Supporting information:

Donor-acceptor π-conjugated aggregation-induced emission molecules for reversible nanometer-scale data storage

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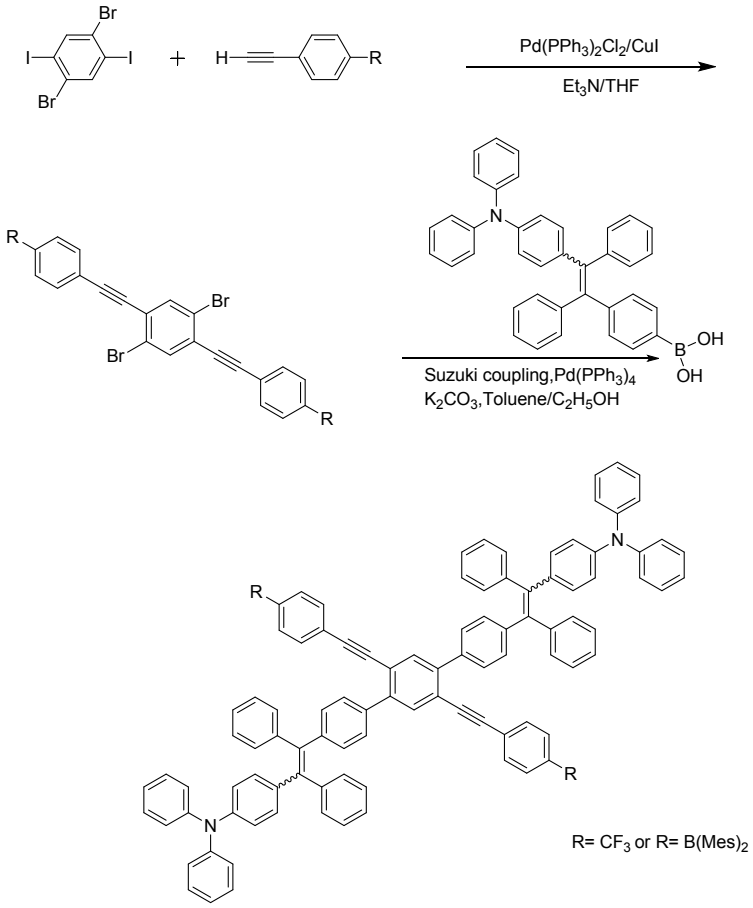
Experimental section

All experiments were carried out under a nitrogen atmosphere unless otherwise noted. TPE units were prepared by the similar procedure as previously reported[1]. All solvents were dried by normal procedure and distilled under an inert atmosphere before use. ^{1}H and ^{13}C NMR spectra were measured on a Bruker 400 MHz spectrometer. UV/Vis absorption spectra and fluorescence spectra measurement were performed at room temperature with a Varian 50Conc spectrometer and a PerkinElmer LS55 spectrometer, respectively. HRMS were determined on a Bruker Solarix 9.4 T mass spectrometer. The absolute fluorescent quantum yield was determined by a Hamamatsu Quantaurus-QY C11347 integrated sphere system. The single crystal X-ray diffraction measurement was performed at 173 K with a Rigaku Saturn 724+ CCD diffractometer equipped with a sealed tube MoKα radiation source.

Synthetic route:



Synthetic method

To a 50 mL flask was charged with 1,4-dibromo-2,5-diiodobenzene, $Pd(PPh_3)_2Cl_2$, and CuI under N_2 atmosphere, then (4-ethynylphenyl)dimesitylborane or 1-ethynyl-4-(trifluoromethyl)benzene was added. The THF and Et_3N mixture (3:1) were injected. The mixture was stirred at r.t. for 10h. After concentrated, NH_4Cl solution (10 mL) was added and the mixture was extracted with dichloromethane. The combined organic layers were washed with brine (20 mL), dried over $MgSO_4$, filtered, and concentrated under reduced pressure. The residue was purified by a silica gel column chromatography to afford the title compound in about 70-80% yield.

Compound **1**

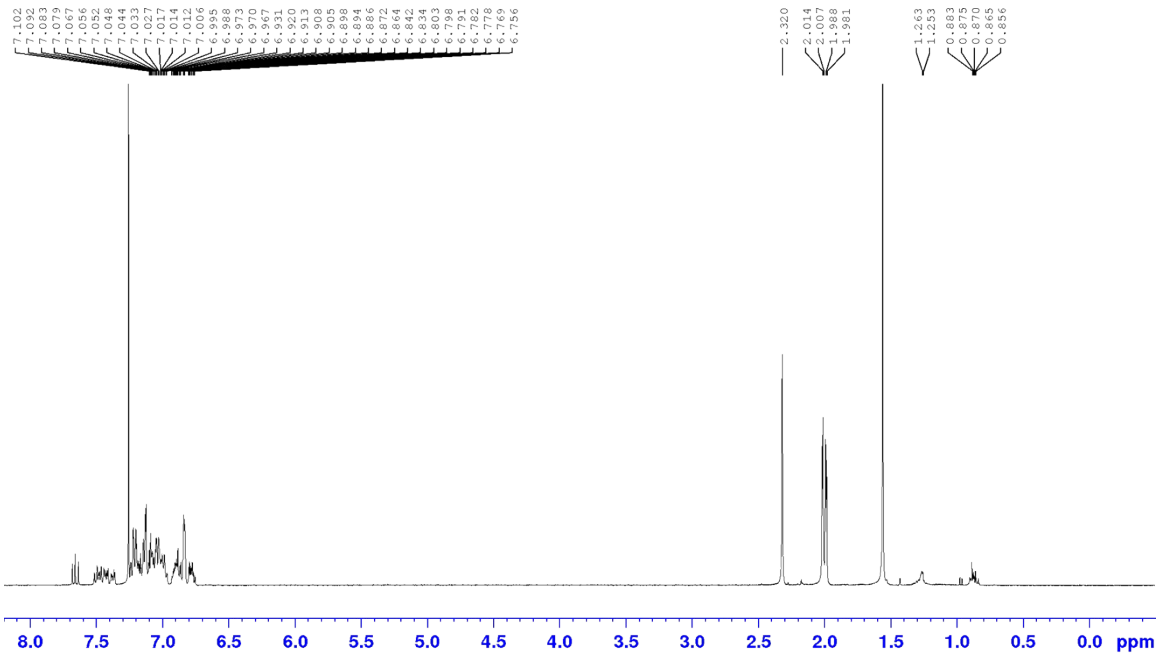
(((2,5-dibromo-1,4-phenylene)bis(ethyne-2,1-diyl))bis(4,1-phenylene))bis(dimesitylborane) reacted with (4-(2-(4-(diphenylamino)phenyl)-1,2-diphenylvinyl)phenyl)boronic acid under $Pd(PPh_3)_4$, and K_2CO_3 in N_2 atmosphere, ^1H NMR (400 MHz, Chloroform-d_6): 7.66 (t, J =10Hz, 2H), 7.52-7.36 (m, 8H), 7.24-6.97(m, 46H), 6.92-6.76(m, 18H), 2.32(s, 12H), 2.00(q, 24H); ^{13}C NMR (100 MHz, Chloroform-d_6): 147.57,147.52, 145.98, 144.06, 143.89, 143.60, 143.43, 142.20, 141.51, 141.09, 140.96, 140.77, 140.15, 140.02, 138.81, 137.93, 137.73, 137.01, 136.10, 133.52, 133.31, 132.18, 131.40, 131.00, 130.78, 130.74, 129.06, 128.60, 128.19, 127.69, 127.61, 126.57, 126.47, 126.34, 124.23, 124.20, 122.74, 122.65, 121.67, 121.44, 94.38,94.22,

91.50, 23.42, 21.21; HRMS (MALDI), calcd. : $C_{134}H_{110}B_2N_2$: 1768.888315, Found: 1768.887398.

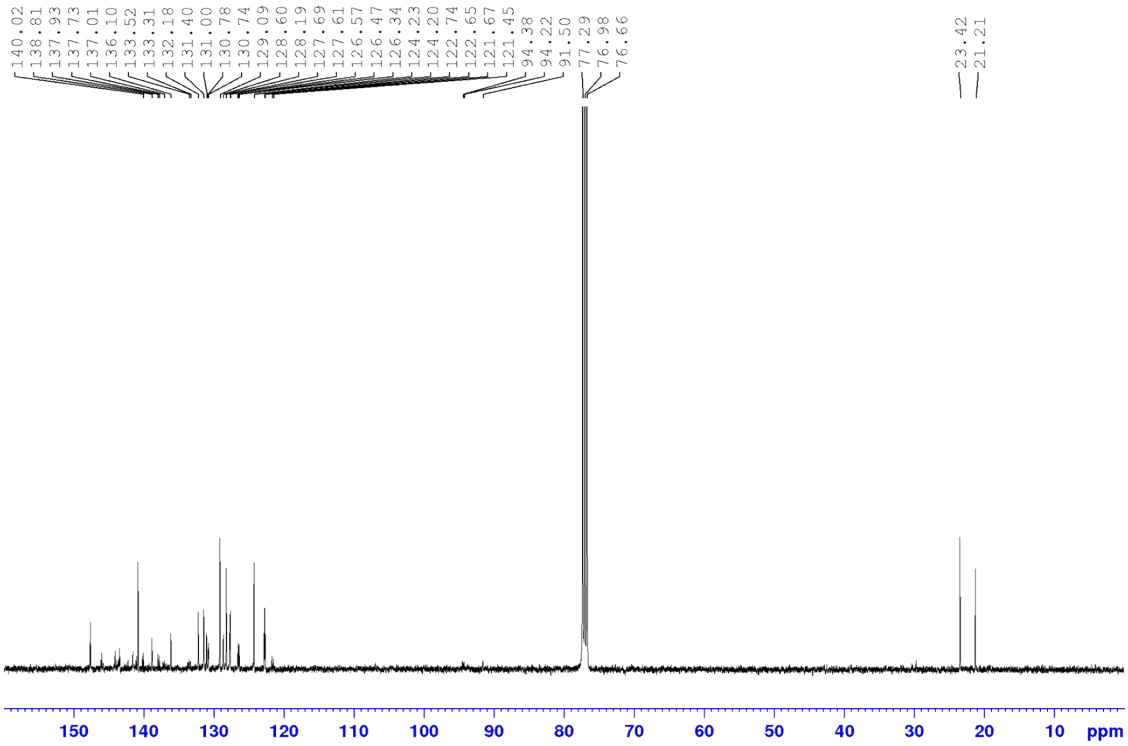
Compound **2**

4,4'-(2,5-dibromo-1,4-phenylene)bis(ethyne-2,1-diyl))bis((trifluoromethyl)benzene) reacted with (4-(2-(4-(diphenylamino)phenyl)-1,2-diphenylvinyl)phenyl)boronic acid under $Pd(PPh_3)_4$, and K_2CO_3 in N_2 atmosphere,

^{1}H NMR (400 MHz, Chloroform-d_6): 7.70(t, J =10Hz, 2H), 7.56-7.45(m, 8H), 7.37-7.33(m, 4H), 7.24-7.09(m, 42H), 6.95-6.88(m, 6H), 6.82-6.77(m, 4H); ^{13}C NMR (100 MHz, Chloroform-d_6): 147.72,147.64, 146.28, 144.28, 143.96, 143.83, 143.64, 143.49, 142.95, 142.82, 142.46, 141.46, 141.30, 140.12, 140.03, 137.87, 137.75, 137.13, 136.93, 133.88, 133.75, 132.60, 132.33, 131.73, 131.71, 131.62, 131.57, 131.52,131.24, 131.01, 130.20，129.92, 129.28, 128.94, 128.71, 127.84, 127.04, 126.70, 126.60, 125.41, 124.49, 124.43, 122.97, 122.89, 122.83, 122.58, 121.66, 121.44, 92.66, 91.68; HRMS (MALDI), calcd. : $C_{100}H_{66}F_6N_2$: 1408.512471, Found: 1408.511854.



^{1}H spectrum of compound **1** (li-hk-70)



^{13}C spectrum of compound **1** (li-hk-70)

MALDI,LI-HK-70,20151224

Analysis Info

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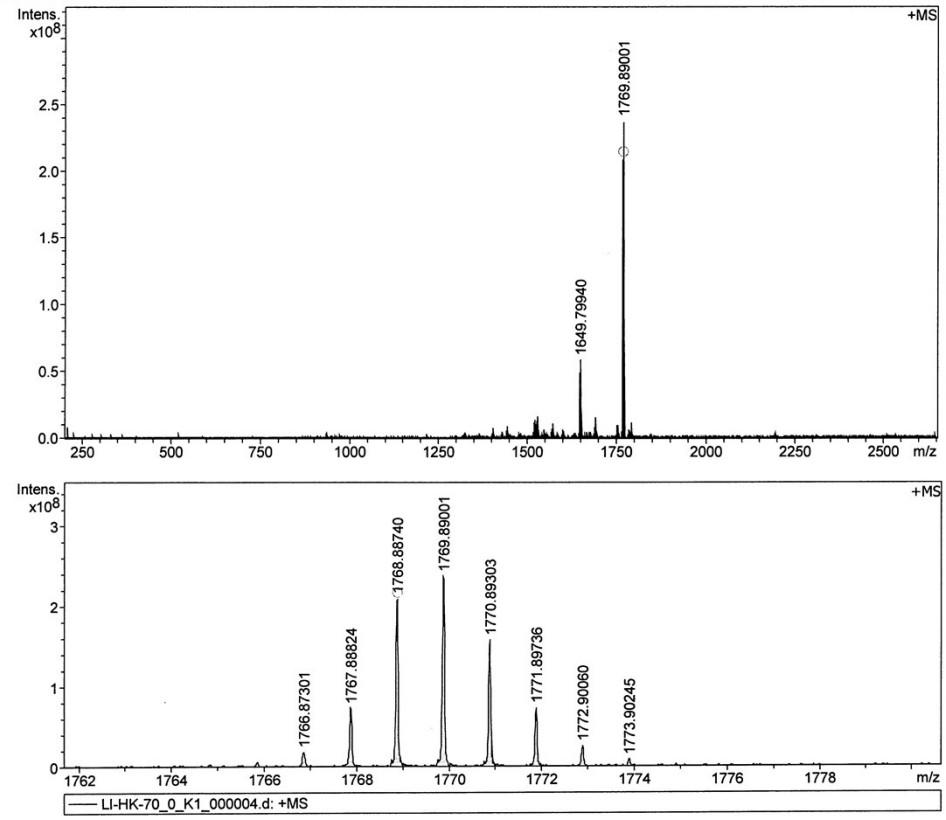
Method	MALDI_P_100-3000	Operator	
Sample Name		Instrument	solariX
Comment			

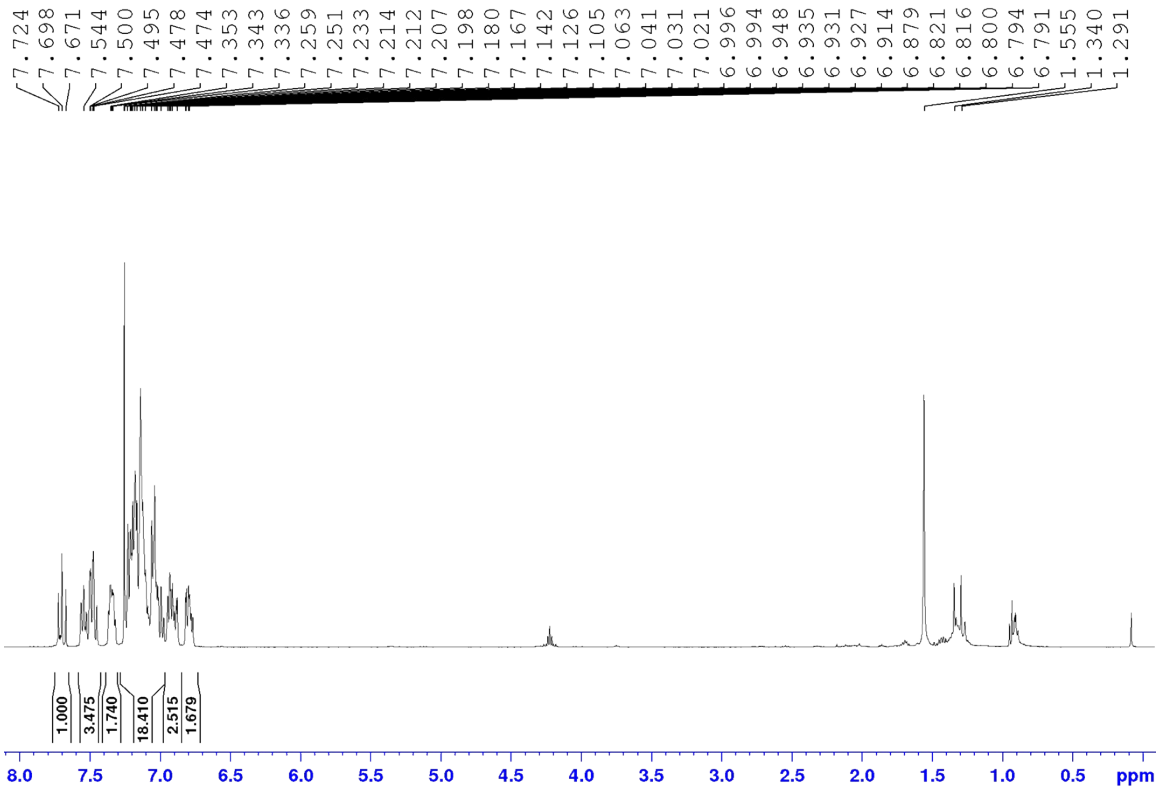
Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	5	Calibration Date	Thu Dec 24 04:38:36
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	2048576
Broadband Low Mass	202.1 m/z	No. of Laser Shots	10	Data Processing Size	2097152
Broadband High Mass	2650.0 m/z	Laser Power	29.6 lp	Apodization	Sine-Bell Multiplication
Source Accumulation	0.001 sec	Laser Shot Frequency	0.020 sec		
Ion Accumulation Time	0.300 sec				

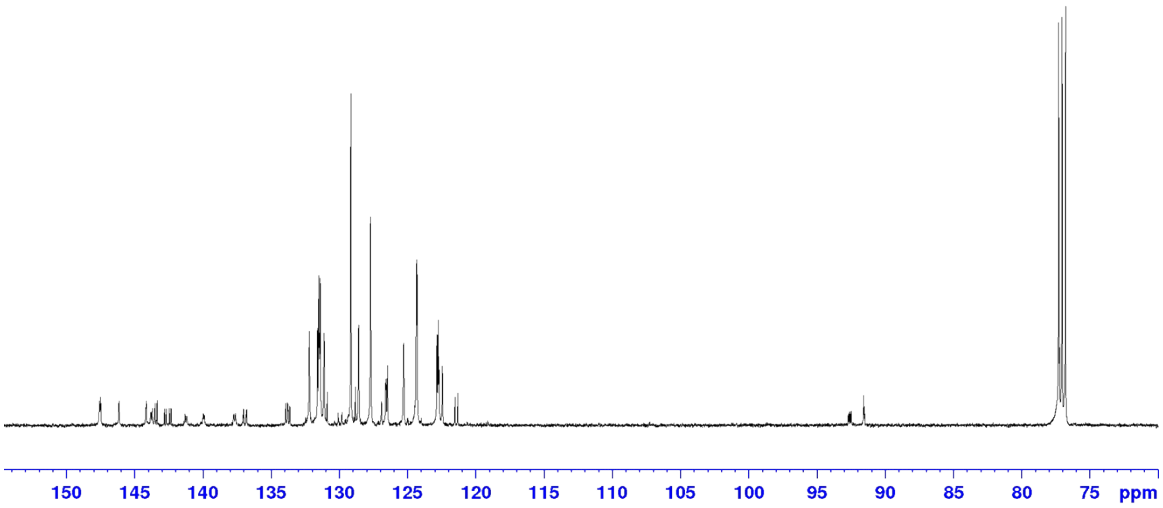


Meas. m/z	#	Ion Formula	Score	m/z	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
1768.887396	1	C134H110B2N2	100.00	1768.888315	0.4	18.2	82.0	odd	ok

HRMS of compound **1** (li-hk-70)



^{1}H spectrum of compound **2** (li-hk-74)



^{13}C spectrum of compound **2** (li-hk-74)

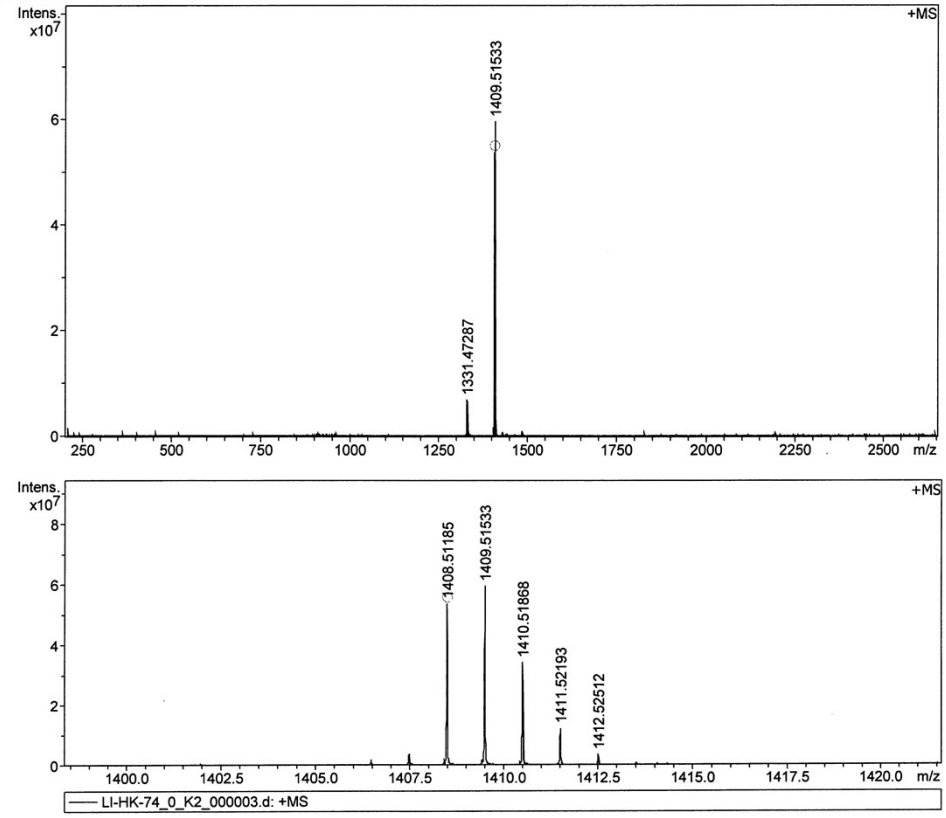
MALDI,LI-HK-74,20151224

Analysis Info

Analysis Name	D:\Data\MALDI\2015\1224\LI-HK-74_0_K2_000003.d	Acquisition Date	12/24/2015 4:52:46 PM
Method	MALDI_P_100-3000	Operator	
Sample Name		Instrument	solariX
Comment			

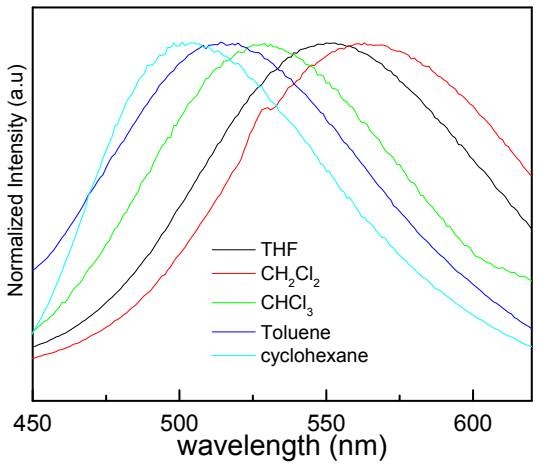
Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	5	Calibration Date	Thu Dec 24 04:38:36
Polarity	Positive	No. of Cell Fills	1	Data Acquisition Size	2097152
Broadband Low Mass	202.1 m/z	No. of Laser Shots	10	Data Processing Size	4194304
Broadband High Mass	2650.0 m/z	Laser Power	23.2 lp	Apodization	Sine-Bell Multiplication
Source Accumulation	0.001 sec	Laser Shot Frequency	0.020 sec		
Ion Accumulation Time	0.300 sec				

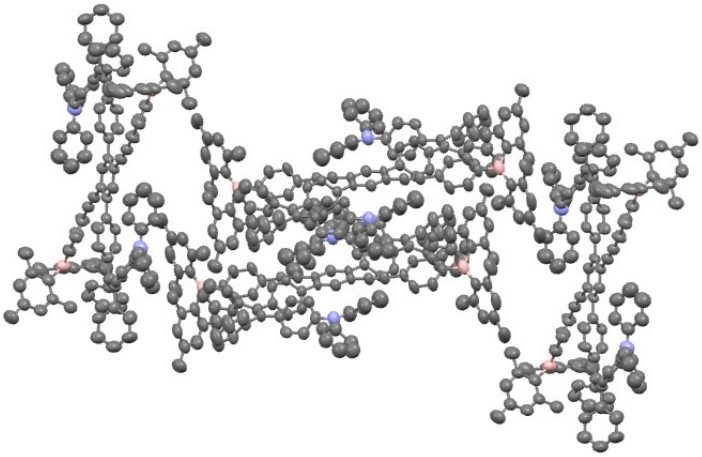


Meas. m/z	#	Ion Formula	Score	m/z	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
1408.511854	1	C100H66F6N2	100.00	1408.512471	0.4	15.7	66.0	odd	ok

HRMS of compound **2** (li-hk-74)



Sup. 2 Fluorescent spectra of the compound **2** in different solvents ($\lambda_{ex.}$= 370 nm)



Sup.3 The single crystal packing mode of compound **1** shows that the donating triphenylamine group of one molecule can easily interact with the dimesitylboryl group of neighboring molecule.

Reference

(1) J. Zhou, Z. Chang, Y. Jiang, B. He, M. Du, P. Lu, Y. N. Hong, H. S. Kwok, A. Qin, H. Qiu, Z. Zhao, B.Z. Tang, Chem. Comm.. 2013, 49, 2491.