

トリアジン骨格を有する分子ローターを用いた結晶内の分子間ギア運動の開発とその精密制御

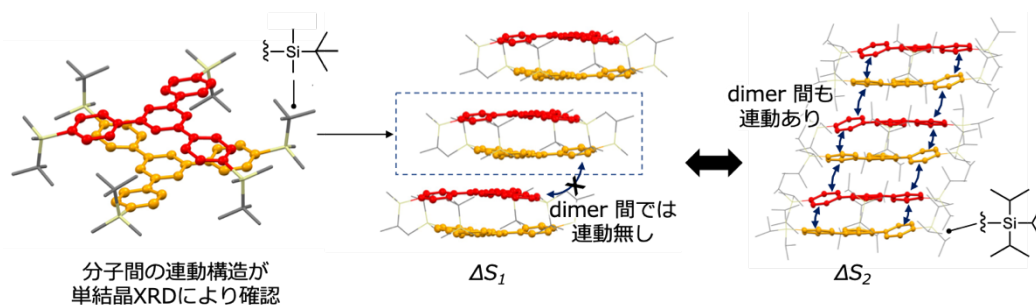
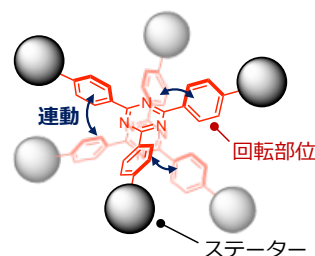
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Development of crystalline molecular gears by utilizing tri-phenyl triazine based rotors (¹Graduate School of Engineering, Hokkaido University, ²WPI-ICReDD, Hokkaido University, ³NanoMaterials Research Institute, Kanazawa University) ○Mingoo Jin,^{1,2} Ryunosuke Kitsu,¹ Natsumi Hamnyo,¹ Motohiro Mizuno,³ Hajime Ito^{1,2}

Crystalline molecular gear showing molecular correlated-rotation in crystalline media have attracted many interests because of the high potential for application to molecular machines.¹⁾ However, it is difficult to design the molecular gears in crystal due to unpredictable crystal packing. Recently, we have developed a crystalline molecular gear by utilizing inter-molecular packing manner of a 2,4,6-triaryl-1,3,5-triazine molecular rotors in crystal. In this work, we have designed and investigated the series of triazine-based crystalline molecular gears, which consist of phenyl-rings as a rotator with bulky silyl groups as a stator. The molecular rotors formed inter-locked dimer structure in crystal, having the correlated geometry between the phenylenes, confirmed by single crystal XRD. Interestingly, introducing different silyl-group could alter the inter-dimer packing manner. The geared rotations were observed by several solid-state NMR studies and the DFT calculation, which will be described in the presentation.

Keywords : Aziridine; Iminoiodinane; Metal Free; Iodine; Ammonium Iodide

結晶中で分子やその一部が隣り合う分子と互いに連動してギア運動を示す結晶を結晶性分子ギアと言う。この結晶は分子マシンへの応用が期待されているが、その設計指針は未だない¹⁾。本研究では、トリアリールトリアジン骨格を有する分子が結晶内で分子間の連動回転を示すことおよびその連動構造を精密に調整することに成功した(右図と下図)。本発表では、その分子間連動運動の詳細および関連する結晶構造について報告する。



1) Liepuoniute, I.; Jellen, M. J.; Garcia-Garibay, M. A. *Chem. Sci.* **2020**, *11*, 12994.