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SINGLE CRYSTAL X-RAY LABORATORY AT THE INSTITUTE OF PHYSICAL CHEMISTRY STU IN BRATISLAVA

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X-ray laboratory was established in 2005 with the support of structural funds INTERREG IIIA as a National Laboratory for obtaining single crystal diffraction data. Laboratory is of service for both academic and commercial users. According the statute the academic users can obtain the data by covering the running cost of the measuring time. For non-crystallographers the laboratory offers the help from the solving the crystal structure up to preparing the crystallographic part for publication. The laboratory is equipped with GEMINI R diffractometer and low temperature attachment for data collection at 100 K.

There are two main goals of the laboratory. The first, to produce the data collection for 'routine' single crystal analysis, the second, the high accurate data for study of electronic structure.

Nowadays, the single crystal structure analysis of well crystallized samples is quite straightforward and take only some hours. As the diffractometers and software are better and better, the problems which seems to be problematic in the past are possible to be solved at this time. Our laboratory is able to solve the crystal structure of very small, weak diffracting crystals, merohedric twins and the absolute structure of small organic molecules. To demonstrate our results in these branches we can show the next examples:

1. The smallest crystal of composition $C_{15}H_{14}O_2$ with the crystal dimension of 0.033 0.038 0.242 mm was solved with R-value of 4.18% for 1166 observed diffractions.
2. The software development in the merohedric twins makes this much more easy. As an example we can show the crystal structure of N,N'-Diphenylsuberamide, $C_{20}H_{24}N_2O_2$ [1].
3. The absolute structure of natural (+)-calvine, $C_{14}H_{25}N_1O_2$ [2] was determined.

Data collection for electronic structure studies should have a high redundancy. Crystal quality should be excellent and the experiment lasts for two – three weeks. These results are still in the stage of improvements. Anyway, some results which have been already published can be presented:

4. Electronic structure in tetrakis ($_2$-Acetato) -diaqua -di-copper(II) complex [3].
5. Electronic structure in of $[RuCl_3(indazole)_2NO]$ [4].

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2. P.Kubizna, I. Špánik, J. Kožíšek , P. Szolcsányi, Tetrahedron, **66**, (2010), 2351.
3. J. Kožíšek, L. Perašinová, M. Breza, *Acta Cryst*. **A64,** (2008), C128.
4. J. Kožíšek, M. Fronc, M. Breza, K. Schiessl, V.B. Arion, *Acta Cryst*. **A65,** (2009), S303.