Supporting information:

Multicarbazolyl Substituted TTM Radicals: Red-shift of Fluorescent Emission with Enhanced Luminescent Efficiency

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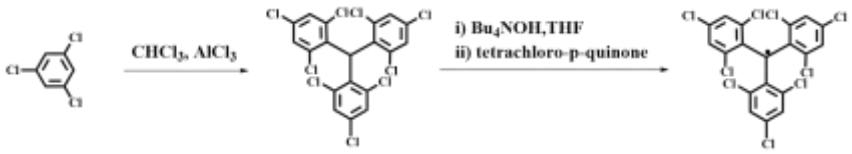
Contents

1. Materials synthesis

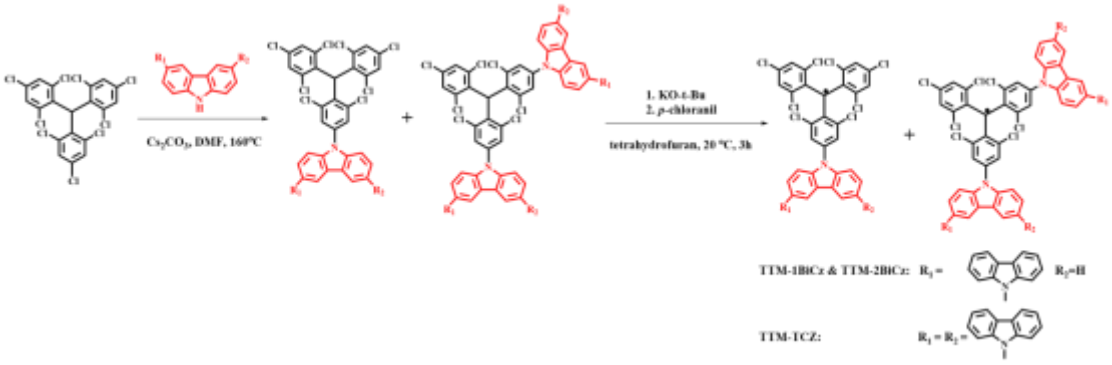
General: All chemical reagents and solvents, unless otherwise stated, were purchased from commercial sources and used without further purification. Tetrahydrofuran (THF) was distilled before use. Column chromatography was performed using silica gel (200-300 mesh). The concentration of sample solutions used for the optical measurements is around 10^{-4} mol/L.

Ultraviolet-visible (UV-vis) spectra were recorded by a Shimadzu UV-2550 spectrophotometer. Fluorescence spectra of radicals were performed using a Shimadzu 5301PC spectrofluorometer. Relative PLQYs were measured using a Shimadzu UV-2550 spectrofluorometer and an Edinburgh fluorescence spectrometer (FLS980). The fluorescence lifetimes were measured using the FLS980. EPR spectra of radicals in the solid state were recorded on a JES-FA200 at ambient temperature. IR spectra of radicals were recorded with a Brucker VERTEX 80V. Mass spectra of all compounds were measured on a Thermo Fisher ITQ1100 mass detector.

The TTM radical [1, 2] and multicarbazole[3] were prepared as reported (Scheme 1).The stepwise synthetic methods for the radicals are outlined in Scheme 2. Since the synthesis of the TTM radical derivatives are similar, general produces are given as below.



Scheme 1. Synthesis of the TTM radical



Scheme 2. Synthesis of the TTM radical derivatives

(1) General synthesis of radical precursor H compounds (mixtures of H compound and radical):

HTTM (1.00 g, 1.81 mmol), multicarbazole (2.00 mmol) and Cs_2CO_3 (1.00 g, 3.07 mmol) were dissolved in DMF solution (20 ml). The mixture was stirred at 95 °C for 48 h under argon atmosphere and in the dark. After the reaction, the mixture was cool to room temperature, the resulting mixture was poured into (1 M) hydrochloric acid solution, and the precipitate was filtered. The crude product was adsorbed in silica gel and purified by silica gel column chromatography using (petroleum ether: dichloromethane = 5:1v/v). The desired products H compounds (mixtures of H compound and radical) were obtained. **MS (m/z):** HTTM 553.65 $[M]^+$, HTTM-1BiCz 850.19 $[M]^+$, HTTM-2BiCz 1145.25 $[M+1]^+$, HTTM-TCz 1011.28 $[M-4]^+$

(2) General procedure to synthesize radicals from H compounds.

Under argon atmosphere and in the dark, the H compound (1.00 equiv.) was dissolved in dry THF (40 ml). Then KO^{t}Bu (2.00 equiv.) was added, at which point the solution immediately become claret-colored. The solution was stirred for 1.5 h in the dark at room temperature, and then p-chloranil (2.7 equiv.) was added. The solution was stirred for an additional 1.5 h. After the reaction was complete, the solvent was removed under vacuum, and the crude product was purified by silica gel column chromatography (using petroleum ether: dichloromethane = 5:1v/v). The crude products were recrystallized twice from dichloromethane and methanol.**MS (m/z):**TTM 552.89 $[M]^+$, TTM-1BiCz 849.26 $[M]^+$, TTM-2BiCz 1144.91 $[M]^+$, TTM-TCz 1013.54 $[M-1]^+$;

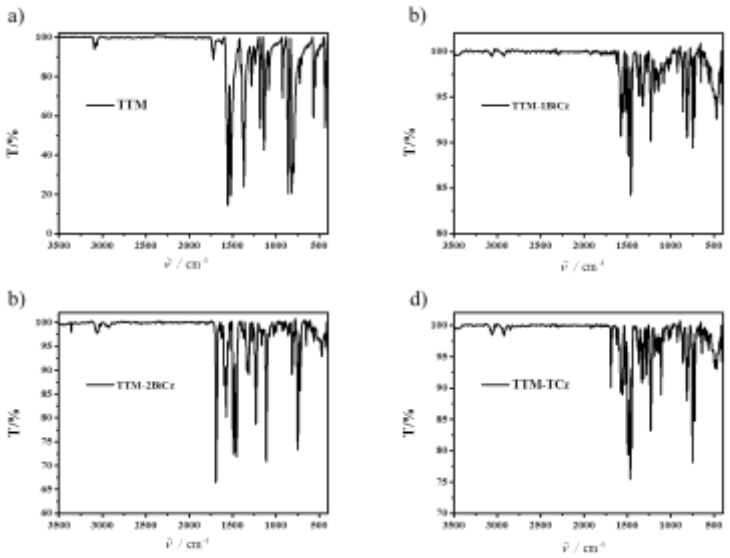


Fig.S1 Infrared absorption spectra of the TTM radicals: a) TTM; b) TTM-1BiCz; c) TTM-2BiCz; d) TTM-TCz.

2. Electron Paramagnetic Resonance (EPR) spectra of the radicals

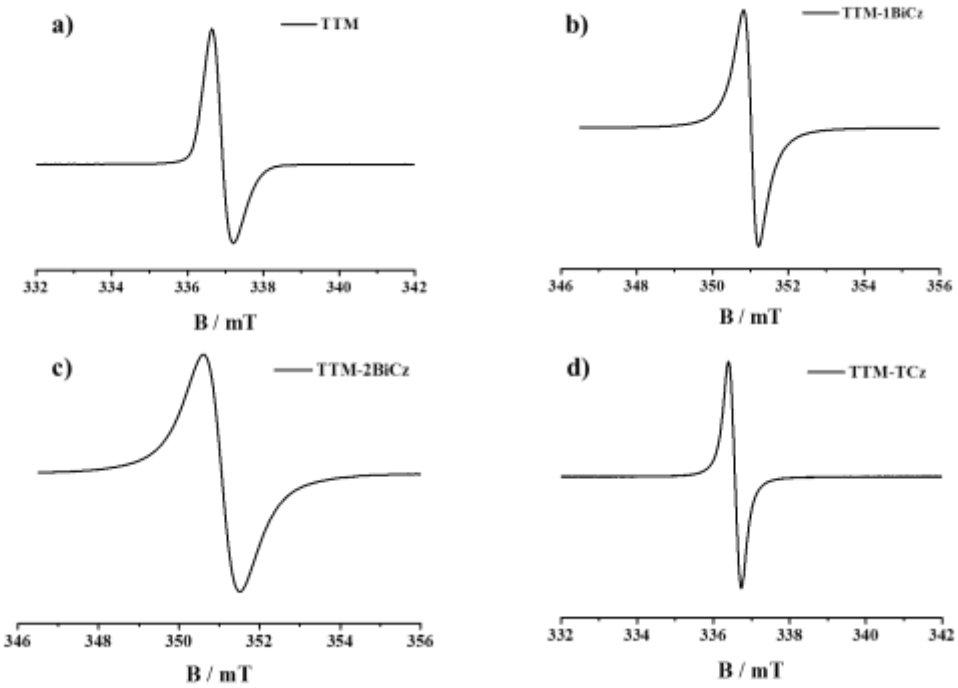


Fig. S2 EPR spectra (room temperature) of the TTM radicals: a) TTM; b) TTM-1BiCz; c) TTM-2BiCz; d) TTM-TCz.

3. Photophysical parameters of TTM radical and derivatives in different solvents

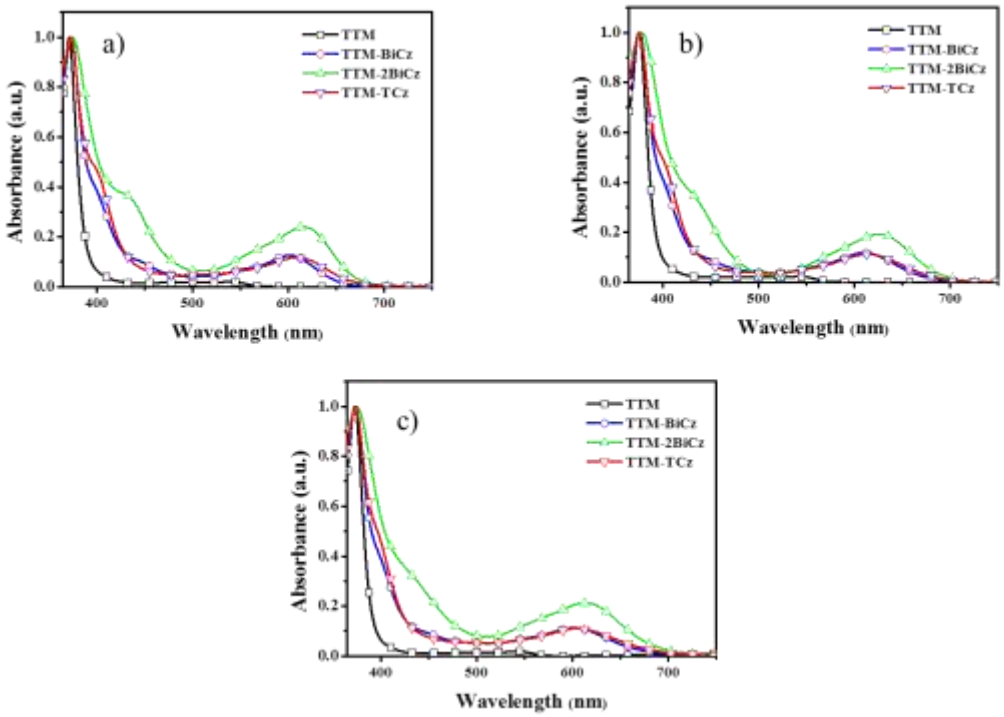


Fig. S3 UV−vis spectra of TTM radicals in different solvents: a) cyclohexane; b) toluene; c) THF.

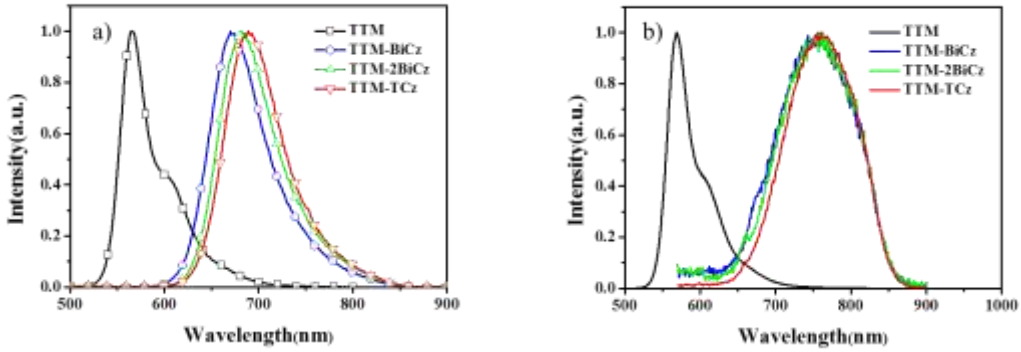


Fig. S4 PL spectra of PTM radicals in different solvents: a) cyclohexane; b) toluene.

Table S1. Photophysical parameters of TTM radical and derivatives in different solvents

Adduct	solvent	λ_{abs} (nm)	λ_{em} (nm) [a]	τ (ns) [b]
TTM	cyclohexene	371, 540	565	6.54
	toluene	375, 542	569	7.09
	THF	372, 543	568	-[c]
TTM-BiCz	cyclohexene	373, 400, 601	671	9.86
	toluene	376, 610	751	-[c]
	THF	374, 603	-[c]	-[c]
TTm-2BiCz	cyclohexene	374, 400, 617	681	7.12
	toluene	378, 627	758	-[c]
	THF	375, 616	-[c]	-[c]
TTM-TCz	cyclohexene	373, 435, 612	689	16.8
	toluene	375, 616	762	-[c]
	THF	373, 609	-[c]	-[c]

a) All are excited at their maximum absorption around 370 nm; b) The lifetimes in solution were measured using Edinburgh fluorescence spectrometer (FLS980) under the laser excitation at 378.8 nm and a pulse width of 68.9 ps; c) When excited in toluene and tetrahydrofuran (THF), some emissions of substituted radicals were too weak to measure.

The PLQYs (Φ_f) of the substituted radicals in cyclohexane were measured by reference method using R6G in ethanol as a standard.[4]

1. V. Gamero, D. Velasco, S. Latorre, F. López-Calahorra, E. Brillas and L. Juliá, *Tetrahedron letters*, 2006, **47**, 2305-2309.
2. Q. Peng, A. Obolda, M. Zhang and F. Li, *Angewandte Chemie International Edition*, 2015, **54**, 7091-7095.
3. M. P. Gaj, A. Wei, C. Fuentes-Hernandez, Y. Zhang, R. Reit, W. Voit, S. R. Marder and B. Kippelen, *Organic Electronics*, 2015, **25**, 151-155.
4. C. Würth, M. Grabolle, J. Pauli, M. Spieles, U. Resch-Genger, Analytical chemistry 2011, 83, 3431-3439.

4. DFT calculation results of the radicals

Computational details

DFT calculations were executed using the Gaussian09 program package. Calculations were performed using the unrestricted Becke three-parameter hybrid functional with Lee–Yang–Parr correlation functional (B3LYP). Frequency calculations were carried out to ensure that the optimized geometries were minima on the potential energy surface, in which no imaginary frequencies were observed in any of the compounds. TD-DFT calculations were performed using UB3LYP to calculate the first 20 doublet transitions.

TTM (UB3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.252720	-2.017587	-0.896749
2	6	0	1.562984	-3.373353	-0.906543
3	6	0	0.927097	-4.216572	-0.001763
4	6	0	-0.003630	-3.718919	0.903854
5	6	0	-0.290856	-2.358062	0.895734
6	6	0	0.316432	-1.439352	-0.000020
7	1	0	2.273636	-3.762913	-1.623795
8	1	0	-0.484886	-4.371505	1.620634
9	6	0	0.000223	0.000339	0.001019
10	6	0	1.088271	0.995115	0.001494
11	6	0	1.122544	2.094101	-0.896244
12	6	0	2.185378	0.929792	0.899800
13	6	0	2.141795	3.040353	-0.905351
14	6	0	3.220429	1.858779	0.909062
15	6	0	3.188178	2.912309	0.001804
16	1	0	2.125357	3.849751	-1.623602
17	1	0	4.024861	1.768779	1.627416
18	6	0	-1.405812	0.445753	0.000183
19	6	0	-2.371050	-0.068092	-0.904422
20	6	0	-1.900257	1.421954	0.903842
21	6	0	-3.700469	0.340478	-0.914334
22	6	0	-3.222618	1.852964	0.912387
23	6	0	-4.115848	1.303623	-0.001135
24	1	0	-4.390919	-0.073517	-1.637557
25	1	0	-3.549629	2.589484	1.634762
26	17	0	-1.397526	-1.813149	2.142439

27	17	0	2.029289	-1.056880	-2.141858
28	17	0	-1.921006	-1.208189	-2.158834
29	17	0	-0.876697	2.096296	2.157991
30	17	0	-0.095454	2.284361	-2.143621
31	17	0	2.263991	-0.301328	2.146414
32	17	0	-5.783432	1.831049	-0.001642
33	17	0	4.479920	4.091288	0.001448
34	17	0	1.302592	-5.924731	-0.003135

Dipole moment (field-independent basis, Debye):

X= 0.0027 Y= 0.0003 Z= 0.0003

Tot= 0.0027

TTM-1BiCz (UB3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.379570	0.189025	0.998828
2	6	0	-3.773247	1.633468	0.637991
3	6	0	-2.800969	2.533276	0.201822
4	6	0	-5.102938	2.042218	0.747820
5	6	0	-3.157848	3.841620	-0.125815
6	6	0	-5.459579	3.350398	0.420697
7	6	0	-4.487046	4.250077	-0.016531
8	1	0	-2.391212	4.550758	-0.470102
9	1	0	-6.507446	3.672847	0.507158
10	6	0	-2.048093	-0.167007	0.311798
11	6	0	-0.847800	-0.046517	1.011798
12	6	0	-2.042499	-0.609879	-1.011474
13	6	0	0.358327	-0.369847	0.389555
14	6	0	-0.836580	-0.932661	-1.633655
15	6	0	0.363903	-0.813020	-0.932986
16	1	0	1.304504	-0.275207	0.941763
17	1	0	-0.831839	-1.281718	-2.676541
18	6	0	-4.478782	-0.777459	0.520037
19	6	0	-4.983672	-0.672850	-0.775866
20	6	0	-4.970016	-1.757809	1.383067
21	6	0	-5.978937	-1.548991	-1.209796
22	6	0	-5.965378	-2.633401	0.949327
23	6	0	-6.469618	-2.529259	-0.347325
24	1	0	-6.376549	-1.466633	-2.231688
25	1	0	-6.352741	-3.406133	1.629260

26	17	0	-6.329570	0.906484	1.298352
27	17	0	-1.123849	2.018030	0.062579
28	17	0	-4.937482	5.900579	-0.429508
29	17	0	-4.363995	0.563091	-1.864925
30	17	0	-4.332711	-1.889449	3.018338
31	17	0	-7.725349	-3.634464	-0.894374
32	17	0	-0.854407	0.511460	2.680995
33	17	0	-3.557352	-0.761711	-1.894519
34	6	0	2.053137	-2.613689	-1.398869
35	6	0	2.846106	-0.428776	-0.996906
36	6	0	1.363782	-3.755211	-1.760795
37	6	0	3.300742	-2.708869	-0.708595
38	6	0	3.064827	0.932007	-0.898386
39	6	0	3.791938	-1.355479	-0.459624
40	6	0	1.913551	-5.004709	-1.437017
41	1	0	0.403745	-3.693351	-2.291844
42	6	0	3.835930	-3.946551	-0.393034
43	6	0	4.231243	1.381939	-0.261723
44	1	0	2.344050	1.653225	-1.308055
45	6	0	4.940796	-0.902346	0.167030
46	6	0	3.128555	-5.098279	-0.764837
47	1	0	1.373262	-5.920075	-1.720332
48	1	0	4.794828	-4.027973	0.137735
49	6	0	5.153049	0.480093	0.261501
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51	1	0	5.672986	-1.608714	0.582691
52	1	0	3.543236	-6.087307	-0.519975
53	7	0	1.695141	-1.169739	-1.620123
54	6	0	7.198215	1.924749	0.053575
55	6	0	7.397312	-0.114701	1.222004
56	6	0	6.812132	3.122752	-0.516516
57	6	0	8.504268	1.396289	-0.185193
58	6	0	7.239182	-1.252455	1.989979
59	6	0	8.627603	0.133010	0.538575
60	6	0	7.726990	3.806145	-1.331581
61	1	0	5.810308	3.538080	-0.339424
62	6	0	9.400857	2.077722	-0.991194
63	6	0	8.308811	-2.155480	2.083502
64	1	0	6.297414	-1.452629	2.519607
65	6	0	9.678291	-0.763825	0.636757
66	6	0	8.999152	3.292204	-1.564571
67	1	0	7.430209	4.760781	-1.790566
68	1	0	10.407014	1.677766	-1.179642
69	6	0	9.507427	-1.914817	1.418508

70	1	0	8.193851	-3.064665	2.691981
71	1	0	10.627581	-0.580371	0.114238
72	1	0	9.702279	3.843071	-2.206639
73	1	0	10.334612	-2.634856	1.504534
74	7	0	6.425335	1.001593	0.954989

Dipole moment (field-independent basis, Debye):

X= 3.4294 Y= -3.1121 Z= -6.1550

Tot= 7.7026

TTM-2BiCz (UB3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.023910	2.532577	-0.985045
2	6	0	-1.118326	1.740704	-0.245591
3	6	0	-0.790855	0.570264	0.438554
4	6	0	-2.437958	2.194100	-0.260388
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6	6	0	-3.429163	1.477066	0.409621
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9	1	0	-4.469282	1.834131	0.398139
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12	6	0	1.815604	2.814661	0.748142
13	6	0	3.390917	0.874019	-0.491519
14	6	0	3.064187	2.487628	1.276941
15	6	0	3.852093	1.517517	0.656860
16	1	0	4.011723	0.109156	-0.980118
17	1	0	3.427887	2.994539	2.182611
18	6	0	-0.275709	4.041802	-0.810581
19	6	0	-0.544275	4.562536	0.455092
20	6	0	-0.235542	4.888437	-1.919099
21	6	0	-0.771592	5.929946	0.613167
22	6	0	-0.463283	6.255438	-1.761057
23	6	0	-0.730943	6.776318	-0.494782
24	1	0	-0.982876	6.340365	1.611194
25	1	0	-0.431703	6.922946	-2.634505
26	17	0	-2.850831	3.671083	-1.123903
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29	17	0	0.103302	4.230937	-3.516121
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35	6	0	6.477757	3.374235	0.655642
36	6	0	7.268649	1.171265	-0.033695
37	6	0	5.007685	-1.442462	1.151264
38	6	0	6.844215	-0.219522	0.109451
39	6	0	7.590608	3.931764	0.008304
40	1	0	5.752324	4.022178	1.166942
41	6	0	8.364231	1.730311	-0.670115
42	6	0	5.587429	-2.631297	0.683424
43	1	0	4.075423	-1.472089	1.732223
44	6	0	7.409542	-1.398029	-0.348179
45	6	0	8.517502	3.123463	-0.643104
46	1	0	7.728160	5.023117	0.018430
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49	1	0	5.098644	-3.591673	0.904438
50	1	0	8.341486	-1.388010	-0.930599
51	1	0	9.383666	3.579630	-1.144866
52	7	0	5.230700	1.156871	1.240791
53	6	0	7.607448	-4.890910	0.580206
54	6	0	8.766222	-3.712655	-1.102999
55	6	0	6.693109	-5.449450	1.452726
56	6	0	8.996771	-5.208346	0.685407
57	6	0	9.178974	-2.921685	-2.158119
58	6	0	9.714546	-4.478520	-0.357224
59	6	0	7.156943	-6.331588	2.440154
60	1	0	5.622581	-5.212214	1.380606
61	6	0	9.445698	-6.080181	1.663277
62	6	0	10.544143	-2.887171	-2.479719
63	1	0	8.458152	-2.328813	-2.738137
64	6	0	11.060236	-4.438547	-0.681906
65	6	0	8.509814	-6.641309	2.543249
66	1	0	6.437786	-6.782057	3.140129
67	1	0	10.512560	-6.329186	1.750632
68	6	0	11.468312	-3.632997	-1.754136
69	1	0	10.883920	-2.260696	-3.317670
70	1	0	11.795660	-5.024699	-0.113215
71	1	0	8.853888	-7.335372	3.324264
72	1	0	12.534484	-3.592804	-2.022005

73	7	0	7.382754	-3.929155	-0.554099
74	6	0	-5.007534	-1.315757	0.879551
75	6	0	-5.216362	0.436590	2.444764
76	6	0	-4.602234	-2.333248	0.037104
77	6	0	-6.378981	-0.917052	0.926669
78	6	0	-5.050179	1.426070	3.394810
79	6	0	-6.508341	0.168384	1.896216
80	6	0	-5.562998	-2.963791	-0.767676
81	1	0	-3.550238	-2.647700	-0.006895
82	6	0	-7.320566	-1.545091	0.128642
83	6	0	-6.173330	2.158685	3.807258
84	1	0	-4.061190	1.640496	3.823094
85	6	0	-7.611559	0.896437	2.309433
86	6	0	-6.898846	-2.576142	-0.722345
87	1	0	-5.251450	-3.775062	-1.442102
88	1	0	-8.377118	-1.244099	0.159147
89	6	0	-7.431980	1.897886	3.273780
90	1	0	-6.052552	2.948933	4.562904
91	1	0	-8.608432	0.696105	1.892369
92	1	0	-8.300499	2.483113	3.610345
93	6	0	-9.311455	-2.722146	-1.408615
94	6	0	-8.087631	-4.730751	-1.229800
95	6	0	-9.773058	-1.434478	-1.603833
96	6	0	-10.193480	-3.745176	-0.942253
97	6	0	-7.147587	-5.743421	-1.220123
98	6	0	-9.435418	-4.989364	-0.831507
99	6	0	-11.121366	-1.154741	-1.335251
100	1	0	-9.103376	-0.640355	-1.962169
101	6	0	-11.522975	-3.459963	-0.679658
102	6	0	-7.543944	-7.025921	-0.812202
103	1	0	-6.108563	-5.555431	-1.524414
104	6	0	-9.817862	-6.258551	-0.430508
105	6	0	-11.981034	-2.150498	-0.881099
106	1	0	-11.499592	-0.133006	-1.487162
107	1	0	-12.207469	-4.241269	-0.320690
108	6	0	-8.856418	-7.278699	-0.424479
109	1	0	-6.803751	-7.839589	-0.800410
110	1	0	-10.852456	-6.465399	-0.122838
111	1	0	-13.035026	-1.911315	-0.676194
112	1	0	-9.147769	-8.291183	-0.108122
113	7	0	-4.195808	-0.484468	1.834626
114	7	0	-7.932555	-3.285597	-1.616615

Dipole moment (field-independent basis, Debye):

X= 3.9979 Y= 1.5560 Z= 6.0153
Tot= 7.3884

TTM-TCz (UB3LYP/6-31G(d))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.196097	0.079222	0.860686
2	6	0	4.966260	1.234083	0.193794
3	6	0	6.322254	1.089695	-0.101000
4	6	0	4.308211	2.424369	-0.115624
5	6	0	7.020123	2.135657	-0.704460
6	6	0	5.005915	3.470384	-0.720167
7	6	0	6.361697	3.326277	-1.014487
8	1	0	8.089082	2.022153	-0.936278
9	1	0	4.486713	4.408606	-0.964388
10	6	0	4.931320	-1.247970	0.596856
11	6	0	5.806094	-1.762993	1.553931
12	6	0	4.722640	-1.935230	-0.598835
13	6	0	6.472510	-2.964668	1.314998
14	6	0	5.388429	-3.137784	-0.837576
15	6	0	6.263370	-3.652504	0.119022
16	1	0	7.162511	-3.370359	2.069061
17	1	0	5.223383	-3.679647	-1.780242
18	6	0	2.774325	0.003924	0.273751
19	6	0	1.672846	-0.094284	1.124381
20	6	0	2.587726	0.034012	-1.108213
21	6	0	0.385140	-0.163063	0.593058
22	6	0	1.299627	-0.033785	-1.639827
23	6	0	0.198396	-0.132448	-0.789478
24	1	0	-0.483065	-0.241105	1.263451
25	1	0	1.152780	-0.009626	-2.729473
26	6	0	-2.058373	0.962466	-0.934819
27	6	0	-1.974842	-1.392700	-0.832658
28	6	0	-1.858912	2.313218	-1.146853
29	6	0	-3.195211	0.504446	-0.200059
30	6	0	-1.679630	-2.739218	-0.927602
31	6	0	-3.143481	-0.954406	-0.136792
32	6	0	-2.793395	3.221431	-0.627033
33	1	0	-0.988201	2.676137	-1.710470
34	6	0	-4.112563	1.408170	0.309458
35	6	0	-2.549005	-3.662840	-0.328091

36	1	0	-0.783668	-3.087030	-1.460314
37	6	0	-3.996211	-1.873260	0.451814
38	6	0	-3.900847	2.776194	0.088598
39	1	0	-2.644490	4.299111	-0.789846
40	1	0	-4.989287	1.063727	0.875625
41	6	0	-3.687519	-3.236841	0.349499
42	1	0	-2.323597	-4.737309	-0.397279
43	1	0	-4.896935	-1.544080	0.988629
44	6	0	-4.541880	-5.599036	0.294063
45	6	0	-6.067650	-3.882047	0.830899
46	6	0	-3.456125	-6.436288	0.122539
47	6	0	-5.820599	-5.952680	-0.236848
48	6	0	-6.729254	-2.752831	1.274102
49	6	0	-6.765706	-4.889143	0.095697
50	6	0	-3.636107	-7.636436	-0.581431
51	1	0	-2.468515	-6.174019	0.526707
52	6	0	-5.989041	-7.139431	-0.930469
53	6	0	-8.095925	-2.617381	0.987451
54	1	0	-6.202069	-1.972375	1.840200
55	6	0	-8.114908	-4.747187	-0.182513
56	6	0	-4.881117	-7.981620	-1.098744
57	1	0	-2.778570	-8.310527	-0.723928
58	1	0	-6.969251	-7.418360	-1.341828
59	6	0	-8.776573	-3.597876	0.271795
60	1	0	-8.632572	-1.722323	1.335248
61	1	0	-8.658768	-5.517304	-0.747287
62	1	0	-5.002062	-8.927166	-1.647752
63	1	0	-9.848303	-3.473458	0.057301
64	6	0	-5.628824	4.515746	-0.460058
65	6	0	-4.214181	4.904277	1.387115
66	6	0	-6.435680	4.007939	-1.460253
67	6	0	-5.374846	5.919522	-0.376624
68	6	0	-3.400807	4.841401	2.502349
69	6	0	-4.498595	6.160193	0.767573
70	6	0	-6.997865	4.897346	-2.388275
71	1	0	-6.637522	2.930255	-1.533518
72	6	0	-5.934006	6.790132	-1.297081
73	6	0	-2.862467	6.032984	3.010899
74	1	0	-3.175673	3.880960	2.986467
75	6	0	-3.963001	7.331503	1.276562
76	6	0	-6.751070	6.264611	-2.307688
77	1	0	-7.641785	4.503991	-3.188721
78	1	0	-5.743339	7.870952	-1.239605
79	6	0	-3.139231	7.256556	2.408331

80	1	0	-2.213420	5.994633	3.898225
81	1	0	-4.177090	8.301235	0.805799
82	1	0	-7.201196	6.945873	-3.044820
83	1	0	-2.707795	8.179928	2.822261
84	7	0	-1.223589	-0.208328	-1.375823
85	7	0	-4.624810	-4.272486	0.997978
86	7	0	-4.911029	3.795156	0.647926
87	17	0	3.977048	0.158184	-2.181509
88	17	0	1.908915	-0.133453	2.868037
89	17	0	6.070002	-0.894797	3.061972
90	17	0	3.618947	-1.285900	-1.806242
91	17	0	7.104434	-5.168927	-0.182093
92	17	0	7.242656	4.645930	-1.776082
93	17	0	7.152412	-0.411962	0.290747
94	17	0	2.597557	2.606682	0.255889

Dipole moment (field-independent basis, Debye):

X= -1.3967 Y= -3.8591 Z= -6.0745

Tot= 7.3310

5.Extracted results of TD-DFT calculation.

TTM (UB3LYP/6-31G(d))

Excited State 1: 2.214-A 2.6538 eV 467.20 nm f=0.0225 <S**2>=0.976
137A ->138A 0.28870
133B ->137B -0.23514
135B ->137B 0.12892
136B ->137B 0.87169
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -4869.24555561
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.214-A 2.6556 eV 466.88 nm f=0.0222 <S**2>=0.975
137A ->139A 0.28581
132B ->137B -0.22933
135B ->137B 0.87405
136B ->137B -0.12965

Excited State 3: 2.110-A 2.9244 eV 423.97 nm f=0.0052 <S**2>=0.863
137A ->138A -0.11258
137A ->140A -0.12074
132B ->137B -0.11252
133B ->137B 0.55300
134B ->137B 0.75520
136B ->137B 0.21714

Excited State 4: 2.126-A 2.9277 eV 423.48 nm f=0.0030 <S**2>=0.880
137A ->138A -0.13390
137A ->139A -0.14672
132B ->137B 0.81289
133B ->137B 0.35217
134B ->137B -0.16254
135B ->137B 0.31130

Excited State 5: 2.115-A 2.9284 eV 423.38 nm f=0.0043 <S**2>=0.868
137A ->139A 0.12082
132B ->137B -0.36642
133B ->137B 0.61226
134B ->137B -0.59587
135B ->137B -0.10050
136B ->137B 0.23698

Excited State 6:	2.356-A	3.0870 eV	401.63 nm	f=0.0000	<S**2>=1.138
132A ->139A	0.10039				
133A ->138A	0.10259				
135A ->139A	0.12022				
136A ->138A	-0.12123				
137A ->146A	-0.24467				
131B ->137B	0.87188				
134B ->140B	-0.10789				
135B ->138B	0.10040				
136B ->139B	0.10194				
Excited State 7:	2.375-A	3.3459 eV	370.56 nm	f=0.1780	<S**2>=1.160
133A ->140A	-0.11920				
134A ->142A	-0.12111				
137A ->138A	0.28867				
137A ->139A	0.74305				
131B ->138B	0.10853				
132B ->137B	0.32264				
135B ->137B	-0.29397				
135B ->138B	0.10623				
136B ->139B	-0.10022				
Excited State 8:	2.370-A	3.3471 eV	370.42 nm	f=0.1813	<S**2>=1.155
132A ->140A	0.11939				
134A ->141A	0.12198				
137A ->138A	0.74374				
137A ->139A	-0.28890				
131B ->139B	0.10935				
133B ->137B	0.32441				
135B ->139B	-0.10091				
136B ->137B	-0.29393				
136B ->138B	-0.10178				
Excited State 9:	2.206-A	3.5902 eV	345.34 nm	f=0.0109	<S**2>=0.967
137A ->140A	0.95776				
134B ->137B	0.16943				
Excited State 10:	3.250-A	3.6830 eV	336.64 nm	f=0.0000	<S**2>=2.391
132A ->139A	-0.15898				
132A ->141A	-0.22306				
133A ->138A	-0.16002				
133A ->142A	-0.22204				
134A ->140A	-0.32024				
135A ->138A	-0.10136				

135A ->139A -0.14185
135A ->141A 0.17233
136A ->138A 0.13874
136A ->139A -0.10132
136A ->142A -0.17435
131B ->137B 0.40755
131B ->146B 0.11796
132B ->138B 0.17080
132B ->141B 0.20386
133B ->139B 0.17209
133B ->142B 0.20369
134B ->140B 0.28989
135B ->138B -0.21751
135B ->141B 0.16171
136B ->139B -0.21575
136B ->142B 0.16375

Excited State 11: 2.335-A 3.7762 eV 328.33 nm f=0.0060 <S**2>=1.113
133A ->140A 0.13028
137A ->139A 0.15757
137A ->141A 0.90808
132B ->137B 0.10809
133B ->140B -0.12563

Excited State 12: 2.336-A 3.7792 eV 328.07 nm f=0.0057 <S**2>=1.114
132A ->140A -0.13026
137A ->138A 0.15605
137A ->142A 0.90827
132B ->140B 0.12511
133B ->137B 0.10553

Excited State 13: 3.152-A 3.8755 eV 319.92 nm f=0.0134 <S**2>=2.233
131A ->139A 0.10281
132A ->141A 0.19092
133A ->140A 0.26044
133A ->142A -0.19018
134A ->142A 0.29399
135A ->139A -0.15282
136A ->138A -0.15174
136A ->140A 0.21578
137A ->138A 0.13738
137A ->139A 0.37954
137A ->141A -0.24944
131B ->138B -0.10879

132B ->141B -0.19150
133B ->140B -0.27569
133B ->142B 0.19360
134B ->142B -0.29898
135B ->138B -0.12930
136B ->139B 0.12890
136B ->140B -0.21355

Excited State 14: 3.155-A 3.8778 eV 319.72 nm f=0.0134 <S**2>=2.239
131A ->138A 0.10258
132A ->140A -0.26393
132A ->142A -0.18986
133A ->141A -0.18696
134A ->141A -0.29829
135A ->138A 0.14972
135A ->140A 0.21431
136A ->139A -0.15122
137A ->138A 0.37666
137A ->139A -0.13707
137A ->142A -0.24867
131B ->139B -0.10898
132B ->140B 0.27700
132B ->142B 0.19148
133B ->141B 0.18454
134B ->141B 0.30700
135B ->139B 0.12597
135B ->140B 0.21211
136B ->138B 0.12758

Excited State 15: 3.309-A 4.3056 eV 287.96 nm f=0.0000 <S**2>=2.488
132A ->141A -0.20034
133A ->142A -0.20195
134A ->140A -0.27041
135A ->138A 0.18643
135A ->139A 0.25836
136A ->138A -0.25629
136A ->139A 0.18500
137A ->146A -0.19417
126B ->137B 0.29253
131B ->137B -0.11270
132B ->138B -0.10893
132B ->141B 0.20382
133B ->139B -0.10850
133B ->142B 0.20579

134B ->140B 0.27403
135B ->138B 0.33238
136B ->139B 0.33060
136B ->142B 0.10128

Excited State 16: 2.483-A 4.3187 eV 287.09 nm f=0.0192 <S**2>=1.292
131A ->139A -0.10904
133A ->138A -0.10006
135A ->139A 0.17855
136A ->138A 0.17751
137A ->139A -0.11757
137A ->144A 0.23983
137A ->145A -0.16304
129B ->137B -0.47715
130B ->137B 0.63563
131B ->138B 0.14064
135B ->138B 0.12976
136B ->139B -0.12962

Excited State 17: 2.468-A 4.3196 eV 287.03 nm f=0.0200 <S**2>=1.273
131A ->138A -0.10991
135A ->138A -0.17233
136A ->139A 0.17729
137A ->138A -0.11827
137A ->144A -0.16285
137A ->145A -0.23664
129B ->137B 0.63990
130B ->137B 0.48232
131B ->139B 0.14171
135B ->139B -0.12426
136B ->138B -0.12810

Excited State 18: 2.217-A 4.3434 eV 285.45 nm f=0.0011 <S**2>=0.979
137A ->143A 0.96322

Excited State 19: 2.374-A 4.4706 eV 277.33 nm f=0.0190 <S**2>=1.159
135A ->139A 0.10426
136A ->138A 0.11143
137A ->144A 0.68059
137A ->145A -0.32460
128B ->137B -0.15518
129B ->137B 0.34252
130B ->137B -0.33745
134B ->142B -0.10148

135B ->138B 0.10963
136B ->139B -0.11194
136B ->140B -0.10671

Excited State 20: 2.374-A 4.4728 eV 277.19 nm f=0.0192 <S**2>=1.159
135A ->138A 0.11195
137A ->144A 0.33523
137A ->145A 0.68880
127B ->137B 0.11624
129B ->137B 0.33045
130B ->137B 0.33905
134B ->141B -0.10338
135B ->139B 0.11599
135B ->140B -0.10855

TTM-1BiCz (UB3LYP/6-31G(d))

Excited State 1: 2.059-A 1.5485 eV 800.66 nm f=0.0304 <S**2>=0.810
212B ->215B -0.11728
214B ->215B 0.99087
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -5442.23589231
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.056-A 2.0148 eV 615.38 nm f=0.0006 <S**2>=0.807
213B ->215B 0.99712

Excited State 3: 2.080-A 2.0744 eV 597.68 nm f=0.0714 <S**2>=0.831
212B ->215B 0.96881
214B ->215B 0.12374

Excited State 4: 2.074-A 2.4183 eV 512.70 nm f=0.0005 <S**2>=0.825
211B ->215B 0.99416

Excited State 5: 2.212-A 2.6528 eV 467.36 nm f=0.0190 <S**2>=0.973
212A ->217A 0.14081
214A ->217A 0.26759
206B ->215B 0.21350
207B ->215B -0.11875
209B ->215B 0.87232

Excited State 6: 2.226-A 2.7754 eV 446.73 nm f=0.0005 <S**2>=0.989
214A ->216A -0.30724

215A ->216A -0.12400
204B ->215B 0.37795
208B ->215B 0.78635
212B ->215B -0.15778

Excited State 7: 2.115-A 2.9100 eV 426.07 nm f=0.0037 <S**2>=0.869
214A ->217A -0.15159
214A ->218A 0.10952
205B ->215B 0.42559
206B ->215B -0.21957
207B ->215B 0.77936
209B ->215B 0.27291

Excited State 8: 2.126-A 2.9329 eV 422.73 nm f=0.0031 <S**2>=0.880
214A ->216A -0.13771
214A ->217A 0.12233
204B ->215B 0.28579
205B ->215B -0.31091
206B ->215B 0.66525
207B ->215B 0.41887
208B ->215B -0.25079
209B ->215B -0.20965

Excited State 9: 2.158-A 2.9371 eV 422.12 nm f=0.0025 <S**2>=0.914
214A ->216A -0.24991
215A ->216A -0.12590
204B ->215B 0.61964
205B ->215B -0.10711
206B ->215B -0.41577
207B ->215B -0.18822
208B ->215B -0.49091

Excited State 10: 2.069-A 3.0657 eV 404.42 nm f=0.0000 <S**2>=0.820
210B ->215B 0.99501

Excited State 11: 2.673-A 3.1016 eV 399.74 nm f=0.1254 <S**2>=1.537
204A ->216A 0.13752
211A ->219A 0.12036
214A ->216A 0.39553
214A ->226A 0.14430
215A ->216A 0.41084
202B ->215B 0.50258
204B ->215B 0.33466
204B ->216B 0.10011

211B ->219B -0.12230
212B ->216B 0.12843
214B ->216B -0.11478

Excited State 12: 3.396-A 3.1431 eV 394.47 nm f=0.0073 <S**2>=2.633
202A ->230A 0.10593
211A ->219A 0.51004
212A ->225A -0.14070
214A ->216A -0.13853
215A ->219A 0.28785
215A ->225A 0.14224
201B ->230B 0.10447
202B ->215B -0.15995
211B ->218B -0.10485
211B ->219B -0.49751
212B ->225B 0.15475
214B ->219B -0.26176
214B ->225B -0.11533

Excited State 13: 3.473-A 3.1824 eV 389.59 nm f=0.0000 <S**2>=2.766
203A ->237A -0.13527
210A ->222A 0.15427
213A ->222A 0.59671
215A ->228A -0.24051
203B ->237B 0.13602
210B ->222B -0.15423
210B ->231B -0.10051
213B ->222B -0.59677
214B ->228B 0.24946

Excited State 14: 3.376-A 3.2141 eV 385.75 nm f=0.0001 <S**2>=2.599
211A ->219A -0.10336
212A ->219A -0.29247
214A ->219A 0.19634
215A ->219A 0.55276
215A ->225A -0.13511
202B ->215B 0.21336
211B ->219B 0.11701
212B ->219B 0.33257
214B ->218B -0.10475
214B ->219B -0.45797
214B ->225B 0.10807

Excited State 15: 2.405-A 3.2732 eV 378.79 nm f=0.1652 <S**2>=1.196

209A ->217A -0.10432
212A ->226A 0.10948
214A ->216A -0.36566
215A ->216A -0.41980
215A ->219A -0.11850
202B ->215B 0.60340
204B ->215B -0.28999
205B ->215B 0.19315
208B ->215B -0.12361

Excited State 16: 2.298-A 3.3018 eV 375.50 nm f=0.1569 <S**2>=1.071
212A ->217A 0.23499
214A ->217A 0.68853
215A ->217A 0.38274
205B ->215B 0.16268
206B ->215B -0.29445
207B ->215B 0.12893
209B ->215B -0.26803

Excited State 17: 3.470-A 3.3446 eV 370.70 nm f=0.0013 <S**2>=2.760
210A ->228A 0.13449
214A ->222A 0.18054
215A ->222A -0.64272
210B ->228B -0.13476
212B ->222B 0.13175
214B ->222B 0.65643

Excited State 18: 2.772-A 3.4268 eV 361.80 nm f=0.0364 <S**2>=1.672
211A ->219A -0.16756
212A ->216A -0.15475
214A ->216A -0.25775
215A ->216A 0.25629
202B ->215B -0.15039
205B ->215B 0.54604
206B ->215B 0.27484
207B ->215B -0.23686
211B ->219B 0.14035
212B ->216B 0.13765
214B ->216B -0.48772

Excited State 19: 2.671-A 3.4384 eV 360.58 nm f=0.0455 <S**2>=1.534
212A ->216A 0.17411
214A ->216A 0.30424
215A ->216A -0.23467

204B ->215B 0.31881
205B ->215B 0.52209
206B ->215B 0.27423
207B ->215B -0.23731
212B ->216B -0.15751
214B ->216B 0.44725

Excited State 20: 2.485-A 3.4657 eV 357.75 nm f=0.0078 <S**2>=1.294
212A ->218A 0.10056
214A ->218A 0.68525
214A ->220A -0.18765
215A ->217A -0.13750
215A ->218A 0.54630
215A ->220A -0.20511
205B ->215B -0.14116
206B ->215B -0.11242

TTM-2BiCz (UB3LYP/6-31G(d))

Excited State 1: 2.060-A 1.5297 eV 810.50 nm f=0.0436 <S**2>=0.811
288B -> 293B 0.13223
292B -> 293B 0.98668
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -6015.18626592
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.058-A 1.5486 eV 800.65 nm f=0.0210 <S**2>=0.809
291B -> 293B 0.99097

Excited State 3: 2.056-A 2.0038 eV 618.73 nm f=0.0011 <S**2>=0.807
289B -> 293B 0.20338
290B -> 293B 0.97435

Excited State 4: 2.056-A 2.0049 eV 618.39 nm f=0.0013 <S**2>=0.807
289B -> 293B 0.97205
290B -> 293B -0.21147

Excited State 5: 2.080-A 2.0389 eV 608.09 nm f=0.1011 <S**2>=0.831
276B -> 293B -0.12043
288B -> 293B 0.96064
289B -> 293B 0.11235
292B -> 293B -0.13700

Excited State 6:	2.075-A	2.1140 eV	586.49 nm	f=0.0307	<S**2>=0.826
287B -> 293B	0.97579				
291B -> 293B	-0.10282				
Excited State 7:	2.073-A	2.4143 eV	513.55 nm	f=0.0004	<S**2>=0.824
286B -> 293B	0.99437				
Excited State 8:	2.073-A	2.4166 eV	513.06 nm	f=0.0003	<S**2>=0.824
285B -> 293B	0.99420				
Excited State 9:	2.213-A	2.7116 eV	457.24 nm	f=0.0036	<S**2>=0.974
287A -> 295A	0.12461				
291A -> 295A	0.26530				
293A -> 295A	0.13794				
277B -> 293B	-0.16057				
279B -> 293B	0.30316				
282B -> 293B	0.82063				
287B -> 293B	-0.12492				
Excited State 10:	2.253-A	2.8300 eV	438.10 nm	f=0.0302	<S**2>=1.019
291A -> 294A	0.34920				
293A -> 294A	0.24387				
276B -> 293B	0.34518				
278B -> 293B	0.13940				
280B -> 293B	0.26419				
281B -> 293B	0.68849				
288B -> 293B	0.17216				
Excited State 11:	2.148-A	2.9110 eV	425.92 nm	f=0.0137	<S**2>=0.903
291A -> 294A	0.21717				
291A -> 296A	-0.12776				
293A -> 294A	0.17068				
276B -> 293B	0.27191				
278B -> 293B	-0.27054				
280B -> 293B	0.62439				
281B -> 293B	-0.55225				
Excited State 12:	2.150-A	2.9231 eV	424.16 nm	f=0.0004	<S**2>=0.906
291A -> 295A	-0.24951				
293A -> 295A	-0.15411				
277B -> 293B	0.65838				
279B -> 293B	-0.44076				
282B -> 293B	0.45759				

Excited State 13:	2.201-A	2.9425 eV	421.35 nm	f=0.0268	<S**2>=0.961
291A -> 294A	-0.31943				
293A -> 294A	-0.25537				
276B -> 293B	-0.41776				
278B -> 293B	-0.23233				
280B -> 293B	0.62012				
281B -> 293B	0.36515				
Excited State 14:	2.068-A	3.0552 eV	405.82 nm	f=0.0006	<S**2>=0.819
284B -> 293B	0.98965				
Excited State 15:	2.067-A	3.0561 eV	405.70 nm	f=0.0002	<S**2>=0.818
283B -> 293B	0.99100				
Excited State 16:	2.979-A	3.1213 eV	397.21 nm	f=0.0777	<S**2>=1.968
276A -> 294A	-0.10973				
285A -> 297A	-0.13786				
286A -> 297A	0.11128				
286A -> 298A	-0.15998				
288A -> 294A	-0.18937				
291A -> 295A	0.30176				
292A -> 294A	0.27508				
293A -> 295A	0.34558				
293A -> 304A	-0.13497				
273B -> 293B	0.34370				
276B -> 294B	0.11171				
277B -> 293B	0.13038				
279B -> 293B	-0.24255				
285B -> 297B	0.17579				
286B -> 298B	0.17939				
288B -> 294B	-0.13763				
292B -> 294B	-0.17720				
Excited State 17:	3.422-A	3.1396 eV	394.91 nm	f=0.0051	<S**2>=2.678
285A -> 297A	-0.26601				
285A -> 298A	0.20506				
286A -> 297A	0.25609				
286A -> 298A	0.25530				
287A -> 297A	-0.10810				
287A -> 298A	0.10965				
288A -> 304A	-0.11098				
292A -> 297A	0.14767				
292A -> 304A	0.12093				
293A -> 294A	-0.15542				

293A -> 297A -0.11940
293A -> 298A 0.13611
293A -> 305A 0.13230
276B -> 293B 0.14803
285B -> 297B 0.32366
285B -> 298B -0.19408
286B -> 297B -0.18958
286B -> 298B -0.28650
287B -> 305B 0.12762
288B -> 304B -0.12454
291B -> 294B -0.10785
291B -> 298B 0.13941
291B -> 305B 0.10155
292B -> 297B -0.15256
292B -> 304B -0.11302

Excited State 18: 3.254-A 3.1478 eV 393.87 nm f=0.0331 <S**2>=2.397
285A -> 297A 0.22939
285A -> 298A 0.17789
286A -> 297A -0.16483
286A -> 298A 0.27060
288A -> 294A -0.13006
288A -> 305A -0.11041
291A -> 295A 0.22740
291A -> 306A -0.10550
292A -> 297A -0.14106
292A -> 298A 0.14780
293A -> 295A 0.17045
293A -> 297A 0.15247
293A -> 298A 0.16857
273B -> 293B 0.23119
277B -> 293B 0.15356
285B -> 297B -0.27161
286B -> 297B -0.12809
286B -> 298B -0.30383
288B -> 305B -0.10750
291B -> 297B 0.18812
292B -> 298B -0.19850

Excited State 19: 2.962-A 3.1795 eV 389.94 nm f=0.1231 <S**2>=1.944
289A -> 301A -0.15180
290A -> 302A 0.28930
291A -> 294A -0.23857
292A -> 295A -0.10465

292A -> 297A -0.13372
292A -> 298A -0.10484
293A -> 294A -0.38683
293A -> 297A 0.12246
293A -> 298A -0.16524
276B -> 293B 0.48246
278B -> 293B 0.10960
287B -> 298B -0.10371
288B -> 297B 0.10425
289B -> 301B 0.15348
290B -> 302B -0.29061
291B -> 298B -0.14179
292B -> 297B 0.15220

Excited State 20: 3.220-A 3.1836 eV 389.45 nm f=0.0653 <S**2>=2.341
284A -> 302A -0.11768
289A -> 301A -0.20778
290A -> 302A 0.45357
291A -> 294A 0.17984
292A -> 310A -0.12365
293A -> 294A 0.27168
293A -> 310A -0.13261
276B -> 293B -0.34115
284B -> 302B 0.11819
289B -> 301B 0.20697
290B -> 302B -0.45299
291B -> 310B -0.11246
292B -> 310B 0.15292

TTM-TCz (UB3LYP/6-31G(d))
Excited State 1: 2.060-A 1.4812 eV 837.07 nm f=0.0399 <S**2>=0.811
253B -> 258B -0.10277
257B -> 258B 0.99309
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -5958.50969794
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.058-A 1.6147 eV 767.87 nm f=0.0019 <S**2>=0.809
256B -> 258B 0.99884

Excited State 3: 2.056-A 1.9885 eV 623.51 nm f=0.0000 <S**2>=0.807
255B -> 258B 0.99497

Excited State 4:	2.056-A	1.9890 eV	623.36 nm	f=0.0000	<S**2>=0.807
254B -> 258B	0.99497				

Excited State 5:	2.090-A	2.2314 eV	555.63 nm	f=0.0658	<S**2>=0.842
254A -> 259A	-0.10019				
245B -> 258B	-0.12093				
248B -> 258B	-0.12355				
253B -> 258B	0.96009				
257B -> 258B	0.11121				

Excited State 6:	2.078-A	2.5508 eV	486.06 nm	f=0.0001	<S**2>=0.830
252B -> 258B	0.99230				

Excited State 7:	2.205-A	2.6412 eV	469.43 nm	f=0.0208	<S**2>=0.966
253A -> 260A	0.10383				
254A -> 260A	0.26689				
246B -> 258B	0.19854				
249B -> 258B	0.89157				

Excited State 8:	2.210-A	2.7783 eV	446.26 nm	f=0.0011	<S**2>=0.972
254A -> 259A	0.28678				
258A -> 259A	-0.12727				
245B -> 258B	0.38782				
248B -> 258B	0.78514				
253B -> 258B	0.20605				

Excited State 9:	2.098-A	2.9132 eV	425.59 nm	f=0.0060	<S**2>=0.850
254A -> 262A	-0.14346				
246B -> 258B	-0.11099				
247B -> 258B	0.95798				

Excited State 10:	2.175-A	2.9206 eV	424.52 nm	f=0.0021	<S**2>=0.933
254A -> 259A	0.28130				
258A -> 259A	-0.16509				
245B -> 258B	0.70848				
248B -> 258B	-0.55646				

Excited State 11:	2.132-A	2.9279 eV	423.45 nm	f=0.0017	<S**2>=0.886
254A -> 260A	0.20142				
244B -> 258B	0.23528				
246B -> 258B	0.86231				
247B -> 258B	0.10985				
249B -> 258B	-0.28727				

Excited State 12:	3.417-A	3.0359 eV	408.40 nm	f=0.0018	<S**2>=2.668
253A -> 261A	0.24305				
258A -> 261A	0.66565				
251B -> 258B	-0.10198				
253B -> 261B	-0.26324				
257B -> 261B	0.58768				
Excited State 13:	2.083-A	3.0382 eV	408.08 nm	f=0.0001	<S**2>=0.835
251B -> 258B	0.98976				
Excited State 14:	2.085-A	3.0434 eV	407.39 nm	f=0.0000	<S**2>=0.837
250B -> 258B	0.98831				
Excited State 15:	2.641-A	3.0852 eV	401.87 nm	f=0.1653	<S**2>=1.494
244A -> 259A	-0.13608				
253A -> 259A	0.11082				
254A -> 259A	-0.37079				
254A -> 270A	-0.11778				
258A -> 259A	0.53134				
241B -> 258B	-0.45145				
245B -> 258B	0.35538				
245B -> 259B	0.10142				
253B -> 259B	-0.11482				
257B -> 259B	0.12117				
Excited State 16:	3.444-A	3.1120 eV	398.41 nm	f=0.0000	<S**2>=2.715
252A -> 261A	0.50104				
253A -> 267A	-0.17031				
257A -> 259A	0.14246				
257A -> 261A	0.25066				
258A -> 267A	-0.22435				
240B -> 275B	0.12090				
244B -> 261B	0.10508				
250B -> 258B	-0.12130				
252B -> 259B	-0.10625				
252B -> 261B	-0.49512				
253B -> 267B	-0.18146				
256B -> 259B	-0.13677				
256B -> 261B	-0.24393				
257B -> 267B	0.20881				
Excited State 17:	3.475-A	3.1810 eV	389.76 nm	f=0.0000	<S**2>=2.768
250A -> 266A	-0.10574				
255A -> 265A	0.26706				

256A -> 265A -0.15427
256A -> 266A 0.49927
257A -> 273A -0.15049
257A -> 274A 0.10716
258A -> 274A -0.16621
250B -> 266B 0.10551
254B -> 265B -0.31470
254B -> 266B 0.19950
255B -> 265B 0.10107
255B -> 266B -0.46010
256B -> 272B 0.15438
257B -> 273B -0.17025

Excited State 18: 3.474-A 3.1812 eV 389.74 nm f=0.0000 <S**2>=2.767
250A -> 265A 0.10930
255A -> 265A -0.44485
255A -> 266A -0.29009
256A -> 265A -0.25462
256A -> 266A 0.10887
257A -> 273A 0.10123
257A -> 274A 0.14933
258A -> 273A 0.16928
250B -> 265B -0.10845
254B -> 265B 0.33534
254B -> 266B 0.33100
255B -> 265B 0.37231
256B -> 273B -0.15366
257B -> 272B 0.17194

Excited State 19: 2.515-A 3.2613 eV 380.17 nm f=0.0912 <S**2>=1.331
249A -> 260A 0.10473
254A -> 259A -0.12947
254A -> 270A 0.13043
258A -> 259A 0.51918
241B -> 258B 0.69724
245B -> 258B 0.23085

Excited State 20: 2.332-A 3.3049 eV 375.15 nm f=0.1447 <S**2>=1.109
247A -> 264A 0.10599
253A -> 260A 0.15806
254A -> 260A 0.66067
256A -> 260A 0.11644
258A -> 260A -0.46058
246B -> 258B -0.32283

249B -> 258B -0.27560