Replacement of the CCD detector in single crystal X-ray diffractometer by HyPix-6000HE Hybrid Photon Counting (HPC) detector

The main goal of the project is to replace the old type of CCD detector in a monocrystalline X-ray single crystal diffractometer with a HyPix-6000HE Hybrid Photon Counting (HPC) detector. The HyPix-6000HE is the newest HPC detector offered by Rigaku Oxford Diffraction and is based on hybrid pixel technology, which combines pixelated silicon sensors with CMOS-based readout electronics. Key features of the HyPix-6000HE include direct detection of X-rays and single photon counting, extremely fast readout time, high counting rates, no dark current or readout noise, and single point spread function. The HyPix-6000HE is designed for low maintenance with air cooling. Thanks to all the above mentioned advantages this detector allows one to collect single crystal X-ray data of a far better quality than using older CCD type detectors. The quality of X-ray data is crucial for the quality of our quantum crystallographic and structural research such as experimental charge density studies of drugs and important biochemical molecules, charge density studies of minerals and other crystals under pressure, development and applications of Hirshfeld Atom Refinement (HAR) and Experimental Wavefunction Refinement (XWR) in studies of macromolecules, relativistic and correlation effects in heavy atom crystals, quest for new polymorphs of ice, crystals of hydrogen storage materials, electronic and structural properties high temperature superconductors, new supramolecular compounds and many other interesting systems.

I would like to emphasize that the diffractometer, the modernization of which we propose, is not only used for research by members of the Crystallochemistry Lab., Laboratory for Structural Research both at the Chemistry Department, Laboratory for Biochemical and Structural Research at CNBCh but it is also used for service purposes as a part of the Core Facility for Crystallographic and Biophysical Research to Support the Development of Medicinal Products which has been established at CNBCh UW. Thus, it serves a really large community of users. In fact, we use 3 different single crystal diffractometers (with Ag, Mo and Mo/Cu microfocus tubes) at CNBCh for ambitious crystallographic research. Let me present some statistics regarding the use of these pieces of equipment since their installation in 2013. All statistics are based on experimental log files as we register all measurements and can easily be verified.

Diffractometer/Microfocus tube	Ag	Mo	Mo/Cu	Total
Period of time	2013-2020	2013-2020	2013-2020	ca. 7.5 years
Number of full experiments	524	1178	2038	3740
Number of preexperiments	2002	5924	9365	17291
Total number of hours of data collection / h	14390	21919	26340	62649
Total time of preexperiments / h	356	734	1101	2191

So within the past ca. 7.5 years, we have done ca. 3740 full single crystal X-ray data collections and a significant part of them (ca. 40-50%) were high resolution data collections for the purposes of quantum crystallographic research. We have established structures and experimental electron densities for at least 2000 of new crystals. From the very beginning, when I got my first monocrystalline diffractometer in the early 90's of the previous century, I was convinced that apart from ambitious strictly scientific state-of-the-art research applications, a very expensive equipment should be used in its spare time for a wide range of users from the department, our University, other scientific institutions in Poland and abroad as well as for commercial companies. However, we always give priority to ambitious scientific projects and use this equipment for service in its spare time only.

There are several group of users of this equipment. Firstly, these are members of my (Krzysztof Woźniak) research group and research groups of other group leaders at the Chemistry Department and CNBCh who rooted from my group (prof. Paulina Dominiak, dr hab. Anna Makal, dr Maria Górna). Except the group leaders, this group of users include: D. Trzybiński, R. Gajda, M. Malińska, A. Hoser, Sz. Sutuła, S. Pawlędzio, M. Wanat, D. Tchoń, M. Cabaj, U. Budniak, S. Bojarowski, P. Kumar, J. Kutner, F. Sanjuan-Szklarz, B. Gruza, M. Ziemniak, K. Polak, A. Huć, A. Wrobel, M. Kisiała, S. Kandasamy, M. Archangelskis, M. Woińska + many others in the past.

The second group of beneficiaries of our diffactometers are some other researchers from our Department and from the other departments of our University. These are among others: K. Grela, M. Chmielewski, M. Barbasiewicz, E. Górecka, A. Szadkowska, T. Jaroń, P. Malinowski, P. Jolly, P. Kwiatkowski, R. Siciński, J. Mieczkowski. D. Pawlak, R. Kamiński, K. Jarzembska. K. Chmurski, E. Megiel, M. Wierzbicka, + a group of researchers from Geology Department (J. Parafiniuk, B. Bagiński, R. Macdonald, M. Stachowicz), + many others.

The next group of users comes from other scientific institutions in Poland: J. Zakrzewski (UŁ), K. Kowalski (UŁ), D. Plażuk (UŁ), L. Dobrzańska (UMK), J. Poznański, A. Mieczkowski, and K. Mieczkowska (IBB), Z. Rafiński (UMK), S. Popiel (WAT), M. Makowski (UG), O. Demczuk (IF, Warsaw), B. Korybut-Daszkiewicz (IChO), M. Woźny (IChO), T. Biernat (UG), P. Niedziałkowski (UG), P. Kaszyński (UŁ), K. Trzcińska and M. Łaszcz (IF), M. Czerniuk (WUM), A. Kutner (WUM), W. Paszkowicz (IF), I. Zarzyka (PRz), D. Gryko (IChO) + quite a few researchers from Warsaw Technical University (S. Podsiadło, K. Durka, J. Serwatowski, S. Luliński, G. Matyszczak, Z. Ochal, P. Guńka), L. Pajchel (WUM), Ł. Kurpaska(IBJ), M. Gagoś (UMCS), L. Mazur (UMCS), D. Kamiński (UMCS), A. Kozieł (UMCS), I. Galuskina and E. Galuskin (UŚ), W. Maruszak and P. Rudzki (Celon Pharma) + others.

Finally, I want to name our collaborators from abroad who also benefited from data collected using our diffractometers: Prof. W. Priebe (USA), Prof. W. Minor (USA), Prof. D. Haynes (South Africa), Prof. A. Korlyukov (Russia), Prof. D. Hasa (Italy), Prof. J. Henn (Germany), Prof. E. Zschech (Germany), Dr. M. Gutmann (UK), Prof. S. Grabowsky (Switzerland), Prof. A. Pawlukojć (Dubna, Russia), Dr. M. Kelland (Norway), Dr. F. White (Rigaku), Prof. A. Haddad (Tunisia), Dr A. Harchani (Tunisia), Prof. A. Beheshti (Iran), Dr. S. Soleymani (Iran), Prof. T. Sedaghat (Iran), Dr. S. Varughese (India), Prof. V. R. Pedireddi (India), Prof. Y. Lampeka (Ukraine). We also have collaboration with several companies including: WPD Pharmaceuticals, Pharmaceutical Research Institute, OncoArendi Therapeutics, Pikralida, Cellis, Leaderna Biostructures, Celon Pharma.

As our groups of the primary users of the diffractometers (K. Woźniak, P. Dominiak, A. Makal) — publish for last years, all together, ca. 40 papers per year and ca. 70-80% of them contain structural and electron density results obtained with our single crystal diffractometers, more than 210 papers have been published by us (by our "supergroup"). As we also have had quite a few users who wanted just crystallographic service and they later use results of crystallographic studies in their papers without us as co-authors, I estimate that at least 250 papers have been published in which data from our diffractometers have been analysed and used. Our intense research activities also mean many bachelor, MsS, PhD, habilitation degrees and even professorships. Thanks to these activities we also have had ca. 20 different grants, which has helped us to be so productive.

In conclusion, the proposed upgrade of the single crystal detector when granted – will serve not only us, singular researches and our research groups' members, but it will be of a great help to the whole crystallographic community of users of our diffractometers. This is particularly important for the state-of-the-art quantum crystallographic research which requires the best possible quality of data which can be achieved with this new HyPix-6000HE Hybrid Photon Counting (HPC) detector. Also studies of subtle phase transitions, quantitative studies of electron densities and their changes under variable pressure or temperature, studies of superconductive crystals, H-storage materials etc require the highest possible quality of the diffracted data and the new detector will allow to get such data.