The Noncovalent Approach in The Design of Luminescent Crystalline Rotors

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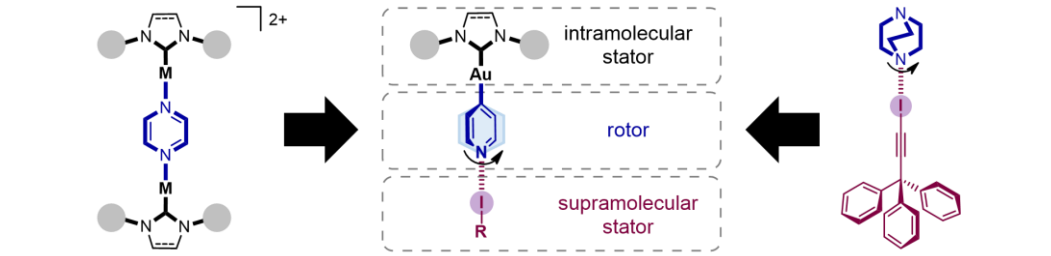
This work is aimed at the development of amphidynamic luminescent co-crystals based on the principles of the rational design of organometallic luminophores and noncovalent crystal engineering to produce materials that combine both luminescence and rotational motion. In pursuit of a new concept in the development of amphidynamic crystalline materials, we implemented the strategy of encapsulation of molecular rotor by two types of stators: intramolecular organometallic stator and supramolecular halogen bonding stator. The background of this work is based on the encapsulation approach utilized previously for semi-closed shell NHC metal complexes[1] and halogen bonding crystal engineering of DABCO-based molecular rotors.[2]

Therefore, we have developed the half-closed NHC gold(I) aryl complexes which could act as halogen bond acceptors and co-crystallized them with three types of organic halogen bond donors: iodopentafluorobenzene, 1,4-diiodotetrafluorobenzene, 1,3,5-triiodotrifluorobenzene. The several co-crystals with different ratios of components were obtained and characterized by single-crystal X-ray diffraction and luminescence spectroscopy in the solid state. All co-crystals display the strong dependence of the luminescence intensity on temperature which suggests the presence of rotational dynamics in the solid state.



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