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ChemTech

International Journal of ChemTech Research
CODEN (USA): IJCRGG ISSN: 0974-4290
Vol.8, No.7, pp 172-176, 2015

Efficient green light-emitting diodes based on Substituted triphenylamine derivatives and its structural elucidation

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Abstract: In continuation of our blue light emissive preliminary work, here we report x-ray crystallographic structure of green emissive (OLED) molecule 4,4'-Bis(a-cyano-b-chlorostyr-b-yl)-triphenylamine(CLT,**3**), the structure of compound **3** was well characterized by IR ,NMR and elemental analysis an unambiguously elucidated by x-ray crystallography (**Fig-I** and **Table –II**).

Key words : OLED, Fluorescence ,Triphenylamine, Imidazole.

Introduction

Now a days bright and efficient organic light – emitting devices (OLED) have attracted considerable interest due to their potential application to flat panel display[1,2]. When constructed a light – emitting compounds for OLED devices three main points should be very important : emission color, emission efficiency and device time.In most of the OLED technology, there are two types of compounds : conjugated organic polymers[3-5] and molecular species such as Alq[6,7] . For full-color display applications, efficient blue, green and red emitters with excellent color purity are required. A great effort has been devoted to improve the efficiencies of the electroluminescent (EL) devices through ingenious device configurations, electrode modification and new efficient materials discoveries[8-10]. To a mixture of 4,4'-diformyl triphenylamine **1** and KOH in EtOH was added 4-halophenylacetonitrile under nitrogen atmosphere. The reaction mixture was stirred at room temperature. After the disappearance of the starting material, the separated green color solid was filtered and the crude product was washed with EtOH and recrystallized two times with Chloroform-Methanol (4:1) to give the final compounds **2-4** shown **Scheme-I**

In this paper, we wish to report a x-ray crystallography structure of compound **3** were shown in **Fig I** and **Table –I.**

Experimental

All melting points are uncorrected. IR spectra were recorded on Shimadzu FT-IR 8300 model and BOMEM (Hartmann&Braun). ^{1}H and ^{13}C-NMR spectra were recorded on JEOL GMX 400 MHz,Varian 400 MHz, with CDCl$_3$ and DMSO-d_6 as the solvent with tetramethylsilane as the internal standard. Mass spectra were taken using Hewlett-Packard 5985(70ev), Shimadzu QP 1000A. HRMS(High Resolution Mass Spectra) data were recorded on Thermo Finnigan (Model : MAT 95XL). Absorption and emission measurements were carried out using a Hitachi U-3300 absorption spectrophotometer and a Hitachi F-4500 fluorescence spectrophotometer respectively. The thermal data were carried out using a Seiko SII-EXSTAR 600-DSC-6200 differential scanning calorimeter. The redox potentials of the compound (**2**) were determined by cyclic voltammetry (CV) using an electrochemical analyzer CHI 600A.

Synthesis Part

4,4’-Bis(a-cyano-b-flurostyr-b-yl)-triphenylamine (2)

To a mixture of 4,4’-diformyl triphenylamine **1**[15](0.5g , 0.166mmole) and KOH (0.2 g excess) in 30 ml of dry EtOH was added 4-fluorophenylacetonitrile(0.44g ,0.33 mmole)under nitrogen atmosphere. The reaction mixture was stirred at room temperature. After the disappearance of the starting material, the separated green color solid was filtered and the crude product was washed with EtOH and recrystallized two times with Chloroform-Methanol (4:1) to give the product **2**[16] .

Yield:0.62g (70%) ; m.p:180 -183°C ; IR (KBr):2212,1583,1510,1300,832 Cm^{-1};

^{1}H-NMR(400MHz,$CDCl_3$)d =7.08-7.36(m,15H),7.58-7.63(m,4H),7.77-7.80(d.4H,J=12Hz); ^{13}C-NMR(100MHz,$CDCl_3$)d=164.28,148.74,145.81,

141.20,130.88,130.62,129.87, 127.63, 126.47,125.44,122.97,118.33,116.19, 115.90,107.92.Ms:(m/z%) 535(100),419(10),418(20),417(10),310(5),285(8),267(15). Anal.calcd for

$C_{36}H_{23}N_3F_2$:C,80.73; H,4.32; N,7.84.Found: C,80.64: H,4.42; N,8.17

4,4’-Bis(a-cyano-b-chlorostyr-b-yl)-triphenylamine(3)

Synthesis of compound **3,** was carried out by following the procedure for **2.**

Yield:0.75g(80%) ; m.p:174-176 °C ; IR(KBr):2210,1580,1510,1300,800 Cm^{-1}; UV :l_{max} 492nm ; Flu:l_{max} 520nm(CH_2Cl_2) ; Flu:l_{max}542nm(solid state);

^{1}H-NMR(400MHz,$CDCl_3$)d=7.13-7.40(m,15H),7.56-7.58(m,4H),7.79-7.81(d,4H,J=8.9Hz);^{13}C-MNR (100MHz, $CDCl_3$) d=148.91,145.78,141.54,134.79,

133.29,130.79,129.92,129.20,127.90,126.99,126,56,125.57,122.99,118.13,107.88.

MS:m/z(%) 570(29),569(15),567(5),282(5),261(50); Anal.calcd for $C_{36}H_{23}N_3Cl_2$:C,76.05; H,4.07; N,7.39. Found: C,76.24: H,4.42; N,6.87.

4,4’-Bis(a-cyano-b-bromostyr-b-yl)-triphenylamine (4)

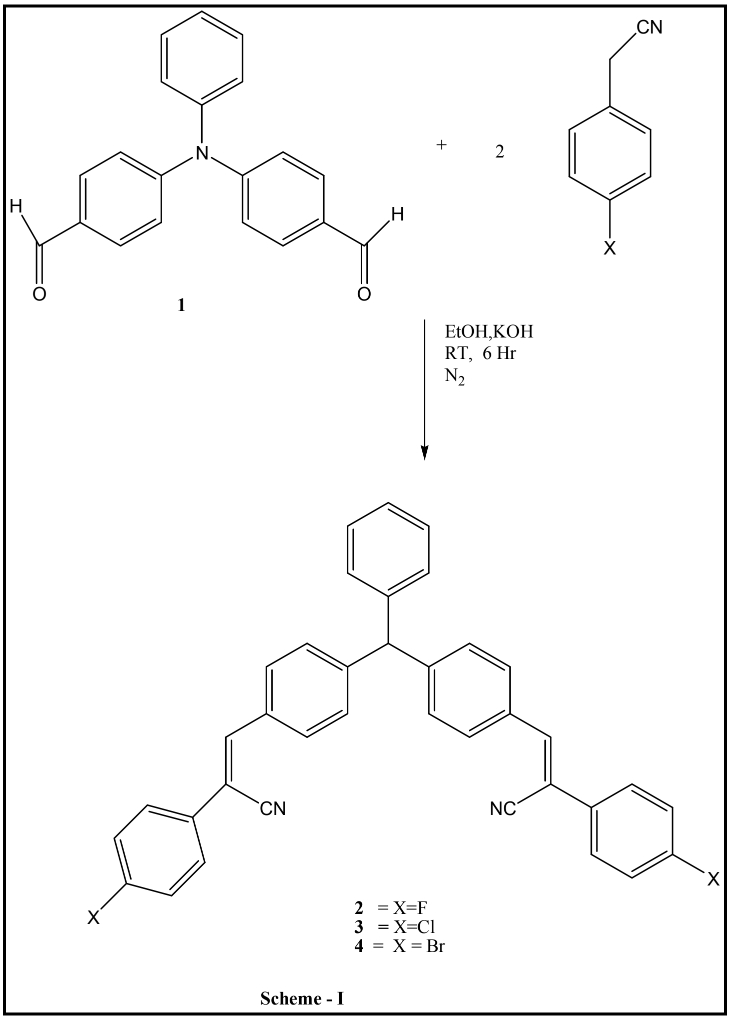
Synthesis of compound **4,** was carried out by following the procedure for **2.**

Yield:0.75g(61%) ; m.p: 187-189 °C ; IR(KBr): 2210,1580,1510,1300,800 Cm^{-1}.

UV :l_{max} 490 nm ; Flu:l_{max} 525nm(CH_2Cl_2); Flu:l_{max}545nm(solid state);^{1}H-NMR(400MHz,$CDCl_3$) d= 7.13-7.40 (m,15H),7.56-7.58 (m,4H),7.78- 7.82(d,4H,J=8.9Hz); ^{13}C-MNR(100MHz,$CDCl_3$) d=147.91,144.78,140.54,134.69,

133.99,130.09,129.12,129.50,127.90,126.19,126,16,124.57,122.19,117.13,107.88;

Anal.calcd for $C_{36}H_{23}N_3Br_2$: C,65.77; H,3.53; N,6.39.Found: C,65.34: H,3.42; N,6.87.



Scheme - I

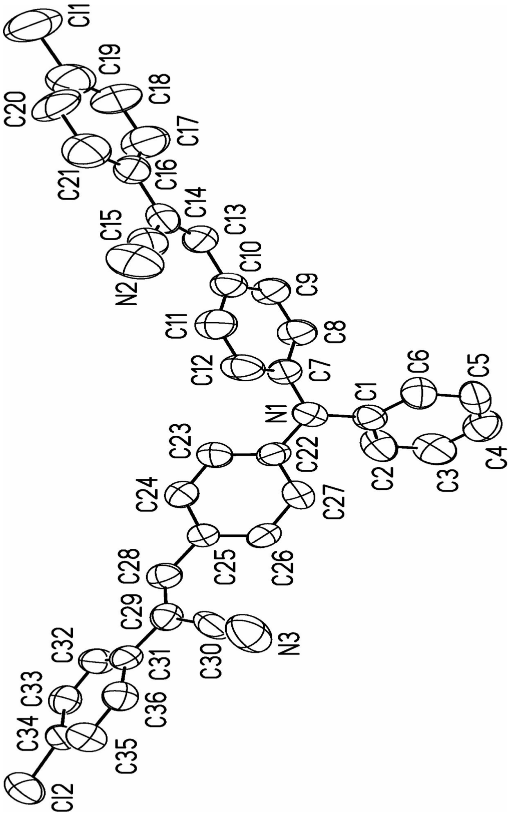


Fig.1 Molecular structure of compound 3 , showing 50% displacement ellipsoids

Table I Crystallographic data for the compound 3

Formula weight	w568.47
Empirical formula	$C_{36} H_{23} Cl_2 N_3$
Crystal system	Monoclinic
Space group	C2/c
a, Å	60.465(4)
b, Å	9.5460(6)
c, Å	28.2074(16)
α, °	90
β, °	117.279(1)
γ, °	90
volume , Å^3	14470.4(15)
Z	20
D_{cal} gcm^{-3}	1.305
μ, mm^{-1}	0.255
T, °C	296(2)K
λÅ	0.71073
number of unique data[1>2σ (1)]	17366
number of variables	925
R_1^a	0.0379
WR_2^a	0.0386
Goodness-of-fit	0.620

Conclusion

To a mixture of 4,4'-diformyl triphenylamine **1** and KOH was added 4-halophenylacetonitrile under nitrogen atmosphere under the refluxing condition, the separated green color solid was filtered and the crude product was washed with EtOH and recrystallized two times with Chloroform-Methanol (4:1) to give the final compounds **2-4** shown **Scheme-I**. In this paper, we wish to report a x-ray crystallography structure of compound **3** were shown in **Fig I** and **Table -I**

Acknowledgement

We thank the National Science Council of the Republic of China for the financial support of this research work, and Prof V.T. Ramakrishnan for generous support for all work.

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