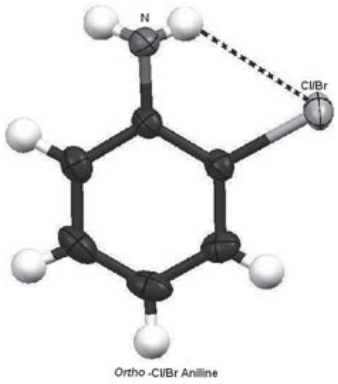
lattices and establishes that indeed fluorine has a directing influence in molecular assembly. In order to evaluate the propensity of interactions in halogens in general *ortho* chloro and *ortho* bromo anilines were crystallized from their respective liquids via *in situ* cryocrystallization method. The crystal structures are isostructural belonging to a trigonal system, space group $P\,3_1$. The crystal packing is due to intramolecular N-H…Cl or Br and intermolecular N-H...N hydrogen bonds. However, in the case of *ortho* bromo aninline short Br...Br contacts (3.64 Å) are observed suggesting that this interaction is a consequence of the size of Br atom.



Ortho -Cl/Br Aniline

1. Deepak Chopra and T. N. Guru Row,*Journal of the Indian Institute of Science*, 2007,**87**, 167

Keywords: cryocrystallography, *in-situ* structure determination, intermolecualr interactions

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Relation of DLS distribution of protein samples with thermal stability

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With the rise of ultimate methods such as X-ray crystallography and NMR, the number of proteins, of which complete quaternary structure was confirmed, has rapidly increased. To be analyzed by X-ray spectroscopy, protein purification is very important to evaluate the detail of its structure. Sample separation is often used by gel permeation chromatography and it's been checked by poly acrylamide electrophoresis, such as SDS-PAGE, however it is required for crystallography to be purified as a level of quaternary structure of proteins. So we often use the system of dynamic light scattering (DLS). It is expected that protein quality is accepted by result of the DLS distribution below 20% for crystallography, but it's not always. Various kinds of proteins have various kinds of strutures and stiffness for thermal stability, and DLS distribution depends on the aspect ratio of particle or stiffness of the surface. In this study, we discuss relation of DLS distribution of proteins with thermal stability and other factors.

Keywords: dynamic light scattering, polydispersity, protein stability

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Microseed matrix screening: A modified version

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The crystallization of purified proteins has remained one of the bottlenecks for the determination of protein structures by X-ray diffraction methods. The crystallization process can be considered composed of two sequential processes. The first is an initial nucleation step and the second subsequent growth of crystal nuclei to well ordered crystals. A method that influences the first step of this process "Microseed Martix Screening" has recently been published. The method is further development of the work by Ireton and Stoddard [2] aims at influencing the nucleation event in crystallization screens. We report the implementation of and experience of with this method in our laboratory. The seed-bead method is used for preparation of the seed stocks. The protein, reservoir solution and seed stock are pipetted simultaneously using a three-bore dispensing tip mounted on the Oryx 8 robot (Douglas Instruments), setting up screening crystallization experiments with seed stock solution added. The authors of [1] used the method with 5 test proteins and observed that the number of crystals hits increase from 1-9 to 21-63. We have also observed an increased number of crystal hits, but that include both protein crystals ad nonobvious salt crystals. Salts crystals can lead the crystallization experiments astray and consume valuabe time and sample. We have therefore modified the method to inlude two control experiments: 1) Crystallization experiments with the Izit Dye for positive indentification of protin crystals and 2) Crystallization experiments with protein buffer for positive identification of salt crystals.

1. Allan D'Arcy, Frederic Villard and May March Acta Cryst. (2007) D63, p550-554
2. G.A., Ireton and Barry L. Stoddard Acta Cryst (2004) D60, 601-605.

Keywords: crystallization strategies, microseeding, protein crystallization

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An open and flexible robotic system designed towards autonomous protein crystal harvesting

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Process automation with robotic mounting equipment has become an essential element of modern crystallography facilities, resulting in efficient utilization of valuable X-ray resources. However, serious rate-limiting manual operations persist in the crystal harvesting process. Based on experience gained during development of an operator-assisting universal micromanipulation robot (UMR) prototype, we discuss progress and challenges ahead for the design of a fully autonomous, integrated system capable of reliable harvesting of protein microcrystals. Harvesting of micron-sized objects requires a sophisticated mechanical system, and autonomy means that a capable real-time machine vision system embedded in powerful control software must be developed. The vision system and the mechanical system interact in a complex way, and the demands on the optical system pose additional and formidable design challenges. Real time image processing interfaced with mechanical control and