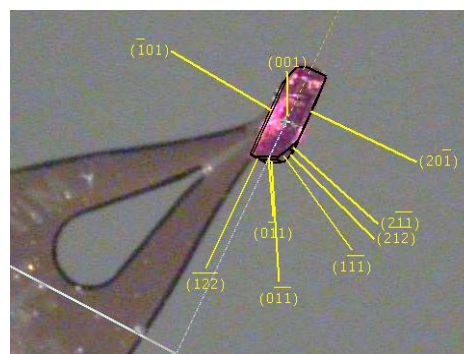
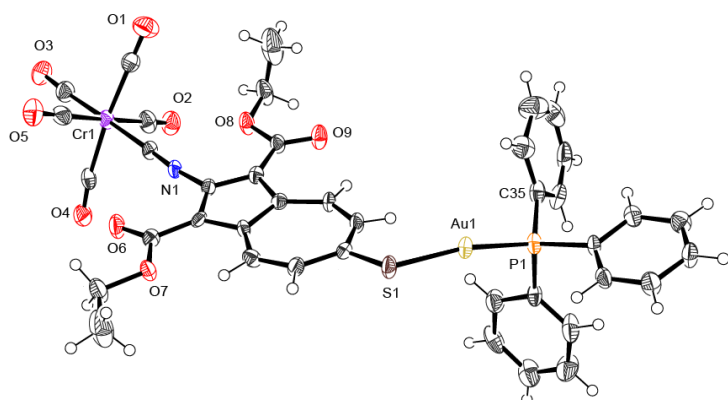


Biazulene-based organometallics relevant to molecular electronics

Azulene is a nonbenzenoid polycyclic aromatic hydrocarbon (PAH) comprised of an edge sharing combination of 5- and 7-membered sp^2 -carbon rings. The toxicology, carcinogenicity, and mutagenicity profiles of azulene are far more favorable compared to those of its benzenoid isomer naphthalene. Indeed, the former has 10 times lower acute oral toxicity and, unlike the latter, is not on the *California Proposition 65* list of carcinogens. Substances incorporating the azulenic motif offer unique opportunities in the realm of molecular and optoelectronic applications. The Barybin group has recently pioneered the design of unusual azulenic linkers and demonstrated their superiority in charge delocalization compared to similar benzenoid bridges. The X-ray structure of the first PAH π -linker equipped with both thiolate and isocyanide junctions is illustrated below. Given the robust redox profile of the 6,6'-biazulenyl moiety, our 2019 NSF-REU participant will engage in synthetic design of a non-symmetrically anchored linear biazulenic linker and then will work on assessment of its electron delocalization capabilities within electron-rich metal/organic frameworks. The student will acquire experience in organic, coordination, and organometallic syntheses (including air-free manipulations) and learn the basics of operation and interpretation of many techniques such as electrochemistry, electronic spectroscopy, X-ray crystallography, multinuclear NMR, FTIR, and magnetic measurements.



Relevant references

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