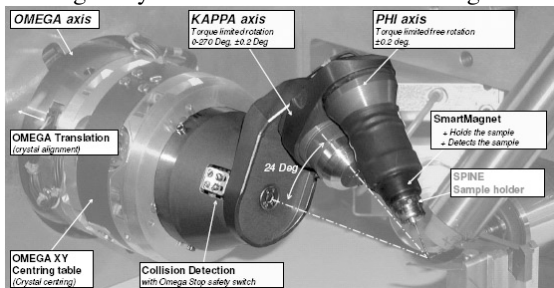


W0204

Routine Crystal Reorientation. S. Brockhauser¹, F. Cipriani¹, S. McSweeney², R. Ravelli¹, The DNA Collaboration (www.dna.ac.uk) ¹EMBL-Grenoble, France, ²ESRF, Grenoble, France.

Macromolecular crystallographers (MX) in general use simple single-axis goniometers for data collection, and most automation and remote data collection efforts exclude the use of multi-axis goniometers. However, the call for more degrees of freedom to re-orient the sample has never completely faded. The reimplementation of “old” methods of collecting truly redundant data is becoming more and more important with the increased use of very small anomalous signals for solving macromolecular structures.



The construction of a MiniKappa Goniometer Head has allowed us to reduce one of the major risks of traditional multi-axes goniometers: that of collisions. This small device offers routine crystal re-orientation and fast data collection sweeps without stability problems. A comprehensive software package that includes modules for calibration, 3D virtual beamline simulation, crystal re-orientation calculation, automated sample re-centring as well as smart

multi-pass strategy calculation is being developed and integrated with the data collection system DNA (automated collection of data).

We will present the general use of DNA for service data collection with particular emphasis on exploitation of multi-axes goniometers.

Work funded in part by BIOXHIT.