New Journal of Chemistry

Supporting information for:

Schiff-bases Containing Triphenylamine and Pyrrole Units: Synthesis and Electrochromic, Acidochromic Properties

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Captions

Fig. S1 (a) ^{1}H-NMR, (b) ^{13}C-NMR and (c) aromatic region of the H-H COSY spectrum of SB5 in DMSO-d_6.

Fi g. S2 Acidochromic absorption change of SB1~SB4.

Fig. S3 Relationship between $(I-I_0)/I_0$ and pH value at their new peaks of SB1~SB4.

Fig. S4 relationship between A and $(A_{HA}-A)/[H^+]$ at their new peaks of SB1~SB4.

Fig. S5 CV curves of SB3~SB5 in CH_3CN containing 0.1 M $LiClO_4$ at a scan rate of 50 mV·s−1.

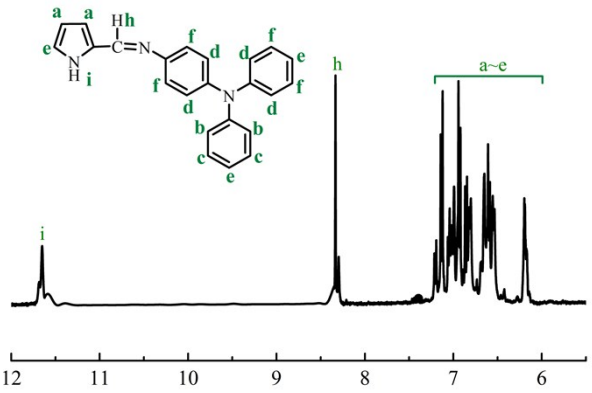
Fig. S6 Electronic absorption change of SB1~SB4 in CH_3CN containing 0.1 M $LiClO_4$ as the supporting electrolyte.

Fig. S7 ^{1}H-NMR spectrum of pyrrole-2-aldehyde.

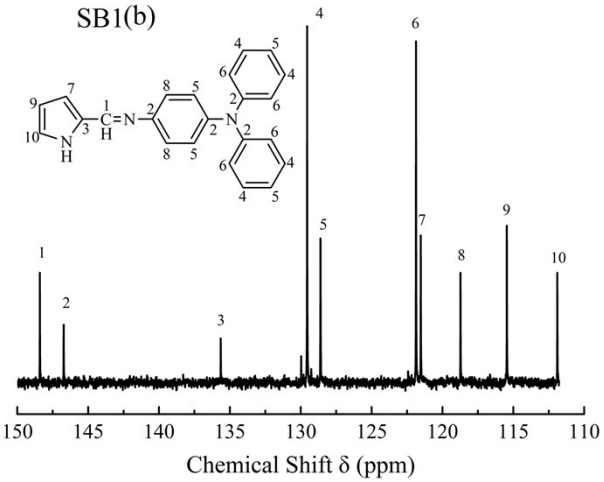
Fig. S8 FT-IR spectrum of pyrrole-2-aldehyde.

Scheme S1 Synthetic route of complex and pyrrole-2-aldehyde.

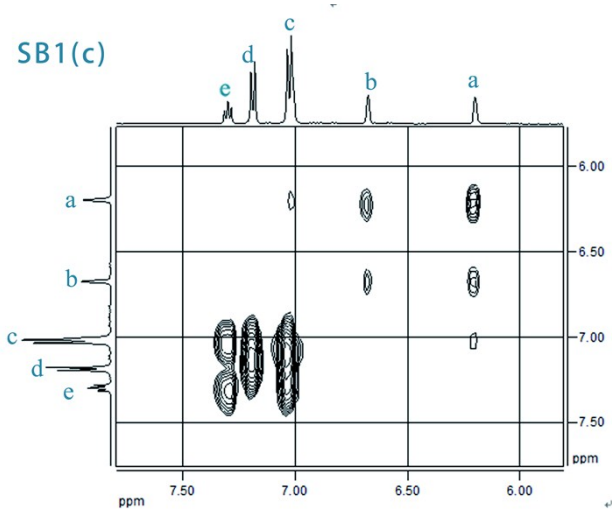
SB1(a)

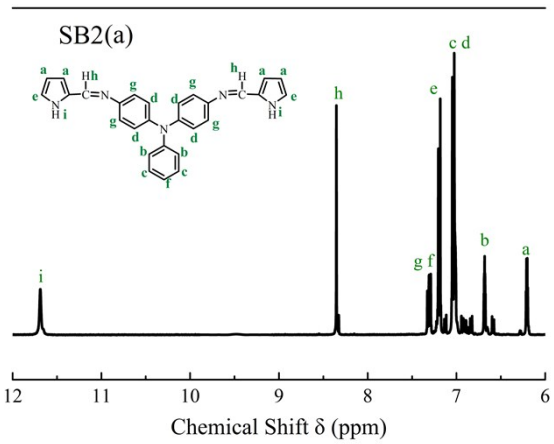


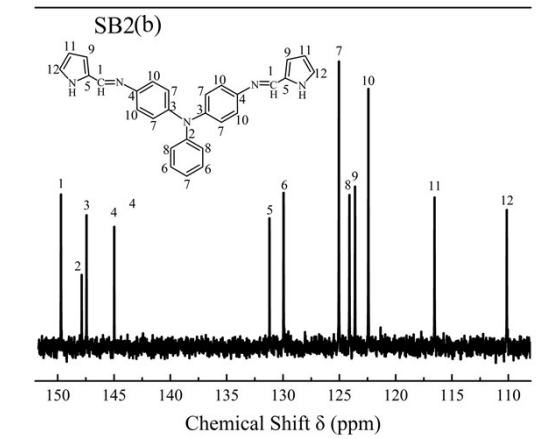
SB1(b)

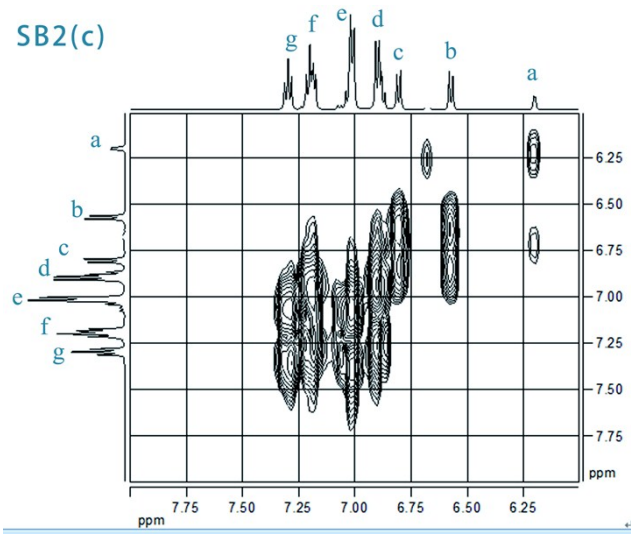


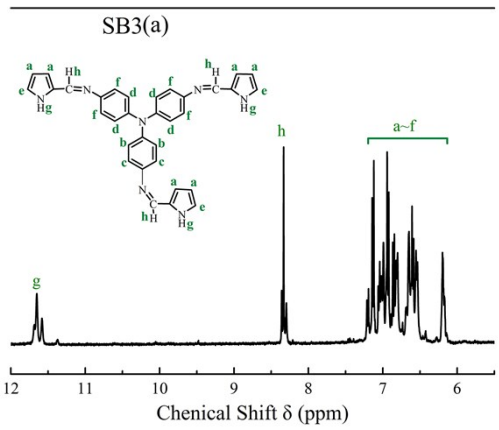
SB1(c)

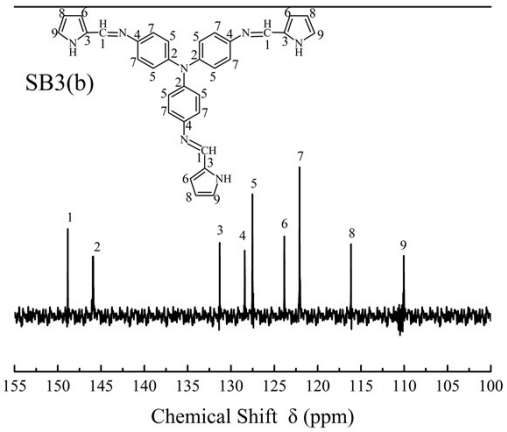


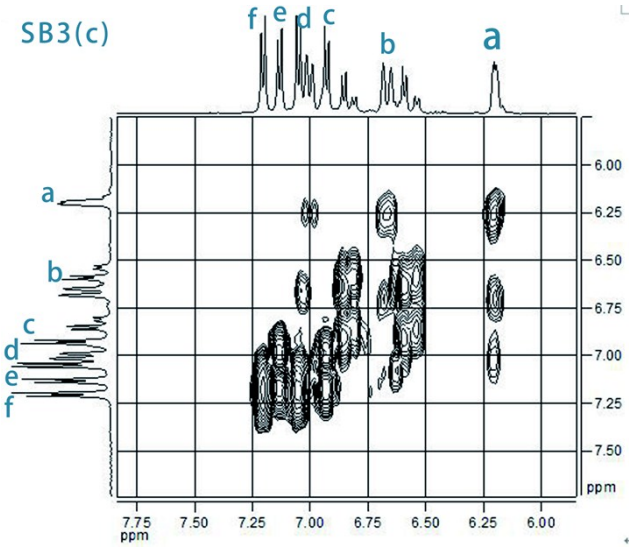

SB2(a)
i
h
g f
e
c d
b
a
12
11
10
9
8
7
6
Chemical Shift δ (ppm)


SB2(b)
150
145
140
135
130
125
120
115
110
Chemical Shift δ (ppm)


SB2(c)
g
f
e
d
c
b
a
6.25
6.50
6.75
7.00
7.25
7.50
7.75
ppm
7.75
7.50
7.25
7.00
6.75
6.50
6.25
ppm


SB3(a)
a~f
h
g
12
11
10
9
8
7
6
Chenical Shift δ (ppm)


SB3(b)
155
150
145
140
135
130
125
120
115
110
105
100
Chemical Shift δ (ppm)


SB3(c)
f
e
d
c
b
a
6.00
6.25
6.50
6.75
7.00
7.25
7.50
ppm
7.75
7.50
7.25
7.00
6.75
6.50
6.25
6.00
ppm

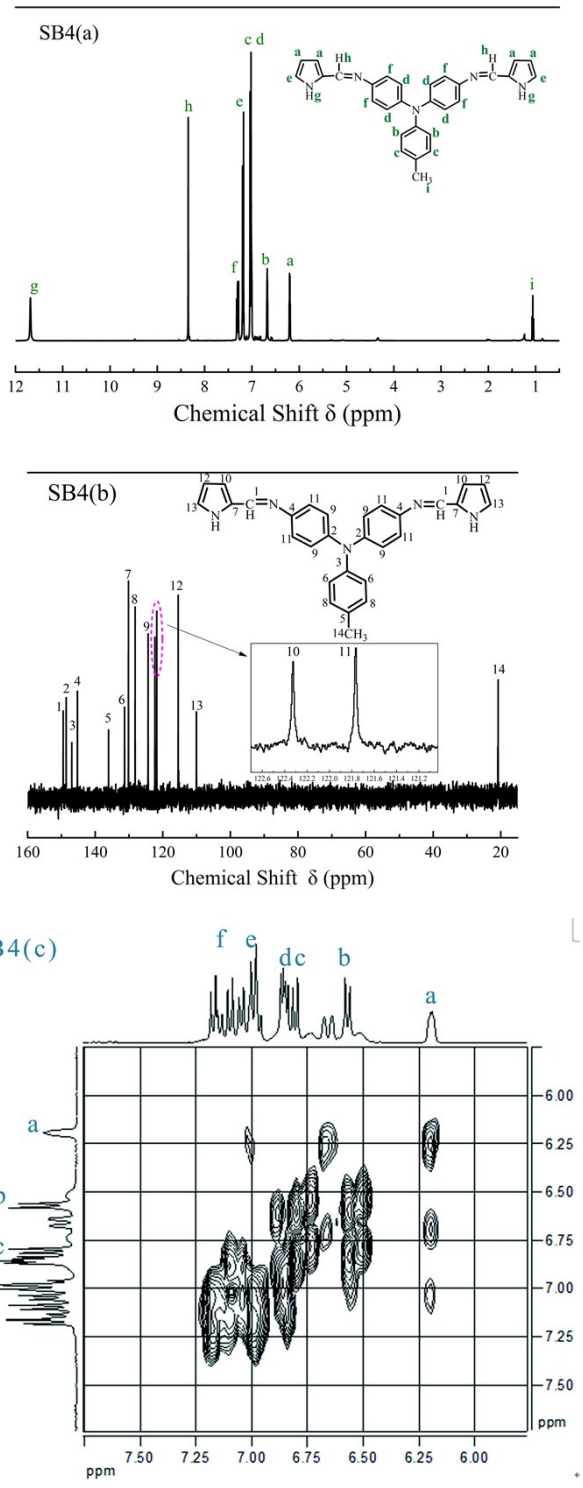
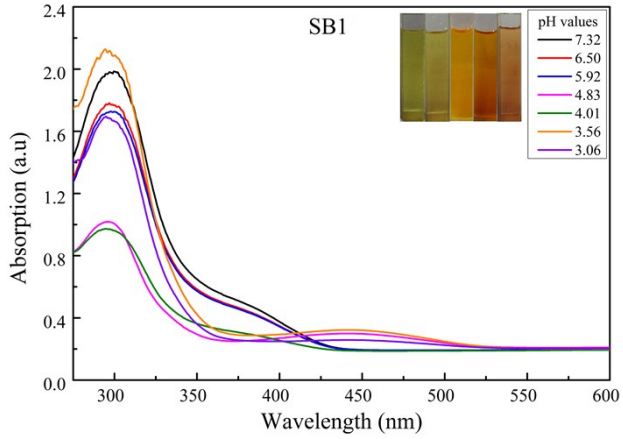
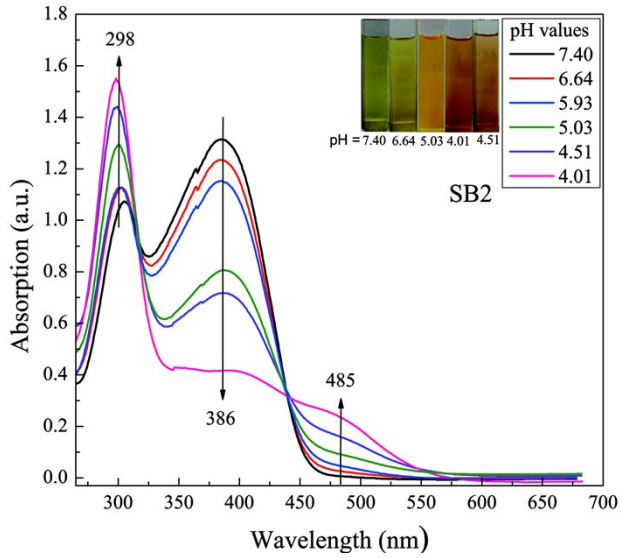
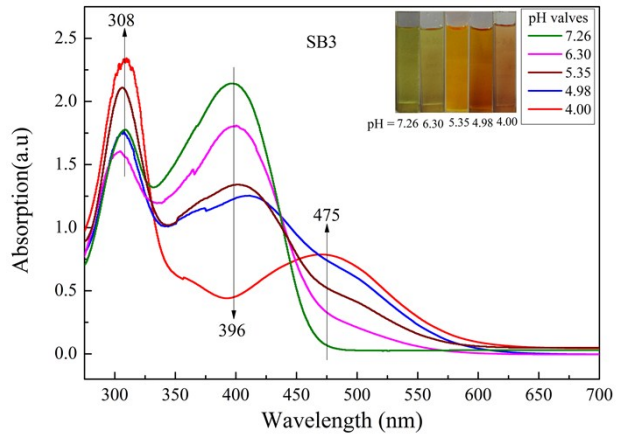
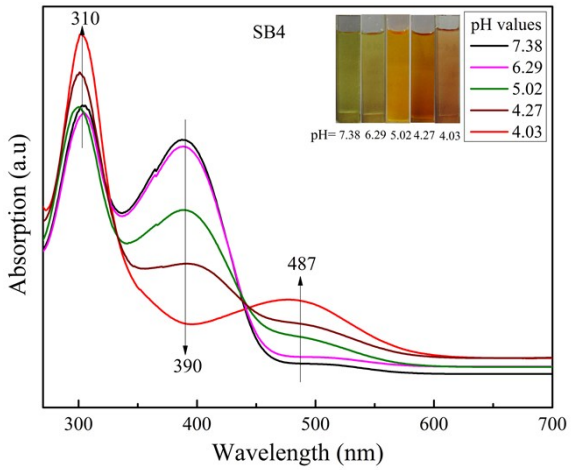


Fig. S1 (a) ^{1}H-NMR, (b) ^{13}C-NMR and (c) aromatic region of the H-H COSY spectrum of SB5 in DMSO-d_6.

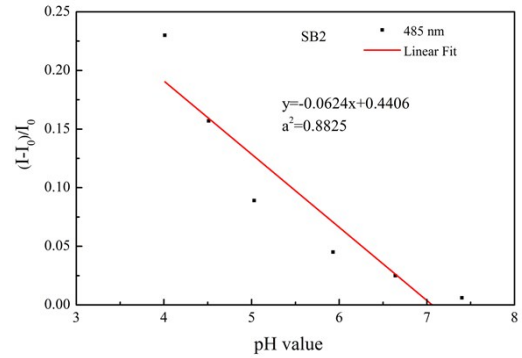

SB1
pH values
7.32
6.50
5.92
4.83
4.01
3.56
3.06
Absorption (a.u)
Wavelength (nm)

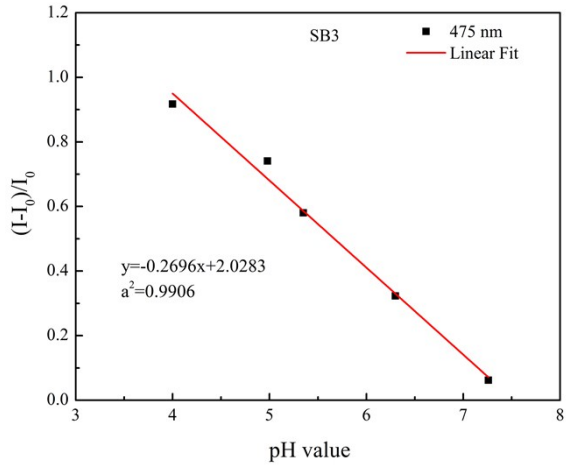

298
386
485
SB2
pH values
7.40
6.64
5.93
5.03
4.51
4.01
pH = 7.40 6.64 5.03 4.01 4.51
Absorption (a.u.)
Wavelength (nm)


308
396
475
SB3
pH valves
7.26
6.30
5.35
4.98
4.00
pH = 7.26 6.30 5.35 4.98 4.00
Absorption(a.u)
Wavelength (nm)



Fi g. S2 Acidochromic absorption change of SB1~SB4.





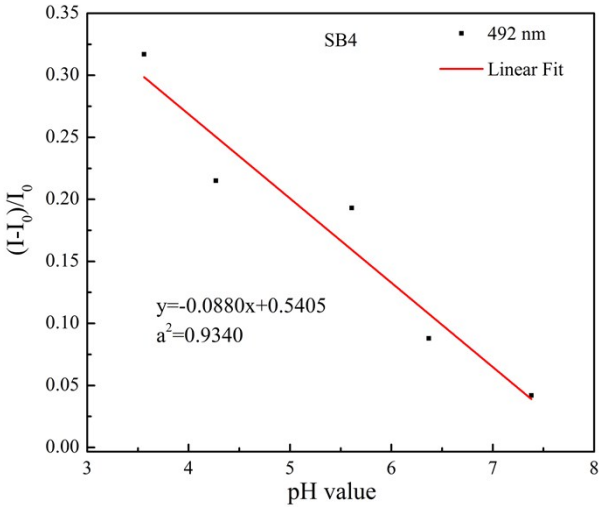
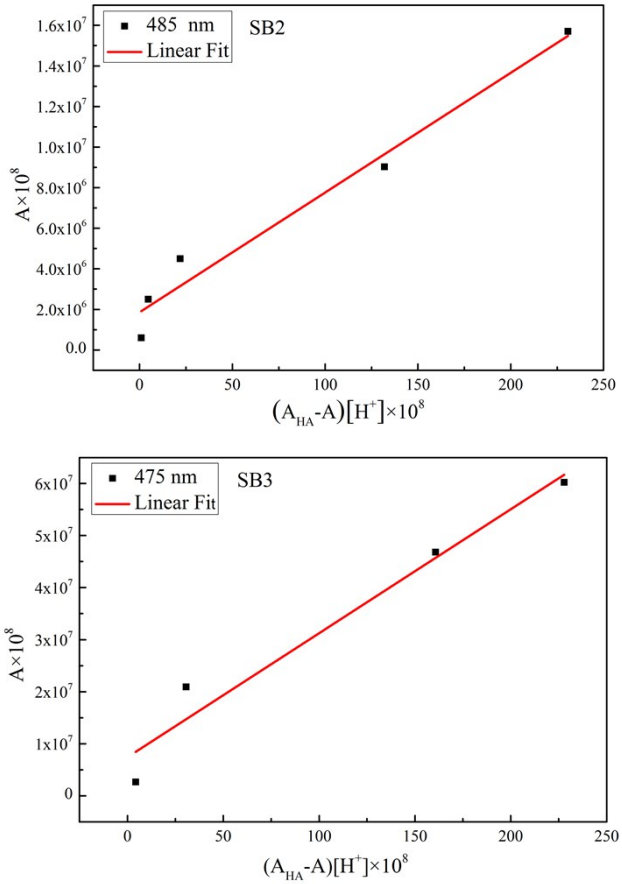


Fig. S3 Relationship between $(I-I_0)/I_0$ and pH value at their new peaks of SB1~SB4.



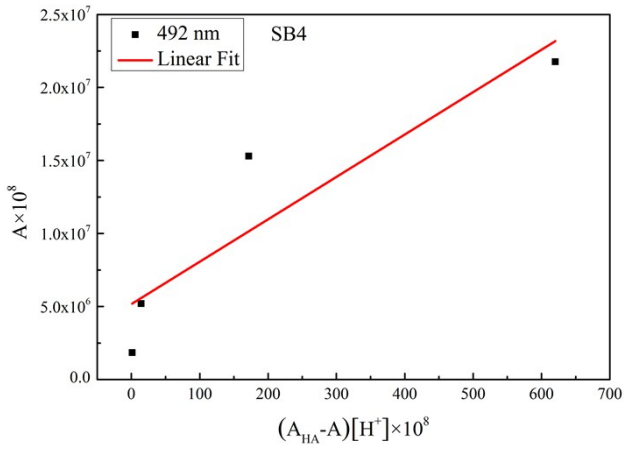
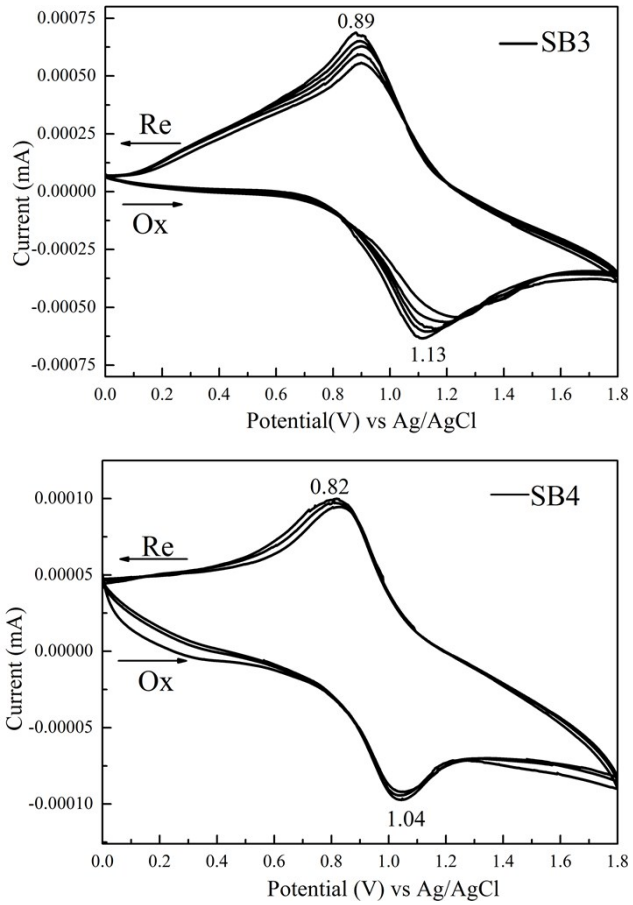


Fig. S4 The relationship between A and $(A_{HA}-A)/[H^+]$ at their new peaks of SB1~SB4.



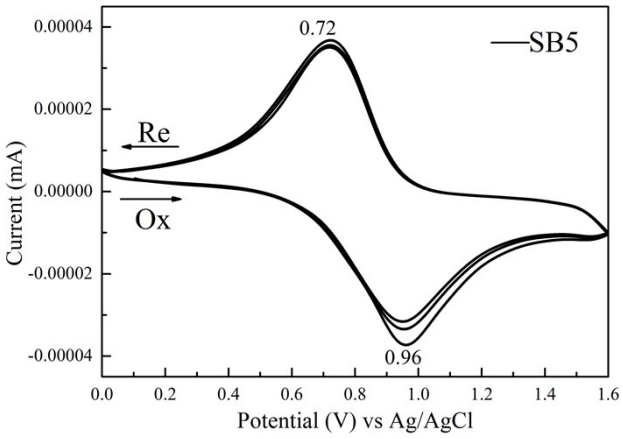
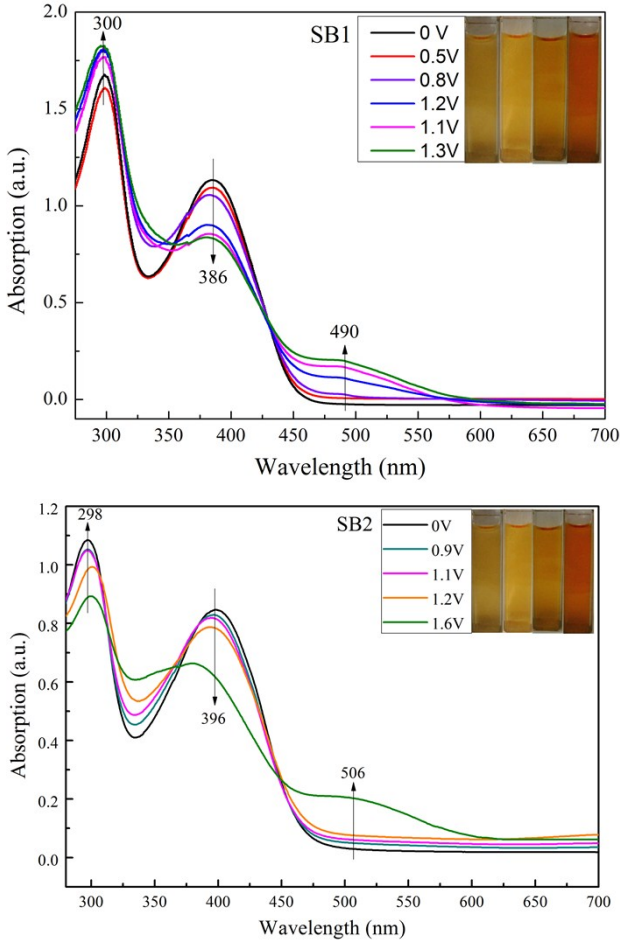


Fig. S5 CV curves of SB3~SB5 in CH_3CN containing 0.1 M $LiClO_4$ at a scan rate of 50 mV·s−1.



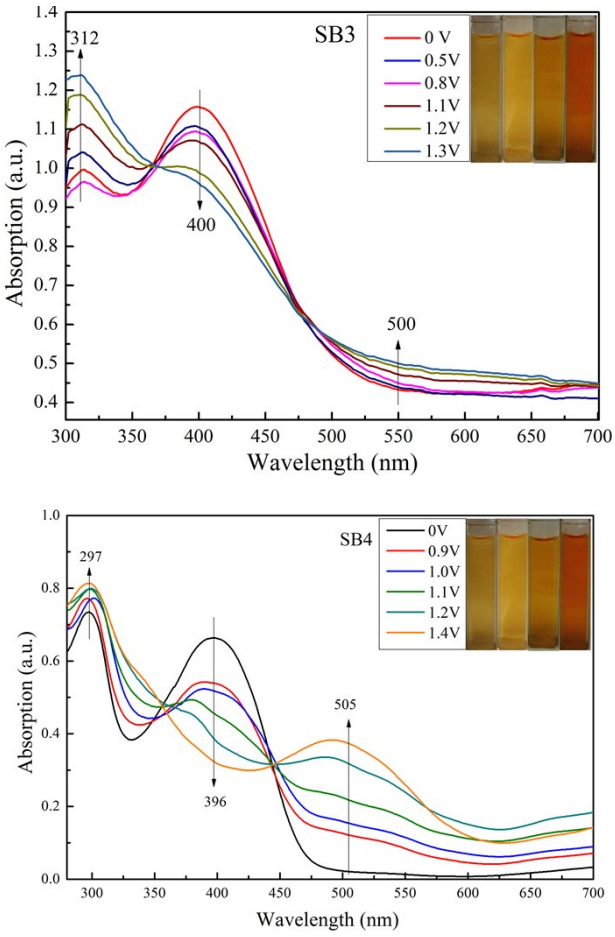


Fig. S6 Electronic absorption change of SB1~SB4 in CH_3CN containing 0.1 M $LiClO_4$ as the supporting electrolyte.

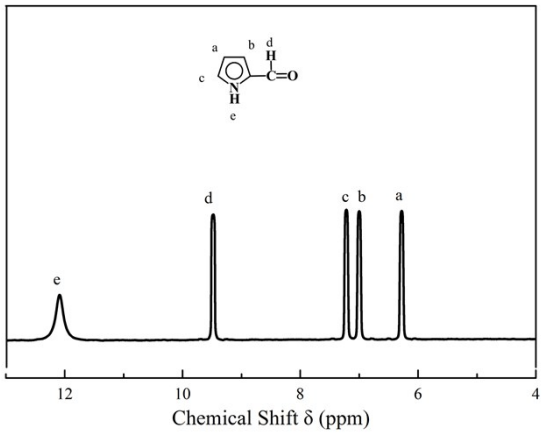


Fig. S7 ^{1}H-NMR spectrum of pyrrole-2-aldehyde.

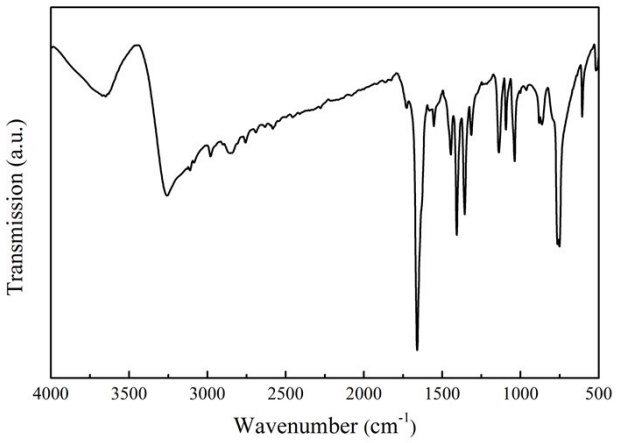
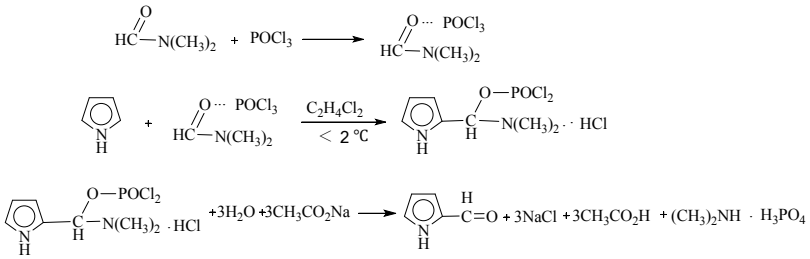


Fig. S8 FT-IR spectrum of pyrrole-2-aldehyde.

The synthesis process of pyrrole-2-aldehyde

6.0 ml (5.6900 g, 0.778 mol) DMF was introduced into a 250-ml three-neck round-bottom flask with stirred in ice salt solution under nitrogen for 15min, 7 ml (11.5000 g, 0.075 mol) $POCl_3$ was added slowly into the equipment, while DMF and $POCl_3$ formed complex, the synthesis routes as shown in Scheme S1. Later the solution was colorless and transparent. 5 ml (4.8011 g, 0.072 mol) pyrrole dissolved in $C_2H_4Cl_2$ (30 ml) were added in dropwise. The mixture was heated with stirring at 90°C under nitrogen for 20 min. Then, the produce was poured into saturated solution of sodium acetate with quickly stirred; the pH value was adjusted by sodium hydroxide solution to near 7. The solution was extracted by diethyl ether to separate the organic phase, and then the organic solvent was removed by rotary evaporation.



Scheme S1. Synthetic route of complex and pyrrole-2-aldehyde