

Supporting information

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for

AIE-Active Organoboron Complexes with Highly Efficient Solid-State Luminescence and Their Application as Gas

Sensitive Materials

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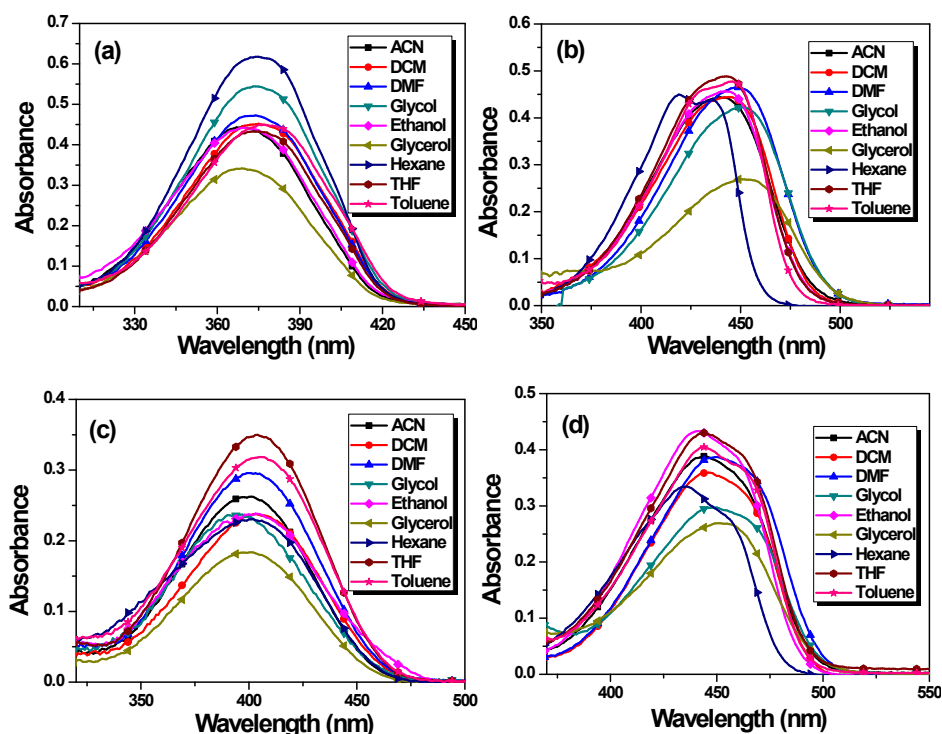


Figure S1. Absorption spectra of compound 3 (a), compound 4 (b), compound 5 (c) and compound 6 (d) in various solvents.

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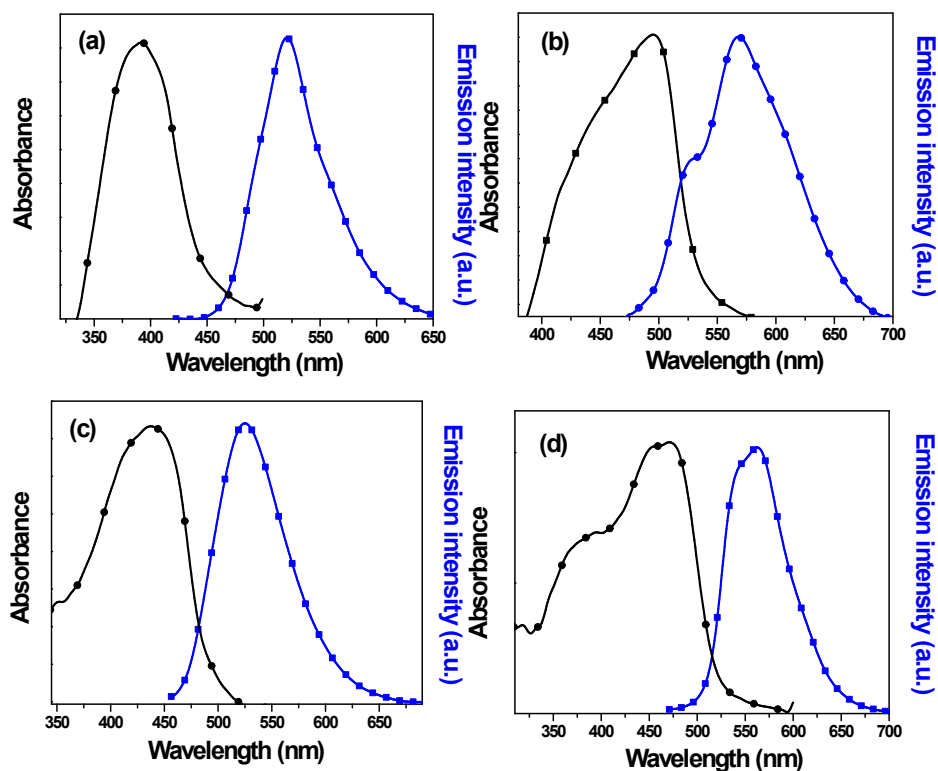


Figure S2. Absorption and emission of compound 3 (a), compound 4 (b), compound 5 (c) and compound 6 (d) in the solid state.

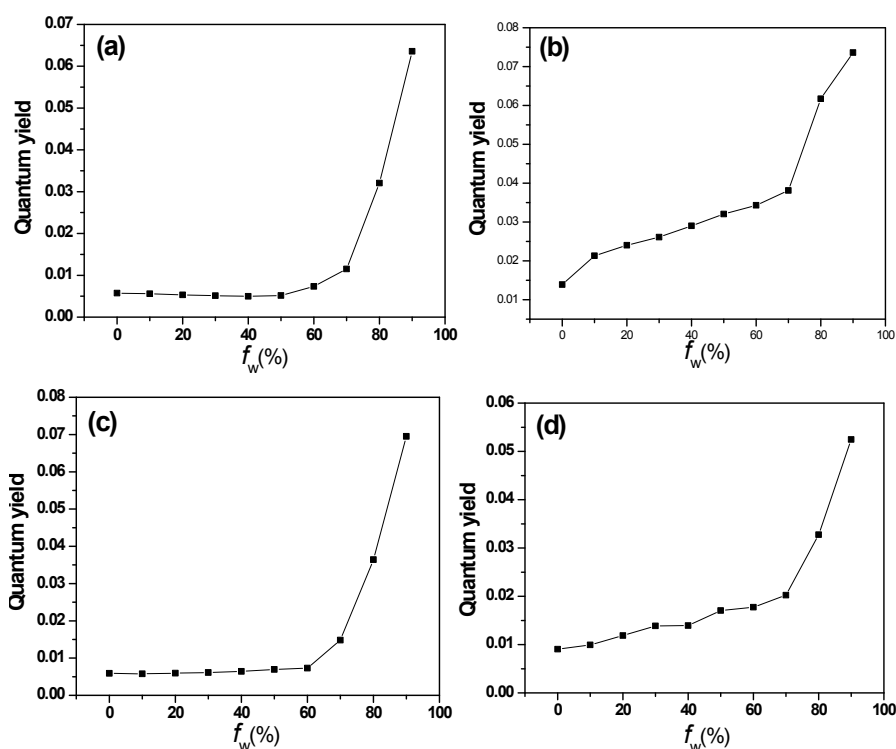


Figure S3. Changes in the quantum yields of compound 3 (a), compound 4 (b), compound 5 (c) and compound 6 (d) in THF/water mixtures (10 μ M) with varied volumetric fractions of water (f_w).

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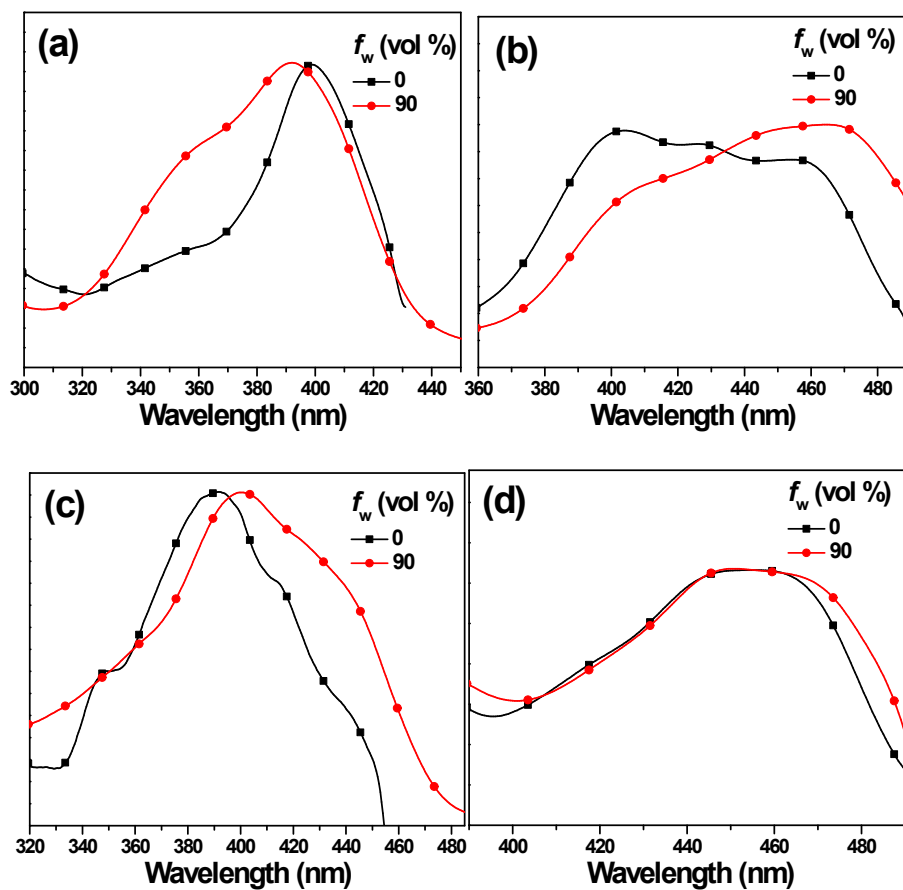


Figure S4. Normalized emission spectra of compounds 3 (a), 4 (b), 5 (c) and 6 (d) in THF/water mixtures (10 μ M) with f_w of 90%.

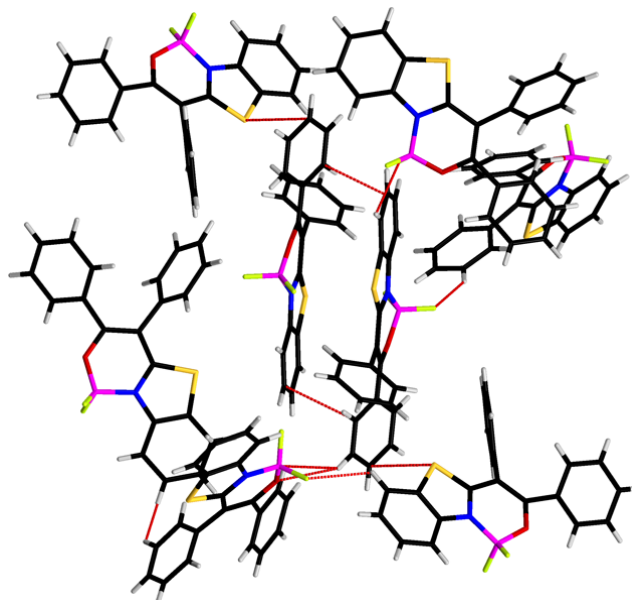


Figure S5. Crystal packing structures of compound 3. The red dotted lines show intermolecular C-H...F and C-H... π interactions within 3.

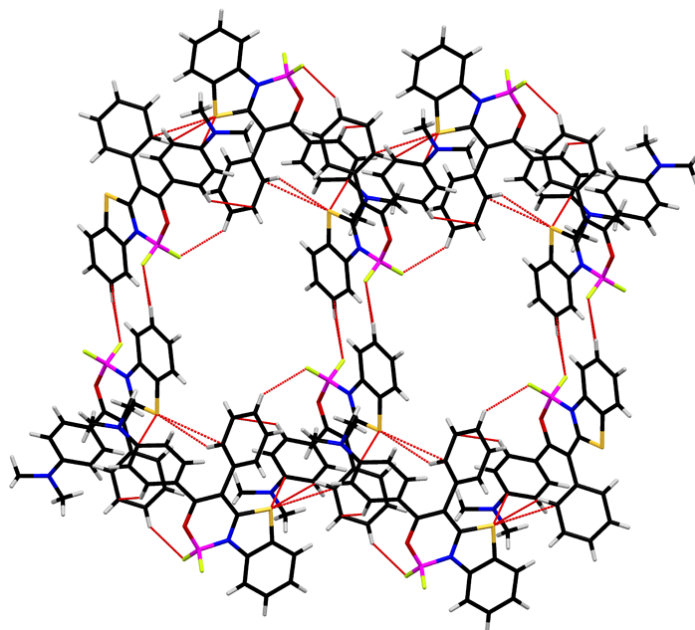


Figure S6. Crystal packing structures of compound **4**. The red dotted lines show intermolecular C-H...F and C-H... π interactions within **4**.

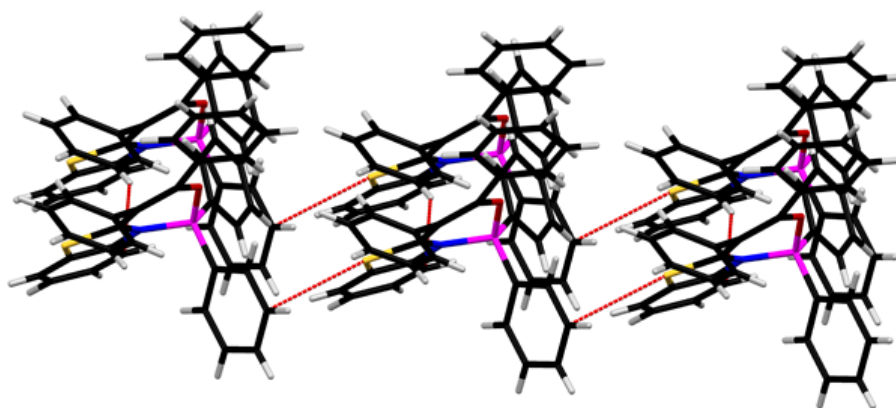


Figure S7. Crystal packing structures of compound **5**. The red dotted lines show intermolecular C-H...S and C-H... π interactions within **5**.

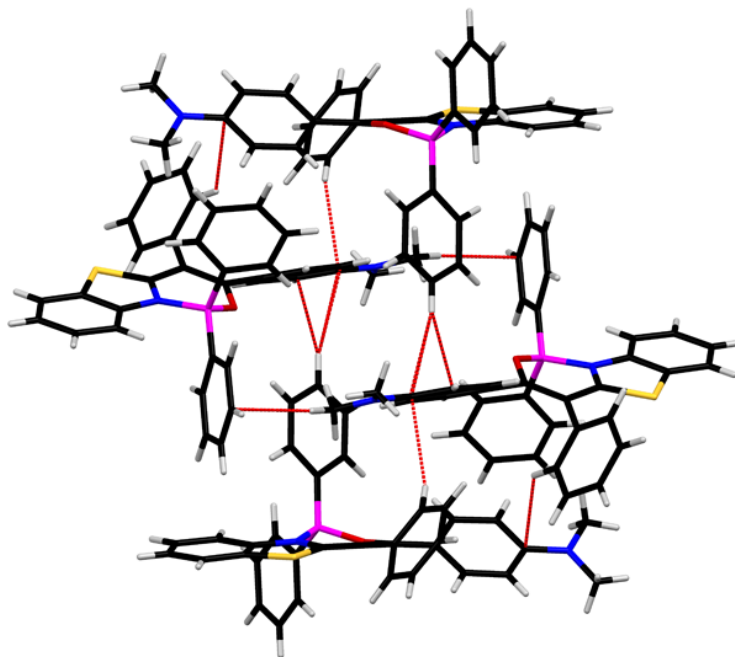


Figure S8. Crystal packing structures of compound **6**. The red dotted lines show intermolecular C–H... π interactions within **6**.

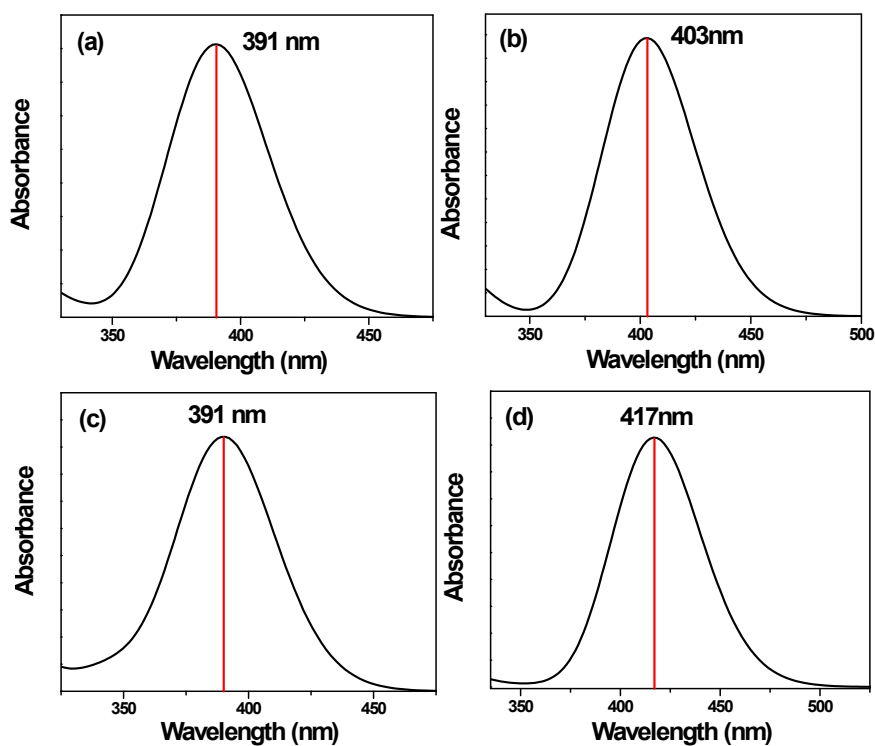


Figure S9. Calculated absorption spectra of compound **3** (a), compound **4** (b), compound **5** (c) and compound **6** (d)

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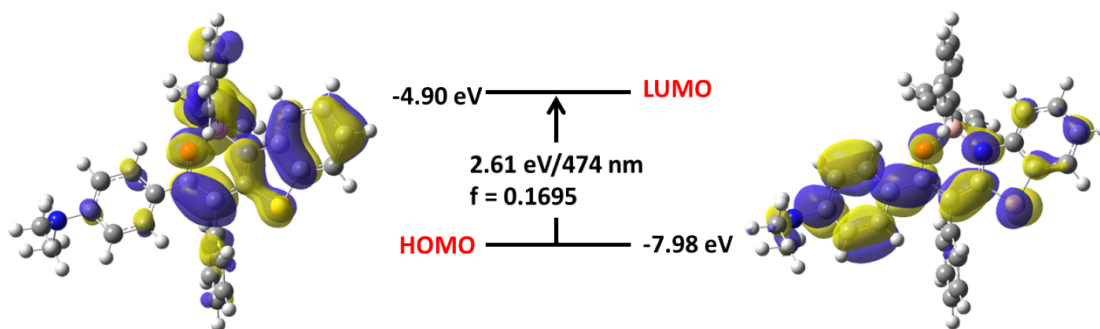


Figure S10. Molecular orbital amplitude plots and energy levels of HOMOs and LUMOs of compound **6+H+** calculated by using B3LYP/6-31G(d, p) basis set with G03 Program..

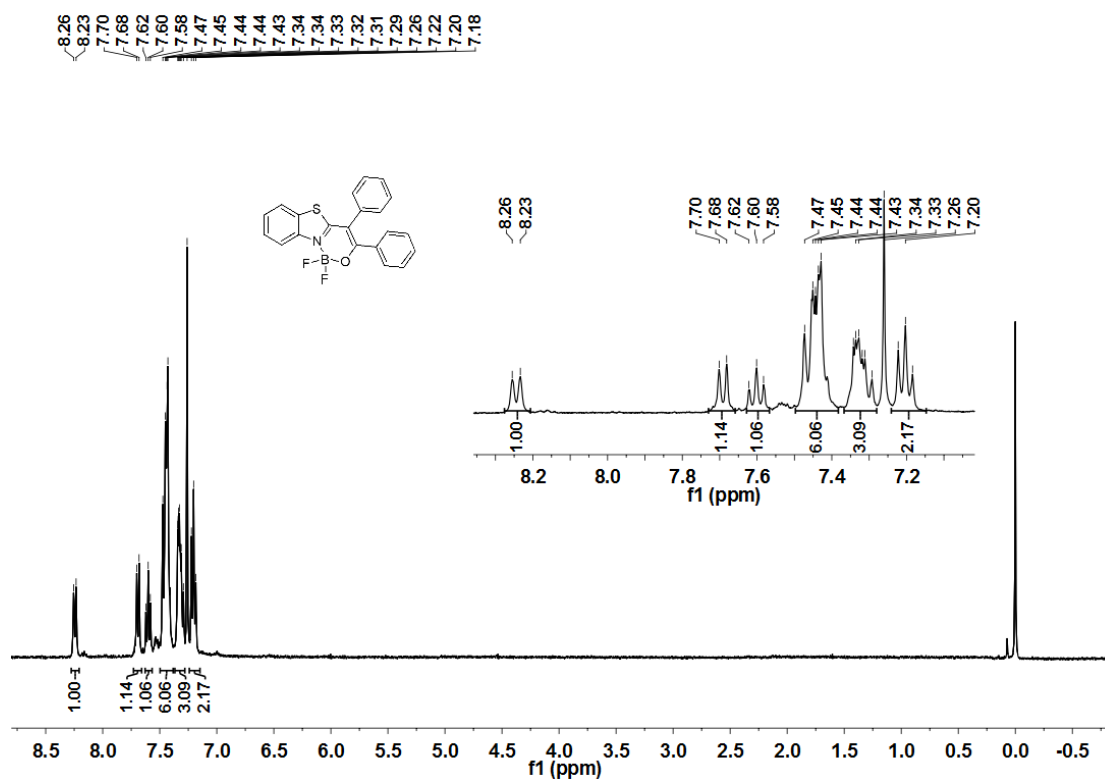


Figure S11. ^1H NMR spectrum of compound **3** in CDCl_3 .

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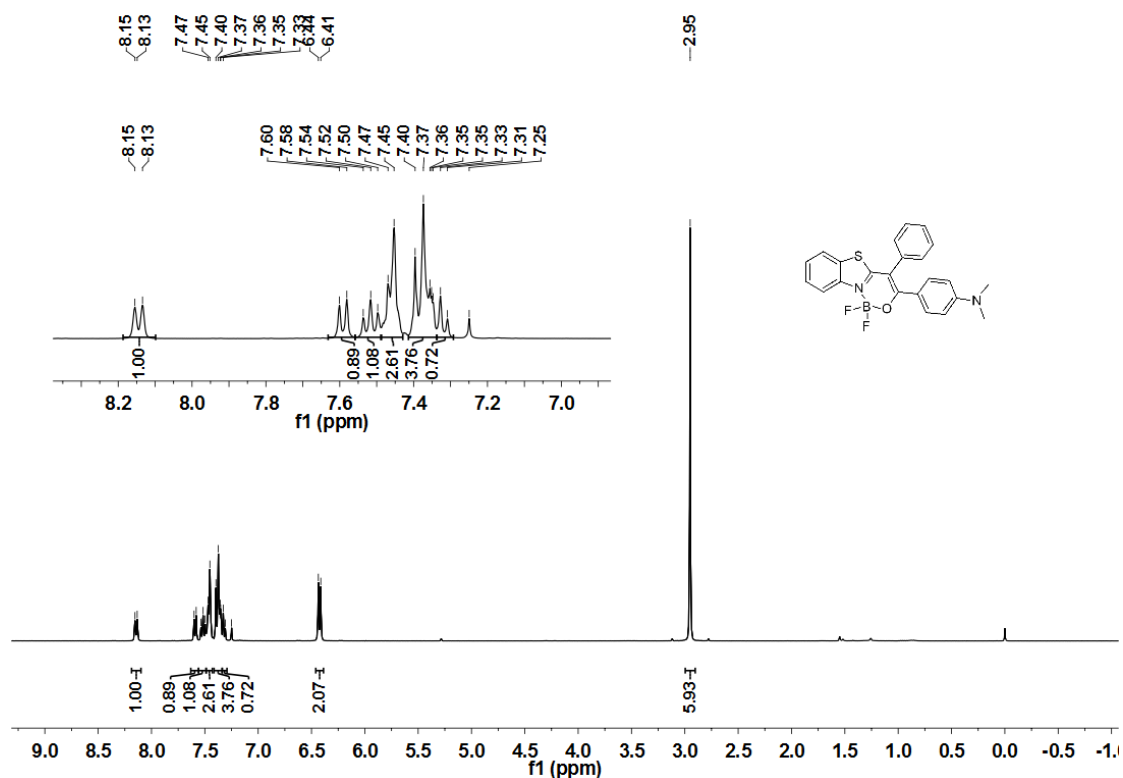


Figure S12. ^1H NMR spectrum of compound **4** in CDCl_3 .

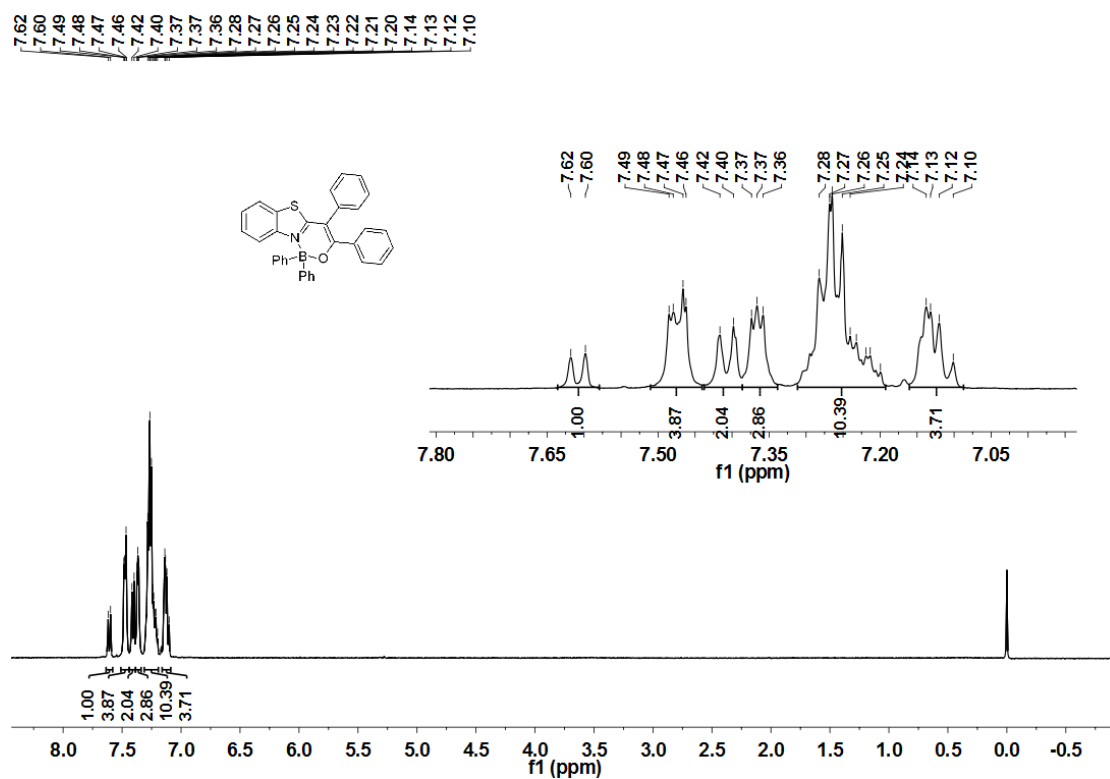
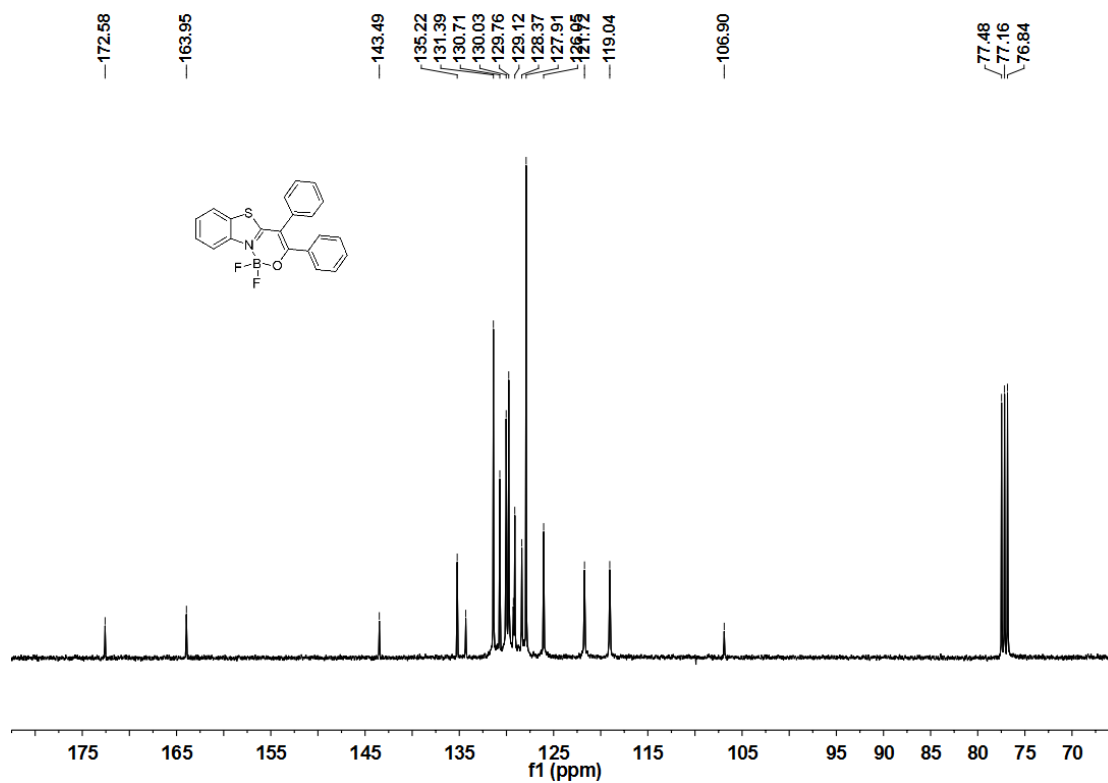
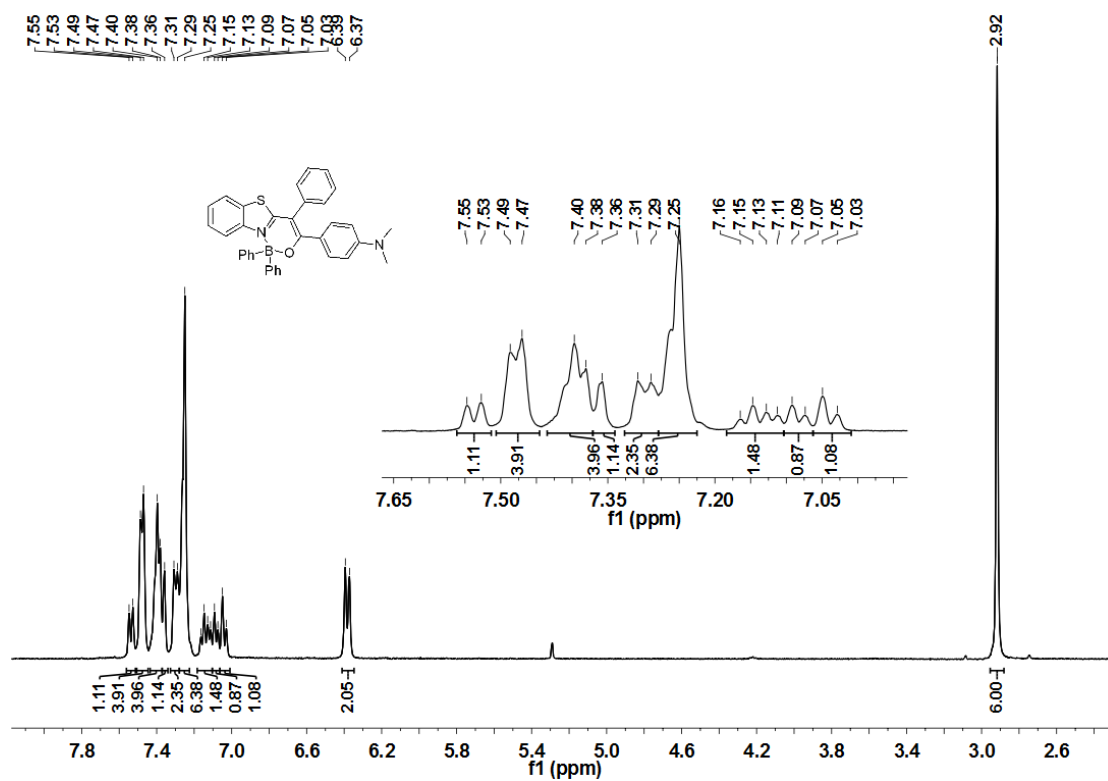
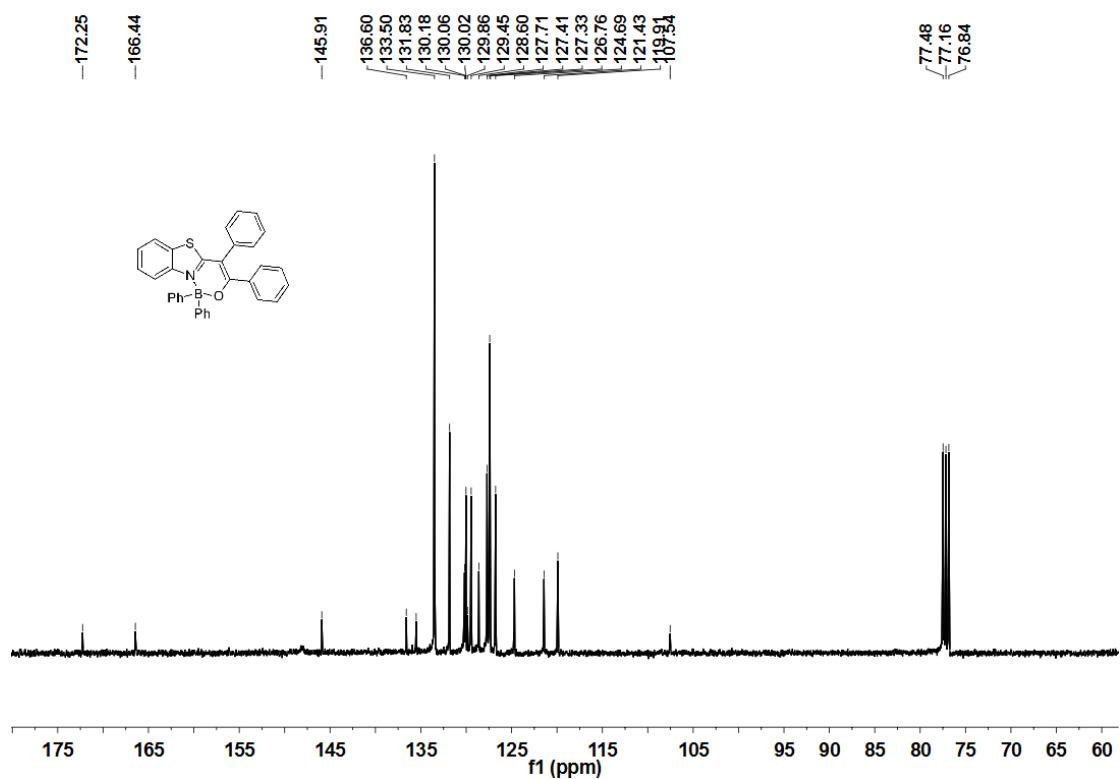
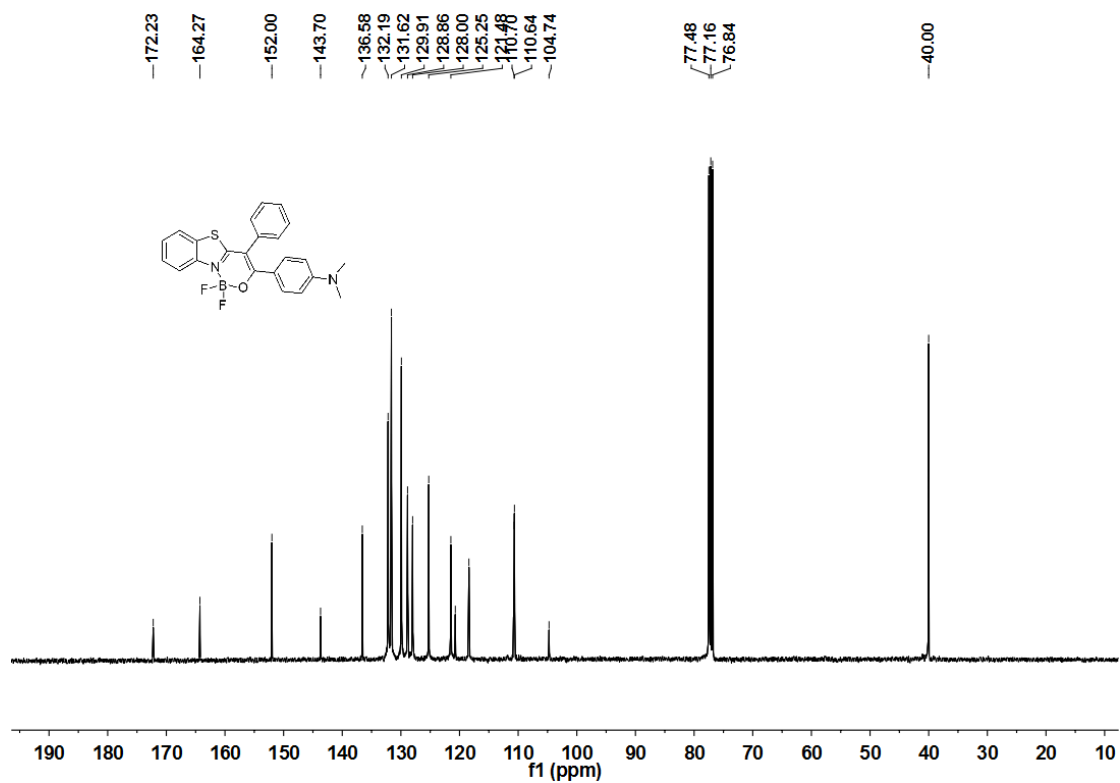


Figure S13. ^1H NMR spectrum of compound **5** in CDCl_3 .

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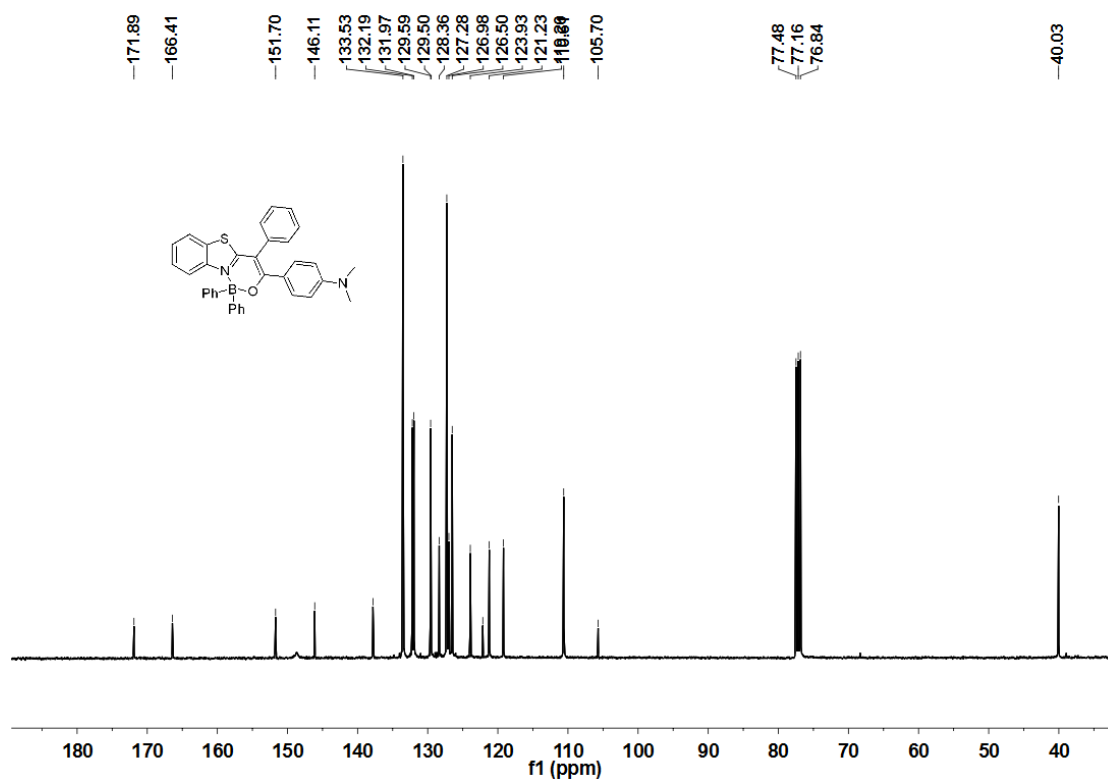


Figure S18. ^{13}C NMR spectrum of compound **6** in CDCl_3 .