DIMAS: A web-based service crystallography submission and data management system

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The Department of Chemistry at the University of Durham, UK has a long and prestigious reputation in the field of single crystal x-ray crystallography. As the premier technique allowing full structural identification of crystalline materials, crystallographers at Durham University work with researchers in numerous fields including materials science, chemistry, physics, biology, and engineering.\textsuperscript{[1]}

In collaboration with OlexSys Ltd.\textsuperscript{[2]} and Labsafe\textsuperscript{[3]} we have developed a web-based platform to allow researchers to submit crystalline samples for x-ray diffraction analysis to the in-house crystallography service. DIMAS guides users through the process of submitting samples allowing them to include details about the synthesis and crystallisation conditions. There is an imbedded chemical drawing module to input the expected compound and users can keep track of all their submissions in one convenient location.

Following collection, a full set of crystallographic files, including data reduction outputs, structure solution and refinement files, as well as rendered images of the structures can be uploaded. DIMAS automatically extracts the relevant unit cell parameters, symmetry and data statistics as well as allowing the user to download the archived files and giving research group leaders oversight over their research group data.

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\textsuperscript{[1]} https://crystallographygroup.webspace.durham.ac.uk/
\textsuperscript{[2]} https://www.olexsys.org/
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