

MS33-P09 | PRIOR EVALUATION OF GUEST EXCHANGE IN CRYSTALLINE FRAMEWORK USING PRELIMINARY DIFFRACTION DATA

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The demand for accurate structure determination of guest molecule in crystalline host framework is rapidly increasing nowadays [1]. Sufficient guest exchange in crystalline framework is a crucial step to achieve definitive structural characterization of a guest molecule by crystal structure analysis. However, degree of guest exchange in a grain of crystal specimen is hardly evaluated until finishing X-ray diffraction data collection and structural analysis with spending a lot of time.

Here we show an analytical methodology for evaluation of guest exchange in crystalline framework using a small preliminary diffraction data. In this methodology, Bayesian inference is adopted for statistically estimating an intrinsic parameter, which represents thermal nature peculiar to a guest molecule, in diffraction data. Just applying this methodology to a few hundreds of diffraction data covering a possibly-wide resolution range for sample screening, guest molecules in crystalline frameworks were successfully distinguished.

Since efficiency of guest exchange is related to unique characters in crystal (e.g., grain size, surface conditions, and crystallinity), crystal specimens are usually nonuniform in degree of guest exchange. We will propose this methodology as a fundamental technology to select the promising crystal for accurate structural characterization of guest molecule in crystalline framework.

[1] M. Hoshino, A. Khutia, H. Xing, Y. Inokuma, M. Fujita, *IUCrJ*, 3, 139-151 (2016).