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# Supplementary Information for *J. Mater. Chem.*

## Cruciform DPVBi: Synthesis, Morphology, Optical and Electroluminescent Properties

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# The structure characterization of octaethyl biphenyl-2,2',5,5' -tetrayltetrakis(met-hylene)tetraphosphonate (tetra(phosphonate)) and 2,5,2',5'-tetrakis(2,2-diphenylvinyl)biphenyl (TDPVBi)

## 1. $^{1}$H-NMR spectrum of tetra(phosphonate):

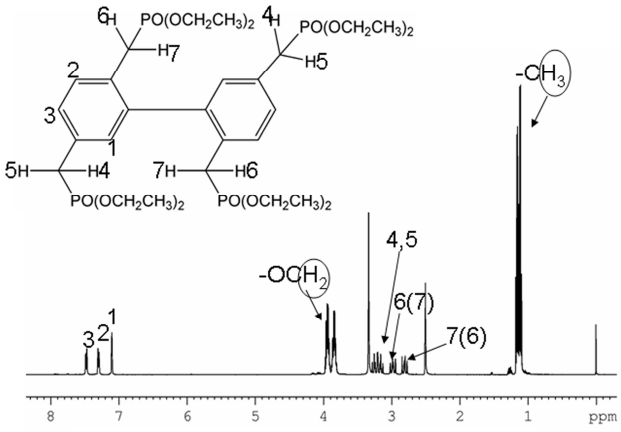


**Fig. S1** The $^{1}$H-NMR (500 MHz, 25 °C, DMSO-$d_6$, TMS, ppm) spectrum of tetra(phosphonate).

## 2. $^{13}$C-NMR spectrum of tetra(phosphonate):

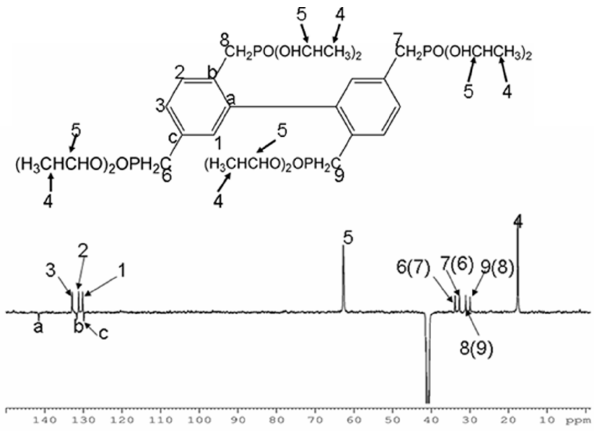

**Fig. S2** The $^{13}$C-NMR (125 MHz, 25 °C, DMSO-$d_6$) spectrum of tetra(phosphonate).

## 3. Two-dimensional COSY spectrum of TDPVBi:

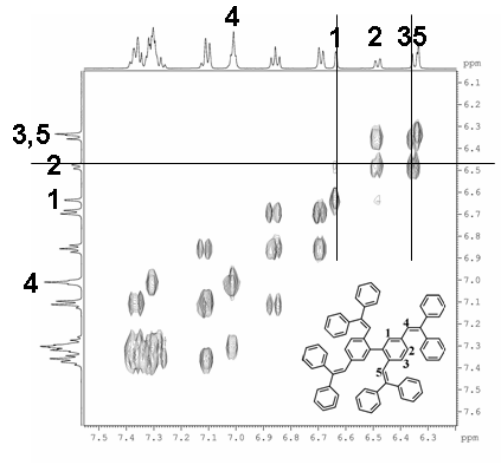


**Fig. S3** The two-dimensional COSY spectrum of **TDPVBi.**

As shown in **Fig. S3,** the neighbor protons $H_3$, $H_2$ with a strong H-H correlation and $H_1$, $H_2$ with a weak H-H correlation can be seen from two-dimensional COSY spectrum. These protons in central phenyl can be made sure by two-dimensional COSY spectrum, which is corresponding with $^1$H NMR. Some of the protons of around phenyls exhibit so complex H-H correlation, which can not be made sure by two-dimensional COSY spectrum.

## 4. $^{13}$C-NMR spectrum of TDPVBi:

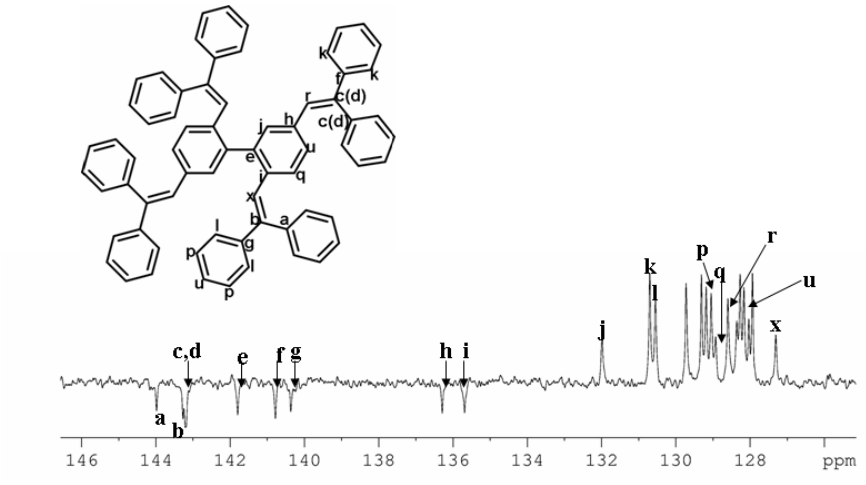


**Fig. S4** The $^{13}$C-NMR spectrum of **TDPVBi.**

Combined analysis of $^{1}$H NMR spectrum, two-dimensional COSY spectrum and HMBC spectrum, the $^{13}$C-NMR spectrum can be signed except some of the phenyls around. It is noted that C-a ($\delta$ 143.98) and C-g ($\delta$ 140.37), C-x ($\delta$ 127.31) and C-r ($\delta$ 128.59), C-f ($\delta$ 140.78) and C-c (d) ($\delta$ 143.20) are different, which reflect the twist structure of the molecule.

## 5. MALDI-TOF mass spectrum of TDPVBi:

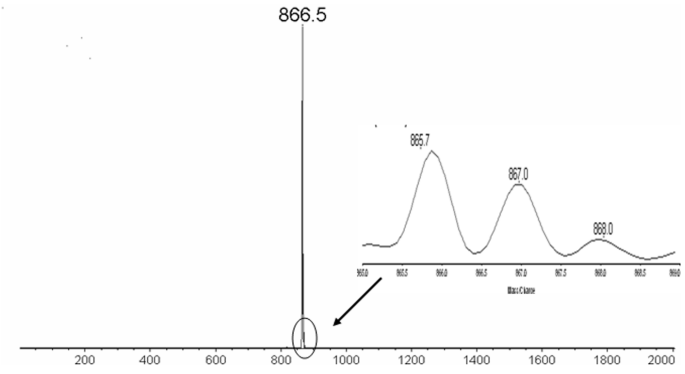


**Fig. S5** The matrix assisted MALDI-TOF mass spectrum of **TDPVBi.** $[M + H]^+$ peak of **TDPVBi** at 866.50, which is in good agreement with the calculated value of 866.39 based on the $C_{68}H_{50}$ molecular formula of **TDPVBi**.