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Synthesis, Structure, and Electroluminescence of BR_2q (R = Et, Ph, 2-Naphthyl and q = 8-Hydroxyquinolato)

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Three 8-hydroxyquinolato (q) boron compounds $B(C_2H_5)_2q$ (**1**), BPh_2q (**2**), and B(2-naph)$_2$q (**3**) have been synthesized by the reaction of 8-hydroxyquinoline with an appropriate BR_3 compound. Compounds **1**−**3** have a tetrahedral geometry as demonstrated by the structure of **1** determined by a single-crystal X-ray diffraction analysis. Compounds **1**−**3** emit a green-blue color at $\lambda_{max} = 495-500$ nm when irradiated by UV light. The electroluminescent (EL) properties of **2** and **3** were examined by fabricating EL devices using **2** and **3** as the light-emitting layer, respectively. The devices of **2** produce a yellow-green light with broad emission spectra, attributed to the formation of an exciplex of **2** with the *N*,*N*′-di-1-naphthyl-*N*,*N*′-diphenylbenzidine (NPB) in the hole transport layer while the intrinsic EL emission of compound **3** was observed. Both **2** and **3** were found to be good electron transport materials in EL devices.

Introduction

Organic and organometallic/coordination luminescent compounds have been playing an important role in organic light-emitting devices (LEDs).[1,2] A typical organic light-emitting device consists of three layers: an electron transport layer, a light-emitting layer, and a hole transport layer, sandwiched between a transparent indium−tin oxide (ITO) anode and a metallic cathode (such as Al, Mg) via vacuum deposition. The most well-known electron transport material used in organic LEDs known to date is Alq_3 in which three 8-hydroxyquinolato (q) ligands chelate to the Al(III) ion in an octahedral environment.[3] Additionally, Alq_3 is also a good green emitter in organic LEDs. In a recent study on blue luminescent materials based on 7-azaindole, we revealed that boron compounds in general are more stable than the corresponding aluminum compounds.[4] Our investigation on boron chelate compounds with 8-hydroxyquinoline was therefore motivated by their potential application as electron transport materials in organic LEDs. In this report, the synthesis, structure, and electroluminescent properties of three 8-hydroxyquinolinlato compounds of boron are presented.

Experimental Section

All syntheses were carried out under a nitrogen atmosphere. Solvents were freshly distilled over appropriate drying agents prior to use. 8-Hydroxyquinoline, $B(C_2H_5)_3$, BPh_3, BBr_3, and 2-bromonaphthalene were purchased from Aldrich Chemical Co. NMR spectra were recorded on a Bruker AM 400 spectrometer. Elemental analyses were performed by Canadian Microanalytical Service, Delta, British Columbia. Excitation and emission spectra were recorded on a Photon Technologies International QM1 spectrometer. Mass spectra were recorded on a Fisons V6 Quattro spectrometer using EI methods. Elemental analyses were performed by Canadian Microanalytical Service, Ltd., Delta, British Columibia.

Synthesis of $B(C_2H_5)_2q$ (1). 8-Hydroxyquinoline (0.580 g, 4 mmol) was dissolved in 20 mL of tetrahydrofuran (THF). Triethylborane (4 mL, 4 mmol, 1.0 M in hexanes) was then added. The solution became yellow immediately with green luminescence and was stirred for 5 h at 25 °C. The solution mixture was concentrated by vacuum to about 5 mL and separated by silica gel thin layer chromatography (TLC) plates using a solvent mixture of hexane/ethyl acetate in a 1:0.2 ratio. The product was collected by washing the silica gel using CH_2Cl_2. The solution was concentrated by vacuum. After a few

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days standing, yellow thin plate crystals of **1** formed in 28% yield with mp 43 °C. ^{1}H NMR ($CDCl_3$, ppm, 298 K): δ 8.28 (d, $^3J = 8.0$ Hz, 1H), 8.24 (d, $^3J = 4.4$ Hz, 1H), 7.52−7.57 (m, 2H), 7.10 (d, $^3J = 8.4$ Hz, 1H), 6.96 (d, $^3J = 8.0$ Hz, 1H), 0.71−0.78 (m, 4H, ethyl), 0.65 (t, $^3J = 7.2$ Hz, 6H, ethyl). ^{13}C NMR ($CDCl_3$, ppm, 298 K): δ 137.66, 132.78, 128.46, 122.45, 111.07, 108.56, 15.33 (ethyl), 8.34 (ethyl) (the peaks due to 8-hydroxyquinline are not specified.). MS: $m/z = 213.1$ (M^+). Elemental analysis for compound **1** was not performed because its low melting point and high volatility (sublimes at ambient temperature and 1 atm) makes it difficult to obtain satisfactory results.

Synthesis of BPh_2q (2). 8-Hydroxyquinoline (0.871 g, 6 mmol) was dissolved in 20 mL of CH_2Cl_2. Triphenylborane (1.452 g, 6 mmol) was added in the above stirred solution. The solution became yellow with green luminescence after being stirred for a few minutes. The solution was stirred for 5 h at 25 °C. The reaction mixture was concentrated by vacuum. Precipitation occurred after 5 mL of hexanes was added to the solution. The mixture was filtered, and the solid residue was sublimed under vacuum (0.1 mmHg) at 100 °C to remove the starting materials. A yellow powder of compound **2** was obtained in the bottom of the sublimer in 75% yield with mp 205 °C. ^{1}H NMR ($CDCl_3$, ppm, 298 K): δ 8.55 (d, $^3J = 4.4$ Hz, 1H), 8.36 (d, $^3J = 7.5$ Hz, 1H), 7.62 (t, $^3J = 8.1$ Hz, 1H), 7.58 (t, $^3J = 5.1$ Hz, 1H), 7.42 (dd, $^3J = 6.4$ Hz, $^4J = 1.4$ Hz, 4H, Ph), 7.26 (d, $^3J = 1.9$ Hz, 1H), 7.22 (m, 6H, Ph), 7.15 (d, $^3J = 7.7$ Hz, 1H). ^{13}C NMR ($CDCl_3$, ppm, 298 K): δ 139.29, 138.75, 132.94, 131.99 (Ph), 127.55 (Ph), 126.99 (Ph), 122.80, 112.13, 109.70. MS: $m/z = 309.2$ (M^+). Elem. anal. Calcd for $C_{21}H_{16}NOB/0.15CH_2Cl_2$ (compound **2** cocrystallizes with CH_2Cl_2; the vacuum-dried sample used for elemental analysis appears to contain 15% CH_2Cl_2.): C, 78.84; H, 5.06; N, 4.34. Found: C, 79.02; H, 4.98; N, 4.12.

Synthesis of B(2-Naph)$_2$q (3). To the solution of 0.219 g (9.0 mmol) of Mg in 40 mL of THF was added 1.8634 g (9.0 mmol) of 2-bromonaphthalene in 20 mL of THF slowly in1 h at 25 °C. After being stirred for 10 h, the solution became dark and all Mg disappeared. BBr_3 (3.0 mL, 3.0 mmol, 1.0 M in hexane) was then added. Upon addition of BBr_3 the mixture became a brown color. The solution was evaporated to dryness under vacuum, and 40 mL of toluene was added to extract the product. After filtration, the solution was concentrated by vacuum and 0.436 g of (3 mmol) of 8-hydroxyquinoline was added. The reaction mixture became yellow immediately with green luminescence. After being stirred for 4 h, the reaction mixture was concentrated under vacuum. After standing for a few days, yellow crystals of compound **3** were obtained in 56% yield with mp 214 °C. ^{1}H NMR ($CDCl_3$, ppm, 298 K): δ 8.68 (d, $^3J = 3.3$ Hz, 1H), 8.44 (d, $^3J = 7.2$ Hz, 1H), 7.90 (s, 2H, naph), 7.64−7.75 (m, 8H, quinoline and naph), 7.60 (d, $^3J = 6.3$ Hz, 1H), 7.36−7.39 (m, 4H, naph), 7.21−7.29 (m, 2H, naph), 7.16 (d, $^3J = 7.2$ Hz, 1H). ^{13}C NMR ($CDCl_3$, ppm, 298 K): δ 139.48, 138.92, 133.33, 133.04 (naph), 131.29 (naph), 130.12 (naph), 128.04 (naph), 127.57 (naph), 126.89 (naph), 125.32 (naph), 122.80, 112.39, 109.95. MS: $m/z = 409.3$ (M^+). Elem. anal. Calcd for $C_{29}H_{20}NOB$ C, 85.12; H, 4.89; N, 3.42. Found: C, 83.43; H, 4.93; N, 3.29. This sample from a different batch of syntheses (crsytals and sublimed powders) was analyzed twice and consistently showed the low carbon content. The cause of it is unknown to us.

X-ray Crystallography Analysis. The single crystal of **1** obtained from THF/hexane solution was mounted on a brass pin, and the data were collected on a Siemens SMART CCD diffractometer with graphite-monochromated Mo Kα radiation operated at 50 kV and 35 mA at −100 °C over the 2θ range of 3.4−46.6°. No significant decay was observed during the data collection. Data were processed on a Pentium PC using Siemens SHELXTL software package (version 5.0).[5] The crystal belongs to an orthorhombic space group, *Pbca*, uniquely determined by systematic absences. The structure was solved by direct methods. All non-hydrogen atoms were refined anisotropically. The positions of hydrogen atoms were calculated, and their contributions in structural factor calculations were included. The crystal data are summarized in Table 1. Selected bond lengths and angles are given in Table 2.

Table 1. Crystallographic Data of 1

formula	$C_{13}H_{16}NOB$
fw	213.1
space group	*Pbca*
a/Å	13.248(3)
b/Å	7.782(2)
c/Å	23.206(5)
V/Å^3	2392.3(9)
Z	8
D_c/(g cm^{-3})	1.183
μ/cm^{-1}	0.73
$2\theta_{max}$/deg	46.6
reflns measd	10199
reflns used (R_{int})	1733 (0.146)
no. of variables	209
final R [$I > 2\sigma(I)$]	$R_1{}^a = 0.0732$, $R_{w2}{}^b = 0.1427$
R (all data)	$R_1 = 0.1249$, $R_{w2} = 0.1642$
goodness-of-fit on F^2	1.015

[a] $R_1 = \sum|F_o| - |F_c|/\sum|F_o|$ [b] $R_{w2} = [\sum w[(F_o{}^2 - F_c{}^2)^2]/\sum[w(F_o{}^2)^2]]^{1/2}$. $w = 1/[\sigma^2(F_o{}^2) + (0.075P)^2]$, where $P = [\max(F_o{}^2,0) + 2F_c{}^2]/3$.

Table 2. Selected Bond Lengths (Å) and Angles (°) for 1

O(1)−C(1)	1.337(4)	N(1)−B(1)	1.636(5)
O(1)−B(1)	1.543(5)	B(1)−C(12)	1.585(6)
N(1)−C(8)	1.338(5)	B(1)−C(10)	1.589(7)
N(1)−C(9)	1.347(4)		
C(1)−O(1)−B(1)	111.8(3)	O(1)−B(1)−C(10)	110.8(3)
C(8)−N(1)−C(9)	118.7(3)	C(12)−B(1)−C(10)	118.1(4)
C(8)−N(1)−B(1)	132.4(3)	O(1)−B(1)−N(1)	97.0(3)
C(9)−N(1)−B(1)	108.9(3)	C(12)−B(1)−N(1)	108.6(3)
O(1)−B(1)−C(12)	110.9(3)	C(10)−B(1)−N(1)	109.3(3)

Fabrication of Electroluminescent Devices. The EL devices using **2** as the emitting layer were fabricated on an indium−tin oxide (ITO) substrate, which was cleaned by an ultraviolet ozone cleaner immediately before use. Organic layers and a metal cathode composed of magnesium silver alloy ($Mg_{0.9}Ag_{0.1}$) were deposited on the substrate by conventional vapor vacuum deposition. Prior to the deposition, all the organic materials were purified via a train sublimation method.[6] *N*,*N*′-Di-1-naphthyl-*N*,*N*′-diphenylbenzidine (NPB) doped with 1% of 9,10-diphenylanthracence (DPA) was employed as the hole transport layer in all devices. The device structures and the thickness of each layer are listed in Table 3. To obtain the photoluminescence (PL) spectra, a thin film (100 nm) deposited on a quartz substrate was measured with a fluorescence spectrophotometer. The current/voltage characteristics were measured using a Keithley 238 current/voltage unit. The light intensity of the EL device was measured by a Minolta Chroma meter CS100. The EL spectrum was obtained by an in-house setup made up of a series of electronic components including a monochromator (Instruments SA Inc), a photomultiplier tube, and a photon counter. The device structure for **3** consists of 30 nm of TPD (*N*, *N*′-diphenyl-*N*,*N*′-bis(3-methylphenyl)-1,1′-biphenyl-4,4′-diamine) as a hole transport layer, 30 nm of **3** as an emissive layer, 10 nm of PBD (2-(4-biphenylyl)-5-(4-*tert*-butylphenyl)-1,3−4 oxadiazole) as the hole blocking layer, and thermally evaporated calcium (60 nm) and aluminum (120 nm) layers as a cathode. The active device area of **3** is 1.0 × 5.0 mm^2. The EL spectra and the luminance for the device of **3** were measured by using a Photo Research-650 SpectraColorimeter. PL measurements of **3** were carried out on thermally evaporated thin films using a Fluorolog-3 fluorescence spectrometer (ISA Jobin Yvon-SPEX).

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Table 3. Properties of EL Devices for Compound 2 at 25 mA/cm^2

					efficiency		
device structure	thickness, nm	luminance, cd/m^2	λ_{max}/nm	voltage/V	int QE/%	lum/W	cd/A
A: NPB:DPA/BPh$_2$q	75/75	80	565	12.4	0.69	0.08	0.32
B: NPB:DPA/BPh$_2$q/Alq$_3$	75/75/10	100	575	12.3	1.24	0.1	0.40
C: NPB:DPA/Alq$_3$	75/75	783	540	8.8	11.5	1.12	3.13
D: NPB:DPA/Alq$_3$/BPh$_2$q	75/75/10	501	550	10.6	7.0	0.59	2.0

Results and Discussion

Synthesis and Structure. Three boron compounds, B(C$_2$H$_5$)$_2$q (**1**), BPh$_2$q (**2**), and B(2-naph)$_2$q (**3**) were obtained readily from the reaction of 8-hydroxyquinoline with the corresponding BR$_3$. For compounds **1** and **2**, the starting materials can be obtained from commercial sources. For compound **3**, the starting material B(2-naph)$_3$ was synthesized by first making 2-naph−Mg−Br via a Grignard reaction of magnesium metal with 2-boromonaphthalene in THF, and the subsequent reaction of 2-naph−Mg−Br with BBr$_3$ in a 3:1 ratio. An alternative approach for the synthesis of compound **2** where tetraphenyldiboroxide is reacted with 8-hydroxyquinoline was reported by Hohaus and Umland.[7] All three compounds have a bright yellow-green color and are stable under air. Compound **1** is very soluble in solvents such as dichloromethane and hexanes with a very low melting point (45 °C) and sublimes readily. In contrast, compounds **2** and **3** have a melting point above 200 °C but can also be sublimed under vacuum. The free 8-hydroxyquinoline ligand has a melting point of 76 °C. The low melting point of compound **1** could be attributed to the following: (1) the lack of intermolecular hydrogen bonds in **1** which are present in the free ligand in the solid state; (2) poor packing of molecules of **1** in the solid state. Point 2 could also explain the dramatic increase of melting points of compounds **2** and **3**, in comparison to that of **1**. The aromatic phenyl and 2-naphthyl groups in compounds **2** and **3** likely increase the melting point of the compound by enhancing intermolecular interaction via weak intermolecular $\pi-\pi$ interactions, thus improving the packing of the molecules in the solid state. To further understand the low melting point of compound **1**, we examined the crystal structure of **1** by a single-crystal X-ray diffraction analysis. Attempts to grow single crystals of **2** and **3** suitable for X-ray diffraction studies were unsuccessful.

As shown in Figure 1, compound **1** has a tetrahedral structure, typical of boron compounds. The B−N and B−C bond lengths are similar to those reported previously.[8,9] Unit cell packing diagrams given in Figure 2 show that compound **1** has a chain arrangement in the solid state. Within each chain, there is a π stacking interaction between two 8-hydroxyquinolinato ligands of two neighboring molecules with an averaged atomic separation distance of ~3.6 Å. The π stacking interaction is, however, localized between two molecules. The low melting point of **1** can therefore be attributed to the lack of extended π stacking interactions in the solid state.

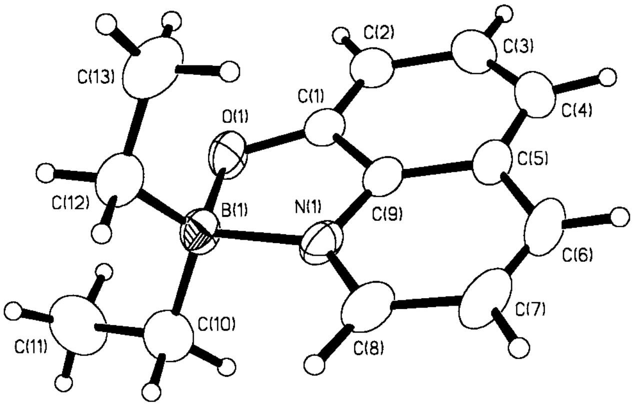

Figure 1. Diagram showing the molecular structure of **1** with labeling scheme and 50% thermal ellipsoids.

Photoluminescent and Electroluminescent Properties[10] of 1−3. Compounds **1**−**3** exhibit a bright blue-green luminescence in solution and the solid state with the emission maxima for the three compounds at the solid-state being at 498, 495, and 500 nm, respectively. In comparison to that of Alq$_3$, compounds **1**−**3** have a blue shift in emission energy.

The electroluminescent properties of compounds **2** and **3** were investigated (the EL properties of compound **1** were not studied because of its low melting point.). For compound **2**, two EL devices (**A** and **B**) were fabricated. Compound **2** in device **A** serves as both emitter and the electron transport layer, while in device **B**, where an Alq$_3$ electron transport layer was added, it functions only as the emitter. In all devices, NPB doped with 1% DPA was used as the hole transport layer (the doping is to minimize the degradation of the hole transport layer, a strategy commonly used in EL device fabrication[2e,4a]). The size of the EL cell is 8 mm^2. More detailed device structures are shown in Table 3. Their EL performance characteristics were examined in comparison with a control device based on Alq$_3$ (device **C**). Both devices **A** and **B** displayed similar EL spectra, as shown in Figure 3, indicating that the light emission originates from the same emitter species. In comparison with the PL of compound **2**, however, the EL spectra of **A** and **B** exhibit very broad emission bands and a large red shift with a peak at about 570 nm. The EL spectra of **A** and **B** also do not match the PL spectrum of the hole transport layer (NPB:1%DPA). It is therefore believed that the EL emissions of both devices originate from an exciplex between compound **2** and NPB in the

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(10) We learned recently that a British research team reported their investigation on the EL properties of BPh$_2$q, prepared by methods described in ref 7: Anderson, S.; Hudson, A. J.; Weaver, M. S. *The 2nd International Conference on Electroluminescence from Molecular Materials and Related Phenomena*; Sheffield, U.K.; May 1999; Elsevier: New York, 1999; Abstract P-90.

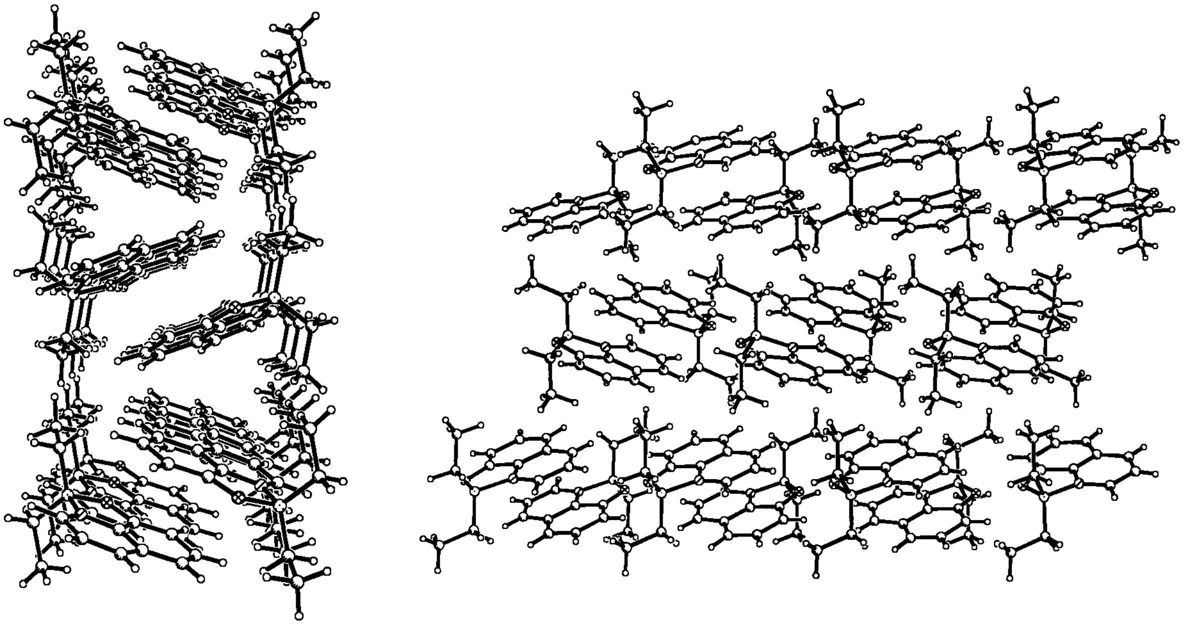

Figure 2. Packing diagram showing the intermolecular interaction of **1** in the solid state: left, a side view; right, a front view.

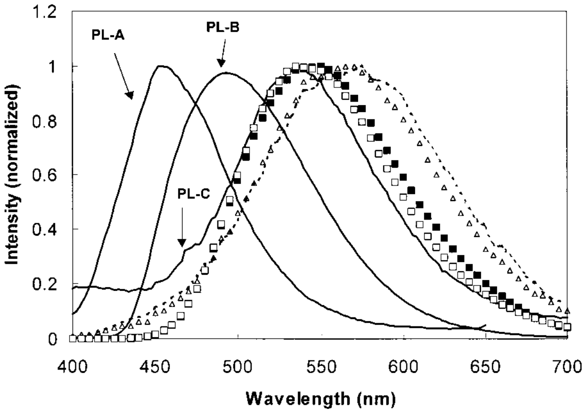

Figure 3. PL spectra (solid lines) of films: NPB:1% DPA (PL-A), BPh_2q (PL-B), and 50% NPB:50% BPh_2q (PL-C); EL spectra of device **A** (triangle), device **B** (dashed line), device **C** (solid square), and device **D** (empty square).

hole transport layer. An exciplex is a transient donor–acceptor complex between the excited state of the donor and the ground state of the acceptor.[11] A few examples of exciplex emissions in electroluminescent devices have been reported previously.[12] The dramatic red shift of emission energy of devices **A** and **B** in comparison to that of the PL emission of BPh_2q ($\lambda_{max} = 495$ nm, Figure 3) implies that the HOMO level of the NPB:1% DPA layer must be higher than that of the BPh_2q layer. The PL spectrum (Figure 3) of a film containing 50% NPB and 50% compound **2** obtained by vacuum co-deposition matches approximately the EL spectrum of the device, confirming that the exciplex formation is indeed between the NPB layer and compound **2**. The fact that device **A** produces a similar EL emission despite the absence of the Alq_3 electron transport layer suggests that in addition to forming an exciplex with the hole transport layer, compound **2** can also function as an electron transport material in EL devices.

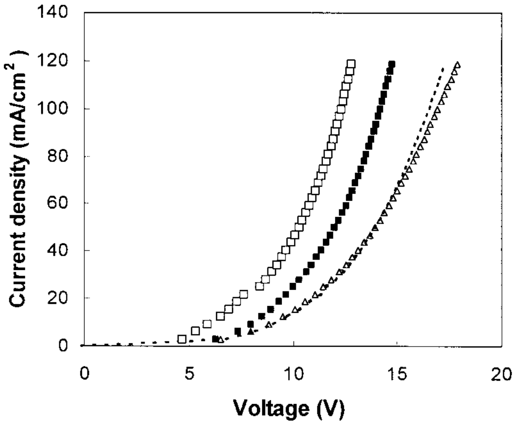

Figure 4. $J-V$ characteristics of devices **A** (triangle), **B** (dashed line), **C** (solid square), and **D** (empty square).

Figure 4 shows the current/voltage ($J-V$) plots of the EL devices. Interestingly, device **A** displays $J-V$ characteristics very similar to those of device **B** which contains an Alq_3 electron transport layer, suggesting that compound **2** functions as an excellent electron transport material. To further establish the electron transport properties of compound **2**, device **D** with compound **2** as the electron transport layer and Alq_3 as the light emitting layer was fabricated. This device provides green light similar to device **C** with an emission peak at 550 nm, attributable to the intrinsic emission of Alq_3, further supporting that compound **2** can indeed function as an electron transport material. Figure 5 provides the luminance/current ($J-L$) plots for all devices. Likewise, devices **A** and **B** show very similar $J-L$ characteristics. The EL performance is poorer than that of devices **C** and **D**. The numerical data of device efficiency for all four devices are summarized in Table 3. The poor efficiency of devices **A** and **B** could be attributed to the formation of an exciplex in these devices. In fact, a similar effect of an exciplex emission

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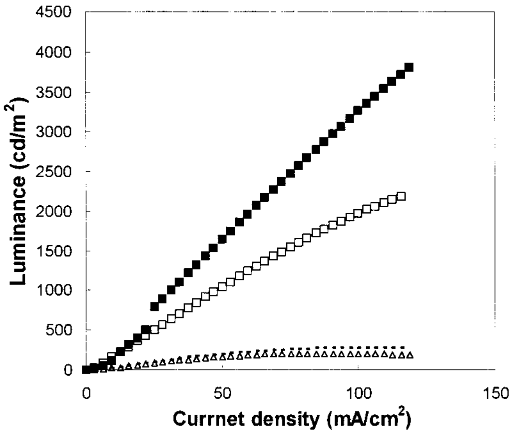

Figure 5. *J*−*L* characteristics of devices **A** (triangle), **B** (dashed line), **C** (solid square), and **D** (empty square).

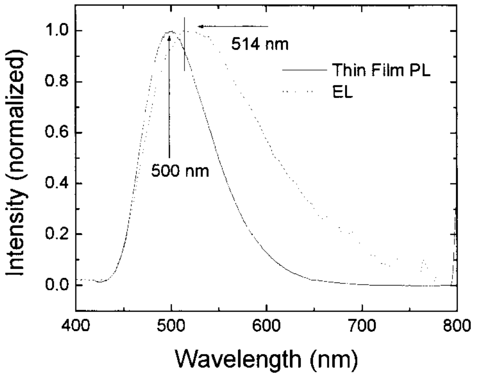

Figure 6. PL and EL spectra of compound **3**.

on the EL quantum efficiency has been observed by Adachi and co-workers.[13] Attempts to achieve the intrinsic EL emission of compound **2** were unsuccessful. The intrinsic EL emission from compound **3** was, however, observed when an EL device structure using TPD as the hole transporting layer and compound **3** as the emitting layer/electron transporting layer was constructed. The PL and EL spectra of compound **3** shown in Figure 6 confirmed that the observed EL of the device is indeed from compound **3**. The *J*−*V* and *L*−*V* curves for the device of compound **3** are shown in Figures 7 and 8, respectively. Further investigation on the performance of compound **3** in EL devices is currently being conducted in our laboratory, and the results will be described in a subsequent report.

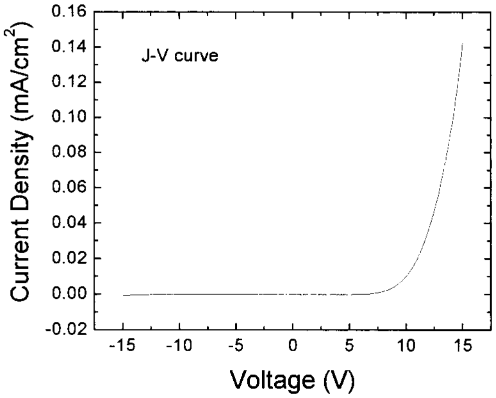

Figure 7. *J*−*V* curve of the EL device of **3**.

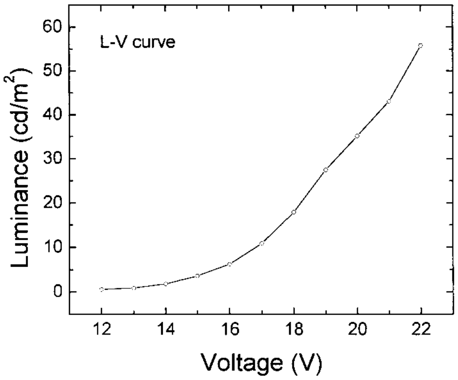

Figure 8. *L*−*V* curve of the EL device of **3**.

Conclusion

8-Hydroxyquinoline boron complexes have been synthesized for EL applications. These boron compounds provide bright green-blue photoluminescence. The replacement of an aliphatic group by an aromatic group in the complex significantly increases the melting point of the compound, due to perhaps the increased intermolecular interactions in the solid state. EL devices based on BPh_2q and $B(2\text{-naph})_2q$ were fabricated. The devices with **2** as the emitter produced an exciplex emission originating from the hole transporting layer and compound **2**. The attempts to obtain the intrinsic EL emission of compound **2** were unsuccessful. The intrinsic EL emission from compound **3** was observed when TPD was used as the hole transporting layer. In addition to being promising emitters, the new boron compounds were found to possess excellent electron transport properties. Therefore, further study of these boron compounds may lead to a new class of electron transport materials for organic LEDs.

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[13] Tamoto, N.; Adachi, C.; Nagai, K. *Chem. Mater.* **1997**, *9*, 1077.