

Structural Analysis of Porous MOF Crystals

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1. Background

Metal-organic frameworks (MOFs) or porous coordination polymers (PCPs) possessing large surface areas and highly ordered structures, have demonstrated unique superiority in various fields, such as, storage/separation, luminescence, catalysis, and so on. Recently, we designed and synthesized a new azolate ligand (az), and used it to construct several new MOF crystals. However, we can not analyze the crystal structure owing to the very weak signal of single crystal X-ray diffraction obtained from conventional single crystal diffraction apparatus. According to the results of the last experiment (No. 2019ND601), this problem has been well solved by using synchrotron radiation experiments at Aichi Synchrotron Radiation (AichiSR) center. We therefore want to test some more MOF crystals at AichiSR.

2. Experiments

Five kinds of crystals were carried out for single crystal X-ray diffraction experiments on BL2S1. With a lot of effort, four crystals were successfully measured (Figure 1). Diffraction data was collected at room temperature through using synchrotron radiation at a wavelength of 0.75 Å.

3. Results and Discussion

Based on the results of the data collected at the beamline, a preliminary structural analysis was performed, and the initial phase could be solved in the process of testing. These crystals have a similar structure with Zn-az measured last time (No. 2019ND601). Afterwards, structural analysis was further performed, and it was confirmed that high quality data without any problems were obtained.

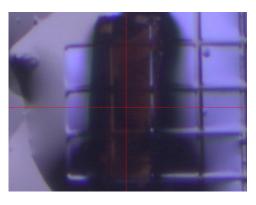


Figure 1. Optical microscope image of single crystal used in measurements.

4. References

- (1) Scofield, M. E.; Liu, H.; Wong, S. S. Chem. Soc. Rev. 2015, 44, 5836.
- Q.; Zaworotko, M. J.; Chen, B. Science 2016, 353, 141.
- (3) Lin, R.-B.; Liu, S.-Y.; Ye, J.-W.; Li, X.-Y.; Zhang, J.-P. Adv. Sci. 2016, 3, 1500434.
- (4) Yu, X.; Cohen, S. M. J. Am. Chem. Soc. 2016, 138, 12320.
- (5) Schoedel, A.; Li, M.; Li, D.; O'Keeffe, M.; Yaghi, O. M. Chem. Rev. 2016.