QuantumBox: The future of crystallography

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QuantumBox is a collaborative community project which brings together all the tools that are required to perform modern small-molecule crystallographic analyses accessibly, reliably and with ease.

Interoperability: The data management system underlying QuantumBox ensures that many ‘standard’ crystallographic packages can operate securely on the same data. This covers the entire crystallographic workflow including data integration, primary structure solution and refinement as well as cutting-edge modern refinement techniques and extending into charge density analysis and properties calculations.

Beyond IAM: In going beyond the Independent Atom Model, QuantumBox opens the world of quantum crystallography to ‘routine’ structure analyses. Modern experimental diffraction data contains so much more information than was conceivable in the past – and together with equally unprecedented cheap and accessible computing power, crystal structures can be so much more than those based on techniques that were developed many decades ago.

Resilience: Inherent to QuantumBox is a desire to protect contributing software as well as resulting structures from falling into oblivion as time goes by. By linking their crystallographic software to QuantumBox, authors can ensure that their contribution to the field of crystallography will endure. Equally, when authoring a crystal structure of any kind through QuantumBox, a full version history is maintained so that every step along the analysis can be repeated using the correct version of the various software that was used during creation.

Reusability: QuantumBox evolves by constantly increasing the number of reusable functions which are available for use by all participating existing software – or from which entirely new crystallographic software can be built. This is achieved by contributing the Quantum Crystallographic Toolbox (qctbx) to the well-established cctbx [1] project.

Organisation: The project has been funded for three years (starting in September 2022) and is led by the University of Southampton and Durham University. This publicly funded project is open source and free to use for everyone. Anyone with an interest in contributing their software – be it a large and complex software system or a single function is welcome to join QuantumBox. Professional research software engineers will work with contributors to ensure that the integration will be carried out sustainably and with maximum effect. QuantumBox has been endorsed and has the full support of the relevant European and IUCr commissions in quantum crystallography. The governing body of the project, together with the crystallographic expertise available in Southampton and Durham ensures that this really will be the future of crystallography.

For the latest information regarding QuantumBox, please refer to our website at: https://qubox.org/

¹ https://cci.lbl.gov/docs/cctbx/

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