**Electronic Supplementary Information**

# Carbazolyl-contained phenol-pyridyl boron complexes: syntheses, structures, photoluminescent and electroluminescent properties

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**Content**

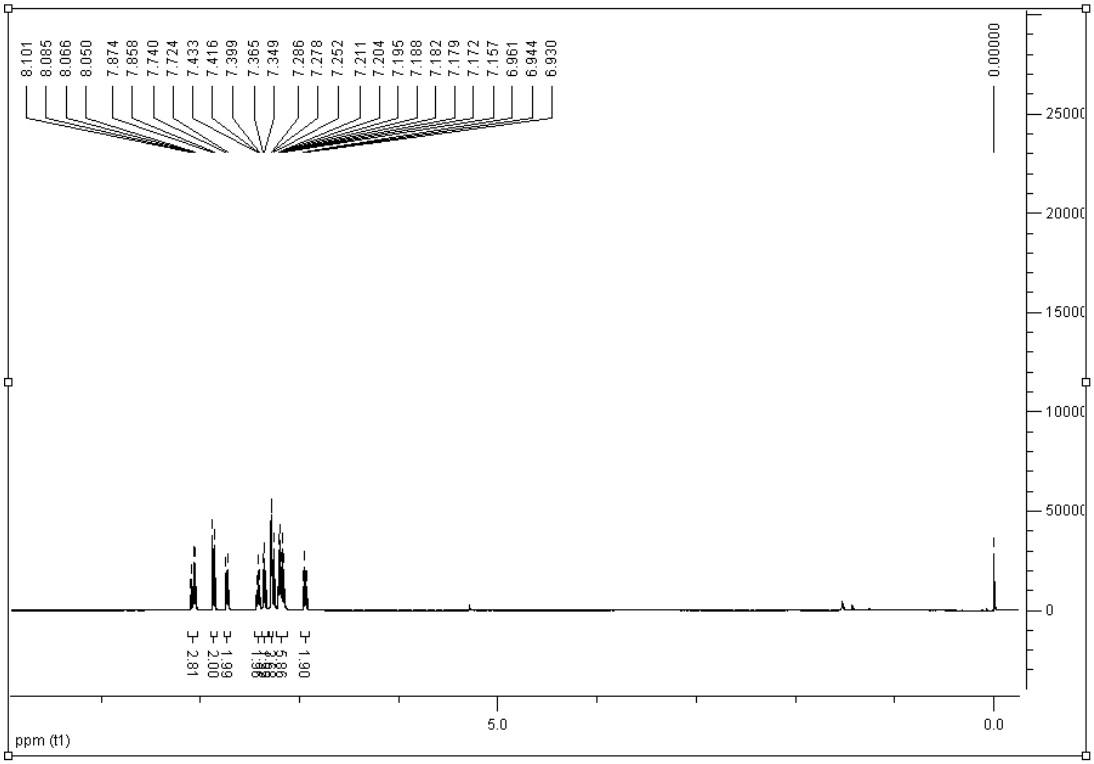


**Fig. S1** $^{1}$H NMR spectrum of complex **1**.

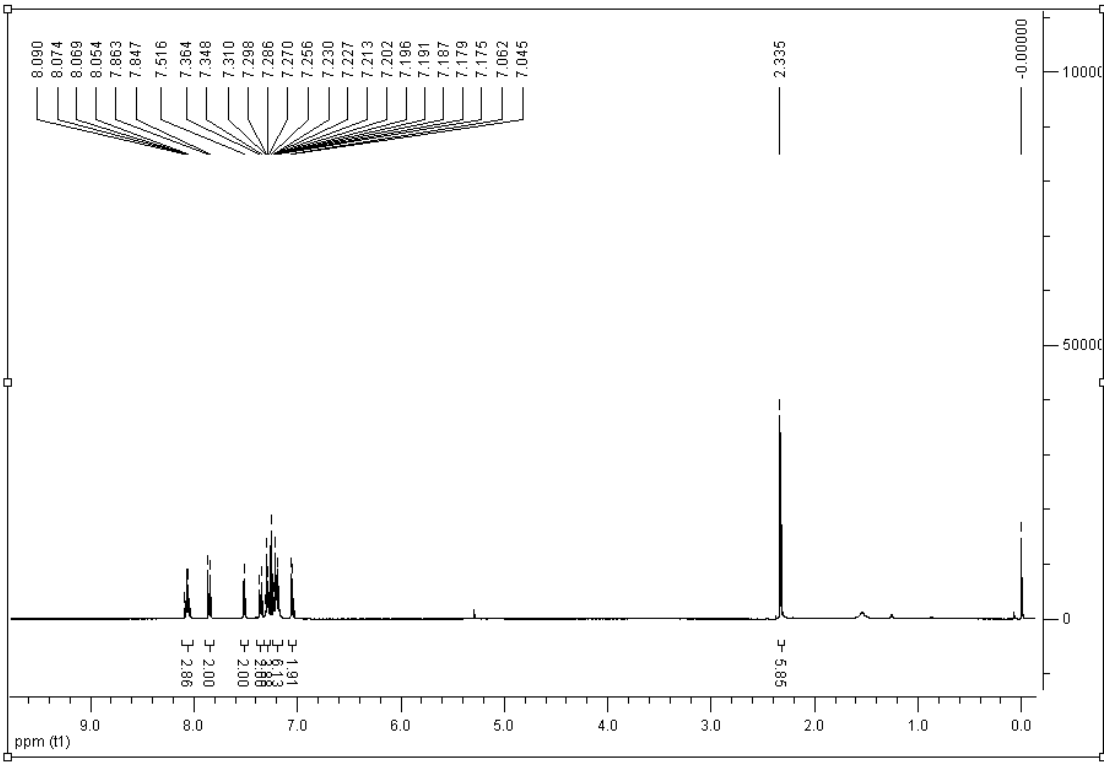


**Fig. S2** $^{1}$H NMR spectrum of complex **2**.

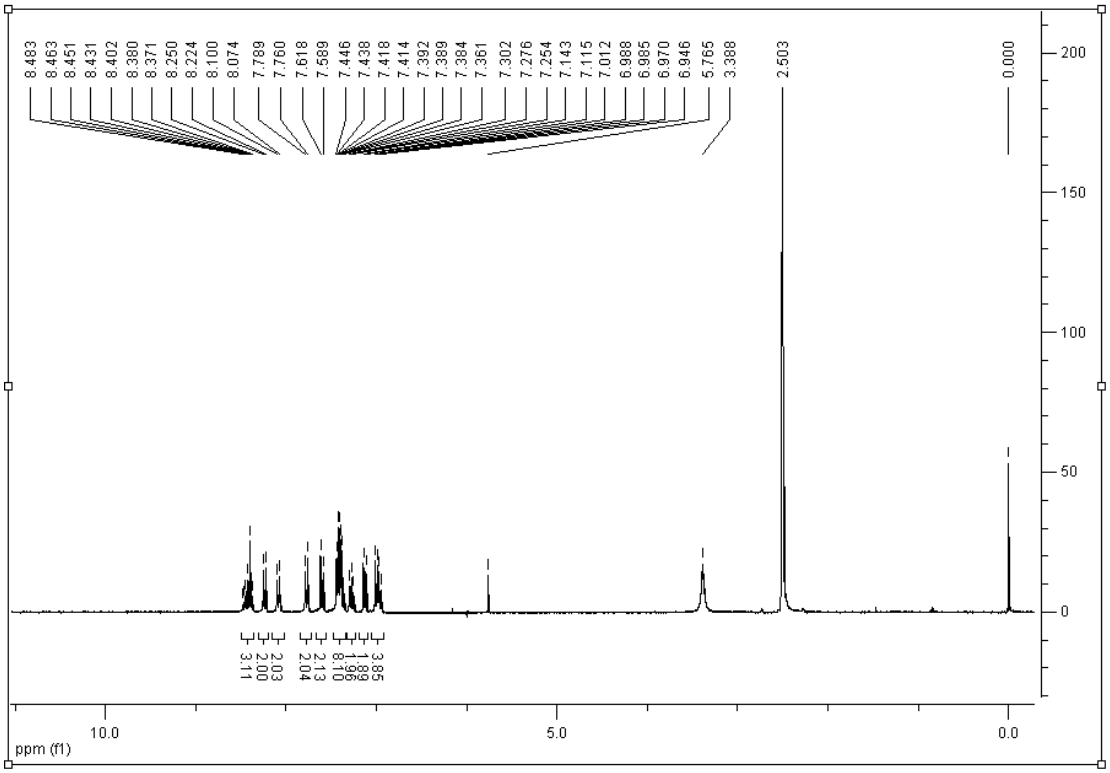


**Fig. S3** $^{1}$H NMR spectrum of complex **3**.

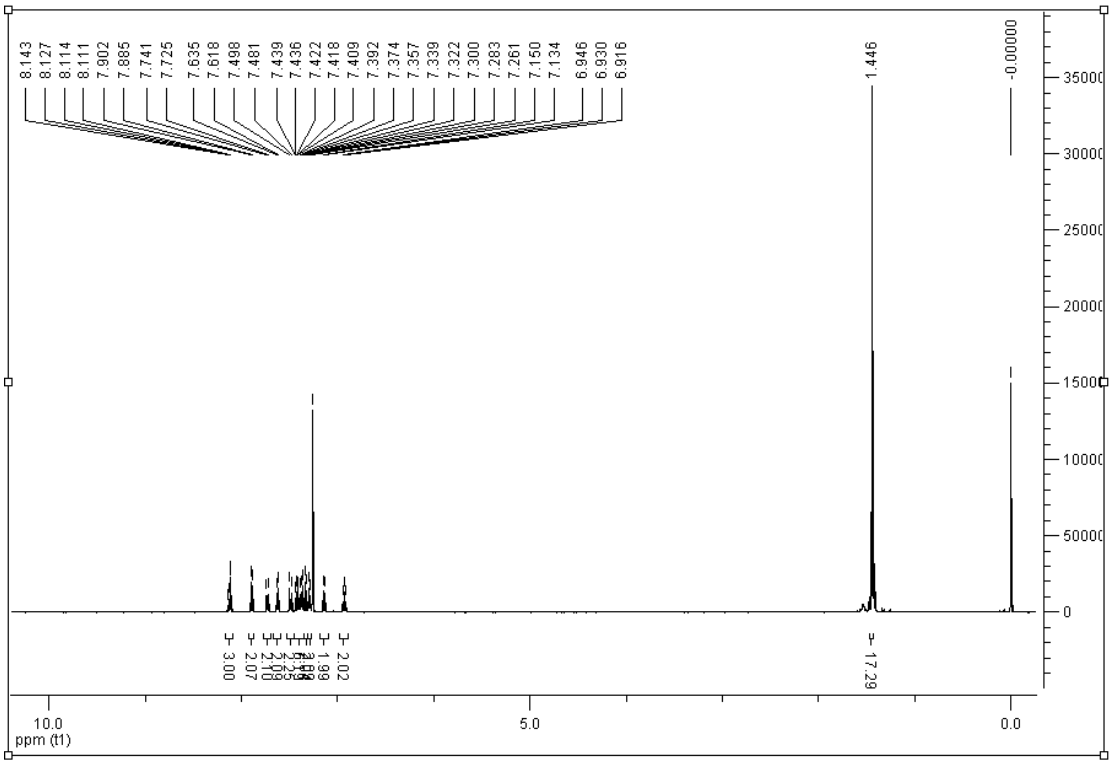


**Fig. S4** $^{1}$H NMR spectrum of complex **4**.

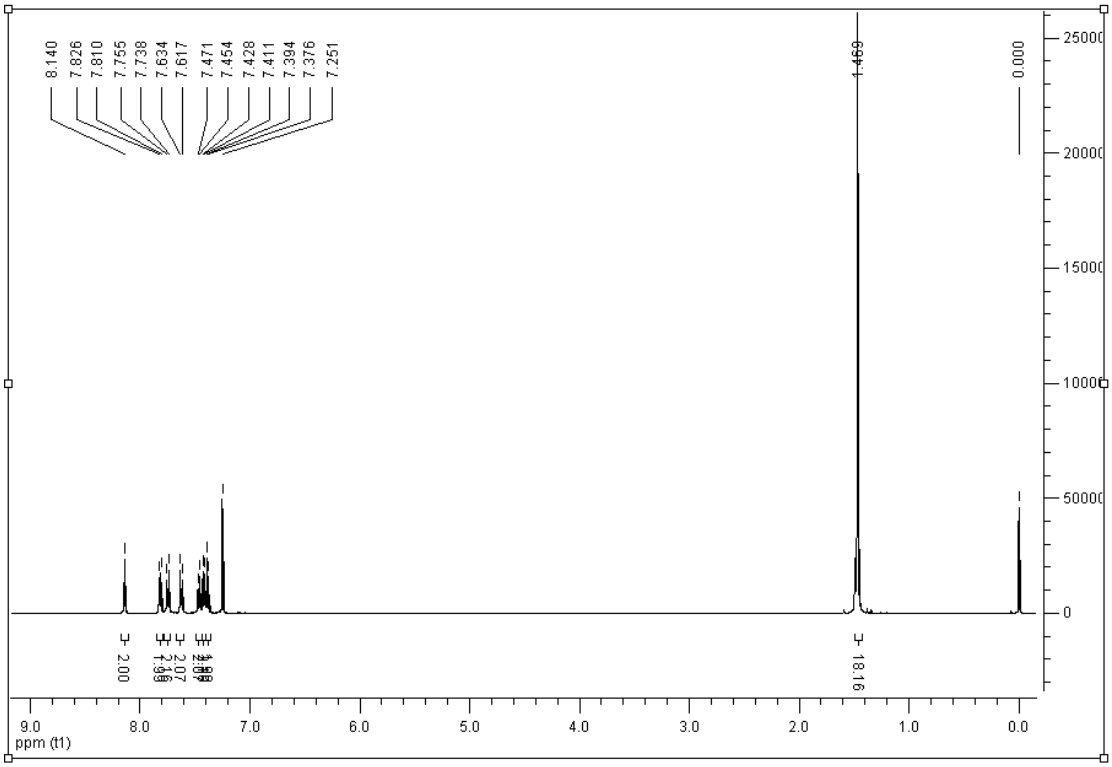


**Fig. S5** $^{1}$H NMR spectrum of compound **7**.

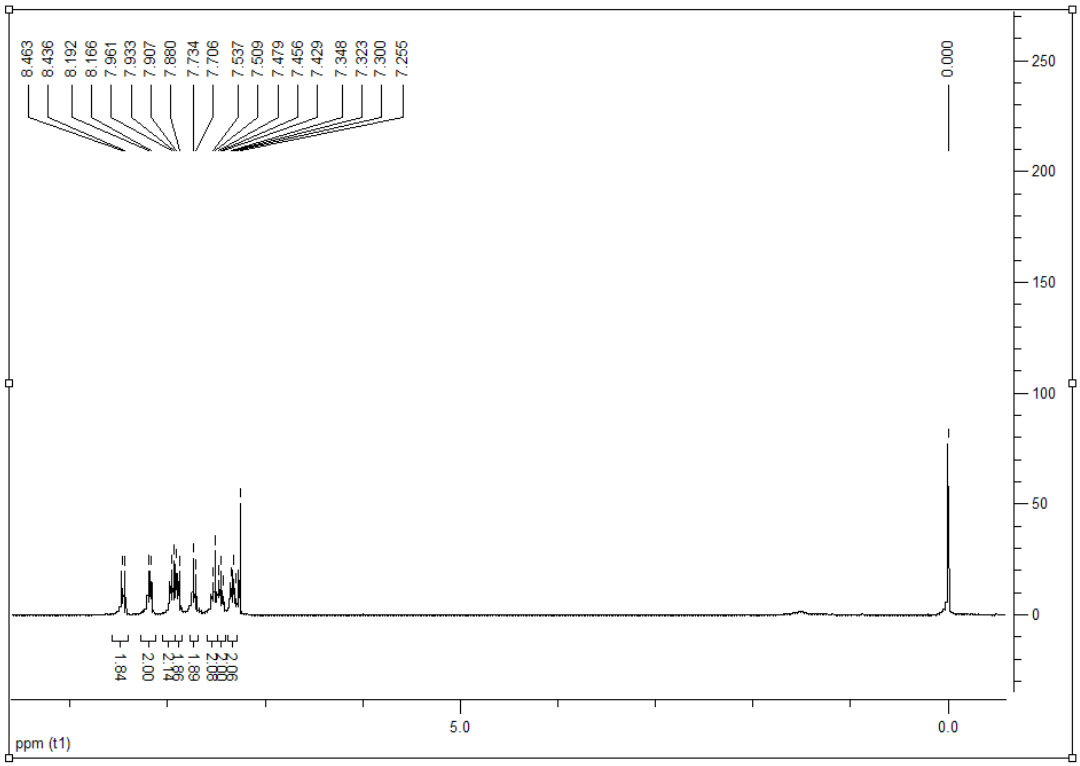


**Fig. S6** $^{1}$H NMR spectrum of compound **8**.

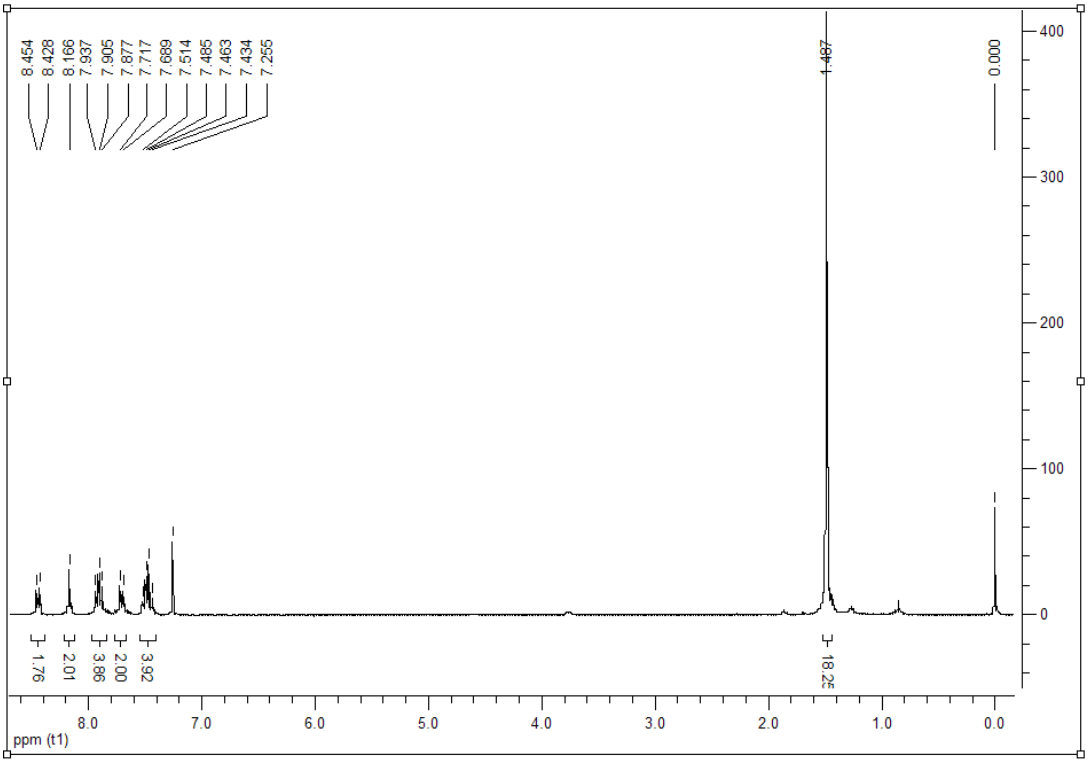


**Fig. S7** $^{1}$H NMR spectrum of compound **9**.

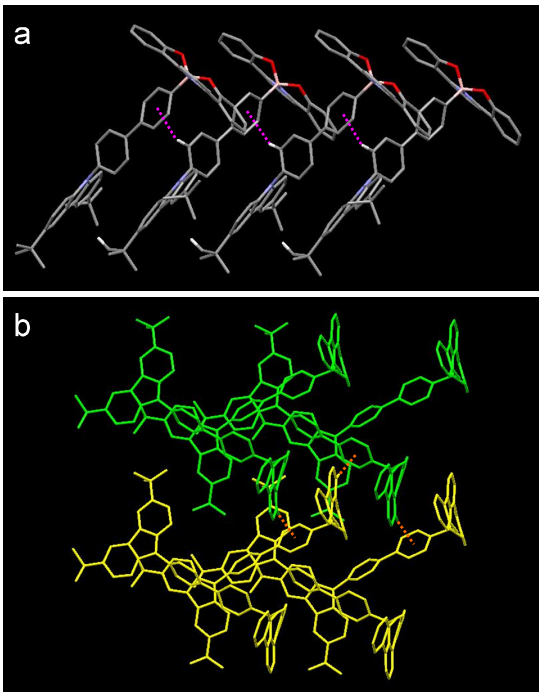


**Fig. S8** (a) View of the molecular chain in the crystal of complex **4**, pink line: C(28)–H(28)···π hydrogen bond (C···π-ring centroid = 3.82 Å, C···π-ring plane = 3.62 Å, C–H···π-ring centroid = 158.3°). (b) View of the interactions between molecular chains, orange line: C(10)–H(10)···π hydrogen bond (C···π-ring centroid = 3.45 Å, C···π-ring plane = 3.44 Å, C–H···π-ring centroid = 150.1°).

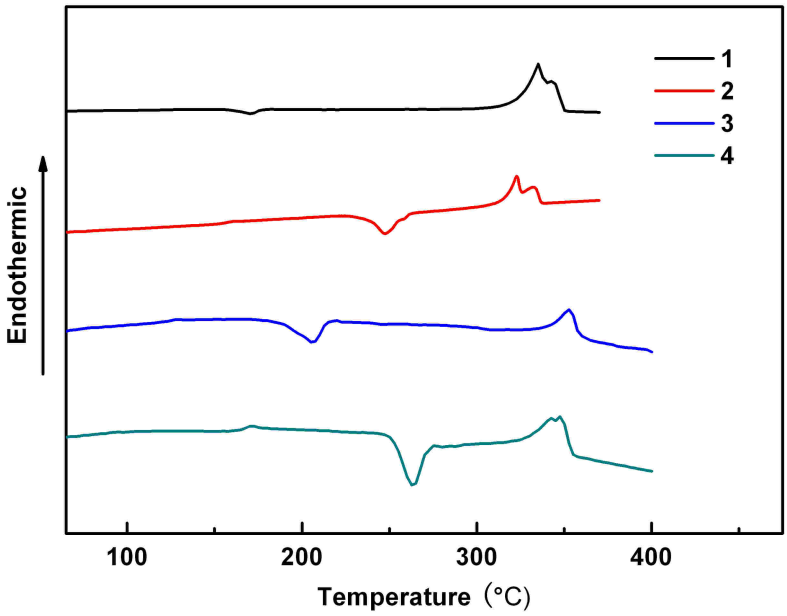


**Fig. S9** DSC thermograms for the second heating cycle.

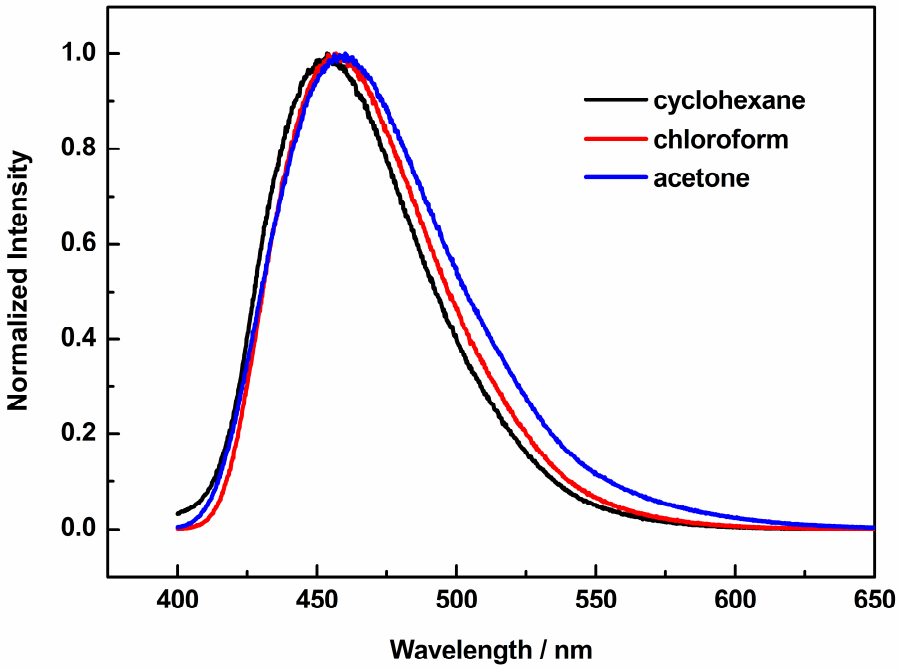


**Fig. S10** Emission spectra of complex **1** in different solvents.

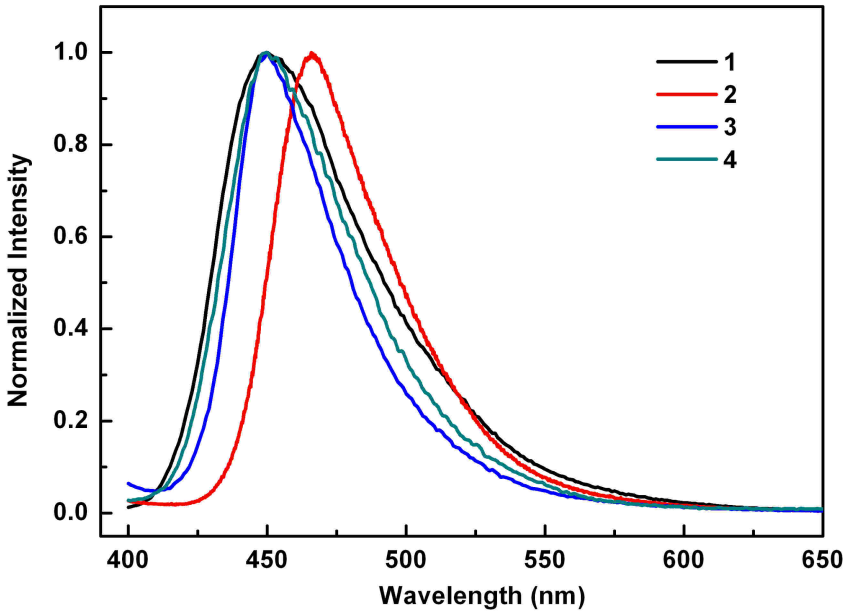


**Fig. S11** Emission spectra of complexes **1**–**4** in the solid state.

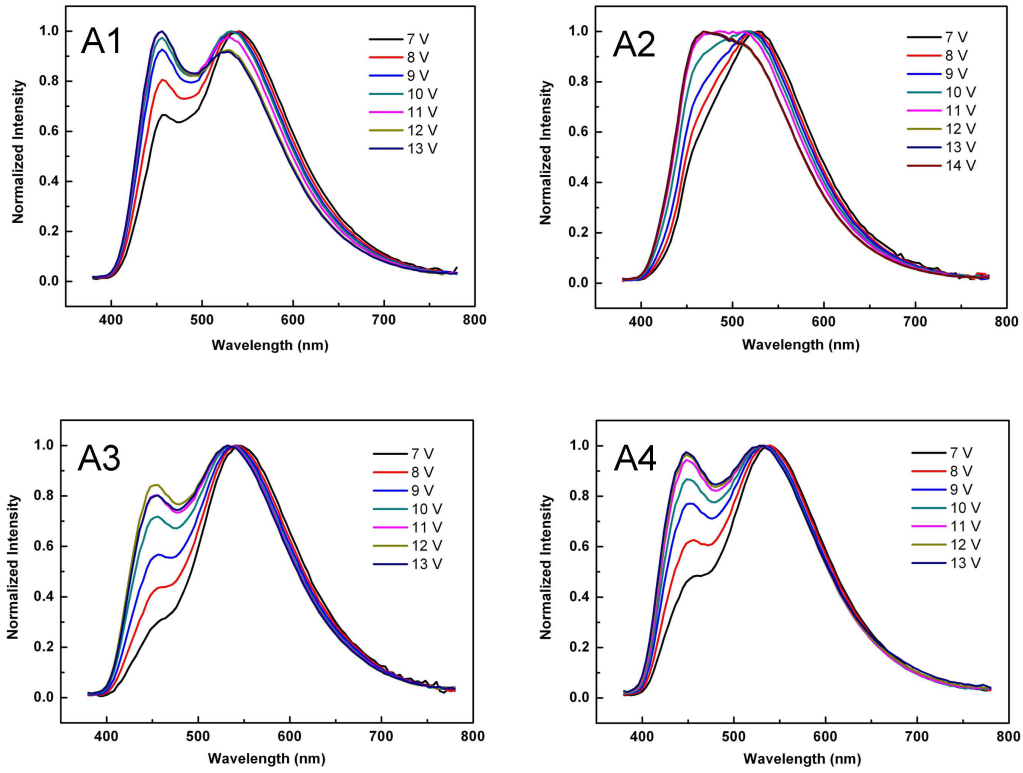


**Fig. S12** EL spectra of devices A1–A4.

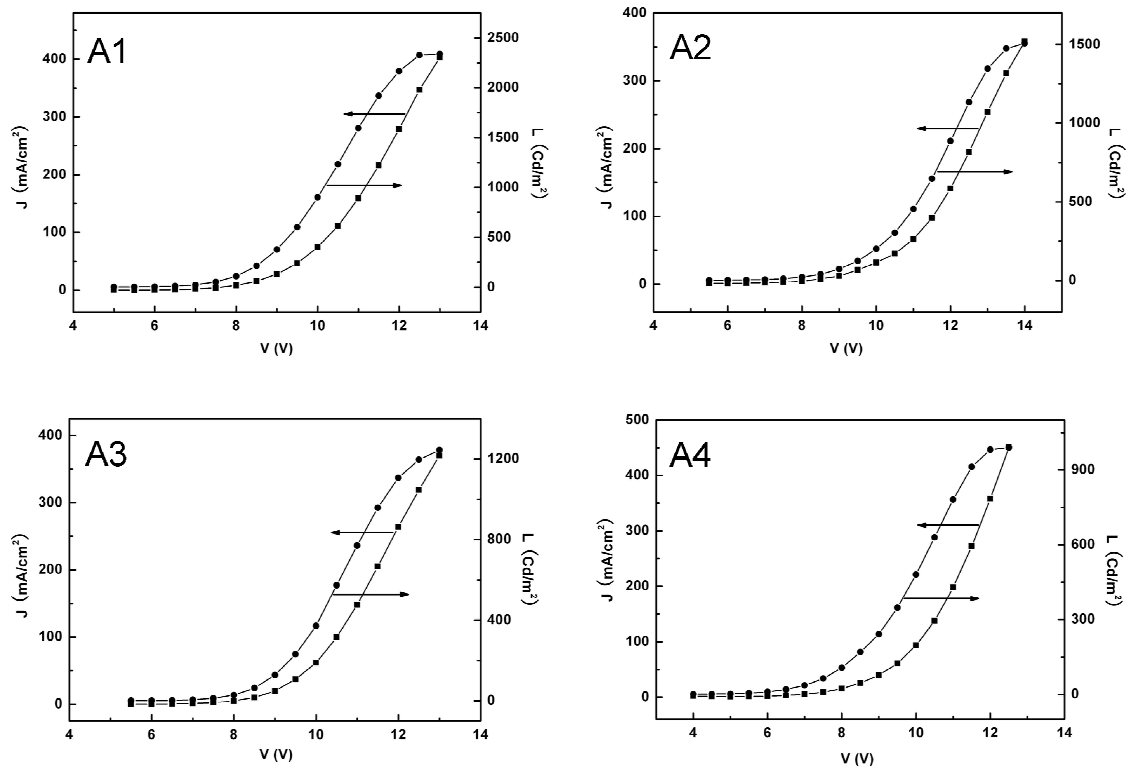


**Fig. S13** *J–V* and *L–V* curves of the EL devices.

**Table S1** Crystal data for complexes **1**, **2** and **4**

| | **1** | **2** | **4** |
|---|---|---|---|
| formula | $C_{35}H_{23}BN_2O_2$ | $C_{37}H_{27}BN_2O_2{\cdot}CHCl_3$ | $C_{49}H_{43}BN_2O_2{\cdot}CHCl_3$ |
| fw | 514.36 | 661.78 | 822.03 |
| crystal system | *Monoclinic* | *Monoclinic* | *Monoclinic* |
| space group | *P2(1)/n* | *P2(1)/c* | *P2(1)/c* |
| *a* (Å) | 11.376(2) | 10.324(2) | 32.791(7) |
| *b* (Å) | 19.307(4) | 29.638(6) | 11.692(2) |
| *c* (Å) | 12.927(3) | 1.364(2) | 11.615(2) |
| $\alpha$ (deg) | 90 | 90 | 90 |
| $\beta$ (deg) | 111.60(3) | 106.61(3) | 90.69(3) |
| $\gamma$ (deg) | 90 | 90 | 90 |
| *V* (Å$^3$) | 2640.0(9) | 3332.3(12) | 4452.8(15) |
| *Z* | 4 | 4 | 4 |
| $D_c$ (g cm$^{-3}$) | 1.294 | 1.319 | 1.226 |
| $\theta_{max}$ (deg) | 27.47 | 25.00 | 25.00 |
| no. of reflns meads | 25300 | 25586 | 32755 |
| no. of reflns used | 6013 | 5764 | 7586 |
| no. of parameters | 361 | 417 | 529 |
| $R_{int}$ | 0.0491 | 0.0489 | 0.0994 |
| final *R* [I > 2σ(I)] | | | |
| R1 | 0.0531 | 0.0833 | 0.1057 |
| wR2 | 0.1266 | 0.2607 | 0.2585 |

**Table S2** Selected bond lengths (Å) and angles (deg) for **1**, **2** and **4**

| | | | |
|---|---|---|---|
| Complex **1** | | | |
| O(1)-B(1) | 1.454(2) | O(1)-B(1)-O(2) | 104.93(13) |
| O(2)-B(1) | 1.455(2) | O(1)-B(1)-N(1) | 108.10(12) |
| N(1)-B(1) | 1.606(2) | O(2)-B(1)-N(1) | 107.36(12) |
| C(18)-B(1) | 1.618(2) | O(1)-B(1)-C(18) | 113.93(13) |
| O(1)-C(1) | 1.3518(18) | O(2)-B(1)-C(18) | 113.40(12) |
| O(2)-C(17) | 1.3510(19) | N(1)-B(1)-C(18) | 108.80(13) |
| C(7)-C(6) | 1.460(2) | C(1)-O(1)-B(1) | 119.36(13) |
| C(11)-C(12) | 1.463(3) | C(17)-O(2)-B(1) | 117.46(13) |
| N(2)-C(21) | 1.4320(18) | | |
| Complex **2** | | | |
| O(1)-B(1) | 1.443(5) | O(1)-B(1)-O(2) | 105.0(3) |
| O(2)-B(1) | 1.460(5) | O(1)-B(1)-N(1) | 108.1(3) |
| N(1)-B(1) | 1.607(5) | O(2)-B(1)-N(1) | 108.3(3) |
| C(18)-B(1) | 1.643(5) | O(1)-B(1)-C(18) | 113.2(3) |
| O(1)-C(1) | 1.351(4) | O(2)-B(1)-C(18) | 112.4(3) |
| O(2)-C(17) | 1.470(4) | N(1)-B(1)-C(18) | 109.5(3) |
| C(7)-C(6) | 1.619(5) | C(1)-O(1)-B(1) | 115.9(3) |
| C(11)-C(12) | 1.466(5) | C(17)-O(2)-B(1) | 118.6(3) |
| N(2)-C(21) | 1.426(5) | | |
| Complex **4** | | | |
| O(1)-B(1) | 1.455(8) | O(1)-B(1)-O(2) | 105.4(5) |
| O(2)-B(1) | 1.445(7) | O(1)-B(1)-N(1) | 106.8(5) |
| N(1)-B(1) | 1.625(8) | O(2)-B(1)-N(1) | 107.1(5) |
| C(18)-B(1) | 1.598(8) | O(1)-B(1)-C(18) | 112.4(5) |
| O(1)-C(1) | 1.358(7) | O(2)-B(1)-C(18) | 114.0(5) |
| O(2)-C(17) | 1.346(8) | N(1)-B(1)-C(18) | 110.6(4) |
| C(7)-C(6) | 1.457(9) | C(1)-O(1)-B(1) | 115.4(4) |
| C(11)-C(12) | 1.482(9) | C(17)-O(2)-B(1) | 116.3(5) |
| C(21)-C(24) | 1.488(7) | | |
| N(2)-C(27) | 1.409(6) | | |

**Table S3** Selected torsion angles (deg) for complexes **1**, **2** and **4**

| | |
|---|---|
| Complex **1** | |
| C(1)-C(6)-C(7)-N(1) | 15.93 |
| N(1)-C(11)-C(12)-C(17) | –18.73 |
| C(19)-C(18)-B(1)-N(1) | –55.63 |
| C(20)-C(21)-N(2)-C(24) | –70.91 |
| Complex **2** | |
| C(1)-C(6)-C(7)-N(1) | 15.16 |
| N(1)-C(11)-C(12)-C(17) | –12.44 |
| C(19)-C(18)-B(1)-N(1) | 0.42 |
| C(20)-C(21)-N(2)-C(24) | –108.02 |
| Complex **4** | |
| C(1)-C(6)-C(7)-N(1) | 18.63 |
| N(1)-C(11)-C(12)-C(17) | –20.79 |
| C(19)-C(18)-B(1)-N(1) | 35.41 |
| C(20)-C(21)-C(24)-C(25) | 21.91 |
| C(26)-C(27)-N(2)-C(30) | –62.19 |

**Table S4** Calculated HOMO and LUMO energy levels of **1**–**4**[a]

| complex | HOMO (eV) | LUMO (eV) |
|---|---|---|
| **1** | –5.06 (–5.58) | –2.12 (–2.85) |
| **2** | –5.04 (–5.56) | –2.05 (–2.83) |
| **3** | –5.15 (–5.60) | –2.08 (–2.84) |
| **4** | –4.98 (–5.47) | –2.06 (–2.83) |

[a] Values in parentheses are obtained from the electrochemical data.

**Table S5** CIE coordinates of devices A1–A4

| device | CIE coordinates | | | | | | |
|---|---|---|---|---|---|---|---|
| | 7 V | 8 V | 9 V | 10 V | 11 V | 12 V | 13 V |
| A1 | 0.32, 0.41 | 0.30, 0.38 | 0.29, 0.36 | 0.28, 0.36 | 0.27, 0.35 | 0.27, 0.34 | 0.27, 0.34 |
| A2 | 0.30, 0.43 | 0.29, 0.42 | 0.28, 0.40 | 0.26, 0.37 | 0.25, 0.35 | 0.25, 0.34 | 0.25, 0.34 |
| A3 | 0.36, 0.47 | 0.34, 0.44 | 0.32, 0.41 | 0.30, 0.39 | 0.29, 0.37 | 0.29, 0.37 | 0.29, 0.37 |
| A4 | 0.33, 0.43 | 0.31, 0.40 | 0.29, 0.38 | 0.28, 0.36 | 0.28, 0.35 | 0.28, 0.34 | 0.28, 0.34 |