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Synthesis of Tetraphenylene Derivatives by the Scholl Reaction

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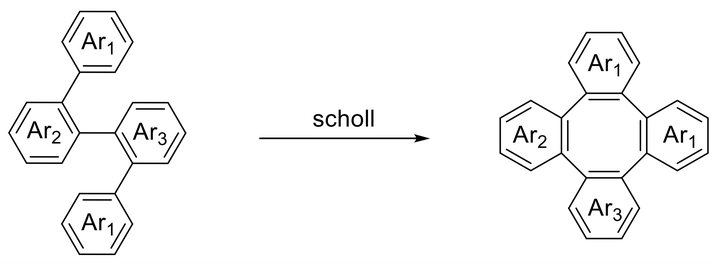
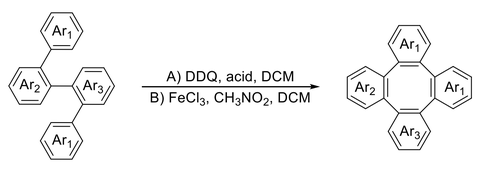
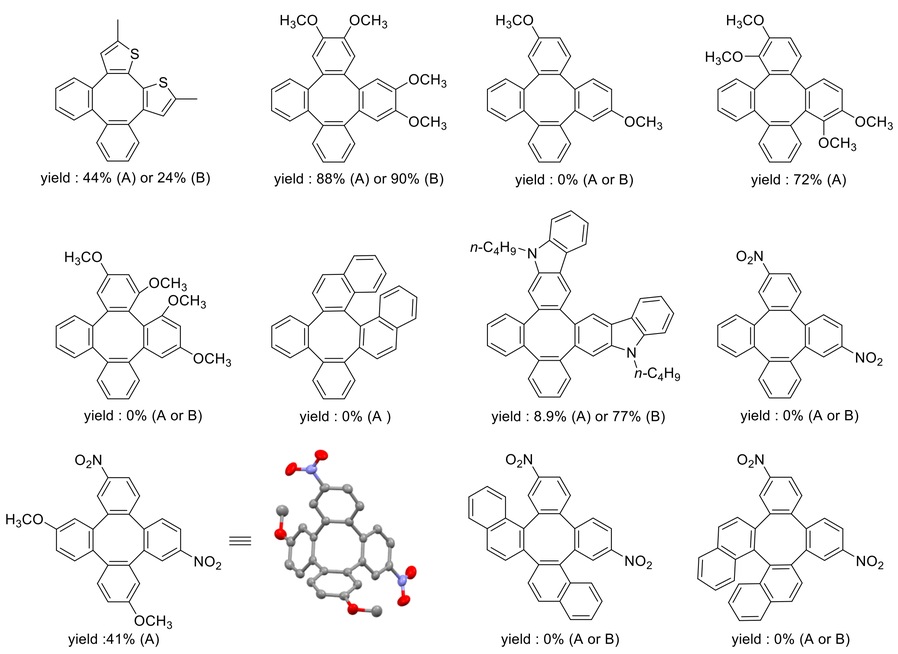
Introduction

The Scholl reaction is a powerful method to synthesize polycyclic aromatics enabling oxidative aryl−aryl coupling without requiring prefunctionalization of the aryl groups and allowing multiple carbon−carbon bonds to be formed in one synthetic operation. Six-membered carbocycles are commonly formed in Scholl reactions, while direct formation of five-, seven-, or eight-membered rings, particularly in a predictable manner, is still unusual.[1] This presentation describes a newly developed method to form an eight-membered ring in tetraphenylene derivatives by a regioselective Scholl reaction of quaterphenyl derivatives. It is found that this reaction requires the two terminal aryl groups in the quaterphenyl substrate to be much electron-richer than the two internal arylene groups, and an action mechanism is proposed for this Scholl reaction on the basis of DFT calculations.

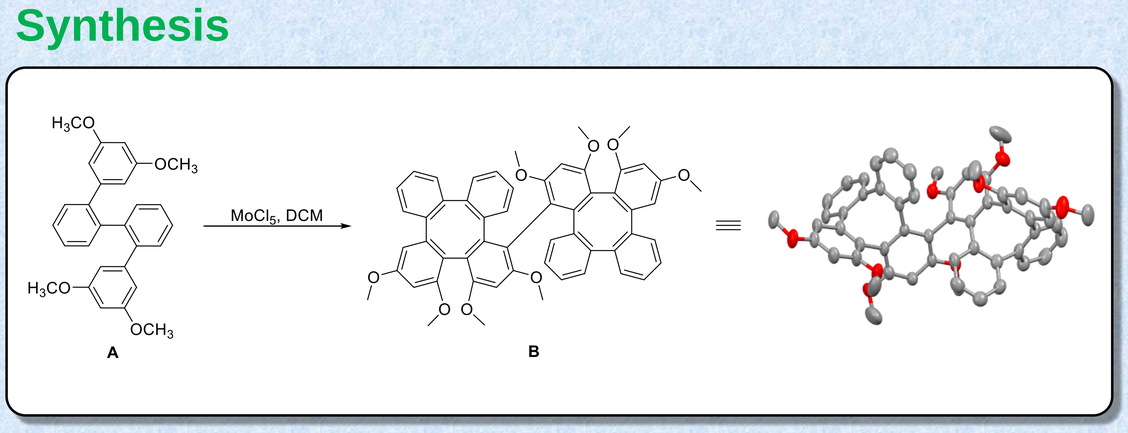


Synthesis

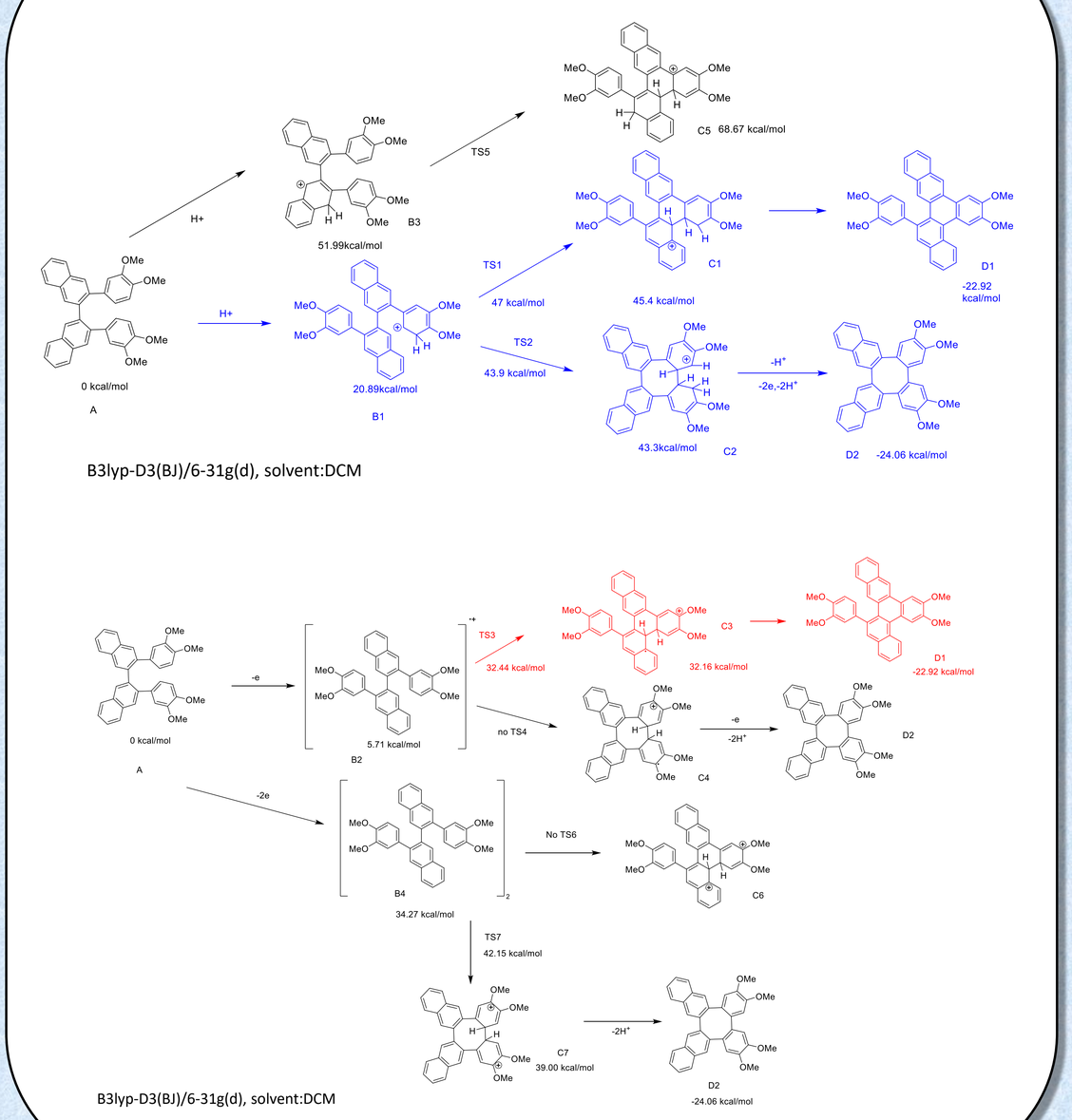




Synthesis



Density Functional Theory



Conclusions

In conclusion, we have discovered a new method to synthesize tetraphenylene derivatives by the Scholl reaction of quaterphenyl derivatives, in which two terminal aryl groups need to be much electron-richer than the two internal arylene groups. We also studied the reaction mechanism by DFT calculations and found that this Scholl reaction may undergoes cation mechanism. The radical cation mechanism tends to form six-membered rings. This method broadens the way to obtain tetraphenylene derivative by directly constructing an eight-membered ring.

Reference

(1) Zhang, Y.; Pun, S.; Miao, Q. *Chem. Rev.* **2022**, *122*, 14554-14593.

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