

Electronic Supplementary Information

Highly efficient triazine/carbazole-based host material for green phosphorescent organic light-emitting diodes with low efficiency roll-off

Mingming Hu,^a Yang Liu,^a Yi Chen,^a Wenxuan Song,^a Lei Gao,^c Haichuan Mu,^{*b}

Jinhai Huang^d and Jianhua Su^{*a}

^aKey Laboratory for Advanced Materials and Institute of Fine Chemicals, East China University of Science & Technology, Shanghai 200237, PR China. Email: bbsjh@ecust.edu.cn.

^bDepartment of Physics, School of Science, East China University of Science and Technology, 130 Meilong Road, Shanghai 200237, PR China. Email: hcmu@ecust.edu.cn.

^cSchool of Chemistry and Chemical Engineering, Queen's University, Belfast.

^dShanghai Taoe Chemical Technology Co., Ltd, Shanghai, PR China.

Contents

1. ¹ H and HRMS	S2
2. EL spectra of two materials under different driving voltages	S4

Content

1. ^1H , ^{13}C NMR and HRMS

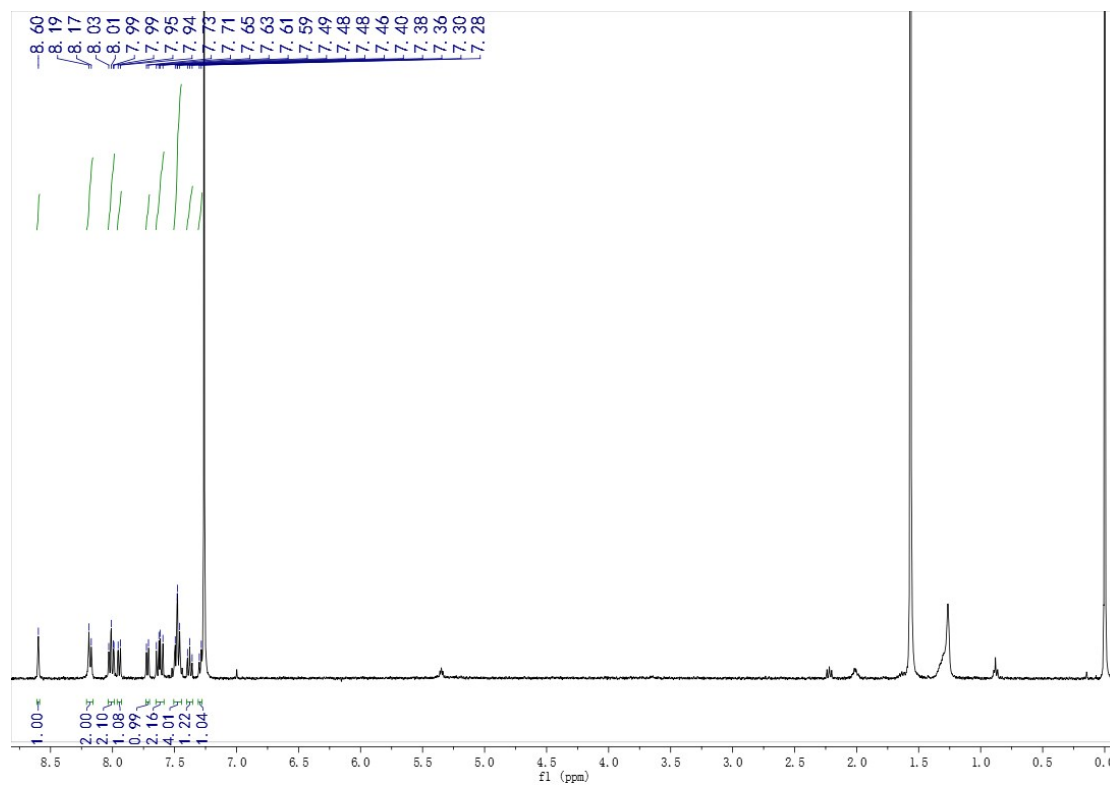


Fig. S1 ^1H NMR of (3)

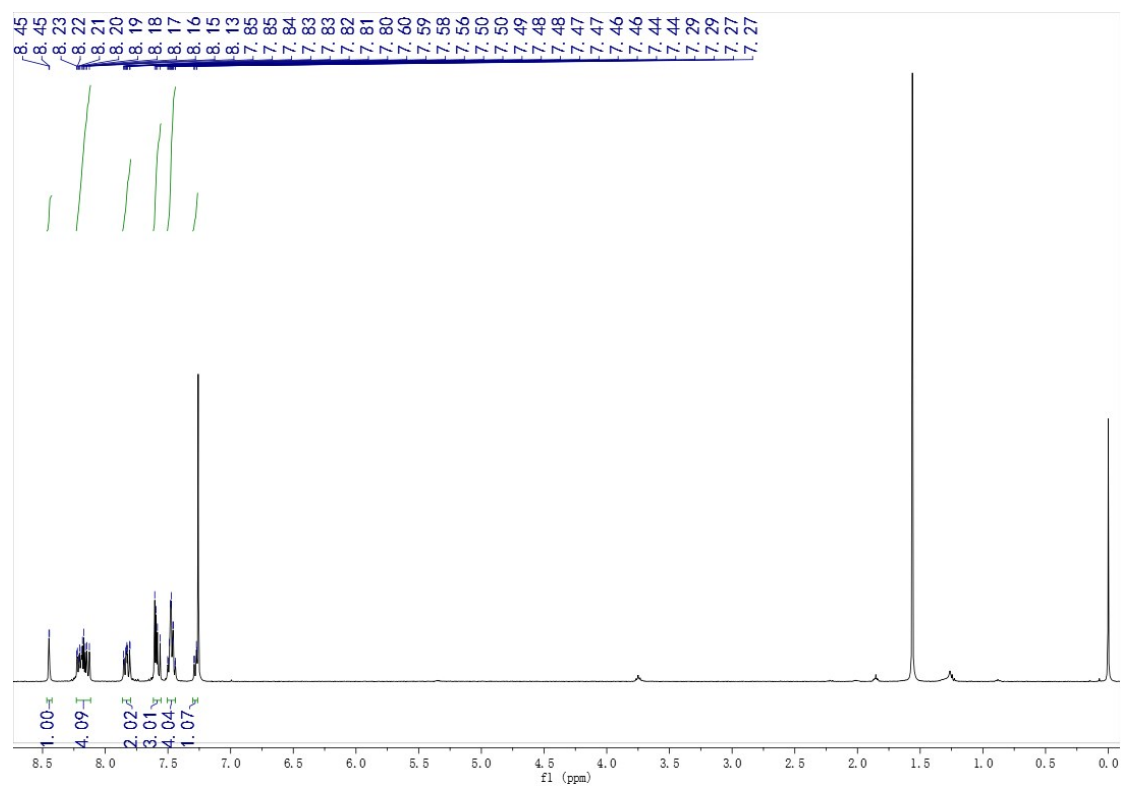


Fig. S2 ^1H NMR of (5)

Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

C: 0-24 H: 0-20 N: 0-1 O: 0-1

H-TIAN

ECUST institute of Fine Chem

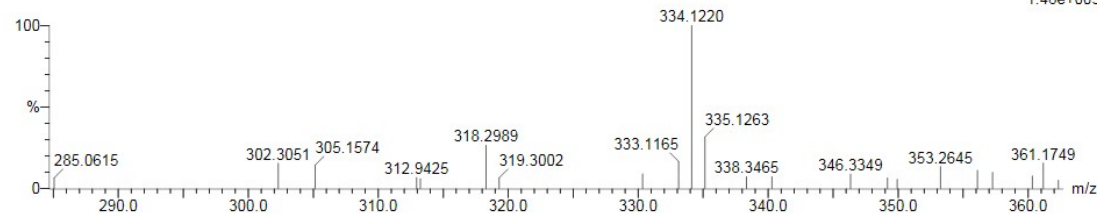
01-Dec-2016

23:29:32

1: TOF MS ES+

1.46e+003

TH-HMM-1 26 (0.890) Cm (25:27)



Minimum:

Maximum:

300.0

500.0

-1.5

100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
334.1220	334.1232	-1.2	-3.6	17.5	20.3	0.0	C24 H16 N O

Fig. S3 Mass spectrometry of (3)

Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

C: 0-24 H: 0-14 N: 0-1 S: 0-1

H-TIAN

ECUST institute of Fine Chem

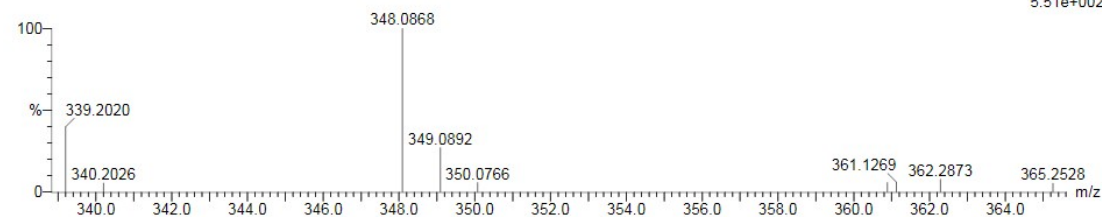
29-Nov-2016

15:54:19

1: TOF MS ES-

5.51e+002

TH-HMM-88 47 (1.105) Cm (47)



Minimum:

Maximum:

300.0

500.0

-1.5

100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
348.0868	348.0847	2.1	6.0	18.5	9.9	0.0	C24 H14 N S

Fig. S4 Mass spectrometry of (5)

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Even Electron Ions

24 formula(e) evaluated with 2 results within limits (up to 1 closest results for each mass)

Elements Used:

C: 0-44 H: 0-33 N: 0-4 O: 0-1

H-TIAN

ECUST institute of Fine Chem

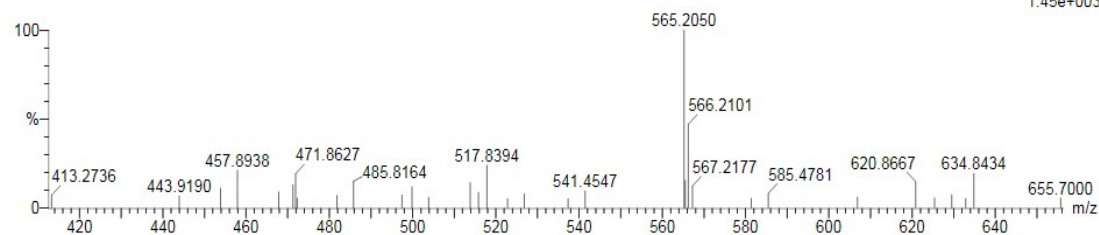
26-Sep-2016

20:24:27

1: TOF MS ES+

1.45e+003

TH-HMM-15 169 (1.129) Cm (164:169)



Minimum:

Maximum: 300.0 50.0 -1.5

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
565.2050	565.2028	2.2	3.9	29.5	20.7	0.0	C39 H25 N4 O

Fig. S5 Mass spectrometry of BFTC



Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

13 formula(e) evaluated with 6 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

C: 0-39 H: 0-68 N: 0-4 S: 0-1

H-TIAN

ECUST institute of Fine Chem

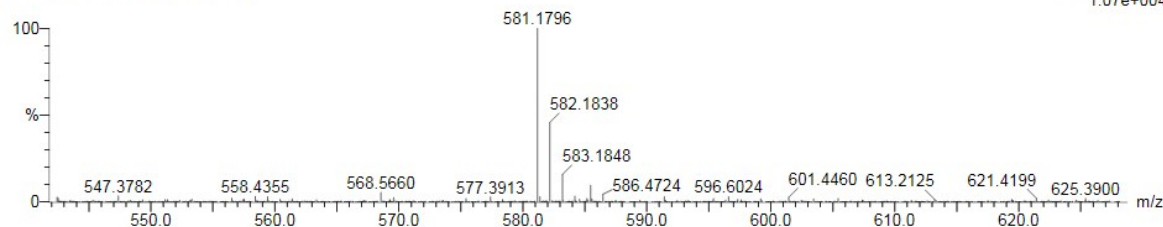
19-Nov-2016

17:14:17

1: TOF MS ES+

1.07e+004

TH-HMM-1 46 (0.666) Cm (45:49)



Minimum:

Maximum: 300.0 500.0 -1.5

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
581.1796	581.1800	-0.4	-0.7	29.5	190.8	0.0	C39 H25 N4 S

Fig. S6 Mass spectrometry of BTTC

2. EL spectra of four materials under different driving voltages

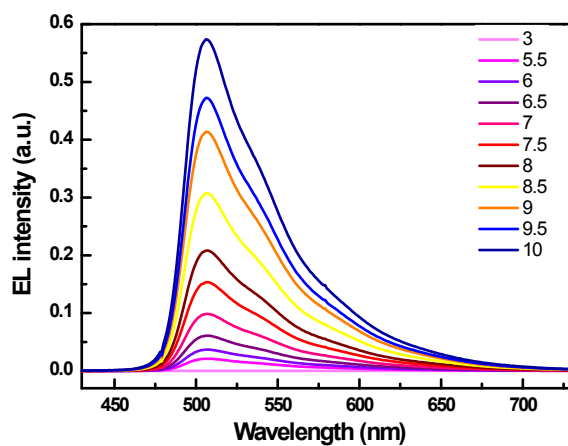


Fig. S7 EL spectra of BFTC under different driving voltages

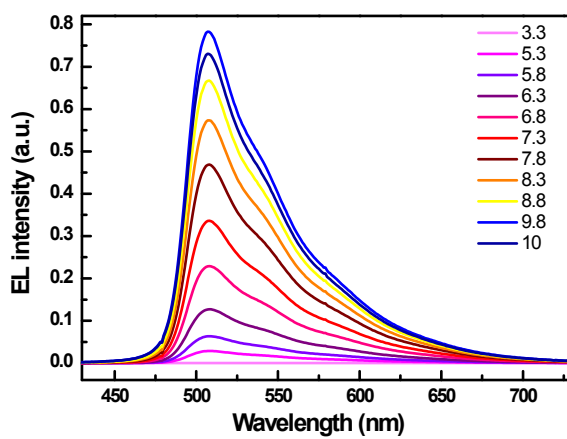


Fig. S8 EL spectra of BTTC under different driving voltages