Multi-Dynamic Crystalline Molecular Rotors by N-Heterocyclic Carbene Binuclear Au(I) Complex with Solvated THF

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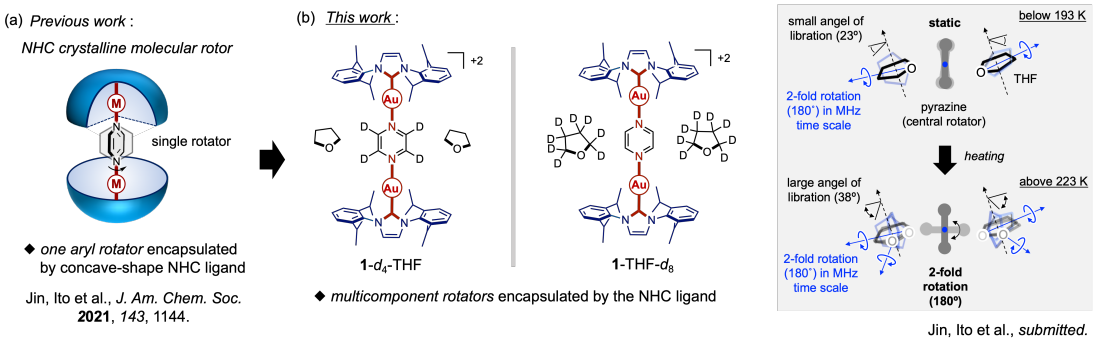
The design of molecular rotation in crystalline media has attracted much interest not only in the field of molecular machines but also in solid-state functional materials, because the rotation-induced molecular geometry alteration can provide an avenue for switching the physical properties of solid compounds.[1] The general blueprint of this design is based on the combination of a rotator moiety with a bulky and rigid domain as a stator that is used to construct the ordered frame as well as the local space that can undergoes molecular rotation. Many examples have utilized a single-component rotator that generally shows a simple rotational dynamics.[1] To broaden the application of crystalline molecular rotors, realizing larger complexity of molecular motions in the solid-state is important because the multiple molecular dynamics in crystals have a high potential to integrate various functions such as photophysical or dielectric properties

Here, we report multi-dynamic molecular rotations in crystals using a concave-shape *N*-heterocyclic carbene (NHC) binuclear Au(I) complex rotor bearing pyrazine and tetrahydrofuran (THF) molecules as multicomponent rotators. Single-crystal X-ray diffraction (XRD) measurements revealed that two THF molecules are located near the central pyrazine encapsulated by two bulky NHC ligands. From ^{2}H solid-state NMR analysis, it was observed that the pyrazine rotated in a 2-fold site exchange with a 180° rotational angle and a 31 kJ mol^{-1} energy barrier, while the THF molecules showed a 23°–38° libration with a lower energy barrier (14 kJ mol^{-1}). Interestingly, the pyrazine rotation was accelerated when the THF molecules rotated in fast site exchange with a large angle of libration, suggesting that the rotators exhibit multi-dynamics in a correlated manner



1) C. S. Vogelsberg, M. A. Garcia-Garibay, *Chem. Soc. Rev.* **2012**, *41*, 1892–1910.