226 -> 235	0.10931				
226 -> 249	0.11192				
Excited State 18:	Triplet-A	5.0386 eV	246.07 nm	f=n.d.	<S**2>=2.000
219 -> 238	0.17416				
220 -> 235	0.16370				
223 -> 229	0.25708				
223 -> 235	0.11638				
224 -> 230	-0.25798				
224 -> 232	-0.10784				
224 -> 295	0.10027				
225 -> 235	0.10320				
225 -> 249	0.10894				
226 -> 238	0.10960				
Excited State 19:	Singlet-A	5.0592 eV	245.07 nm	f=1.6383	<S**2>=0.000
225 -> 230	0.31652				
226 -> 229	0.31614				
227 -> 232	0.32738				
228 -> 231	0.31337				
Excited State 20:	Triplet-A	5.0698 eV	244.55 nm	f=n.d.	<S**2>=2.000
217 -> 234	-0.13409				
218 -> 233	0.14091				
218 -> 234	0.10478				
221 -> 231	-0.11623				
222 -> 230	-0.13818				
222 -> 231	-0.25193				
222 -> 232	0.25426				
222 -> 273	-0.10049				
Excited State 21:	Triplet-A	5.0698 eV	244.55 nm	f=n.d.	<S**2>=2.000
217 -> 233	-0.13070				
218 -> 233	-0.10216				
218 -> 234	0.14441				
221 -> 230	-0.13915				
221 -> 231	0.25166				
221 -> 232	0.25451				
221 -> 273	-0.10050				
222 -> 231	-0.11631				
Excited State 22:	Singlet-A	5.0765 eV	244.23 nm	f=0.0000	<S**2>=0.000
225 -> 229	-0.29703				
226 -> 230	-0.28977				
227 -> 231	0.33742				
228 -> 232	0.34236				
Excited State 23:	Singlet-A	5.1004 eV	243.09 nm	f=0.0029	<S**2>=0.000
225 -> 230	0.16797				
225 -> 232	0.24857				
226 -> 229	0.21578				
226 -> 231	-0.22444				
227 -> 230	0.24280				
227 -> 232	-0.20562				
228 -> 229	-0.21593				
228 -> 231	-0.23642				
Excited State 24:	Singlet-A	5.1012 eV	243.05 nm	f=0.0000	<S**2>=0.000
223 -> 235	-0.10391				
225 -> 229	0.25646				
225 -> 231	-0.20736				
226 -> 230	0.18085				
226 -> 232	0.25561				
227 -> 229	0.21289				
227 -> 231	0.21604				
228 -> 230	-0.25077				
228 -> 232	0.16223				

Excited State	25:	Triplet-A	5.1107 eV	242.60 nm	f=n.d.	<S**2>=2.000
	217 -> 230	-0.13155				
	218 -> 231	0.10348				
	219 -> 230	0.11808				
	219 -> 232	0.12904				
	220 -> 229	0.17334				
	223 -> 249	0.10808				
	225 -> 233	0.10594				
	225 -> 235	0.10648				
	226 -> 238	0.13498				
	227 -> 235	0.10313				
	228 -> 234	0.12758				
Excited State	26:	Triplet-A	5.1114 eV	242.56 nm	f=n.d.	<S**2>=2.000
	217 -> 229	0.11969				
	217 -> 231	0.10709				
	218 -> 230	-0.11390				
	218 -> 232	0.10586				
	219 -> 229	-0.12687				
	219 -> 231	0.11024				
	220 -> 230	-0.12153				
	220 -> 232	-0.11529				
	225 -> 238	-0.12184				
	226 -> 233	-0.11655				
	227 -> 234	0.14643				
	228 -> 233	-0.10318				
	228 -> 235	0.10893				
Excited State	27:	Triplet-A	5.1159 eV	242.35 nm	f=n.d.	<S**2>=2.000
	217 -> 232	-0.16950				
	218 -> 231	-0.17558				
	219 -> 230	0.16774				
	220 -> 229	0.17167				
	225 -> 235	0.11914				
	226 -> 234	-0.10293				
	227 -> 233	0.15798				
	228 -> 234	-0.13820				
Excited State	28:	Triplet-A	5.1164 eV	242.33 nm	f=n.d.	<S**2>=2.000
	217 -> 231	-0.15645				
	218 -> 232	-0.15907				
	219 -> 229	-0.18387				
	220 -> 230	-0.18275				
	226 -> 235	-0.13399				
	227 -> 234	-0.12567				
	228 -> 233	0.14451				
Excited State	29:	Triplet-A	5.2195 eV	237.54 nm	f=n.d.	<S**2>=2.000
	213 -> 287	-0.10609				
	214 -> 286	-0.10103				
	215 -> 264	0.12814				
	215 -> 265	-0.21539				
	216 -> 264	0.20961				
Excited State	30:	Triplet-A	5.2195 eV	237.54 nm	f=n.d.	<S**2>=2.000
	214 -> 287	0.10896				
	215 -> 264	0.20962				
	216 -> 264	-0.12825				
	216 -> 265	-0.21540				
Excited State	31:	Triplet-A	5.2691 eV	235.31 nm	f=n.d.	<S**2>=2.000
	214 -> 230	-0.10197				
	215 -> 231	-0.12590				
	215 -> 232	0.13493				
	216 -> 231	-0.10496				
	216 -> 232	0.11939				
	227 -> 264	-0.15716				
	227 -> 265	0.14403				
	228 -> 264	0.14710				
	228 -> 265	-0.14301				

Excited State	32:	Triplet-A	5.2691 eV	235.30 nm	f=n.d.	<S**2>=2.000
	213 -> 230	-0.10342				
	215 -> 231	-0.10514				
	215 -> 232	-0.11973				
	216 -> 231	0.12561				
	216 -> 232	0.13502				
	227 -> 264	-0.14558				
	227 -> 265	-0.14127				
	228 -> 264	-0.15882				
	228 -> 265	-0.14556				
Excited State	33:	Triplet-A	5.2945 eV	234.18 nm	f=n.d.	<S**2>=2.000
	213 -> 264	-0.14665				
	213 -> 265	0.13636				
	214 -> 264	0.14830				
	214 -> 265	-0.14394				
	215 -> 274	0.10334				
	215 -> 279	0.10458				
	215 -> 286	-0.10630				
	215 -> 287	0.10728				
Excited State	34:	Triplet-A	5.2946 eV	234.17 nm	f=n.d.	<S**2>=2.000
	213 -> 264	0.14849				
	213 -> 265	0.14408				
	214 -> 264	0.14654				
	214 -> 265	0.13609				
	216 -> 274	-0.10302				
	216 -> 279	0.10455				
	216 -> 287	-0.11370				
Excited State	35:	Triplet-A	5.3059 eV	233.67 nm	f=n.d.	<S**2>=2.000
	213 -> 232	0.10006				
	214 -> 232	-0.10495				
	215 -> 229	0.12294				
	215 -> 230	0.13301				
	216 -> 229	0.10466				
	216 -> 230	0.11616				
	225 -> 264	-0.14125				
	225 -> 265	0.13323				
	226 -> 264	-0.13999				
	226 -> 265	0.13536				
Excited State	36:	Triplet-A	5.3060 eV	233.67 nm	f=n.d.	<S**2>=2.000
	213 -> 232	0.10497				
	214 -> 232	0.10024				
	215 -> 229	-0.10290				
	215 -> 230	0.11735				
	216 -> 229	0.12153				
	216 -> 230	-0.13490				
	225 -> 264	0.13942				
	225 -> 265	0.13486				
	226 -> 264	-0.14196				
	226 -> 265	-0.13364				
Excited State	37:	Singlet-A	5.4820 eV	226.17 nm	f=0.0000	<S**2>=0.000
	219 -> 230	0.13991				
	220 -> 229	0.18559				
	223 -> 229	-0.20941				
	223 -> 235	-0.21644				
	224 -> 230	0.24441				
	224 -> 238	0.16706				
	225 -> 235	-0.16309				
	226 -> 230	-0.12213				
	226 -> 238	-0.16542				
	227 -> 235	-0.10388				
Excited State	38:	Singlet-A	5.4838 eV	226.09 nm	f=0.6481	<S**2>=0.000
	219 -> 229	-0.13673				
	220 -> 230	-0.12572				
	221 -> 234	-0.11674				

222	->	231	-0.10692						
222	->	233	-0.10446						
223	->	230	0.19414						
223	->	238	0.16115						
224	->	229	-0.16464						
224	->	235	-0.18989						
225	->	238	0.16460						
226	->	233	0.12740						
226	->	235	0.16327						
227	->	234	-0.11853						
228	->	235	-0.13043						
Excited State	39:	Singlet-A	5.5039 eV	225.27 nm	f=0.0000	<S**2>=0.000			
217	->	232	0.15269						
218	->	231	0.16546						
221	->	231	0.20412						
221	->	232	0.10422						
221	->	233	0.14968						
222	->	230	0.11792						
222	->	231	0.11548						
222	->	232	-0.18412						
222	->	234	0.17247						
226	->	234	-0.11118						
227	->	233	0.18074						
228	->	234	-0.16834						
Excited State	40:	Singlet-A	5.5060 eV	225.18 nm	f=0.0269	<S**2>=0.000			
217	->	231	-0.14475						
218	->	232	-0.14898						
219	->	229	-0.12191						
220	->	230	-0.12295						
221	->	230	0.10215						
221	->	231	-0.10323						
221	->	232	-0.16627						
221	->	234	0.14869						
222	->	231	0.18288						
222	->	233	0.12835						
223	->	230	0.14490						
224	->	229	-0.13275						
226	->	235	0.13882						
227	->	234	0.14859						
228	->	233	-0.16754						
Excited State	41:	Triplet-A	5.6432 eV	219.71 nm	f=n.d.	<S**2>=2.000			
215	->	264	-0.11893						
216	->	265	0.11244						
226	->	238	0.10800						
227	->	233	-0.12366						
227	->	235	0.11695						
228	->	234	0.16474						
Excited State	42:	Triplet-A	5.6435 eV	219.69 nm	f=n.d.	<S**2>=2.000			
215	->	265	0.11231						
216	->	264	-0.11871						
225	->	238	0.11154						
227	->	234	-0.16874						
228	->	233	0.12176						
228	->	235	-0.11920						

Table S5 First TD- ω B97X/6-311++G(d,p) triplet and singlet electronic transitions computed for the $\pi\cdots\pi$ dimer of TT-CCH (Figure 6c) at the optimized ground state geometry.

Excitation energies and oscillator strengths:

Excited State	1:	Triplet-A	3.2352 eV	383.23 nm	f=n.d.	<S**2>=2.000			
109	->	115	-0.10924						
113	->	115	0.42638						
113	->	116	0.22274						
114	->	115	-0.37909						
114	->	116	-0.13068						

Excited State	2:	Triplet-A	3.2508 eV	381.40 nm	f=n.d.	<S**2>=2.000
113 ->115		-0.18184				
113 ->116		0.30640				
114 ->115		-0.18664				
114 ->116		0.47296				
Excited State	3:	Triplet-A	3.9357 eV	315.02 nm	f=n.d.	<S**2>=2.000
109 ->116		0.16651				
110 ->115		-0.12474				
111 ->120		0.28394				
112 ->117		0.37028				
112 ->120		0.25213				
Excited State	4:	Triplet-A	3.9464 eV	314.17 nm	f=n.d.	<S**2>=2.000
109 ->115		-0.16471				
109 ->120		0.10403				
110 ->115		0.12650				
110 ->116		0.11767				
111 ->117		0.39249				
111 ->120		-0.19552				
112 ->120		0.27089				
Excited State	5:	Triplet-A	4.0809 eV	303.82 nm	f=n.d.	<S**2>=2.000
109 ->117		0.27680				
110 ->120		0.26966				
111 ->115		-0.18976				
111 ->131		-0.11700				
112 ->116		0.20927				
112 ->126		-0.13961				
113 ->117		0.17296				
114 ->120		0.13936				
Excited State	6:	Triplet-A	4.0956 eV	302.72 nm	f=n.d.	<S**2>=2.000
109 ->120		0.25003				
110 ->117		0.31376				
111 ->115		0.14673				
111 ->116		0.16056				
111 ->126		-0.14000				
112 ->115		-0.18196				
112 ->131		-0.12555				
113 ->120		0.16309				
114 ->117		0.12848				
Excited State	7:	Triplet-A	4.7964 eV	258.49 nm	f=n.d.	<S**2>=2.000
103 ->115		-0.11661				
107 ->135		0.12350				
110 ->115		-0.12753				
111 ->115		0.20713				
113 ->115		0.12242				
113 ->117		0.16961				
113 ->120		-0.12037				
113 ->126		-0.12639				
113 ->131		0.12688				
113 ->137		-0.12279				
114 ->117		-0.12118				
114 ->120		0.10267				
114 ->131		-0.11256				
Excited State	8:	Triplet-A	4.7995 eV	258.33 nm	f=n.d.	<S**2>=2.000
100 ->116		-0.10304				
104 ->116		0.10636				
111 ->116		0.11131				
112 ->115		-0.10785				
112 ->116		0.21965				
113 ->120		-0.11478				
114 ->117		-0.15142				
114 ->120		-0.14106				
114 ->126		0.14583				
114 ->138		-0.12481				

Excited State	9:	Triplet-A	5.0565 eV	245.20 nm	f=n.d.	<S**2>=2.000
109 ->117		-0.16025				
110 ->115		0.16658				
110 ->117		0.13275				
110 ->120		-0.12309				
110 ->137		-0.12774				
111 ->115		-0.30096				
111 ->137		0.12444				
112 ->115		0.15315				
112 ->116		0.14072				
Excited State	10:	Singlet-A	5.0597 eV	245.04 nm	f=0.0129	<S**2>=0.000
111 ->117		-0.11503				
113 ->115		0.46061				
114 ->115		-0.22434				
114 ->116		-0.39484				
Excited State	11:	Triplet-A	5.0636 eV	244.85 nm	f=n.d.	<S**2>=2.000
109 ->116		-0.12458				
109 ->120		-0.13760				
110 ->116		-0.12694				
110 ->117		-0.12250				
111 ->116		0.14161				
112 ->115		-0.19771				
112 ->116		0.30054				
112 ->138		0.17085				
112 ->147		-0.10150				
114 ->126		-0.11356				
Excited State	12:	Triplet-A	5.0949 eV	243.35 nm	f=n.d.	<S**2>=2.000
109 ->116		-0.14142				
109 ->120		0.11670				
109 ->131		0.10326				
110 ->116		-0.12037				
113 ->117		0.11551				
113 ->120		0.15162				
114 ->117		0.16640				
114 ->120		0.16042				
Excited State	13:	Triplet-A	5.1180 eV	242.25 nm	f=n.d.	<S**2>=2.000
109 ->115		-0.15287				
110 ->115		0.20248				
111 ->117		-0.10943				
111 ->131		0.12225				
113 ->117		0.19242				
113 ->120		-0.13378				
114 ->117		-0.16162				
114 ->120		0.14230				
Excited State	14:	Singlet-A	5.1229 eV	242.02 nm	f=0.3578	<S**2>=0.000
111 ->120		-0.12377				
112 ->117		-0.14888				
113 ->116		-0.37015				
114 ->115		0.39416				
114 ->116		-0.31904				
Excited State	15:	Triplet-A	5.2350 eV	236.84 nm	f=n.d.	<S**2>=2.000
97 ->135		-0.13096				
107 ->132		-0.12655				
107 ->134		0.16145				
107 ->135		-0.28527				
108 ->135		-0.11313				
108 ->136		0.11412				
114 ->117		-0.10279				
Excited State	16:	Triplet-A	5.2408 eV	236.58 nm	f=n.d.	<S**2>=2.000
98 ->134		-0.10326				
107 ->135		-0.17946				
108 ->133		-0.15060				
108 ->134		0.23617				
108 ->136		-0.20233				

109	->117	-0.10010					
113	->117	0.10449					
114	->120	0.11836					
Excited State	17:	Triplet-A	5.2783 eV	234.89 nm	f=n.d.	<S**2>=2.000	
103	->135	-0.13348					
104	->135	0.10136					
107	->115	0.26997					
107	->116	0.13308					
109	->135	0.10486					
113	->132	-0.12373					
113	->134	0.10795					
113	->135	-0.25469					
114	->134	-0.12359					
114	->135	0.20076					
Excited State	18:	Triplet-A	5.2899 eV	234.38 nm	f=n.d.	<S**2>=2.000	
108	->115	-0.10675					
108	->116	0.25873					
113	->133	-0.10436					
113	->134	0.15661					
113	->136	-0.13298					
114	->133	-0.13990					
114	->134	0.19394					
114	->135	0.13468					
114	->136	-0.19507					
Excited State	19:	Singlet-A	5.4563 eV	227.23 nm	f=0.0038	<S**2>=0.000	
109	->115	-0.11835					
110	->115	0.11788					
110	->116	0.17888					
111	->115	-0.16762					
111	->116	-0.16956					
111	->117	0.21407					
112	->115	0.27540					
112	->116	-0.18828					
112	->120	0.20490					
113	->120	0.14415					
114	->117	0.20901					
Excited State	20:	Singlet-A	5.5007 eV	225.40 nm	f=0.2488	<S**2>=0.000	
109	->116	-0.14552					
110	->115	0.20987					
111	->115	-0.27909					
111	->120	-0.16095					
112	->116	0.29867					
112	->117	-0.18989					
113	->117	-0.19549					
114	->115	-0.10450					
114	->120	-0.20074					
Excited State	21:	Triplet-A	5.6720 eV	218.59 nm	f=n.d.	<S**2>=2.000	
103	->120	-0.10357					
104	->117	-0.11348					
107	->135	-0.12238					
112	->115	0.10564					
113	->117	-0.10118					
113	->120	0.16991					
113	->137	-0.13367					
114	->117	0.16370					
114	->137	0.10218					
Excited State	22:	Triplet-A	5.6778 eV	218.37 nm	f=n.d.	<S**2>=2.000	
104	->120	-0.10287					
112	->116	-0.10150					
112	->147	-0.12063					
113	->117	0.15650					
113	->138	-0.13045					
114	->120	0.16829					
114	->138	-0.13356					

Excited State	23:	Singlet-A	5.7678 eV	214.96 nm	f=0.0003	<S**2>=0.000
104	->135	0.11568				
107	->115	-0.16874				
110	->135	-0.10207				
113	->129	0.10046				
113	->134	0.20510				
113	->135	-0.21661				
114	->132	0.15620				
114	->135	0.28366				
114	->136	-0.12094				
Excited State	24:	Singlet-A	5.7759 eV	214.66 nm	f=0.0010	<S**2>=0.000
103	->135	0.10276				
104	->134	0.10356				
108	->116	-0.13206				
113	->132	0.12897				
113	->135	0.21915				
113	->136	-0.15486				
114	->133	-0.16552				
114	->134	0.28471				
114	->136	-0.19563				
Excited State	25:	Triplet-A	5.7949 eV	213.96 nm	f=n.d.	<S**2>=2.000
107	->115	0.41800				
107	->116	0.18671				
107	->131	-0.10661				
113	->135	0.17152				
114	->135	-0.15338				
Excited State	26:	Singlet-A	5.8065 eV	213.53 nm	f=0.0035	<S**2>=0.000
109	->115	-0.14791				
109	->120	0.14310				
111	->115	0.16293				
111	->116	0.27486				
111	->117	0.36074				
112	->115	-0.25629				
112	->116	0.12322				
112	->120	0.26030				
Excited State	27:	Triplet-A	5.8274 eV	212.76 nm	f=n.d.	<S**2>=2.000
108	->115	-0.20450				
108	->116	0.43991				
108	->129	-0.10169				
114	->134	-0.15024				
114	->136	0.13301				
Excited State	28:	Singlet-A	5.8466 eV	212.06 nm	f=0.3741	<S**2>=0.000
109	->116	0.15800				
110	->115	-0.13510				
111	->115	-0.24195				
111	->120	0.27704				
112	->116	0.20244				
112	->117	0.33195				
112	->120	0.14362				
113	->117	-0.16135				
114	->120	-0.13795				
Excited State	29:	Triplet-A	5.8915 eV	210.45 nm	f=n.d.	<S**2>=2.000
96	->115	-0.13383				
103	->115	-0.10475				
104	->115	0.11586				
107	->135	-0.15344				
110	->120	0.10740				
110	->137	-0.14781				
111	->115	0.12645				
Excited State	30:	Triplet-A	5.8948 eV	210.33 nm	f=n.d.	<S**2>=2.000
94	->116	-0.11753				
96	->116	0.13502				
100	->116	0.10949				
104	->116	-0.12586				

108 ->134	0.10998
108 ->136	-0.10408
109 ->138	-0.13599
110 ->138	-0.12901
112 ->138	0.11751
112 ->147	-0.11652
114 ->117	-0.10923

Table S6 First TD- ω B97X/6-311++G(d,p) triplet and singlet electronic transitions computed for the $\pi\cdots\pi$ tetramer of TT-CCH (Figure 6d) at the optimized ground state geometry.

Excitation energies and oscillator strengths:

Excited State	1:	Triplet-A	3.2367 eV	383.06 nm	f=n.d.	<S**2>=2.000
225 -> 229		0.17936				
225 -> 230		0.25012				
225 -> 231		-0.22809				
225 -> 232		0.10529				
226 -> 229		-0.17928				
226 -> 230		-0.20565				
227 -> 229		0.27545				
227 -> 230		0.15009				
228 -> 229		-0.21392				
Excited State	2:	Triplet-A	3.2398 eV	382.69 nm	f=n.d.	<S**2>=2.000
225 -> 229		-0.17259				
225 -> 230		-0.13968				
225 -> 232		0.12774				
226 -> 229		0.16975				
226 -> 231		-0.10341				
226 -> 232		0.20432				
227 -> 231		0.20391				
227 -> 232		-0.11610				
228 -> 229		-0.20913				
228 -> 230		0.30360				
228 -> 232		-0.12019				
Excited State	3:	Triplet-A	3.2426 eV	382.36 nm	f=n.d.	<S**2>=2.000
225 -> 229		0.26246				
225 -> 231		0.10699				
226 -> 230		-0.19245				
226 -> 232		0.13865				
227 -> 229		-0.15373				
227 -> 230		0.16094				
227 -> 231		-0.17053				
228 -> 230		0.10877				
228 -> 231		0.25709				
228 -> 232		-0.25456				
Excited State	4:	Triplet-A	3.2525 eV	381.20 nm	f=n.d.	<S**2>=2.000
226 -> 230		0.15152				
226 -> 231		0.22224				
226 -> 232		0.21608				
227 -> 230		0.14042				
227 -> 231		0.24655				
227 -> 232		0.27687				
228 -> 231		0.17243				
228 -> 232		0.23006				
Excited State	5:	Triplet-A	3.9335 eV	315.20 nm	f=n.d.	<S**2>=2.000
219 -> 232		0.10158				
220 -> 230		-0.11163				
222 -> 238		0.18235				
222 -> 241		-0.26612				
223 -> 235		0.16957				
223 -> 238		0.16783				
224 -> 233		-0.20355				
224 -> 235		0.22559				
Excited State	6:	Triplet-A	3.9389 eV	314.77 nm	f=n.d.	<S**2>=2.000

217 -> 231	-0.10843					
221 -> 235	-0.10875					
221 -> 238	0.15267					
221 -> 241	0.10105					
222 -> 235	-0.17661					
222 -> 238	-0.13832					
223 -> 233	0.25603					
223 -> 241	0.19455					
224 -> 233	-0.13940					
224 -> 238	-0.14509					
Excited State	7:	Triplet-A	3.9432 eV	314.43 nm	f=n.d.	<S**2>=2.000
218 -> 229	0.11505					
220 -> 232	0.10092					
221 -> 233	0.12596					
221 -> 235	0.17301					
221 -> 238	-0.15019					
222 -> 233	0.19601					
222 -> 235	-0.17525					
224 -> 235	0.11975					
224 -> 241	0.23208					
Excited State	8:	Triplet-A	3.9461 eV	314.19 nm	f=n.d.	<S**2>=2.000
217 -> 229	-0.14849					
218 -> 230	0.11853					
221 -> 233	0.25649					
221 -> 235	0.22131					
221 -> 238	-0.11595					
222 -> 233	-0.11425					
223 -> 233	0.11535					
223 -> 238	0.18714					
224 -> 241	-0.15970					
Excited State	9:	Triplet-A	4.0753 eV	304.23 nm	f=n.d.	<S**2>=2.000
217 -> 233	-0.13380					
218 -> 235	0.11570					
219 -> 235	0.16441					
219 -> 238	0.13420					
220 -> 238	-0.11138					
220 -> 241	0.21152					
222 -> 230	0.14821					
222 -> 258	-0.10209					
223 -> 231	0.11936					
224 -> 232	0.13883					
224 -> 249	-0.10620					
225 -> 233	-0.10818					
226 -> 235	0.12724					
Excited State	10:	Triplet-A	4.0827 eV	303.68 nm	f=n.d.	<S**2>=2.000
217 -> 233	-0.17780					
217 -> 235	-0.11741					
218 -> 238	-0.17362					
219 -> 241	0.14187					
220 -> 238	0.11502					
221 -> 229	0.14773					
222 -> 231	-0.11685					
223 -> 250	0.10444					
225 -> 233	-0.12551					
Excited State	11:	Triplet-A	4.0915 eV	303.03 nm	f=n.d.	<S**2>=2.000
217 -> 235	-0.11066					
217 -> 238	0.12997					
218 -> 233	0.17349					
218 -> 235	0.11561					
218 -> 241	-0.10973					
219 -> 241	-0.12404					
220 -> 235	-0.16272					
221 -> 229	0.10823					
221 -> 230	0.12194					
221 -> 250	-0.11217					
222 -> 232	0.10293					

224 -> 230	0.11807					
226 -> 241	-0.10718					
Excited State 12:	Triplet-A	4.0997 eV	302.42 nm	f=n.d.	<S**2>=2.000	
217 -> 238	-0.11613					
217 -> 241	-0.15412					
218 -> 233	-0.10157					
218 -> 235	-0.13022					
219 -> 233	0.14019					
219 -> 238	0.10534					
220 -> 233	0.15802					
220 -> 235	-0.10768					
222 -> 232	0.10781					
223 -> 229	0.10789					
223 -> 231	0.10812					
224 -> 229	-0.12078					
224 -> 230	0.10646					
225 -> 241	-0.12617					
Excited State 13:	Triplet-A	4.7728 eV	259.77 nm	f=n.d.	<S**2>=2.000	
222 -> 229	-0.10050					
223 -> 229	0.12216					
223 -> 231	0.12619					
225 -> 233	0.12336					
227 -> 233	-0.10296					
228 -> 241	0.11361					
Excited State 14:	Triplet-A	4.7756 eV	259.62 nm	f=n.d.	<S**2>=2.000	
222 -> 232	0.10250					
224 -> 230	0.11666					
225 -> 229	0.10855					
228 -> 233	0.13324					
Excited State 15:	Triplet-A	4.7940 eV	258.62 nm	f=n.d.	<S**2>=2.000	
213 -> 265	-0.10074					
221 -> 229	0.16299					
221 -> 230	0.15269					
225 -> 233	0.10194					
225 -> 235	0.11527					
225 -> 250	0.11641					
Excited State 16:	Triplet-A	4.7994 eV	258.33 nm	f=n.d.	<S**2>=2.000	
222 -> 231	-0.11821					
222 -> 232	-0.11993					
223 -> 231	-0.10409					
223 -> 232	-0.10502					
227 -> 253	0.10325					
Excited State 17:	Singlet-A	5.0307 eV	246.45 nm	f=0.0007	<S**2>=0.000	
225 -> 229	-0.28588					
226 -> 230	0.25260					
227 -> 229	0.11276					
227 -> 230	-0.14633					
227 -> 231	0.24489					
228 -> 231	-0.20897					
228 -> 232	0.31839					
Excited State 18:	Triplet-A	5.0350 eV	246.25 nm	f=n.d.	<S**2>=2.000	
220 -> 230	-0.10348					
222 -> 229	0.10278					
222 -> 230	-0.11983					
223 -> 229	-0.10178					
223 -> 231	-0.10286					
224 -> 230	0.14852					
224 -> 232	-0.17545					
Excited State 19:	Triplet-A	5.0372 eV	246.14 nm	f=n.d.	<S**2>=2.000	
223 -> 229	-0.15713					
223 -> 231	-0.15413					
224 -> 229	0.15383					
224 -> 230	-0.13463					

Excited State	20:	Triplet-A	5.0550 eV	245.27 nm	f=n.d.	<S**2>=2.000
	218 -> 230	0.10489				
	218 -> 233	-0.11080				
	218 -> 235	-0.11394				
	221 -> 229	0.25038				
	221 -> 230	0.22114				
	221 -> 231	-0.11746				
	221 -> 271	0.10650				
Excited State	21:	Triplet-A	5.0600 eV	245.03 nm	f=n.d.	<S**2>=2.000
	220 -> 235	0.10273				
	222 -> 231	0.13904				
	222 -> 232	0.16212				
	223 -> 231	0.13807				
	223 -> 232	0.14047				
	224 -> 230	0.10614				
	224 -> 231	0.13999				
	224 -> 232	0.12272				
Excited State	22:	Singlet-A	5.0611 eV	244.98 nm	f=0.0018	<S**2>=0.000
	225 -> 229	-0.19901				
	225 -> 230	-0.20700				
	226 -> 229	0.23545				
	226 -> 231	-0.19481				
	227 -> 230	-0.15639				
	227 -> 232	-0.21185				
	228 -> 229	-0.13031				
	228 -> 230	0.24655				
	228 -> 231	-0.13880				
	228 -> 232	-0.18004				
Excited State	23:	Triplet-A	5.0874 eV	243.71 nm	f=n.d.	<S**2>=2.000
	220 -> 232	0.11670				
	224 -> 241	-0.10151				
	226 -> 241	-0.12154				
	228 -> 233	-0.13141				
	228 -> 235	0.12682				
Excited State	24:	Triplet-A	5.0903 eV	243.57 nm	f=n.d.	<S**2>=2.000
	219 -> 232	-0.11056				
	220 -> 230	0.11474				
	220 -> 231	0.11393				
	226 -> 235	0.12665				
	227 -> 238	0.10117				
	227 -> 241	-0.10880				
Excited State	25:	Triplet-A	5.0928 eV	243.45 nm	f=n.d.	<S**2>=2.000
	217 -> 229	0.10642				
	217 -> 250	0.10182				
	227 -> 233	0.11951				
Excited State	26:	Singlet-A	5.0950 eV	243.34 nm	f=0.2046	<S**2>=0.000
	225 -> 230	0.19372				
	225 -> 231	-0.24821				
	225 -> 232	0.10840				
	226 -> 229	-0.12589				
	226 -> 230	-0.22046				
	227 -> 229	0.31458				
	227 -> 232	-0.13793				
	228 -> 229	-0.25325				
	228 -> 231	-0.13678				
Excited State	27:	Triplet-A	5.1167 eV	242.31 nm	f=n.d.	<S**2>=2.000
	217 -> 229	-0.11118				
	217 -> 230	-0.10587				
	218 -> 229	0.15224				
	218 -> 230	0.12921				
	221 -> 250	0.11382				
	221 -> 255	0.11009				
	221 -> 256	-0.10258				

225 -> 233	-0.11186					
225 -> 235	-0.11555					
Excited State 28:	Singlet-A	5.1191 eV	242.20 nm	f=0.4661	<S**2>=0.000	
222 -> 241	-0.10228					
225 -> 232	0.10162					
226 -> 231	0.17643					
226 -> 232	0.28624					
227 -> 230	0.18590					
227 -> 231	0.26949					
227 -> 232	0.17994					
228 -> 229	-0.17352					
228 -> 230	0.24196					
228 -> 231	0.16951					
Excited State 29:	Triplet-A	5.2285 eV	237.13 nm	f=n.d.	<S**2>=2.000	
214 -> 262	-0.12080					
214 -> 263	-0.14470					
214 -> 265	-0.10938					
216 -> 262	-0.16034					
Excited State 30:	Triplet-A	5.2327 eV	236.94 nm	f=n.d.	<S**2>=2.000	
213 -> 265	0.12755					
214 -> 262	0.12779					
215 -> 263	-0.10128					
216 -> 262	-0.12998					
216 -> 263	0.11078					
216 -> 266	0.12562					
Excited State 31:	Triplet-A	5.2371 eV	236.74 nm	f=n.d.	<S**2>=2.000	
213 -> 261	-0.13052					
213 -> 263	-0.12452					
213 -> 265	0.24009					
214 -> 262	-0.11610					
Excited State 32:	Triplet-A	5.2410 eV	236.57 nm	f=n.d.	<S**2>=2.000	
196 -> 264	0.14659					
215 -> 262	0.11703					
215 -> 264	-0.26485					
215 -> 266	-0.12996					
216 -> 263	0.12296					
216 -> 264	-0.15540					
Excited State 33:	Triplet-A	5.2790 eV	234.86 nm	f=n.d.	<S**2>=2.000	
213 -> 229	0.18062					
213 -> 230	0.17790					
213 -> 231	-0.10574					
225 -> 261	0.11214					
225 -> 265	-0.18086					
226 -> 265	0.13023					
228 -> 263	-0.10831					
Excited State 34:	Triplet-A	5.2800 eV	234.82 nm	f=n.d.	<S**2>=2.000	
215 -> 232	0.10273					
216 -> 230	0.14961					
216 -> 232	-0.12559					
226 -> 262	0.12159					
226 -> 263	-0.11556					
228 -> 262	-0.12457					
228 -> 263	0.15030					
228 -> 265	0.10460					
228 -> 266	0.11997					
Excited State 35:	Triplet-A	5.2821 eV	234.73 nm	f=n.d.	<S**2>=2.000	
214 -> 229	0.15657					
214 -> 231	0.16851					
225 -> 263	-0.12811					
227 -> 265	0.11213					
228 -> 262	-0.16293					
Excited State 36:	Triplet-A	5.2892 eV	234.41 nm	f=n.d.	<S**2>=2.000	

207 -> 264	-0.10074				
215 -> 231	0.14843				
215 -> 232	0.15710				
216 -> 232	0.11812				
226 -> 264	-0.18178				
227 -> 264	-0.20911				
228 -> 264	-0.15483				
Excited State 37:	Singlet-A	5.4201 eV	228.75 nm	f=0.0002	<S**2>=0.000
219 -> 231	-0.11140				
220 -> 232	0.14601				
222 -> 232	0.14939				
222 -> 233	0.12120				
223 -> 229	0.14878				
223 -> 231	0.16103				
223 -> 238	-0.11274				
224 -> 229	-0.17843				
224 -> 230	0.20050				
224 -> 241	0.17696				
225 -> 229	0.12960				
228 -> 233	0.15506				
Excited State 38:	Singlet-A	5.4489 eV	227.54 nm	f=0.0008	<S**2>=0.000
221 -> 229	-0.11258				
221 -> 230	-0.10248				
222 -> 229	-0.10449				
222 -> 232	-0.10612				
223 -> 229	0.18985				
223 -> 232	-0.12783				
223 -> 241	-0.10605				
224 -> 230	-0.14724				
224 -> 231	-0.16095				
224 -> 238	0.11331				
227 -> 233	-0.13663				
228 -> 235	0.11873				
Excited State 39:	Singlet-A	5.4825 eV	226.15 nm	f=0.0098	<S**2>=0.000
218 -> 229	0.12448				
221 -> 229	0.20008				
221 -> 230	0.15420				
221 -> 235	0.10972				
222 -> 231	-0.14144				
223 -> 230	-0.12845				
223 -> 232	-0.12426				
224 -> 231	-0.11174				
224 -> 232	-0.14109				
224 -> 235	0.10643				
226 -> 233	-0.10383				
227 -> 235	0.11768				
228 -> 238	0.10246				
Excited State 40:	Singlet-A	5.4945 eV	225.65 nm	f=0.4595	<S**2>=0.000
220 -> 230	0.10192				
221 -> 229	0.14847				
221 -> 230	0.12673				
222 -> 230	0.15608				
223 -> 231	0.19820				
224 -> 232	0.20579				
224 -> 233	0.13547				
226 -> 235	-0.13887				
227 -> 238	-0.13850				
228 -> 241	0.13888				
Excited State 41:	Triplet-A	5.6655 eV	218.84 nm	f=n.d.	<S**2>=2.000
223 -> 284	-0.10677				
225 -> 241	-0.10051				
228 -> 233	-0.11066				
Excited State 42:	Triplet-A	5.6673 eV	218.77 nm	f=n.d.	<S**2>=2.000
226 -> 241	-0.10569				
228 -> 241	0.10902				

Table S7 First TD- ω B97X/6-311++G(d,p) triplet and singlet electronic transitions computed for the tetramer comprising two π - π stacked H-bonded dimers of TT-CCH (Figure 6e) at the optimized ground state geometry.

Excitation energies and oscillator strengths:

Excited State	1:	Triplet-A	3.2106 eV	386.17 nm	f=n.d.	<S**2>=2.000
225 -> 230		0.36311				
225 -> 231		0.13979				
226 -> 229		0.41725				
226 -> 232		0.11811				
227 -> 230		-0.20932				
Excited State	2:	Triplet-A	3.2109 eV	386.13 nm	f=n.d.	<S**2>=2.000
225 -> 229		0.38190				
226 -> 230		0.42059				
226 -> 231		0.12541				
227 -> 229		-0.18177				
Excited State	3:	Triplet-A	3.2212 eV	384.90 nm	f=n.d.	<S**2>=2.000
225 -> 232		0.16921				
227 -> 229		-0.13077				
227 -> 232		0.36476				
228 -> 230		-0.13207				
228 -> 231		0.41485				
Excited State	4:	Triplet-A	3.2234 eV	384.63 nm	f=n.d.	<S**2>=2.000
225 -> 230		-0.11685				
225 -> 231		0.14557				
227 -> 231		0.39339				
228 -> 229		-0.11875				
228 -> 232		0.39535				
Excited State	5:	Triplet-A	3.9412 eV	314.58 nm	f=n.d.	<S**2>=2.000
219 -> 232		-0.14977				
220 -> 231		0.13139				
223 -> 234		-0.19911				
223 -> 239		0.24255				
223 -> 240		0.21201				
224 -> 233		0.22686				
224 -> 238		0.28465				
Excited State	6:	Triplet-A	3.9432 eV	314.43 nm	f=n.d.	<S**2>=2.000
219 -> 231		-0.14012				
220 -> 232		0.13336				
223 -> 233		0.22850				
223 -> 238		0.29984				
224 -> 234		-0.18581				
224 -> 239		0.23161				
224 -> 240		0.20447				
Excited State	7:	Triplet-A	3.9611 eV	313.01 nm	f=n.d.	<S**2>=2.000
217 -> 229		-0.11306				
218 -> 229		-0.10345				
218 -> 230		-0.11910				
221 -> 233		-0.18341				
221 -> 234		0.25793				
221 -> 238		0.13368				
222 -> 233		0.20658				
222 -> 234		-0.21344				
222 -> 238		-0.14964				
Excited State	8:	Triplet-A	3.9611 eV	313.01 nm	f=n.d.	<S**2>=2.000
217 -> 230		0.11460				
218 -> 229		0.11828				
218 -> 230		-0.10484				
221 -> 233		0.23577				
221 -> 234		0.18152				
221 -> 238		-0.14625				
222 -> 233		0.21770				

222 -> 234	0.22924				
222 -> 238	-0.13460				
222 -> 240	0.10062				
Excited State 9:	Triplet-A	4.0987 eV	302.49 nm	f=n.d.	<S**2>=2.000
217 -> 233	-0.13089				
219 -> 234	0.16068				
219 -> 239	-0.17676				
219 -> 240	-0.14956				
220 -> 233	0.10526				
220 -> 238	0.21890				
223 -> 232	0.18625				
224 -> 231	0.17504				
224 -> 255	-0.10792				
Excited State 10:	Triplet-A	4.0989 eV	302.48 nm	f=n.d.	<S**2>=2.000
217 -> 234	0.13106				
219 -> 233	-0.15379				
219 -> 238	-0.21790				
220 -> 234	-0.10122				
220 -> 239	0.17466				
220 -> 240	0.15161				
223 -> 231	0.18182				
223 -> 255	-0.12634				
224 -> 232	0.16221				
Excited State 11:	Triplet-A	4.1131 eV	301.44 nm	f=n.d.	<S**2>=2.000
217 -> 233	-0.18470				
217 -> 238	0.16768				
218 -> 234	0.23409				
218 -> 239	0.10036				
218 -> 240	0.10093				
220 -> 233	-0.16375				
221 -> 230	-0.17679				
221 -> 252	-0.13766				
222 -> 229	0.18537				
222 -> 248	0.11462				
226 -> 234	0.10184				
Excited State 12:	Triplet-A	4.1131 eV	301.44 nm	f=n.d.	<S**2>=2.000
217 -> 234	-0.19224				
217 -> 239	-0.11350				
217 -> 240	-0.11032				
218 -> 233	0.23005				
218 -> 238	-0.15150				
220 -> 234	-0.15538				
221 -> 229	0.18356				
221 -> 248	0.11731				
222 -> 230	-0.17821				
222 -> 252	-0.13609				
Excited State 13:	Triplet-A	4.7658 eV	260.15 nm	f=n.d.	<S**2>=2.000
211 -> 232	0.13299				
212 -> 231	0.10109				
223 -> 232	0.11373				
224 -> 231	0.16428				
227 -> 232	-0.12044				
227 -> 238	0.14549				
227 -> 248	-0.13507				
228 -> 234	-0.11558				
228 -> 239	0.10447				
228 -> 255	0.13772				
228 -> 275	0.11029				
Excited State 14:	Triplet-A	4.7673 eV	260.07 nm	f=n.d.	<S**2>=2.000
211 -> 231	0.11452				
212 -> 232	0.11221				
224 -> 232	0.16408				
227 -> 230	0.11332				
227 -> 234	-0.10478				
227 -> 239	0.11715				

227 -> 255	0.12916				
227 -> 275	0.10239				
228 -> 238	0.13656				
228 -> 248	-0.13169				
Excited State 15:	Triplet-A	4.7871 eV	259.00 nm	f=n.d.	<S**2>=2.000
208 -> 230	0.12273				
221 -> 230	0.15226				
222 -> 229	-0.14391				
225 -> 233	-0.11632				
225 -> 238	0.11066				
225 -> 248	0.14015				
226 -> 234	0.17143				
226 -> 252	0.17585				
226 -> 270	0.10334				
Excited State 16:	Triplet-A	4.7884 eV	258.93 nm	f=n.d.	<S**2>=2.000
208 -> 229	-0.11579				
221 -> 229	-0.14661				
222 -> 230	0.13961				
225 -> 230	-0.10191				
225 -> 234	-0.13267				
225 -> 252	-0.14496				
226 -> 233	0.11991				
226 -> 238	-0.13167				
226 -> 248	-0.14303				
227 -> 234	0.11804				
Excited State 17:	Singlet-A	4.9960 eV	248.16 nm	f=0.0000	<S**2>=0.000
225 -> 229	-0.28782				
226 -> 230	-0.27601				
227 -> 232	0.33822				
228 -> 230	-0.12844				
228 -> 231	0.35201				
Excited State 18:	Triplet-A	5.0347 eV	246.26 nm	f=n.d.	<S**2>=2.000
217 -> 234	0.14331				
218 -> 229	0.12022				
218 -> 233	-0.12798				
221 -> 229	0.26746				
221 -> 272	0.10901				
222 -> 230	-0.25401				
222 -> 270	-0.12717				
Excited State 19:	Triplet-A	5.0349 eV	246.25 nm	f=n.d.	<S**2>=2.000
217 -> 233	0.12435				
218 -> 230	-0.11999				
218 -> 234	-0.15757				
218 -> 270	-0.10846				
221 -> 230	-0.25600				
221 -> 270	-0.12933				
222 -> 229	0.26526				
222 -> 272	0.10652				
226 -> 252	0.10696				
Excited State 20:	Singlet-A	5.0368 eV	246.16 nm	f=0.3358	<S**2>=0.000
225 -> 230	0.39417				
226 -> 229	0.43374				
226 -> 232	0.12735				
227 -> 230	-0.18097				
227 -> 231	-0.11657				
Excited State 21:	Triplet-A	5.0471 eV	245.65 nm	f=n.d.	<S**2>=2.000
219 -> 238	0.14012				
220 -> 234	0.10011				
223 -> 230	-0.10127				
223 -> 231	0.28064				
224 -> 229	-0.10231				
224 -> 232	0.24939				
Excited State 22:	Triplet-A	5.0493 eV	245.55 nm	f=n.d.	<S**2>=2.000

219 -> 234	-0.10302					
220 -> 232	0.12159					
220 -> 238	-0.10802					
223 -> 229	-0.10735					
223 -> 232	0.23825					
224 -> 231	0.27778					
Excited State 23:	Triplet-A	5.0633 eV	244.87 nm	f=n.d.	<S**2>=2.000	
219 -> 229	0.10498					
219 -> 232	-0.15167					
220 -> 231	0.17268					
223 -> 255	0.11512					
228 -> 233	-0.14454					
228 -> 238	-0.19209					
Excited State 24:	Triplet-A	5.0651 eV	244.78 nm	f=n.d.	<S**2>=2.000	
219 -> 231	-0.16410					
219 -> 255	0.11298					
220 -> 232	0.12430					
220 -> 233	0.10654					
220 -> 238	0.10014					
223 -> 238	-0.11490					
227 -> 238	-0.11187					
228 -> 234	0.10786					
228 -> 239	-0.15406					
228 -> 240	-0.13716					
Excited State 25:	Singlet-A	5.0729 eV	244.41 nm	f=0.0000	<S**2>=0.000	
225 -> 229	0.26413					
225 -> 232	0.18642					
226 -> 230	0.33384					
227 -> 229	-0.24095					
227 -> 232	0.17088					
228 -> 230	-0.11691					
228 -> 231	0.24471					
Excited State 26:	Singlet-A	5.0905 eV	243.56 nm	f=0.8068	<S**2>=0.000	
225 -> 231	0.18304					
227 -> 230	-0.18112					
227 -> 231	0.37785					
228 -> 229	-0.14406					
228 -> 232	0.40807					
Excited State 27:	Triplet-A	5.1120 eV	242.53 nm	f=n.d.	<S**2>=2.000	
217 -> 229	0.16755					
217 -> 233	0.10120					
218 -> 230	0.18285					
221 -> 252	-0.11860					
222 -> 233	0.10501					
225 -> 233	0.16701					
226 -> 234	-0.18535					
Excited State 28:	Triplet-A	5.1125 eV	242.51 nm	f=n.d.	<S**2>=2.000	
217 -> 230	0.16868					
218 -> 229	0.18624					
218 -> 233	0.10420					
221 -> 233	-0.10421					
222 -> 252	0.12172					
225 -> 234	-0.16501					
226 -> 233	0.18656					
226 -> 238	-0.11429					
Excited State 29:	Triplet-A	5.2117 eV	237.90 nm	f=n.d.	<S**2>=2.000	
215 -> 261	-0.11632					
215 -> 265	-0.23091					
216 -> 259	-0.14300					
216 -> 260	0.11199					
216 -> 264	0.18573					
Excited State 30:	Triplet-A	5.2133 eV	237.82 nm	f=n.d.	<S**2>=2.000	
215 -> 259	-0.14214					

215 -> 260	0.11273				
215 -> 264	0.18735				
216 -> 261	-0.11441				
216 -> 265	-0.23065				
Excited State 31:	Triplet-A	5.2532 eV	236.02 nm	f=n.d.	<S**2>=2.000
213 -> 231	-0.12563				
214 -> 229	0.10843				
215 -> 230	-0.12731				
215 -> 231	0.13242				
216 -> 232	0.17130				
227 -> 261	-0.11019				
227 -> 265	-0.20347				
228 -> 259	-0.12611				
228 -> 264	0.13687				
228 -> 271	-0.10320				
Excited State 32:	Triplet-A	5.2567 eV	235.86 nm	f=n.d.	<S**2>=2.000
213 -> 229	0.10388				
214 -> 231	-0.12025				
215 -> 232	0.17087				
216 -> 230	-0.12303				
216 -> 231	0.14223				
226 -> 265	-0.10390				
227 -> 259	-0.14005				
227 -> 260	0.10546				
227 -> 264	0.16402				
228 -> 265	-0.18204				
228 -> 273	0.10103				
Excited State 33:	Triplet-A	5.2874 eV	234.49 nm	f=n.d.	<S**2>=2.000
213 -> 259	0.11242				
213 -> 260	-0.10109				
213 -> 264	-0.16427				
214 -> 265	0.19958				
215 -> 271	-0.10069				
215 -> 282	0.12041				
216 -> 273	0.12017				
Excited State 34:	Triplet-A	5.2884 eV	234.44 nm	f=n.d.	<S**2>=2.000
213 -> 265	0.19439				
214 -> 259	0.11666				
214 -> 264	-0.16624				
215 -> 273	0.12067				
216 -> 282	0.12026				
Excited State 35:	Triplet-A	5.2948 eV	234.16 nm	f=n.d.	<S**2>=2.000
213 -> 229	0.13818				
214 -> 230	-0.17369				
215 -> 229	0.17331				
216 -> 230	-0.11788				
216 -> 231	-0.13200				
225 -> 259	0.11260				
225 -> 260	-0.10374				
225 -> 264	-0.17103				
226 -> 265	-0.17602				
Excited State 36:	Triplet-A	5.2973 eV	234.05 nm	f=n.d.	<S**2>=2.000
213 -> 230	-0.16826				
214 -> 229	0.14264				
215 -> 230	-0.12215				
215 -> 231	-0.13475				
216 -> 229	0.16566				
225 -> 265	0.19498				
226 -> 264	0.15739				
Excited State 37:	Singlet-A	5.4420 eV	227.83 nm	f=0.0000	<S**2>=0.000
219 -> 231	-0.13321				
220 -> 232	0.14424				
223 -> 229	-0.11310				
223 -> 232	0.17953				

223 -> 233	0.19390				
223 -> 238	0.17508				
224 -> 231	0.27149				
224 -> 239	0.11936				
224 -> 240	0.11477				
225 -> 238	0.10060				
228 -> 231	0.12530				
228 -> 234	-0.11822				
228 -> 239	0.14137				
228 -> 240	0.12336				
Excited State 38:	Singlet-A	5.4635 eV	226.93 nm	f=0.1241	<S**2>=0.000
219 -> 232	-0.11951				
220 -> 231	0.15112				
221 -> 229	0.11835				
222 -> 230	-0.12440				
223 -> 231	0.24205				
223 -> 239	0.14449				
223 -> 240	0.13732				
224 -> 229	-0.12252				
224 -> 232	0.18786				
224 -> 233	0.14365				
224 -> 238	0.11937				
228 -> 233	0.16185				
228 -> 238	0.17940				
Excited State 39:	Singlet-A	5.4830 eV	226.12 nm	f=0.4785	<S**2>=0.000
217 -> 230	0.11624				
218 -> 229	0.15683				
220 -> 230	0.12842				
221 -> 229	0.23149				
221 -> 233	0.18125				
222 -> 230	-0.21338				
222 -> 231	-0.12825				
222 -> 234	0.14350				
225 -> 234	0.16600				
226 -> 233	-0.15939				
226 -> 238	0.10195				
228 -> 238	-0.10121				
Excited State 40:	Singlet-A	5.4897 eV	225.85 nm	f=0.0000	<S**2>=0.000
217 -> 229	0.12428				
218 -> 230	0.16332				
220 -> 229	0.13252				
221 -> 230	0.23644				
221 -> 231	0.11909				
221 -> 234	-0.13232				
222 -> 229	-0.23552				
222 -> 233	-0.18836				
224 -> 231	-0.10943				
225 -> 233	-0.15157				
226 -> 234	0.16783				
Excited State 41:	Triplet-A	5.6259 eV	220.38 nm	f=n.d.	<S**2>=2.000
215 -> 265	-0.10770				
225 -> 234	-0.10820				
227 -> 239	0.12309				
227 -> 240	0.10650				
228 -> 233	0.12496				
228 -> 238	0.14692				
Excited State 42:	Triplet-A	5.6301 eV	220.22 nm	f=n.d.	<S**2>=2.000
216 -> 265	0.10877				
225 -> 238	-0.11420				
227 -> 233	-0.14123				
227 -> 238	-0.10091				
228 -> 239	-0.11600				
228 -> 240	-0.10021				