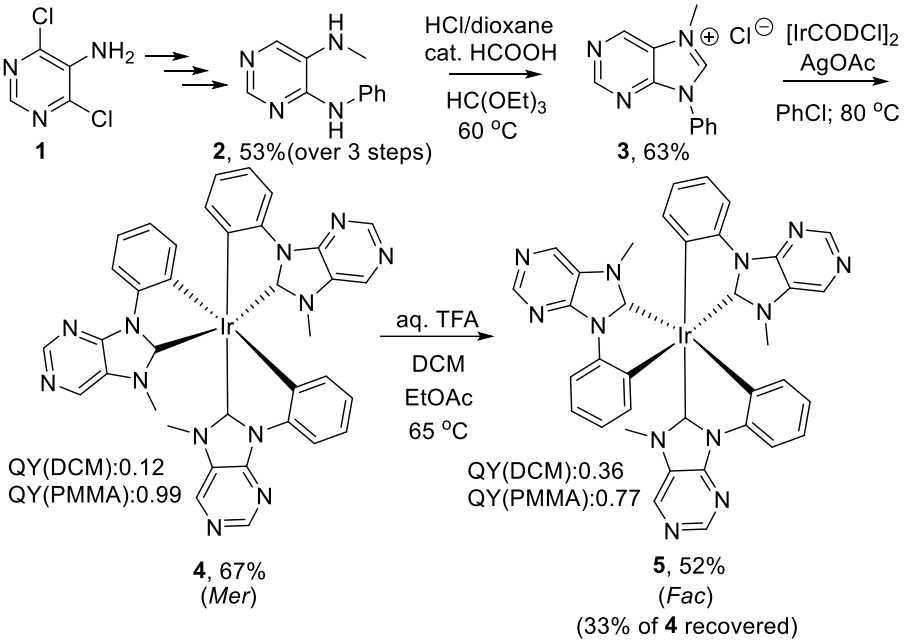
Synthesis of Phosphorescent Iridium Complexes with Purine Ligands and their Photophysical Properties

Research towards more efficient emitters in organic light-emitting diodes (OLED) continues, and especially for structures, that emit light in the high energy blue region. One of the approaches for achieving highly efficient emitters is using phosphorescent transition metal complexes, that utilize excited triplet states for emission. To the best of our knowledge, there are few publications that have prepared iridium complexes with purine carbenes and examined their photophysical properties.[1] Further research of such compounds is important for achieving optimal emitters for OLEDs.

The carbene precursor **3** was prepared from a functionalized pyrimidine derivative **1** via *de novo* purine synthesis. We utilized alkylation, S_NAr reaction, Pd catalyzed hydrodehalogenation and ring closure with orthoester to prepare compound **3**. *Mer* isomer **4** was selectively synthesized in a AgOAc mediated reaction, while *fac* isomer **5** was achieved in an acid catalyzed isomerization. XRD structures proved the identity of both isomers.[2] They emitted blue light, with *mer* isomer showing a bathochromic shift compared to *fac* isomer in DCM solution and in the mixture with PMMA. Emission also exhibited a bathochromic shift, when comparing PMMA doped solid state to DCM solution.



1. a) Qin, Y.; Yang, X.; Jin, J.; Li, D.; Zhou, X.; Zheng, Z.; Sun, Y.; Wong, W.-Y.; Chi, Y.; Su, S.-J. *Adv. Optical Mater.* **2022**, *10*, 2201633. b) Jin, J.; Zhu, Z.; Yan, J.; Zhou, X.; Cao, C.; Chou, P.-T.; Zhang, Y.-X.; Zheng, Z.; Lee, C.-S.; Chi, Y. *Adv. Photonics Res.* **2022**, *3*, 2100381.
2. Sebris, A.; Guzauskas, M.; Mahmoudi, M.; Volyniuk, D.; Grazulevicius, J. V.; Mishnev, A.; Novosjolova, I.; Turks, M.; Jonusauskas, G.; Traskovskis, K. *J. Mater. Chem. C*, **2023**, *11*, 14608.