< Supporting Information >

Integration of Fine-Tuned Chiral Donor with Hybrid Long/Short-Range Charge-Transfer for High-Performance Circularly Polarized Electroluminescence

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1. General Informations

^{1}H and ^{13}C nuclear magnetic resonance (NMR) spectra were acquired at room temperature using a Bruker AV 500M NMR spectrometer, with $CDCl_3$ as the solvent and tetramethylsilane as the internal standard. High-resolution mass spectrometry (HRMS) was performed using a Thermo Scientific LTQ Orbitrap XL mass spectrometer equipped with an electron spray ionization ion source. Thermogravimetric analysis (TGA) was conducted on a TA Q50 instrument under a nitrogen atmosphere, with a uniform heating rate of 10°C per minute from room temperature to 800°C. The degradation temperature (T_d) was determined based on a 5% weight loss criterion. Cyclic voltammetry (CV) measurements were executed using a CHI600 electrochemical analyzer (Chenhua, China) at room temperature. A conventional three-electrode system comprising a glassy carbon working electrode, a platinum wire auxiliary electrode, and an Ag/AgCl standard electrode as the reference electrode was employed. The supporting electrolyte consisted of 0.1 M tetrabutylammonium hexafluorophosphate (n-Bu_4NPF_6) in anhydrous dichloromethane solution, and ferrocene served as an internal standard during the measurements. UV-Vis spectra in solution were recorded using a UV-3100 spectrophotometer at room temperature. Room-temperature photoluminescence spectra and phosphorescence spectra were measured with a Hitachi F-7000 fluorescence spectrophotometer, using a xenon lamp as the light source. Absolute fluorescence quantum yields (Φ_{PL}) were determined using a Quantaurus-QY measurement system (C9920-02, Hamamatsu Photonics) equipped with a calibrated integrating sphere. During the Φ_{PL} measurements, the integrating sphere was purged with pure and dry argon to maintain an inert environment. The lifetimes of fluorescence and delayed fluorescence were measured using a PicoQuant Fluotime300 instrument under an argon atmosphere. Circular dichroism (CD) spectra were collected with a ChirascanTM circular dichroic spectropolarimeter, while circularly polarized luminescence (CPPL and CPEL) spectra were recorded using a Jasco CPL-300 spectrometer.

2 Theoretical Calculations

The geometrical and electronic properties of these CP-TADF molecules at ground-states were computed by using DFT within the Gaussian 16 software package at the B3LYP/def2-svp level, which incorporates Grimme's dispersion correction.[1] Energy levels of excited states, including singlets and triplets, and the optimal geometrical configuration of the S_1 were determined through time-dependent DFT (TD-DFT) at the PBE0/Def2-svp level. NTO analysis was conducted using the Multiwfn 3.8 program.[2] Spin-orbit coupling constants

between the S_1 and T_n (n = 1, 2, 3) states were computed by using PySOC, with parameter settings in accordance with their TD-DFT calculations. All computations were performed in the gas phase and visualized using GaussView 6.0 and VMD 1.9.3.[3]

3 Device Fabrication and Characterization

The ITO-coated glass substrates (sheet resistance: 15 Ω square^{-1}) underwent consecutive ultrasonic cleaning with acetone/isopropanol, nitrogen gas drying, and a 20-minute UV-ozone treatment. Post-treatment, the substrates entered the deposition system. Organic layers, including HAT-CN, TAPC, TCTA, mCBP, emitting layers (R/S-BACzBO 20 or 30 wt% in PPF), POT2T, ANT-BIZ, and a Liq layer, were thermally evaporated at 5×10-5 Pa with deposition rates of 0.2-3 Å/s. The cathode Al layer was deposited at 3 Å/s. Device measurements, including J-V-L properties, external quantum efficiency, and electroluminescence spectra, were conducted using a Keithley 2400 source meter and an absolute EQE measurement system (C9920-12, Hamamatsu Photonics, Japan). The device's emitting area is 0.09 cm2.

4. Materials Synthesis and Characterization

***Synthesis of M-1*:** The synthetic process was referred to the reported literature.[4]

***Synthesis of M-2*:** The synthetic process was referred to the reported literature.[5]

***Synthesis of R/S-BA-1*:** The synthetic process was referred to the reported literature.[6]

***Synthesis of R-BA-2*:** To a round-bottom flask was added ***R*-BA-1** (1.33 g, 3 mmol), NaH (180 mg, 7.5 mmol) and 60 ml dry DMF. The mixture was stirred at room temperature under argon for 30 minutes，followed by the addition of **M-1** (705 mg, 3 mmol). The reaction mixture was then stirred at room temperature for additional 12h. After then, the mixture was poured into water, and the crude product was collected by filtration and washed with water. The crude product was further purified by column chromatography on silica gel (eluent: petroleum ether/dichloromethane = 4:1, *v*/*v*) to afford ***R*-BA-2** as a yellow powder with the yield of 60%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 9.0 Hz, 1H), 7.46 (d, *J* = 7.3 Hz, 1H), 7.41 (d, *J* = 8.9 Hz, 1H), 7.30 (t, *J* = 7.4 Hz, 1H), 7.22-7.12(m,3H), 7.07-6.94 (m, 3H), 6.94-6.83 (m, 2H), 6.76 (t, *J* = 7.6 Hz, 1H), 6.63-6.41 (m, 5H),5.86 (d, *J* = 8.0 Hz, 1H), 5.59 (d, *J* = 8.6 Hz, 1H), 2.68-2.56 (m, 2H), 2.42-2.17 (m, 4H), 1.81-1.61 (m, 2H), 1.52-1.31 (m, 8H). HRMS:(ESI) m/z calcd for $C_{44}H_{38}N_3O_2^+$ $[M+H]^+$: 640.2959; found: 640.2957.

Synthesis of *R*-BACz: To a round-bottom flask was added ***R*-BA-2** (1.43 g, 3 mmol), PPh_3 (3.14 g, 12 mmol) and 60 ml dry *o*-DCB. The mixture was stirred at 220 °C under argon for 48h. After cooling to room temperature, the solvent was removed under reduced pressure and the crude product was further purified by column chromatography on silica gel (eluent: petroleum ether/dichloromethane = 3:1, v/v) to afford ***R*-BACz** as a white powder with the yield of 80%.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.57 (d, *J* = 8.0 Hz, 1H), 7.43 (d, *J* = 8.5 Hz, 1H), 7.35 (d, *J* = 8.1, 1H), 7.30-7.20 (m, 2H), 7.15 (d, *J* = 7.9 Hz, 2H), 7.03 (d, *J* = 8.6 Hz, 1H), 6.93-6.67 (m, 6H), 6.56 – 6.28 (m, 4H), 5.92 (s, 1H), 5.59 (d, *J* = 8.0, Hz, 1H), 2.68-2.57 (m, 2H), 2.51-2.26 (m, 4H), 2.14-1.84 (m, 2H) , 1.54-1.41 (m, 8H). HRMS:(ESI) m/z calcd for $C_{44}H_{38}N_3^+$ $[M+H]^+$: 608.3061; found: 608.3065.

Synthesis of *R*-BACzBO: To a round-bottom flask was added ***R*-BACz** (607 mg, 1 mmol), **M-2** (348mg, 1 mmol), Tris(dibenzylideneacetone)dipalladium (45 mg, 0.05 mmol), sodium *tert*-butoxide (192 mg, 2 mmol), tri-*tert*-butylphosphine tetrafluoroborate (28 mg, 0.1 mmol) and 20 mL dry toluene. The mixture was stirred at 110 °C under argon for 12h. After cooling down to room temperature, the suspension was extracted with dichloromethane and water, and the combined organic layers were evacuated to drynessand. The crude product was further purified by column chromatography on silica gel (eluent: petroleum ether/dichloromethane = 4:1, v/v) to afford ***R*-BACzBO** as faint yellow powder with the yield of 60%. ^{1}H NMR (500 MHz, CD_2Cl_2) δ 8.74 (dd, *J* = 7.8, 1.7 Hz, 2H), 7.79 – 7.72 (m, 3H), 7.67-7.54 (m, 3H), 7.50 (s, 2H), 7.44 (t, *J* = 7.4 Hz, 3H), 7.30 (t, *J* = 8.3 Hz, 1H), 7.22-7.14 (m, 2H), 7.09 (t, *J* = 8.5 Hz, 1H), 7.04-6.64 (m, 6H), 6.63-6.39 (m, 3H), 5.67 (m, 3H), 5.32-5.30 (m, 1H), 2.71-2.57 (m, 2H), 2.52-2.30 (m, 4H), 2.14-1.92 (m, 2H), 1.61-1.43 (m, 6H), 1.20-0.92 (m, 2H).^{13}C NMR (126 MHz, CD_2Cl_2) δ 161.95, 159.79, 149.50, 142.39, 140.80, 139.98, 139.34, 139.16, 138.49, 137.84, 137.50, 135.97, 135.27, 130.95, 130.66, 129.70, 129.28, 128.44, 126.80, 124.53, 124.47, 123.79, 123.54, 119.75, 118.24, 30.74, 30.68, 28.56, 28.53, 24.13, 24.06, 23.48, 23.41. HRMS:(ESI) m/z calcd for $C_{62}H_{47}BN_3O_2^+$ $[M+H]+$: 876.3756; found: 876.3750.

Synthesis of *S*-BA-1: The synthetic process was referred to the reported literature.[3]

Synthesis of *S*-BA-2: This compound was synthesized according to the same procedure of ***R*-BA-2**.^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.9 Hz, 1H), 7.46 (d, *J* = 7.7 Hz, 1H), 7.41 (d, *J* = 8.9 Hz, 1H), 7.30 (t, *J* = 7.6 Hz, 1H), 7.18 (d, *J* = 18.8 Hz, 2H), 7.06-6.90 (m, 3H), 6.90-6.87 (m, 2H), 6.76 (t, *J* = 7.6 Hz, 1H), 6.69 (t, *J* = 7.3 Hz, 1H), 6.59 (d, *J* = 7.8 Hz, 1H), 6.57-6.41 (m, 3H), 6.36-6.15 (m, 2H), 5.87 (d, *J* = 8.0 Hz, 1H), 5.59 (d, *J* = 8.6 Hz, 1H), 2.68-

2.54 (m, 2H), 2.49-2.11 (m, 4H), 1.81-1.69 (m, 2H), 1.49-1.17 (m, 8H). HRMS:(ESI) m/z calcd for $C_{44}H_{38}N_3O_2^+$ $[M+H]^+$: 640.2959; found: 640.2956.

Synthesis of *S*-BACz: This compound was synthesized according to the same procedure of ***R*-BACz**.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.57 (d, *J* = 8.0 Hz, 1H), 7.43 (d, *J* = 8.5 Hz, 1H), 7.35 (d, *J* = 8.1, 1H), 7.30-7.20 (m, 2H), 7.15 (d, *J* = 7.9 Hz, 2H), 7.03 (d, *J* = 8.6 Hz, 1H), 6.94-6.65 (m, 6H), 6.56-6.28 (m, 4H), 5.92 (s, 1H), 5.59 (d, *J* = 8.0, Hz, 1H), 2.70-2.53 (m, 2H), 2.47-2.11 (m, 4H), 2.16-1.94 (m, 2H)1.72-1.40 (m, 8H). HRMS:(ESI) m/z calcd for $C_{44}H_{38}N_3^+$ $[M+H]^+$: 608.3061; found: 608.3063.

Synthesis of *S*-BACzBO: This compound was synthesized according to the same procedure of ***S*-BACzBO**. ^{1}H NMR (500 MHz, CD_2Cl_2) δ 8.74 (dd, *J* = 7.8, 1.7 Hz, 2H), 7.79-7.72 (m, 3H), 7.67-7.54 (m, 3H), 7.50 (s, 2H), 7.44 (t, *J* = 7.4 Hz, 3H), 7.30 (t, *J* = 8.3 Hz, 1H), 7.22-7.14 (m, 2H), 7.09 (t, *J* = 8.5 Hz, 1H), 7.04-6.64 (m, 6H), 6.63 – 6.39 (m, 3H), 5.67 (m, 3H), 5.32-5.30 (m, 1H), 2.71-2.57 (m, 2H), 2.52-2.30 (m, 4H), 2.14-1.92 (m, 2H), 1.61-1.43 (m, 6H), 1.20-1.05 (m, 2H). ^{13}C NMR (126 MHz, CD_2Cl_2) δ 162.21, 160.05, 149.75, 142.39, 140.80, 139.98, 139.34, 139.16, 138.49, 137.84, 137.50, 135.97, 135.27, 130.95, 130.66, 129.70, 129.28, 128.44, 126.80, 124.53, 124.47, 123.79, 123.54, 119.75, 118.24, 30.74, 30.68, 28.56, 28.53, 24.38, 24.32, 23.74, 23.67. HRMS:(ESI) m/z calcd for $C_{62}H_{47}BN_3O_2^+$ $[M+H]$+: 876.3756; found: 876.3751.

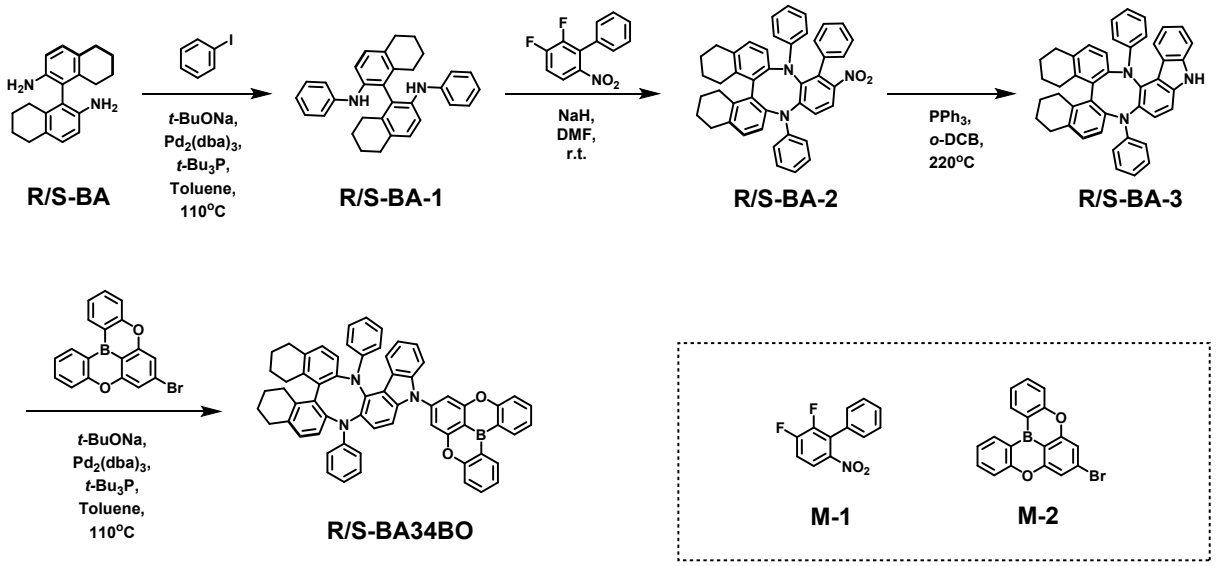


Figure S1. Synthetic routes of the *R*-BACzBO and *S*-BACzBO.

5. Thermal properties

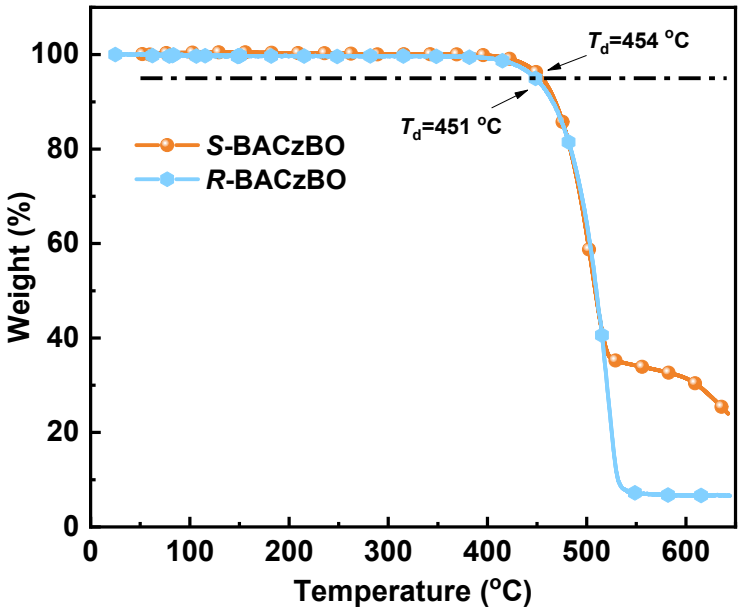


Figure S2. TGA curves of *R*-BACzBO and *S*-BACzBO.

6. Electrochemical properties

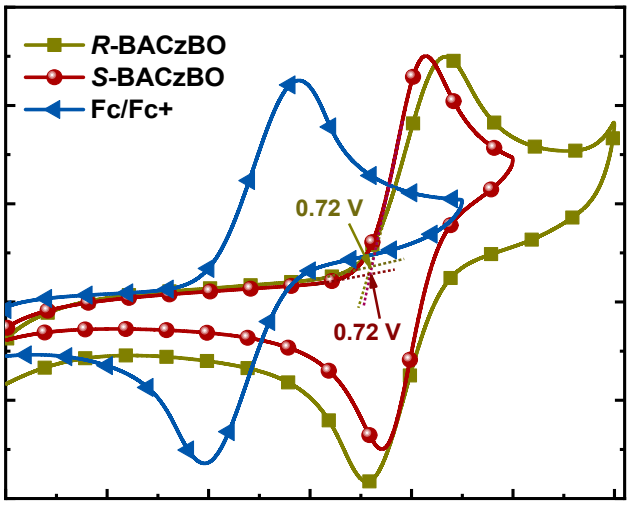


Figure S3. CV curves (oxidation process) of the *R*-BACzBO and *S*-BACzBO.

7. Theoretical simulations

Table S1. Summary of the key TD-DFT data for *R*-BACzBO at the PBE0/Def2-svp level.

Molecules	Transition model	Wavelength (nm)	Energy gap (eV)	Oscillator Strength	Relevant orbitals
***R*-BACzBO**	$S_0 \rightarrow T_1$	453	2.75	0.000	HOMO-2→LUMO (4.6%) HOMO-1→LUMO+1 (5.1%) HOMO→LUMO (74.4%)
	$S_0 \rightarrow S_1$	435	2.85	0.1260	HOMO→LUMO (97.5%)
	$S_0 \rightarrow T_2$	434	2.86	0.000	HOMO-4→LUMO+1 (15.8%) HOMO-1→LUMO+1 (35.2%) HOMO→LUMO (11.8%)
	$S_0 \rightarrow T_3$	415	2.99	0.000	HOMO-4→LUMO+1 (2.7%) HOMO-2→LUMO+1 (3.5%) HOMO→LUMO+1 (76.8%)

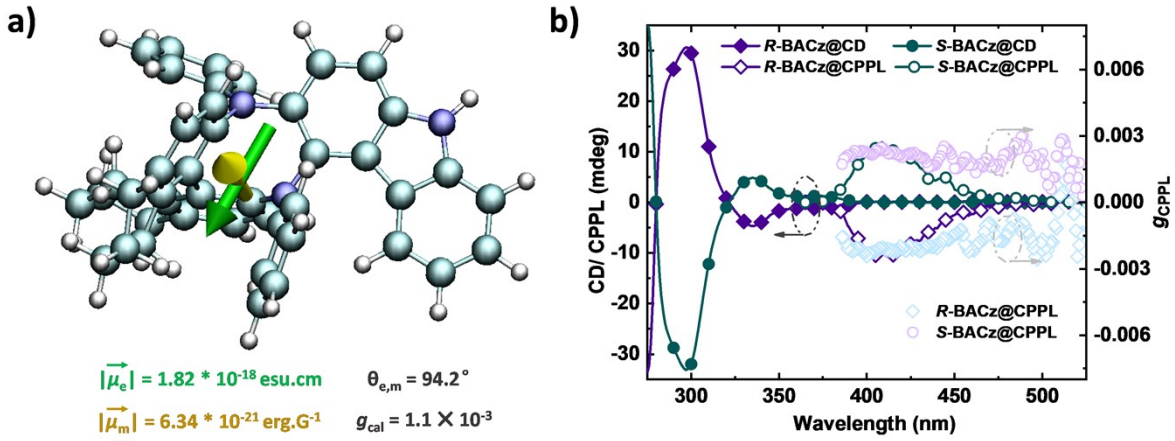
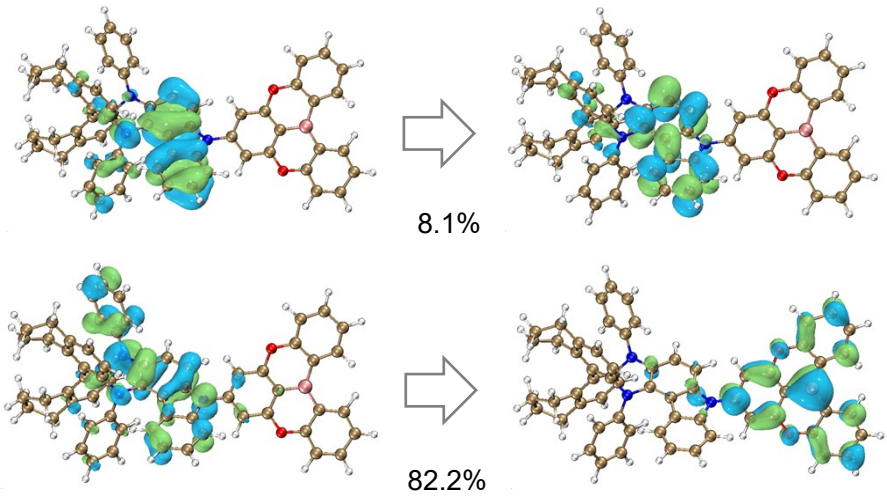
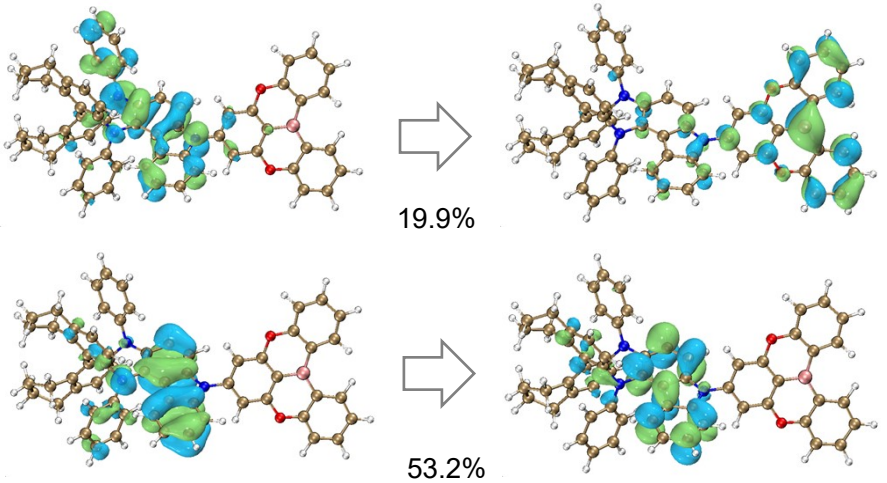
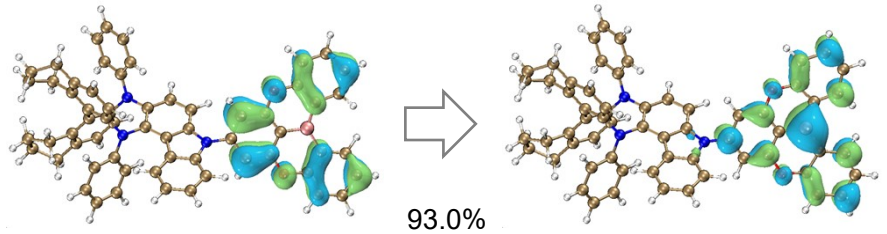
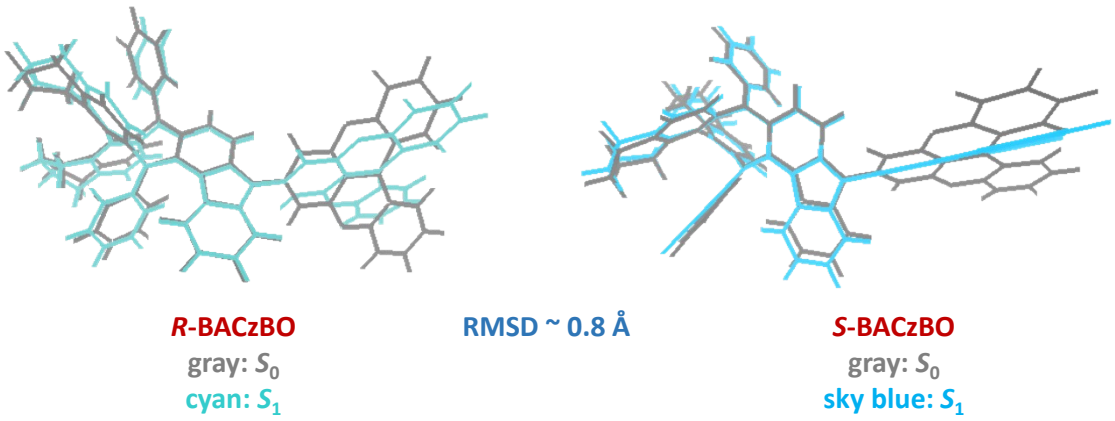


Figure S4. a) Optimized geometrical configuration of the new generated chiral donor *R*-BACz at singlet excited state and the calculated parameters associated with CPL properties, b) the CD and CPL spectra of the key intermediate *R*-BACz and *S*-BACz.

Table S2. Analysis of natural transition orbitals for the three lowest triplet states.

Transition model	Visualized natural transition orbitals (hole→electron)
$S_0 \rightarrow T_1$	
$S_0 \rightarrow T_2$	
$S_0 \rightarrow T_3$	



FigureS5. The comparison of optimized geometrical configurations of the *R*-BACzBO and *S*-BACzBO from S_0 to S_1.

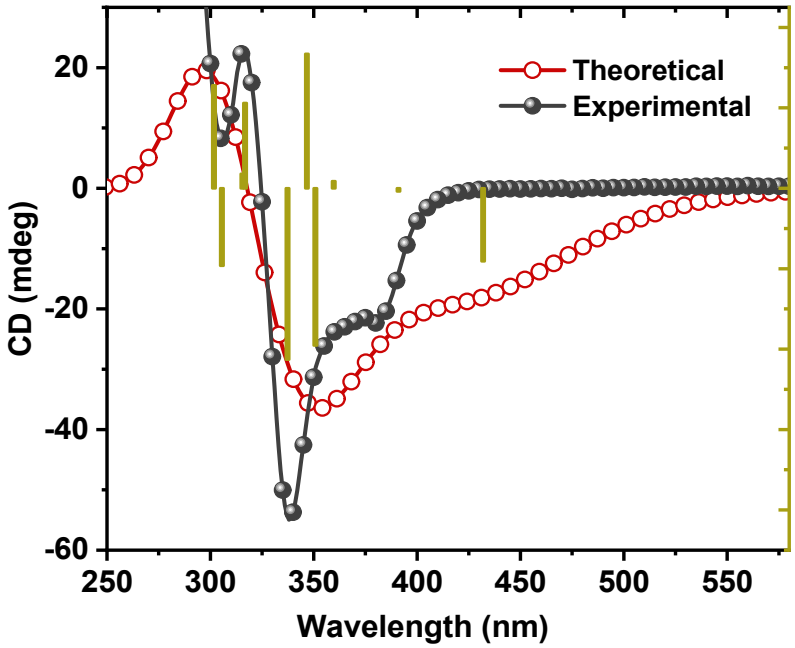


Figure S6. a) The comparison of CD spectra of the *R*-BACzBO between the experimental and theoretical results.

8. Photophysical and circularly polarized luminescence properties

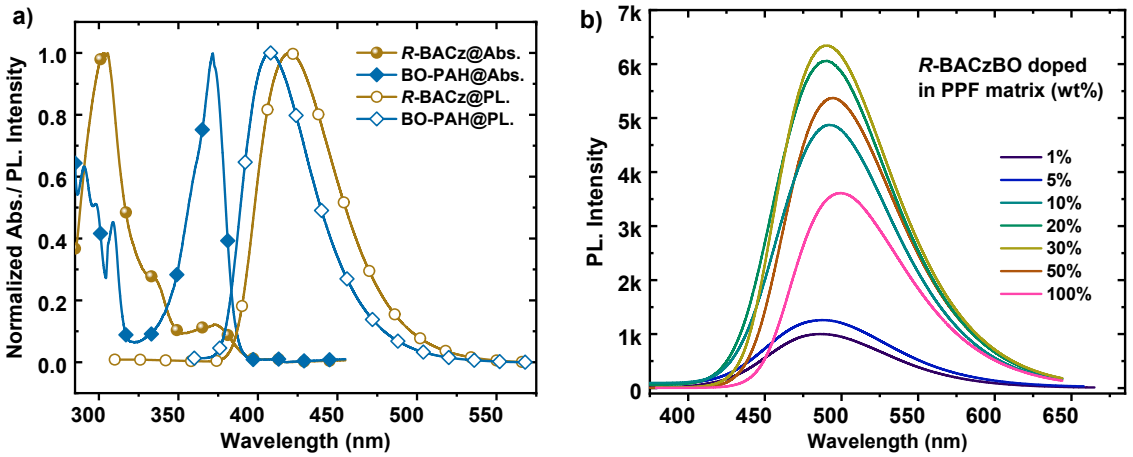


Figure S7. a) The UV-Vis absorption and photoluminescence spectra of the individual segments, *R*-BACz and BO-PAH, b) the photoluminescence spectra of the *R*-BACzBO doped in dibenzo[*b*,*d*]furan-2,8-diylbis(diphenylphosphine oxide) (PPF) matrix under various doping ratio.

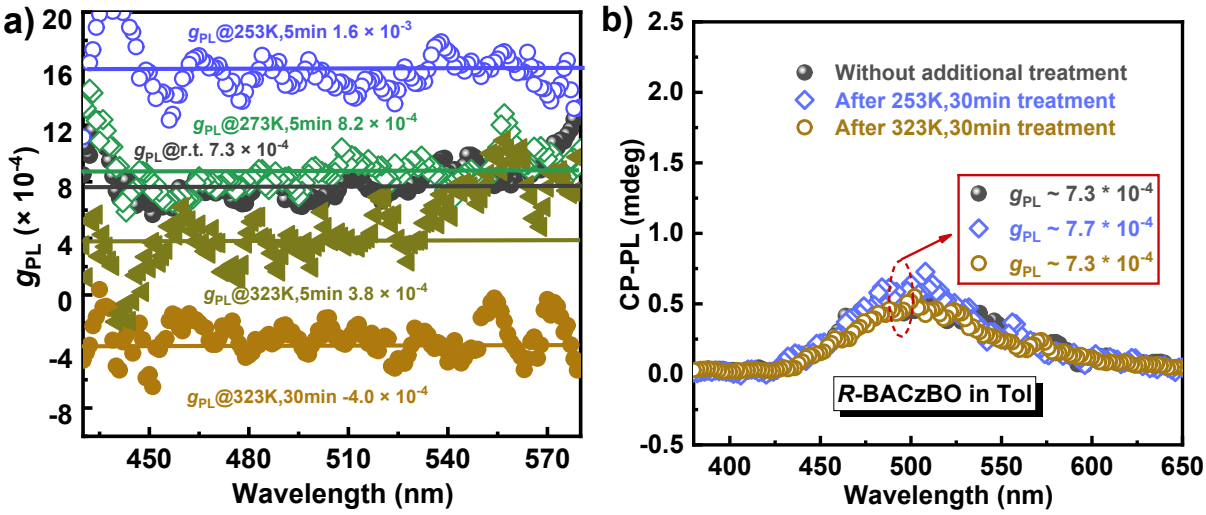


Figure S8. a) A scatter plot showing the results of gPL under various temperature conditions. b) CPPL spectra of the same sample following sequential cold and hot treatments.

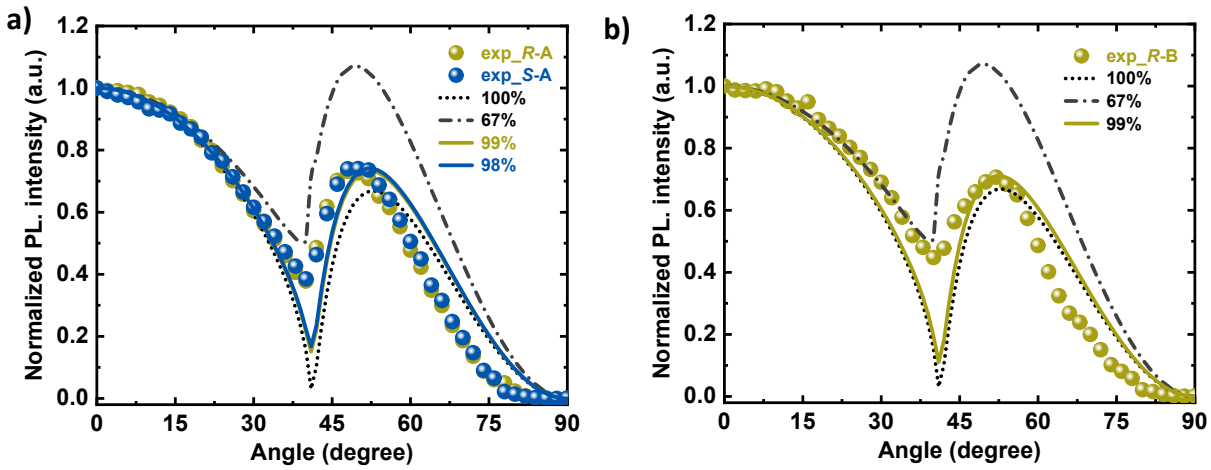


Figure S9. The angle-dependent *p*-polarized PL. intensity and simulation curves of the emitting layers for g) *R*/*S*-A and h) *R*-B.

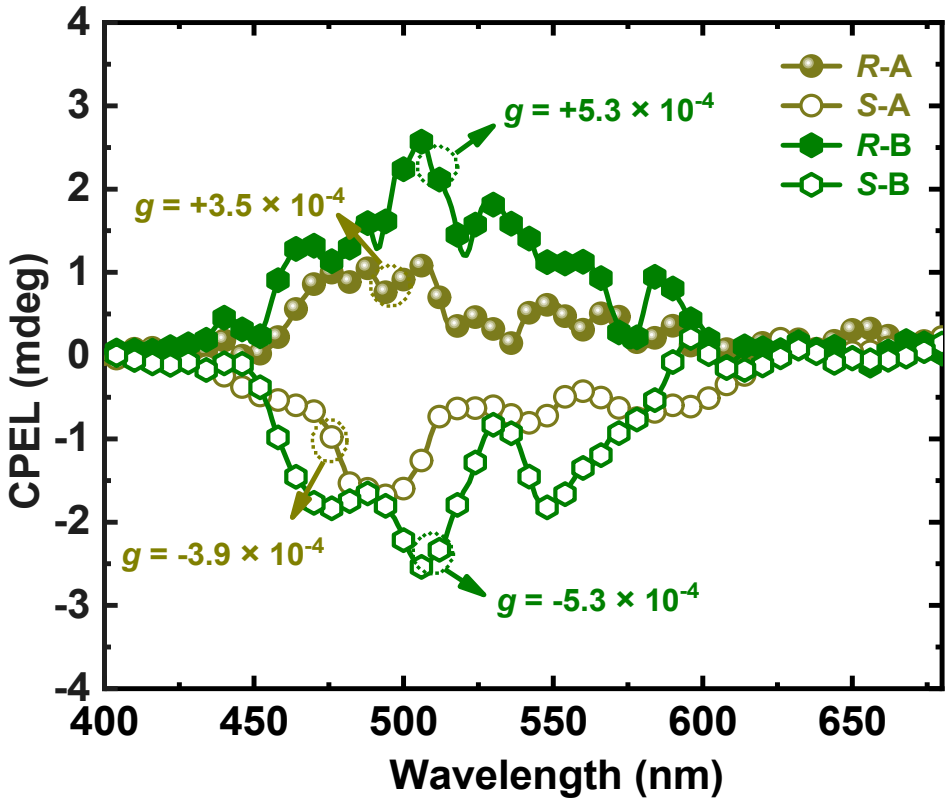


Figure S10. The CPEL spectra and g_{EL} scatter plots of device *R*/*S*-A and *R*-B.

9. Cartesian coordinates of these optimized geometries.

Table S3. Cartesian coordinates of *R*-BACzBO at the optimized S_0 geometry.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.288403	-0.724446	0.766219
2	6	0	1.187694	-0.127045	0.142018
3	6	0	1.157154	0.839005	-0.871531
4	6	0	-0.002599	-0.671348	0.690944
5	6	0	-1.256991	-0.226343	0.225492
6	6	0	-1.290072	0.732793	-0.809424
7	6	0	-0.087931	1.253378	-1.330809
8	6	0	1.820502	-1.636070	1.720500
9	6	0	2.543050	-2.423454	2.622748
10	6	0	1.820995	-3.223752	3.508663
11	6	0	0.414996	-3.236286	3.502322
12	6	0	-0.303567	-2.441492	2.610899
13	6	0	0.396988	-1.627033	1.707191
14	1	0	-0.158819	1.991878	-2.131221
15	1	0	3.632795	-2.407342	2.641843
16	1	0	-1.391661	-2.455025	2.614430
17	7	0	-2.455202	-0.730146	0.788818
18	6	0	-3.429797	0.220968	1.234054
19	6	0	-4.547131	0.499578	0.415769
20	6	0	-3.254562	0.882017	2.449051
21	6	0	-5.488329	1.446039	0.841889
22	6	0	-4.553755	-0.139133	-0.927286
23	6	0	-4.198624	1.822873	2.868136
24	1	0	-2.379926	0.645060	3.057760
25	6	0	-5.312415	2.107198	2.076230
26	6	0	-6.678976	1.877662	0.026556
27	6	0	-3.467183	0.178174	-1.772655
28	6	0	-5.470161	-1.121514	-1.325448
29	1	0	-4.065474	2.342214	3.820841
30	6	0	-6.360995	3.121029	2.449846
31	6	0	-7.969021	1.879862	0.868967
32	1	0	-6.484467	2.901325	-0.335461
33	7	0	-2.526924	1.171926	-1.351065
34	6	0	-3.294847	-0.487941	-2.985384
35	6	0	-5.297589	-1.785344	-2.558565
36	6	0	-6.627397	-1.588495	-0.481902
37	6	0	-7.776773	2.543352	2.259177
38	1	0	-6.219146	3.467422	3.485010
39	1	0	-8.762129	2.392447	0.302224
40	6	0	-4.211568	-1.467313	-3.375848
41	1	0	-2.443656	-0.225890	-3.616450
42	6	0	-6.316477	-2.839344	-2.901981

43	6	0	-7.933530	-1.640620	-1.297451
44	1	0	-6.391207	-2.602595	-0.117560
45	1	0	-7.951889	1.798627	3.051667
46	1	0	-4.079544	-1.989971	-4.326948
47	6	0	-7.747995	-2.311752	-2.684995
48	1	0	-6.184424	-3.188877	-3.937397
49	1	0	-8.698337	-2.172320	-0.709772
50	1	0	-7.968168	-1.582522	-3.480610
51	6	0	-2.970486	2.490400	-1.151417
52	6	0	-2.415223	3.304869	-0.146993
53	6	0	-4.011781	3.009207	-1.943819
54	6	0	-2.905041	4.592354	0.065133
55	1	0	-1.621016	2.909968	0.486089
56	6	0	-4.494862	4.297498	-1.719499
57	1	0	-4.446781	2.386820	-2.726630
58	6	0	-3.951123	5.100545	-0.711937
59	1	0	-2.470579	5.201556	0.861937
60	1	0	-5.306156	4.678899	-2.345209
61	1	0	-4.332396	6.109131	-0.538650
62	6	0	-2.847383	-2.063166	0.572950
63	6	0	-2.247978	-2.847246	-0.427718
64	6	0	-3.860045	-2.632862	1.366512
65	6	0	-2.666906	-4.160051	-0.635658
66	1	0	-1.469986	-2.413710	-1.055344
67	6	0	-4.273800	-3.945814	1.145361
68	1	0	-4.327257	-2.032343	2.147872
69	6	0	-3.685219	-4.720984	0.141514
70	1	0	-2.196267	-4.748881	-1.426954
71	1	0	-5.064683	-4.368198	1.770717
72	1	0	-4.010293	-5.749563	-0.028318
73	1	0	2.362841	-3.849276	4.222088
74	1	0	-0.121601	-3.876170	4.206145
75	1	0	2.073062	1.241556	-1.302866
76	6	0	3.644116	-0.441115	0.494874
77	6	0	4.528617	-1.497690	0.232174
78	6	0	4.086321	0.890220	0.495512
79	6	0	5.867276	-1.200491	-0.021991
80	1	0	4.182436	-2.529598	0.206657
81	6	0	5.428668	1.148075	0.218651
82	1	0	3.408814	1.710282	0.727113
83	6	0	6.355572	0.120349	-0.042038
84	8	0	6.692592	-2.245923	-0.267144
85	8	0	5.818577	2.445028	0.224619
86	5	0	7.818624	0.423224	-0.330466
87	6	0	8.016674	-2.093554	-0.571948
88	6	0	7.111989	2.834534	0.013006
89	6	0	8.170038	1.933004	-0.262225
90	6	0	8.669981	-0.837703	-0.635258
91	6	0	8.684393	-3.302023	-0.821799
92	6	0	7.307567	4.221587	0.093435
93	6	0	9.447300	2.518189	-0.437583

94	6	0	10.042085	-0.874541	-0.982468
95	6	0	10.032595	-3.282875	-1.151186
96	1	0	8.120710	-4.233746	-0.752945
97	6	0	8.579441	4.744731	-0.094091
98	1	0	6.447554	4.858580	0.306041
99	6	0	9.660061	3.888349	-0.358575
100	1	0	10.301658	1.872411	-0.636231
101	6	0	10.718410	-2.060777	-1.236029
102	1	0	10.592500	0.062060	-1.061491
103	1	0	10.555365	-4.222089	-1.347255
104	1	0	8.735389	5.824353	-0.031279
105	1	0	10.662579	4.297564	-0.500008
106	1	0	11.777574	-2.043239	-1.501300
107	1	0	-6.749301	-0.965615	0.413409
108	1	0	-8.308046	-0.613355	-1.430818
109	1	0	-8.464836	-3.137848	-2.814230
110	1	0	-6.150706	-3.717212	-2.250554
111	1	0	-6.797532	1.256945	-0.870738
112	1	0	-8.308269	0.840047	0.999641
113	1	0	-6.240998	4.008762	1.801823
114	1	0	-8.520227	3.341159	2.413281

Table S4. Cartesian coordinates of *S*-BACzBO at the optimized S_0 geometry.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.221515	-0.801154	-0.744916
2	6	0	1.121889	-0.193675	-0.127786
3	6	0	1.098887	0.847773	0.808372
4	6	0	-0.071018	-0.732818	-0.675557
5	6	0	-1.323886	-0.246498	-0.243171
6	6	0	-1.349364	0.763849	0.743394
7	6	0	-0.141979	1.305978	1.232770
8	6	0	1.751043	-1.714600	-1.695251
9	6	0	2.471782	-2.573695	-2.531217
10	6	0	1.749304	-3.401196	-3.391177
11	6	0	0.343917	-3.378387	-3.415601
12	6	0	-0.373052	-2.539097	-2.564609
13	6	0	0.326995	-1.698731	-1.684285
14	1	0	-0.206033	2.100068	1.978682
15	1	0	3.561179	-2.601436	-2.510515
16	1	0	2.290101	-4.079616	-4.055342
17	1	0	-1.460568	-2.546910	-2.575847
18	1	0	-0.194471	-4.035556	-4.101927
19	7	0	-2.523348	-0.747826	-0.804673
20	6	0	-3.474036	0.205728	-1.294984

21	6	0	-2.921001	-2.078481	-0.589227
22	6	0	-4.581976	0.562196	-0.499445
23	6	0	-3.259640	0.825226	-2.526393
24	6	0	-3.857740	-2.678608	-1.450553
25	6	0	-2.387053	-2.836710	0.466688
26	6	0	-5.471543	1.563862	-0.937251
27	6	0	-4.623407	-0.044087	0.862635
28	6	0	-4.149200	1.803146	-2.962574
29	1	0	-2.390484	0.537807	-3.120998
30	6	0	-4.262379	-3.997277	-1.244152
31	1	0	-4.264403	-2.099002	-2.280506
32	6	0	-2.795760	-4.154598	0.660740
33	1	0	-1.666408	-2.378584	1.143538
34	6	0	-5.250061	2.185838	-2.185210
35	6	0	-6.561548	2.062564	-0.006957
36	6	0	-3.545461	0.285558	1.707859
37	6	0	-5.554543	-1.028334	1.252014
38	1	0	-3.980274	2.297541	-3.923173
39	6	0	-3.739378	-4.745940	-0.185813
40	1	0	-4.993547	-4.444386	-1.922543
41	1	0	-2.377646	-4.723957	1.494606
42	6	0	-6.169887	3.277630	-2.695427
43	6	0	-7.616865	2.931274	-0.690053
44	1	0	-7.035744	1.221284	0.516367
45	7	0	-2.577263	1.241993	1.266028
46	6	0	-3.389089	-0.359986	2.934651
47	6	0	-5.391391	-1.675297	2.495996
48	6	0	-6.631285	-1.476173	0.281444
49	1	0	-4.056617	-5.778684	-0.027097
50	6	0	-6.949536	3.975734	-1.582465
51	1	0	-5.580536	4.005416	-3.276091
52	1	0	-8.285538	2.301543	-1.305056
53	6	0	-2.955917	2.585393	1.102931
54	6	0	-4.310608	-1.330100	3.318141
55	1	0	-2.539672	-0.099587	3.568796
56	6	0	-6.351268	-2.755043	2.955404
57	6	0	-7.726675	-2.332881	0.915318
58	1	0	-7.070867	-0.609728	-0.230934
59	1	0	-6.258731	4.586144	-0.974564
60	6	0	-3.875131	3.171188	1.992896
61	6	0	-2.446277	3.362678	0.046368
62	1	0	-4.186063	-1.846098	4.274188
63	6	0	-7.111976	-3.411561	1.804812
64	1	0	-5.796325	-3.508333	3.537425
65	1	0	-8.397506	-1.699383	1.523965
66	6	0	-4.284247	4.493144	1.816756
67	1	0	-4.268938	2.575913	2.817888
68	6	0	-2.860152	4.682911	-0.118051
69	1	0	-1.747921	2.913096	-0.659463
70	1	0	-6.416454	-4.025904	1.206385
71	6	0	-3.785348	5.259648	0.759318

72	1	0	-5.000905	4.928663	2.517882
73	1	0	-2.465077	5.264486	-0.954914
74	1	0	-4.107901	6.294119	0.623589
75	1	0	2.018443	1.284035	1.197428
76	6	0	3.575386	-0.526526	-0.460037
77	6	0	4.015590	-0.540688	0.872146
78	6	0	4.459994	-0.241518	-1.511065
79	6	0	5.355146	-0.257580	1.136462
80	1	0	3.337529	-0.787076	1.687524
81	6	0	5.795850	0.019213	-1.207505
82	1	0	4.116302	-0.201878	-2.543201
83	6	0	6.282021	0.024154	0.114260
84	8	0	5.742831	-0.278254	2.434091
85	8	0	6.620961	0.286412	-2.247859
86	5	0	7.741949	0.319861	0.423771
87	6	0	7.034685	-0.066058	2.828413
88	6	0	7.941402	0.603148	-2.088422
89	6	0	8.591985	0.653924	-0.830589
90	6	0	8.092313	0.228751	1.932618
91	6	0	7.229357	-0.167448	4.214220
92	6	0	8.608388	0.879328	-3.291555
93	6	0	9.959833	1.018145	-0.859230
94	6	0	9.368349	0.399735	2.521653
95	6	0	8.499917	0.017349	4.741592
96	1	0	6.369777	-0.394254	4.846893
97	6	0	9.952666	1.223963	-3.264669
98	1	0	8.047157	0.818744	-4.225334
99	6	0	10.635226	1.298135	-2.040069
100	1	0	10.507250	1.090016	0.079735
101	6	0	9.580247	0.299716	3.890609
102	1	0	10.222533	0.611273	1.879709
103	1	0	8.655130	-0.061988	5.820238
104	1	0	10.474749	1.440722	-4.199712
105	1	0	11.691043	1.575983	-2.016334
106	1	0	10.581862	0.438385	4.302978
107	1	0	-6.066130	2.652282	0.780980
108	1	0	-8.250673	3.410282	0.073483
109	1	0	-7.694626	4.662268	-2.015863
110	1	0	-6.886856	2.830398	-3.410038
111	1	0	-6.132366	-2.058876	-0.509172
112	1	0	-8.349611	-2.779735	0.123819
113	1	0	-7.886116	-4.088709	2.200381
114	1	0	-7.079407	-2.306191	3.657593

Table S5. Cartesian coordinates of *R*-BACzBO at the optimized S_1 geometry.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	2.232376	-0.716086	0.941217
2	6	0	1.166602	-0.249160	0.240198
3	6	0	1.182644	0.576426	-0.907881
4	6	0	-0.049551	-0.659448	0.883228
5	6	0	-1.272473	-0.253271	0.343628
6	6	0	-1.252022	0.517409	-0.863678
7	6	0	-0.027946	0.966018	-1.435508
8	6	0	1.770054	-1.426227	2.050690
9	6	0	2.520736	-2.063851	3.037879
10	6	0	1.817504	-2.695171	4.065750
11	6	0	0.412182	-2.685475	4.102551
12	6	0	-0.334556	-2.046732	3.108655
13	6	0	0.346975	-1.407616	2.063693
14	1	0	-0.070191	1.575067	-2.339211
15	1	0	3.609922	-2.057161	2.995382
16	1	0	-1.422086	-2.052364	3.152521
17	7	0	-2.502476	-0.512687	0.975710
18	6	0	-3.406608	0.587424	1.167327
19	6	0	-4.516054	0.723665	0.301999
20	6	0	-3.173040	1.518725	2.176885
21	6	0	-5.383973	1.809693	0.460505
22	6	0	-4.563715	-0.240362	-0.826124
23	6	0	-4.053775	2.593301	2.339472
24	1	0	-2.310772	1.388344	2.833216
25	6	0	-5.154510	2.744603	1.493859
26	6	0	-6.535099	2.106931	-0.463908
27	6	0	-3.430729	-0.246311	-1.664920
28	6	0	-5.522926	-1.246977	-0.980338
29	1	0	-3.878768	3.322049	3.134768
30	6	0	-6.137597	3.879903	1.602857
31	6	0	-7.826915	2.425041	0.315843
32	1	0	-6.257320	2.986120	-1.071634
33	7	0	-2.458874	0.802051	-1.503561
34	6	0	-3.235348	-1.236609	-2.624356
35	6	0	-5.351798	-2.232071	-1.979312
36	6	0	-6.726753	-1.405307	-0.091400
37	6	0	-7.583872	3.353768	1.534782
38	1	0	-5.973897	4.450737	2.529028
39	1	0	-8.553434	2.876829	-0.376911
40	6	0	-4.212625	-2.222764	-2.786480
41	1	0	-2.340173	-1.216659	-3.248071
42	6	0	-6.431429	-3.275397	-2.081447
43	6	0	-8.012612	-1.609926	-0.916163
44	1	0	-6.558698	-2.293576	0.541176
45	1	0	-7.788671	2.802974	2.466103
46	1	0	-4.080393	-2.996802	-3.545879
47	6	0	-7.827128	-2.622457	-2.077721
48	1	0	-6.292864	-3.895333	-2.979603
49	1	0	-8.816161	-1.938946	-0.239727
50	1	0	-7.967024	-2.109537	-3.042110

51	6	0	-2.814345	2.105223	-1.866338
52	6	0	-2.284726	3.205536	-1.159409
53	6	0	-3.759951	2.321171	-2.889618
54	6	0	-2.692704	4.494658	-1.481351
55	1	0	-1.595076	3.031181	-0.334025
56	6	0	-4.161141	3.616775	-3.197046
57	1	0	-4.166050	1.468595	-3.433346
58	6	0	-3.631419	4.709271	-2.498597
59	1	0	-2.290935	5.340260	-0.919831
60	1	0	-4.889417	3.778778	-3.994237
61	1	0	-3.951239	5.723739	-2.743644
62	6	0	-2.971082	-1.826161	1.172993
63	6	0	-2.437060	-2.899964	0.441109
64	6	0	-4.009301	-2.068036	2.089739
65	6	0	-2.944087	-4.185529	0.617257
66	1	0	-1.636258	-2.721195	-0.275794
67	6	0	-4.513564	-3.357816	2.251139
68	1	0	-4.421260	-1.239344	2.666129
69	6	0	-3.988847	-4.425150	1.515667
70	1	0	-2.521574	-5.008843	0.037019
71	1	0	-5.321641	-3.529933	2.966104
72	1	0	-4.382988	-5.434612	1.647824
73	1	0	2.371835	-3.204635	4.856869
74	1	0	-0.106635	-3.187057	4.922075
75	1	0	2.131853	0.870888	-1.353435
76	6	0	3.615462	-0.476500	0.615080
77	6	0	4.278053	-1.365407	-0.242696
78	6	0	4.261352	0.643386	1.157563
79	6	0	5.614298	-1.107358	-0.556433
80	1	0	3.776914	-2.238699	-0.660481
81	6	0	5.597918	0.863209	0.817984
82	1	0	3.747250	1.332002	1.828301
83	6	0	6.312976	0.005330	-0.043558
84	8	0	6.225934	-1.986846	-1.392430
85	8	0	6.192610	1.959687	1.357256
86	5	0	7.775263	0.269261	-0.404634
87	6	0	7.540972	-1.842582	-1.805511
88	6	0	7.517728	2.290013	1.121042
89	6	0	8.369068	1.525079	0.274968
90	6	0	8.375450	-0.771772	-1.377947
91	6	0	7.968640	-2.841904	-2.676120
92	6	0	7.937079	3.438850	1.787244
93	6	0	9.694420	2.023171	0.163989
94	6	0	9.689082	-0.794502	-1.917276
95	6	0	9.278463	-2.820650	-3.177186
96	1	0	7.263327	-3.628743	-2.950701
97	6	0	9.256598	3.891088	1.640629
98	1	0	7.218003	3.965762	2.417542
99	6	0	10.132671	3.172348	0.823884
100	1	0	10.405629	1.483680	-0.460922
101	6	0	10.135114	-1.786932	-2.791473

102	1	0	10.382348	-0.000755	-1.640283
103	1	0	9.616327	-3.604134	-3.859360
104	1	0	9.587676	4.791900	2.162446
105	1	0	11.166097	3.507357	0.699785
106	1	0	11.159024	-1.751941	-3.173556
107	1	0	-6.831995	-0.557522	0.597486
108	1	0	-8.331730	-0.636723	-1.321422
109	1	0	-8.595192	-3.409240	-2.031334
110	1	0	-6.344174	-3.954971	-1.214099
111	1	0	-6.700323	1.287968	-1.176148
112	1	0	-8.276155	1.479178	0.657045
113	1	0	-5.967371	4.583327	0.766707
114	1	0	-8.282165	4.204327	1.517459

Table S6. Cartesian coordinates of *S*-BACzBO at the optimized S_1 geometry.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.160037	-0.836637	-0.863955
2	6	0	1.094385	-0.294979	-0.220772
3	6	0	1.116104	0.655420	0.827232
4	6	0	-0.122724	-0.770153	-0.815332
5	6	0	-1.345055	-0.300962	-0.323427
6	6	0	-1.319493	0.597339	0.797716
7	6	0	-0.090314	1.105582	1.309741
8	6	0	1.699079	-1.661738	-1.890708
9	6	0	2.453929	-2.401125	-2.800600
10	6	0	1.755580	-3.136894	-3.759695
11	6	0	0.350836	-3.127181	-3.804207
12	6	0	-0.399661	-2.385446	-2.887448
13	6	0	0.275798	-1.641435	-1.909930
14	1	0	-0.127709	1.810148	2.141044
15	1	0	3.542843	-2.389999	-2.753099
16	1	0	2.312690	-3.727917	-4.489719
17	1	0	-1.486103	-2.394260	-2.940946
18	1	0	-0.166042	-3.710319	-4.569171
19	7	0	-2.574900	-0.614248	-0.926475
20	6	0	-3.468668	0.471450	-1.222538
21	6	0	-3.031087	-1.941220	-1.043304
22	6	0	-4.560509	0.725476	-0.367111
23	6	0	-3.210384	1.306545	-2.308380
24	6	0	-3.998026	-2.266765	-2.010254
25	6	0	-2.541782	-2.947017	-0.193844
26	6	0	-5.379576	1.849168	-0.580813
27	6	0	-4.624566	-0.142322	0.841131
28	6	0	-4.044792	2.399478	-2.536900
29	1	0	-2.357545	1.095585	-2.955936

30	6	0	-4.477151	-3.572786	-2.108429
31	1	0	-4.366856	-1.490443	-2.681429
32	6	0	-3.023345	-4.249314	-0.305313
33	1	0	-1.795321	-2.700371	0.560694
34	6	0	-5.122169	2.687478	-1.688742
35	6	0	-6.417884	2.231223	0.456644
36	6	0	-3.498348	-0.072802	1.678881
37	6	0	-5.585928	-1.148978	1.047711
38	1	0	-3.845861	3.059258	-3.385316
39	6	0	-3.997856	-4.571786	-1.255694
40	1	0	-5.229471	-3.811748	-2.863702
41	1	0	-2.637586	-5.019906	0.365771
42	6	0	-5.983227	3.902794	-1.968056
43	6	0	-7.428490	3.270117	-0.027670
44	1	0	-6.932226	1.336294	0.833366
45	7	0	-2.512287	0.943347	1.424406
46	6	0	-3.303613	-0.985534	2.713284
47	6	0	-5.407336	-2.060549	2.113674
48	6	0	-6.714221	-1.328006	0.051135
49	1	0	-4.372358	-5.593962	-1.337168
50	6	0	-6.712732	4.422486	-0.729726
51	1	0	-5.363022	4.692929	-2.420063
52	1	0	-8.140927	2.802105	-0.730450
53	6	0	-2.823332	2.277144	1.731733
54	6	0	-4.270953	-1.964295	2.927846
55	1	0	-2.410224	-0.919854	3.336458
56	6	0	-6.409535	-3.165843	2.374351
57	6	0	-7.828354	-2.258555	0.529823
58	1	0	-7.125516	-0.351528	-0.239510
59	1	0	-5.985648	4.878390	-0.034046
60	6	0	-3.644885	2.577366	2.834739
61	6	0	-2.364763	3.314269	0.895650
62	1	0	-4.133453	-2.687132	3.735635
63	6	0	-7.238726	-3.526818	1.143049
64	1	0	-5.880284	-4.048725	2.765980
65	1	0	-8.450411	-1.744819	1.284699
66	6	0	-3.992694	3.899716	3.097068
67	1	0	-3.997748	1.769865	3.476235
68	6	0	-2.721384	4.630422	1.168834
69	1	0	-1.771873	3.068860	0.014529
70	1	0	-6.595402	-4.029759	0.399746
71	6	0	-3.535340	4.931012	2.268203
72	1	0	-4.623732	4.129099	3.958053
73	1	0	-2.377460	5.428200	0.507660
74	1	0	-3.814325	5.965616	2.476316
75	1	0	2.067725	0.993586	1.234928
76	6	0	3.543136	-0.562091	-0.565394
77	6	0	4.203895	-1.347408	0.389326
78	6	0	4.190257	0.487759	-1.232089
79	6	0	5.539995	-1.055777	0.673020
80	1	0	3.701746	-2.166770	0.903914

81	6	0	5.526682	0.744027	-0.918520
82	1	0	3.677409	1.095344	-1.977872
83	6	0	6.240200	-0.009858	0.036549
84	8	0	6.149717	-1.833448	1.605580
85	8	0	6.122727	1.770794	-1.579512
86	5	0	7.702342	0.292756	0.366533
87	6	0	7.465628	-1.645974	1.998292
88	6	0	7.446861	2.127604	-1.378668
89	6	0	8.296670	1.464481	-0.449291
90	6	0	8.301725	-0.632451	1.451013
91	6	0	7.892203	-2.540815	2.976422
92	6	0	7.866754	3.194216	-2.169552
93	6	0	9.620877	1.974391	-0.391260
94	6	0	9.616263	-0.597328	1.987428
95	6	0	9.202788	-2.465907	3.470265
96	1	0	7.185533	-3.289680	3.339456
97	6	0	9.185293	3.662122	-2.071447
98	1	0	7.148879	3.645351	-2.857382
99	6	0	10.059702	3.042114	-1.175832
100	1	0	10.330609	1.511029	0.293526
101	6	0	10.061326	-1.485082	2.968203
102	1	0	10.311299	0.157402	1.620470
103	1	0	9.539839	-3.167520	4.236744
104	1	0	9.516825	4.498501	-2.691061
105	1	0	11.092221	3.390886	-1.087230
106	1	0	11.086011	-1.409646	3.342265
107	1	0	-5.872091	2.637359	1.325755
108	1	0	-8.021899	3.634053	0.825754
109	1	0	-7.422829	5.214127	-1.015423
110	1	0	-6.730708	3.630665	-2.736643
111	1	0	-6.267866	-1.741618	-0.868208
112	1	0	-8.493890	-2.498830	-0.314005
113	1	0	-8.031969	-4.238816	1.419204
114	1	0	-7.088867	-2.836842	3.183034

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