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Supporting information

A Luminescent Organic Radical with Two Pyridyl Groups: High Photostability, Dual Stimuli-Responsive Property, and Theoretical Analyses of Photophysical Processes

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Table S1. Selected angles in the crystal of bisPyTM

Angles	
C4C1C9	118.80(17)°
C4C1C15	120.13(17)°
C9C1C15	121.05(19)°
Dihedral angle between C4C9C15 plain and	
(3,5-dichloropyridyl including N1)	54.58°
(3,5-dichloropyridyl including N2)	40.07°
(2,4,6-trichlorophenyl)	50.07°

Table S2. Hyperfine coupling constants (hccs) used for ESR simulation and DFT-calculated values

hcc / mT	N	H
Sim.	0.108	0.108
Calcd.	0.1174	0.1341
	0.1174	0.1515
		0.1412

Table S3. Absolute photoluminescence quantum yield in various solvents

Solvent	ϕ (bisPyTM)
chloroform	1.2 %
dichloromethane	1.1 %
hexane	0.9 %
cyclohexane	0.9 %
acetonitrile	0.7 %
ethylacetate	0.7 %
acetone	0.5 %
diethyl ether	0.5 %
ethanol	0.4 %
methanol	0.4 %
tetrahydrofuran	0.3 %
toluene	0.2 %

Table S4. Crystallographic data of bisPyTM

Empirical formula	$C_{17}H_6Cl_7N_2$
Fw / g mol^{-1}	486.42
Crystal system	monoclinic
Space group	$P2_1/n$
Crystal size / mm	0.20×0.18×0.03
Temperature / K	113
a / Å	8.7015(13)
b / Å	14.840(3)
c / Å	14.860(3)
α / °	90
β / °	105.5165(15)
γ / °	90
V / Å^3	1848.9(5)
r_{calced} / g cm^{-3}	1.747
l / Å	0.7107
μ / mm^{-1}	1.077
Reflections collected	14405
Independent reflections	4208
Parameters	235
R_{int}	0.0226
$R1^a$	0.0344
$wR2^b$	0.0888
GoF^c	1.062

$^aR_1 = \Sigma||F^o|-|F^c||/\Sigma|F^o|$ ($I>2\sigma(I)$). $^bwR_2 = [\Sigma(w(F^{o2}-F^{c2})^2/\Sigma w(F^{o2})^2]^{1/2}$ ($I>2\sigma(I)$).
^{c}GoF = $[\Sigma(w(F^{o2}-F^{c2})^2/\Sigma(N^r-N^p)^2)$.

Table S5 Absorption coefficients (at 355 nm) and emission maximum wavelengths of bisPyTM in various solvents

Solvents	ε / $10^4 M^{-1}cm^{-1}$	λ_{em} / nm
chloroform	1.65	658
dichloromethane	1.78	650
hexane	1.85	652
cyclohexane	1.46	653
acetonitrile	2.19	673
ethylacetate	1.41	674
acetone	1.36	676
diethyl ether	1.76	659
ethanol	1.48	669
methanol	1.23	673
tetrahydrofuran	1.37	657
toluene	1.58	666

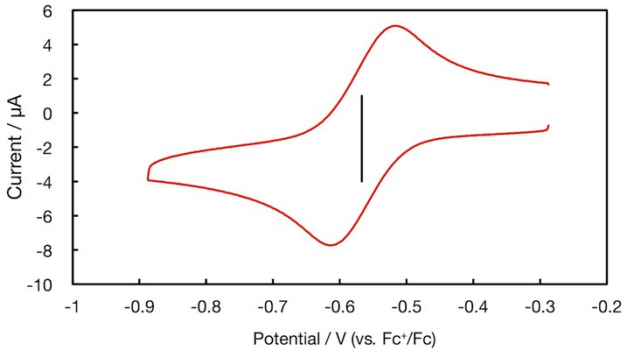


Figure S1. Cyclic voltammogram of bisPyTM.

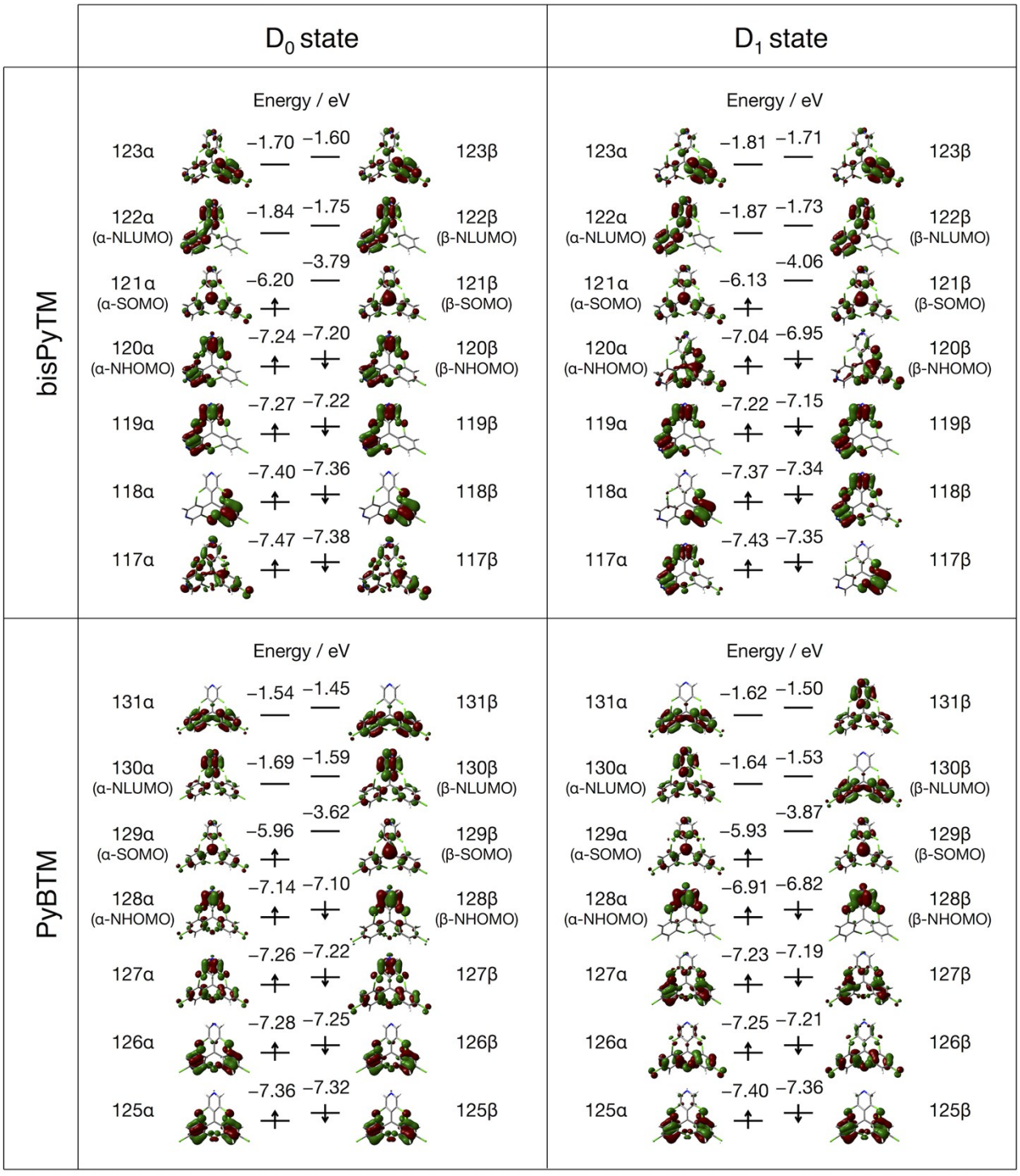


Figure S2. Molecular orbitals of bisPyTM and PyBTM in D_0 and D_1 states calculated using DFT (UB3LYP/6-31G(d,p) 6D 10F) in vacuum.

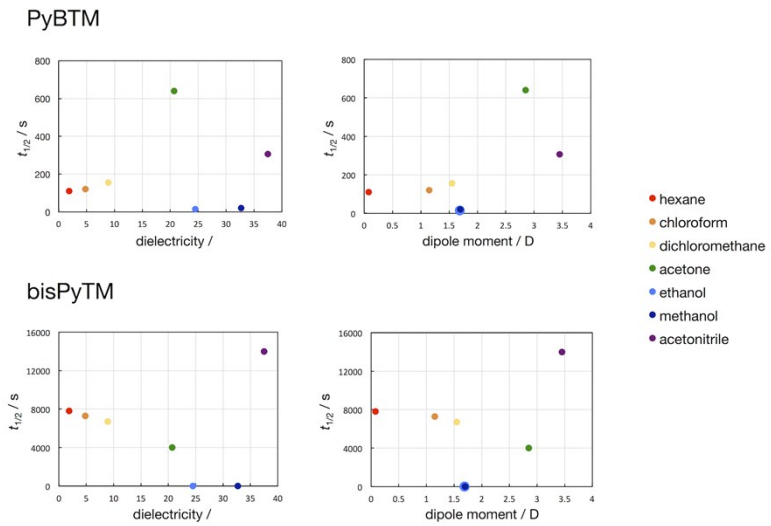


Figure S3. Relationship between photostability and solvent parameters.

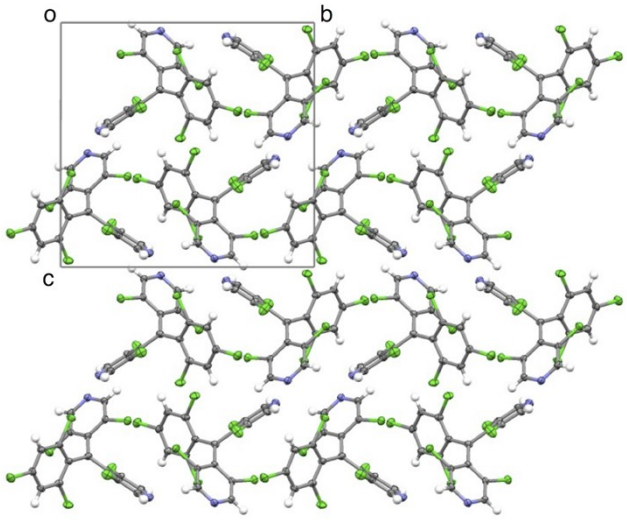


Figure S4. Crystal structure viewed along *a*-axis of bisPyTM with thermal ellipsoids set at 50% probability.

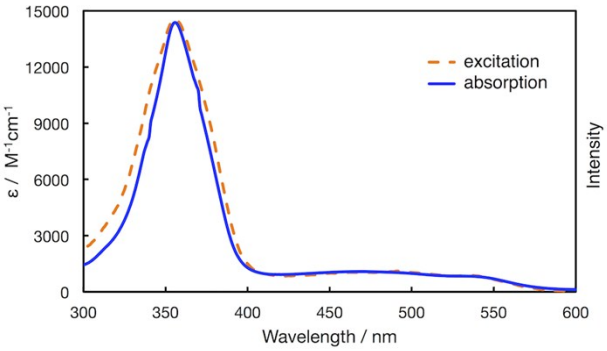


Figure S5. Excitation spectrum for emission wavelength at 650 nm and absorption spectrum of bisPyTM.

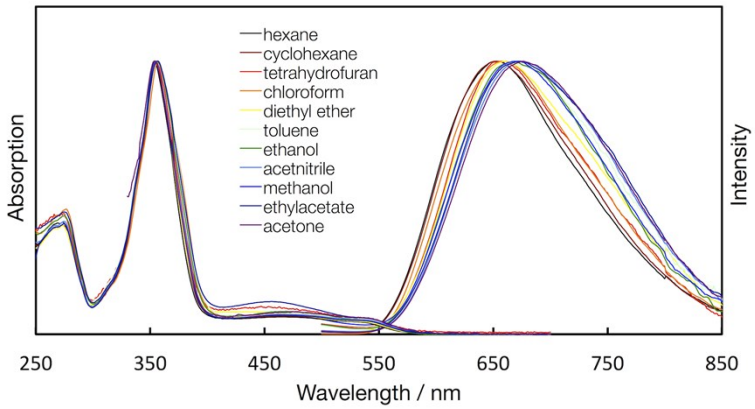


Figure S6. Absorption and emission spectra of bisPyTM in various solvents.

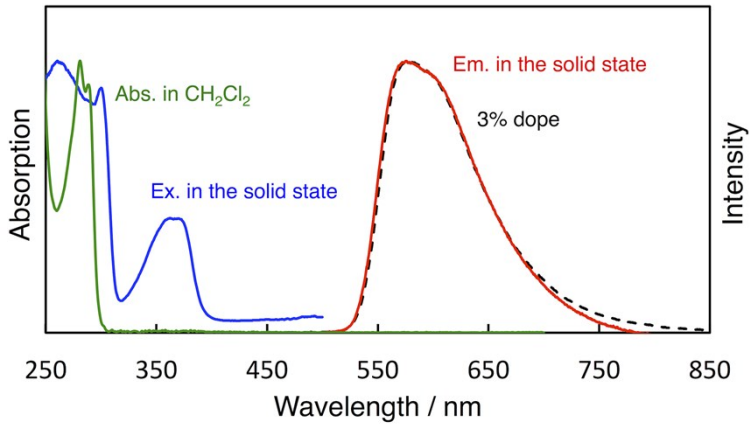
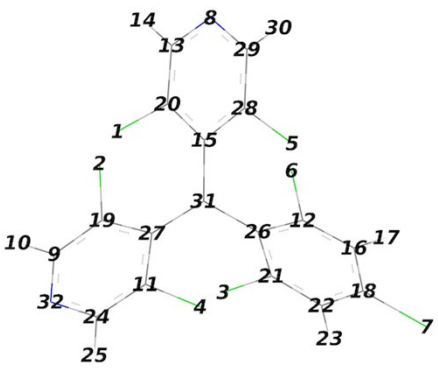
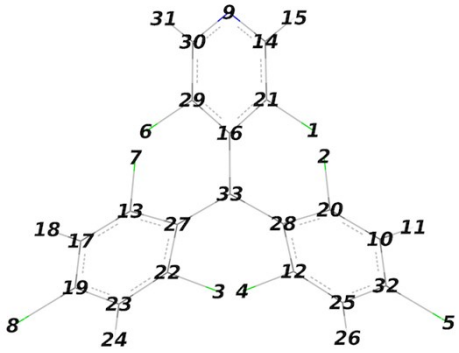


Figure S7.Emission (red) and excitation (blue) spectra of freshly prepared *αH*-bisPyTM crystals, and an absorption spectrum of freshly prepared *αH*-bisPyTM in dichloromethane. Black dashed line indicates the emission spectra of *αH*-bisPyTM crystals doped with 3 wt % of bisPyTM. We found that it was very difficult to prepare perfectly non-doped *αH*-bisPyTM crystals (= 0% doped crystal), because tiny amount of bisPyTM (< 0.2 wt %) was always contaminated in *αH*-bisPyTM. The freshly prepared *αH*-bisPyTM crystals displayed bisPyBTM-based emission while no emission from *αH*-bisPyTM was observed.

Simulated bond lengths, bond angles, dihedral angles of bisPyTM and PyBTM by DFT calculations

The numbers representing the atoms of bisPyTM (left) and PyBTM(right) in DFT calculations.





Bond lengths of bisPyTM

atoms	D_0 state	D_1 state
1,20	1.7514	1.7571
2,19	1.7514	1.7572
3,21	1.7539	1.7351
4,11	1.7513	1.7555
5,28	1.7513	1.7554
6,12	1.7539	1.7351
7,18	1.7488	1.7289
8,13	1.3347	1.3399
8,29	1.3346	1.3361
9,10	1.0861	1.0866
9,19	1.3936	1.3898
9,32	1.3347	1.3399
11,24	1.3939	1.3899
11,27	1.4156	1.4254
12,16	1.3903	1.3787
12,26	1.4188	1.4551
13,14	1.0861	1.0866
13,20	1.3936	1.3898
15,20	1.4155	1.4262
15,28	1.4156	1.4254

15,31	1.4751	1.4458
16,17	1.0822	1.0824
16,18	1.3913	1.4041
18,22	1.3913	1.4041
19,27	1.4155	1.4263
21,22	1.3903	1.3788
21,26	1.4188	1.4552
22,23	1.0822	1.0824
24,25	1.0861	1.0864
24,32	1.3346	1.3361
26,31	1.4735	1.4711
27,31	1.4751	1.4457
28,29	1.3939	1.3898
29,30	1.0861	1.0864

Bond angles of bisPyTM

atoms	D_0 state	D_1 state
13,8,29	117.5422	116.5374
10,9,19	119.5589	119.0583
10,9,32	117.414	116.9434
19,9,32	123.0237	123.9718
4,11,24	116.5756	117.1808
4,11,27	122.065	119.3982
24,11,27	121.2746	123.3693
6,12,16	115.8007	117.5346
6,12,26	120.9253	119.1123
16,12,26	123.1749	123.3415
8,13,14	117.414	116.9446
8,13,20	123.0237	123.9699
14,13,20	119.5589	119.059
20,15,28	113.7557	111.3281
20,15,31	123.1485	125.3255
28,15,31	123.0957	123.2739
12,16,17	120.2483	120.5069
12,16,18	118.8017	119.0545
17,16,18	120.9385	120.4003
7,18,16	119.4406	119.3073

7,18,22	119.4406	119.3149
16,18,22	121.1189	121.3779
2,19,9	116.6502	116.1935
2,19,27	121.9322	121.5757
9,19,27	121.3319	122.05
1,20,13	116.6502	116.1968
1,20,15	121.9322	121.5747
13,20,15	121.3319	122.048
3,21,22	115.8007	117.5397
3,21,26	120.9253	119.1056
22,21,26	123.1749	123.3431
18,22,21	118.8017	119.0495
18,22,23	120.9386	120.3989
21,22,23	120.2483	120.5131
11,24,25	119.5224	119.7505
11,24,32	123.071	122.7214
25,24,32	117.4032	117.4994
12,26,21	114.9276	113.7437
12,26,31	122.5362	123.125
21,26,31	122.5362	123.1314
11,27,19	113.7557	111.3231
11,27,31	123.0958	123.2773
19,27,31	123.1485	125.3274
5,28,15	122.065	119.3987
5,28,29	116.5756	117.1825
15,28,29	121.2746	123.3673
8,29,28	123.071	122.7203
8,29,30	117.4032	117.5005
28,29,30	119.5224	119.7506
15,31,26	120.1366	118.8764
15,31,27	119.7268	122.2297
26,31,27	120.1366	118.8939
9,32,24	117.5422	116.5352

Dihedral angles of bisPyTM

atoms	D_0 state	D_1 state

29,8,13,14	-179.4666	-177.7671
29,8,13,20	-0.1403	0.338
13,8,29,28	-0.1432	-1.7025
13,8,29,30	-179.4771	-179.7492
10,9,19,2	2.9212	3.8673
10,9,19,27	179.6166	179.0514
32,9,19,2	-176.3914	-174.1991
32,9,19,27	0.304	0.985
10,9,32,24	-179.4666	-177.759
19,9,32,24	-0.1402	0.345
4,11,24,25	2.8723	2.4777
4,11,24,32	-176.4482	-175.5243
27,11,24,25	179.5893	179.842
27,11,24,32	0.2688	1.8399
4,11,27,19	176.4349	176.8491
4,11,27,31	-3.5193	-6.0955
24,11,27,19	-0.1003	-0.4597
24,11,27,31	179.9456	176.5957
6,12,16,17	2.5462	1.8617
6,12,16,18	-176.2348	-175.8975
26,12,16,17	178.9512	-179.3884
26,12,16,18	0.1702	2.8525
6,12,26,21	176.1401	177.2594
6,12,26,31	-3.8599	-2.7539
16,12,26,21	-0.0867	-1.4718
16,12,26,31	179.9134	178.5149
8,13,20,1	-176.3914	-174.2048
8,13,20,15	0.3041	0.9824
14,13,20,1	2.9211	3.8628
14,13,20,15	179.6166	179.0499
28,15,20,1	176.3522	174.0803
28,15,20,13	-0.1674	-0.8502
31,15,20,1	-3.6936	-2.8975
31,15,20,13	179.7867	-177.828
20,15,28,5	176.4347	176.8426
20,15,28,29	-0.1003	-0.4696
31,15,28,5	-3.5195	-6.1066
31,15,28,29	179.9455	176.5813
20,15,31,26	131.669	140.103
20,15,31,27	-48.331	-39.8931

28,15,31,26	-48.3811	-36.5294
28,15,31,27	131.6189	143.4745
12,16,18,7	179.9181	178.6288
12,16,18,22	-0.0819	-1.3764
17,16,18,7	1.1459	0.8672
17,16,18,22	-178.8542	-179.138
7,18,22,21	179.9182	178.5915
7,18,22,23	1.1459	0.8377
16,18,22,21	-0.0818	-1.4034
16,18,22,23	-178.8541	-179.1572
2,19,27,11	176.3521	174.0665
2,19,27,31	-3.6937	-2.9161
9,19,27,11	-0.1675	-0.8606
9,19,27,31	179.7867	-177.8432
3,21,22,18	-176.2347	-175.8938
3,21,22,23	2.5463	1.8574
26,21,22,18	0.1703	2.854
26,21,22,23	178.9513	-179.3948
3,21,26,12	176.1399	177.2786
3,21,26,31	-3.8602	-2.7081
22,21,26,12	-0.0869	-1.4506
22,21,26,31	179.9131	178.5627
11,24,32,9	-0.1432	-1.7101
25,24,32,9	-179.4772	-179.7546
12,26,31,15	-49.573	-53.3534
12,26,31,27	130.427	126.6429
21,26,31,15	130.427	126.6321
21,26,31,27	-49.573	-53.3717
11,27,31,15	131.619	143.5156
11,27,31,26	-48.381	-36.4805
19,27,31,15	-48.3309	-39.847
19,27,31,26	131.6691	140.1569
5,28,29,8	-176.448	-175.5265
5,28,29,30	2.8724	2.4779
15,28,29,8	0.2689	1.8411
15,28,29,30	179.5893	179.8455

Bond lengths of PyBTM

atoms	D_0 state	D_1 state
1,21	1.7524	1.7564
2,20	1.755	1.7508
3,22	1.7549	1.7434
4,12	1.7549	1.7432
5,32	1.7497	1.7414
6,29	1.7524	1.7565
7,13	1.755	1.751
8,19	1.7497	1.7416
9,14	1.3349	1.3377
9,30	1.3349	1.3377
10,11	1.0822	1.0827
10,20	1.3904	1.3821
10,32	1.391	1.4039
12,25	1.3906	1.3845
12,28	1.419	1.4488
13,17	1.3904	1.3822
13,27	1.419	1.4395
14,15	1.0861	1.0865
14,21	1.3935	1.3912
16,21	1.4161	1.4231
16,29	1.4161	1.4231
16,33	1.4748	1.4518
17,18	1.0822	1.0827
17,19	1.391	1.4037
19,23	1.391	1.3943
20,28	1.419	1.4397
22,23	1.3906	1.3846
22,27	1.419	1.4484
23,24	1.0822	1.0824
25,26	1.0822	1.0824
25,32	1.391	1.3944
27,33	1.4742	1.4528
28,33	1.4742	1.4529
29,30	1.3935	1.3912
30,31	1.0861	1.0865

Bond angles of PyBTM

atoms	D_0 state	D_1 state
14,9,30	117.4339	116.6356
11,10,20	120.2562	120.1064
11,10,32	120.9445	120.2138
20,10,32	118.7873	119.6338
4,12,25	115.6145	116.8936
4,12,28	121.0434	118.7205
25,12,28	123.2453	124.3776
7,13,17	115.6684	116.1163
7,13,27	120.9337	120.2724
17,13,27	123.3007	123.4702
9,14,15	117.384	117.2314
9,14,21	123.0882	123.284
15,14,21	119.5239	119.4522
21,16,29	113.5613	111.6574
21,16,33	123.2192	124.1593
29,16,33	123.2195	124.1833
13,17,18	120.2561	120.1024
13,17,19	118.7881	119.6333
18,17,19	120.9438	120.2184
8,19,17	119.4581	119.3418
8,19,23	119.4709	119.8576
17,19,23	121.071	120.8003
2,20,10	115.6693	116.1379
2,20,28	120.9323	120.2564
10,20,28	123.3011	123.465
1,21,14	116.4665	116.694
1,21,16	122.0318	120.6135
14,21,16	121.4135	122.5626
3,22,23	115.6137	116.8768
3,22,27	121.0435	118.7251
23,22,27	123.2459	124.3896
19,23,22	118.832	118.5631
19,23,24	120.9252	120.91
22,23,24	120.2313	120.4713
12,25,26	120.2314	120.4724
12,25,32	118.8321	118.5664

26,25,32	120.9249	120.9056
13,27,22	114.7617	113.0758
13,27,33	122.6058	124.2907
22,27,33	122.6325	122.6254
12,28,20	114.7623	113.081
12,28,33	122.6333	122.6278
20,28,33	122.6044	124.2833
6,29,16	122.0317	120.6337
6,29,30	116.4664	116.685
16,29,30	121.4137	122.551
9,30,29	123.0881	123.2952
9,30,31	117.3843	117.2265
29,30,31	119.5239	119.4461
5,32,10	119.4579	119.338
5,32,25	119.4708	119.8546
10,32,25	121.0713	120.8072
16,33,27	119.8666	119.6496
16,33,28	119.8634	119.6268
27,33,28	120.2699	120.7236

Dihedral angles of PyBTM

atoms	D_0 state	D_1 state
30,9,14,15	-179.4589	-178.4924
30,9,14,21	-0.1735	-0.578
14,9,30,29	-0.1733	-0.5613
14,9,30,31	-179.4591	-178.4814
11,10,20,2	2.567	3.0852
11,10,20,28	179.0048	178.7742
32,10,20,2	-176.1869	-174.4541
32,10,20,28	0.251	1.2349
11,10,32,5	1.1236	1.8887
11,10,32,25	-178.8539	-177.9453
20,10,32,5	179.8686	179.4253
20,10,32,25	-0.1089	-0.4086
4,12,25,26	2.5325	1.5938
4,12,25,32	-176.2416	-175.7185
28,12,25,26	178.9818	-179.4697
28,12,25,32	0.2076	3.218

4,12,28,20	176.1871	176.5639
4,12,28,33	-3.833	-4.4177
25,12,28,20	-0.0756	-2.3546
25,12,28,33	179.9043	176.6638
7,13,17,18	2.564	3.0936
7,13,17,19	-176.1894	-174.4471
27,13,17,18	179.0027	178.7769
27,13,17,19	0.2492	1.2362
7,13,27,22	176.1059	175.5412
7,13,27,33	-3.8689	-3.4502
17,13,27,22	-0.1517	0.0295
17,13,27,33	179.8736	-178.9619
9,14,21,1	-176.3004	-174.7019
9,14,21,16	0.3507	1.1723
15,14,21,1	2.9703	3.1684
15,14,21,16	179.6214	179.0427
29,16,21,1	176.3	175.1725
29,16,21,14	-0.1634	-0.5443
33,16,21,1	-3.6995	-4.8358
33,16,21,14	179.837	179.4474
21,16,29,6	176.3007	175.1639
21,16,29,30	-0.1644	-0.548
33,16,29,6	-3.6997	-4.8278
33,16,29,30	179.8352	179.4602
21,16,33,27	132.0363	139.1278
21,16,33,28	-47.9612	-40.8602
29,16,33,27	-47.9632	-40.8815
29,16,33,28	132.0392	139.1305
13,17,19,8	179.8664	179.4498
13,17,19,23	-0.1121	-0.3797
18,17,19,8	1.1218	1.912
18,17,19,23	-178.8567	-177.9176
8,19,23,22	179.9134	178.4357
8,19,23,24	1.1477	1.1345
17,19,23,22	-0.1081	-1.7356
17,19,23,24	-178.8738	-179.0368
2,20,28,12	176.0987	175.5891
2,20,28,33	-3.8813	-3.4104
10,20,28,12	-0.1581	0.0699
10,20,28,33	179.862	-178.9296

3,22,23,19	-176.2398	-175.7382
3,22,23,24	2.5347	1.5752
27,22,23,19	0.2097	3.188
27,22,23,24	178.9842	-179.4986
3,22,27,13	176.1808	176.6088
3,22,27,33	-3.8445	-4.3806
23,22,27,13	-0.0822	-2.299
23,22,27,33	179.8925	176.7116
12,25,32,5	179.9113	178.4456
12,25,32,10	-0.1112	-1.7213
26,25,32,5	1.1459	1.1454
26,25,32,10	-178.8766	-179.0215
13,27,33,16	-49.1887	-45.3428
13,27,33,28	130.8089	134.6451
22,27,33,16	130.8386	135.759
22,27,33,28	-49.1639	-44.2531
12,28,33,16	130.8226	135.6133
12,28,33,27	-49.1749	-44.3746
20,28,33,16	-49.199	-45.4796
20,28,33,27	130.8035	134.5325
6,29,30,9	-176.3016	-174.7052
6,29,30,31	2.9696	3.171
16,29,30,9	0.3511	1.1656
16,29,30,31	179.6223	179.0418

Cartesian coordinates of all the optimized geometries by DFT calculations

bisPyTM (UB3LYP/6-31G(d,p)6D10F) (ground state in a vacuum)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-2.696032	0.408861	-2.130627
2	17	0	-2.696064	-0.408591	2.130612
3	17	0	1.061614	-1.708106	2.174670
4	17	0	0.383585	-2.215729	-2.118028
5	17	0	0.383784	2.215709	2.118014
6	17	0	1.061750	1.708038	-2.174707
7	17	0	5.663014	-0.000244	-0.000039
8	7	0	-2.572571	3.747861	-0.014990
9	6	0	-2.884769	-2.763083	0.858596
10	1	0	-3.699737	-2.941457	1.554380
11	6	0	-0.840922	-2.345100	-0.873454
12	6	0	1.839139	0.772131	-0.913663
13	6	0	-2.884525	2.763368	-0.858605
14	1	0	-3.699478	2.941817	-1.554387
15	6	0	-1.137068	1.275768	-0.005725
16	6	0	3.229684	0.782666	-0.923148
17	1	0	3.763933	1.377186	-1.652791
18	6	0	3.915432	-0.000165	-0.000031
19	6	0	-2.209573	-1.544027	0.890248
20	6	0	-2.209437	1.544252	-0.890263
21	6	0	1.839076	-0.772270	0.913619
22	6	0	3.229620	-0.782932	0.923092
23	1	0	3.763822	-1.377502	1.652730
24	6	0	-1.565856	-3.535234	-0.832774
25	1	0	-1.319234	-4.335320	-1.524991
26	6	0	1.076290	-0.000035	-0.000019
27	6	0	-1.137181	-1.275641	0.005708
28	6	0	-0.840711	2.345195	0.873440
29	6	0	-1.565539	3.535395	0.832765
30	1	0	-1.318846	4.335457	1.524986
31	6	0	-0.397403	0.000030	-0.000013
32	7	0	-2.572906	-3.747607	0.014984

bisPyTM (UB3LYP/6-31g(d,p)6D10F) (lowest excited state in a vacuum)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-3.071063	0.434461	-1.822878
2	17	0	-3.068518	-0.436003	1.825509
3	17	0	0.986700	-1.662866	2.196163
4	17	0	0.680250	-2.215920	-1.832105
5	17	0	0.681189	2.218308	1.829174
6	17	0	0.987958	1.664487	-2.194173
7	17	0	5.591163	-0.001935	0.000276
8	7	0	-2.460120	3.861185	0.064849
9	6	0	-2.942309	-2.838549	0.649190
10	1	0	-3.830238	-3.031605	1.245080
11	6	0	-0.712669	-2.391558	-0.776562
12	6	0	1.788110	0.759004	-0.950370
13	6	0	-2.943907	2.837822	-0.648668
14	1	0	-3.832404	3.030168	-1.243943
15	6	0	-1.177496	1.265978	0.036352
16	6	0	3.168770	0.784192	-0.935328
17	1	0	3.712767	1.375444	-1.660953
18	6	0	3.856783	-0.000859	0.000309
19	6	0	-2.356491	-1.577633	0.701652
20	6	0	-2.358032	1.576922	-0.700540
21	6	0	1.787391	-0.758710	0.951578
22	6	0	3.167962	-0.785138	0.936262
23	1	0	3.711558	-1.376765	1.661887
24	6	0	-1.341053	-3.631781	-0.756675
25	1	0	-0.940360	-4.450544	-1.348118
26	6	0	0.991589	0.000318	0.000581
27	6	0	-1.177032	-1.265810	-0.036452
28	6	0	-0.712622	2.392756	0.774812
29	6	0	-1.341178	3.632930	0.754346
30	1	0	-0.939935	4.452315	1.344560
31	6	0	-0.479161	0.000342	0.000130
32	7	0	-2.459101	-3.860970	-0.065959

bisPyTM (UB3LYP/6-31g(d,p)6D10F) (ground state in dichloromethane)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-2.688146	0.409536	-2.136257
2	17	0	-2.688168	-0.409271	2.136247
3	17	0	1.059438	-1.704346	2.177615
4	17	0	0.377408	-2.211042	-2.123315
5	17	0	0.377614	2.211029	2.123289
6	17	0	1.059578	1.704282	-2.177648
7	17	0	5.663184	-0.000247	-0.000037
8	7	0	-2.573438	3.746971	-0.015843
9	6	0	-2.883824	-2.762855	0.862850
10	1	0	-3.696690	-2.941383	1.560652
11	6	0	-0.843899	-2.343853	-0.875142
12	6	0	1.840323	0.771137	-0.914317
13	6	0	-2.883584	2.763138	-0.862857
14	1	0	-3.696439	2.941738	-1.560654
15	6	0	-1.136843	1.275730	-0.006233
16	6	0	3.230539	0.782412	-0.925033
17	1	0	3.765296	1.375781	-1.655196
18	6	0	3.914349	-0.000165	-0.000029
19	6	0	-2.206995	-1.545046	0.892850
20	6	0	-2.206864	1.545268	-0.892863
21	6	0	1.840260	-0.771275	0.914277
22	6	0	3.230475	-0.782679	0.924982
23	1	0	3.765182	-1.376097	1.655141
24	6	0	-1.568116	-3.534139	-0.835466
25	1	0	-1.323412	-4.332872	-1.529513
26	6	0	1.077217	-0.000035	-0.000018
27	6	0	-1.136956	-1.275604	0.006213
28	6	0	-0.843686	2.343952	0.875123
29	6	0	-1.567798	3.534302	0.835451
30	1	0	-1.323018	4.333013	1.529499
31	6	0	-0.396323	0.000030	-0.000013
32	7	0	-2.573771	-3.746718	0.015834

bisPyTM (UB3LYP/6-31g(d,p)6D10F) (lowest excited state in dichloromethane)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-3.064091	0.434579	-1.827730
2	17	0	-3.064901	-0.434111	1.826986
3	17	0	0.984853	-1.652568	2.203053
4	17	0	0.683015	-2.217731	-1.831467
5	17	0	0.682526	2.216036	1.832963
6	17	0	0.983879	1.651680	-2.203801
7	17	0	5.585826	0.001844	0.000160
8	7	0	-2.464759	3.858151	0.074734
9	6	0	-2.946369	-2.834494	0.644108
10	1	0	-3.836556	-3.024508	1.237541
11	6	0	-0.712704	-2.391331	-0.781007
12	6	0	1.790893	0.756281	-0.955721
13	6	0	-2.945243	2.834820	-0.644482
14	1	0	-3.835074	3.025284	-1.238303
15	6	0	-1.173442	1.265095	0.038254
16	6	0	3.169274	0.783119	-0.941647
17	1	0	3.714901	1.370127	-1.669243
18	6	0	3.856967	0.000739	-0.000068
19	6	0	-2.354267	-1.578305	0.698520
20	6	0	-2.353573	1.578404	-0.698839
21	6	0	1.791441	-0.756466	0.955262
22	6	0	3.169901	-0.782337	0.941278
23	1	0	3.715994	-1.368996	1.668815
24	6	0	-1.345132	-3.628854	-0.764836
25	1	0	-0.944021	-4.447040	-1.356443
26	6	0	0.995896	-0.000257	-0.000203
27	6	0	-1.173656	-1.265503	-0.038085
28	6	0	-0.712511	2.390473	0.781765
29	6	0	-1.344459	3.628238	0.765537
30	1	0	-0.943378	4.446131	1.357580
31	6	0	-0.475177	-0.000330	0.000017
32	7	0	-2.465931	-3.858182	-0.074672

PyBTM (UB3LYP/6-31g(d,p)6D10F) (ground state in a vacuum)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	1.801933	1.890771	2.111356
2	17	0	2.125382	1.140738	-2.162530
3	17	0	-0.410804	-1.866068	-2.155860
4	17	0	0.411772	-1.864619	2.156862
5	17	0	5.259212	-2.648701	-0.009520
6	17	0	-1.803179	1.888491	-2.112487
7	17	0	-2.126177	1.140696	2.161848
8	17	0	-5.257781	-2.651792	0.010967
9	7	0	-0.001467	4.704812	-0.001365
10	6	0	3.540167	-0.750260	-0.921150
11	1	0	4.301794	-0.493146	-1.645770
12	6	0	1.553671	-1.423794	0.901700
13	6	0	-2.328244	-0.069368	0.909656
14	6	0	0.769780	4.012221	0.837616
15	1	0	1.390689	4.577912	1.526565
16	6	0	-0.000612	1.843285	-0.000550
17	6	0	-3.539852	-0.751830	0.921532
18	1	0	-4.301629	-0.494758	1.646007
19	6	0	-3.741747	-1.781060	0.007960
20	6	0	2.328158	-0.068504	-0.909657
21	6	0	0.798830	2.619159	0.874025
22	6	0	-1.552962	-1.425216	-0.900944
23	6	0	-2.753651	-2.127151	-0.907708
24	1	0	-2.917982	-2.915832	-1.630355
25	6	0	2.754773	-2.125018	0.908858
26	1	0	2.919567	-2.913198	1.631947
27	6	0	-1.277935	-0.366252	0.002694
28	6	0	1.278022	-0.365498	-0.002531
29	6	0	-0.800516	2.618182	-0.875568
30	6	0	-0.772298	4.011283	-0.839952
31	1	0	-1.393545	4.576209	-1.529223
32	6	0	3.742667	-1.778859	-0.007002
33	6	0	-0.000173	0.368889	-0.000127

PyBTM (UB3LYP/6-31g(d,p)6D10F) (lowest excited state in a vacuum)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	2.148695	2.014049	1.736237
2	17	0	2.239144	1.181851	-2.057398
3	17	0	-0.328022	-1.797492	-2.195099
4	17	0	0.328296	-1.796926	2.195400
5	17	0	5.151003	-2.810963	0.053730
6	17	0	-2.147954	2.013966	-1.736747
7	17	0	-2.239455	1.182692	2.056489
8	17	0	-5.150940	-2.810854	-0.053709
9	7	0	-0.000361	4.791582	0.000450
10	6	0	3.538016	-0.806435	-0.838227
11	1	0	4.323726	-0.566834	-1.542970
12	6	0	1.497599	-1.408964	0.943696
13	6	0	-2.353187	-0.077434	0.834368
14	6	0	0.920634	4.088098	0.650262
15	1	0	1.598802	4.631932	1.301896
16	6	0	0.000133	1.839628	0.000018
17	6	0	-3.538118	-0.805998	0.837812
18	1	0	-4.323945	-0.566125	1.542333
19	6	0	-3.676264	-1.864682	-0.052206
20	6	0	2.353102	-0.077840	-0.834821
21	6	0	0.981212	2.672189	0.644678
22	6	0	-1.497395	-1.409141	-0.943597
23	6	0	-2.657418	-2.175901	-0.947868
24	1	0	-2.773193	-2.983069	-1.659729
25	6	0	2.657620	-2.175739	0.948071
26	1	0	2.773489	-2.982682	1.660169
27	6	0	-1.262232	-0.330448	-0.046057
28	6	0	1.262359	-0.330548	0.045891
29	6	0	-0.981085	2.672170	-0.644639
30	6	0	-0.921134	4.088136	-0.649597
31	1	0	-1.599548	4.631997	-1.300953
32	6	0	3.676309	-1.864805	0.052151
33	6	0	0.000072	0.421575	-0.000033

PyBTM (UB3LYP/6-31g(d,p)6D10F) (ground state in dichloromethane)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	1.790843	1.888710	2.120152
2	17	0	2.121719	1.141060	-2.164530
3	17	0	-0.411461	-1.864014	-2.157363
4	17	0	0.412367	-1.862435	2.158344
5	17	0	5.259749	-2.648217	-0.012761
6	17	0	-1.792062	1.886800	-2.121279
7	17	0	-2.122902	1.141466	2.163349
8	17	0	-5.258179	-2.651721	0.014484
9	7	0	-0.001332	4.704753	-0.001229
10	6	0	3.540727	-0.749419	-0.923784
11	1	0	4.302114	-0.492667	-1.648726
12	6	0	1.555356	-1.423806	0.901051
13	6	0	-2.328628	-0.069603	0.910006
14	6	0	0.767184	4.012001	0.842172
15	1	0	1.385130	4.577085	1.533917
16	6	0	-0.000593	1.842986	-0.000560
17	6	0	-3.540508	-0.750994	0.924039
18	1	0	-4.302080	-0.494239	1.648784
19	6	0	-3.740966	-1.780193	0.009955
20	6	0	2.328366	-0.068874	-0.910251
21	6	0	0.794500	2.619207	0.877325
22	6	0	-1.554693	-1.425321	-0.900318
23	6	0	-2.754722	-2.127962	-0.907234
24	1	0	-2.919982	-2.917018	-1.629232
25	6	0	2.755880	-2.125598	0.908490
26	1	0	2.921684	-2.914023	1.631052
27	6	0	-1.278461	-0.366287	0.002907
28	6	0	1.278431	-0.365584	-0.002903
29	6	0	-0.796079	2.618388	-0.878812
30	6	0	-0.769487	4.011211	-0.844309
31	1	0	-1.387731	4.575650	-1.536314
32	6	0	3.741903	-1.777785	-0.008922
33	6	0	-0.000225	0.368168	-0.000203

PyBTM (UB3LYP/6-31g(d,p)6D10F) (lowest excited state in dichloromethane)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	1.999562	1.902810	1.911835
2	17	0	2.250830	1.280610	-2.029010
3	17	0	-0.278280	-1.936059	-2.002002
4	17	0	0.281118	-1.932035	2.006460
5	17	0	5.203686	-2.716446	-0.007936
6	17	0	-1.999932	1.905591	-1.911698
7	17	0	-2.253740	1.282587	2.026003
8	17	0	-5.204467	-2.716346	0.005617
9	7	0	0.000749	4.740943	0.001162
10	6	0	3.569697	-0.705911	-0.836590
11	1	0	4.370844	-0.426350	-1.509030
12	6	0	1.507403	-1.466035	0.858556
13	6	0	-2.384146	0.003223	0.837629
14	6	0	0.866029	4.037940	0.740343
15	1	0	1.556907	4.598259	1.364179
16	6	0	-0.000168	1.848439	0.000217
17	6	0	-3.570964	-0.705249	0.834081
18	1	0	-4.372821	-0.424740	1.505276
19	6	0	-3.710945	-1.820578	-0.006566
20	6	0	2.383031	0.002559	-0.839664
21	6	0	0.887701	2.647285	0.774028
22	6	0	-1.506406	-1.467589	-0.856737
23	6	0	-2.669807	-2.218276	-0.844383
24	1	0	-2.781331	-3.068766	-1.504624
25	6	0	2.670653	-2.216783	0.845426
26	1	0	2.783177	-3.066347	1.506690
27	6	0	-1.262919	-0.321957	-0.004573
28	6	0	1.262621	-0.321682	0.004377
29	6	0	-0.887543	2.648229	-0.773190
30	6	0	-0.864850	4.038844	-0.738555
31	1	0	-1.555328	4.599998	-1.362085
32	6	0	3.710600	-1.820381	0.005396
33	6	0	-0.000274	0.396652	-0.000083

Abstracted results of TDDFT calculations

bisPyTM (UB3LYP/6-31g(d,p)6D10F) (ground state in a vacuum)

121A is SOMO.

Excited State 1:	2.124-A	2.5067 eV	494.62 nm	f=0.0066	<S**2>=0.878
121A ->123A	0.12819				
117B ->121B	0.31417				
120B ->121B	0.91989				
Excited State 2:	2.112-A	2.5690 eV	482.62 nm	f=0.0055	<S**2>=0.865
119B ->121B	0.97802				
Excited State 3:	2.150-A	2.6601 eV	466.08 nm	f=0.0254	<S**2>=0.906
121A ->123A	0.18501				
117B ->121B	0.89008				
120B ->121B	-0.34783				
Excited State 4:	2.102-A	2.7100 eV	457.50 nm	f=0.0045	<S**2>=0.855
114B ->121B	-0.14851				
116B ->121B	0.15332				
118B ->121B	0.95182				
Excited State 5:	2.216-A	2.8628 eV	433.09 nm	f=0.0063	<S**2>=0.978
121A ->122A	0.28465				
114B ->121B	-0.42476				
116B ->121B	0.77007				
118B ->121B	-0.24718				
Excited State 6:	2.251-A	2.9908 eV	414.55 nm	f=0.0021	<S**2>=1.017
121A ->123A	0.14848				
115B ->121B	0.93311				
116B ->122B	0.16639				
117B ->121B	-0.11239				
Excited State 7:	2.277-A	3.0197 eV	410.58 nm	f=0.0006	<S**2>=1.046
121A ->122A	-0.24035				
114B ->121B	0.73168				
115B ->122B	0.15702				
116B ->121B	0.54354				

Excited State 8:	2.462-A	3.2475 eV	381.78 nm	f=0.0028	<S**2>=1.266
114A ->122A	0.15970				
116A ->122A	-0.11176				
117A ->123A	-0.11575				
119A ->125A	-0.13661				
120A ->126A	0.14474				
121A ->123A	-0.21377				
121A ->128A	-0.19551				
112B ->121B	-0.11507				
113B ->121B	0.80622				
114B ->122B	0.12197				
116B ->122B	-0.10664				
119B ->125B	-0.14342				
120B ->126B	0.14685				

Excited State 9:	2.685-A	3.4234 eV	362.16 nm	f=0.1105	<S**2>=1.552
117A ->123A	-0.13762				
118A ->124A	-0.25637				
118A ->125A	0.14748				
121A ->123A	0.72115				
113B ->121B	0.18342				
115B ->121B	-0.22144				
115B ->123B	0.12151				
117B ->121B	-0.24510				
117B ->123B	0.22356				
118B ->124B	-0.21414				
118B ->125B	0.12644				
120B ->123B	0.11407				

Excited State 10:	2.214-A	3.4554 eV	358.81 nm	f=0.1086	<S**2>=0.976
119A ->126A	0.11797				
121A ->122A	0.82180				
114B ->121B	0.45149				
116B ->121B	-0.15078				

bisPyTM (UB3LYP/6-31g(d,p)6D10F) (lowest excited state in a vacuum)

121A is SOMO.

Excited State	1:	2.085-A	1.9718 eV	628.80 nm	f=0.0189	<S**2>=0.837
121A ->123A		0.12597				
120B ->121B		0.97920				
Excited State	2:	2.087-A	2.2380 eV	554.00 nm	f=0.0068	<S**2>=0.839
119B ->121B		0.98141				
Excited State	3:	2.106-A	2.4217 eV	511.96 nm	f=0.0184	<S**2>=0.859
118B ->121B		0.97613				
Excited State	4:	2.086-A	2.4400 eV	508.14 nm	f=0.0048	<S**2>=0.838
121A ->122A		-0.12448				
114B ->121B		0.15308				
116B ->121B		0.21081				
117B ->121B		0.93743				
119B ->121B		0.11038				
Excited State	5:	2.146-A	2.6641 eV	465.39 nm	f=0.0111	<S**2>=0.901
121A ->122A		-0.25642				
114B ->121B		0.35005				
116B ->121B		0.81742				
117B ->121B		-0.29882				
Excited State	6:	2.194-A	2.7359 eV	453.17 nm	f=0.0007	<S**2>=0.954
114B ->122B		-0.10990				
115B ->121B		0.95969				
116B ->122B		0.13795				
Excited State	7:	2.202-A	2.7640 eV	448.56 nm	f=0.0025	<S**2>=0.962
121A ->122A		-0.17510				
114B ->121B		0.83043				
115B ->122B		-0.16695				
116B ->121B		-0.44550				
Excited State	8:	2.709-A	3.1163 eV	397.85 nm	f=0.0462	<S**2>=1.584
118A ->124A		-0.15388				
118A ->126A		0.10825				
120A ->123A		-0.18856				
120A ->128A		0.10701				

121A ->123A 0.69312
112B ->121B 0.13952
113B ->121B -0.35326
115B ->121B -0.10547
117B ->124B -0.12932
118B ->121B -0.11249
120B ->121B -0.15995
120B ->123B 0.34808

Excited State 9: 2.592-A 3.1753 eV 390.46 nm f=0.0123 <S**2>=1.430
114A ->122A 0.10730
116A ->122A 0.10122
117A ->123A -0.11537
120A ->123A -0.26306
121A ->123A 0.16258
121A ->128A -0.19945
113B ->121B 0.77644
118B ->123B 0.10188
120B ->123B 0.25304

Excited State 10: 2.190-A 3.4233 eV 362.18 nm f=0.1473 <S**2>=0.949
119A ->125A 0.13035
121A ->122A 0.85401
104B ->121B -0.11862
114B ->121B 0.34324
116B ->121B 0.20708

bisPyTM (UB3LYP/6-31g(d,p)6D10F) (ground state in dichloromethane)

121A is SOMO.

Excited State 1: 2.123-A 2.4985 eV 496.24 nm f=0.0153 <S**2>=0.877
121A ->123A 0.13266
117B ->121B 0.34752
120B ->121B 0.90635

Excited State 2: 2.114-A 2.5802 eV 480.52 nm f=0.0065 <S**2>=0.867
119B ->121B 0.97803

Excited State 3:	2.139-A	2.6509 eV	467.70 nm	f=0.0335	<S**2>=0.894
121A ->123A	0.15048				
117B ->121B	0.88797				
120B ->121B	-0.37871				
Excited State 4:	2.087-A	2.6624 eV	465.69 nm	f=0.0070	<S**2>=0.839
118B ->121B	0.97675				
Excited State 5:	2.246-A	2.8738 eV	431.42 nm	f=0.0087	<S**2>=1.011
121A ->122A	-0.32698				
114B ->121B	0.42580				
116B ->121B	0.76897				
118B ->121B	-0.13843				
Excited State 6:	2.247-A	3.0643 eV	404.61 nm	f=0.0016	<S**2>=1.012
121A ->123A	0.12048				
114B ->122B	0.11516				
115B ->121B	0.94049				
116B ->122B	-0.14531				
Excited State 7:	2.270-A	3.0949 eV	400.61 nm	f=0.0002	<S**2>=1.038
121A ->122A	-0.22224				
114B ->121B	0.73876				
115B ->122B	0.18045				
116B ->121B	-0.54852				
Excited State 8:	2.468-A	3.2519 eV	381.27 nm	f=0.0066	<S**2>=1.273
114A ->122A	0.13589				
116A ->122A	0.14612				
117A ->123A	-0.10594				
119A ->124A	0.11351				
119A ->125A	0.11048				
120A ->126A	-0.14484				
121A ->123A	-0.28447				
121A ->128A	-0.17646				
112B ->121B	-0.12066				
113B ->121B	0.78459				
116B ->122B	0.13888				
117B ->121B	0.10899				
119B ->124B	-0.12238				

119B ->125B -0.11997
120B ->126B 0.14089

Excited State 9: 2.706-A 3.4123 eV 363.35 nm f=0.1338 <S**2>=1.580
117A ->123A -0.15288
118A ->124A -0.21383
118A ->125A 0.18169
121A ->123A 0.71367
121A ->128A -0.10664
113B ->121B 0.24568
115B ->121B -0.19244
117B ->121B -0.21812
117B ->123B 0.22620
118B ->124B 0.19157
118B ->125B -0.16786
120B ->123B 0.13269

Excited State 10: 2.172-A 3.4200 eV 362.53 nm f=0.1412 <S**2>=0.930
121A ->122A 0.83159
114B ->121B 0.44211
116B ->121B 0.20067

bisPyTM (UB3LYP/6-31g(d,p)6D10F) (lowest excited state in dichloromethane)

121A is SOMO.

Excited State 1: 2.078-A 1.9295 eV 642.56 nm f=0.0290 <S**2>=0.830
121A ->123A 0.11490
120B ->121B 0.98150

Excited State 2: 2.088-A 2.2450 eV 552.26 nm f=0.0096 <S**2>=0.840
118B ->121B 0.12697
119B ->121B 0.97842

Excited State 3: 2.076-A 2.4019 eV 516.20 nm f=0.0040 <S**2>=0.828
116B ->121B -0.19168
118B ->121B 0.95277
119B ->121B -0.13746

Excited State 4:	2.104-A	2.4186 eV	512.62 nm	f=0.0239	<S**2>=0.857
117B ->121B	0.97908				

Excited State 5:	2.158-A	2.6550 eV	466.99 nm	f=0.0181	<S**2>=0.915
121A ->122A	-0.28745				
114B ->121B	0.27503				
116B ->121B	0.84884				
118B ->121B	0.24435				

Excited State 6:	2.199-A	2.8183 eV	439.92 nm	f=0.0006	<S**2>=0.959
114B ->122B	-0.14808				
115B ->121B	0.95796				

Excited State 7:	2.198-A	2.8459 eV	435.65 nm	f=0.0009	<S**2>=0.958
121A ->122A	-0.13118				
114B ->121B	0.88503				
115B ->122B	-0.17983				
116B ->121B	-0.35321				

Excited State 8:	2.791-A	3.0968 eV	400.37 nm	f=0.0646	<S**2>=1.698
118A ->124A	0.12963				
118A ->126A	0.13844				
120A ->123A	-0.21807				
120A ->128A	0.11355				
121A ->123A	0.71670				
112B ->121B	0.13036				
113B ->121B	0.25790				
115B ->121B	-0.11588				
118B ->124B	-0.11809				
118B ->126B	-0.11130				
120B ->121B	-0.15591				
120B ->123B	0.38083				
120B ->130B	-0.10191				

Excited State 9:	2.515-A	3.1750 eV	390.51 nm	f=0.0096	<S**2>=1.332
116A ->122A	-0.13950				
119A ->124A	-0.10704				
120A ->123A	0.24440				
121A ->128A	0.19784				
112B ->121B	0.12874				

113B ->121B 0.80851
116B ->122B 0.12411
117B ->125B 0.10500
119B ->124B -0.11027
120B ->123B -0.21431

Excited State 10: 2.153-A 3.3673 eV 368.20 nm f=0.1940 <S**2>=0.909
119A ->125A 0.10318
121A ->122A 0.87146
104B ->121B -0.10242
114B ->121B 0.27272
116B ->121B 0.28511

PyBTM (UB3LYP/6-31g(d,p)6D10F) (ground state in a vacuum)

129A is SOMO.

Excited State 1: 2.154-A 2.5550 eV 485.27 nm f=0.0191 <S**2>=0.910
129A ->131A -0.19971
125B ->129B 0.12069
127B ->129B 0.36779
128B ->129B 0.87229

Excited State 2: 2.147-A 2.6992 eV 459.34 nm f=0.0199 <S**2>=0.902
128A ->130A -0.10488
129A ->131A -0.15802
125B ->129B 0.14564
127B ->129B 0.84910
128B ->129B -0.43169

Excited State 3: 2.175-A 2.7048 eV 458.39 nm f=0.0064 <S**2>=0.933
129A ->130A 0.23427
124B ->129B 0.44217
126B ->129B 0.82173

Excited State 4: 2.097-A 2.8434 eV 436.04 nm f=0.0066 <S**2>=0.849
129A ->132A -0.10178
125B ->129B 0.95024

127B ->129B -0.22113

Excited State 5: 2.156-A 2.8648 eV 432.78 nm f=0.0066 <S**2>=0.912
129A ->130A 0.25054
124B ->129B 0.76776
126B ->129B -0.53440

Excited State 6: 2.275-A 3.0604 eV 405.13 nm f=0.0003 <S**2>=1.044
123A ->130A 0.10282
129A ->131A 0.16555
123B ->129B 0.92760
123B ->130B -0.20412

Excited State 7: 2.389-A 3.1813 eV 389.73 nm f=0.0075 <S**2>=1.177
124A ->130A 0.19007
127A ->134A 0.10230
128A ->134A 0.13897
129A ->130A 0.32472
129A ->137A 0.20023
122B ->129B 0.77306
122B ->130B -0.10150
124B ->129B -0.20395
128B ->134B -0.14479

Excited State 8: 2.404-A 3.3825 eV 366.54 nm f=0.1196 <S**2>=1.195
125A ->132A 0.13238
126A ->133A -0.14350
129A ->130A 0.75367
122B ->129B -0.32205
124B ->129B -0.36225
125B ->132B -0.10374
126B ->133B -0.10724
127B ->131B -0.13447
128B ->131B -0.10702

Excited State 9: 2.547-A 3.3885 eV 365.90 nm f=0.1520 <S**2>=1.372
125A ->133A 0.17224
126A ->132A -0.17861
129A ->131A 0.76399
123B ->129B -0.23074

124B ->131B 0.15622
125B ->129B 0.16055
125B ->133B 0.14223
126B ->132B 0.13351
127B ->129B 0.24228
127B ->130B -0.10682
128B ->129B 0.14499

Excited State 10: 2.259-A 3.7203 eV 333.27 nm f=0.0095 <S**2>=1.025
129A ->132A 0.94872
125B ->129B 0.11248

PyBTM (UB3LYP/6-31g(d,p)6D10F) (lowest excited state in a vacuum)

129A is SOMO.

Excited State 1: 2.092-A 2.0384 eV 608.25 nm f=0.0027 <S**2>=0.844
128B ->129B 0.98100

Excited State 2: 2.129-A 2.4045 eV 515.64 nm f=0.0181 <S**2>=0.883
129A ->130A 0.20317
124B ->129B 0.25283
127B ->129B 0.91691

Excited State 3: 2.129-A 2.4491 eV 506.24 nm f=0.0429 <S**2>=0.883
129A ->131A -0.20086
125B ->129B 0.17005
126B ->129B 0.93911

Excited State 4: 2.088-A 2.6661 eV 465.04 nm f=0.0074 <S**2>=0.840
123B ->129B 0.10515
125B ->129B 0.95551
126B ->129B -0.19907

Excited State 5: 2.108-A 2.6772 eV 463.11 nm f=0.0114 <S**2>=0.861
129A ->130A 0.19258
124B ->129B 0.90583
127B ->129B -0.32258

Excited State 6: 2.172-A 2.8117 eV 440.96 nm f=0.0006 <S**2>=0.929

123B ->129B	0.95570
123B ->131B	0.15997
125B ->129B	-0.11804

Excited State 7: 2.374-A 3.1011 eV 399.80 nm f=0.0111 <S**2>=1.159

124A ->130A	-0.13302
127A ->130A	-0.10174
128A ->133A	0.21951
129A ->130A	0.33778
129A ->137A	-0.18650
111B ->129B	-0.10330
120B ->129B	0.11182
122B ->129B	0.75179
124B ->129B	-0.18946
127B ->129B	-0.13250
128B ->133B	0.22163

Excited State 8: 2.579-A 3.2986 eV 375.87 nm f=0.1131 <S**2>=1.413

124A ->132A	0.10041
125A ->134A	-0.15798
126A ->130A	0.13794
127A ->132A	-0.15162
129A ->131A	0.79703
123B ->129B	0.10037
124B ->130B	-0.13644
125B ->129B	0.13383
125B ->134B	-0.13747
126B ->129B	0.23654
126B ->131B	0.15169
127B ->130B	-0.16073
127B ->132B	0.11701

Excited State 9: 2.669-A 3.3826 eV 366.53 nm f=0.1258 <S**2>=1.531

125A ->131A	-0.12542
125A ->132A	0.16701
126A ->131A	0.18287
127A ->134A	0.17404
128A ->131A	-0.11283
129A ->130A	0.69044

129A ->137A 0.10842
122B ->129B -0.28366
124B ->129B -0.24083
124B ->131B -0.11040
124B ->134B -0.11036
125B ->132B -0.15280
126B ->130B 0.23087
127B ->129B -0.14697
127B ->134B 0.12410

Excited State 10: 3.194-A 3.5611 eV 348.16 nm f=0.0015 <S**2>=2.300
125A ->133A -0.14714
126A ->132A -0.10037
128A ->132A -0.23839
128A ->133A 0.48710
122B ->129B -0.46410
125B ->133B 0.11558
128B ->132B -0.17684
128B ->133B 0.51469

PyBTM (UB3LYP/6-31g(d,p)6D10F) (ground state in dichloromethane)

129A is SOMO.

Excited State 1: 2.152-A 2.5462 eV 486.93 nm f=0.0349 <S**2>=0.908
129A ->131A 0.19782
125B ->129B -0.16979
126B ->129B 0.23380
128B ->129B 0.90971

Excited State 2: 2.156-A 2.6913 eV 460.69 nm f=0.0069 <S**2>=0.912
129A ->130A 0.20183
124B ->129B 0.42923
127B ->129B 0.84194

Excited State 3: 2.142-A 2.7223 eV 455.44 nm f=0.0222 <S**2>=0.897
129A ->131A 0.11656
125B ->129B -0.22284
126B ->129B 0.89403

128B ->129B -0.30902

Excited State 4: 2.094-A 2.8077 eV 441.59 nm f=0.0101 <S**2>=0.846
125B ->129B 0.92781
126B ->129B 0.29035
128B ->129B 0.12739

Excited State 5: 2.160-A 2.8359 eV 437.19 nm f=0.0115 <S**2>=0.916
129A ->130A 0.24802
124B ->129B 0.78307
127B ->129B -0.50831

Excited State 6: 2.292-A 3.1639 eV 391.87 nm f=0.0004 <S**2>=1.064
123A ->130A 0.10735
129A ->131A 0.19478
123B ->129B 0.91957
123B ->130B -0.21273

Excited State 7: 2.364-A 3.1746 eV 390.55 nm f=0.0218 <S**2>=1.148
124A ->130A 0.19311
126A ->134A -0.12342
128A ->134A 0.10337
129A ->130A 0.44419
129A ->137A 0.17626
122B ->129B 0.71351
122B ->130B -0.11076
124B ->129B -0.24892
126B ->134B 0.11892
128B ->134B -0.10598

Excited State 8: 2.416-A 3.3538 eV 369.68 nm f=0.1422 <S**2>=1.209
125A ->131A 0.11095
125A ->132A 0.10938
127A ->133A -0.13798
128A ->131A -0.12655
129A ->130A 0.71986
129A ->137A -0.11602
122B ->129B -0.43493
124B ->129B -0.30590
127B ->133B 0.11373

128B ->131B 0.13300

Excited State 9: 2.557-A 3.3796 eV 366.86 nm f=0.1867 <S**2>=1.385
125A ->133A 0.15508
127A ->132A -0.17169
129A ->131A 0.76642
123B ->129B -0.25765
124B ->131B 0.15904
125B ->129B 0.17044
125B ->133B -0.13920
126B ->129B -0.16042
127B ->132B 0.13852
128B ->129B -0.19084
128B ->130B 0.10653

Excited State 10: 3.118-A 3.7390 eV 331.60 nm f=0.0115 <S**2>=2.180
124A ->130A -0.16278
125A ->131A 0.14291
125A ->132A 0.23048
125A ->134A -0.14338
126A ->132A 0.22968
127A ->133A -0.30903
128A ->131A -0.17768
128A ->134A -0.14927
129A ->130A -0.26286
122B ->129B 0.42454
124B ->129B -0.10369
124B ->130B 0.19076
125B ->131B -0.14309
125B ->132B -0.23739
125B ->134B 0.12999
126B ->131B 0.12566
126B ->132B -0.18797
127B ->133B 0.28661
128B ->131B 0.19146
128B ->134B 0.13515

PyBTM (UB3LYP/6-31g(d,p)6D10F) (lowest excited state in dichloromethane)

129A is SOMO.

Excited State 1:	2.104-A	2.1687 eV	571.69 nm	f=0.0457	<S**2>=0.856
129A ->131A	-0.19083				
128B ->129B	0.96425				
Excited State 2:	2.133-A	2.4358 eV	509.01 nm	f=0.0180	<S**2>=0.887
129A ->130A	0.23285				
124B ->129B	0.31412				
126B ->129B	0.89020				
Excited State 3:	2.093-A	2.4603 eV	503.95 nm	f=0.0138	<S**2>=0.845
127B ->129B	0.98329				
Excited State 4:	2.103-A	2.6477 eV	468.27 nm	f=0.0168	<S**2>=0.855
129A ->131A	-0.14622				
125B ->129B	0.96593				
Excited State 5:	2.106-A	2.6657 eV	465.10 nm	f=0.0094	<S**2>=0.859
129A ->130A	0.18945				
124B ->129B	0.87870				
126B ->129B	-0.38509				
Excited State 6:	2.232-A	2.9978 eV	413.58 nm	f=0.0014	<S**2>=0.996
129A ->131A	-0.19059				
123B ->129B	0.93340				
123B ->130B	0.20350				
Excited State 7:	2.247-A	3.0932 eV	400.83 nm	f=0.0363	<S**2>=1.012
124A ->130A	0.15093				
126A ->130A	0.11218				
127A ->134A	0.10967				
129A ->130A	-0.49214				
129A ->137A	0.16580				
120B ->129B	-0.10057				
122B ->129B	0.73164				
124B ->129B	0.17062				
126B ->129B	0.13509				
127B ->134B	0.10223				

Excited State 8: 2.432-A 3.1939 eV 388.19 nm f=0.2134 <S**2>=1.229

126A ->132A	-0.10380
128A ->130A	-0.11921
129A ->131A	0.82283
123B ->129B	0.23172
124B ->131B	-0.12176
125B ->129B	0.16706
126B ->131B	-0.11436
128B ->129B	0.21945
128B ->130B	0.14934

Excited State 9: 2.440-A 3.2202 eV 385.03 nm f=0.1545 <S**2>=1.239

126A ->133A	-0.10632
128A ->131A	-0.20391
129A ->130A	0.69949
129A ->137A	0.12656
122B ->129B	0.45270
124B ->129B	-0.25815
126B ->129B	-0.13275
128B ->131B	0.21911

Excited State 10: 3.122-A 3.6470 eV 339.96 nm f=0.0156 <S**2>=2.187

124A ->130A	-0.19029
124A ->133A	-0.11831
125A ->131A	0.10405
125A ->132A	-0.12236
125A ->134A	0.14461
126A ->133A	0.20976
127A ->132A	-0.23067
128A ->131A	0.35028
128A ->134A	-0.10416
129A ->130A	0.29057
122B ->129B	0.40586
124B ->130B	0.19004
124B ->133B	0.14721
125B ->131B	-0.10301
125B ->132B	0.12992
125B ->134B	-0.13269
126B ->130B	0.15404
126B ->133B	-0.17197

127B ->132B	-0.20061
128B ->131B	-0.36298

Fermi constant couplings by DFT calculation

bisPyTM (UB3LYP/6-31g(d,p)6D10F) (ground state in a vacuum)

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	Cl(35)	0.00075	0.33008	0.11778	0.11010
2	Cl(35)	0.00075	0.33010	0.11779	0.11011
3	Cl(35)	0.00082	0.35762	0.12761	0.11929
4	Cl(35)	0.00055	0.23979	0.08556	0.07999
5	Cl(35)	0.00055	0.23982	0.08557	0.08000
6	Cl(35)	0.00082	0.35764	0.12762	0.11930
7	Cl(35)	0.00207	0.90764	0.32387	0.30276
8	N(14)	0.01018	3.29073	1.17422	1.09767
9	C(13)	-0.00548	-6.15594	-2.19659	-2.05340
10	H(1)	0.00084	3.75804	1.34096	1.25355
11	C(13)	0.02731	30.69819	10.95388	10.23981
12	C(13)	0.02862	32.17003	11.47907	10.73077
13	C(13)	-0.00548	-6.15576	-2.19653	-2.05334
14	H(1)	0.00084	3.75800	1.34095	1.25353
15	C(13)	-0.02910	-32.71837	-11.67473	-10.91367
16	C(13)	-0.00592	-6.64986	-2.37284	-2.21816
17	H(1)	0.00095	4.24479	1.51465	1.41591
18	C(13)	0.01030	11.57812	4.13136	3.86205
19	C(13)	0.02746	30.87395	11.01659	10.29844
20	C(13)	0.02746	30.87396	11.01660	10.29844
21	C(13)	0.02862	32.17008	11.47908	10.73078
22	C(13)	-0.00592	-6.64985	-2.37283	-2.21815
23	H(1)	0.00095	4.24479	1.51465	1.41591
24	C(13)	-0.00520	-5.84803	-2.08672	-1.95069
25	H(1)	0.00089	3.95670	1.41185	1.31981
26	C(13)	-0.02952	-33.19053	-11.84321	-11.07117
27	C(13)	-0.02910	-32.71857	-11.67480	-10.91374
28	C(13)	0.02731	30.69809	10.95384	10.23978
29	C(13)	-0.00520	-5.84786	-2.08666	-1.95064
30	H(1)	0.00089	3.95667	1.41184	1.31980
31	C(13)	0.09331	104.90279	37.43192	34.99180
32	N(14)	0.01018	3.29081	1.17424	1.09770

Spin density by DFT calculation

bisPyTM (UB3LYP/6-31g(d,p)6D10F) (ground state in a vacuum)

1	Cl	0.004672
2	Cl	0.004672
3	Cl	0.003887
4	Cl	0.003811
5	Cl	0.003811
6	Cl	0.003887
7	Cl	0.007707
8	N	0.069617
9	C	-0.041933
10	H	0.002189
11	C	0.094733
12	C	0.092385
13	C	-0.041932
14	H	0.002189
15	C	-0.118650
16	C	-0.045783
17	H	0.002301
18	C	0.081260
19	C	0.094683
20	C	0.094681
21	C	0.092386
22	C	-0.045783
23	H	0.002301
24	C	-0.041541
25	H	0.002307
26	C	-0.121159
27	C	-0.118652
28	C	0.094732
29	C	-0.041540
30	H	0.002307
31	C	0.786832
32	N	0.069619

Sum of Mulliken atomic densities = 1.00000