**Supporting Information**

**Multiple Resonance Deep-red Emitters with Hybridized π-bonding/ non-bonding Orbitals to Surpass the Energy Gap Law**

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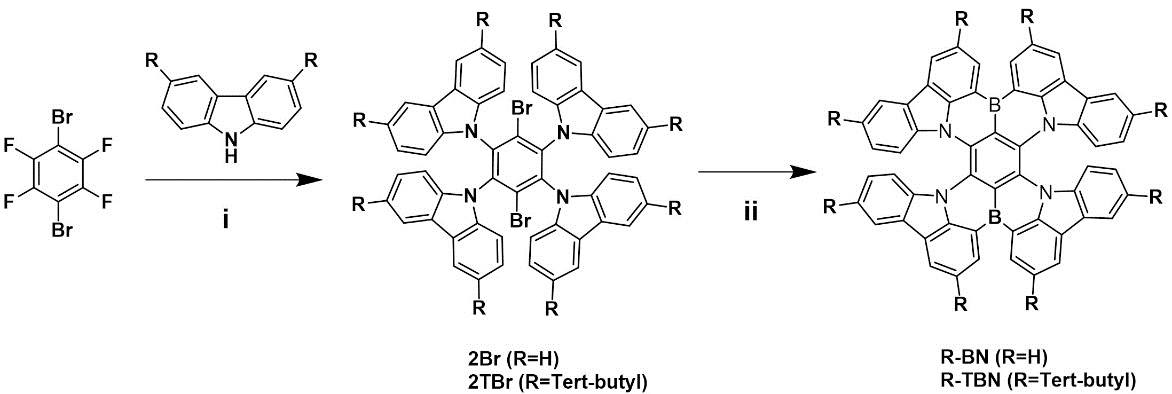
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**1. Experimental Section**

**1.1 General Information.** All commercially available reagents were used as received unless otherwise stated. All reactions were carried out using Schlenk techniques under a nitrogen atmosphere. 600/400 MHz 1H-NMR and 150 MHz 13C-NMR spectra were measured by a JEOL JNM-ECS600 spectrometer at room temperature in deuterated dichloromethane and chloroform respectively with tetramethyl silane as the internal standard. MALDI-TOF-MS data was performed on a Shimadzu AXIMA Performance MALDI-TOF instrument in positive detection modes. Elemental analysis was obtained with a CE-440 Elemental Analyzer.

**1.2 Synthesis.**

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**Scheme S1.** Synthetic procedures: i) Cs2CO3, DMF, 150℃, 12 h; ii) n-BuLi, t-BuPh, 0℃, 30 min, then 60℃, 24 h; 2. BBr3, -40℃, 0.5 h, then RT, 0.5 h; 3. NEt(i-Pr)2, 0℃, then 120℃,5 h.

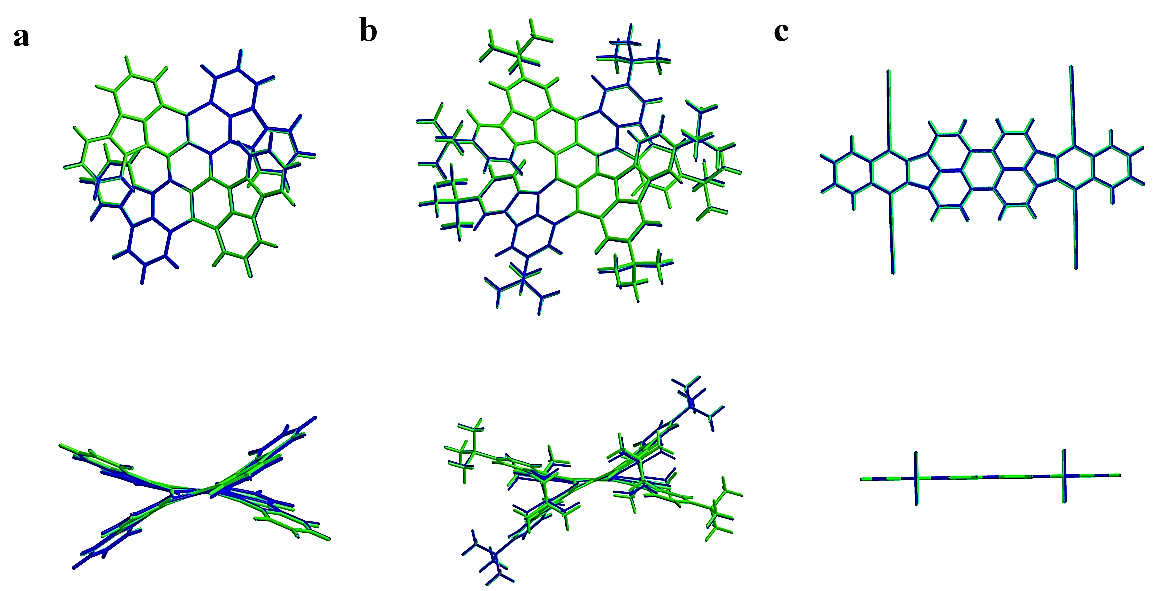
**Synthesis of 2Br:** *9,9',9'',9'''-(3,6-dibromobenzene-1,2,4,5-tetrayl)tetrakis(9H-carbazole)*: Under argon atmosphere carbazole (9.78g, 58.47 mmol) was added to a two necked round bottom flask equipped with a reflux condenser. Addition of cesium carbonate (38.10 g, 116.93mmol) followed by DMF (50 ml) resulted in a suspension, which was stirred for 30 min at room temperature. Afterwards, 5-bromo-2-chloro-1,3-difluorobenzene (3.00g, 9.74 mmol) was poured in all in once and reaction mixture was stirred at 155°C for 12 hours. The mixture was diluted with water and the crude product was recrystallized from hot ethanol. **2Br** (7.52g, 8.39mmol, 86%) was obtained as white solid. 1H NMR (400 MHz, Chloroform-*d*) *δ*: 7.80-7.77 (d, 8H), 7.26-7.24 (d, 8H),7.13-7.09 (t, 16H). MALDI-TOF: Calculated: 896.69, Found: 897.06. Anal. Calcd (%) for C54H32Br2N4: C, 72.33; H, 3.60; Br, 17.82; N, 6.25; Found: C, 72.22; H, 3.81; Br, 17.77; N, 6.20.

**Synthesis of 2TBr:** *9,9',9'',9'''-(3,6-dibromobenzene-1,2,4,5-tetrayl)tetrakis(3,6-di-tert-butyl-9H-carbazole)*: **2TBr** was synthesized according to the same procedure as for **2Br** by using 3,6-Di-tert-butylcarbazole (10.89 g, 38.98 mmol) instead carbazole. After recrystallization from hot ethanol, **2TBr** (8.02 g, 5.96 mmol, 94%) was obtained as white solid. 1H NMR (400 MHz, Chloroform-*d*) *δ*: 7.60 (d, *J* = 1.8 Hz, 8H), 7.09 (s, 8H), 6.95 (s, 8H), 1.37 (s, 72H). MALDI-TOF: Calculated: 1345.55, Found: 1345.63. Anal. Calcd (%) C86H96Br2N4: C, 76.77; H, 7.19; Br, 11.88; N, 4.16; Found: C, 76.61; H, 7.32; Br, 11.78; N, 4.29.

**Synthesis of R-BN:**A solution of n-butyllithium in pentane (7.9 mL, 1.70 M, 13.38 mmol) was added slowly to a solution of **2Br** (2.0 g, 2.2 mmol) in tert-butylbenzene (20 mL) at 0 ºC under a nitrogen atmosphere. After stirring at 60 ºC for 24 h, pentane was removed in vacuo. After addition of boron tribromide (2.5 mL, 26.8 mmol) at –40 ºC, the reaction mixture was stirred at room temperature for 0.5 h. *N,N*-Diisopropylethylamine (7.0 mL, 40.2 mmol) was added at 0 ºC and then the reaction mixture was allowed to warm to room temperature. After stirring at 120 ºC for 5 h, the reaction mixture was cooled to room temperature. An aqueous solution of sodium acetate (5.0 g in 50 mL) and dichloromethane (100 mL) was added to the reaction mixture. The aqueous layer was separated and extracted with dichloromethane (100 mL). The combined organic layers were dried with magnesium sulphate, filtered, and evaporated under reduced pressure. The crude product was purified by column chromatography (silica, CH2Cl2 / petroleum ether = 50:1) and recrystallized from CH2Cl2 and methanol as a grey powder (0.64 g, yield: 38%).1H NMR (600 MHz, Chloroform-*d*) δ 9.26 (d, *J* = 7.5 Hz, 1H), 8.50 (d, *J* = 7.3 Hz, 1H), 7.96 – 7.87 (m, 2H), 6.97 (t, *J* = 7.3 Hz, 1H), 6.68 (t, *J* = 7.7 Hz, 1H), 6.47 (d, *J* = 8.4 Hz, 1H). 13C NMR (151 MHz, Chloroform-*d*) *δ*: 141.93, 139.19, 133.20, 126.08, 125.07, 124.77, 122.85, 122.17, 121.88, 120.25, 111.53. MALDI-TOF: Calculated: 754.47, Found: 754.33. Anal. Calcd (%) for C54H28B2N4: C, 85.97; H, 3.74; B, 2.87; N, 7.43; Found: C, 85.84; H, 3.85; B, 2.66; N, 7.65.

**Synthesis of R-TBN:** **R-TBN**was synthesized according to the same procedure as for **R-BN** by using **2TBr** (2.0 g, 1.5 mmol) instead **2Br** (2.0 g, 2.2 mmol). **R-TBN** (0.72 g, yield: 40%) was obtained as a grey solid. 1H NMR (600 MHz, Chloroform-*d*) *δ*: 9.05 (s, 2H), 8.43 (s, 2H), 8.38 (s, 2H), 8.35 (d, J = 8.7 Hz, 2H), 8.24 (s, 2H), 7.69 – 7.63 (m, 3H), 7.58 – 7.52 (m, 2H), 7.23 – 7.18 (m, 1H), 1.66 (s, 18H), 1.54 (s, 18H). 13C NMR (600 MHz, CDCl3) 13C NMR (151 MHz, Chloroform-*d*) *δ*: 145.01, 144.33, 138.03, 129.39, 127.76, 125.15, 124.63, 123.45, 122.23, 121.80, 115.90, 111.60, 35.50, 34.59, 32.47, 31.74. MALDI-TOF: Calculated: 1203.33, Found: 1203.63. Anal. Calcd (%) C86H92B2N4: C, 85.84; H, 7.71; B, 1.80; N, 4.66; Found: C, 85.95; H, 7.67; B, 1.60; N, 4.78.

1. **Supplementary figures** **and tables**

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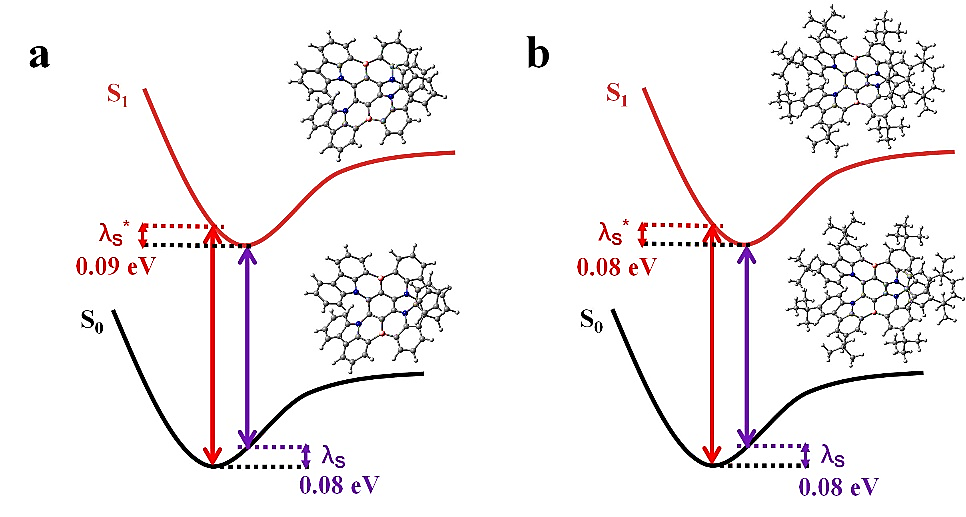
**Figure S1.** Comparison of the optimized structures of R-BN (a), R-TBN (b) and DBP (c) in the S0 (blue) and S1 (green) states.

**Table S1.** Summary of Franck-Condon analysis on the S0–S1 transition of R-BN, R-TBN and DBP at the (TD)B3LYP/6-31G(d) level.

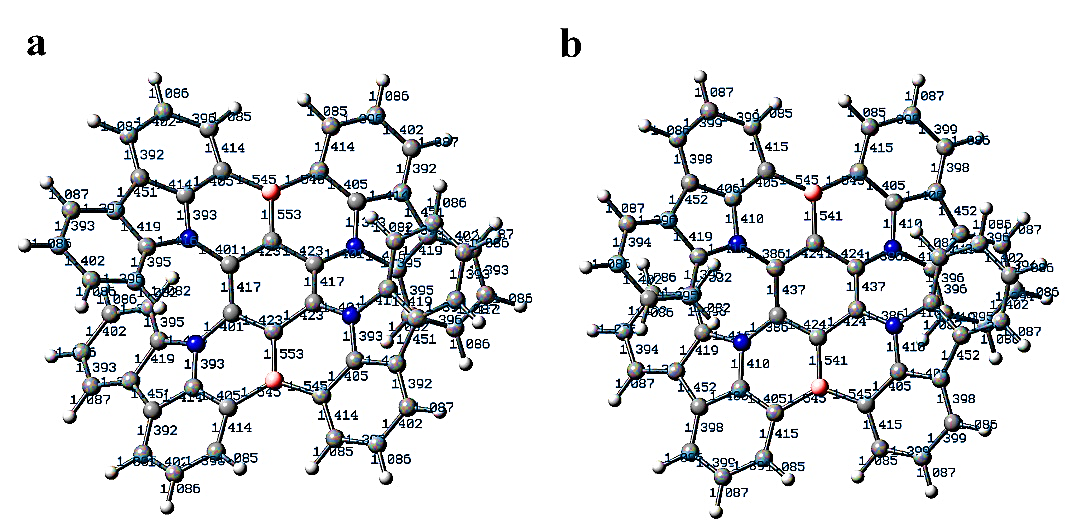
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| --- | --- | --- | --- | --- | --- |
| compound | transition  (S0 → S1) | frequency  (cm–1) | Relative frequency  (cm–1) | line  density | dipole strength  (a.u.) |
| R-BN | 0 → 0 | 14956.9714 | 0 | 13480 | 0.8182 |
|  | 0 → 71 | 15032.4336 | 75.4622 | 4687 | 0.2832 |
|  | 0 → 131 | 15077.5726 | 120.6012 | 4369 | 0.2632 |
|  | 0 → 13171 | 15153.0348 | 196.0634 | 1498 | 0.090 |
|  | 0 → 251 | 15188.3327 | 231.3613 | 3996 | 0.2390 |
|  | 0 → 291 | 15234.8884 | 277.9170 | 2747 | 0.1638 |
|  | 0 → 25171 | 15263.7948 | 306.8234 | 1308 | 0.0788 |
|  | 0 → 351 | 15298.6372 | 341.6658 | 2384 | 0.1415 |
|  | 0 → 251131 | 15308.9339 | 351.9625 | 1269 | 0.0753 |
|  | 0 → 391 | 15338.8585 | 381.8871 | 2183 | 0.1293 |
| R-TBN | 0 → 0 | 14566.8524 | 0 | 11350 | 0.7078 |
|  | 0 → 51 | 14587.8708 | 21.0184 | 1699 | 0.1058 |
|  | 0 → 81 | 14598.2666 | 31.4142 | 2559 | 0.1593 |
|  | 0 → 161 | 14605.9974 | 39.1450 | 1834 | 0.1141 |
|  | 0 → 201 | 14630.8225 | 63.9701 | 1967 | 0.1221 |
|  | 0 → 231 | 14645.6301 | 78.7777 | 1686 | 0.1046 |
|  | 0 → 311 | 14681.261 | 114.4086 | 1524 | 0.09429 |
|  | 0 → 841 | 14887.6385 | 320.7861 | 2259 | 0.1378 |
| DBP | 0 → 0 | 15023.5961 | 0 | 146200 | 8.839 |
|  | 0 →22 | 15037.1235 | 13.5274 | 15590 | 0.9416 |
|  | 0 →32 | 15043.9355 | 20.3394 | 9765 | 0.5896 |
|  | 0 → 221 | 15177.641 | 154.0449 | 30890 | 1.848 |
|  | 0 → 531 | 15461.1973 | 437.6012 | 6338 | 0.3723 |
|  | 0 → 611 | 15523.3474 | 499.7513 | 6316 | 0.3695 |
|  | 0 →1951 | 16327.7259 | 1304.1298 | 29590 | 1.646 |
|  | 0 →1951221 | 16481.7708 | 1458.1747 | 6412 | 0.3533 |
|  | 0 → 2231 | 16498.7421 | 1475.1460 | 7756 | 0.4270 |
|  | 0 →2311 | 16528.5489 | 1504.9528 | 21520 | 1.182 |
|  | 0 →2511 | 16667.3484 | 1643.7523 | 20020 | 1.091 |

**Table S2.** Summary of Franck-Condon analysis on the S1–S0 transition of R-BN, R-TBN and DBP at the (TD)B3LYP/6-31G(d) level.

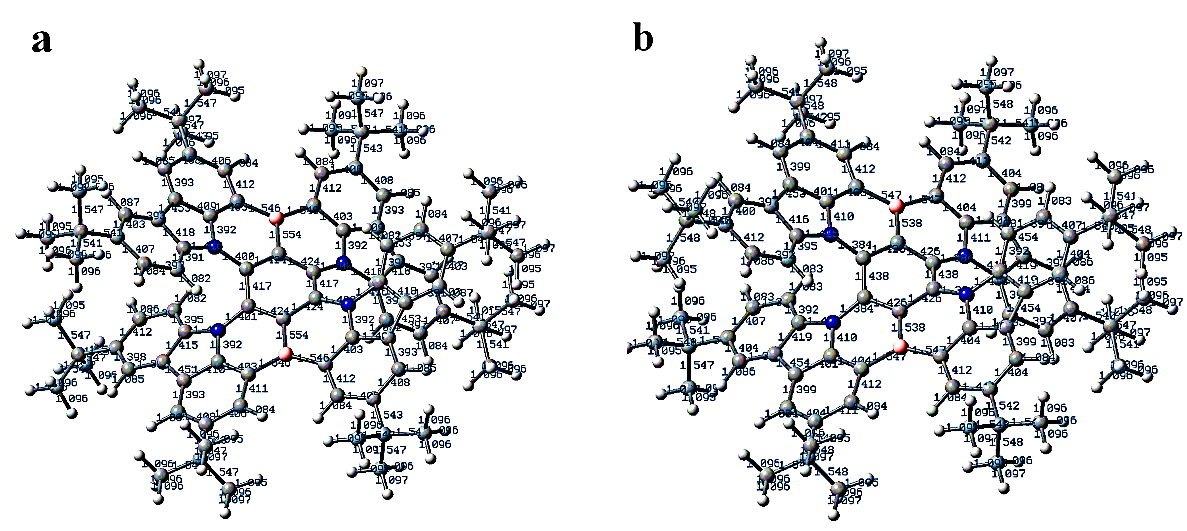
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| --- | --- | --- | --- | --- | --- |
| compound | transition  (S1 → S0) | frequency  (cm–1) | Relative frequency  (cm–1) | line  density | dipole strength  (a.u.) |
| R-BN | 0 → 0 | 13710.5293 | 0 | 74.62 | 0.8276 |
|  | 0 → 81 | 13630.9448 | -79.5845 | 22.91 | 0.2601 |
|  | 0 →141 | 13586.9042 | -123.6251 | 18.65 | 0.2145 |
|  | 0 → 261 | 13476.5627 | -233.9666 | 17.40 | 0.2068 |
|  | 0 → 301 | 13422.6493 | -287.8800 | 9.990 | 0.1206 |
|  | 0 → 371 | 13365.728 | -344.8013 | 13.14 | 0.1614 |
|  | 0 → 401 | 13333.2926 | -377.2367 | 13.26 | 0.1645 |
|  | 0 → 461 | 13256.1938 | -454.3355 | 5.917 | 0.0751 |
| R-TBN | 0 → 0 | 13256.0205 | 0 | 51.95 | 0.6593 |
|  | 0 → 11 | 13250.1384 | -5.8821 | 7.627 | 0.09697 |
|  | 0 → 81 | 13223.1886 | -32.8319 | 12.01 | 0.1540 |
|  | 0 → 161 | 13216.6104 | -39.4101 | 8.911 | 0.1145 |
|  | 0 → 231 | 13175.6878 | -80.3327 | 7.610 | 0.09901 |
|  | 0 → 911 | 12924.0378 | -331.9827 | 9.978 | 0.1402 |
| DBP | 0 → 0 | 13714 | 0 | 755.9 | 8.374 |
|  | 0 → 32 | 13673.3388 | -40.6612 | 31.15 | 0.3494 |
|  | 0 →42 | 13669.2258 | -44.7742 | 47.94 | 0.5381 |
|  | 0 →52 | 13668.8963 | -45.1037 | 58.99 | 0.6622 |
|  | 0 → 221 | 13560.3158 | -153.6842 | 152.3 | 1.765 |
|  | 0 → 521 | 13275.6291 | -438.3709 | 32.03 | 0.4041 |
|  | 0 → 2021 | 12386.3699 | -1327.6301 | 91.22 | 1.519 |
|  | 0 →2171 | 12294.9559 | -1419.0441 | 35.58 | 0.6103 |
|  | 0 → 2201 | 12252.0906 | -1461.9094 | 21.80 | 0.3797 |
|  | 0 → 2241 | 12227.7905 | -1486.2095 | 60.14 | 1.054 |
|  | 0 → 2501 | 12070.1554 | -1643.8446 | 27.37 | 0.5055 |

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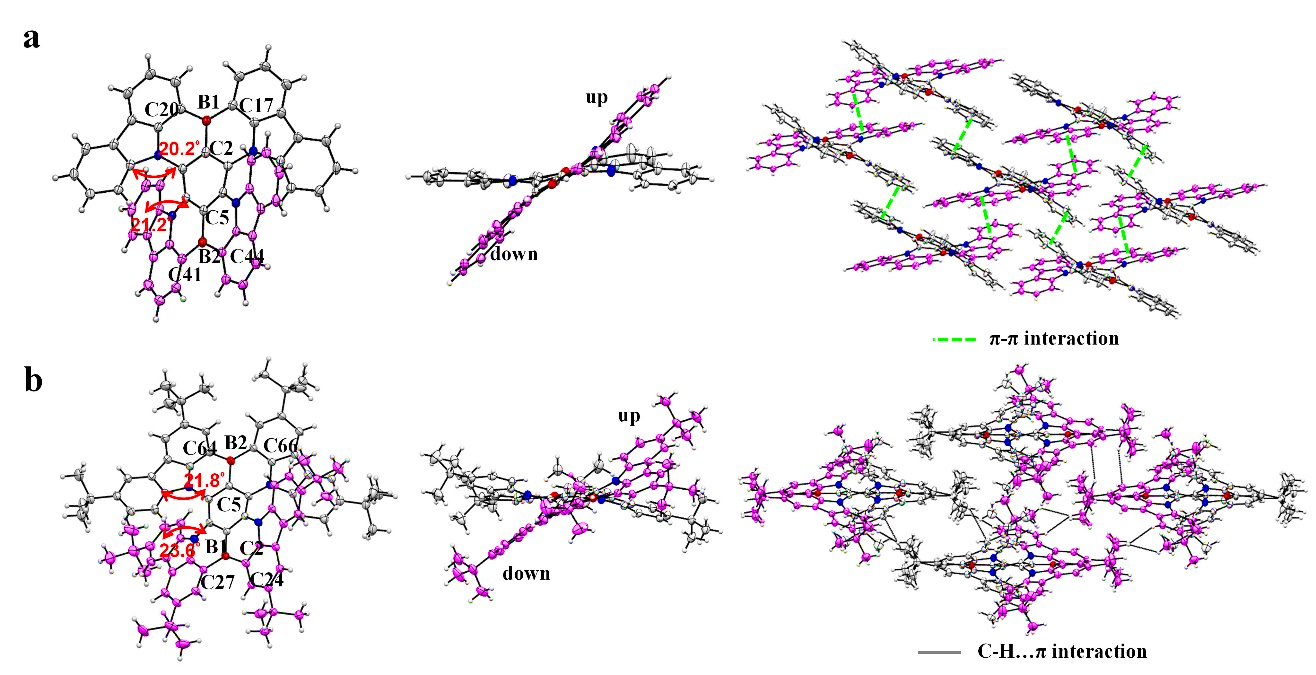
**Figure S2.** The optimized S0 and S1 structures, reorganization (*λ*S) and structural relaxation (*λ*S\*) energies of (a) R-BN and (b) R-TBN.



**Figure S3.** Bond lengths of the optimized structures of R-BN in the (a) S0 and (b) S1 states.

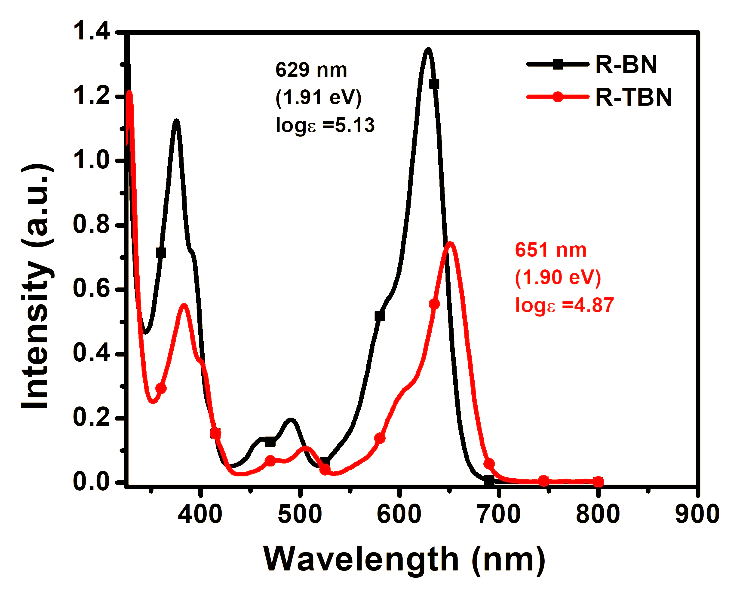


**Figure S4.** Bond lengths of the optimized structures of R-TBN in the (a) S0 and (b) S1 states.

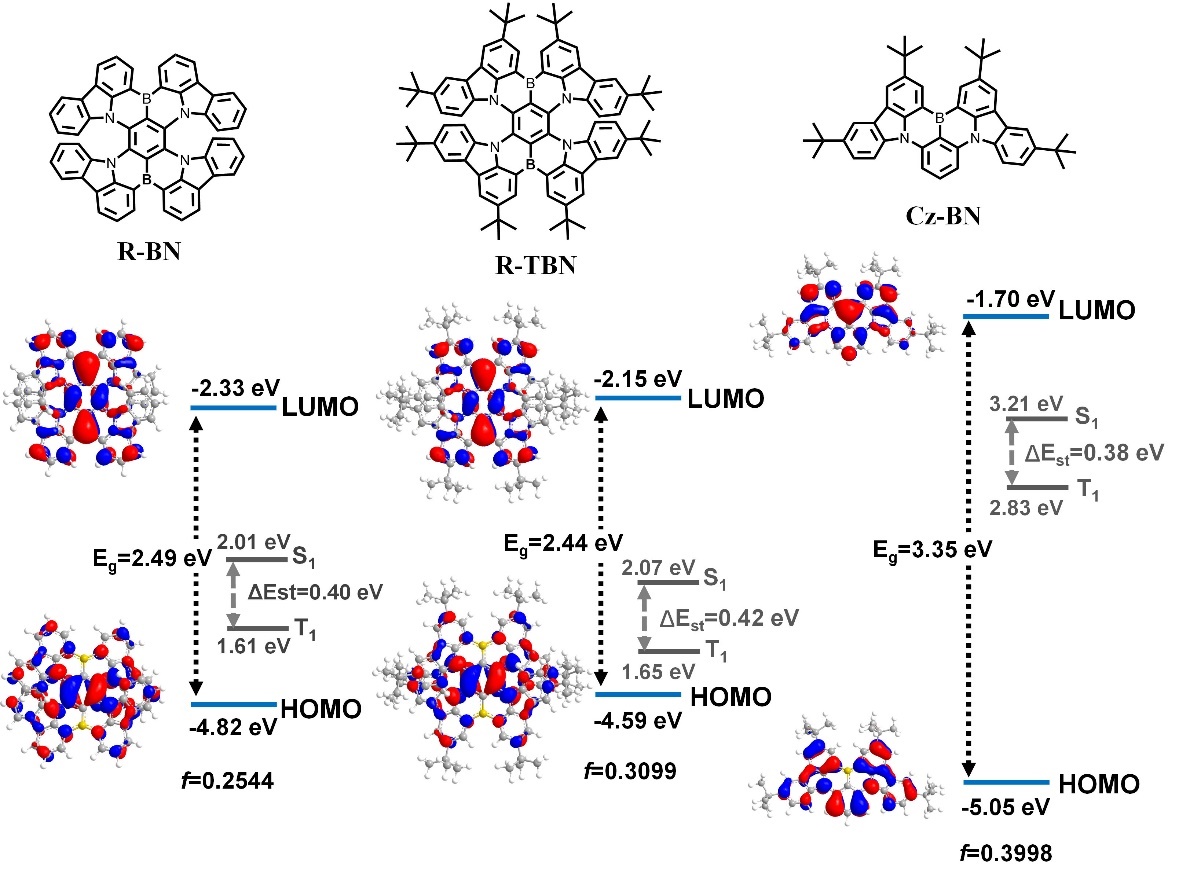
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**Figure S5.** Crystal structures and molecular packing patterns of R-BN (a) and R-TBN (b).

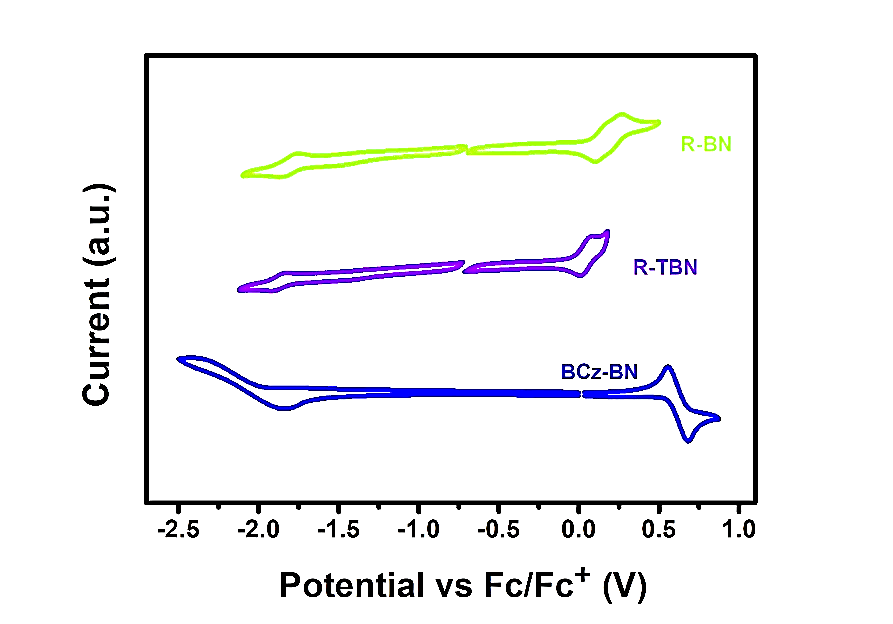
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| **Table S3.** Summary of TD-DFT calculation for R-BN, R-TBN, BCz-BN and DBPat the S0, S1, and T1 structures at the B3LYP/6-31G(d) level. | | | | | | |
| compound | Optimized structure | transition | Wavelength  (nm) | Energy  (eV) | Oscillator  strength | coefficient of HOMO-LUMO |
| R-BN | S0 | S0-S1 | 600.08 | 2.0661 | 0.2544 | 0.70423 |
|  |  | S0-T1 | 751.25 | 1.6504 | 0.0000 | 0.69848 |
|  | S1 | S1-S0 | 673.43 | 1.8411 | 0.2227 | 0.70526 |
|  | T1 | T1-S0 | 930.49 | 1.3325 | 0.0000 | 0.69992 |
| R-TBN | S0 | S0-S1 | 616.54 | 2.0110 | 0.3099 | 0.70448 |
|  |  | S0-T1 | 770.21 | 1.6098 | 0.0000 | 0.69827 |
|  | S1 | S1-S0 | 688.05 | 1.8020 | 0.2759 | 0.70539 |
|  | T1 | T1-S0 | 943.98 | 1.3134 | 0.0000 | 0.69968 |
| BCz-BN | S0 | S0-S1 | 433.92 | 2.8573 | 0.4125 | 0.70146 |
|  |  | S0-T1 | 505.55 | 2.4525 | 0.0000 | 0.68612 |
|  | S1 | S1-S0 | 453.96 | 2.7312 | 0.3558 | 0.70194 |
|  | T1 | T1-S0 | 530.09 | 2.3389 | 0.0000 | 0.68082 |
| DBP | S0 | S0-S1 | 572.91 | 2.1641 | 1.2005 | 0.70306 |
|  |  | S0-T1 | 1011.99 | 1.2251 | 0.0000 | 0.69114 |
|  | S1 | S1-S0 | 640.46 | 1.9359 | 1.1841 | 0.70522 |
|  | T1 | S0-T1 | 1396.04 | 0.8881 | 0.0000 | 0.70696 |

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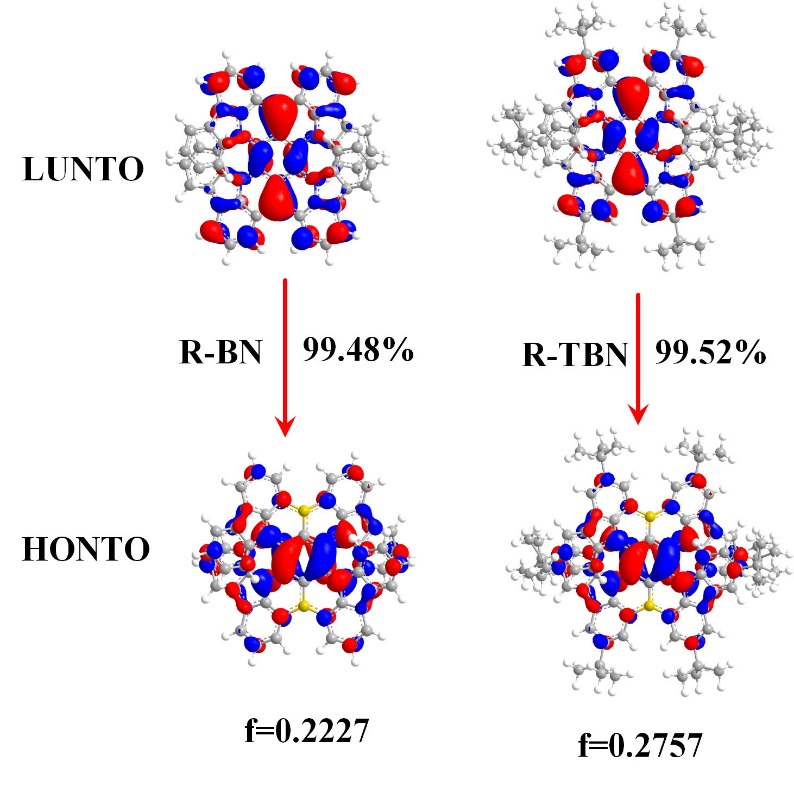
**Figure S6.** Absorption spectra of R-BN (black) and R-TBN (red) in toluene (0.01 mM solution at 298 K) with absorption maxima (nm, eV) and absorption coefficient at absorption maxima.



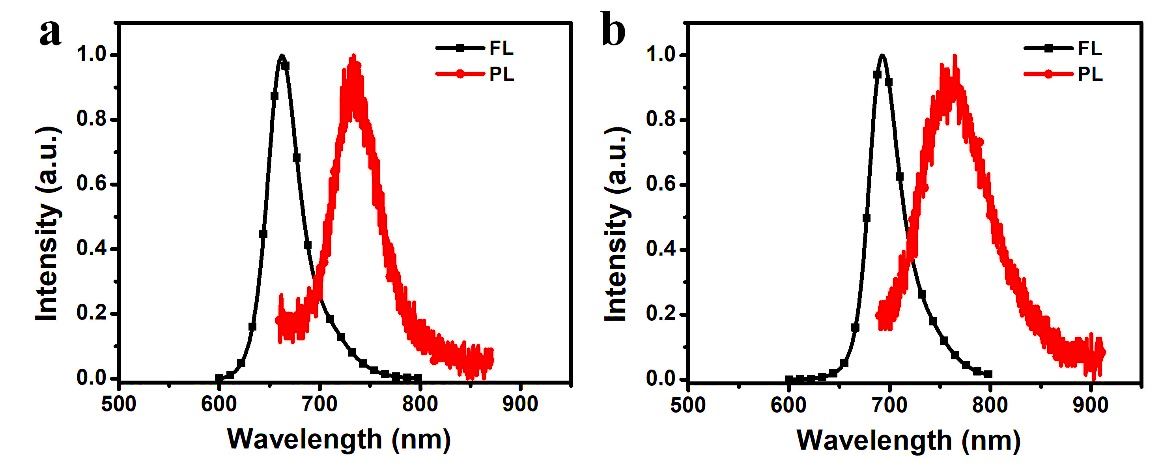
**Figure S7.** HOMO–LUMO distributions and the state levels of R-BN, R-TBN and BCz-BN.

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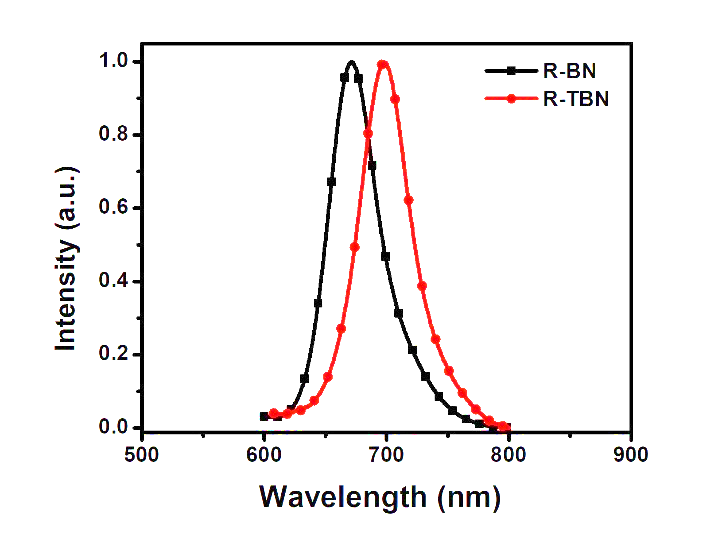
**Figure S8.** Cyclic Voltammograms of R-BN (green line), T-TBN ([purple](http://www.baidu.com/link?url=9fE0pAAXZZW0yaNeh4Se1hXYCfQoB39va8TlgQvSClbyjCGbjfIAgLgVelKefhpKTkVy5Xe-sc7JP4_ICo597xHfb7-JFaKjpXArwZJ10qO&wd=&eqid=986064ee000e58d4000000035f7c2364) line) and BCz-BN (blue line).

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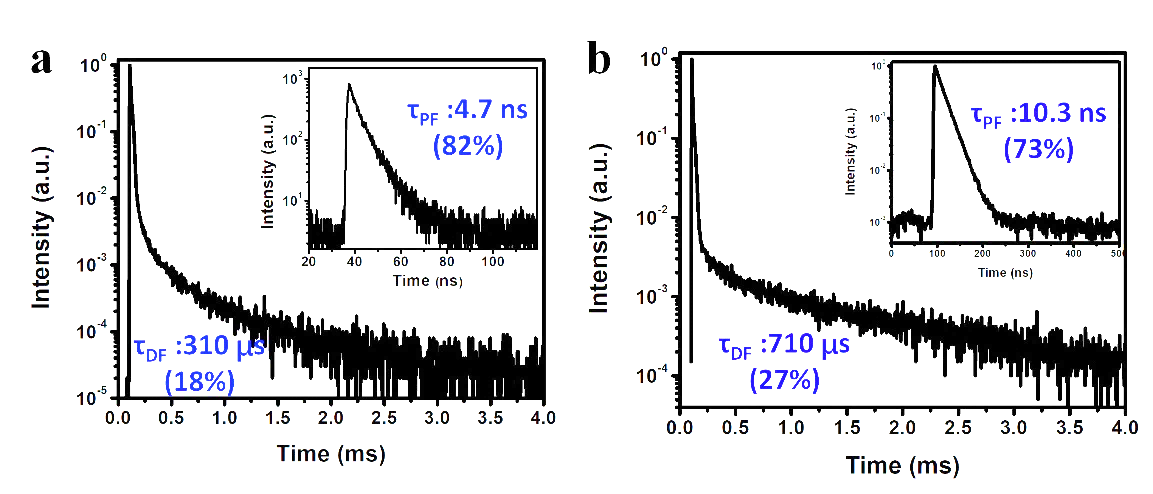
**Figure S9.** Highest occupied and lowest unoccupied natural transition orbitals (HONTOs and LUNTOs) of R-BNs for the S1 state.



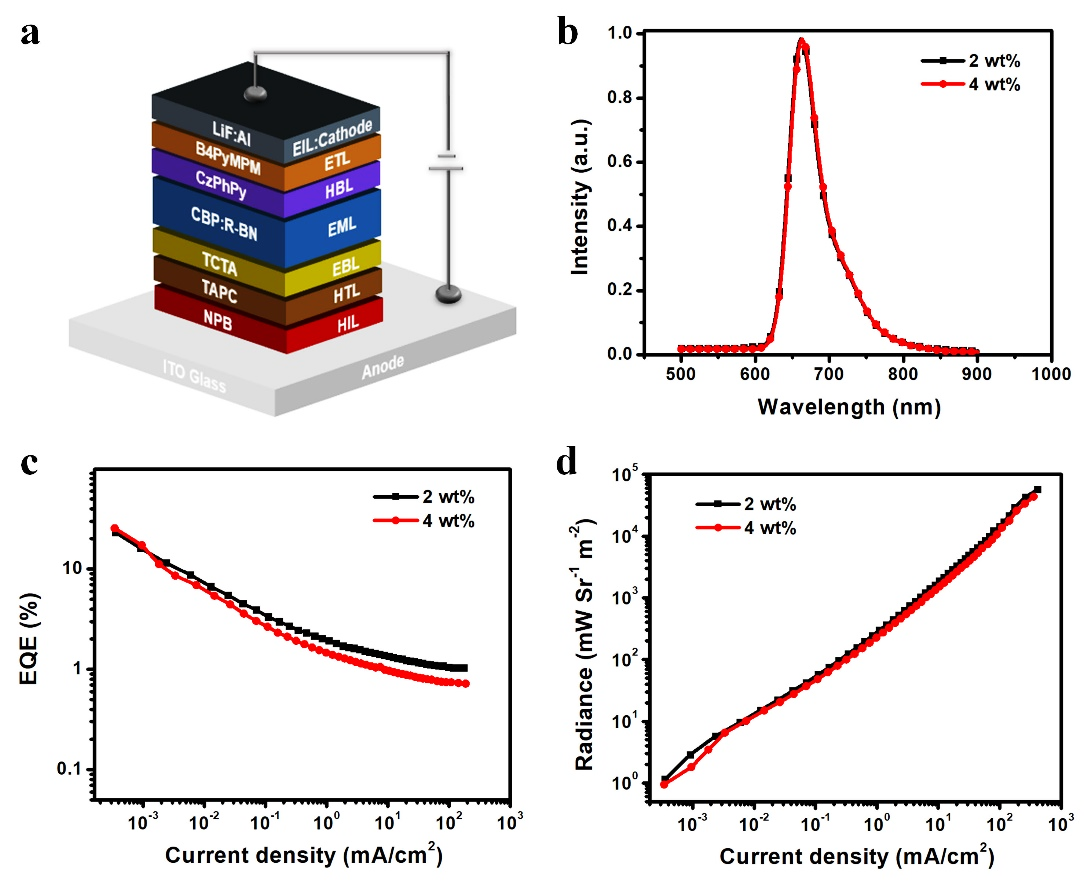
**Figure S10.** Fluorescence and Phosphorescence spectra of the R-BN (a) and R-TBN (b) in toluene.



**Figure S11.** The normalized PL spectrum of 3 wt%-doped films of R-BN (black) and R-TBN (red) in CBP.

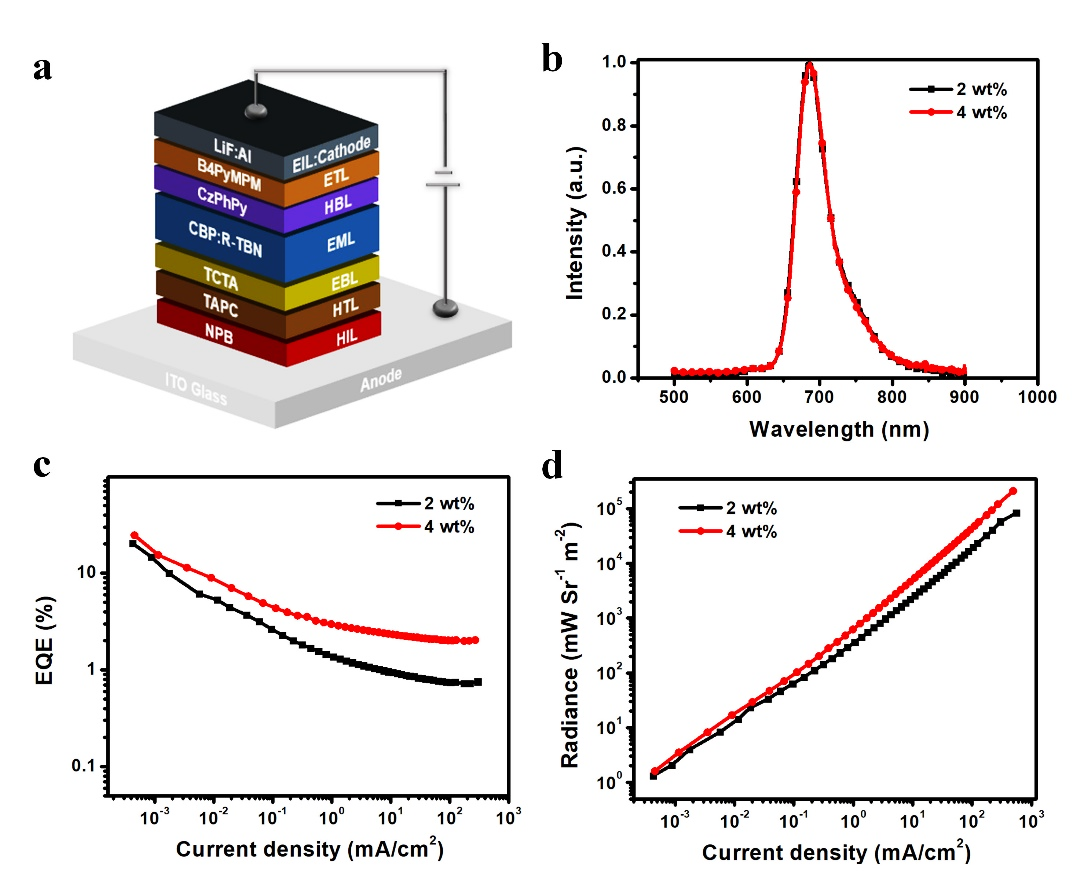


**Figure S12.** Transient decay spectra of a CBP film (3 wt%, dispersed) of R-BN (a) and R-TBN (b)at 300 K.



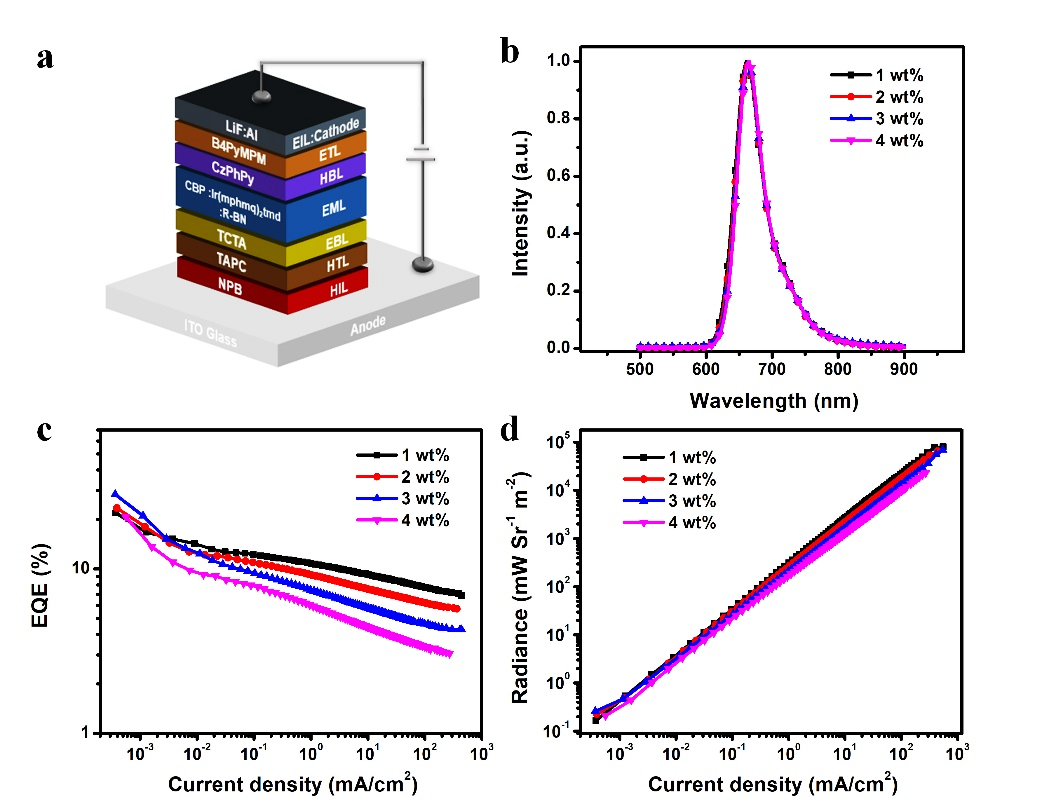
**Figure S13.** a) The energy level diagrams of the R-BN doped in CBP devices. b) The EL spectra of the devices. c) EQE versus current density characteristics. d) Radiance versus current density characteristics.

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| **Table S4.** Summary of the EL data of DR/NIR OLEDs based on R-BN doped in CBP with different doping concentrations. | | | | | |
| Device | λELa)[nm] | FWHMb)[nm] | EQEmaxc)[%] | Radianced)[mW Sr-1 m-2] | CIE (x,y)e) |
| 2 wt% R-BN | 662 | 49 | 23.1 | 0.6 × 105 | 0.718,0.280 |
| 4 wt% R-BN | 663 | 48 | 25.6 | 0.4 × 105 | 0.720,0.279 |
| a)Maximum electroluminescence wavelength. b)Full width at half maximum of electroluminescence. c)Maximum external quantum efficiencies. d)Maximum radiance. e)Recorded at 10 mA cm-2. | | | | | |

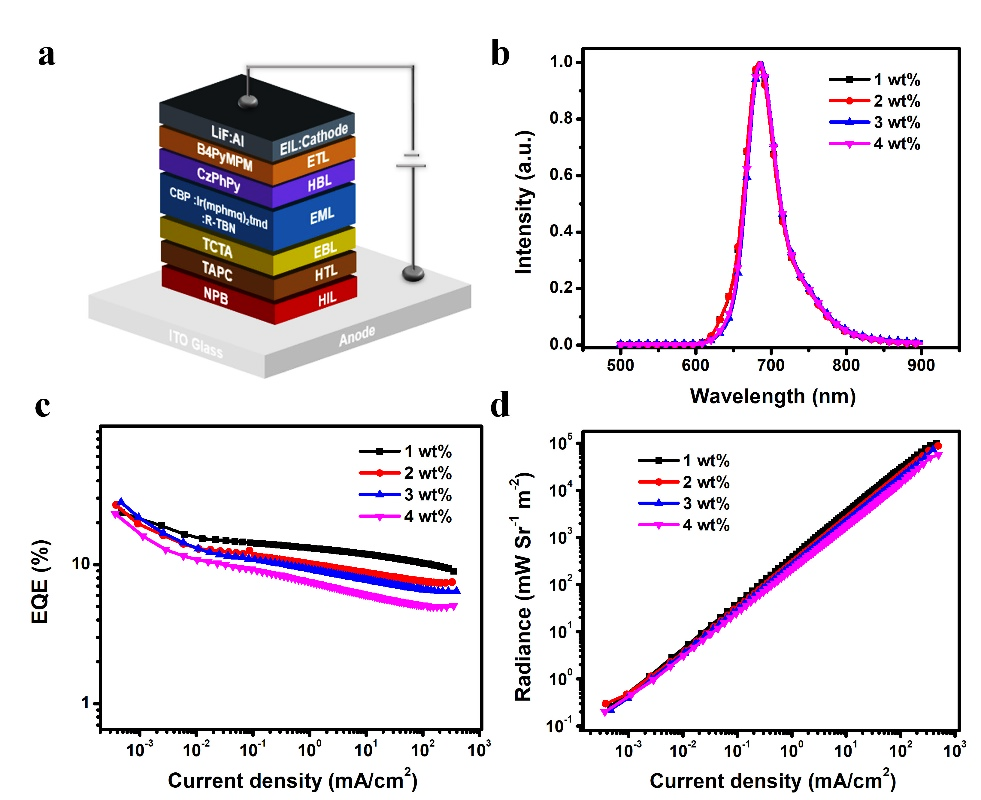
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**Figure S14.** a) The energy level diagrams of the R-TBN doped in CBP devices. b) The EL spectra of the devices. c) EQE versus current density characteristics. d) Radiance versus current density characteristics.

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| --- | --- | --- | --- | --- | --- |
| **Table S5.** Summary of the EL data of DR/NIR OLEDs based on R-TBN doped in CBP with different doping concentrations. | | | | | |
| Device | λELa)[nm] | FWHMb)[nm] | EQEmaxc)[%] | Radianced)[mW Sr-1 m-2] | CIE (x,y)e) |
| 2 wt% R-TBN | 686 | 49 | 20.3 | 0.8 × 105 | 0.721,0.278 |
| 4 wt% R-TBN | 686 | 48 | 24.7 | 2.1 × 105 | 0.722,0.278 |
| a)Maximum electroluminescence wavelength. b)Full width at half maximum of electroluminescence. c)Maximum external quantum efficiencies. d)Maximum radiance. e)Recorded at 10 mA cm-2. | | | | | |



**Figure S15.** a) The energy level diagrams of the R-BN doped in CBP and Ir(mphmq)2tmd devices. b) The EL spectra of the devices. c) EQE versus current density characteristics. d) Radiance versus current density characteristics.

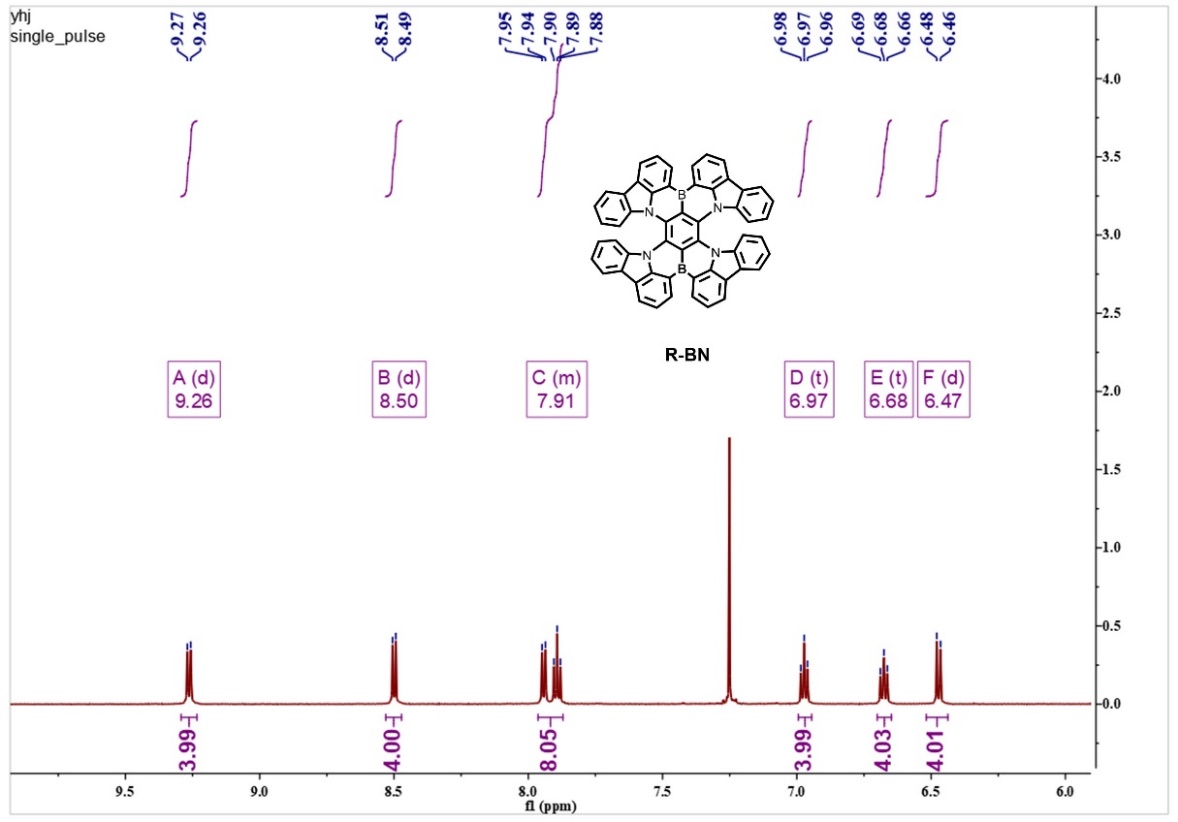


**Figure S16.** a) The energy level diagrams of the R-TBN doped in CBP and Ir(mphmq)2tmd devices. b) The EL spectra of the devices. c) EQE versus current density characteristics. d) Radiance versus current density characteristics.

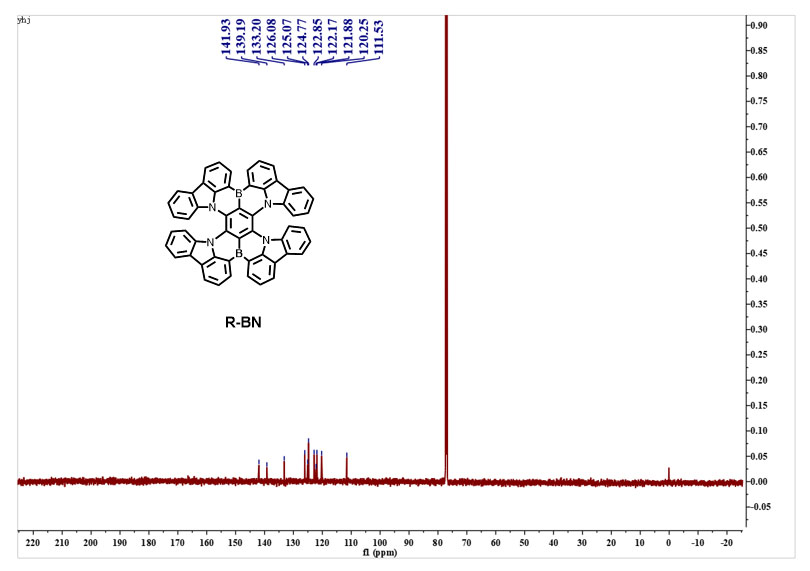
|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Table S6.** Summary of the EL data of DR/NIR OLEDs based on R-BNs doped in CBP and Ir(mphmq)2tmd with different doping concentrations. | | | | | |
| Device | λELa)[nm] | FWHMb)[nm] | EQEmaxc)[%] | Radianced)[mW Sr-1 m-2] | CIE (x,y)e) |
| 1 wt% R-BN | 661 | 50 | 21.9 | 7.5 × 105 | 0.716,0.282 |
| 2 wt% R-BN | 662 | 49 | 23.4 | 6.1 × 105 | 0.718,0.282 |
| 3 wt% R-BN | 664 | 48 | 28.4 | 6.5 × 105 | 0.719,0.280 |
| 4 wt% R-BN | 664 | 48 | 20.8 | 2.1 × 105 | 0.720,0.280 |
| 1 wt% R-TBN | 684 | 49 | 23.7 | 10.3 × 105 | 0.718,0.280 |
| 2 wt% R-TBN | 684 | 49 | 26.8 | 9.0 × 105 | 0.718,0.280 |
| 3 wt% R-TBN | 686 | 49 | 28.1 | 7.3 × 105 | 0.721,0.278 |
| 4 wt% R-TBN | 686 | 48 | 23.2 | 5.8 × 105 | 0.722,0.278 |
| a)Maximum electroluminescence wavelength. b)Full width at half maximum of electroluminescence. c)Maximum external quantum efficiencies. d)Maximum radiance. e)Recorded at 10 mA cm-2. | | | | | |

|  |  |  |  |
| --- | --- | --- | --- |
| **Table S7.** The DR/NIR OLEDs devices published to date with the emission maxima > 650 nm and the corresponding citations. | | | |
| EL λem (nm) | EQEmax (nm) | CIE (x,y) | Reference |
| 656 | 12.8 | 0.66,0.34 | 1 |
| 670 | 15 | 0.64,0.36 | 1 |
| 693 | 10.19 | - | 2 |
| 696 | 9.7 | - | 2 |
| 700 | 9.4 | 0.68,0.31 | 3 |
| 728 | 3.9 | 0.69,0.31 | 3 |
| 668 | 9.8 | 0.68,0.32 | 4 |
| 710 | 2.1 | 0.70,0.29 | 4 |
| 728 | 0.064 | 0.70,0.29 | 5 |
| 715 | 0.254 | 0.69,0.30 | 5 |
| 721 | 9.69 | - | 6 |
| 700 | 14.1 | - | 7 |
| 711 | 3.5 | - | 7 |
| 680 | 5.2 | 0.68,0.32 | 8 |
| 652 | 12.3 | 0.67,0.33 | 9 |
| 670 | 3.18 | 0.64,0.36 | 10 |
| 691 | 2.22 | 0.65,0.36 | 10 |
| 693 | 2.1 | 0.68,0.35 | 10 |
| 696 | 1.43 | 0.68,0.35 | 10 |
| 664 | 4.7 | 0.68,0.32 | 11 |
| 676 | 3.7 | 0.68,0.31 | 11 |
| 692 | 4.3 | 0.70,0.30 | 11 |
| 712 | 6.57 | 0.68,0.29 | 12 |
| **664** | **28.4** | **0.719,0.280** | **This work** |
| **686** | **28.1** | **0.721,0.278** | **This work** |

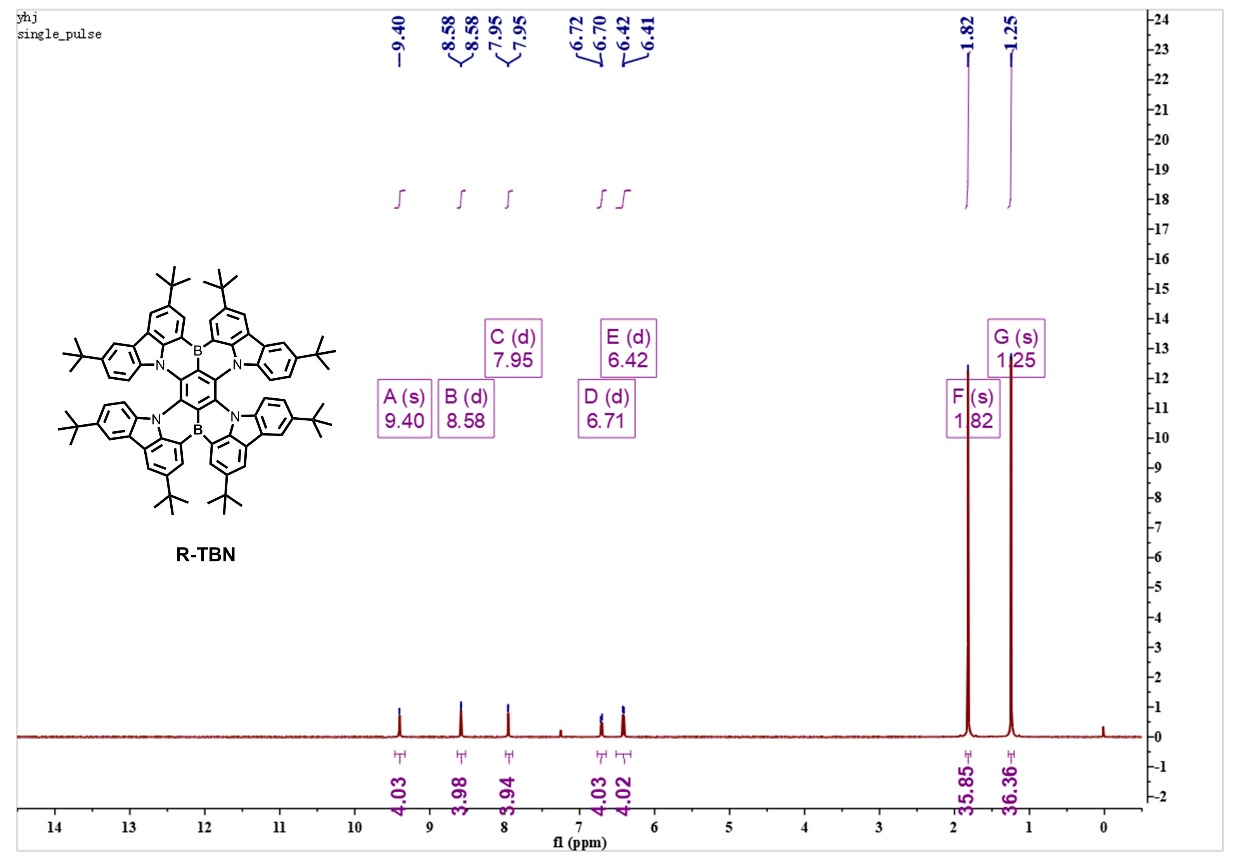
|  |  |  |
| --- | --- | --- |
| **Table S8.** Crystal Data and Structure Refinements of R-BNs Crystals. | | |
|  | R-BN | R-TBN |
| empirical formula | C54 H28 B2 N4 | C86 H92 B2 N4 |
| formula wt | 754.42 | 1203.25 |
| crystal system | Triclinic | Triclinic |
| *T* (K) | 99.99(10) | 99.99(10) |
| space group | P -1 | P -1 |
| *a*/Å | 8.0866(4) | 10.18637(18) |
| *b*/Å | 14.5879(5) | 17.8059(3) |
| *c*/Å | 15.5387(3) | 22.3062(3) |
| *α*/ ° | 91.985(2) | 106.4002(13) |
| β/ ° | 93.541(3) | 92.1304(13) |
| *γ*/ ° | 90.822(3) | 100.0691(15) |
| *V/*Å3 | 1828.23(12) | 3805.37(11) |
| *Z* | 2 | 2 |
| density, mg/m3 | 1.370 | 1.050 |
| absorption coefficient, mm-1 | 0.618 | 0.450 |
| *F (000)* | 780.0 | 1292.0 |
| θ range/Å | 4.090-66.573 | 3.773-75.274 |
| no. of reflcns collected | 6460 | 13444 |
| no. of unique reflns | 5129 | 15298 |
| *R*(int) | 0.0716 | 0.0459 |
| GOF | 1.049 | 1.042 |
| *R1* [*I* > *2σ*(*I*)] | 0.0469 | 0.0739 |
| *wR2* [*I* > *2σ*(*I*)] | 0.1176 | 0.1918 |
| *R1* (all data) | 0.1384 | 0.0812 |
| *wR2* (all data) | 0.1239 | 0.1969 |



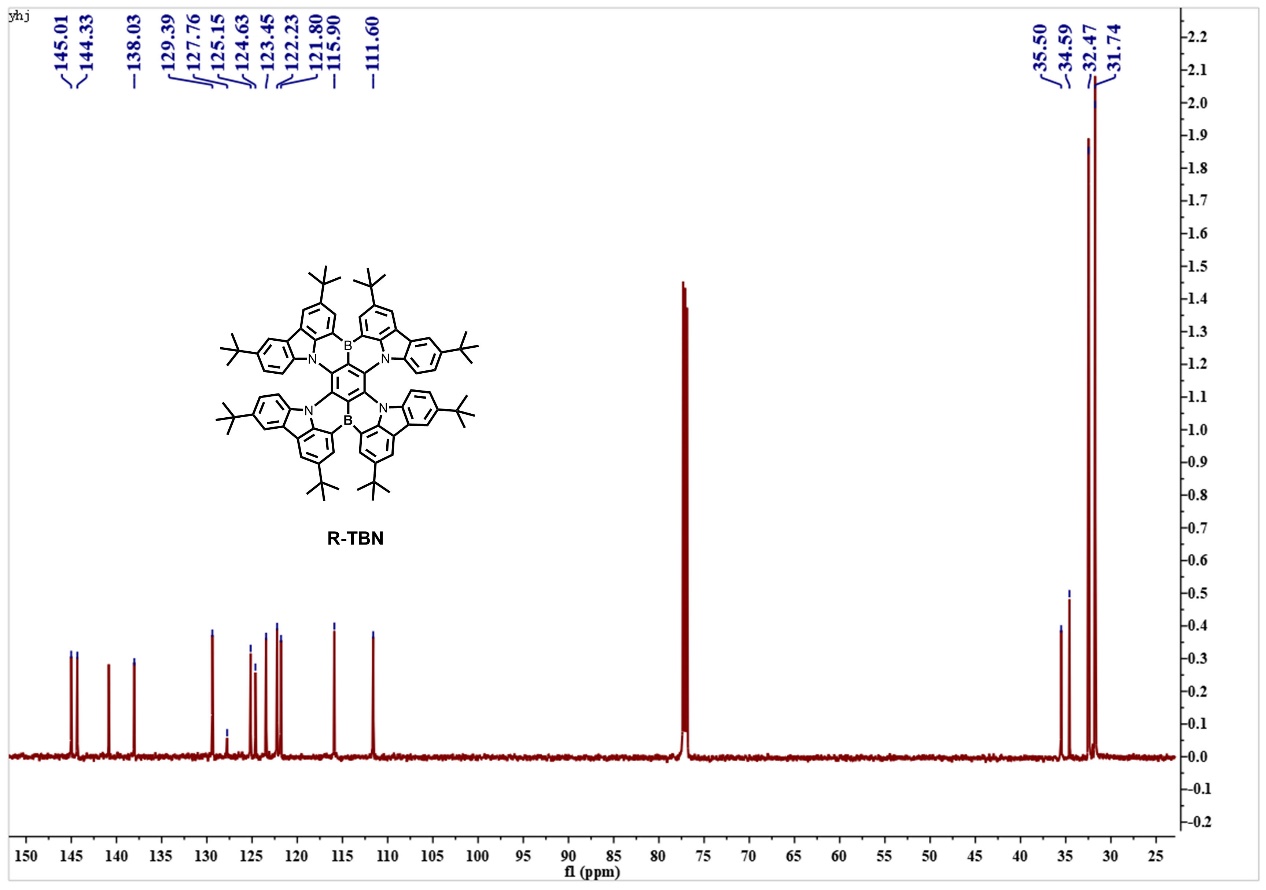
**Figure S17.** 1H NMR spectrum of R-BN in CDCl3.



**Figure S18.** 13C NMR spectrum of R-BN in CDCl3.



**Figure S19.** 1H NMR spectrum of R-TBN in CDCl3.



**Figure S20.** 13C NMR spectrum of R-TBN in CDCl3.

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|  |  |
| --- | --- |
| **Cartesian coordinates** |  |
| **R-TBN (S0)** |  |
| C -0.0306 -1.3143 -0.1366  C 1.1675 -0.7481 0.1402  C 1.1876 0.6001 0.3183  C -0.0086 1.2282 0.4052  C -1.1909 0.6633 0.0705  C -1.2208 -0.6889 0.0081  C 1.3683 3.2827 1.3449  C 1.6696 4.4687 1.8957  C -1.3749 3.4483 0.7527  C -1.6589 4.7354 1.0072  C -2.8085 5.3186 0.6085  C -3.6818 4.5498 -0.0727  C -3.3854 3.2693 -0.3216  C -2.2455 2.696 0.0763  C 2.3202 2.5448 0.7747  C 3.5484 3.0663 0.7022  C 3.859 4.2631 1.2132  C 2.9154 4.9858 1.8513  N -2.1693 1.4535 -0.2257  N 2.2374 1.3549 0.3094  C -3.2265 1.2336 -0.9311  C 3.3974 1.1513 -0.2167  C 3.8657 0.209 -1.0533  C 5.1458 0.2103 -1.4604  C 6.0288 1.1583 -1.0914  C 5.5382 2.169 -0.3494  C 4.2572 2.1518 0.0408  C -4.0359 2.3056 -0.9732  C -5.224 2.3345 -1.5904  C -5.6621 1.2505 -2.2578  C -4.8051 0.2141 -2.3313  C -3.6167 0.206 -1.7052  B -0.0682 2.6369 1.1478  C -3.1393 6.7887 0.8987  C 3.2702 6.3497 2.4578  C 7.4773 1.1142 -1.591  C -7.0111 1.2041 -2.9838  C -2.0311 7.5471 1.6663  C -3.3626 7.5373 -0.4342  C -4.4224 6.8589 1.7559  C 2.0827 7.063 3.1454  C 4.3729 6.1619 3.523  C -7.4747 -0.9202 2.0902  C -2.1399 -7.5339 -1.7098  C -3.8002 -7.4396 0.1387  C -4.4436 -6.7227 -2.1963  C -8.08 0.4421 1.6773  C -8.4102 -2.0129 1.5242  C -7.4723 -1.0358 3.6285  B -0.0431 -2.7216 -0.8838  H 0.8634 5.0201 2.3881  H -0.9244 5.3222 1.5627  H -4.6368 4.959 -0.4324  H 4.89 4.6332 1.1183  H 3.215 -0.5674 -1.4801  H 5.4546 -0.5931 -2.1481  H 6.1597 3.0302 -0.0699  H -5.8158 3.2585 -1.5463  H -5.0568 -0.6664 -2.9438  H -2.9708 -0.6616 -1.8973  H -2.3185 8.6075 1.8484  H -1.8374 7.103 2.669  H -1.0756 7.5774 1.0951  H -3.5757 8.6167 -0.2628  H -4.2226 7.1374 -1.0149  H -2.4592 7.4716 -1.0827  H -4.2917 6.304 2.713  H -4.6839 7.911 2.01  H -5.3084 6.4299 1.2382  H 2.3923 8.044 3.572  H 1.2572 7.2828 2.4308  H 1.6753 6.4691 3.9947  H 4.6399 7.1292 4.0056  H 5.3154 5.7517 3.0982  H 4.0358 5.4668 4.3255  H 3.0094 7.4134 0.5458  H 4.0196 8.2998 1.7392  H 4.7069 6.9144 0.8541  H 9.156 -0.3237 -1.6708  H 8.009 -0.6084 -0.3202  H 7.5861 -1.0791 -1.9985  H 8.5216 1.4503 -3.5058  H 7.0596 2.4714 -3.2763  H 6.8916 0.733 -3.6936  H 8.4021 1.9458 0.238  H 9.4625 2.0039 -1.2021  H -4.1261 -6.1836 -3.1179  H -4.715 -7.7617 -2.4908  H -5.379 -6.2429 -1.8329  H -9.1527 0.5154 1.9662  H -7.5799 1.3097 2.1595  H -8.0197 0.5896 0.5757 | C 3.7794 7.288 1.341  C 8.0804 -0.2949 -1.3852  C 7.4866 1.4587 -3.095  C 8.4073 2.1116 -0.8632  C -7.9684 2.3452 -2.5701  C -6.7569 1.3134 -4.5014  C -7.743 -0.1241 -2.6788  C 3.6135 -0.4886 1.9161  C 4.8112 -0.5541 2.5206  C 3.2347 -1.4094 1.0128  C 4.0709 -2.4547 0.8916  C 5.2701 -2.5378 1.482  C 5.69 -1.5496 2.2944  N 2.1626 -1.5558 0.3108  C 2.2581 -2.7488 -0.1445  C 1.3713 -3.4413 -0.859  C 1.6841 -4.6571 -1.3327  C 2.8619 -5.2555 -1.0577  C 3.7383 -4.5662 -0.2986  C 3.4262 -3.3374 0.129  C 7.0406 -1.5798 3.0188  C 3.2264 -6.6514 -1.5795  C 6.7916 -1.9191 4.5033  C 8.0212 -2.6271 2.4436  C 7.7421 -0.2052 2.9192  C 2.1107 -7.3237 -2.413  C 4.4776 -6.548 -2.4788  C 3.5208 -7.5832 -0.3826  C -1.435 -3.4646 -0.7039  C -1.7381 -4.7376 -1.0033  C -2.3629 -2.6656 -0.1732  C -3.5793 -3.1786 0.0355  C -3.8961 -4.4439 -0.2615  C -2.9647 -5.2599 -0.795  N -2.273 -1.427 0.1412  C -3.4169 -1.1506 0.6692  C -3.8734 -0.1012 1.3747  C -5.1454 -0.0462 1.8025  C -6.0311 -1.0382 1.5891  C -5.5474 -2.146 0.9966  C -4.276 -2.1801 0.5776  C -3.3192 -6.7132 -1.1373  H 8.1351 3.1715 -1.0659  H -8.9611 2.2409 -3.0636  H -8.1508 2.3454 -1.4712  H -7.5894 3.3475 -2.8704  H -7.7116 1.2938 -5.0741  H -6.1303 0.4755 -4.8813  H -6.2324 2.2637 -4.7515  H -7.2169 -1.0179 -3.0783  H -7.8673 -0.27 -1.5824  H -8.7581 -0.1439 -3.1358  H 2.9447 0.3223 2.2378  H 5.0488 0.2356 3.2511  H 5.8808 -3.4332 1.305  H 0.9612 -5.1422 -1.996  H 4.715 -4.9938 -0.0298  H 7.7467 -1.9636 5.0741  H 6.1473 -1.1612 5.0026  H 6.2888 -2.9074 4.609  H 9.0132 -2.5733 2.9465  H 8.1997 -2.4656 1.3563  H 7.6656 -3.6706 2.5957  H 7.8584 0.1082 1.8581  H 7.1984 0.606 3.4499  H 8.7584 -0.2323 3.3729  H 2.4164 -8.3388 -2.7539  H 1.1765 -7.4604 -1.8225  H 1.8724 -6.7473 -3.3353  H 4.7591 -7.5407 -2.8975  H 5.3694 -6.1717 -1.9309  H 4.2952 -5.8604 -3.336  H 4.3895 -7.2456 0.2241  H 2.6404 -7.647 0.297  H 3.7594 -8.6167 -0.7216  H -0.9537 -5.3632 -1.4348  H -4.916 -4.8023 -0.0609  H -3.2233 0.7334 1.671  H -5.4469 0.8487 2.3702  H -6.1706 -3.039 0.8553  H -2.4476 -8.5797 -1.9373  H -1.7589 -7.1093 -2.6661  H -1.2963 -7.6078 -0.9866  H -4.0364 -8.5082 -0.0673  H -4.7239 -6.9932 0.5678  H -3.0159 -7.4149 0.9293  H -9.4625 -1.8562 1.8528  H -8.1357 -3.0319 1.8774  H -8.4141 -2.0086 0.4102  H -7.0436 -2.0104 3.9556  H -6.8729 -0.2292 4.1069  H -8.5042 -0.9653 4.0413 |
| **R-TBN (S0)** |  |
| C 1E-5 1.41975 -0.10265  C 1.22419 0.69491 -0.12941  C 1.22418 -0.69493 0.12925  C -1E-5 -1.41976 0.10254  C -1.22418 -0.69491 0.12931  C -1.22418 0.69493 -0.12938  C 1.39972 -3.61734 -0.23524  C 1.75884 -4.96939 -0.45594  C -1.39976 -3.61733 -0.23514  C -1.7589 -4.96939 -0.45578  C -3.04109 -5.48408 -0.21754  C -4.01976 -4.62381 0.32688  C -3.72943 -3.28559 0.55807  C -2.45293 -2.80056 0.1959  C 2.4529 -2.80059 0.19581  C 3.7294 -3.28564 0.55797  C 4.01972 -4.62385 0.3267  C 3.04105 -5.48409 -0.21775  N -2.38107 -1.43339 0.43999  N 2.38105 -1.43343 0.43994  C -3.5512 -1.06481 1.14677  C 3.55118 -1.06488 1.14673  C 3.87553 0.1076 1.82839  C 5.1069 0.16865 2.47598  C 6.03047 -0.89917 2.48299  C 5.65977 -2.08144 1.83534  C 4.42586 -2.17643 1.18573  C -4.42589 -2.17636 1.18578  C -5.65983 -2.08134 1.83535  C -6.03055 -0.89903 2.48294  C 4.01983 4.62376 -0.32664  C 3.72947 3.28557 -0.558  C 7.37937 0.73277 -3.20731  C 3.40891 6.95735 0.48621  C 7.13429 0.42751 -4.70425  C 8.25256 1.99854 -3.11537  C 8.16396 -0.438 -2.56838  C 2.23675 7.76121 1.08028  C 4.58417 7.01728 1.49137  C 3.8329 7.63872 -0.83689  C -1.3997 3.61735 0.23504  C -1.75879 4.96943 0.45566  C -2.4529 2.80059 -0.19594  C -3.72941 3.28564 -0.55807  C -4.0197 4.62388 -0.3269  C -3.04099 5.48414 0.21746  N -2.38107 1.43342 -0.44002  C -3.55123 1.06486 -1.14677  C -3.87563 -0.10764 -1.82839  C -5.10705 -0.16869 -2.4759  C -6.03062 0.89913 -2.48287  C -5.65986 2.08142 -1.83528  C -4.4259 2.17642 -1.18575  C -3.40864 6.95756 0.48561  C -7.37946 0.73278 -3.20708  C -2.23642 7.76144 1.07952  C -3.8326 7.63874 -0.8376  C -4.58388 7.01771 1.49077  C -8.16409 -0.4379 -2.56803  C -8.25261 1.99859 -3.11521  C -7.13445 0.42739 -4.70401  B 3E-5 2.96004 0.1652  H 0.99199 -5.64599 -0.80716  H -0.99206 -5.646 -0.80701  H -5.00321 -5.01009 0.5809  H 5.00318 -5.01014 0.58069  H 3.19785 0.95044 1.87384  H 5.35232 1.08767 3.00015  H 6.31275 -2.94732 1.84611  H -6.31281 -2.9472 1.84612  H -5.35239 1.08781 3.00007  H -3.19789 0.95053 1.87383  H -2.55625 -8.79219 -1.27008  H -1.89359 -7.34031 -2.03156  H 7.7688 2.86301 -3.58442  H 8.35967 -0.24392 -1.50737  H 7.61397 -1.38232 -2.63712  H 9.12805 -0.5747 -3.07401  H 2.55641 8.79199 1.2708  H 1.3816 7.80421 0.39607  H 1.89371 7.34002 2.03208  H 4.86777 8.05873 1.6876  H 5.47106 6.49697 1.11432  H 4.30682 6.55484 2.44559  H 4.69947 7.14717 -1.29162  H 3.01607 7.61672 -1.56723  H 4.10226 8.68711 -0.65832  H -0.99192 5.64603 0.80682  H -5.00315 5.01017 -0.58089  H -3.19797 -0.95048 -1.87386  H -5.3525 -1.08772 -3.00003  H -6.31283 2.9473 -1.84602 | C -5.10696 0.16878 2.47594  C -3.87557 0.1077 1.82839  B -2E-5 -2.96004 -0.16533  C -3.40879 -6.95748 -0.48572  C 3.40874 -6.95747 -0.48602  C 7.37926 -0.73284 3.20732  C -7.37937 -0.73266 3.2072  C -2.23661 -7.76138 -1.0797  C -3.83273 -7.63869 0.83748  C -4.58407 -7.01758 -1.49085  C 2.23658 -7.76132 -1.08009  C 4.58405 -7.01752 -1.49111  C 3.83263 -7.63878 0.83715  C 8.16393 0.43786 2.56837  C 7.13413 -0.42749 4.70424  C 8.2524 -1.99865 3.1155  C -8.25253 -1.99846 3.11537  C -7.1343 -0.42726 4.70411  C -8.164 0.43802 2.56817  C 3.87555 -0.10762 -1.82858  C 5.10694 -0.16868 -2.47611  C 3.55121 1.06484 -1.14687  C 4.42592 2.17637 -1.18578  C 5.65986 2.08137 -1.83534  C 6.03055 0.89911 -2.48303  N 2.38105 1.4334 -0.44013  C 2.45294 2.80055 -0.19592  C 1.39978 3.6173 0.23515  C 1.75894 4.96933 0.45595  C 3.04117 5.484 0.21783  H -1.38145 -7.80426 -0.39549  H -4.10206 -8.6871 0.65904  H -4.6993 -7.14711 1.29217  H -3.01588 -7.61657 1.5678  H -4.30675 -6.55524 -2.44513  H -4.86763 -8.05906 -1.68694  H -5.47096 -6.49725 -1.11384  H 2.55621 -8.79213 -1.27054  H 1.38139 -7.80425 -0.39592  H 1.8936 -7.34018 -2.03194  H 4.86762 -8.05899 -1.68725  H 5.47094 -6.49722 -1.11405  H 4.30677 -6.55513 -2.44538  H 3.01576 -7.61669 1.56745  H 4.10196 -8.68718 0.65866  H 4.6992 -7.14723 1.2919  H 9.128 0.57455 3.07404  H 8.35967 0.24371 1.50738  H 7.61397 1.38221 2.63703  H 8.08853 -0.30039 5.23022  H 6.58655 -1.24575 5.1857  H 6.55311 0.48998 4.84429  H 8.48561 -2.25811 2.07645  H 9.20244 -1.83071 3.63537  H 7.76859 -2.86308 3.58458  H -9.2026 -1.83047 3.63514  H -8.48564 -2.25797 2.07631  H -7.76878 -2.86287 3.58453  H -8.08872 -0.30011 5.23005  H -6.55326 0.4902 4.84414  H -6.58677 -1.24551 5.18563  H -7.61404 1.38238 2.63682  H -8.35969 0.24384 1.50717  H -9.12809 0.57474 3.07377  H 3.19784 -0.95042 -1.8741  H 5.35236 -1.08768 -3.00031  H 6.31286 2.94723 -1.84606  H 0.99211 5.64592 0.80722  H 5.00331 5.01003 -0.58057  H 8.08872 0.3004 -5.23019  H 6.55324 -0.48993 -4.84438  H 6.58677 1.24581 -5.18569  H 9.20261 1.83058 -3.6352  H 8.48572 2.25793 -2.0763  H -2.55602 8.79228 1.26988  H -1.89338 7.3404 2.03139  H -1.38128 7.80428 0.39528  H -4.1019 8.68717 -0.65918  H -4.69921 7.14717 -1.29225  H -3.01578 7.61658 -1.56794  H -4.30654 6.55539 2.44506  H -4.86741 8.0592 1.68684  H -5.4708 6.49739 1.11381  H -9.1282 -0.57459 -3.07361  H -7.61415 -1.38226 -2.63671  H -8.35974 -0.24373 -1.50703  H -9.2027 1.83062 -3.63496  H -7.76886 2.863 -3.58439  H -8.48568 2.25809 -2.07615  H -6.58692 1.24563 -5.18553  H -6.55342 -0.49008 -4.84406  H -8.08889 0.30025 -5.22991 |
| **DBP (S0)** |  |
| C 6.4632 1.3525 -2.8751  C 6.7897 0.0577 -2.6277  C 5.8848 -0.8007 -2.0922  C 4.6464 -0.3273 -1.8485  C 4.2943 0.9294 -2.1924  C 5.1989 1.8043 -2.6753  C 2.9638 1.042 -2.0017  C 3.3621 -2.0053 -0.5262  C 2.1233 -2.2615 -0.0678  C 1.0721 -1.4376 -0.2735  C 1.3049 -0.2915 -0.9458  C 0.3631 0.6349 -1.2188  C 0.7499 1.7276 -1.9135  C 2.0188 1.9407 -2.3069  C -0.8975 0.3966 -0.7959  C -1.1289 -0.7462 -0.1176  C -0.1859 -1.6698 0.1607  C -2.3765 -0.9789 0.3078  C -2.7655 -2.0292 1.0317  C -1.8362 -2.9636 1.271  C -0.5763 -2.7709 0.84  C -1.945 1.2292 -0.9856  C -3.1921 0.9542 -0.5619  C -3.4327 -0.1981 0.0768  C -4.514 -0.8091 0.6029  C -4.0725 -1.8633 1.3208  C -5.8246 -0.4994 0.5445  C -6.6779 -1.2408 1.296  C -6.2183 -2.2341 2.0999  C -4.9037 -2.572 2.1107  C -4.4137 -3.5481 2.909  C -6.2528 0.4884 -0.2747  C 6.1761 -2.0986 -1.8456  C 4.8459 3.0907 -2.9008  C 5.1115 3.7213 -4.0626  C 4.7657 5.003 -4.2619  C 4.1482 5.6922 -3.2919  C 3.8796 5.0873 -2.1262  C 4.2241 3.8034 -1.9391  C -7.0706 1.4743 0.1461  C -7.4962 2.4379 -0.6859  C -7.117 2.4329 -1.9718  C -6.3091 1.4587 -2.4139  C -5.8841 0.5032 -1.5721  C -3.3673 -3.2991 3.7229  C -2.872 -4.2414 4.5408  C -3.4146 -5.467 4.5604  C -4.4556 -5.7367 3.7598  C -4.9473 -4.7856 2.9501  C 5.382 -3.0768 -2.3272  **R-TBN (S1)** | C 7.455 2.1869 -3.2595  C 8.6949 1.77 -3.5464  C 8.9712 0.4674 -3.4515  C 8.0215 -0.36 -2.9966  C 3.5875 -0.8874 -1.2286  C 2.5528 -0.058 -1.3697  C 5.6562 -4.3739 -2.1161  C 6.739 -4.7253 -1.4082  C 7.5425 -3.7696 -0.9201  C 7.2627 -2.4755 -1.1421  C -8.0161 -1.0642 1.2197  C -8.8878 -1.7149 2.0009  C -8.4187 -2.5807 2.9022  C -7.1022 -2.8242 2.9355  H 7.3175 3.2742 -3.3601  H 9.4713 2.4801 -3.8776  H 9.9718 0.0905 -3.7222  H 8.3336 -1.4146 -2.9551  H 4.165 -2.7151 -0.2816  H 2.0264 -3.1984 0.5017  H 0.0371 2.513 -2.208  H 2.2365 2.8414 -2.8983  H -2.0721 -3.9056 1.7861  H 0.1225 -3.5879 1.0759  H -1.8342 2.1973 -1.4974  H -3.9765 1.7059 -0.7292  H 5.586 3.1825 -4.9013  H 4.9809 5.4894 -5.2282  H 3.8644 6.7457 -3.4511  H 3.3821 5.6494 -1.318  H 4.0139 3.3563 -0.9515  H -7.3791 1.5383 1.2043  H -8.1519 3.2418 -0.311  H -7.4659 3.2216 -2.6587  H -6.0007 1.4396 -3.4727  H -5.2477 -0.2979 -1.9875  H -2.9109 -2.2945 3.7648  H -2.0225 -4.0064 5.2041  H -3.0092 -6.245 5.2282  H -4.9014 -6.7457 3.7614  H -5.7819 -5.0626 2.2826  H 4.4986 -2.8348 -2.944  H 4.9953 -5.1532 -2.5315  H 6.9663 -5.7893 -1.2294  H 8.4295 -4.0493 -0.3272  H 7.9321 -1.7222 -0.691  H -8.4893 -0.3745 0.5044  H -9.9718 -1.5269 1.9227  H -9.1104 -3.099 3.5874  H -6.8034 -3.5463 3.7105 |
| C 1E-5 1.41975 -0.10265  C 1.22419 0.69491 -0.12941  C 1.22418 -0.69493 0.12925  C -1E-5 -1.41976 0.10254  C -1.22418 -0.69491 0.12931  C -1.22418 0.69493 -0.12938  C 1.39972 -3.61734 -0.23524  C 1.75884 -4.96939 -0.45594  C -1.39976 -3.61733 -0.23514  C -1.7589 -4.96939 -0.45578  C -3.04109 -5.48408 -0.21754  C -4.01976 -4.62381 0.32688  C -3.72943 -3.28559 0.55807  C -2.45293 -2.80056 0.1959  C 2.4529 -2.80059 0.19581  C 3.7294 -3.28564 0.55797  C 4.01972 -4.62385 0.3267  C 3.04105 -5.48409 -0.21775  N -2.38107 -1.43339 0.43999  N 2.38105 -1.43343 0.43994  C -3.5512 -1.06481 1.14677  C 3.55118 -1.06488 1.14673  C 3.87553 0.1076 1.82839  C 5.1069 0.16865 2.47598  C 6.03047 -0.89917 2.48299  C 5.65977 -2.08144 1.83534  C 4.42586 -2.17643 1.18573  C -4.42589 -2.17636 1.18578  C -5.65983 -2.08134 1.83535  C -6.03055 -0.89903 2.48294  C -5.10696 0.16878 2.47594  C -3.87557 0.1077 1.82839  B -2E-5 -2.96004 -0.16533  C -3.40879 -6.95748 -0.48572  C 3.40874 -6.95747 -0.48602  C 7.37926 -0.73284 3.20732  C -7.37937 -0.73266 3.2072  C -2.23661 -7.76138 -1.0797  C -3.83273 -7.63869 0.83748  C -4.58407 -7.01758 -1.49085  C 2.23658 -7.76132 -1.08009  C 4.58405 -7.01752 -1.49111  C 3.83263 -7.63878 0.83715  C -3.8326 7.63874 -0.8376  C -4.58388 7.01771 1.49077  C -8.16409 -0.4379 -2.56803  C -8.25261 1.99859 -3.11521  C -7.13445 0.42739 -4.70401  B 3E-5 2.96004 0.1652  H 0.99199 -5.64599 -0.80716  H -0.99206 -5.646 -0.80701  H -5.00321 -5.01009 0.5809  H 5.00318 -5.01014 0.58069  H 3.19785 0.95044 1.87384  H 5.35232 1.08767 3.00015  H 6.31275 -2.94732 1.84611  H -6.31281 -2.9472 1.84612  H -5.35239 1.08781 3.00007  H -3.19789 0.95053 1.87383  H -2.55625 -8.79219 -1.27008  H -1.89359 -7.34031 -2.03156  H -1.38145 -7.80426 -0.39549  H -4.10206 -8.6871 0.65904  H -4.6993 -7.14711 1.29217  H -3.01588 -7.61657 1.5678  H -4.30675 -6.55524 -2.44513  H -4.86763 -8.05906 -1.68694  H -5.47096 -6.49725 -1.11384  H 2.55621 -8.79213 -1.27054  H 1.38139 -7.80425 -0.39592  H 1.8936 -7.34018 -2.03194  H 4.86762 -8.05899 -1.68725  H 5.47094 -6.49722 -1.11405  H 4.30677 -6.55513 -2.44538  H 3.01576 -7.61669 1.56745  H 4.10196 -8.68718 0.65866  H 4.6992 -7.14723 1.2919  H 9.128 0.57455 3.07404  H 8.35967 0.24371 1.50738  H 7.61397 1.38221 2.63703  H 8.08853 -0.30039 5.23022  H 6.58655 -1.24575 5.1857  H 6.55311 0.48998 4.84429  H 8.48561 -2.25811 2.07645  H 9.20244 -1.83071 3.63537  H 7.76859 -2.86308 3.58458  H -9.2026 -1.83047 3.63514  H -5.4708 6.49739 1.11381  H -9.1282 -0.57459 -3.07361  H -7.61415 -1.38226 -2.63671  H -8.35974 -0.24373 -1.50703  H -9.2027 1.83062 -3.63496 | C 8.16393 0.43786 2.56837  C 7.13413 -0.42749 4.70424  C 8.2524 -1.99865 3.1155  C -8.25253 -1.99846 3.11537  C -7.1343 -0.42726 4.70411  C -8.164 0.43802 2.56817  C 3.87555 -0.10762 -1.82858  C 5.10694 -0.16868 -2.47611  C 3.55121 1.06484 -1.14687  C 4.42592 2.17637 -1.18578  C 5.65986 2.08137 -1.83534  C 6.03055 0.89911 -2.48303  N 2.38105 1.4334 -0.44013  C 2.45294 2.80055 -0.19592  C 1.39978 3.6173 0.23515  C 1.75894 4.96933 0.45595  C 3.04117 5.484 0.21783  C 4.01983 4.62376 -0.32664  C 3.72947 3.28557 -0.558  C 7.37937 0.73277 -3.20731  C 3.40891 6.95735 0.48621  C 7.13429 0.42751 -4.70425  C 8.25256 1.99854 -3.11537  C 8.16396 -0.438 -2.56838  C 2.23675 7.76121 1.08028  C 4.58417 7.01728 1.49137  C 3.8329 7.63872 -0.83689  C -1.3997 3.61735 0.23504  C -1.75879 4.96943 0.45566  C -2.4529 2.80059 -0.19594  C -3.72941 3.28564 -0.55807  C -4.0197 4.62388 -0.3269  C -3.04099 5.48414 0.21746  N -2.38107 1.43342 -0.44002  C -3.55123 1.06486 -1.14677  C -3.87563 -0.10764 -1.82839  C -5.10705 -0.16869 -2.4759  C -6.03062 0.89913 -2.48287  C -5.65986 2.08142 -1.83528  C -4.4259 2.17642 -1.18575  C -3.40864 6.95756 0.48561  C -7.37946 0.73278 -3.20708  C -2.23642 7.76144 1.07952  H -8.48564 -2.25797 2.07631  H -7.76878 -2.86287 3.58453  H -8.08872 -0.30011 5.23005  H -6.55326 0.4902 4.84414  H -6.58677 -1.24551 5.18563  H -7.61404 1.38238 2.63682  H -8.35969 0.24384 1.50717  H -9.12809 0.57474 3.07377  H 3.19784 -0.95042 -1.8741  H 5.35236 -1.08768 -3.00031  H 6.31286 2.94723 -1.84606  H 0.99211 5.64592 0.80722  H 5.00331 5.01003 -0.58057  H 8.08872 0.3004 -5.23019  H 6.55324 -0.48993 -4.84438  H 6.58677 1.24581 -5.18569  H 9.20261 1.83058 -3.6352  H 8.48572 2.25793 -2.0763  H 7.7688 2.86301 -3.58442  H 8.35967 -0.24392 -1.50737  H 7.61397 -1.38232 -2.63712  H 9.12805 -0.5747 -3.07401  H 2.55641 8.79199 1.2708  H 1.3816 7.80421 0.39607  H 1.89371 7.34002 2.03208  H 4.86777 8.05873 1.6876  H 5.47106 6.49697 1.11432  H 4.30682 6.55484 2.44559  H 4.69947 7.14717 -1.29162  H 3.01607 7.61672 -1.56723  H 4.10226 8.68711 -0.65832  H -0.99192 5.64603 0.80682  H -5.00315 5.01017 -0.58089  H -3.19797 -0.95048 -1.87386  H -5.3525 -1.08772 -3.00003  H -6.31283 2.9473 -1.84602  H -2.55602 8.79228 1.26988  H -1.89338 7.3404 2.03139  H -1.38128 7.80428 0.39528  H -4.1019 8.68717 -0.65918  H -4.69921 7.14717 -1.29225  H -3.01578 7.61658 -1.56794  H -4.30654 6.55539 2.44506  H -4.86741 8.0592 1.68684  H -7.76886 2.863 -3.58439  H -8.48568 2.25809 -2.07615  H -6.58692 1.24563 -5.18553  H -6.55342 -0.49008 -4.84406  H -8.08889 0.30025 -5.22991 |
| **R-BN (S1)** |  |
| C 5E-5 1.42046 -9.4E-4  C 1.22525 0.70235 -0.07965  C 1.2252 -0.70241 0.07961  C -6E-5 -1.42043 9.6E-4  C -1.22523 -0.70234 0.07967  C -1.22518 0.70246 -0.07955  C 1.39795 -3.5831 -0.51384  C 1.75614 -4.91097 -0.84275  C -1.39829 -3.58293 -0.51393  C -1.75655 -4.91078 -0.84287  C -3.04378 -5.4108 -0.63532  C -4.03781 -4.62765 -0.03143  C -3.74013 -3.31079 0.3075  C -2.45851 -2.80723 -0.01564  C 2.45829 -2.80742 -0.01571  C 3.7399 -3.31105 0.3074  C 4.03749 -4.62793 -0.03152  C 3.04337 -5.41104 -0.6353  N -2.38139 -1.46328 0.33654  N 2.38126 -1.46345 0.33648  C -3.54718 -1.14264 1.07347  C 3.54712 -1.14286 1.07331  C 3.84742 -0.01991 1.84459  C 5.07589 0.00766 2.50578  C 5.98246 -1.05806 2.41578  C 5.65823 -2.19796 1.68378  C 4.42934 -2.25329 1.02211  C -4.42947 -2.25302 1.02229  C -5.65841 -2.19759 1.68385  C -5.98262 -1.05765 2.41581  C -5.07596 0.00799 2.50586  C -3.84746 -0.01967 1.84474  H 5.01624 -5.05071 0.18007  H 3.26745 -6.43905 -0.90625  H 3.15331 0.8039 1.94857  H 5.3265 0.87599 3.10862  H 6.93237 -1.00326 2.93971  H 6.33936 -3.04404 1.64715  H -6.33958 -3.04362 1.64718  H -6.93255 -1.00277 2.93968  H -5.32654 0.87635 3.10867  H -3.15329 0.80408 1.9488  H 3.15318 -0.80395 -1.94889  H 5.32637 -0.87614 -3.10893 | B -1.4E-4 -2.93247 -0.38845  C 3.84738 0.01978 -1.84482  C 5.07585 -0.00786 -2.50599  C 3.54719 1.14267 -1.0734  C 4.42954 2.25299 -1.02207  C 5.65844 2.1976 -1.68371  C 5.98256 1.05774 -2.41584  N 2.38136 1.46331 -0.33656  C 2.45852 2.80725 0.01574  C 1.39826 3.58299 0.51393  C 1.75658 4.9108 0.84296  C 3.04386 5.41075 0.63557  C 4.03791 4.62759 0.03174  C 3.7402 3.31076 -0.30727  C -1.39799 3.58314 0.51373  C -1.75612 4.91108 0.84245  C -2.45828 2.80747 0.01555  C -3.73985 3.3111 -0.30767  C -4.0374 4.62804 0.03104  C -3.0433 5.41119 0.63481  N -2.38128 1.46346 -0.33645  C -3.54712 1.14281 -1.07329  C -3.8475 0.01971 -1.84433  C -5.07601 -0.00795 -2.50544  C -5.98256 1.0578 -2.41558  C -5.65824 2.19784 -1.68383  C -4.42929 2.25328 -1.02229  B 1.1E-4 2.93252 0.38843  H 1.00716 -5.58209 -1.24838  H -1.00761 -5.58191 -1.24855  H -3.26795 -6.43878 -0.90627  H -5.01657 -5.05039 0.18021  H 6.33968 3.04358 -1.64695  H 6.93246 1.00289 -2.93976  H 1.00766 5.58196 1.24862  H 3.26803 6.43873 0.90657  H 5.01671 5.05028 -0.17979  H -1.00712 5.58222 1.24801  H -5.01613 5.05083 -0.18066  H -3.26737 6.43924 0.90559  H -3.15341 -0.80413 -1.94823  H -5.32668 -0.8764 -3.10808  H -6.93251 1.00291 -2.93943  H -6.33934 3.04394 -1.64731 |
| **DBP (S1)** |  |
| C -7.42112 0.71909 -1.1E-4  C -7.42112 -0.71909 1E-4  C -6.178 -1.44102 2.2E-4  C -4.9976 -0.72626 1.1E-4  C -4.9976 0.72626 -1E-4  C -6.178 1.44102 -2.2E-4  C -8.66978 1.39663 -1.9E-4  C -9.86265 0.70546 -1E-4  C -9.86265 -0.70546 8E-5  C -8.66978 -1.39663 1.8E-4  C -3.59288 -1.17385 1.9E-4  C -2.79807 0 1E-5  C -3.59288 1.17385 -1.8E-4  C -2.93709 -2.39635 3.8E-4  C -1.5257 -2.4225 3.4E-4  C 4.9976 0.72626 1E-4  C 4.9976 -0.72626 -1.1E-4  C 6.178 1.44102 2.2E-4  C 7.42112 0.71909 1E-4  C 7.42112 -0.71909 -1.1E-4  C 6.178 -1.44102 -2.2E-4  C 6.17417 -2.93729 -4.1E-4  C 6.17417 2.93729 4.1E-4  C -6.17417 -2.93729 4.1E-4  C -6.17417 2.93729 -4.1E-4  C -6.16761 3.65254 1.20638  C -6.14741 5.04831 1.20652  C -6.13599 5.74976 -7.6E-4  C -6.14791 5.04801 -1.20787  C -6.16812 3.65225 -1.20738  C 6.16765 3.65254 -1.20638  C 6.14745 5.04831 -1.20652  C 6.13599 5.74976 7.7E-4  C 6.14788 5.04801 1.20787  C 6.16808 3.65224 1.20738  C 6.16808 -3.65224 -1.20738  C 6.14787 -5.04801 -1.20787  C 6.13599 -5.74976 -7.7E-4  C 6.14745 -5.04831 1.20651  C 6.16765 -3.65254 1.20637  C -6.16807 -3.65224 1.20738  C -6.14787 -5.04801 1.20788  C -6.13599 -5.74976 7.7E-4  C -6.14745 -5.04831 -1.20651  C -6.16766 -3.65254 -1.20637  C 8.66978 1.39663 1.8E-4  C 9.86265 0.70546 9E-5  C 9.86265 -0.70546 -1E-4  C 8.66978 -1.39663 -1.9E-4  H -8.67382 2.4814 -3.3E-4  H -10.80386 1.24871 -1.7E-4 | C -0.73291 -1.26946 9E-5  C -1.39677 0 0  C -0.73291 1.26946 -9E-5  C -1.5257 2.4225 -3.3E-4  C -2.93709 2.39635 -3.8E-4  C 0.73291 1.26946 9E-5  C 1.39677 0 0  C 0.73291 -1.26946 -8E-5  C 2.79807 0 0  C 3.59288 -1.17385 -1.8E-4  C 2.93709 -2.39635 -3.7E-4  C 1.5257 -2.4225 -3.3E-4  C 1.5257 2.4225 3.3E-4  C 2.93709 2.39635 3.8E-4  C 3.59288 1.17385 1.8E-4  H -10.80386 -1.24871 1.4E-4  H -8.67382 -2.4814 3.2E-4  H -3.47965 -3.33486 5.8E-4  H -1.04547 -3.39607 5.1E-4  H -1.04547 3.39607 -5.1E-4  H -3.47965 3.33486 -5.8E-4  H 3.47965 -3.33486 -5.7E-4  H 1.04547 -3.39607 -5E-4  H 1.04547 3.39607 5E-4  H 3.47965 3.33486 5.7E-4  H -6.17307 3.10768 2.14657  H -6.13985 5.58716 2.15043  H -6.11963 6.83641 -9E-4  H -6.14074 5.58664 -2.15191  H -6.17396 3.10716 -2.14744  H 6.17314 3.10769 -2.14657  H 6.13992 5.58716 -2.15043  H 6.11963 6.83641 9.1E-4  H 6.14067 5.58663 2.15191  H 6.1739 3.10715 2.14744  H 6.17389 -3.10716 -2.14744  H 6.14067 -5.58663 -2.15192  H 6.11963 -6.83641 -9.1E-4  H 6.13992 -5.58716 2.15042  H 6.17314 -3.10769 2.14657  H -6.17389 -3.10715 2.14744  H -6.14067 -5.58663 2.15192  H -6.11963 -6.83641 9.1E-4  H -6.13993 -5.58716 -2.15042  H -6.17315 -3.10769 -2.14657  H 8.67382 2.4814 3.2E-4  H 10.80386 1.24871 1.5E-4  H 10.80386 -1.24871 -1.6E-4  H 8.67382 -2.4814 -3.3E-4 |