

## Supplementary Information

### A New Dibenzofuran/Spirobifluorene Hybrids as Thermally Stable Host Materials for Efficient Phosphorescent Organic Light-Emitting Diodes with Low Efficiency Roll-Off

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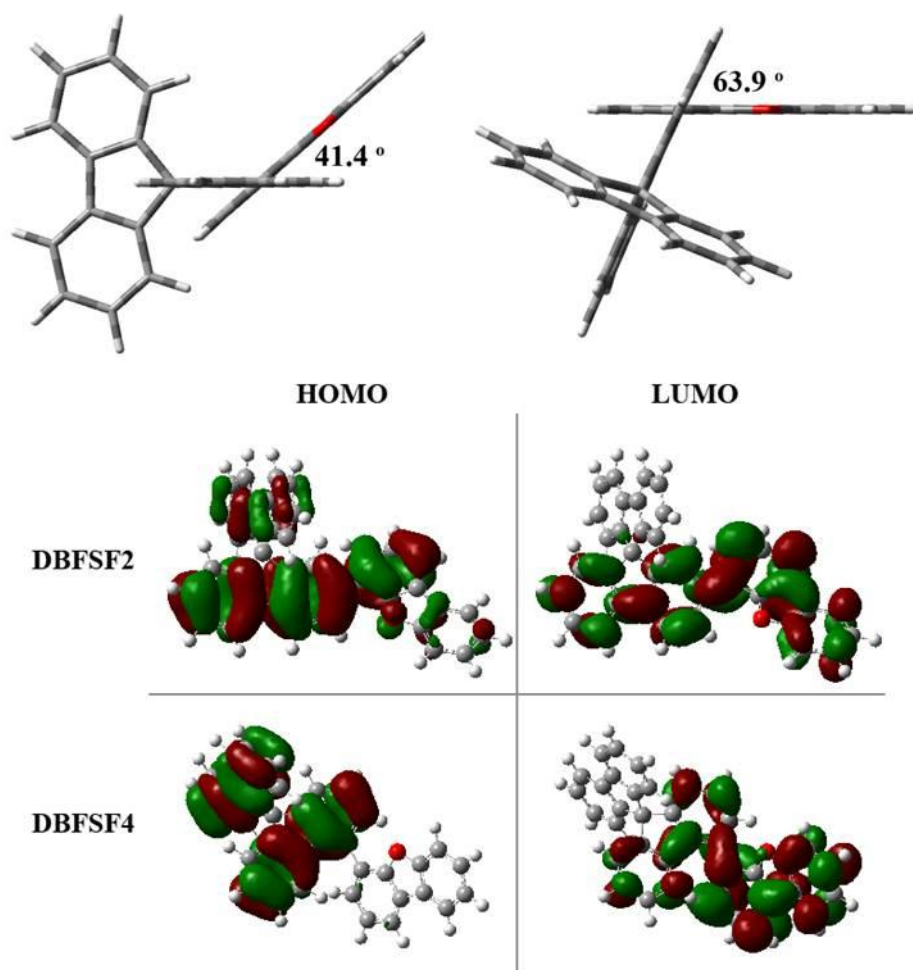
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#### *X-ray structural analysis.*

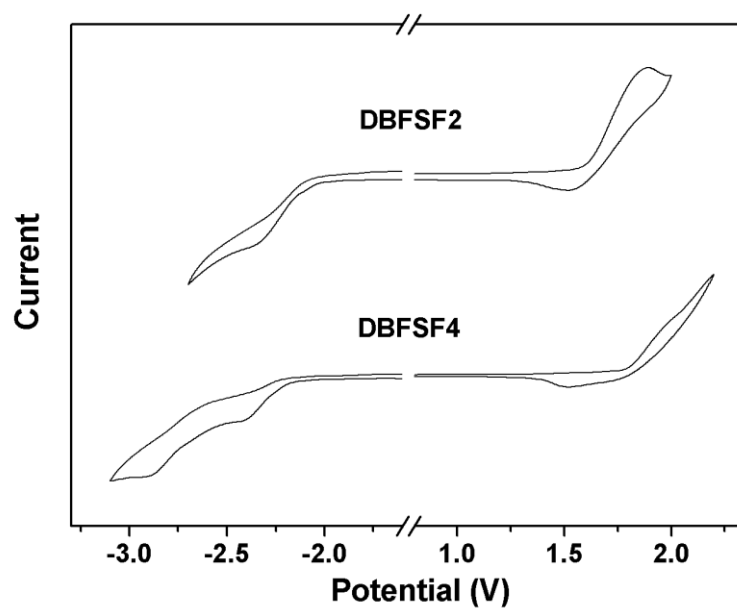
Single-crystal X-ray diffraction data were obtained from a Rigaku Mercury CCD diffractometer using a graphite-monochromated MoK $\alpha$  ( $\lambda=0.71073\text{\AA}$ ) radiation. The data were collected using the  $\omega/2\theta$  scan mode and corrected for Lorentz and polarization effects as well as the absorption during data reduction using Shelxtl 97 software.

Crystal data of DBFSF2 at 293(2) K: C<sub>37</sub>H<sub>22</sub>O,  $M_r = 482.55$ , monoclinic, space group  $P-1$ ,  $D_c = 1.285\text{ g cm}^{-3}$ ,  $Z=4$ ,  $a = 9.9930(6)\text{ \AA}$ ,  $b = 9.7316(4)\text{ \AA}$ ,  $c = 25.6891(12)\text{ \AA}$ ,  $\alpha = 90^\circ$ ,  $\beta = 93.021(4)^\circ$ ,  $\gamma = 90^\circ$ ,  $V = 2494.7(2)\text{ \AA}^3$ ,  $\mu = 0.076\text{ mm}^{-1}$ . Bruker AXS Smart CCD diffractometer, Mo-K $\alpha$  radiation,  $\lambda = 0.7107\text{ \AA}$ , number of reflections measured = 10944, number of independent reflections = 4453,  $R_{\text{int}} = 0.0567$ , final  $R(F) = 0.0624$  ( $I > 2\sigma(I)$ ),  $wR(F^2) = 0.1520$ .

The crystallographic data of DBFSF2 (excluding structure factors) has been deposited to the Cambridge Crystallographic Data Centre with the deposition number CCDC-880571. This data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44) 1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).



**Fig. S1** Optimized geometry and spatial distributions of DBFSF2 and DBFSF4



**Fig. S2** Cyclic voltammograms in  $\text{CH}_2\text{Cl}_2$  for oxidation and DMF for reduction.

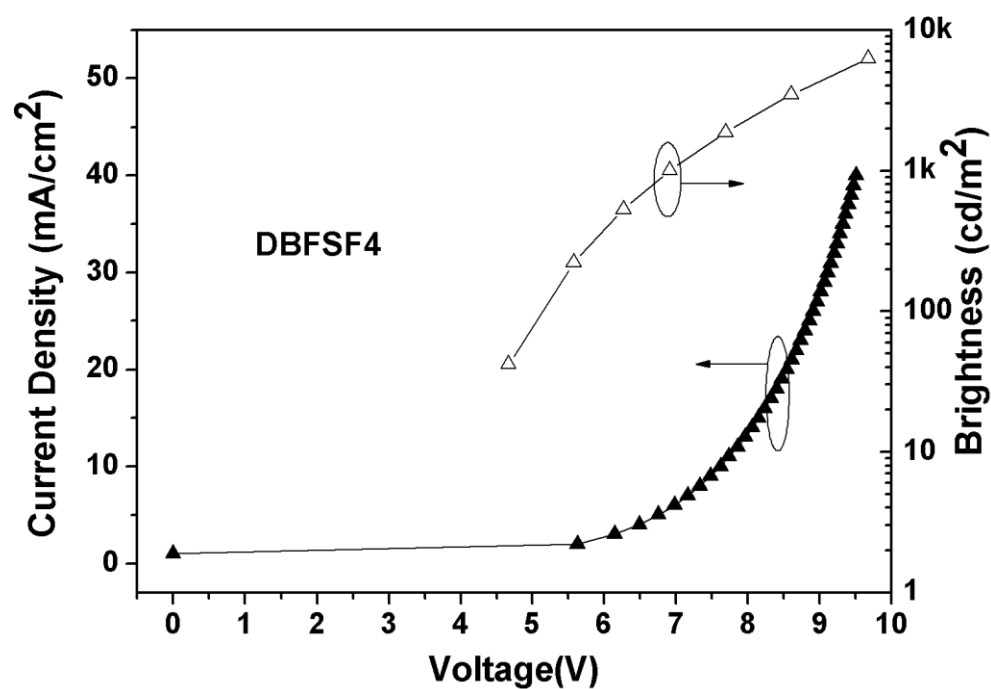


Fig. S3 Current density-voltage-brightness characteristics of Device A.

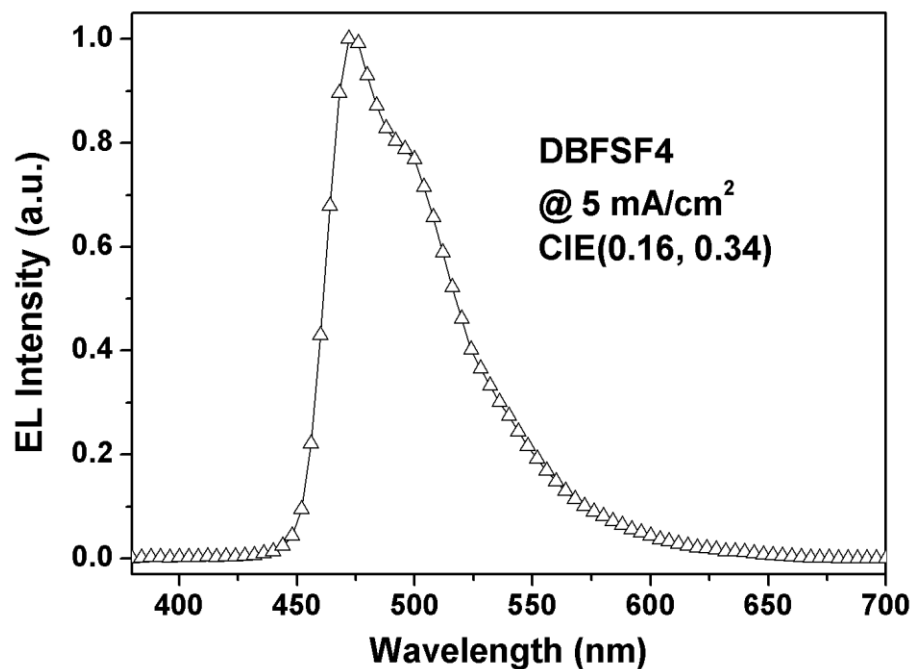


Fig. S4 EL spectrum of Device A.

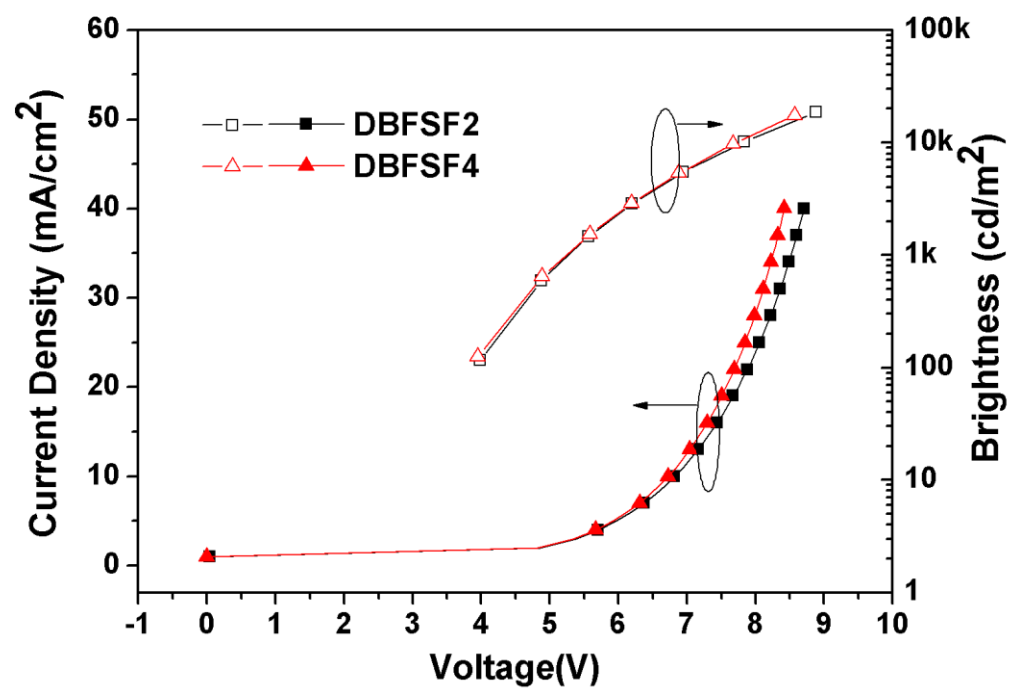


Fig. S5 Current density-voltage-brightness characteristics for Devices B and C.

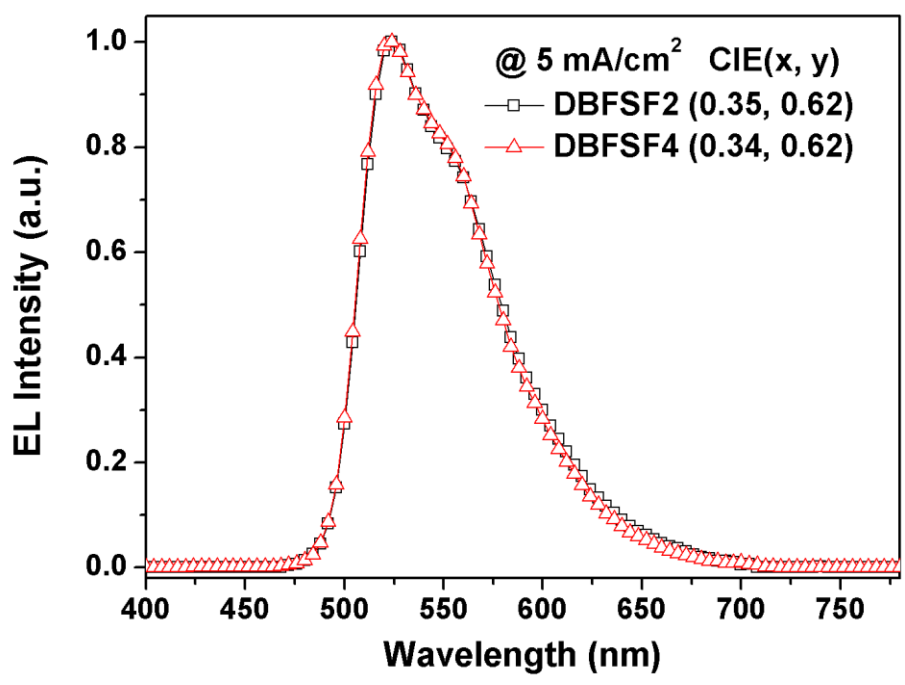
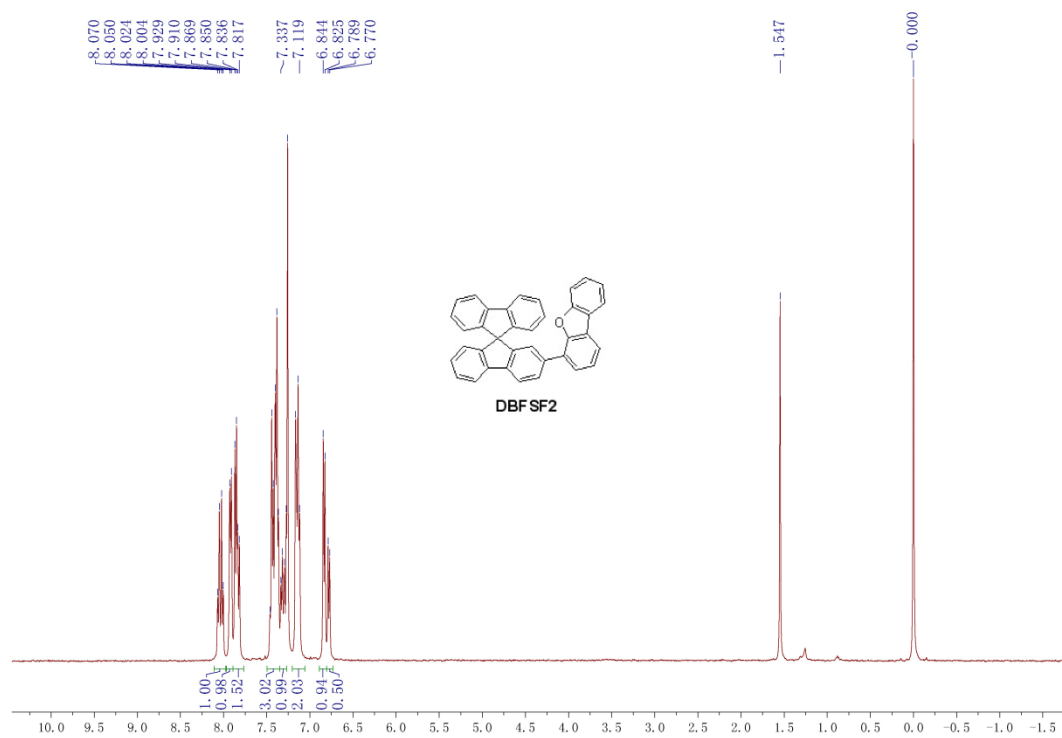
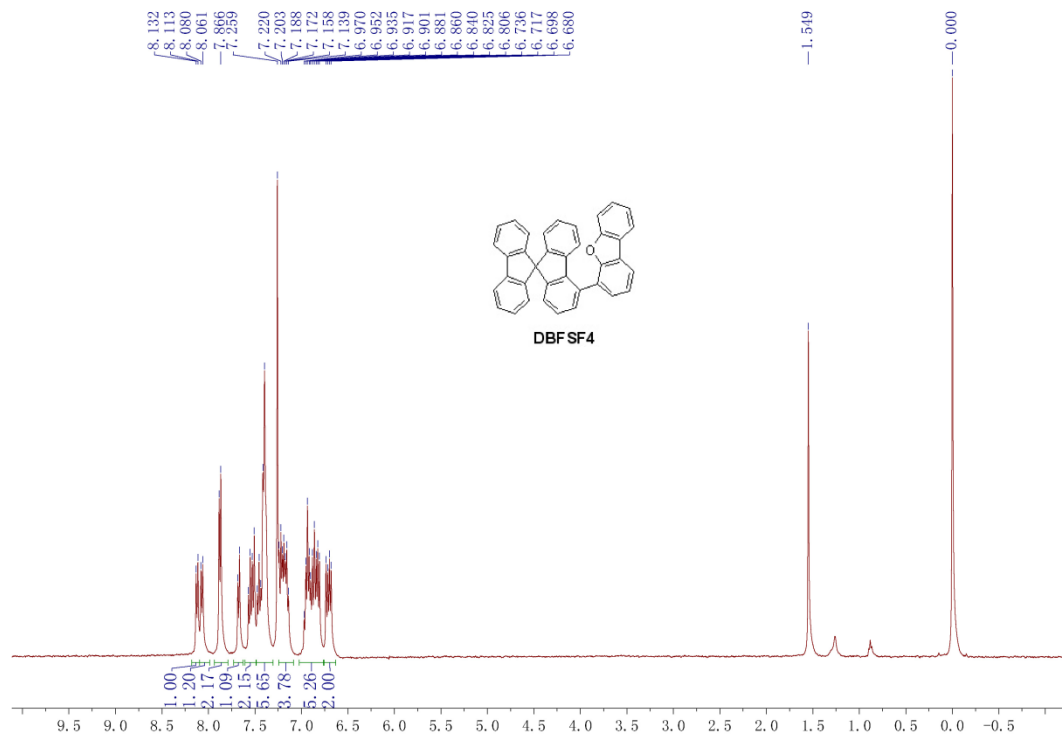


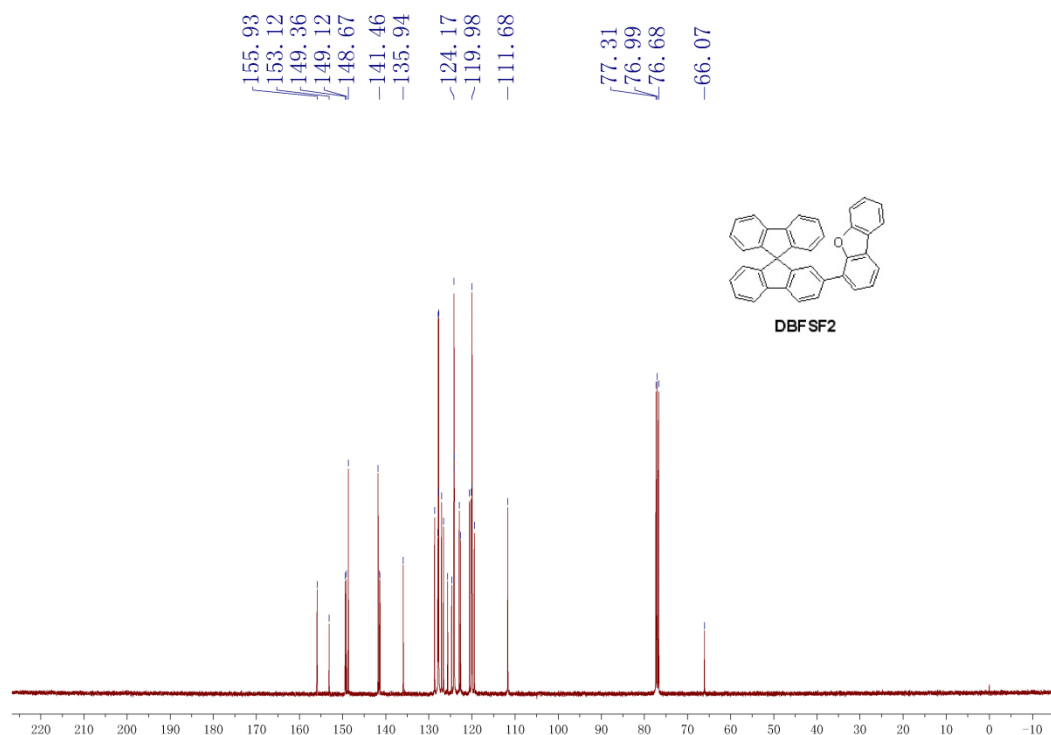
Fig. S6 EL spectra of Devices B and C.



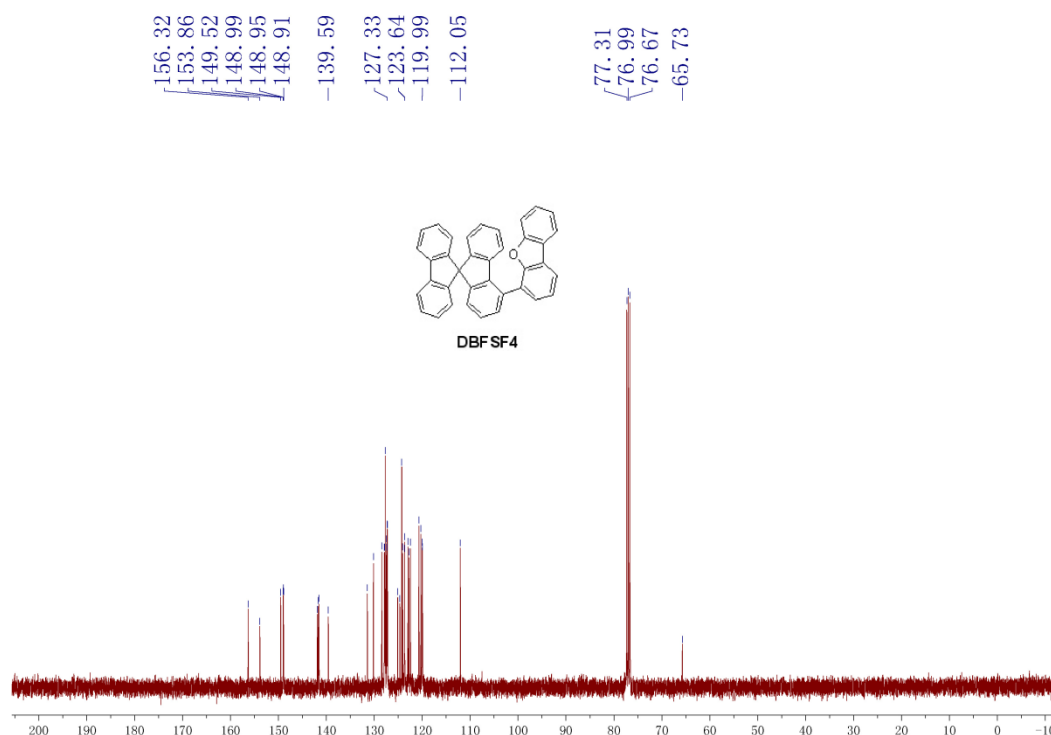
**Fig. S7** <sup>1</sup>H NMR of DBFSF2 in CDCl<sub>3</sub>.



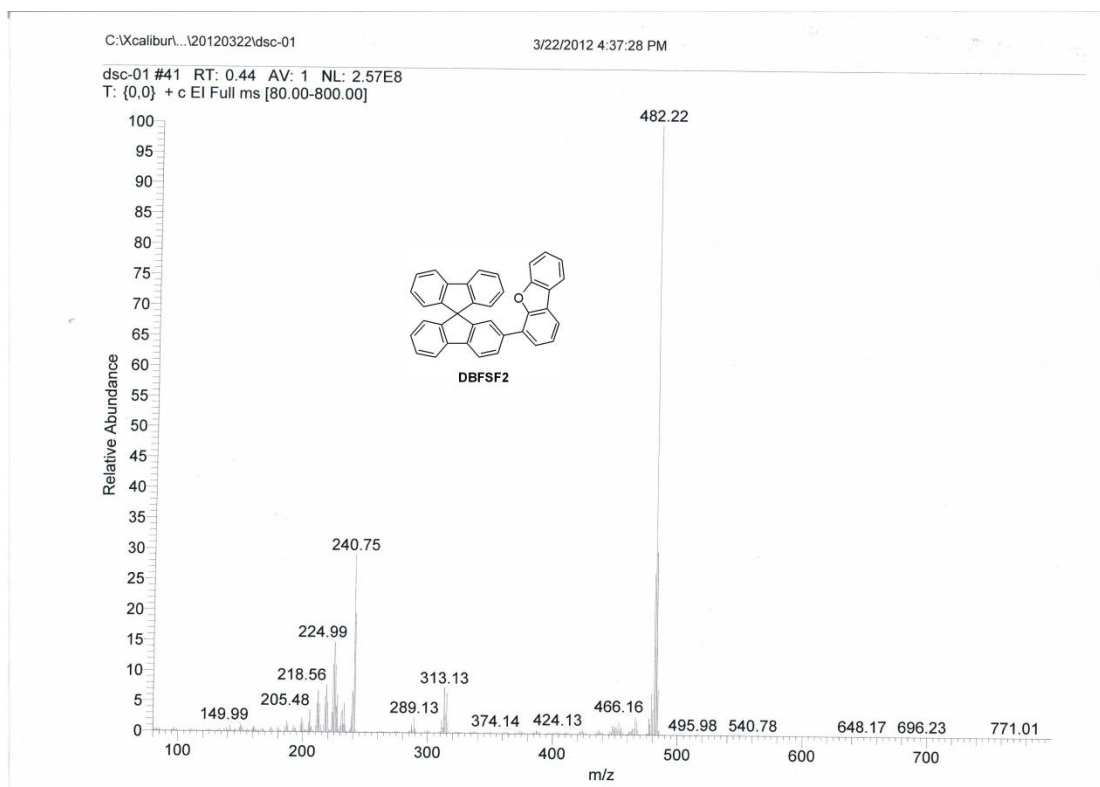
**Fig. S8** <sup>1</sup>H NMR of DBFSF4 in CDCl<sub>3</sub>.



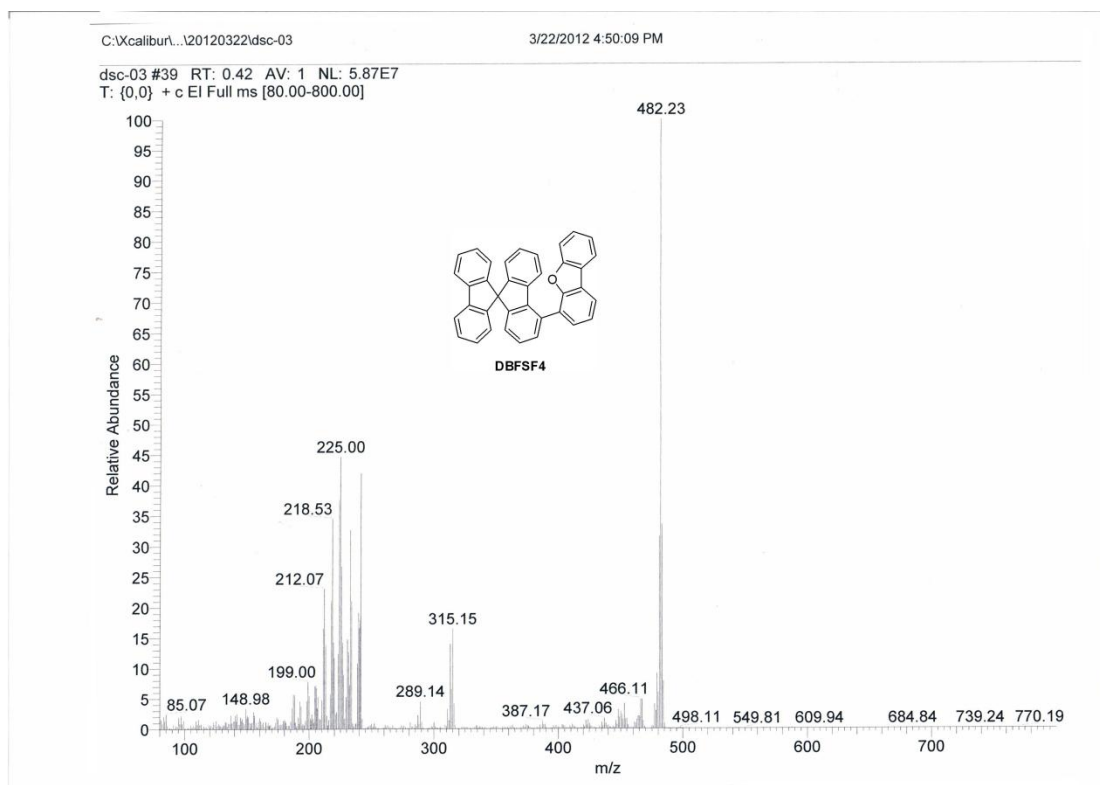
**Fig. S9**  $^{13}\text{C}$  NMR of DBFSF2 in  $\text{CDCl}_3$ .



**Fig. S10**  $^{13}\text{C}$  NMR of DBFSF4 in  $\text{CDCl}_3$ .



**Fig. S11** EI-MS of DBFSF2.



**Fig. S11** EI-MS of DBFSF4.