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BL2S1

Structural Analysis of Metal-Organic Framework Crystals

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1. Background

Metal-organic frameworks (MOFs), also called porous coordination polymers (PCPs), are well-known for their highly designable framework and pore structures,[1] which play an important role in numerous application areas including gas storages,[2] selective adsorption/separation,[3] catalysis,[4] etc. Recently, we designed and synthesized a new azolate ligand (az), and used it to construct new MOF crystals. However, we can't analyze the crystal structure owing to the very weak signal of single crystal X-ray diffraction obtained from the conventional single crystal diffraction apparatus. We believe this problem will be solved very well by using synchrotron radiation experiments at Aichi Synchrotron Radiation (AichiSR) Center.

2. Experiments

Four kinds of crystals (Zn-az, Fe-az, Co-az and Ni-az) were carried out for single crystal X-ray diffraction experiments on BL2S1. With a lot of effort, two crystals of Zn-az 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

The crystal structure of Zn-az can be briefly analyzed from the single crystal diffraction data of these two crystals. Accurate Zn-O and Zn-N bond lengths could be determined from the high-quality crystal data, and the newly synthesized azolate ligand could also be well verified. This result confirmed that the azolate ligand can participate in constructing MOF structure, which plays a great guiding role in the construction of other similar structures.

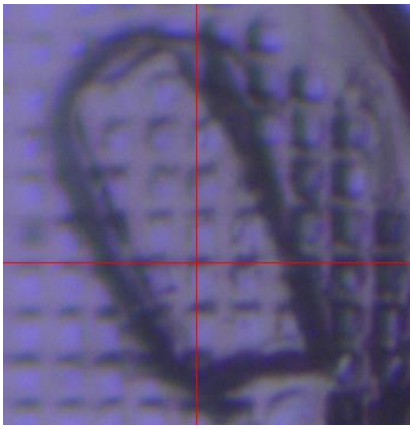

Figure 1. Optical microscope image of single crystal used in measurements.

4. References

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