Electronic Supplementary Material (ESI) for CrystEngComm


**Supporting Information:**

# Crystal structures and solid-state fluorescence of BODIPY dyes based on Λ-shaped Tröger's base

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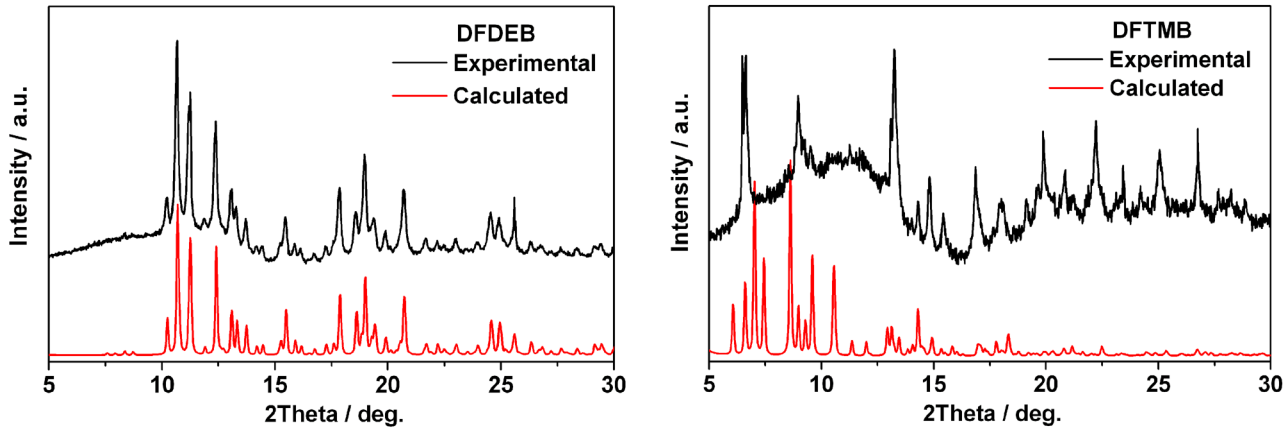


**Fig. S1**. Experimental and calculated powder X-ray diffraction patterns for **DFDEB** (left) and **DFTMB** (right) powders.

**Table S1.** Selected bond lengths (Å) and angles (°) for **DFDEB**.

| | | | |
|---|---|---|---|
| F(1)-B(1) | 1.397(2) | F(3)-B(2) | 1.388(2) |
| F(2)-B(1) | 1.379(2) | F(4)-B(2) | 1.391(2) |
| N(1)-C(16) | 1.349(2) | N(5)-C(46) | 1.343(2) |
| N(1)-C(10) | 1.3998(19) | N(5)-C(42) | 1.400(2) |
| N(1)-B(1) | 1.542(3) | N(5)-B(2) | 1.539(3) |
| N(2)-C(2) | 1.349(2) | N(6)-C(40) | 1.347(2) |
| N(2)-C(8) | 1.4004(19) | N(6)-C(34) | 1.3971(18) |
| N(2)-B(1) | 1.537(2) | N(6)-B(2) | 1.536(2) |
| N(4)-C(27) | 1.4331(18) | N(3)-C(21) | 1.4329(17) |
| N(4)-C(25) | 1.4612(19) | N(3)-C(25) | 1.4562(19) |
| N(4)-C(24) | 1.4718(18) | N(3)-C(26) | 1.4671(18) |
| C(27)-N(4)-C(25) | 110.34(12) | C(25)-N(3)-C(26) | 107.31(11) |
| C(27)-N(4)-C(24) | 113.80(11) | C(21)-N(3)-C(25) | 111.04(12) |
| C(25)-N(4)-C(24) | 106.67(11) | C(21)-N(3)-C(26) | 113.53(11) |
| N(4)-C(24)-C(22) | 111.62(12) | N(3)-C(26)-C(28) | 110.63(12) |
| N(3)-C(25)-N(4) | 111.55(11) | N(2)-B(1)-N(1) | 107.77(13) |
| F(2)-B(1)-F(1) | 108.95(14) | F(2)-B(1)-N(2) | 110.32(15) |
| F(2)-B(1)-N(1) | 110.75(16) | F(1)-B(1)-N(2) | 109.68(16) |
| F(1)-B(1)-N(1) | 109.36(15) | C(2)-N(2)-C(8) | 107.56(14) |
| C(2)-N(2)-B(1) | 127.10(14) | C(8)-N(2)-B(1) | 125.33(14) |
| C(16)-N(1)-C(10) | 107.89(14) | C(16)-N(1)-B(1) | 126.98(14) |
| C(10)-N(1)-B(1) | 124.92(14) | F(3)-B(2)-F(4) | 109.17(15) |
| F(3)-B(2)-N(6) | 110.45(17) | F(4)-B(2)-N(5) | 110.18(17) |
| F(4)-B(2)-N(6) | 109.32(14) | N(6)-B(2)-N(5) | 107.38(14) |
| F(3)-B(2)-N(5) | 110.33(14) | C(46)-N(5)-C(42) | 108.05(15) |
| C(46)-N(5)-B(2) | 126.72(15) | C(42)-N(5)-B(2) | 125.22(14) |
| C(40)-N(6)-C(34) | 107.85(13) | C(40)-N(6)-B(2) | 126.40(14) |
| C(34)-N(6)-B(2) | 125.74(14) | | |

**Table S2.** Selected bond lengths (Å) and angles (°) for **DFTMB**.

| | | | |
|---|---|---|---|
| F(3)-B(1) | 1.388(3) | F(2)-B(2) | 1.389(4) |
| F(4)-B(1) | 1.395(3) | F(1)-B(2) | 1.380(3) |
| N(1)-C(38) | 1.342(3) | N(5)-C(34) | 1.349(3) |
| N(1)-C(19) | 1.400(3) | N(5)-C(24) | 1.399(4) |
| N(1)-B(1) | 1.537(4) | N(5)-B(2) | 1.546(4) |
| N(2)-C(30) | 1.361(3) | N(6)-C(37) | 1.363(3) |
| N(2)-C(12) | 1.395(3) | N(6)-C(14) | 1.392(4) |
| N(2)-B(1) | 1.544(4) | N(6)-B(2) | 1.551(4) |
| N(4)-C(23) | 1.422(3) | N(4)-C | 1.481(3) |
| N(4)-C(40) | 1.454(4) | N(3)-C(15) | 1.443(3) |
| N(3)-C(65) | 1.469(3) | N(3)-C(40) | 1.463(3) |
| C(15)-N(3)-C(40) | 110.5(2) | C(23)-N(4)-C(40) | 111.0(2) |
| C(15)-N(3)-C(65) | 114.1(2) | C(23)-N(4)-C | 112.7(2) |
| C(40)-N(3)-C(65) | 107.0(2) | C(40)-N(4)-C | 108.0(2) |
| N(4)-C(40)-N(3) | 112.1(2) | N(4)-C-C(13) | 110.8(2) |
| N(3)-C(65)-C(48) | 112.2(2) | N(1)-B(1)-N(2) | 106.8(2) |
| F(3)-B(1)-F(4) | 109.1(2) | F(3)-B(1)-N(2) | 109.9(2) |
| F(3)-B(1)-N(1) | 110.1(2) | F(4)-B(1)-N(2) | 110.5(2) |
| F(4)-B(1)-N(1) | 110.4(2) | C(38)-N(1)-C(19) | 108.5(2) |
| C(19)-N(1)-B(1) | 125.5(2) | C(38)-N(1)-B(1) | 126.1(2) |
| C(30)-N(2)-C(12) | 107.6(2) | C(12)-N(2)-B(1) | 126.2(2) |
| C(30)-N(2)-B(1) | 126.0(2) | N(5)-B(2)-N(6) | 106.0(2) |
| F(1)-B(2)-F(2) | 109.9(3) | F(1)-B(2)-N(6) | 110.0(2) |
| F(1)-B(2)-N(5) | 110.4(2) | F(2)-B(2)-N(6) | 110.3(2) |
| F(2)-B(2)-N(5) | 110.2(2) | C(37)-N(6)-C(14) | 108.5(2) |
| C(34)-N(5)-C(24) | 108.0(2) | C(37)-N(6)-B(2) | 125.1(3) |
| C(34)-N(5)-B(2) | 125.8(2) | C(14)-N(6)-B(2) | 126.4(2) |
| C(24)-N(5)-B(2) | 126.1(2) | | |

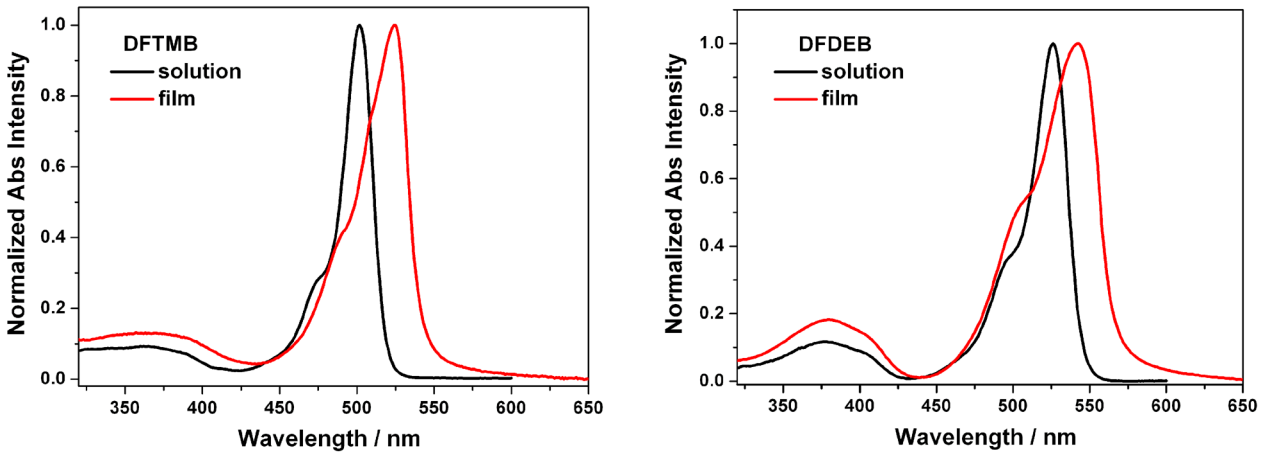


**Fig. S2** Absorption spectra of **DFTMB** (left) and **DFDEB** (right) in $CH_2Cl_2$ solution and thin films.

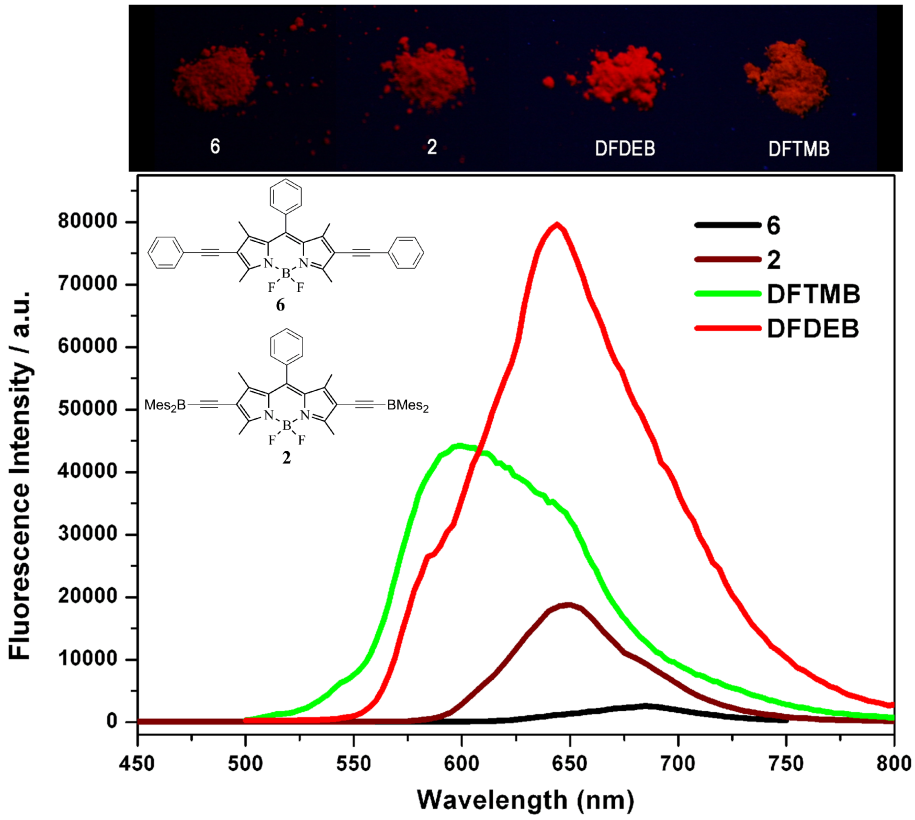


**Fig. S3** Fluorescence spectra of BODIPY dyes **DFDEB**, **DFTMB**, **2** and **6** in powder form. The inset shows the chemical structure of **2** and **6**. The top shows the fluorescence photograph of the powder form (grind to similar graininess before the measurements) of these compounds under 365 nm irradiation. The experiment was carried out under the same conditions