## Accepted Manuscript

Boron-based TADF emitters with improved OLED device efficiency roll-off and long lifetime

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PII: S0143-7208(16)31454-1

DOI: 10.1016/j.dyepig.2017.01.055

Reference: DYPI 5755

To appear in: Dyes and Pigments

Received Date: 21 December 2016

Revised Date: 15 January 2017

Accepted Date: 21 January 2017

Please cite this article as: Bell BM, Clark TP, De Vries TS, Lai Y, Laitar DS, Gallagher TJ, Jeon J-H, Kearns KL, McIntire T, Mukhopadhyay S, Na H-Y, Paine TD, Rachford AA, Boron-based TADF emitters with improved OLED device efficiency roll-off and long lifetime, *Dyes and Pigments* (2017), doi: 10.1016/ j.dyepig.2017.01.055.

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### **1** Boron-Based TADF Emitters with Improved OLED Device Efficiency

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#### **Roll-Off and Long Lifetime**

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9 Keywords: Thermally Activated Delayed Fluorescence, Boron, Efficiency Roll-off, Lifetime, Triplet Energy

#### 10 Abstract

A class of four-coordinate boron complexes is reported that contain both electron-rich and 11 12 electron-poor functional groups. Judicious selection of donor and acceptor moieties with the use of a 13 boron atom as a separating node yields charge transfer complexes capable of thermally activated delayed fluorescence (TADF). Complexes were prepared by a modular method providing access to a 14 15 wide range of emission colors. The singlet (S1) and triplet (T1) energies are independently tuned to achieve a small  $S_1$ - $T_1$  gap. Raising and lowering of  $S_1$  and  $T_1$  states can be predicted using cyclic 16 17 voltammetry, NTO analysis, and spin density distribution as determined using Density Functional Theory; separation of the hole and electron wavefunction for S<sub>1</sub> excitation and delocalization of spin density 18 distribution in the  $T_1$  state can help in achieving negligible  $S_1$ - $T_1$  gap. Although photoluminescent 19 20 quantum yields of the boron complexes in a host matrix are less than 65%, OLED device external quantum efficiencies of up to 8.1% have been achieved at a luminance of 1000  $cd/m^2$ . Selection of a 21

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