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X-ray single crystal diffraction (SCD) analysis has the intrinsic limitation that the target molecules must be obtained as single crystals. Here, we report a new protocol for SCD analysis that does not require the crystallization of the sample. In our method, tiny crystals of porous complexes are soaked in the solution of a target, where the complexes can absorb and orient the target molecules in the pores. The crystallographic analysis clearly determines the absorbed guest structures along with the host frameworks. As the SCD analysis is carried out with only one tiny crystal, the required sample amount is of the nano-to-microgram order. With chiral guests, the space group of the crystal turned into chiral, enabling the determination of absolute configuration of the guests by anomalous scattering effect from the host heavy atoms (Zn and I). In this talk, following a general discussion, the applications of the method for natural product chemistry, synthetic chemistry, and pharmaceutical research will be discussed.

References

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