Supporting Information

Truxene–bridged Bodipy fullerene tetrads without precious metals: study of the energy transfer and application in Triplet−Triplet annihilation upconversion

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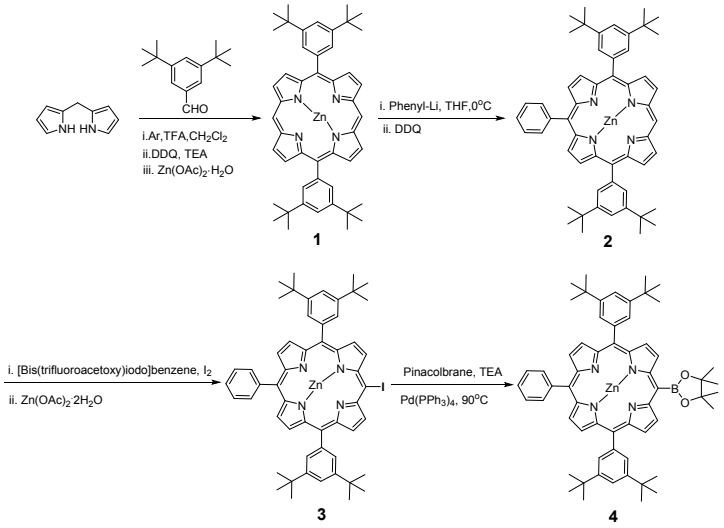
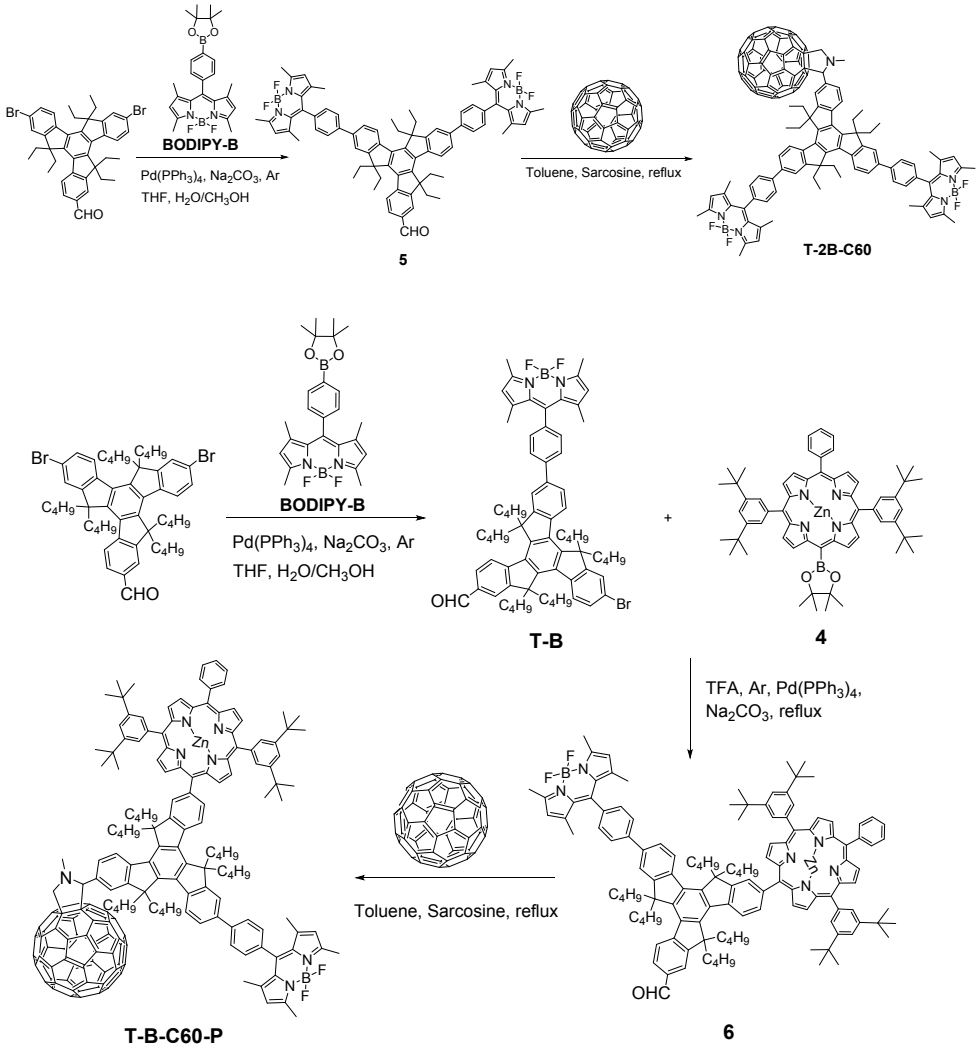


Schem S1 The synthesis route of the porphyrin derivatives **4**



Scheme S2. The synthesis route of the compounds **T-B**, and **T-2B-C_{60}** and **T-B-C_{60}-P**

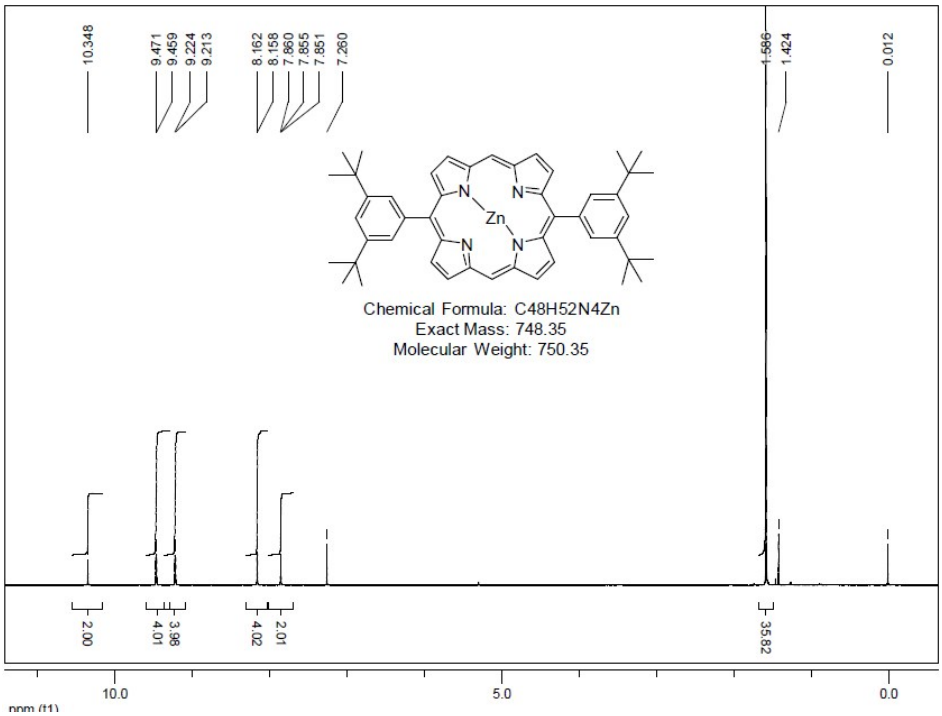


Figure **S1** ^{1}H-NMR spectrum of compound **1** (600 M, $CDCl_3$)

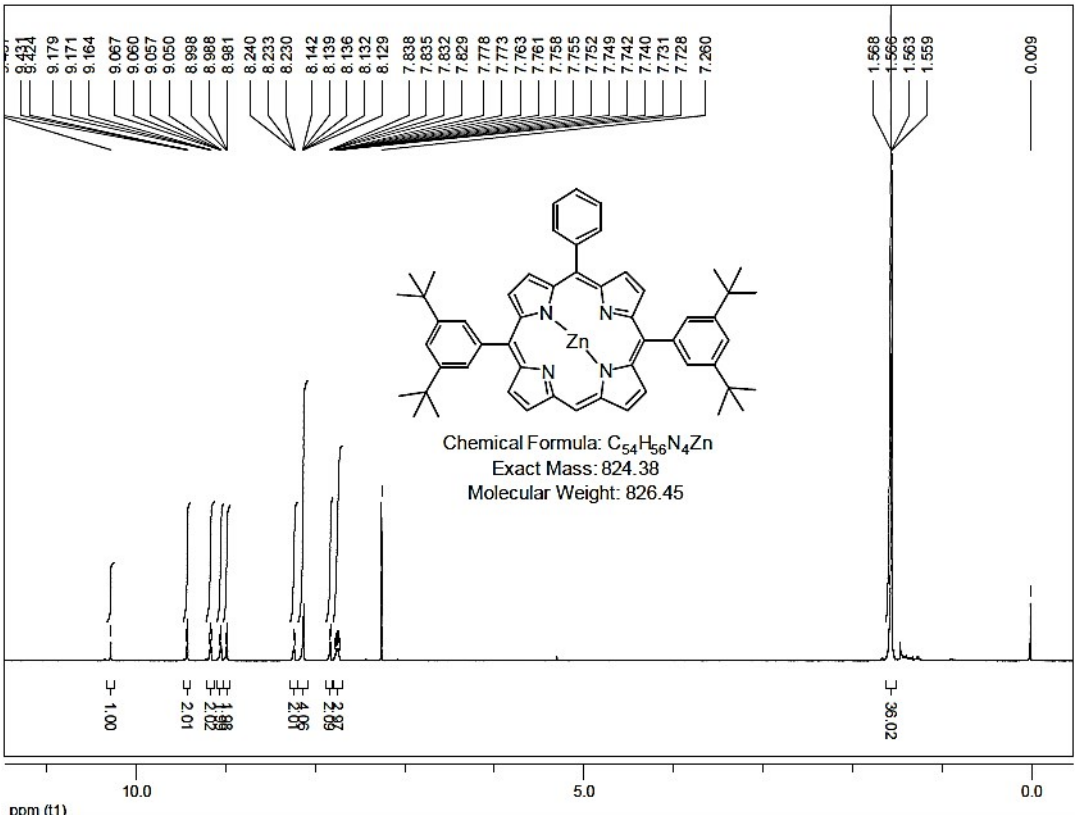


Figure **S2** ^{1}H-NMR spectrum of compound **2** (600 M, $CDCl_3$)

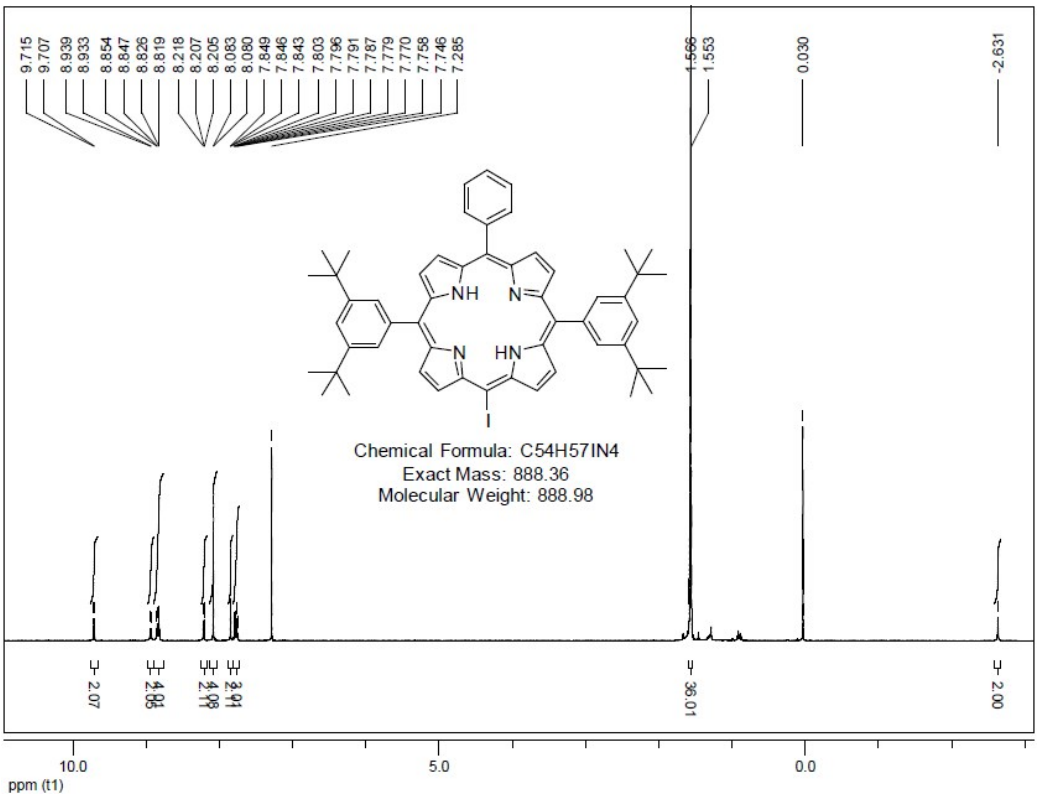


Figure **S3** ^{1}H-NMR spectrum of compound **3** (600 M, $CDCl_3$)

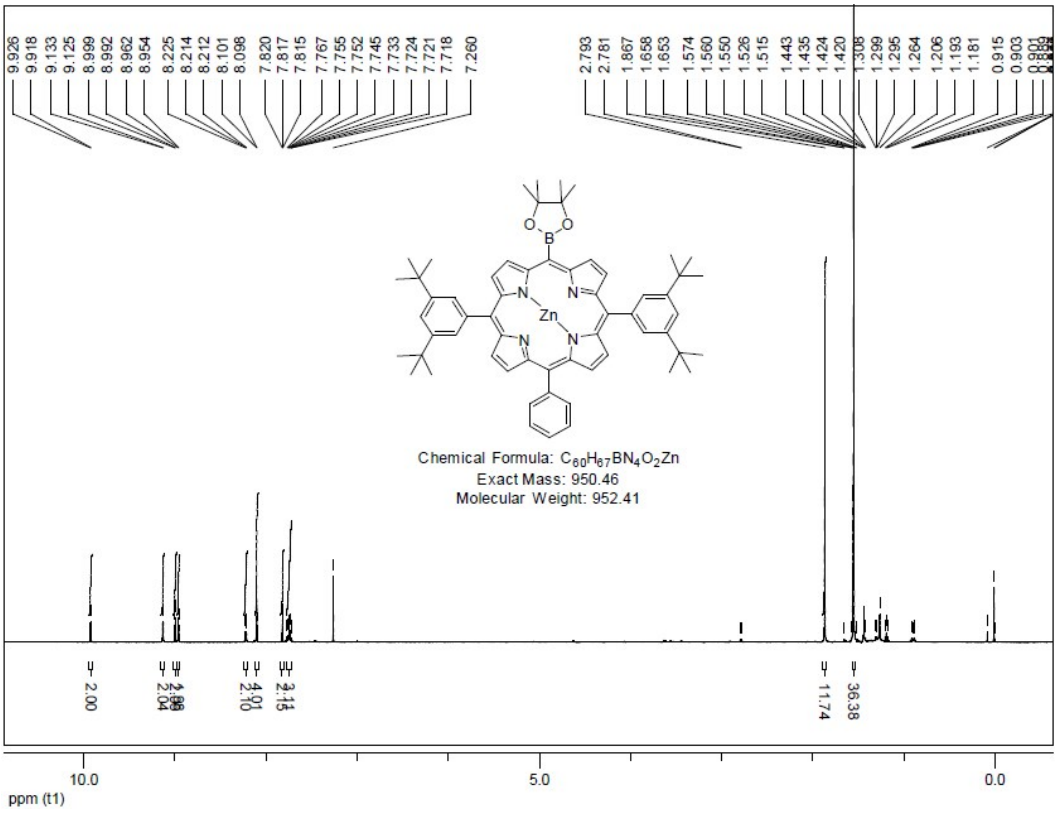


Figure **S4** ^{1}H-NMR spectrum of compound **4** (600 M, $CDCl_3$)

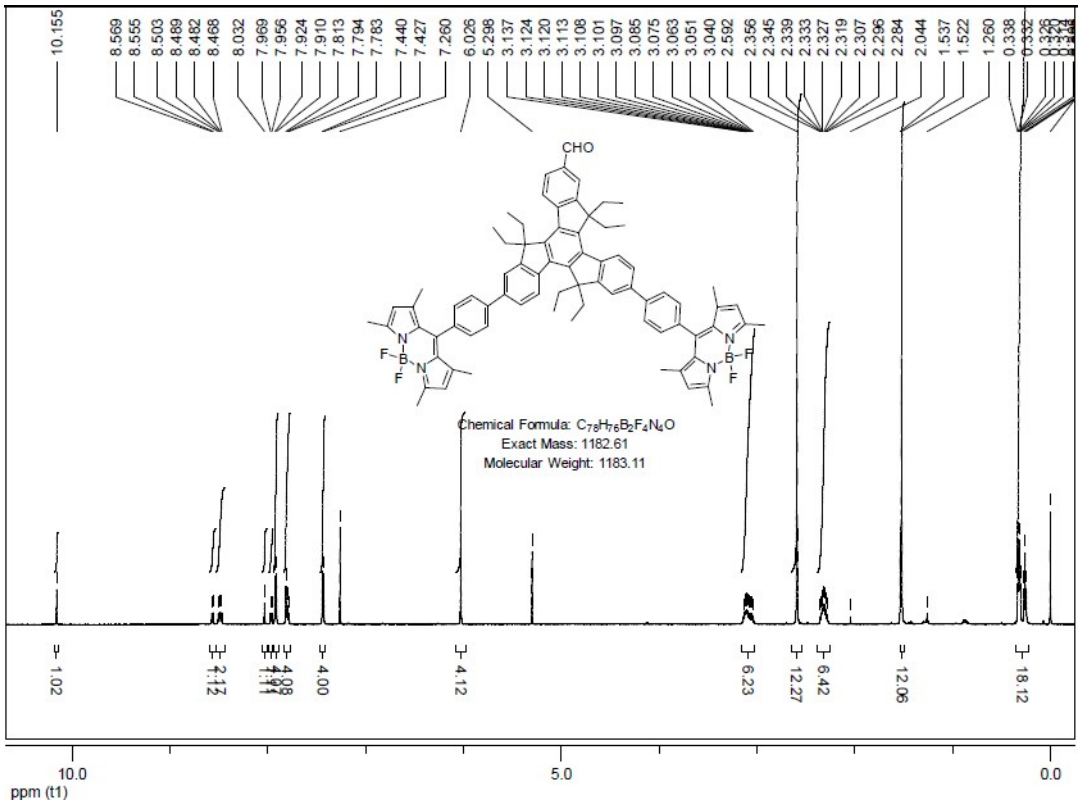


Figure **S5** ^{1}H-NMR spectrum of compound **5** (600 M, $CDCl_3$)

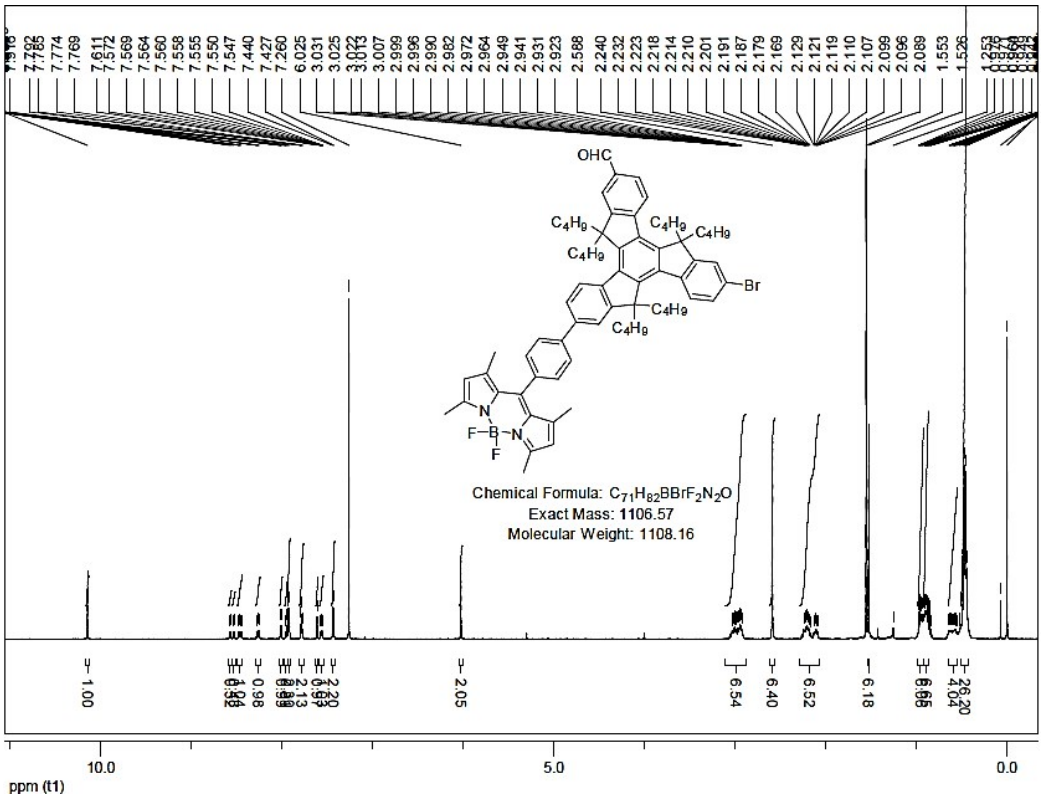


Figure **S6** ^{1}H-NMR spectrum of compound **T-B** (600 M, $CDCl_3$)

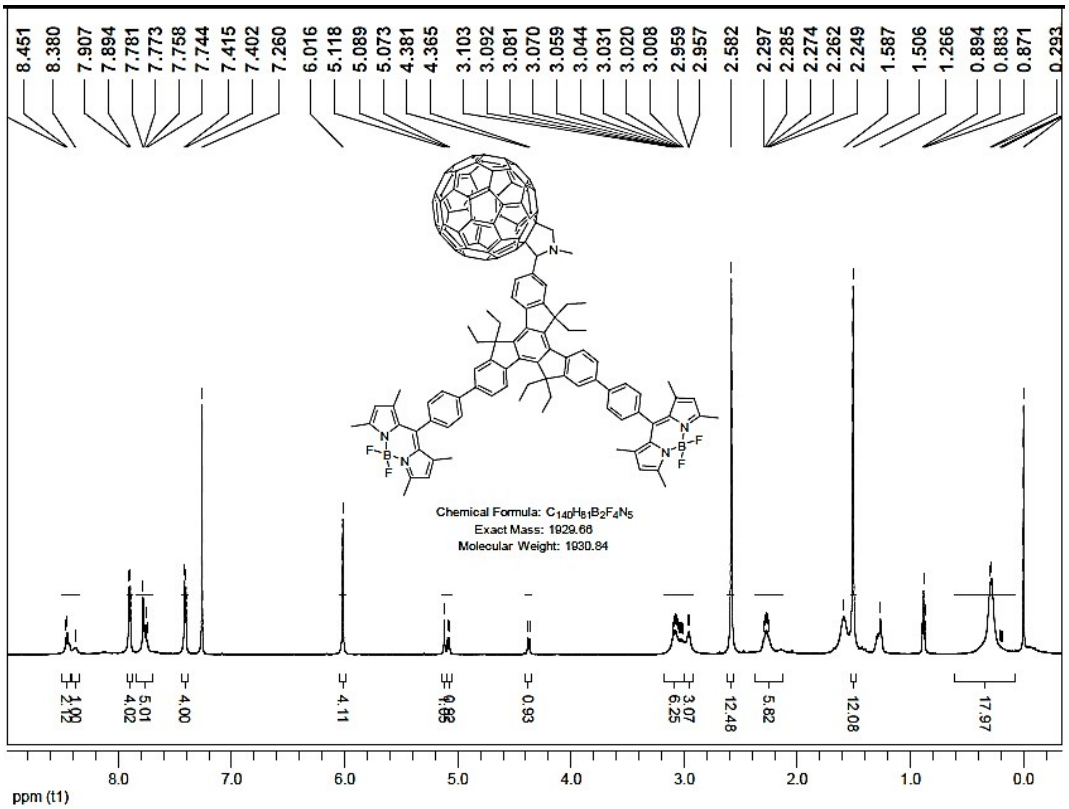


Figure **S7** ^{1}H NMR spectrum of **T-2B-C$_{60}$** (600 M, $CDCl_3$)

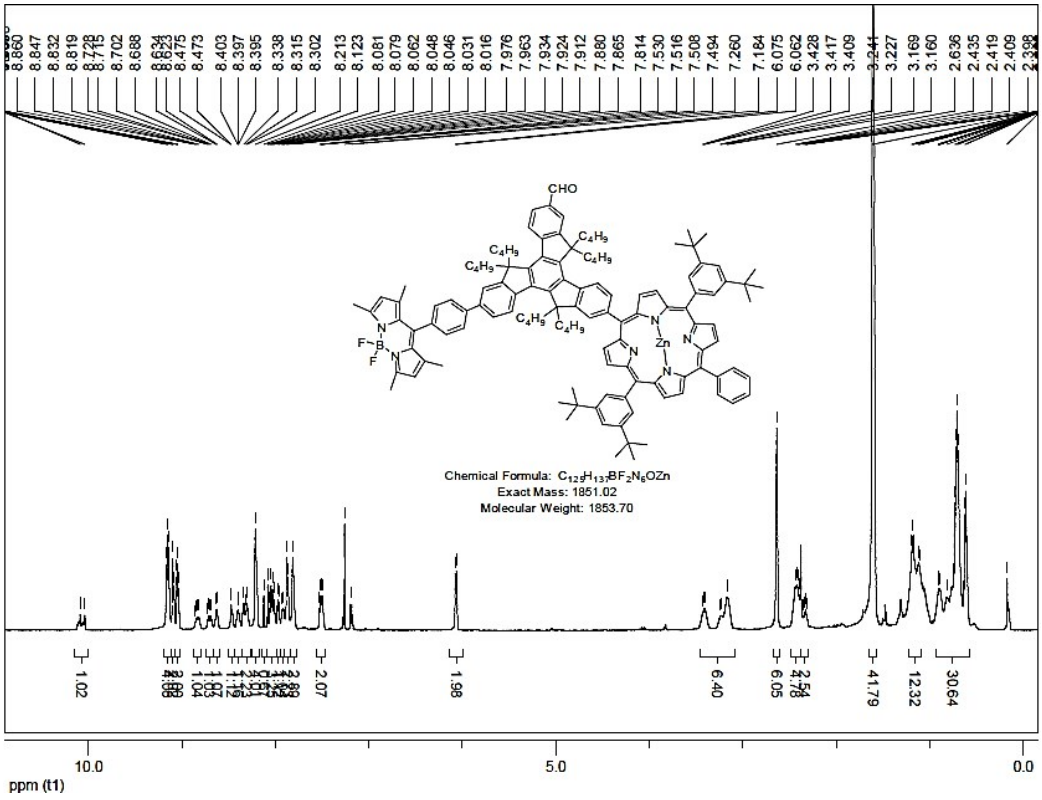


Figure **S8** ^{1}H-NMR spectra of compound **6** (600 M, $CDCl_3$)

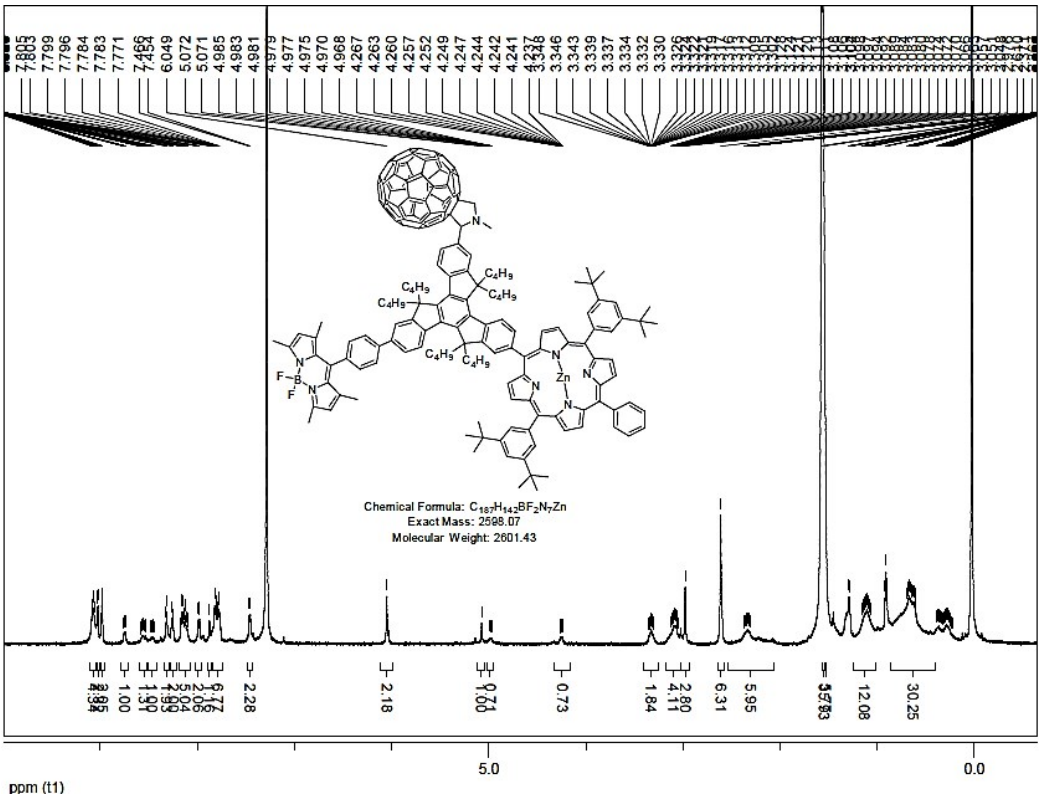


Figure **S9** ^{1}H-NMR spectra of compound **T-B-C_{60}-P** (600 M, $CDCl_3$)

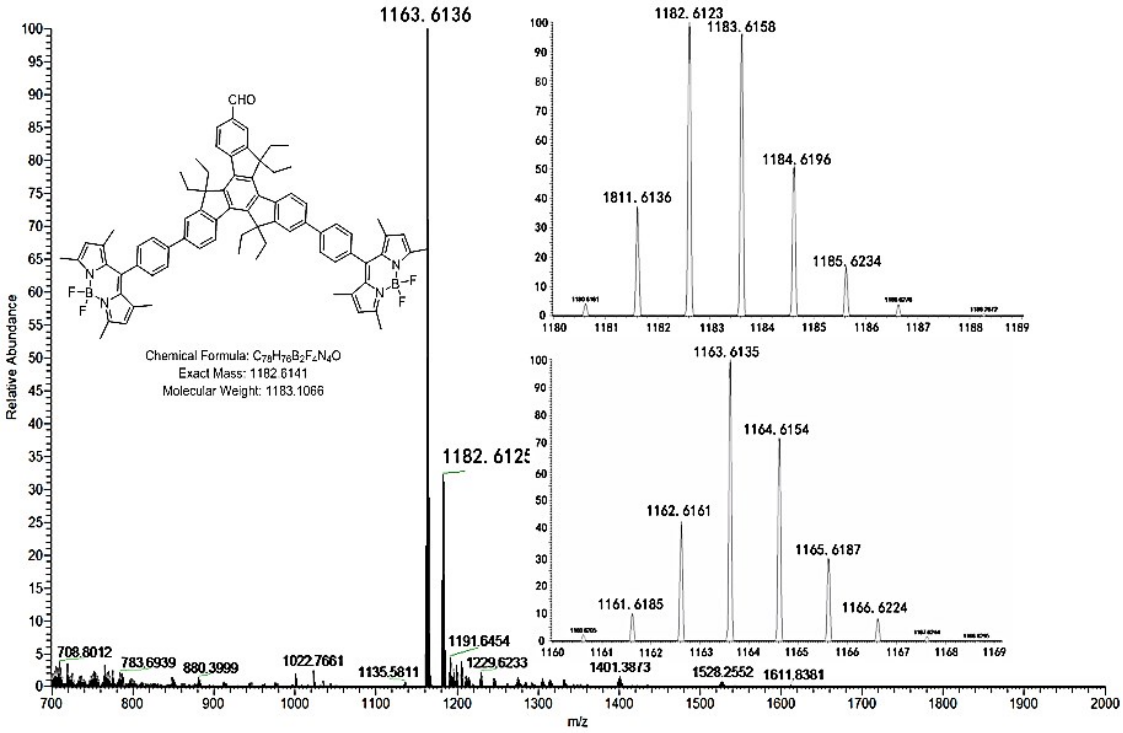


Figure **S10** High resolution mass spectrum of compound **5** (600 M, $CDCl_3$).

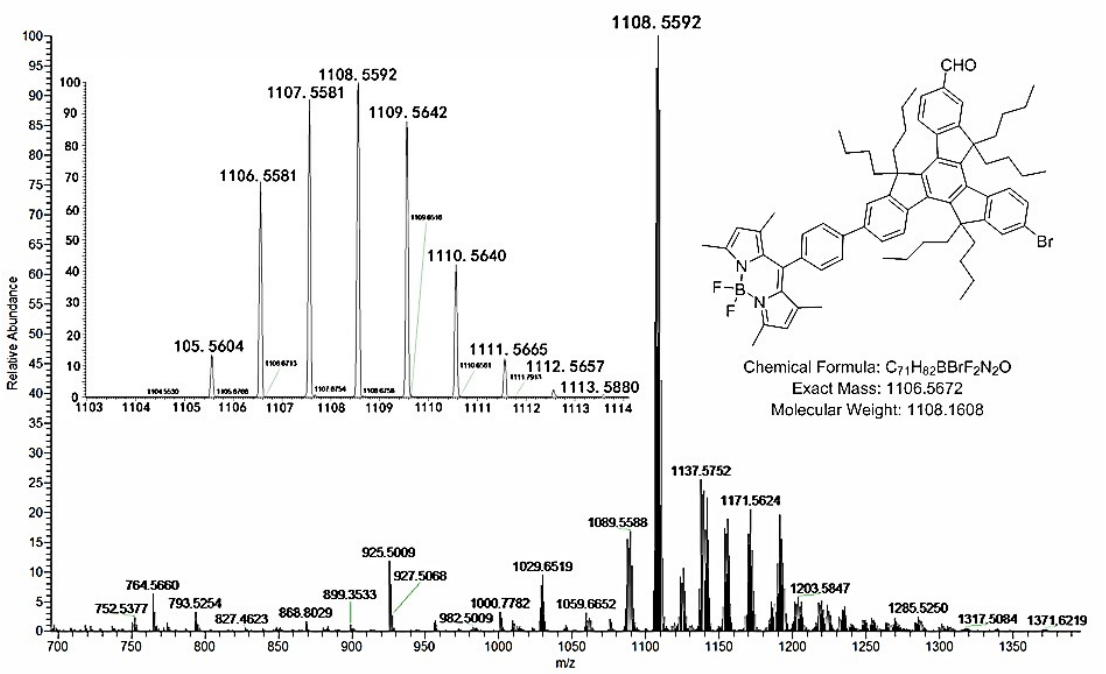


Figure **S11** High resolution mass spectrum of compound **T-B** (600 M, $CDCl_3$).

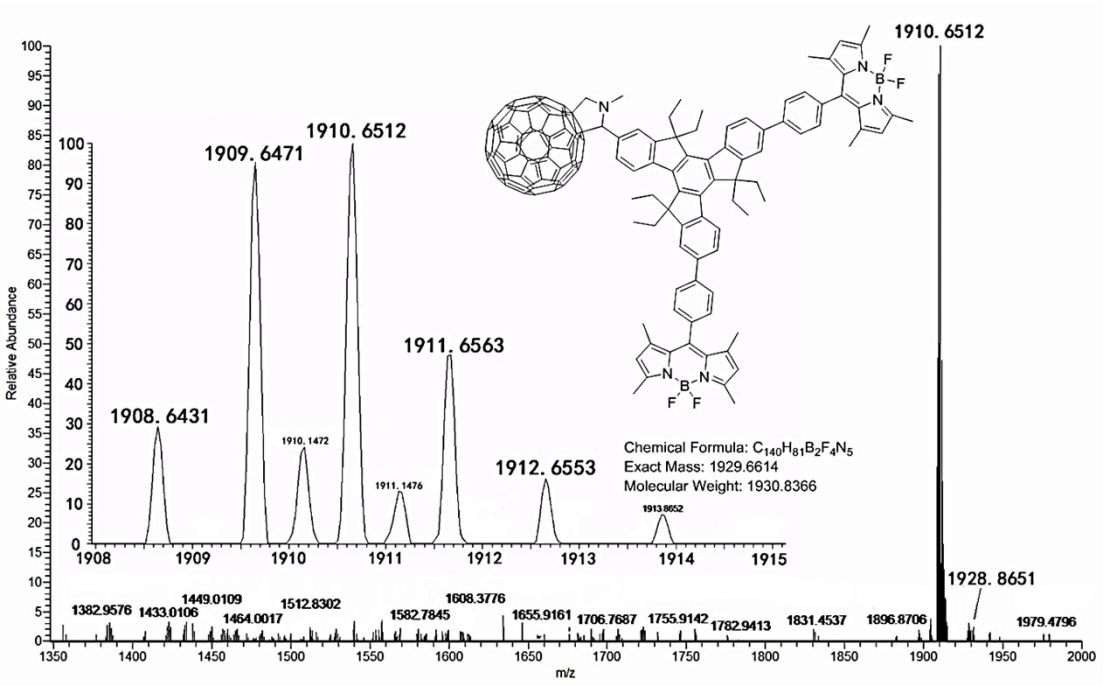


Figure **S12** High resolution mass spectra of compound **T-2B-C_{60}**.

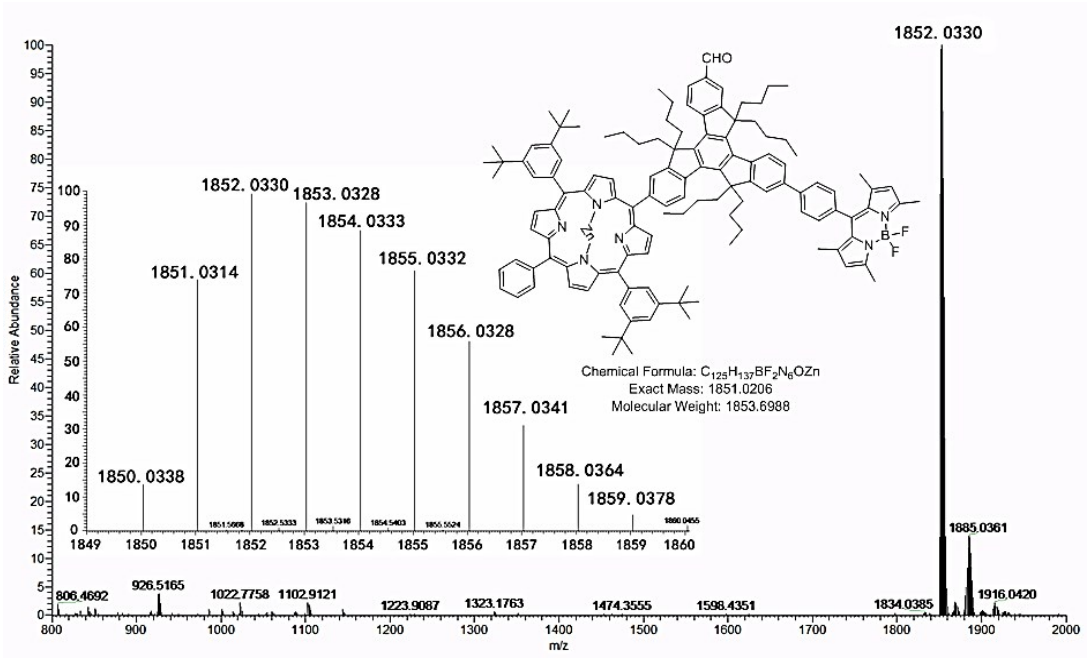


Figure **S13** High resolution mass spectra of compound **6**.

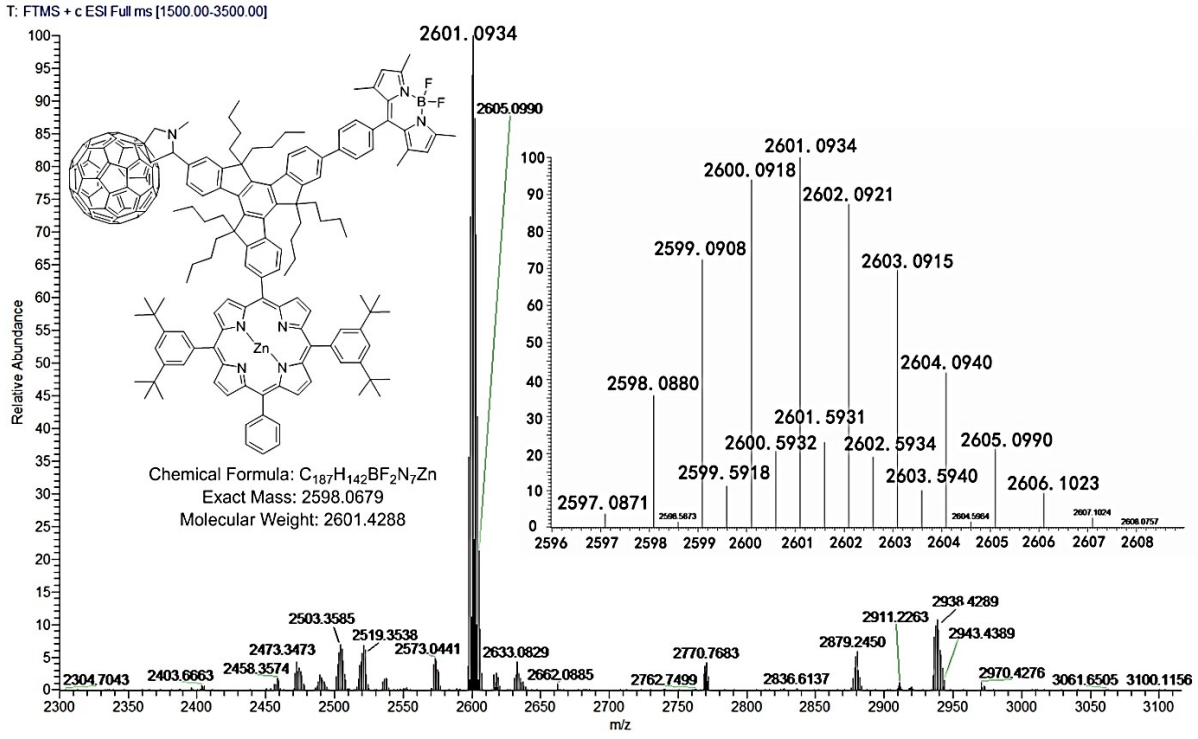


Figure **S14** High resolution mass spectra of compound **T-B-C_{60}-P**.

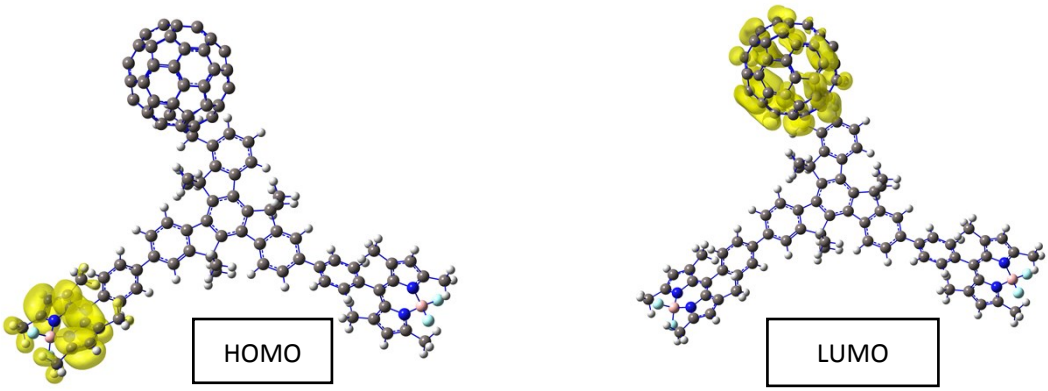


Figure S15. Electron-density maps of the frontier molecular orbitals of **T–2B–C_{60}**

Calculation of the Gibbs free energy changes of the electron transfer

The free energy changes of the intramolecular electron transfer process can be calculated with the Weller equation (Eq. 1 and Eq. 2).

$$\Delta G^{0}{}_{\mathrm{CS}} = e[E_{OX} - E_{RED}] - E_{00} + \Delta G_{\mathrm{S}} \qquad \text{(Eq. 1)}$$

$$\Delta G_{\mathrm{S}} = -\frac{e^2}{4\pi\varepsilon_{\mathrm{S}}\varepsilon_0 R_{\mathrm{CC}}} - \frac{e^2}{8\pi\varepsilon_0}\left(\frac{1}{R_D} + \frac{1}{R_{\mathrm{A}}}\right)\left(\frac{1}{\varepsilon_{REF}} - \frac{1}{\varepsilon_S}\right) \qquad \text{(Eq.2)}$$

Where ΔG_{S} is the static Coulombic energy, which is described by eq. 3. e = electronic charge. E_{OX} = half-wave potential for one-electron oxidation of the electron-donor unit. E_{RED} = half-wave potential for one-electron reduction of the electron-acceptor unit. E_{00} = energy level approximated with the fluorescence emission (for the singlet excited state). ε_{S} = static dielectric constant of the solvent. R_{CC} = center-to-center separation distance between the electron donor and electron acceptor, determined by DFT optimization of the geometry. R_{D} is the radius of the

electron donor. R_A is the radius of the electron acceptor. ε_{REF} is the static dielectric constant of the solvent used for the electrochemical studies. ε_0 is permittivity of free space. The solvents used in the calculation of free energy of the electron transfer is toluene ($\varepsilon_S = 2.38$), and CH_2Cl_2 ($\varepsilon_S = 8.93$).

Energies of the charge-separated states (E_{CS}) and charge recombination energy state ($\Delta G_{(CR)}$) can be calculated with the Eq. 3 and Eq. 4.

$$E_{CS} = e[E_{OX} - E_{RED}] + \Delta G_S \quad \text{(Eq. 3)}$$

$$\Delta G_{CR} = -(\Delta G_{CS} + E_{00}) \quad \text{(Eq. 4)}$$

x,y,z coordinates of the optimized geometries

T-2B-C_{60}

0 1

C	6.62933300	-5.40952800	3.16920200
C	6.20188800	-4.19439800	3.68917600
C	4.39654200	-4.06517400	2.00818400
C	6.93350900	-6.63597000	1.16945900
C	8.24147600	-6.43328700	1.77739000
C	8.05734800	-5.67676000	3.00881800
C	8.98957200	-4.71265800	3.37825400
C	7.18159100	-3.18142900	4.07565400
C	5.32370400	-2.07566600	3.12570300
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C	4.72252000	-5.27334600	0.00721700
C	5.65743200	-5.90145500	-0.81061200
C	6.79409800	-6.59347500	-0.21379300
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C	9.20792600	-6.14511500	-0.47651400

C	7.95979700	-6.34230000	-1.05755600
C	7.53096400	-5.49735100	-2.16677500
C	6.11826700	-5.21920500	-2.00290400
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C	9.42564000	-2.39198500	3.41074900
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H	-3.10326500	2.77274000	1.62370200
C	0.16728500	5.15969000	-0.93461800
H	1.10547400	5.68417100	-1.07387800
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C	-0.91810600	7.36028500	-0.38758200
C	0.14738000	7.94569300	0.31796600
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H	-2.86800700	9.82956500	2.02827400
H	-1.32339200	9.62521300	2.84829000
H	-2.74454300	10.16610100	3.77046200

C	-1.75913200	15.36898300	3.18322900
H	-2.26145900	15.96784800	2.41567100
H	-2.27346500	15.45960500	4.14104300
H	-0.73734500	15.75914800	3.25987500
C	0.38268900	12.04361900	-2.05732600
C	0.81434300	13.21331800	-2.68799500
H	1.28020300	13.29445000	-3.65518300
C	0.52725000	14.28616800	-1.81725100
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