Synthesis and optoelectronic properties of oxadiazole coordinated boron complexes†

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Table S1. Bond lengths [Å] and angles [°] for B-1

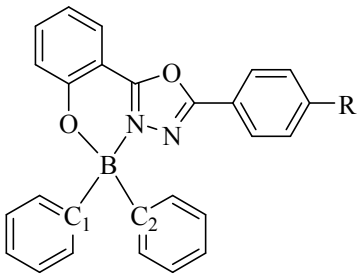
C(1)-C(6)	1.378(5)
C(1)-C(2)	1.388(4)
C(1)-B(1)	1.591(5)
C(2)-C(3)	1.382(5)
C(3)-C(4)	1.354(6)
C(4)-C(5)	1.370(5)
C(5)-C(6)	1.365(5)
C(7)-C(12)	1.377(5)
C(7)-C(8)	1.391(6)
C(8)-C(9)	1.349(6)
C(9)-C(10)	1.351(6)
C(10)-C(11)	1.365(5)
C(11)-C(12)	1.376(5)
C(12)-B(1)	1.591(5)
C(13)-C(14)	1.376(5)
C(13)-C(18)	1.377(4)
C(14)-C(15)	1.374(5)
C(15)-C(16)	1.363(5)
C(16)-C(17)	1.403(4)
C(17)-C(18)	1.394(4)
C(17)-C(26)	1.413(4)
C(18)-O(2)	1.349(4)
C(19)-C(20)	1.374(5)
C(19)-C(24)	1.388(4)
C(19)-C(25)	1.437(4)
C(20)-C(21)	1.365(5)
C(21)-C(22)	1.383(6)
C(22)-C(23)	1.362(6)
C(23)-C(24)	1.377(5)
C(25)-N(1)	1.293(4)

C(25)-O(1)	1.384(4)
C(26)-N(2)	1.307(4)
C(26)-O(1)	1.339(3)
B(1)-O(2)	1.509(4)
B(1)-N(2)	1.610(4)
N(1)-N(2)	1.387(3)

C(6)-C(1)-C(2)	115.0(3)
C(6)-C(1)-B(1)	122.7(3)
C(2)-C(1)-B(1)	122.3(3)
C(3)-C(2)-C(1)	122.0(4)
C(4)-C(3)-C(2)	120.6(4)
C(3)-C(4)-C(5)	119.1(4)
C(6)-C(5)-C(4)	119.6(4)
C(5)-C(6)-C(1)	123.7(3)
C(12)-C(7)-C(8)	122.0(4)
C(9)-C(8)-C(7)	119.8(4)
C(8)-C(9)-C(10)	119.8(4)
C(9)-C(10)-C(11)	119.9(4)
C(10)-C(11)-C(12)	123.2(4)
C(11)-C(12)-C(7)	115.3(3)
C(11)-C(12)-B(1)	122.7(3)
C(7)-C(12)-B(1)	122.0(3)
C(14)-C(13)-C(18)	120.4(4)
C(15)-C(14)-C(13)	120.7(4)
C(16)-C(15)-C(14)	120.5(3)
C(15)-C(16)-C(17)	119.2(3)
C(18)-C(17)-C(16)	120.5(3)
C(18)-C(17)-C(26)	116.3(3)
C(16)-C(17)-C(26)	123.2(3)
O(2)-C(18)-C(13)	119.7(3)
O(2)-C(18)-C(17)	121.4(3)
C(13)-C(18)-C(17)	118.8(3)
C(20)-C(19)-C(24)	119.8(3)
C(20)-C(19)-C(25)	119.0(3)
C(24)-C(19)-C(25)	121.2(3)
C(21)-C(20)-C(19)	120.2(4)
C(20)-C(21)-C(22)	120.0(4)
C(23)-C(22)-C(21)	120.0(4)
C(22)-C(23)-C(24)	120.4(4)
C(23)-C(24)-C(19)	119.5(4)
N(1)-C(25)-O(1)	111.6(3)
N(1)-C(25)-C(19)	128.0(3)
O(1)-C(25)-C(19)	120.4(3)

N(2)-C(26)-O(1)	109.4(3)
N(2)-C(26)-C(17)	123.8(3)
O(1)-C(26)-C(17)	126.9(3)
O(2)-B(1)-C(1)	108.8(3)
O(2)-B(1)-C(12)	112.0(3)
C(1)-B(1)-C(12)	116.6(3)
O(2)-B(1)-N(2)	102.3(2)
C(1)-B(1)-N(2)	108.7(3)
C(12)-B(1)-N(2)	107.4(3)
C(25)-N(1)-N(2)	104.9(2)
C(26)-N(2)-N(1)	109.5(2)
C(26)-N(2)-B(1)	121.7(3)
N(1)-N(2)-B(1)	127.8(2)
C(26)-O(1)-C(25)	104.7(2)
C(18)-O(2)-B(1)	122.4(2)

Table S2. Selected bond distances (Å) from the optimized geometries for the studied complexes and the experimental values for B-1, B-2 and B-3.



	Normal (B-1)		Normal-CH_3 (B-2)		Normal-Ph (B-3)	
	S_0	T_1	S_0	T_1	S_0	T_1
B-N	1.63373	1.55412	1.51572	1.44681	1.51556	1.61461
B-O	1.51567	1.44871	1.63277	1.55284	1.63341	1.51617
B-C1	1.61817	1.65432	1.61832	1.65395	1.61854	1.62554
B-C2	1.61165	1.63486	1.61205	1.63895	1.61198	1.61255

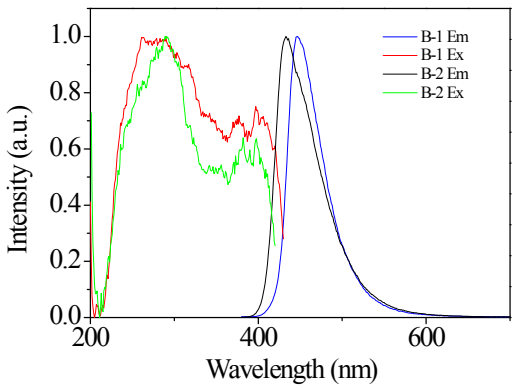


Fig. S1 The excitation and emission spectra of B-1 and B-2 in solid state