In-Situ Studies of Molecular Copper Compounds for Highly Selective Purification of Ethylene

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Purification of ethylene from ethylene-ethane mixtures is an important and challenging industrial process, currently performed by highly energy-intensive cryogenic distillation. We have been studying the reversible reaction of C2H4 with various molecular pyrazolate complexes of copper, and find that they are extremely selective for ethylene vs. ethane.1-4 A typical gas-phase adsorption/desorption reaction, which occurs at 320 K – 343 K at atmospheric pressure, is illustrated in Fig. 1.
We have performed in situ powder diffraction measurements of the repeated adsorption and desorption of ethylene from dense powders of several copper pyrazolate complexes at beamline 17-BM of the Advanced Photon Source.2,3 We have determined previously unknown structures of several of the compounds and monitor the conversion between phases with and without adsorbed ethylene. It is truly remarkable that the subject molecules reversibly pass between trimer and dimer structures in the solid state upon reaction with ethylene.

References
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{3} A. Noonikara-Poyil et al., "A molecular compound for highly selective purification of ethylene," Angew. Chem. Int. Ed. 60, 27184-27188 (2021).

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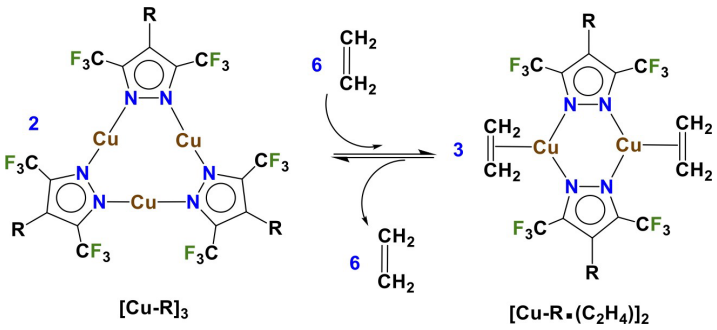

Figure 1. Reversible reaction scheme of {[4-(R)-3,5-(CF3)2Pz]Cu}3 to {[4-(R)-3,5- (CF3)2Pz]Cu(C2H4)}2