π-Conjugated Polycycle Containing Boron

Significance: Triarylboranes have been a subject of extensive studies for electronic applications. This paper reports the synthesis, photophysics and crystal structure of new planarized triarylboranes in which the boron atom is embedded in a 10-ring-fused π-conjugated polycycle. Precursor 6 is obtained via radical-promoted intramolecular homocoupling of 5. The oxidative cyclization only proceeds when using 6b to give the final product, 1, in good yield. The new molecule is reported to be highly stable toward oxygen and water.

Comment: Unlike previously reported triarylboranes, polycycles 1 exhibit a broad absorption band that spans the visible region from 400 nm to 730 nm. The crystal structure shows that the conjugated polycycle is relatively planar and forms a face-to-face π-stacking with a short interplanar distance of 0.35 nm despite the bulky Mes groups.

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