Supporting Information for:

Nanosecond Photochromic Molecular Switching of a Biphenyl-Bridged Imidazole Dimer Revealed by Wide Range Transient Absorption Spectroscopy

Tetsuo Yamaguchi,[a] Michiel F. Hilbers,[b] Paul P. Reinders,[b] Yoichi Kobayashi,[a] Albert M. Brouwer,[b] and Jiro Abe[a,c]*

[a] *Department of Chemistry, School of Science and Engineering, Aoyama Gakuin University, 5-10-1 Fuchinobe, Chuo-ku, Sagamihara, Kanagawa 252-5258, Japan*

[b] *University of Amsterdam, van 't Hoff Institute for Molecular Sciences, P. O. Box 94157, 1090 GD Amsterdam, The Netherlands*

[c] *CREST, Japan Science and Technology Agency, K's Gobancho, 7 Gobancho, Chiyoda-ku, Tokyo 102-0076, Japan*

Email: jiro_abe@chem.aoyama.ac.jp

CONTENTS

1. UV-vis absorption spectrum

The UV-vis absorption spectrum was measured with a Shimadzu UV3150 spectrometer after Ar bubbling over ten minutes. The 1,2'-isomer of imidazole dimers have a small and broad absorption band around 400-450 nm due to the charge transfer from the 6π-imidazole to 4π-imidazole systems with excitation. On the other hand, because bisDMDPI-BP is the 2,2'-isomer and there is no charge transfer process, no absorption band is observed around 400 nm.

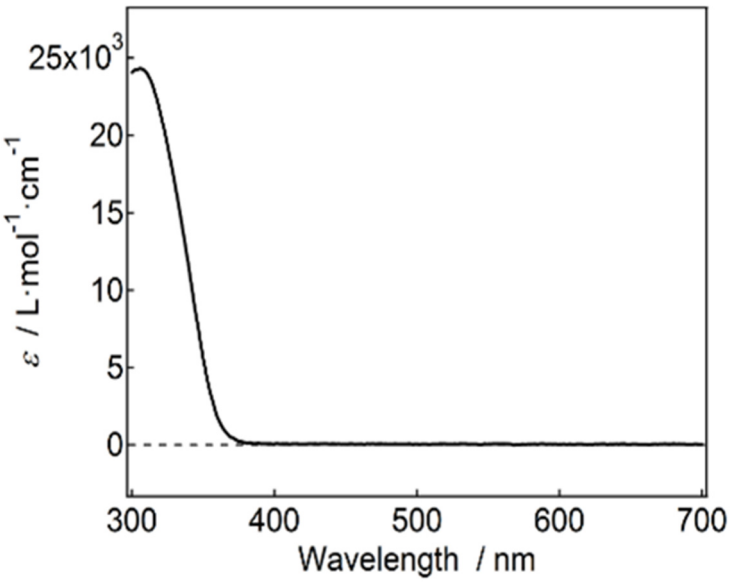

Fig. S1 UV-vis absorption spectrum of bisDMDPI-BP in benzene at room temperature.

2. Durability

The durability of bisDMDPI-BP was examined by repetitive exposures to ns laser pulses. A Continuum Minilite II Q-switched Nd:YAG laser was used for the excitation laser with the third harmonic at 355 nm (pulse duration, 5 ns; power, 8 mJ) and the durability of the sample was analyzed by HPLC system and UV-vis absorption spectrometer. HPLC was carried out on a ODS reversed phase column (Mightysil RP-18 GP, Kanto Chemical Co., Inc.). The HPLC system consists of a pump unit (PU-2080 plus, JASCO), a photodiode array (PDA) detector (MD-2018 plus, JASCO), and a control unit (LC-NetII/ADC, JASCO). UV-vis absorption spectra were measured with a Shimadzu UV3150 spectrometer. Sample solutions were bubbled with argon or oxygen prior to the laser shots.

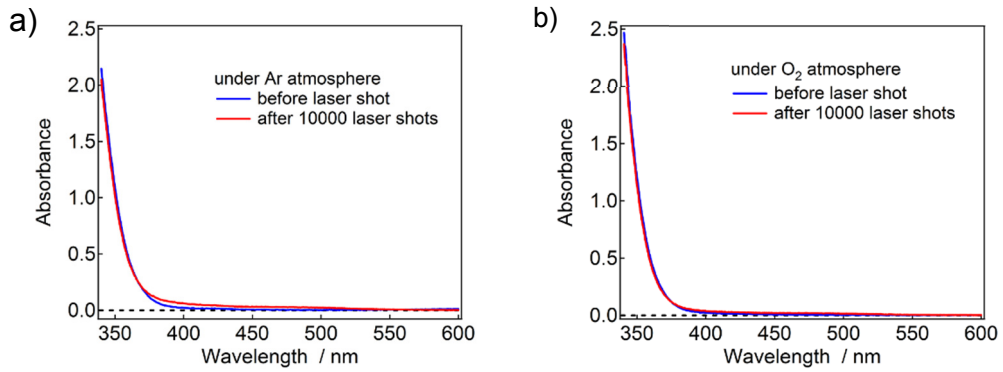

Fig. S2 UV-vis absorption spectra of bisDMDPI-BP in benzene before and after 10000 laser shots (355 nm) under a) Ar (1.9×10^{-4} M) and b) O_2 atmospheres (2.2×10^{-4} M). The blue and red lines show the spectra before and after laser irradiation, respectively.

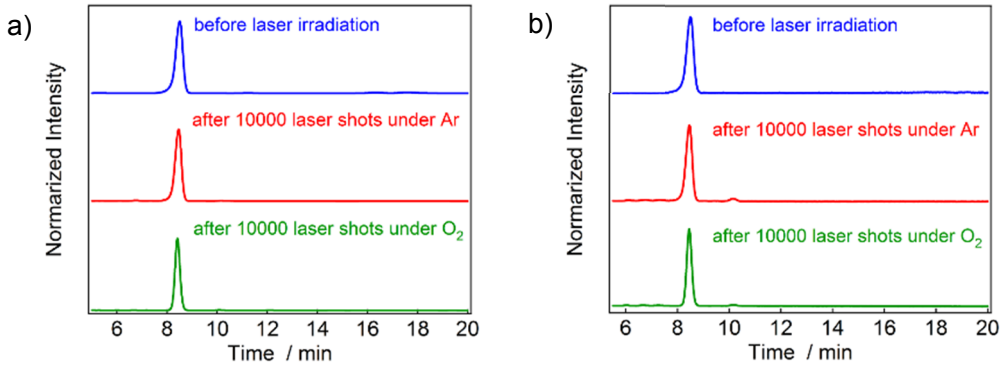

Fig. S3 HPLC chromatograms of bisDMDPI-BP before 355 nm laser shot (blue line), after 10000 laser shots in Ar (red line) and O_2 atmospheres (green line) in benzene. The HPLC analysis was performed using a reverse phase column (eluent, H_2O/acetonitrile = 1/4; flow rate, 1 mL/min; detected at a) 254 and b) 365 nm.

3. Nanosecond transient absorption spectra

Nanosecond transient absorption spectra were measured using an in-house assembled setup. The excitation wavelength of 305 nm was generated using a tunable Nd:YAG-laser system (NT342B, Ekspla) comprising a pump laser (NL300), harmonics generators (SHG, THG) and optical parametric oscillator (OPO). The pulse length is 3-5 ns. The repetition rate of the laser system was 5 Hz. The laser beam homogeneously illuminates the front of a 1 cm quartz cuvette containing the sample solution in an area 1 cm wide and 1 mm high. A high-stability short arc xenon flash lamp (FX-1160, Excelitas Technologies) with a modified PS302 controller (EG&G) running at 10 Hz was used as the probe light. The probe light was split in a signal and a reference beam with a 50/50 beam splitter. The signal beam passed through the sample cell orthogonal to the excitation beam and probed the excited volume immediately behind the front window of the cell in a 1 mm × 1 mm area along the 1 cm path length of the illuminated volume. The sample and reference beams were focused onto the entrance slit of a spectrograph (SpectraPro-150, Princeton Instruments) recorded with an intensified CCD camera (PI-MAX3, Princeton Instruments) using a 2.7-10 ns gate depending on the time step of the measurements. The time delays of laser, flash lamp and camera were generated by a delay generator (Stanford Research System DG535). The whole set-up is controlled with an in-house written program (LabView) and the data were analyzed with macros implemented in Igor Pro 5.03J (WaveMetrics, Inc.).

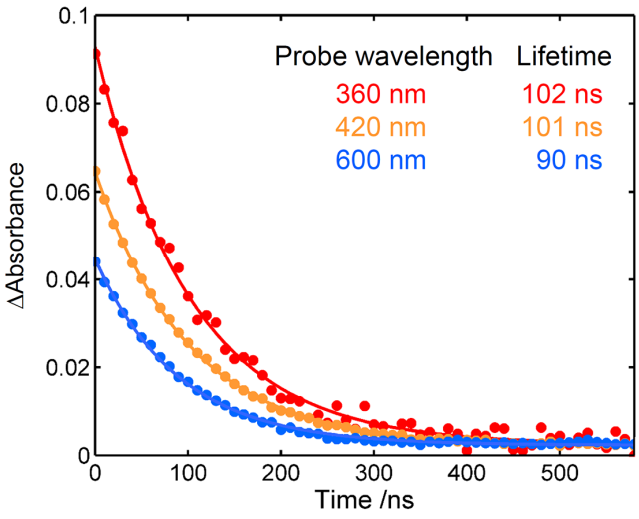

Fig. S4 Decay profiles of the colored species of bisDMDPI-BP in degassed benzene at room temperature (1.1×10^{-4} M, excitation wavelength: 305 nm, pulse duration: 5 ns, excitation intensity: 1.8 mJ). The dots and solid line are experimental data and fittings, respectively.

4. Femtosecond transient absorption spectra[S1]

Fig. S5 shows a time evolution of the transient absorption spectrum. Color represents ΔAbsorbance. As was seen in the Fig. 3a in the main text, the initial transient absorption spectra at 0.3-1.0 ps are obviously broadened. Two possibilities are conceivable for the broadening: transient absorption from the precursor states of the colored species and/or the vibrational cooling from hot states.

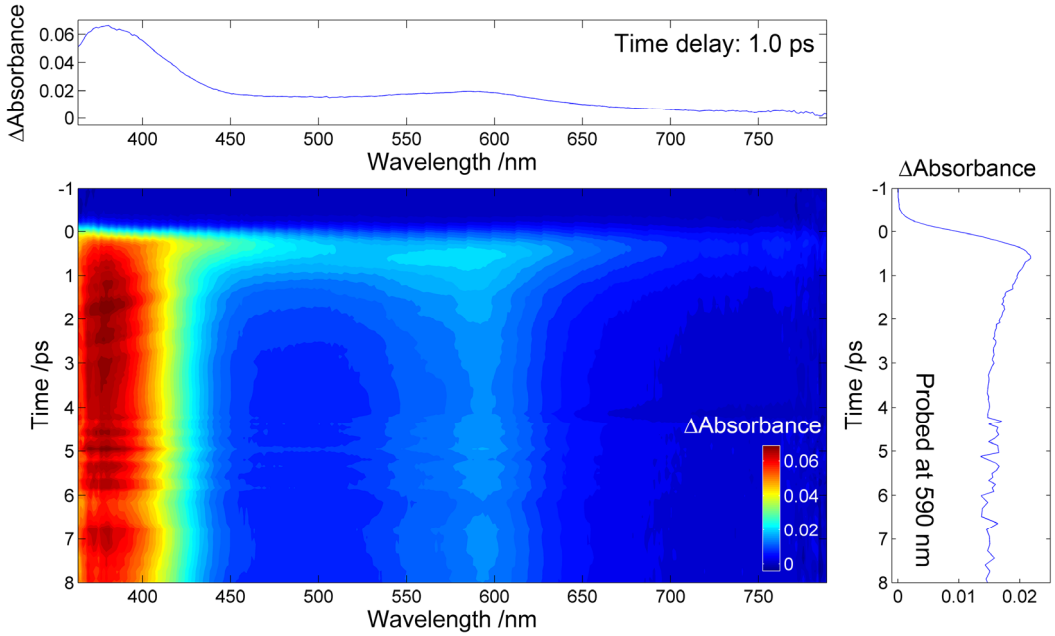

Fig. S5 Time-evolution of the chirp corrected transient absorption spectrum of bisDMPI-BP from 0 to 8 ps in benzene at room temperature (5.5×10^{-4} M, excitation wavelength: 305 nm, pulse duration: 200 fs and laser intensity: 1.8 μJ).

As is described in the main text, the formation process of the colored species after the photoexcitation can be expected as follows: 1) the vibrational relaxation from the Franck-Condon state to the S_1 state, 2) the transition from the S_1 state to the hot state of the colored species, and 3) the vibrational cooling to the ground state of the colored species. In addition to the process 3), the higher excited states of the colored species may also contribute to the generation process of the radicals. All processes are completed within a ps. The time-resolved spectra were analyzed using the TIMP package with the graphical interface program Glotaran, version 1.0.1 (http://glotaran.org).[S2] The instrument response function (IRF) was set to 200 fs. We apply the global analyses to reveal the multi-wavelength kinetics of the transient absorption spectra at the ultrafast time scale. We propose two and three-state sequential models and found out that the three-state sequential model satisfactory explained the kinetics of bisDMPI-BP as shown follows:

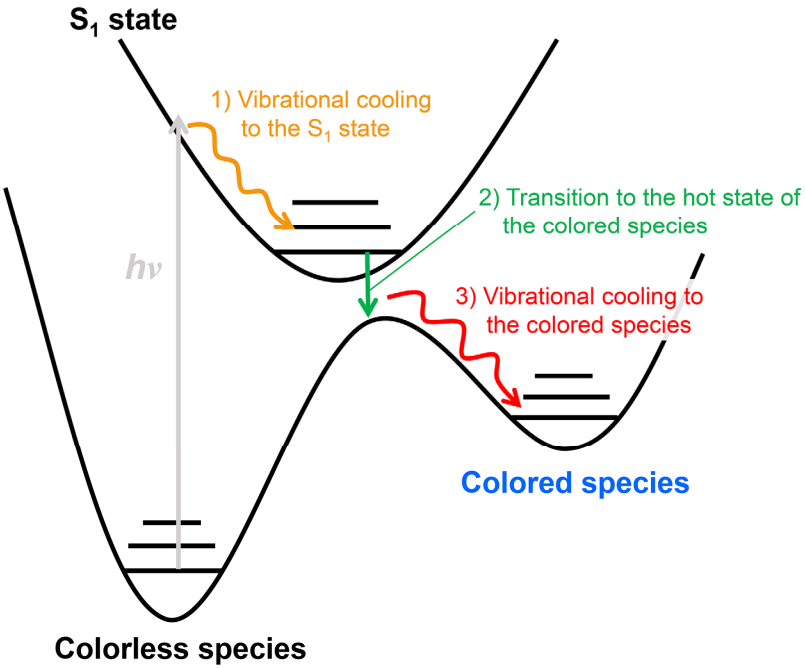

Fig. S6 Plausible energy relaxation pathway of photochromic reaction of the HABI derivatives reported previously.[S2,S3]

a) Two-state sequential model analysis

$$[S_0] \xrightarrow{h\nu} [\text{Component 1}] \xrightarrow{\tau_1} [\text{Colored species}]$$

Firstly, the kinetics were fitted with the two-state sequential model with convolution by the IRF. Figs. S7a and b show evolution associated spectra (EAS) and decays of two components. The component 1 has a broad absorption band and it is quickly converted to the colored species. It is assigned to the transient absorption from the precursor state of the colored species, which is most probably the transient absorption from S_1 state and/or the vibrationally hot state of the colored species. The higher excited states of the colored species may also contribute to the component 1. Another component (denoted as blue) is assigned to the colored species of bisDMDPI-BP because of the strong similarity of the spectral shape to that observed in the ns experiments. The time constants of the decay of the component 1 (τ_1) and the colored species are estimated to be 760 fs and >50 ps, respectively. Fitted spectra at different delay times and fitted decays probed at different wavelengths are shown in Fig. S8. The gray dots and red solid lines indicate the raw data and fitted spectra, respectively. While the simulated transient absorption spectra obtained from the global analyses qualitatively fit with the data (except the spectrum at 0.3 ps), the simulated transient absorption dynamics obviously cannot reproduce the experimental data at 540, 580, and 590 nm (indicated as black arrows). These results suggest that another rise component is necessary to explain the kinetics of bisDMDPI-BP.

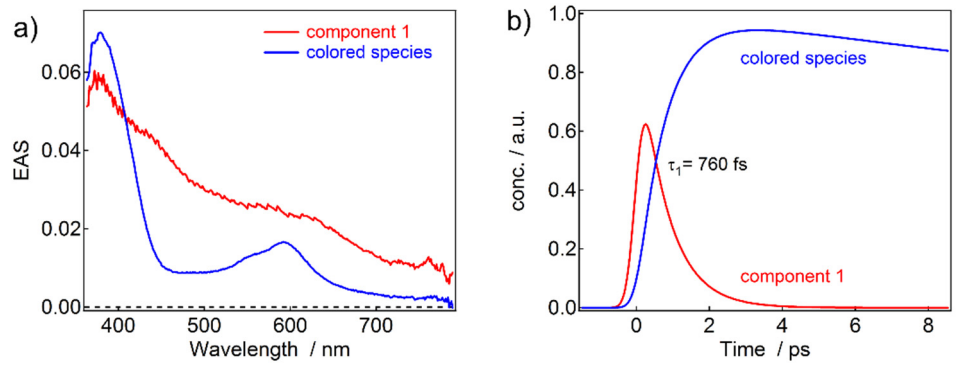

Fig. S7 (a) Evolution associated spectra (EAS) and time profiles of the concentration changes of two components obtained from the global analysis of the two-state sequential model.

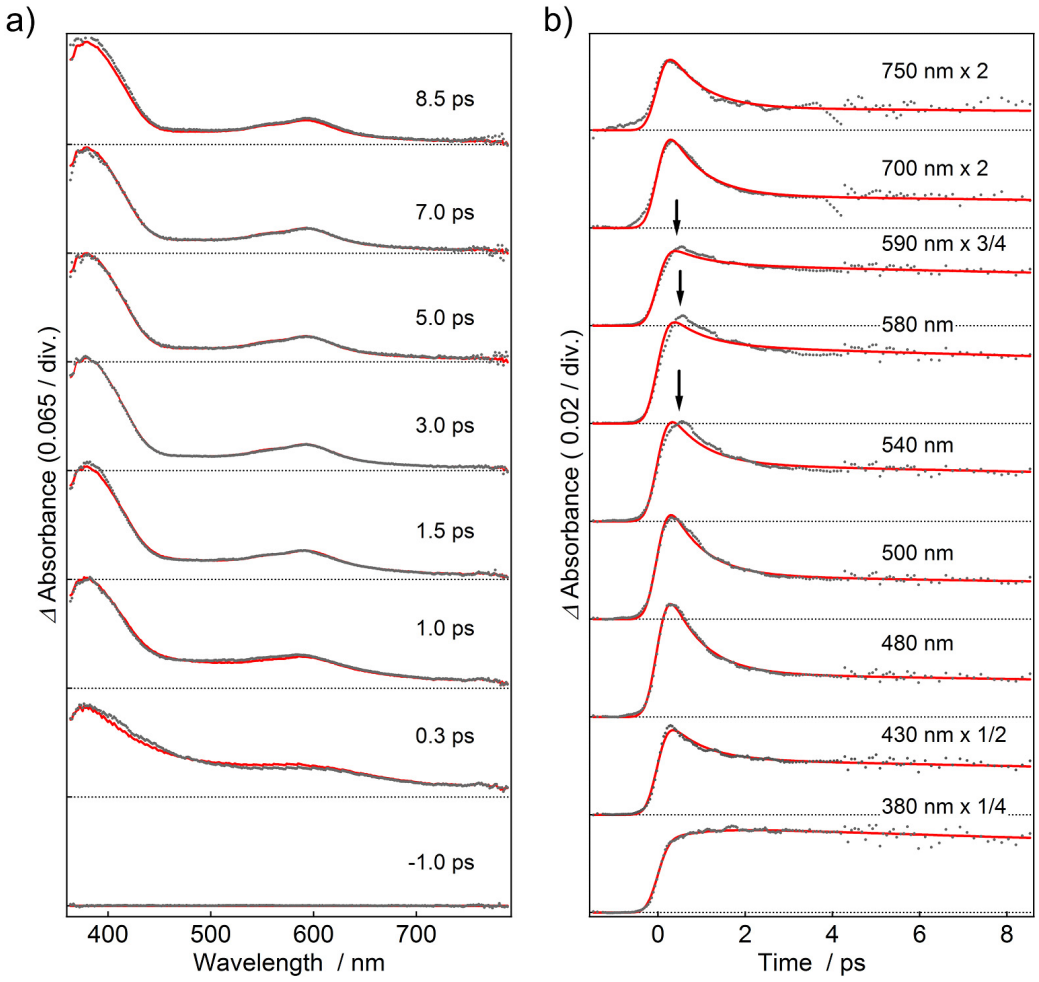

Fig. S8 (left) Transient absorption spectra and (right) dynamics of bisDMDPI-BP. The red curves represent the simulated spectra and decays obtained by global analysis with the two-state sequential model.

b) Three-state sequential model analysis

$$[\text{Ground state}] \xrightarrow{h\nu} [\text{Component 1}] \xrightarrow{\tau_1} [\text{Component 2}] \xrightarrow{\tau_2} [\text{Colored species}]$$

The two-state sequential model assumes that the precursor of the colored species is described as a single component. However, the two-state sequential model does not reproduce the experimental data well. Next, we assume that the precursor state can be split into two states and we fit the kinetics with the three-state sequential model convoluted by the IRF. Figs. S9a and b show EAS and time profiles of each component. Component 1 has a broad absorption band and it is quickly converted to component 2. The spectrum of component 2 has sharp and broad peaks at ~390 and 550 nm and component 2 decays within 2 ps. By following to the relaxation energy diagram shown in Fig. S6, we assigned component 1 to the transient absorption from the S_1 state. Since the spectrum of component 2 is similar to that of the colored species and the spectrum is somewhat shifted and more broadened, component 2 can be assigned to the hot state of the colored species. The component which generates with decreasing the component 2 is assigned to the colored species of bisDMDPI-BP because of the similarity of the spectral shape. The time constants of the decay of the components 1, 2 (τ_1 and τ_2), and colored species are estimated to be 420 fs, 420 fs and >50 ps, respectively. Fitted transient absorption spectra at different delay times and fitted transient absorption dynamics probed at different wavelengths are shown in Fig. S10. The striking difference from the two-state sequential model is that the addition of component 2 satisfactorily reproduces the rise around 520-600 nm.

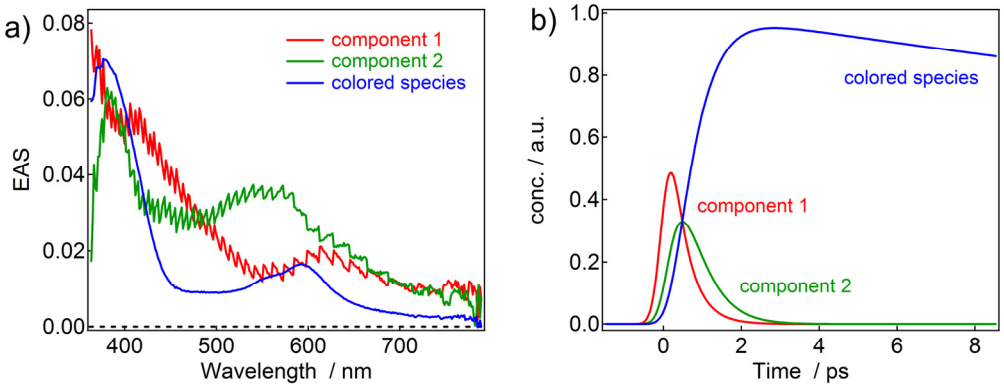

Fig. S9 (a) Evolution Associated Spectra and time profiles of the concentration changes of three components obtained from the global analysis of the three-state sequential model. The τ_1, τ_2, and colored species are 420 fs, 420 fs and >50 ps, respectively.

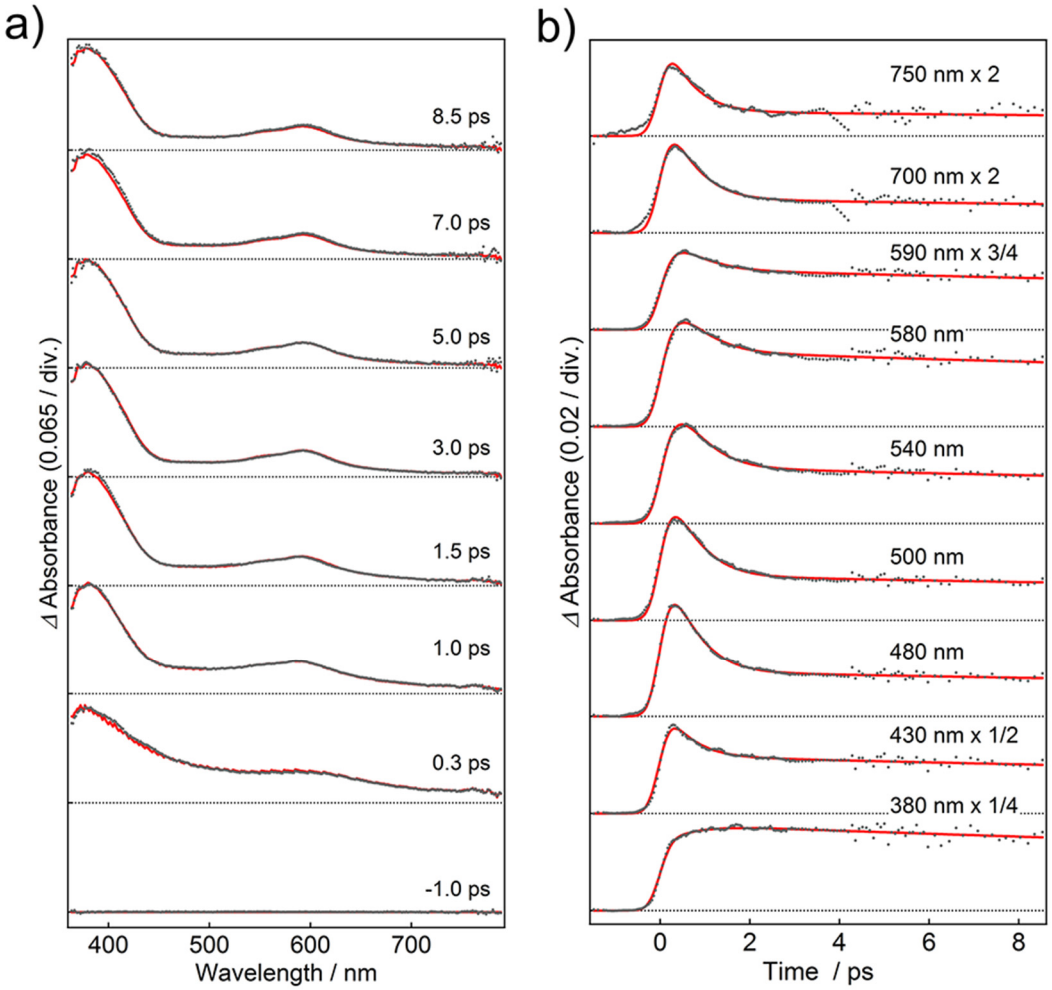

Fig. S10 (left) Transient absorption spectra and (right) dynamics of bisDMDPI-BP. The red curves represent the simulated spectra and decays obtained by global analysis with the three-state sequential model.

5. DFT calculations

All DFT calculations were carried out using the Gaussian 09 program (revision D.01; reference 25 in the main text). The molecular geometries were fully optimized at the MPW1PW91/6-31G(d) level of the theory for the 2,2'-isomer (the colorless isomer) and the UMPW1PW91/6-31G(d) level for the biradical species (the colored isomer) of bisDMDPI-BP, and analytical second derivatives were computed using the vibrational analysis to confirm each stationary point to be a minimum. Zero-point energy (ZPE) corrections were adopted to compare the relative energies for the isomers. It has been reported that the B3LYP functional gives inaccurate results in the system where the medium-range correlation energy, such as van der Waals attraction, is important.[S3), S4)] In the DFT calculation for the biradical species of the bridged imidazole dimer systems, the van der Waals interaction between the radical units should be taken into consideration. Thus we applied the MPW1PW91 level of the theory.

Table S1. Standard orientation of the optimized geometry for the 2,2'-isomer of bisDMDPI-BP.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.560435	-2.935079	-2.770807
2	6	0	-0.449745	-4.106205	-3.514388
3	6	0	-0.091679	-4.160731	-0.731909
4	6	0	-0.384679	-2.956361	-1.392567
5	6	0	0.091595	-4.160730	0.731929
6	6	0	0.384620	-2.956363	1.392583
7	6	0	0.560377	-2.935079	2.770822
8	6	0	0.449662	-4.106199	3.514408
9	6	0	-0.546937	-1.691389	-0.561010
10	6	0	0.546906	-1.691398	0.561021
11	7	0	0.429261	-0.495742	1.363293
12	6	0	1.543843	0.134187	1.236978
13	6	0	2.449292	-0.630093	0.310051
14	7	0	1.856281	-1.702415	-0.075369
15	7	0	-0.429268	-0.495738	-1.363288
16	6	0	-1.543830	0.134223	-1.236963
17	6	0	-2.449311	-0.630054	-0.310061
18	7	0	-1.856314	-1.702376	0.075379
19	6	0	-3.796862	-0.284260	0.165344
20	6	0	-1.798291	1.390879	-1.956571
21	6	0	-4.186784	1.037773	0.425579
22	6	0	-5.441226	1.320662	0.936198
23	6	0	-6.345908	0.285785	1.196485
24	6	0	-5.970269	-1.037560	0.949712
25	6	0	-4.703774	-1.308981	0.447455
26	6	0	-0.733126	2.257757	-2.215352
27	6	0	-0.912219	3.429688	-2.939371
28	6	0	-2.179278	3.745612	-3.438027
29	6	0	-3.251129	2.877639	-3.202216
30	6	0	-3.062226	1.719576	-2.469405

31	6	0	1.798339	1.390830	1.956595
32	6	0	3.796841	-0.284315	-0.165372
33	6	0	0.733191	2.257721	2.215408
34	6	0	0.912314	3.429640	2.939439
35	6	0	2.179388	3.745539	3.438075
36	6	0	3.251221	2.877554	3.202231
37	6	0	3.062288	1.719503	2.469409
38	6	0	4.186776	1.037713	-0.425611
39	6	0	5.441213	1.320587	-0.936251
40	6	0	6.345877	0.285699	-1.196556
41	6	0	5.970224	-1.037641	-0.949780
42	6	0	4.703735	-1.309048	-0.447501
43	8	0	7.550836	0.665135	-1.684268
44	8	0	2.468156	4.856564	4.155181
45	8	0	-2.468017	4.856649	-4.155127
46	8	0	-7.550871	0.665235	1.684177
47	6	0	-8.492631	-0.340863	1.981682
48	6	0	-1.418900	5.754194	-4.441334
49	6	0	1.419056	5.754119	4.441419
50	6	0	8.492580	-0.340973	-1.981786
51	1	0	-0.763570	-1.991088	-3.262480
52	1	0	-0.582507	-4.077258	-4.591166
53	1	0	0.763533	-1.991090	3.262491
54	1	0	0.582426	-4.077250	4.591186
55	1	0	-3.495250	1.852520	0.242591
56	1	0	-5.745192	2.339631	1.147980
57	1	0	-6.649513	-1.857929	1.146714
58	1	0	-4.399140	-2.334519	0.270350
59	1	0	0.250417	1.997974	-1.839930
60	1	0	-0.064806	4.082101	-3.111032
61	1	0	-4.222977	3.132066	-3.609901
62	1	0	-3.902345	1.053472	-2.308581
63	1	0	-0.250363	1.997956	1.840002
64	1	0	0.064913	4.082063	3.111126
65	1	0	4.223081	3.131961	3.609901
66	1	0	3.902395	1.053388	2.308562
67	1	0	3.495254	1.852469	-0.242611
68	1	0	5.745187	2.339553	-1.148036
69	1	0	6.649453	-1.858019	-1.146798
70	1	0	4.399090	-2.334582	-0.270394
71	1	0	-9.373433	0.176052	2.362185
72	1	0	-8.118458	-1.028984	2.748632
73	1	0	-8.768313	-0.912332	1.087503
74	1	0	-1.864468	6.559375	-5.025135
75	1	0	-0.628623	5.275220	-5.030983
76	1	0	-0.983845	6.171190	-3.525404
77	1	0	1.864645	6.559287	5.025221
78	1	0	0.628783	5.275147	5.031076
79	1	0	0.983989	6.171131	3.525502
80	1	0	9.373384	0.175931	-2.362299
81	1	0	8.118390	-1.029089	-2.748733
82	1	0	8.768266	-0.912448	-1.087611
83	6	0	-0.148165	-5.302728	-2.874065
84	1	0	-0.040488	-6.218957	-3.446120

85	6	0	0.036001	-5.323956	-1.496899
86	1	0	0.307982	-6.256011	-1.013113
87	6	0	-0.036110	-5.323948	1.496925
88	1	0	-0.308110	-6.256000	1.013142
89	6	0	0.148057	-5.302719	2.874091
90	1	0	0.040360	-6.218943	3.446150

SCF Done: E(RmPW+HF-PW91) = -2293.90856350 A.U.
Zero-point correction = 0.724147 (Hartree/Particle)
Thermal correction to Energy = 0.768707
Thermal correction to Enthalpy = 0.769652
Thermal correction to Gibbs Free Energy = 0.641461
Sum of electronic and zero-point Energies = -2293.184416
Sum of electronic and thermal Energies = -2293.139856
Sum of electronic and thermal Enthalpies = -2293.138912
Sum of electronic and thermal Free Energies = -2293.267102

Low frequencies --- -4.0428 -2.8882 -1.9784 -0.0013 -0.0008 -0.0005
Low frequencies --- 11.6123 12.8785 13.2809

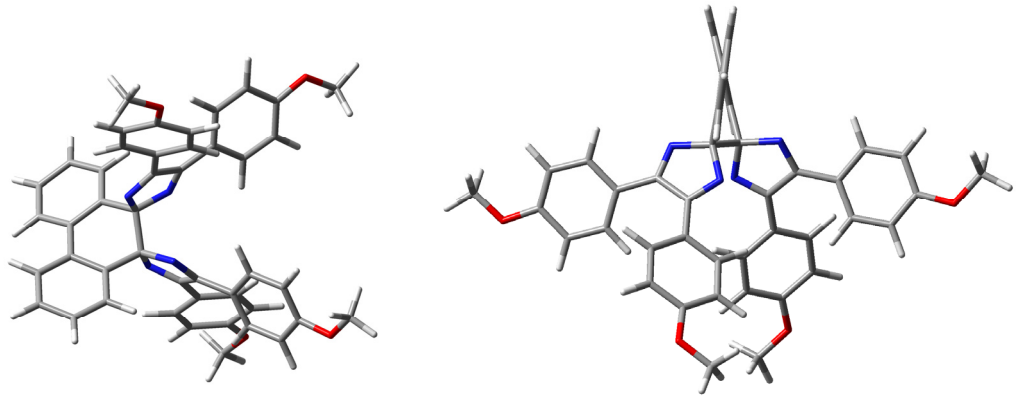

Fig. S11 Optimized structure of the 2,2'-isomer of bisDMDPI-BP.

The Result of the TDDFT calculation

Excited State 1: Singlet-A 3.3414 eV 371.06 nm f=0.0109
186 ->187 0.69080
This state for optimization and/or second-order correction.
Total Energy, E(RPA) = -2293.78576972

Excited State 2: Singlet-A 3.6692 eV 337.90 nm f=0.2356

175 ->187 -0.11303
183 ->187 0.10249
185 ->187 0.65571

Excited State 3: Singlet-A 3.8377 eV 323.07 nm f=0.0174
174 ->187 -0.11735
182 ->187 0.12550
184 ->187 0.48064
186 ->188 -0.43755

Excited State 4: Singlet-A 3.8820 eV 319.39 nm f=0.0177
182 ->187 -0.35099
184 ->187 0.45329
186 ->188 0.34948

Excited State 5: Singlet-A 3.9125 eV 316.89 nm f=0.0791
183 ->187 0.67102
185 ->187 -0.12320

Excited State 6: Singlet-A 3.9662 eV 312.60 nm f=0.0828
174 ->187 -0.12237
182 ->187 0.50960
184 ->187 0.15816
186 ->188 0.39692

Excited State 7: Singlet-A 4.1324 eV 300.03 nm f=0.0439
174 ->188 0.10849
175 ->187 0.17214
176 ->187 -0.11461
181 ->187 0.61803
186 ->187 -0.10244

Excited State 8: Singlet-A 4.1546 eV 298.42 nm f=0.0082
173 ->187 0.11290
174 ->187 0.29376
175 ->188 0.15115

176 ->188 -0.10969
177 ->187 -0.11097
178 ->187 -0.13012
180 ->187 0.37289
182 ->187 0.25259
185 ->188 -0.30112

Excited State 9: Singlet-A 4.2949 eV 288.68 nm f=0.0329
174 ->188 0.18320
175 ->187 0.36834
176 ->187 -0.27956
179 ->187 0.24505
180 ->188 0.14571
181 ->187 -0.27942
183 ->187 0.10091
185 ->187 0.13270

Excited State 10: Singlet-A 4.3231 eV 286.79 nm f=0.0690
180 ->187 0.37176
185 ->188 0.56441

Excited State 11: Singlet-A 4.4116 eV 281.04 nm f=0.0559
184 ->188 0.67890

Excited State 12: Singlet-A 4.4325 eV 279.72 nm f=0.0110
172 ->187 -0.12003
174 ->187 -0.25655
178 ->187 0.16417
180 ->187 0.37582
181 ->188 -0.17276
183 ->188 0.37475
185 ->188 -0.14895

Excited State 13: Singlet-A 4.4868 eV 276.33 nm f=0.0746
182 ->188 0.66828

Excited State	14:	Singlet-A	4.4930 eV	275.95 nm	f=0.1031
174 ->187	0.21269				
178 ->187	-0.16581				
180 ->187	-0.17165				
181 ->188	0.13074				
183 ->188	0.55323				
185 ->188	0.13191				
Excited State	15:	Singlet-A	4.6049 eV	269.24 nm	f=0.2146
181 ->189	0.13079				
186 ->189	0.62082				
Excited State	16:	Singlet-A	4.6686 eV	265.57 nm	f=0.0001
169 ->187	0.14350				
172 ->187	0.20525				
173 ->187	-0.30235				
177 ->187	0.21898				
180 ->187	0.14787				
181 ->188	0.44949				
Excited State	17:	Singlet-A	4.7184 eV	262.77 nm	f=0.0045
174 ->187	0.24957				
178 ->187	0.54919				
179 ->188	-0.16829				
183 ->192	-0.10242				
184 ->193	0.11658				
185 ->194	0.10308				
Excited State	18:	Singlet-A	4.7195 eV	262.71 nm	f=0.0011
175 ->187	-0.22280				
176 ->187	0.15342				
178 ->188	-0.17176				
179 ->187	0.54790				
184 ->192	-0.11600				
Excited State	19:	Singlet-A	4.8370 eV	256.33 nm	f=0.0346

181 ->189 -0.30997
183 ->189 -0.20602
185 ->189 0.15498
186 ->189 0.12064
186 ->191 0.36520
186 ->195 0.22372
186 ->196 -0.29622

Excited State 20: Singlet-A 4.8387 eV 256.23 nm f=0.0004
174 ->187 0.24378
175 ->188 0.10251
176 ->188 0.11519
177 ->187 0.39416
181 ->188 -0.36576
182 ->193 -0.13858
185 ->192 -0.16223

Excited State 21: Singlet-A 4.8451 eV 255.90 nm f=0.0068
175 ->187 0.26735
176 ->187 0.40311
177 ->188 0.18425
180 ->188 0.15463
182 ->192 -0.17842
183 ->193 -0.10247
185 ->189 0.15326
185 ->193 -0.18952
186 ->196 -0.10692

Excited State 22: Singlet-A 4.8631 eV 254.95 nm f=0.0364
180 ->189 -0.20256
184 ->189 -0.20842
186 ->190 0.60314
186 ->197 0.15625

Excited State 23: Singlet-A 4.8882 eV 253.64 nm f=0.0034
175 ->187 -0.20606

180 ->188 0.62071
185 ->189 -0.11141

Excited State 24: Singlet-A 4.9041 eV 252.82 nm f=0.0064
169 ->187 -0.13019
172 ->187 -0.23152
173 ->187 0.38052
177 ->187 0.21973
181 ->188 0.29546
182 ->193 -0.12581
185 ->192 -0.17270

Excited State 25: Singlet-A 4.9344 eV 251.26 nm f=0.1412
176 ->187 -0.12794
185 ->189 0.55016
186 ->191 -0.34697

Excited State 26: Singlet-A 4.9813 eV 248.90 nm f=0.0204
180 ->188 0.11494
181 ->189 0.22272
183 ->189 0.18866
185 ->189 0.33049
186 ->191 0.44368
186 ->195 -0.16657
186 ->196 0.22153

Excited State 27: Singlet-A 5.0078 eV 247.58 nm f=0.0667
180 ->189 0.17697
184 ->189 0.53559
185 ->190 -0.17530
186 ->190 0.27820
186 ->197 -0.14716

Excited State 28: Singlet-A 5.0647 eV 244.80 nm f=0.0033
169 ->188 -0.13819
170 ->187 0.28215

171 ->187 -0.24208
172 ->188 -0.14440
173 ->188 0.24999
174 ->188 0.13469
178 ->188 -0.16728
179 ->187 -0.14997
184 ->192 -0.13504
185 ->193 -0.16969
186 ->193 0.18208

Excited State 29: Singlet-A 5.0802 eV 244.05 nm f=0.0011
174 ->187 -0.13131
175 ->188 0.25123
176 ->188 -0.24069
178 ->187 0.24462
179 ->188 0.31569
183 ->192 0.11966
184 ->193 -0.13312
186 ->192 0.32127

Excited State 30: Singlet-A 5.1079 eV 242.73 nm f=0.0830
177 ->187 0.14679
182 ->189 -0.16726
182 ->191 -0.16716
183 ->190 0.12893
184 ->189 0.17658
184 ->191 -0.15946
185 ->190 0.54186

Excited State 31: Singlet-A 5.1162 eV 242.34 nm f=0.1737
170 ->187 -0.11701
171 ->187 0.13500
178 ->188 -0.16080
179 ->187 -0.18459
183 ->193 0.10314
184 ->190 -0.21109

184 ->192 -0.10960
185 ->191 0.39327
186 ->193 0.26318

Excited State 32: Singlet-A 5.1262 eV 241.87 nm f=0.0171
174 ->187 0.18202
175 ->188 -0.26017
176 ->188 0.19481
177 ->187 -0.17359
179 ->188 -0.16100
184 ->193 -0.11954
185 ->192 -0.12494
186 ->192 0.47826

Excited State 33: Singlet-A 5.1295 eV 241.71 nm f=0.1307
170 ->187 0.18779
171 ->187 -0.10883
172 ->188 -0.11132
174 ->188 -0.11509
176 ->187 -0.10534
178 ->188 0.16815
179 ->187 0.12089
182 ->190 -0.15290
182 ->192 -0.10437
183 ->189 0.10104
183 ->193 -0.10306
184 ->190 -0.12525
185 ->191 0.40826
186 ->193 -0.21847

Excited State 34: Singlet-A 5.1524 eV 240.63 nm f=0.0109
173 ->188 -0.10767
174 ->188 -0.34141
176 ->187 -0.25942
177 ->188 0.15174
178 ->188 0.22563

180 ->188	0.13425				
184 ->192	-0.12018				
185 ->193	-0.14384				
186 ->193	0.35165				
Excited State 35:	Singlet-A	5.1975 eV	238.54 nm	f=0.0057	
172 ->187	-0.26073				
173 ->187	-0.10270				
177 ->187	0.17459				
180 ->189	0.19823				
182 ->189	0.44161				
184 ->189	-0.18652				
185 ->192	0.14740				
186 ->197	-0.15124				
Excited State 36:	Singlet-A	5.2118 eV	237.89 nm	f=0.0056	
173 ->187	0.19782				
175 ->188	-0.13018				
177 ->187	0.30028				
178 ->191	-0.11474				
179 ->190	-0.11370				
182 ->189	-0.18347				
182 ->193	0.15275				
184 ->193	0.13228				
185 ->190	-0.10967				
185 ->192	0.34814				
186 ->192	0.21310				
Excited State 37:	Singlet-A	5.2213 eV	237.46 nm	f=0.0329	
174 ->188	-0.14589				
175 ->187	0.22417				
176 ->187	0.24246				
178 ->190	0.10328				
179 ->191	0.10217				
181 ->189	-0.10867				
182 ->192	0.16925				

183 ->189 0.30146
185 ->193 0.28071
186 ->193 0.22482

Excited State 38: Singlet-A 5.2248 eV 237.30 nm f=0.0001
172 ->187 0.28719
173 ->187 0.22003
180 ->189 -0.23750
182 ->189 0.47081
184 ->189 0.19174
185 ->190 0.12995
186 ->197 0.10810

Excited State 39: Singlet-A 5.2305 eV 237.04 nm f=0.1506
174 ->188 0.21346
175 ->187 -0.18058
181 ->189 -0.13426
182 ->190 -0.18198
183 ->189 0.42890
183 ->191 0.16043
184 ->190 0.17337
185 ->191 -0.11477
186 ->196 -0.11543

Excited State 40: Singlet-A 5.2543 eV 235.97 nm f=0.0107
174 ->187 -0.17840
175 ->188 0.23990
177 ->191 0.10239
178 ->187 -0.16754
179 ->188 -0.15632
180 ->189 0.11757
182 ->193 -0.17415
183 ->192 -0.22793
184 ->193 0.19943
185 ->194 0.13568
186 ->192 0.31113

186 ->197 -0.10103

Table S2. Standard orientation of the optimized geometry for the colored isomer of bisDMDPI-BP.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.562323	1.456930	1.295777
2	7	0	1.868520	-0.729425	1.390837
3	7	0	-1.860009	0.098584	1.514667
4	7	0	-2.681491	-1.860834	0.645153
5	6	0	-1.819862	-1.255413	1.519776
6	6	0	1.766120	0.521962	1.900182
7	6	0	-3.319439	-0.857561	0.061965
8	6	0	-3.008396	1.788418	0.222865
9	6	0	-2.766448	0.405041	0.591382
10	6	0	-4.407759	-1.107655	-0.873201
11	6	0	0.132290	2.661069	4.481172
12	1	0	0.177641	3.697540	4.800152
13	6	0	0.019422	-0.023947	3.641368
14	6	0	-0.951603	-2.041654	2.373426
15	6	0	2.773102	-0.625346	0.422177
16	6	0	-2.690658	2.805289	1.147403
17	1	0	-2.299558	2.517141	2.116327
18	6	0	-3.350463	4.502138	-0.433975
19	6	0	4.726321	2.640994	-0.195444
20	1	0	4.599268	2.974045	0.828310
21	6	0	0.894553	0.884970	2.999259
22	6	0	4.502427	-1.904025	-0.872170
23	1	0	5.190344	-1.068957	-0.809168
24	6	0	4.060216	1.477181	-0.603424
25	6	0	2.395223	-2.940248	-0.334789
26	1	0	1.423405	-2.883750	0.141925
27	6	0	0.927020	2.222520	3.436146
28	1	0	1.597418	2.900689	2.921881
29	6	0	-0.069046	-1.481095	3.328043
30	6	0	5.673801	2.933045	-2.390208
31	6	0	-2.868392	4.134716	0.831014
32	1	0	-2.636200	4.919063	1.542807
33	6	0	-3.640708	3.512373	-1.376231
34	1	0	-3.985710	3.770110	-2.370070
35	6	0	-3.468436	2.174084	-1.043652
36	1	0	-3.668064	1.420542	-1.796494
37	6	0	-1.001307	-3.442041	2.232262
38	1	0	-1.690380	-3.847237	1.500701
39	6	0	3.188256	0.789399	0.339096
40	6	0	3.230937	-1.804766	-0.291016
41	6	0	4.202080	1.073912	-1.943689
42	1	0	3.660632	0.206689	-2.304158
43	6	0	2.799720	-4.097183	-0.965098
44	1	0	2.155000	-4.967818	-1.011941

45	6	0	4.923849	-3.069901	-1.500891
46	1	0	5.918890	-3.110885	-1.926944
47	6	0	5.532932	3.360236	-1.065819
48	1	0	6.042199	4.246929	-0.708052
49	6	0	-0.209076	-4.274137	3.003578
50	1	0	-0.265702	-5.350383	2.875518
51	6	0	-6.558344	-0.553192	-1.854632
52	1	0	-7.420724	0.098127	-1.942524
53	6	0	4.993687	1.788471	-2.822899
54	1	0	5.093861	1.488506	-3.860029
55	6	0	4.067981	-4.172399	-1.559478
56	6	0	-5.516696	-0.250882	-0.998088
57	1	0	-5.573101	0.647508	-0.393993
58	6	0	-4.405862	-2.289943	-1.626086
59	1	0	-3.567963	-2.968818	-1.515540
60	6	0	-6.525983	-1.725200	-2.619618
61	6	0	-5.440337	-2.598581	-2.497903
62	1	0	-5.394099	-3.515519	-3.072945
63	8	0	-7.586329	-1.925883	-3.435918
64	8	0	-3.491154	5.830157	-0.647012
65	8	0	4.370688	-5.349404	-2.153236
66	8	0	6.431361	3.555990	-3.322708
67	6	0	-7.613195	-3.102016	-4.213626
68	1	0	-8.541236	-3.063105	-4.783600
69	1	0	-6.765180	-3.145321	-4.906966
70	1	0	-7.612633	-4.000120	-3.585160
71	6	0	-3.962015	6.255163	-1.906481
72	1	0	-4.004006	7.343103	-1.859398
73	1	0	-3.282178	5.954165	-2.711958
74	1	0	-4.964531	5.863122	-2.113880
75	6	0	7.119348	4.727601	-2.945193
76	1	0	7.652940	5.061753	-3.834741
77	1	0	6.427297	5.513924	-2.622212
78	1	0	7.841144	4.529923	-2.144131
79	6	0	5.636728	-5.481817	-2.759787
80	1	0	6.446312	-5.367209	-2.029631
81	1	0	5.666947	-6.489284	-3.174173
82	1	0	5.773379	-4.754097	-3.568233
83	6	0	-0.717424	1.761317	5.121810
84	1	0	-1.342400	2.086776	5.947678
85	6	0	-0.761549	0.435692	4.701623
86	1	0	-1.424930	-0.265542	5.197620
87	6	0	0.706287	-2.339642	4.107040
88	1	0	1.375187	-1.906740	4.843753
89	6	0	0.650752	-3.720171	3.949853
90	1	0	1.274491	-4.359202	4.566972

SCF Done: E(UmPW1PW91)	=	-2293.89250767	A.U.
Zero-point correction	=	0.721013 (Hartree/Particle)	
Thermal correction to Energy	=	0.766679	
Thermal correction to Enthalpy	=	0.767623	
Thermal correction to Gibbs Free Energy	=	0.634249	
Sum of electronic and zero-point Energies	=	-2293.171495	
Sum of electronic and thermal Energies	=	-2293.125829	
Sum of electronic and thermal Enthalpies	=	-2293.124885	
Sum of electronic and thermal Free Energies	=	-2293.258258	

Low frequencies --- -3.1155 -0.0007 -0.0005 0.0003 1.6661 2.1577

Low frequencies --- 3.8066 7.2528 7.9975

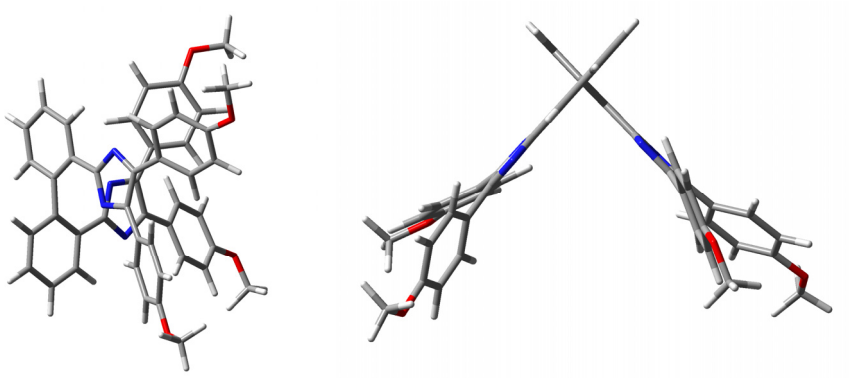

Fig. S12 Optimized structure of the colored isomer of bisDMDPI-BP.

The Result of the TDDFT calculation

Excited State 1: 1.224-A 1.3403 eV 925.07 nm f=0.0003 <S**2>=0.125

186A ->187A 0.33508

186B ->187B 0.93296

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -2293.84325378

Excited State 2: 1.217-A 1.3485 eV 919.45 nm f=0.0002 <S**2>=0.120

186A ->187A 0.93388

186B ->187B -0.33613

Excited State 3:	2.329-A	1.8677 eV	663.84 nm	f=0.0122	<S**2>=1.106
172A ->187A	0.10157				
184A ->187A	0.10183				
185A ->187A	0.39799				
186A ->188A	-0.12276				
172B ->187B	-0.19932				
184B ->187B	0.14674				
185B ->187B	0.82988				

Excited State 4:	2.332-A	1.8715 eV	662.50 nm	f=0.0771	<S**2>=1.109
172A ->187A	0.20894				
184A ->187A	0.19373				
185A ->187A	0.81862				
185B ->187B	-0.40392				
186B ->188B	-0.12494				

Excited State 5:	2.305-A	2.1351 eV	580.71 nm	f=0.0894	<S**2>=1.078
180A ->187A	-0.10639				
182A ->187A	-0.18853				
183A ->187A	-0.26488				
175B ->187B	-0.16625				
176B ->187B	-0.10983				
177B ->187B	0.19096				
179B ->187B	-0.13809				
180B ->187B	-0.30151				
182B ->187B	0.31096				
183B ->187B	0.68095				
184B ->187B	-0.22907				

Excited State 6:	2.301-A	2.1545 eV	575.47 nm	f=0.0431	<S**2>=1.074
175A ->187A	0.20164				
176A ->187A	0.23815				
178A ->187A	-0.11161				
179A ->187A	0.10220				
180A ->187A	0.30701				
181A ->187A	0.19501				

182A ->187A 0.53240
183A ->187A 0.50100
184A ->187A 0.13788
180B ->187B -0.15518
182B ->187B 0.17024
183B ->187B 0.23973

Excited State 7: 2.337-A 2.3036 eV 538.23 nm f=0.1445 <S**2>=1.115
175A ->187A -0.10207
176A ->187A -0.13788
180A ->187A -0.29545
181A ->187A -0.11457
182A ->187A -0.39444
183A ->187A 0.67569
180B ->187B -0.19105
182B ->187B 0.27226
183B ->187B -0.18120
186B ->189B -0.12811

Excited State 8: 2.351-A 2.3521 eV 527.13 nm f=0.1014 <S**2>=1.131
180A ->187A 0.11361
182A ->187A 0.14559
183A ->187A -0.34413
186A ->189A 0.14007
175B ->187B -0.13898
177B ->187B 0.17820
179B ->187B -0.11197
180B ->187B -0.33086
182B ->187B 0.54389
183B ->187B -0.48597
184B ->187B 0.20517

Excited State 9: 2.303-A 2.4850 eV 498.92 nm f=0.0073 <S**2>=1.076
180A ->187A -0.14429
181A ->187A 0.38353
182A ->187A -0.16388

184A ->187A 0.85473
185A ->187A -0.19299

Excited State 10: 2.292-A 2.5106 eV 493.85 nm f=0.0017 <S**2>=1.064
182B ->187B -0.12054
183B ->187B 0.30628
184B ->187B 0.91402
185B ->187B -0.18290

Excited State 11: 2.332-A 2.5346 eV 489.17 nm f=0.0282 <S**2>=1.110
184A ->187A -0.11301
178B ->187B 0.10640
180B ->187B -0.12097
181B ->187B 0.92566
182B ->187B -0.17390

Excited State 12: 2.322-A 2.5867 eV 479.32 nm f=0.0238 <S**2>=1.098
178A ->187A -0.10226
181A ->187A 0.80708
182A ->187A -0.31164
184A ->187A -0.39703
185A ->187A 0.10395
181B ->187B -0.12016

Excited State 13: 2.307-A 2.7990 eV 442.96 nm f=0.0079 <S**2>=1.081
169B ->187B 0.17886
172B ->187B 0.39219
173B ->187B 0.13720
174B ->187B -0.17159
175B ->187B 0.12990
176B ->187B 0.28896
177B ->187B -0.39488
179B ->187B 0.19192
180B ->187B 0.32266
181B ->187B 0.16602
182B ->187B 0.52505

183B ->187B 0.13954
185B ->187B 0.10183

Excited State 14: 2.315-A 2.8136 eV 440.66 nm f=0.0091 <S**2>=1.090
169A ->187A 0.21045
170A ->187A -0.17702
172A ->187A 0.34208
175A ->187A 0.24376
176A ->187A 0.62368
177A ->187A -0.18570
178A ->187A -0.13069
179A ->187A 0.19667
180A ->187A 0.12100
181A ->187A -0.18938
182A ->187A -0.36991
185A ->187A -0.17530

Excited State 15: 2.304-A 2.8913 eV 428.81 nm f=0.0055 <S**2>=1.077
172A ->187A -0.25692
176A ->187A -0.21818
180A ->187A 0.79245
181A ->187A -0.11459
182A ->187A -0.42531
184A ->187A 0.10405

Excited State 16: 2.310-A 2.9130 eV 425.62 nm f=0.0021 <S**2>=1.084
169B ->187B -0.16882
172B ->187B -0.36919
176B ->187B -0.19089
177B ->187B 0.39095
178B ->187B 0.11628
180B ->187B 0.66268
181B ->187B 0.14621
182B ->187B 0.32874
185B ->187B -0.10232

Excited State 17: 2.341-A 3.0074 eV 412.27 nm f=0.0061 <S**2>=1.120

172B ->187B	-0.20103
179B ->187B	0.88629
180B ->187B	-0.30011

Excited State 18: 2.354-A 3.0271 eV 409.58 nm f=0.0029 <S**2>=1.135

172A ->187A	0.15059
176A ->187A	0.20935
177A ->187A	-0.13465
178A ->187A	0.63854
179A ->187A	-0.62441
180A ->187A	0.16999

Excited State 19: 2.456-A 3.0809 eV 402.43 nm f=0.0196 <S**2>=1.258

182A ->189A	-0.11433
186A ->189A	0.20797
186A ->198A	-0.13305
170B ->187B	0.12095
172B ->187B	0.44160
173B ->187B	0.37284
174B ->187B	-0.14259
175B ->187B	-0.10605
177B ->187B	0.46350
178B ->187B	0.31910
179B ->187B	0.16263
181B ->187B	-0.12044
182B ->187B	-0.18672
183B ->191B	-0.10480
185B ->187B	0.10911

Excited State 20: 2.519-A 3.0945 eV 400.66 nm f=0.0082 <S**2>=1.336

171A ->187A	-0.12009
172A ->187A	0.13289
173A ->187A	-0.33105
174A ->187A	-0.15617
175A ->187A	0.27269

177A ->187A 0.46569
178A ->187A 0.45178
179A ->187A 0.25422
181A ->197A -0.10250
183A ->191A -0.12546
182B ->189B 0.13984
184B ->188B 0.11912
186B ->189B -0.21729
186B ->198B 0.16882

Excited State 21: 2.463-A 3.1621 eV 392.10 nm f=0.0085 <S**2>=1.267
182A ->189A 0.10763
186A ->189A -0.17728
186A ->198A 0.12481
170B ->187B 0.11626
172B ->187B 0.46189
173B ->187B -0.38211
174B ->187B 0.20601
175B ->187B -0.44862
176B ->187B -0.20314
178B ->187B -0.16141
179B ->187B 0.19738
180B ->187B 0.20975
182B ->187B -0.10842

Excited State 22: 2.352-A 3.1899 eV 388.68 nm f=0.0182 <S**2>=1.133
172A ->187A 0.74491
175A ->187A -0.36992
176A ->187A -0.27282
179A ->187A 0.14037
180A ->187A 0.23445
181A ->187A 0.15014
182A ->187A 0.14380
185A ->187A -0.13728

Excited State 23: 2.380-A 3.2359 eV 383.16 nm f=0.0107 <S**2>=1.166

186A ->188A 0.14611
186A ->189A -0.14011
172B ->187B 0.28946
173B ->187B -0.25872
175B ->187B 0.77309
176B ->187B -0.24214
177B ->187B 0.26039

Excited State 24: 2.384-A 3.2433 eV 382.28 nm f=0.0120 <S**2>=1.171
172A ->187A 0.18347
173A ->187A 0.37983
174A ->187A 0.29401
175A ->187A 0.66296
176A ->187A -0.36211
177A ->187A 0.17387
186B ->188B -0.16526
186B ->189B 0.14693

Excited State 25: 2.779-A 3.2747 eV 378.61 nm f=0.0138 <S**2>=1.680
175A ->187A 0.12198
183A ->190A -0.12514
185A ->187A 0.12792
185A ->199A -0.11765
186A ->188A 0.45531
175B ->187B -0.13653
182B ->188B 0.11709
183B ->190B 0.10230
184B ->189B 0.11242
184B ->198B 0.12041
186B ->188B 0.63525

Excited State 26: 2.786-A 3.2834 eV 377.60 nm f=0.2376 <S**2>=1.691
182A ->188A 0.11407
184A ->189A -0.10545
184A ->198A -0.12171
185A ->187A -0.10068

186A ->188A 0.64085
175B ->187B -0.10646
178B ->187B -0.11342
179B ->193B -0.10139
183B ->190B 0.11697
185B ->187B 0.14066
185B ->199B 0.12111
186B ->188B -0.45507

Excited State 27: 2.461-A 3.3188 eV 373.58 nm f=0.0242 <S**2>=1.264
171A ->187A -0.13008
172A ->187A 0.13291
173A ->187A -0.22773
175A ->187A 0.14541
178A ->187A -0.31013
179A ->187A -0.41172
180A ->187A 0.10973
183A ->187A -0.11644
186A ->189A -0.16568
173B ->187B -0.18711
176B ->187B 0.22421
178B ->187B 0.48534
186B ->189B -0.26029
186B ->190B -0.10433

Excited State 28: 2.411-A 3.3367 eV 371.58 nm f=0.0536 <S**2>=1.204
171A ->187A 0.11189
173A ->187A 0.21581
175A ->187A -0.15087
178A ->187A 0.28934
179A ->187A 0.36636
186A ->189A -0.16680
173B ->187B -0.22434
176B ->187B 0.26623
178B ->187B 0.58716
186B ->188B -0.10653

186B ->189B 0.18574

Excited State 29: 3.127-A 3.4949 eV 354.76 nm f=0.2529 <S**2>=2.195

169A ->187A 0.12869
173A ->187A 0.12581
174A ->192A -0.12274
178A ->187A 0.13472
183A ->187A -0.12504
183A ->199A 0.10032
184A ->188A -0.24990
185A ->189A -0.10595
185A ->190A 0.23405
186A ->189A 0.31795
186A ->190A 0.12869
186A ->198A 0.13753
169B ->187B -0.13890
174B ->192B 0.12972
175B ->193B 0.10079
179B ->195B -0.11105
183B ->187B 0.13785
184B ->188B -0.26264
185B ->189B -0.11361
185B ->190B 0.21615
186B ->189B -0.29669
186B ->190B -0.13677
186B ->198B -0.14937

Excited State 30: 2.566-A 3.5130 eV 352.93 nm f=0.0302 <S**2>=1.396

168A ->187A -0.20303
169A ->187A 0.69903
170A ->187A -0.31684
176A ->187A -0.19696
178A ->187A 0.18886
181A ->187A 0.10709
184A ->188A 0.16960
185A ->187A 0.11628

186A ->189A -0.14547
185B ->190B -0.16134

Excited State 31: 3.152-A 3.5241 eV 351.82 nm f=0.1284 <S**2>=2.234
169A ->187A 0.34993
170A ->187A -0.14800
174A ->192A -0.12744
175A ->193A -0.10204
183A ->187A 0.14328
184A ->188A -0.22871
185A ->189A 0.11367
185A ->190A -0.23388
186A ->189A 0.20447
186A ->198A 0.13174
169B ->187B 0.11036
174B ->192B -0.14683
175B ->193B 0.10097
179B ->195B -0.11212
183B ->187B 0.11651
184B ->188B 0.24633
185B ->189B -0.11216
185B ->190B 0.22999
186B ->189B 0.23740
186B ->198B 0.13666

Excited State 32: 2.448-A 3.5312 eV 351.11 nm f=0.0396 <S**2>=1.249
186A ->189A -0.10476
168B ->187B -0.22380
169B ->187B 0.78403
170B ->187B -0.28994
176B ->187B -0.11520
177B ->187B 0.14545
179B ->187B -0.12213
185B ->187B -0.12904

Excited State 33: 2.432-A 3.5672 eV 347.56 nm f=0.0087 <S**2>=1.228

169A ->187A 0.12861
174A ->187A 0.13087
175A ->187A -0.15963
176A ->187A 0.30148
177A ->187A 0.77706
178A ->187A -0.23808
179A ->187A -0.26159
185A ->190A 0.10094
184B ->188B -0.10277
186B ->189B 0.10425

Excited State 34: 2.354-A 3.5861 eV 345.74 nm f=0.0068 <S**2>=1.136
174B ->187B 0.12730
176B ->187B 0.73564
177B ->187B 0.46628
178B ->187B -0.39707

Excited State 35: 2.776-A 3.6345 eV 341.14 nm f=0.1567 <S**2>=1.676
173A ->187A -0.32644
174A ->187A -0.18371
175A ->187A 0.12384
180A ->196A 0.11927
182A ->189A 0.11628
183A ->191A 0.12060
184A ->188A -0.13606
185A ->190A 0.12121
186A ->189A -0.30148
186A ->190A -0.12199
169B ->187B -0.18145
173B ->187B 0.45645
174B ->187B -0.20933
176B ->187B -0.16174
181B ->197B 0.11806
183B ->191B 0.15368
185B ->190B 0.14710
186B ->189B 0.22651

Excited State 36: 2.673-A 3.6514 eV 339.55 nm f=0.1516 <S**2>=1.536

173A ->187A	0.46554
174A ->187A	0.28844
175A ->187A	-0.22228
176A ->187A	0.12827
181A ->197A	-0.10464
183A ->191A	-0.14392
186A ->189A	-0.22385
173B ->187B	0.33576
174B ->187B	-0.18609
176B ->187B	-0.16342
180B ->196B	-0.14601
181B ->197B	0.10511
183B ->191B	0.11389
186B ->189B	-0.29698
186B ->190B	-0.12627

Excited State 37: 2.301-A 3.7931 eV 326.87 nm f=0.0043 <S**2>=1.074

171B ->187B	0.14193
173B ->187B	0.36179
174B ->187B	0.86852
175B ->187B	0.12131
177B ->187B	-0.12096
178B ->187B	0.19516

Excited State 38: 2.304-A 3.8139 eV 325.08 nm f=0.0071 <S**2>=1.077

171A ->187A	-0.20101
173A ->187A	-0.40340
174A ->187A	0.84066
175A ->187A	-0.11358
177A ->187A	-0.11496
178A ->187A	0.12495
179A ->187A	0.15073

Excited State 39: 2.849-A 3.8954 eV 318.28 nm f=0.0042 <S**2>=1.780

178A ->193A 0.10820
183A ->193A -0.17472
185A ->191A 0.15529
185A ->195A 0.15419
186A ->192A -0.18724
182B ->192B 0.14719
184B ->189B -0.13600
184B ->194B -0.18692
186B ->188B 0.22700
186B ->192B 0.74657

Excited State 40: 2.858-A 3.8979 eV 318.08 nm f=0.0069 <S**2>=1.792
182A ->192A 0.14354
184A ->189A -0.13458
184A ->194A -0.18328
186A ->188A -0.22914
186A ->192A 0.74002
179B ->193B -0.12721
183B ->193B 0.17514
185B ->191B 0.15957
185B ->195B 0.15533
186B ->192B 0.18203

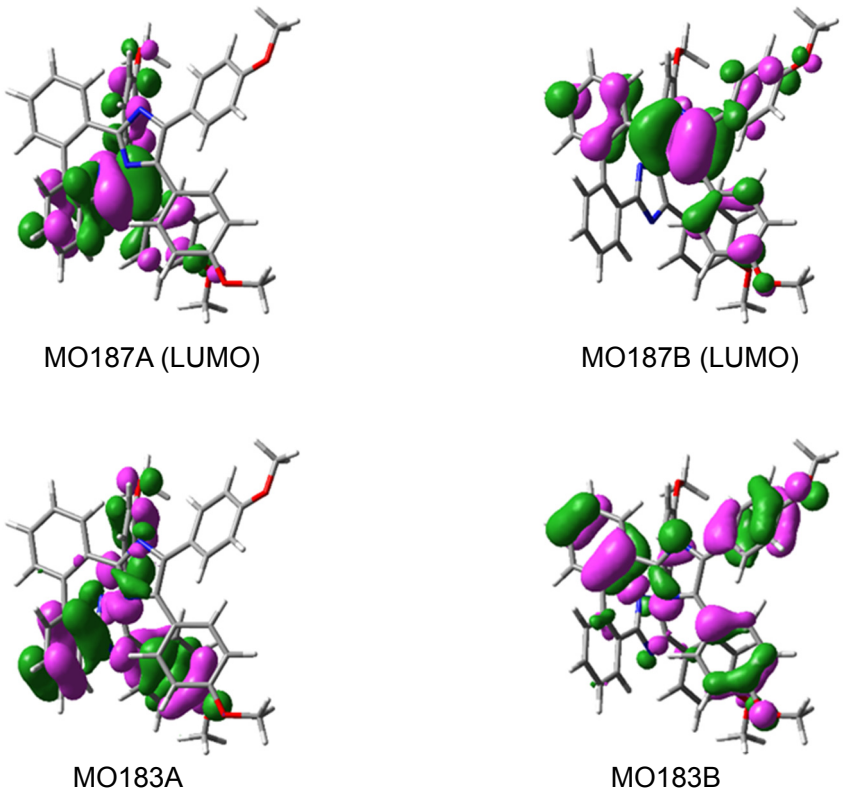

Fig. S13 Relevant molecular orbitals of the colored isomer of bisDMDPI-BP obtained by the UMPW1PW91/6-31G(d) level of the theory.

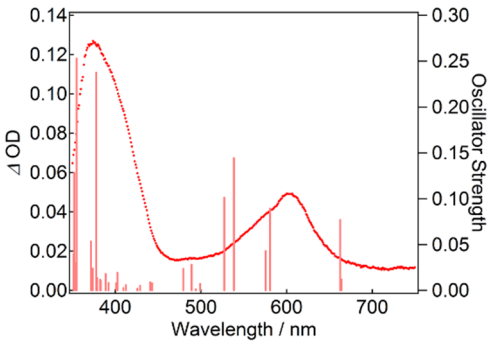

Fig. S14 Transient absorption spectrum (dotted line) and the oscillator strength (vertical lines) obtained by the TDDFT calculations (UMPW1PW91/6-31G(d) //UMPW1PW91/6-31G(d)).

6. Complete reference 25

Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

7. References

S1) A. Jacquart, R. M. Williams, A. M. Brouwer and E. Ishow, *Chem. - Eur. J.*, 2012, **18**, 3706–3720.

S2) J. J. Snellenburg, S. P. Laptenok, R. Seger, K. M. Mullen, and I. H. M. van Stokkum, *J. Stat. Softw.*, 2012, **49**, 1–22.s

S3) Y. Zhao and D. G. Truhlar, *J. Phys. Chem. A*, 2008, **112**, 1095-1099.

S4) Y. Zhao and D. G. Truhlar, *Acc. Chem. Res.*, 2008, **41**, 157-167.