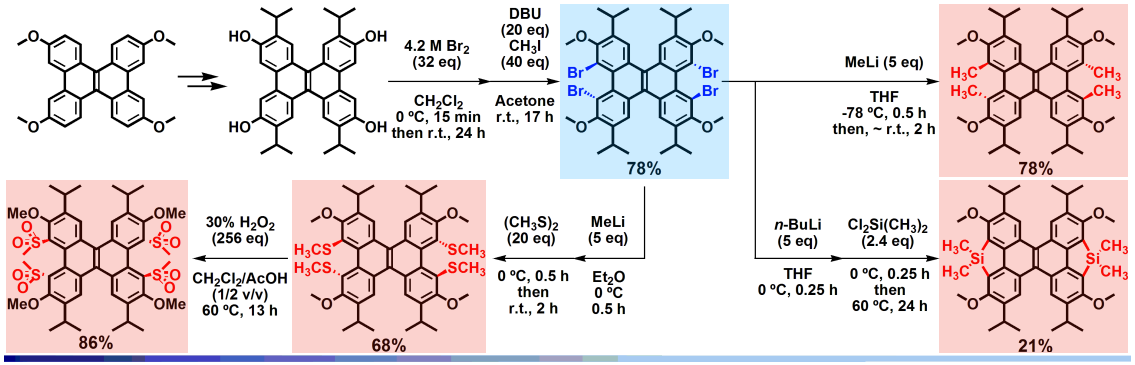
Relevant Synthesis to Manipulating Non-Planarity in a Dibenzo[*g*,*p*]chrysene

N. Yoshida, R. Akasaka, T. Iwasawa*

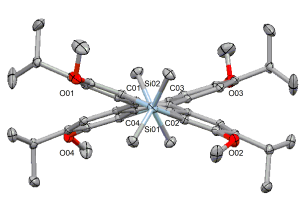
Department of Materials Chemistry, Ryukoku University, Seta, Otsu, Shiga 520-2194, Japan

1. Summary

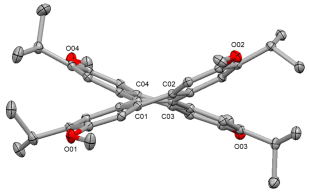
S. Kamiguchi, R. Akasaka, N. Yoshida, T. Imai, Y. Yamaoka, T. Amaya, T. Iwasawa, *Tetrahedron Lett.* **2022**, *92*,153664.



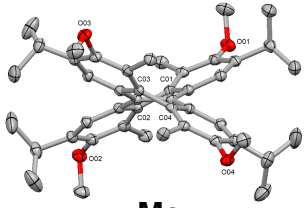
2. Torsion angles (Crystallographic and Computational Data)



-SiMe$_2$
31.2° (31.3°)

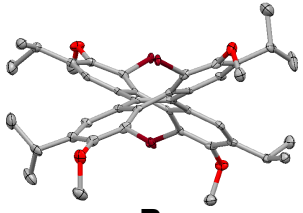


-H
36.7° (39.0°)

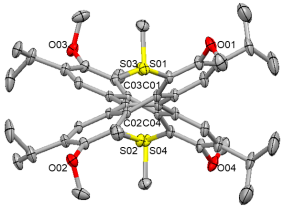


-Me
55.4° (56.5°)

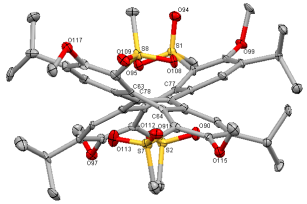
Selected



-Br
56.0° (57.5°)



-SMe
57.2° (56.5°)

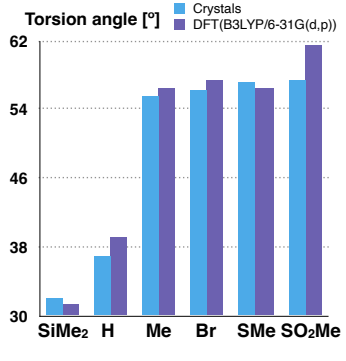


-SO$_2$Me
57.4° (61.4°)

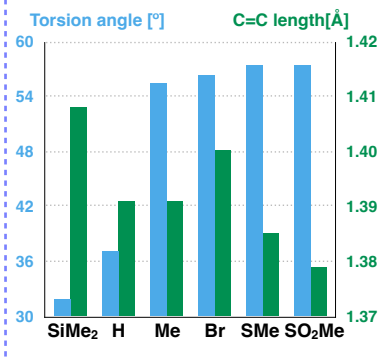
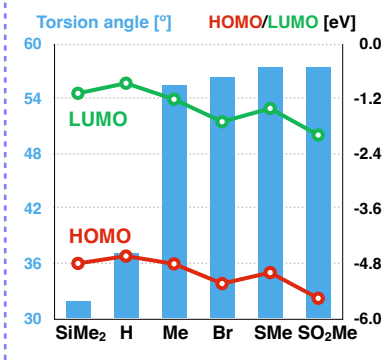
All

3. Correlation between substituents (= torsion angles) and structural features.

Torsion angles



Central C=C bond lengths



HOMO/LUMO levels