Synthesis and Properties of Radial π-Cluster Embedding Anthracene Units

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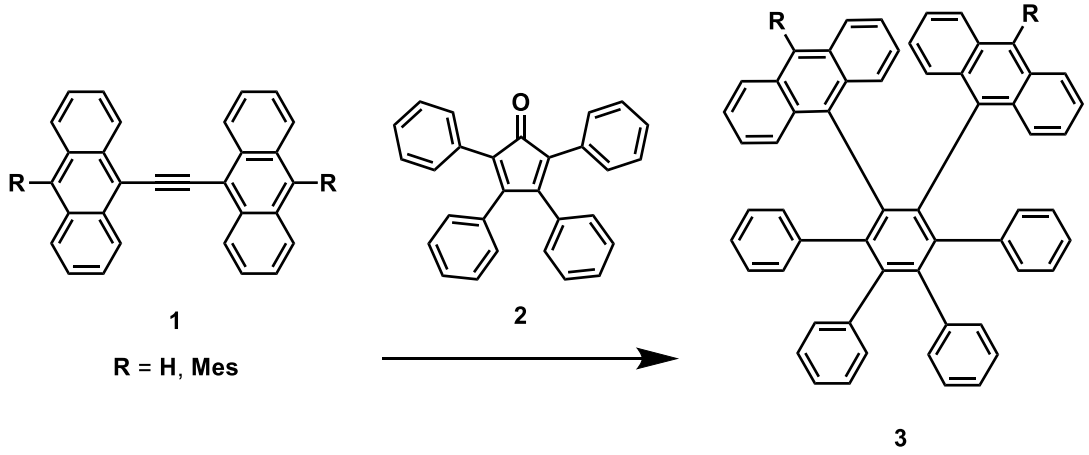
Aromatic π-cluster system possesses a structure in which two or more aromatic rings are positioned closer than the Van der Waals radius of carbon atoms (3.40 Å).[1] Overlap of molecular orbitals of aromatic rings results in a reduced HOMO–LUMO energy gap, enabling the structure to exhibit unique optoelectronic properties that is not usually observed in other π systems.

In this study, a compound called 1,2-*bis*(9-anthryl)-3,4,5,6-tetraphenylbenzene derivative **3** was synthesized. The presence of anthracene units is expected to enhance the optoelectronic properties through excimer (excited-state anthracene dimers) emission. In the case of non-substituted anthracene derivative, photoirradiation of the compound produces a unique anthracene dimeric structure, allowing control over its optoelectronic properties. In addition, the larger π surface of anthracene units is expected to enhance toroidal conjugation, resulting in extended emission lifetime compared to the known compound hexaphenylbenzene. Alongside the non-substituted derivative **3**, a mesityl **Mes** substituted analogue was also synthesized. Introduction of the **Mes** group improves solubility, allowing characterization to be conducted more easily.

In this poster presentation, we will report on the synthesis and characterization of **Mes** substituted and non-substituted derivative **3**.



1) T. Nishiuchi, S. Uno, Y. Hirao, T. Kubo, *J. Org. Chem.* **2016**, 81, 5, 2106–2112.