Supporting Information (SI)

Lattice solvent controlled photochromism of tripyridyl-triazine-based zinc bromide complexes

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Content

1. Figures

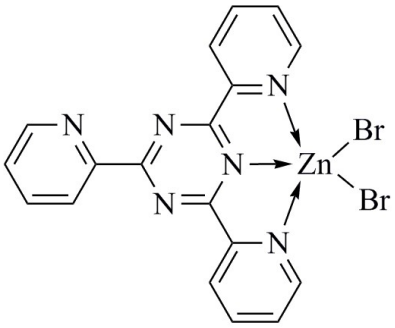

Fig. S1 The Chem Draw type diagram of the chemical formula of [$ZnBr_2$(2-TPT)].

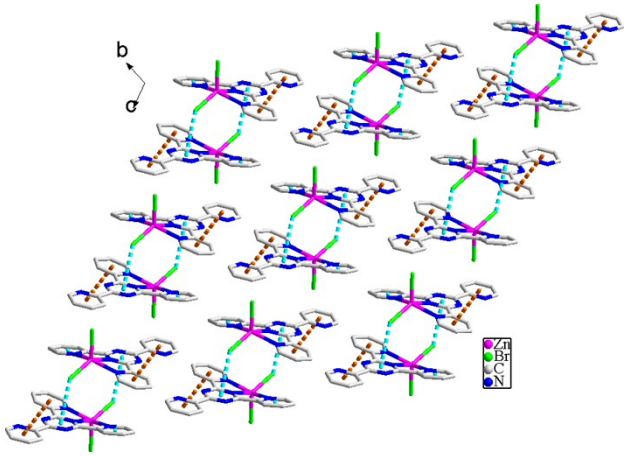

Fig. S2 View of the packing diagram of **1**.

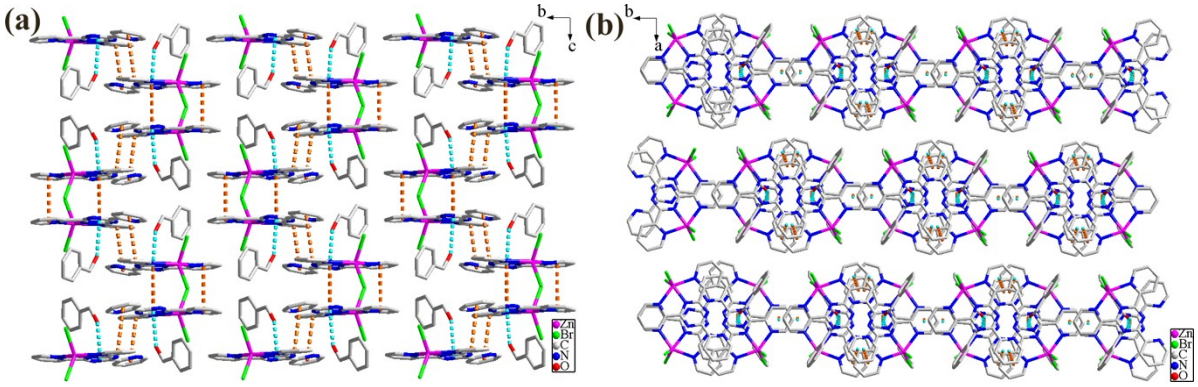

Fig. S3 View of the packing diagram of **2**.

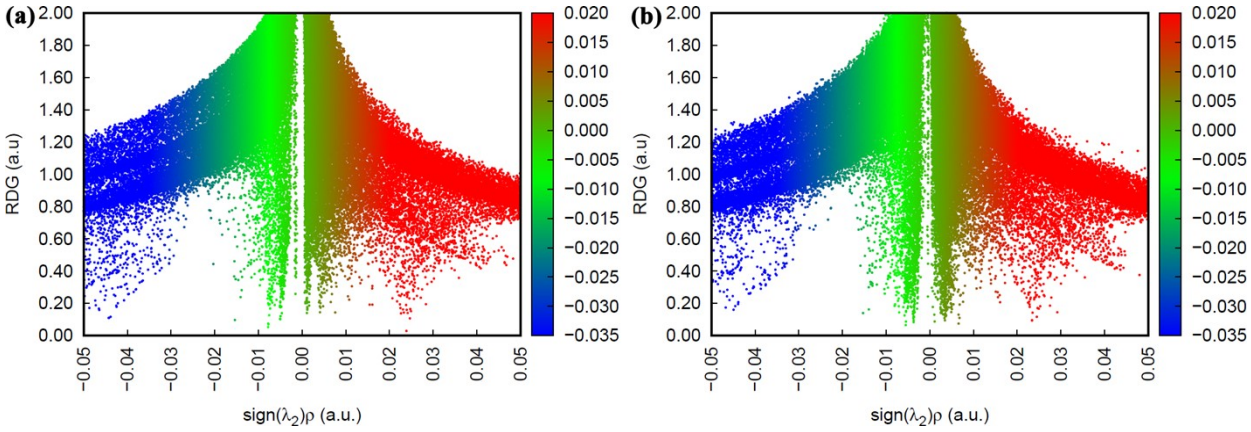

Fig. S4 The scatter graph of **1** (a) and **2** (b).

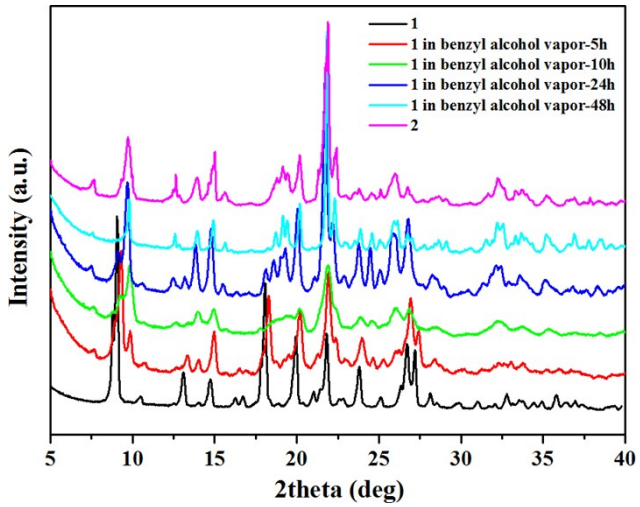

Fig. S5 Powder X-ray diffraction (PXRD) patterns of **1** transform into **2**.

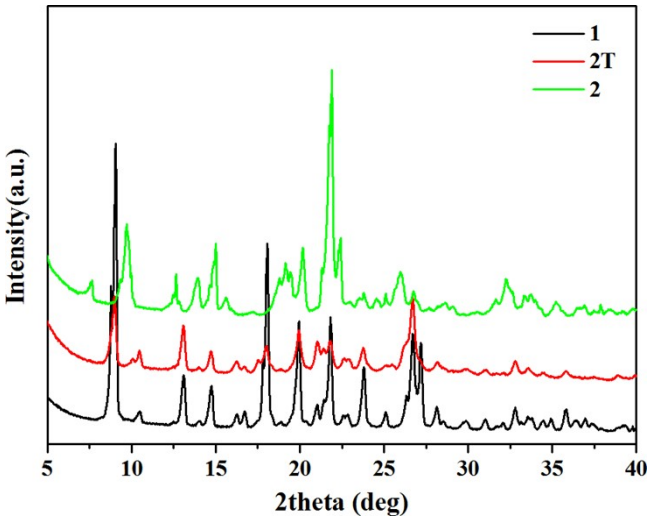

Fig. S6 Powder X-ray diffraction (PXRD) patterns of **2** transform into **1**.

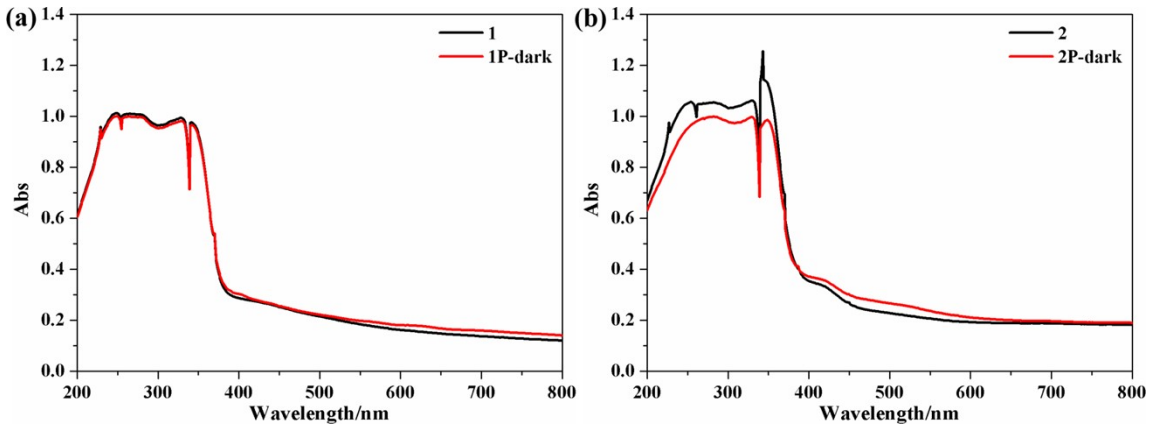

Fig. S7 The comparison UV-vis absorption spectra of **1** and **2** before and after light irradiation.

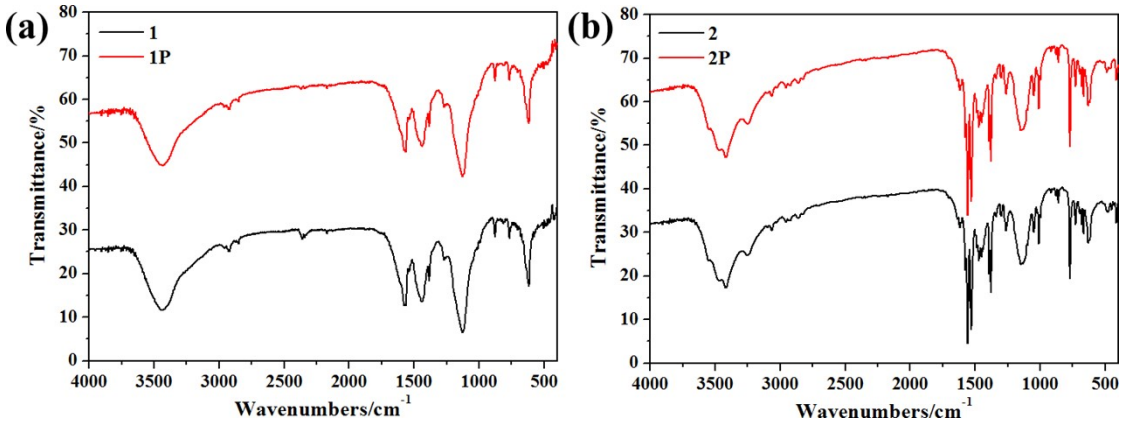

Fig. S8 IR spectra of **1, 1P, 2** and **2P**.

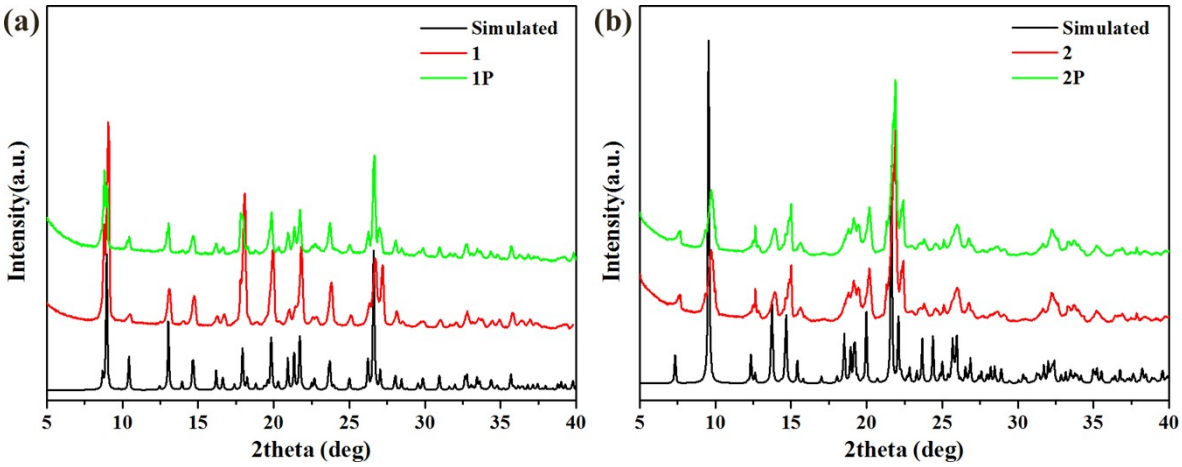

Fig. S9 Powder X-ray diffraction (PXRD) patterns of **1**, **1P**, **2** and **2P** at room temperature.

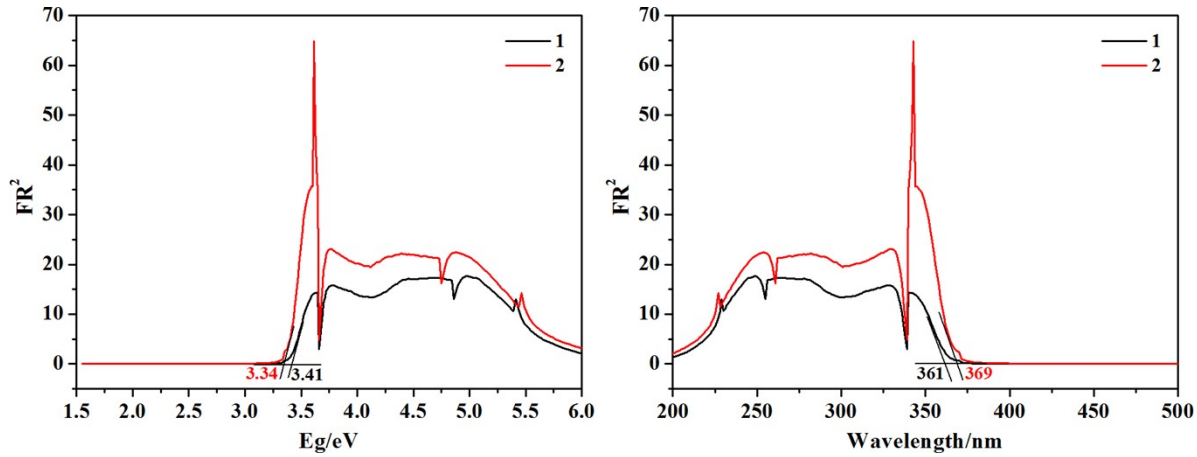

Fig. S10 The comparison of energy gaps and UV-vis absorption spectra of **1** and **2** before irradiation.

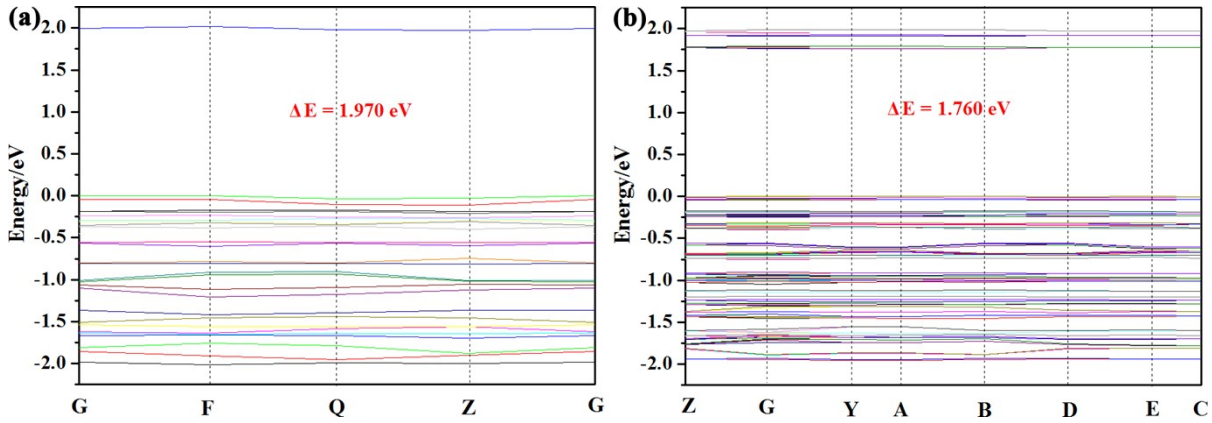

Fig. S11 Calculated band structures of **1** (a) and **2** (b).

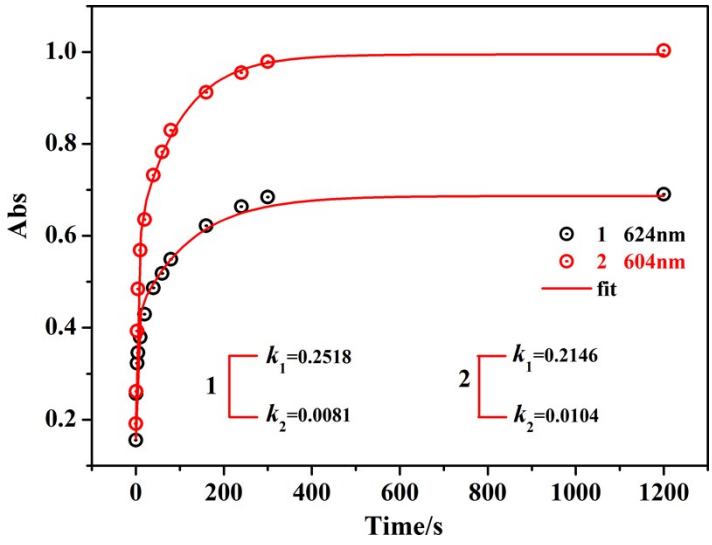

Fig. S12 Abs(*t*) *vs. t* plots for **1-2**. The lines show the fits of the plots according to rate law Abs(*t*) = A_0 + A_1(exp(-k_1t) + exp(-k_2t)) (*inset*: coloration rate constant values of **1-2**). (λ_{max} = 484 nm).

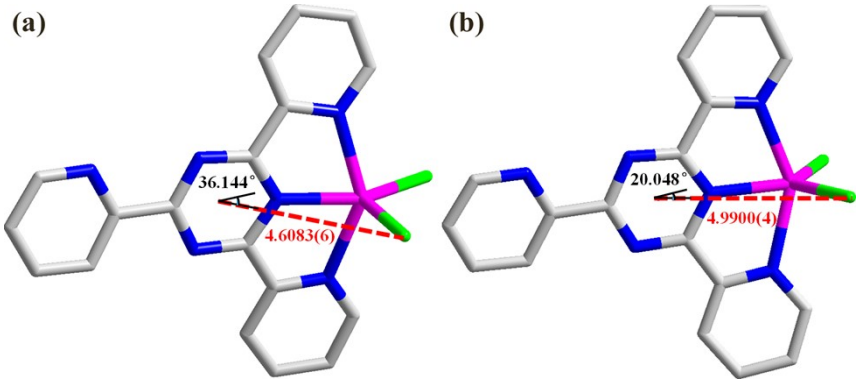

Fig. S13 View of the monomer diagrams of **1** (a) and **2** (b).

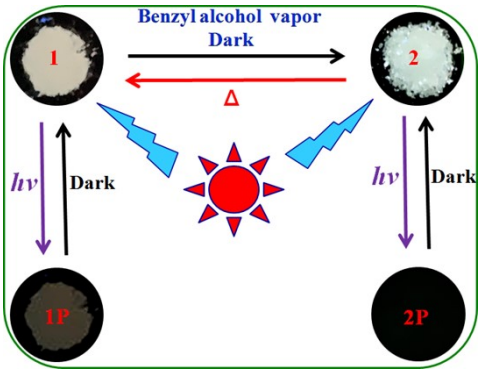

Fig. S14 Photographs showing the fluorescence of **1** and **2**.

2. Tables

Table S1 Crystallographic data and refinement parameters of compounds **1** and **2**.

Compounds	**1**	**2**
CCDC code	1977000	1977001
Temperature (K)	293(2)	273(2)
Empirical formula	$C_{18}H_{12}N_6ZnBr_2$	$C_{25}H_{20}N_6ZnBr_2O$
Formula weight	537.53	645.66
Crystal size (mm)	0.20 x 0.15 x 0.06	0.30 x 0.08 x 0.07
Crystal system	Triclinic	Monoclinic
Space group	*P*-1	*C* 2/*c*
a (Å)	8.6016(10)	24.165(3)
b (Å)	10.7273(16)	14.3269(19)
c (Å)	11.1433(11)	14.6252(19)
α (°)	112.148(12)	90
β (°)	97.577(9)	93.818(4)
γ (°)	92.538(10)	90
V (Å^3)	939.1(2)	5052.2(11)
Z	2	8
D_c (g cm^{-3})	1.901	1.698
F(000)	524	2560
μ (mm^{-1})	1.901	4.166
ϑ range (°)	4.34 to 71.26	2.20 to 28.38
Reflections collected	6184	37018
Unique reflections	3572	6319
R_{int}	0.0743	0.1048
Goodness-of-fit on F^2	0.983	1.075
R_1/wR_2, [$I \geq 2\sigma(I)$][a,b]	0.0650/0.1372	0.0650/0.2765
R_1/wR_2, (all data)	0.1194/0.1820	0.2021/0.3265
$\Delta\rho_{max}/\Delta\rho_{min}$ (e Å^{-3})	0.649/-0.819	1.582/-0.929

Table S2 Selected bond lengths (Å) and angles (°) of **1** and **2.**

Compound **1**			
Zn(1)-N(1)	2.258(7)	Zn(1)-N(2)	2.067(7)
Zn(1)-N(3)	2.305(7)	Zn(1)-Br(1)	2.3777(15)
Zn(1)-Br(2)	2.3889(16)		
N(2)-Zn(1)-N(1)	72.8(3)	N(2)-Zn(1)-N(3)	73.2(3)
N(1)-Zn(1)-N(3)	142.2(3)	N(2)-Zn(1)-Br(1)	140.22(19)
N(1)-Zn(1)-Br(1)	98.82(18)	N(3)-Zn(1)-Br(1)	96.66(19)
N(2)-Zn(1)-Br(2)	106.17(19)	N(1)-Zn(1)-Br(2)	103.78(19)
N(3)-Zn(1)-Br(2)	101.15(19)	Br(1)-Zn(1)-Br(2)	113.56(6)
Compound **2**			
Zn(1)-N(1)	2.281(9)	Zn(1)-N(2)	2.095(8)
Zn(1)-N(3)	2.277(10)	Zn(1)-Br(1)	2.3552(19)
Zn(1)-Br(2)	2.3650(19)		
N(2)-Zn(1)-N(1)	73.1(3)	N(2)-Zn(1)-N(3)	72.5(3)
N(1)-Zn(1)-N(3)	145.6(3)	N(2)-Zn(1)-Br(1)	122.0(2)
N(1)-Zn(1)-Br(1)	100.8(2)	N(3)-Zn(1)-Br(1)	97.9(2)
N(2)-Zn(1)-Br(2)	116.9(2)	N(1)-Zn(1)-Br(2)	95.7(3)
N(3)-Zn(1)-Br(2)	99.0(2)	Br(1)-Zn(1)-Br(2)	121.09(8)

Table S3 Anisotropic displacement parameters U_{ij} ($Å^2 \times 10^3$) for **1** and **2.**

Compound **1**						
Atom	U_{11}	U22	U33	U23	U13	U12
Zn1	37.4(7)	62.2(8)	51.6(7)	17.1(6)	0.5(5)	-1.4(6)
Br1	58.4(7)	87.7(9)	53.5(6)	18.4(6)	-7.8(5)	-3.4(6)
Br2	45.3(6)	105.0(10)	76.1(8)	49.8(7)	7.8(5)	8.3(6)
C1	40(6)	87(8)	64(6)	25(6)	-9(5)	-5(5)
C2	57(7)	78(8)	89(8)	27(7)	3(6)	23(6)
C3	43(5)	60(7)	72(7)	11(5)	5(5)	16(5)
C4	43(5)	50(6)	63(6)	8(5)	3(4)	7(4)
C5	35(5)	53(6)	53(5)	14(4)	5(4)	12(4)
C6	32(4)	46(5)	53(5)	16(4)	-1(4)	-2(4)
C7	31(5)	62(7)	95(8)	28(6)	6(5)	1(4)
C8	56(7)	74(9)	119(11)	21(8)	14(7)	12(6)
C9	80(8)	50(7)	88(8)	11(6)	20(7)	20(6)
C10	53(6)	56(6)	60(6)	13(5)	2(5)	-5(5)
C11	29(4)	54(6)	44(5)	18(4)	2(3)	3(4)
C12	43(5)	46(5)	46(5)	18(4)	1(4)	-9(4)
C13	26(4)	57(6)	52(5)	22(4)	0(3)	0(4)
C14	60(7)	60(7)	78(7)	8(6)	-9(5)	14(5)
C15	58(6)	67(7)	59(6)	12(5)	-10(5)	-21(5)
C16	37(5)	93(9)	67(7)	39(6)	-13(5)	-6(5)
C17	48(6)	57(6)	61(6)	22(5)	1(4)	5(5)
C18	35(5)	47(5)	53(5)	19(4)	0(4)	-2(4)
N1	34(4)	60(5)	54(4)	15(4)	6(3)	4(3)
N2	35(4)	49(5)	50(4)	14(4)	8(3)	4(3)
N3	38(4)	55(5)	58(5)	17(4)	5(3)	2(3)
N4	51(5)	62(6)	61(5)	12(4)	-4(4)	3(4)
N5	37(4)	56(5)	50(4)	18(4)	3(3)	8(3)
N6	36(4)	61(5)	55(5)	16(4)	4(3)	10(3)

Compound **2**						
Atom	U_{11}	U22	U33	U23	U13	U12
Zn1	41.2(7)	57.1(9)	56.3(8)	1.0(6)	5.0(5)	6.3(6)
Br1	62.0(9)	103.8(12)	81.7(10)	22.7(9)	-11.4(7)	5.8(8)
Br2	77.6(10)	71.5(9)	76.2(9)	-14.9(7)	32.5(7)	-7.8(7)
C1	70(9)	61(9)	70(8)	-2(7)	10(7)	-4(7)
C2	97(12)	53(8)	107(12)	19(8)	0(9)	-22(8)
C3	67(9)	75(10)	105(12)	25(9)	-3(8)	-20(8)
C4	61(8)	74(9)	53(7)	10(6)	-6(6)	-14(7)
C5	46(6)	64(8)	39(6)	0(5)	-3(5)	-14(6)
C6	39(6)	60(7)	49(6)	-4(5)	-2(5)	-9(5)
C7	31(5)	69(8)	37(5)	0(5)	-6(4)	7(5)
C8	33(5)	45(6)	40(5)	-2(5)	1(4)	-1(5)
C9	32(5)	54(7)	41(6)	-7(5)	-2(4)	-6(5)
C10	37(6)	56(7)	60(7)	-16(6)	-1(5)	-6(5)
C11	47(7)	57(8)	78(9)	-10(6)	4(6)	-10(6)
C12	23(5)	70(8)	101(10)	1(7)	9(5)	-6(6)
C13	31(6)	61(8)	90(9)	0(7)	3(6)	2(5)
C14	29(5)	74(8)	35(5)	-7(5)	-2(4)	9(5)
C15	39(6)	86(9)	58(7)	-12(6)	2(5)	-6(6)
C16	31(6)	132(15)	65(8)	-6(9)	8(5)	19(8)
C17	47(8)	117(14)	78(10)	-13(9)	-7(7)	36(9)
C18	53(8)	91(10)	67(8)	-23(7)	-3(6)	23(7)
C19	140(15)	91(11)	48(8)	11(8)	-10(9)	-19(11)
C20	135(17)	126(16)	95(14)	2(12)	-37(12)	-65(14)
C21	113(15)	160(20)	92(14)	39(13)	-20(11)	-66(14)
C22	92(11)	142(15)	61(9)	-1(9)	-17(8)	-59(11)
C23	71(9)	85(10)	64(9)	2(7)	6(7)	-16(8)
C24	76(9)	48(7)	62(8)	2(6)	-18(7)	7(6)
C25	114(12)	54(8)	66(9)	4(7)	34(9)	12(8)
N1	45(6)	56(6)	62(6)	7(5)	4(4)	-3(5)
N2	33(4)	50(5)	44(5)	-3(4)	-2(4)	-1(4)

N3	34(5)	56(6)	63(6)	-3(5)	5(4)	5(4)
N4	37(5)	64(6)	43(5)	1(4)	1(4)	-4(4)
N5	37(5)	51(5)	44(5)	-11(4)	0(4)	-6(4)
N6	45(5)	76(8)	56(6)	-9(5)	-2(4)	19(5)
O1	69(6)	134(10)	71(7)	24(6)	-5(5)	-11(6)

Table S4 Hydrogen bonds of compound **1** and **2** (Å and °).

Compound **1**				
D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
C(2)-H(2)...Br(1)#1	0.93	3.04	3.780(11)	137.7
C(7)-H(7)...Br(2)#2	0.93	2.94	3.762(9)	148.9
C(14)-H(14)...Br(1)#3	0.93	3.14	3.995(11)	154.1
C(2)-H(2)...Br(1)#1	0.93	3.04	3.780(11)	137.7
C(7)-H(7)...Br(2)#2	0.93	2.94	3.762(9)	148.9
C(14)-H(14)...Br(1)#3	0.93	3.14	3.995(11)	154.1
C(2)-H(2)...Br(1)#1	0.93	3.04	3.780(11)	137.7
C(7)-H(7)...Br(2)#2	0.93	2.94	3.762(9)	148.9
C(14)-H(14)...Br(1)#3	0.93	3.14	3.995(11)	154.1
C(2)-H(2)...Br(1)#1	0.93	3.04	3.780(11)	137.7
Symmetry code: #1 -x+2,-y+1,-z+1; #2 x-1,y,z; #3 x-1,y-1,z-1				

Compound **2**				
D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
C(4)-H(4)...Br(1)#1	0.93	3.09	3.906(14)	146.8
C(10)-H(10)...O(1)	0.93	2.52	3.441(16)	172.1
C(12)-H(12)...Br(2)#2	0.93	3.07	3.627(12)	120.3
C(13)-H(13)...Br(2)#2	0.93	2.88	3.546(11)	130.0
C(18)-H(18)...Br(2)#3	0.93	2.89	3.721(16)	149.4
Symmetry code: #1 -x,y,-z+1/2; #2 –x+1/2,-y+1/2,-z; #3 -x,-y+1,-z				

Table S5 Selected QTAIM parameters [a.u.] and interaction energies E [kJ·mol^{-1}] for compounds **1** and **2**.

Compounds	Interactions	ρ_{CP}	$\nabla^2\rho$	V_{BCP}	G_{BCP}	H_{BCP}	E
1	n-π	0.0078	0.0243	-0.0039	0.0050	0.0011	-5.10
	π-π	0.0051	0.0128	-0.0021	0.0026	0.0006	-2.72
2	n-π	0.0082	0.0324	-0.0051	0.0066	0.0015	-6.70
	π-π	0.0054	0.0150	-0.0023	0.0030	0.0007	-3.02
	π-π	0.0059	0.0162	-0.0025	0.0033	0.0008	-3.28
	π-π	0.0056	0.0176	-0.0030	0.0037	0.0007	-3.94

Table S6 Reflectivity (R%) of the wavelengths (200-500nm) of compounds **1** and **2.**

Wavelengthes	Compound **1**	Compound **2**
200	1.361197185	2.083747983
201	1.462336764	2.239696486
202	1.572079351	2.390496694
203	1.681291943	2.537626072
204	1.796874132	2.709152124
205	1.92883629	2.894520727
206	2.079305702	3.061744051
207	2.21771774	3.23294619
208	2.37719098	3.416938995
209	2.539381665	3.626682392
210	2.716588303	3.814951316
211	2.912262539	4.032643735
212	3.130518927	4.255628419
213	3.353877444	4.503785749
214	3.555555629	4.746376213
215	3.799980619	5.016266079
216	4.056317397	5.306279247
217	4.310948169	5.635624872
218	4.576563395	5.971813676
219	4.86883109	6.341312445
220	5.216772522	6.743390961
221	5.600494144	7.189881003
222	6.001547228	7.713687963
223	6.48353165	8.35610801
224	6.97833909	9.121696399
225	7.556732479	10.15083216
226	8.28629637	11.67032381
227	9.219651434	14.30256136
228	10.63200039	11.52230575
229	12.97017547	12.06189074

230	10.59474498	12.69720972
231	11.12075509	13.26367253
232	11.70420402	13.87682567
233	12.25150329	14.47452367
234	12.77781022	14.96781962
235	13.22570954	15.54662248
236	13.65660908	16.12766827
237	14.14858674	16.67224819
238	14.58192118	17.19505533
239	15.05293682	17.71305953
240	15.46769949	18.25556108
241	15.83917322	18.69844288
242	16.23709012	19.22585427
243	16.68162205	19.62492802
244	17.07014191	20.06494318
245	17.23365881	20.50270723
246	17.35967074	20.87999327
247	17.44740513	21.17007487
248	17.58469117	21.41661705
249	17.62409774	21.70162877
250	17.53554687	21.85747081
251	17.30140656	22.06282656
252	16.7473746	22.19665356
253	15.97381105	22.35578122
254	14.74857113	22.42958033
255	13.0748456	22.39265263
256	16.77562702	22.233282
257	16.87011805	21.80940951
258	16.98415223	21.12341294
259	17.10848775	20.00944786
260	17.17578339	18.35768633
261	17.23365881	16.19141522

262	17.2529904	21.27541277
263	17.27234191	21.33414296
264	17.34022934	21.36945298
265	17.33051615	21.32238494
266	17.30140656	21.40481702
267	17.23365881	21.4284231
268	17.18541688	21.54681498
269	17.18541688	21.71358003
270	17.15653129	21.71358003
271	17.19505533	21.63004887
272	17.13729902	21.6777445
273	17.07014191	21.79740947
274	17.08930495	21.86950144
275	17.02232063	21.89358107
276	17.07972096	22.0143476
277	17.09889388	22.0143476
278	17.15653129	22.02645809
279	17.10848775	21.97805308
280	16.95557752	22.03857474
281	16.88907479	22.13573025
282	16.7473746	22.17226564
283	16.56013838	22.12356418
284	16.34719243	22.0143476
285	16.07321127	21.97805308
286	15.91085007	21.82141566
287	15.66127362	21.71358003
288	15.41528818	21.64196367
289	15.11278211	21.64196367
290	14.8409691	21.55868737
291	14.54879847	21.41661705
292	14.37602961	21.38123498
293	14.22943625	21.08847889

294	14.09224194	20.83392252
295	13.94829476	20.604974
296	13.76631559	20.45740595
297	13.63320456	20.42349067
298	13.53220713	20.15403121
299	13.41651978	19.88785632
300	13.34754093	19.63581904
301	13.37815818	19.51632382
302	13.41651978	19.6576178
303	13.49354401	19.69035779
304	13.51672978	19.6576178
305	13.48582348	19.7559887
306	13.52446644	19.81083521
307	13.60205545	19.89888186
308	13.69569808	20.04272803
309	13.78205342	20.13172505
310	13.90854834	20.198712
311	14.02809881	20.25469155
312	14.164723	20.37835104
313	14.36784948	20.49137323
314	14.54052855	20.55946409
315	14.65669944	20.7077117
316	14.65669944	20.87999327
317	14.78210935	21.07684608
318	14.88314293	21.20513382
319	14.95084911	21.35767697
320	15.03587804	21.57056581
321	15.14707709	21.70162877
322	15.25038983	21.9901451
323	15.35434719	22.11140429
324	15.45895295	22.28220693
325	15.55541443	22.36806544

326	15.67898084	22.5902528
327	15.81237078	22.75199045
328	15.76779238	22.91479999
329	15.77669884	23.05340413
330	15.65242689	23.09133983
331	15.52027393	22.95252436
332	15.13849668	22.66476818
333	14.5570727	21.84544631
334	13.58650524	20.59358781
335	12.15285016	18.77146919
336	10.21662838	16.10949717
337	7.854595165	12.6170722
338	5.316307717	8.687203256
339	2.938055667	4.906106167
340	14.3433346	34.81362992
341	14.31070753	39.54319843
342	14.29441943	47.70799111
343	14.15665277	64.88697389
344	13.90854834	35.67686968
345	13.62541119	35.6578922
346	13.25607199	35.26154373
347	12.79987286	34.9065034
348	12.25857772	34.29780095
349	11.62978507	33.18096275
350	10.97907549	32.01235806
351	10.23463957	30.48666525
352	9.463098781	28.71755467
353	8.630356399	26.81097327
354	7.779160414	24.57652586
355	6.910477407	22.25773202
356	6.080224033	20.06494318
357	5.272971648	17.81239011

358	4.53277381	15.50273096
359	3.837503963	13.33225627
360	3.204922356	11.2379049
361	2.664902748	9.491126635
362	2.211472145	7.930684592
363	1.819198021	6.620449141
364	1.500041234	5.475623318
365	1.24670545	4.553162898
366	1.038511474	3.832482223
367	0.885812393	3.272099599
368	0.781021937	2.85931735
369	0.731683366	2.583612699
370	0.750345676	2.499266423
371	0.449704078	1.149340829
372	0.280829916	0.9642706
373	0.237946008	0.816764617
374	0.20459748	0.700836488
375	0.176832356	0.605107655
376	0.154939313	0.528808399
377	0.1366765	0.467763018
378	0.121457239	0.417224742
379	0.109733173	0.37583028
380	0.100034151	0.341113123
381	0.092067217	0.31117194
382	0.08603671	0.287102019
383	0.080635049	0.265629396
384	0.075902992	0.248522521
385	0.072256438	0.233768727
386	0.069027358	0.221119798
387	0.06627256	0.210365193
388	0.064749969	0.200678743
389	0.062646928	0.193859697

390	0.061020023	0.171619261
391	0.059842421	0.163936793
392	0.057459313	0.157240089
393	0.05641527	0.151106426
394	0.055543409	0.146000991
395	0.05475992	0.140869549
396	0.053754238	0.136995501
397	0.05314252	0.13320601
398	0.052460807	0.130111676
399	0.051860553	0.12677364
400	0.051265639	0.124536663
401	0.050676031	0.122330887
402	0.05001902	0.120155983
403	0.049729144	0.118438067
404	0.049296773	0.117444911
405	0.048724817	0.115757607
406	0.048369964	0.114643371
407	0.047876538	0.112987844
408	0.047247872	0.111758576
409	0.046832327	0.110539843
410	0.046488207	0.109064486
411	0.046009731	0.108399004
412	0.045738033	0.107209176
413	0.045265553	0.105899197
414	0.04466364	0.104601815
415	0.044597145	0.103189138
416	0.044265818	0.101665153
417	0.043805165	0.100034151
418	0.043348229	0.097932338
419	0.043088784	0.096590898
420	0.04289499	0.09502417
421	0.042509423	0.092887795

422	0.04219017	0.090673726
423	0.041746335	0.088501181
424	0.04149434	0.086147553
425	0.041056181	0.083734641
426	0.040436454	0.081268865
427	0.040129314	0.078963732
428	0.03976313	0.076811313
429	0.039278907	0.074012949
430	0.038739614	0.071678217
431	0.03826506	0.069401299
432	0.037912101	0.066816546
433	0.037561662	0.064484128
434	0.037213728	0.062387831
435	0.036925689	0.06017706
436	0.036696499	0.05794621
437	0.036354775	0.05609701
438	0.036015511	0.053985036
439	0.035511203	0.051935292
440	0.035067519	0.050091694
441	0.034573499	0.048653685
442	0.034138892	0.047109041
443	0.033708511	0.045670304
444	0.033335369	0.044398119
445	0.032703115	0.04289499
446	0.032183331	0.041936106
447	0.031772107	0.040807416
448	0.031213298	0.040129314
449	0.030562682	0.039945898
450	0.029873751	0.040374881
451	0.029776317	0.036015511
452	0.029389025	0.034957269
453	0.029148944	0.034084864

454	0.028673312	0.033335369
455	0.028203675	0.032494431
456	0.027832245	0.031823288
457	0.027464589	0.031466356
458	0.027191308	0.031011984
459	0.026920122	0.030711889
460	0.026517249	0.029101109
461	0.026251254	0.028626079
462	0.026207122	0.028297125
463	0.025207718	0.027832245
464	0.024951888	0.027327686
465	0.02457189	0.027055454
466	0.024154901	0.026695728
467	0.023702513	0.02633969
468	0.023458514	0.026119028
469	0.023216448	0.025768927
470	0.022738072	0.025465558
471	0.022462536	0.025207718
472	0.022150783	0.024951888
473	0.021842361	0.024782447
474	0.021613214	0.024488053
475	0.021348213	0.024321039
476	0.021048414	0.024113503
477	0.020788747	0.02382524
478	0.020458508	0.023620964
479	0.020204448	0.023418036
480	0.019988614	0.023216448
481	0.019774551	0.023096137
482	0.019527037	0.022976305
483	0.019212301	0.022698552
484	0.019004647	0.022540998
485	0.018764561	0.022540998

486	0.018526806	0.022228408
487	0.018358399	0.021919155
488	0.018091388	0.021804041
489	0.01789309	0.021575203
490	0.017566296	0.021499335
491	0.017469155	0.021385917
492	0.017372425	0.021160457
493	0.017180196	0.020936825
494	0.016957991	0.020825691
495	0.016675539	0.020641474
496	0.016427505	0.020385671
497	0.016182303	0.020385671
498	0.016091078	0.020276789
499	0.015909809	0.020060361
500	0.015640838	0.019917063

Table S7 Photochromic kinetic parameters at room temperature of compounds **1** and **2.**

Compounds	A_0	A_1	k_1 (s^{-1})	k_2 (s^{-1})	R
1	0.6868	-0.2645	0.25178	0. 00813	0.97961
2	0.99467	-0.40487	0.21455	0.01037	0.99797