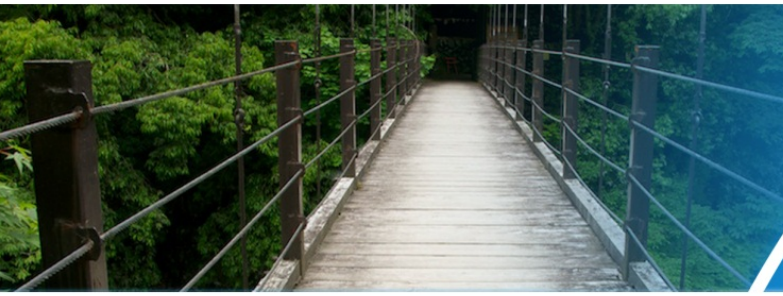

THE BRIDGE
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The XtaLAB mini benchtop system for accessible single crystal X-ray structural analysis

Kyoto University Graduate School of Engineering,
Materials Chemistry Course, Matsubara Laboratory Group

Specialized laboratory equipment and shared usage

The Katsura Campus A Cluster at Kyoto University consists of laboratories belonging to each course including the following studies within the Graduate School of Engineering: Energy & Hydrocarbon Chemistry, Chemical Engineering, Polymer Chemistry, Materials Chemistry, Molecular Engineering, Synthetic Biochemistry, Electrical Engineering, and Electronic Engineering. All laboratories are equipped with their own analytical instruments as well as various analytical instruments for shared usage as research tools by each course.

In February 2013, two XtaLAB minis were installed as specialized laboratory instruments for a materials chemistry course, located in Prof. Matsubara's laboratory, and as shared equipment for the chemical systems and materials engineering courses.

Organic synthesis research using single crystal X-ray structural analysis

The Matsubara laboratory conducts comprehensive organic synthesis reaction planning from four perspectives: reactive site analysis, development of new organic synthesis reactions, new organic materials, and methods in new organic synthesis. These studies are applied to drug development.

As with many general organic synthesis laboratories, the Matsubara laboratory's primary analysis methods are those normally in place in a laboratory, such as NMR, GC-MS, LC-MS, UV, and FTIR. Where single crystal X-ray analysis was required, the laboratory used the large equipment installed as shared equipment with the materials chemistry course. Although X-ray crystal structural analysis is a relatively unfamiliar method of analysis within the area of organic synthesis, here we will hear from Assistant Professor Takuya Kurahashi who selected the XtaLAB mini as his own research tool.

Reasons for choosing XtaLAB mini

- Simple installation
- Compactness of the machine
- Fully automated, requiring no authorized chief X-ray inspection engineer

I had images of previous single crystal X-ray structural analysis instruments only as large machines, so what impressed me about the XtaLAB mini was its compact appearance. Since there is almost no difference in size between analytical instruments used in organic chemical systems such as FTIR and UV, I expected that the instrument being readily available would enable easy measurement and accelerate our research speed. The instrument operates with a power supply of 100V, does not require an authorized chief X-ray inspection engineer, and from measurement to analysis can be conducted entirely automatically if operated according to the flow-bar in automatic measurement/automatic analysis mode.

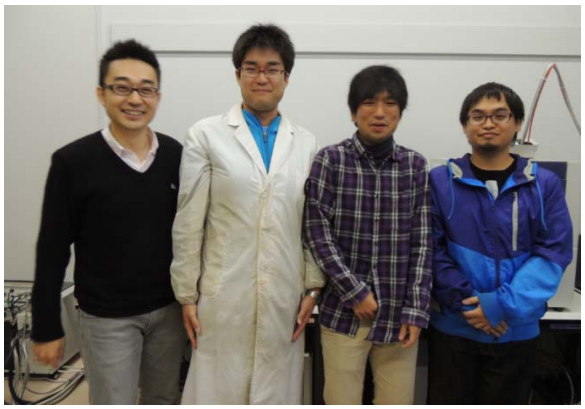
Although the hurdle to using single crystal X-ray structural analysis instruments is thought to be somewhat high, in actuality even laboratory students became able to use the XtaLAB mini soon after its installation. The reason for choosing this particular instrument was that, in ordinary research, I observed the structures of catalysts using transition metals such as platinum and ruthenium and the structures of heterocyclic compounds which used those catalysts; the measurement results obtained using the demonstration instrument were equal to those of the large instrument of another manufacturer that I used in the past.

Towards an instrument enabling accessible single crystal X-ray structural analysis

Professor Seijiro Matsubara proposed usage of this kind of easily usable single crystal X-ray structural analysis instrument as a more accessible instrument that would allow more students to utilize it, and so it was introduced as shared equipment with the chemical systems and materials chemistry courses.

Future hopes: Towards a device based on student usage and more accessible methods

Shortly after the instrument was introduced, an explanatory meeting on the instrument was held for those hoping to use the shared equipment. We could see that there was a high level of interest in the instrument, as more researchers and students participated than expected. After several years, the XtaLAB mini may become a standard piece of equipment in organic synthesis laboratories in the same way as the NMR and GC-MS. In the future, I hope that it will become easier for users to understand proper selection of crystals prior to data collection. I also believe that holding regular seminars for students with no knowledge of crystallography in relation to, for example, alert countermeasures on the CIF check, will make single crystal X-ray structural analysis a more popular and accessible method.



Assistant Professor Takuya Kurahashi was selected for the Advanced Catalytic Transformation Program for Carbonization (ACT-C) of the Japan Strategic Basic Research Programs (JST), and conducts research into the creation of functional catalysts focused on fluctuation in the electronic structures of porphyrin metal complexes, and into the development of advanced catalytic transformation technology through new catalytic reactions. The specialized laboratory equipment was purchased with this research fund.

http://www.jst.go.jp/act-c/research_area/ongoing/kurahashi.html

The shared equipment was purchased with the Ministry of Education, Culture, Sports, Science and Technology's "Grant for the Formation of Excellent Graduate Schools."
http://www.mext.go.jp/a_menu/koutou/kaikaku/takuetsu/

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Click here for more information about the Rigaku XtaLab mini

