MS106.O02

Data quality as a driver for ever more subtle charge density analyses

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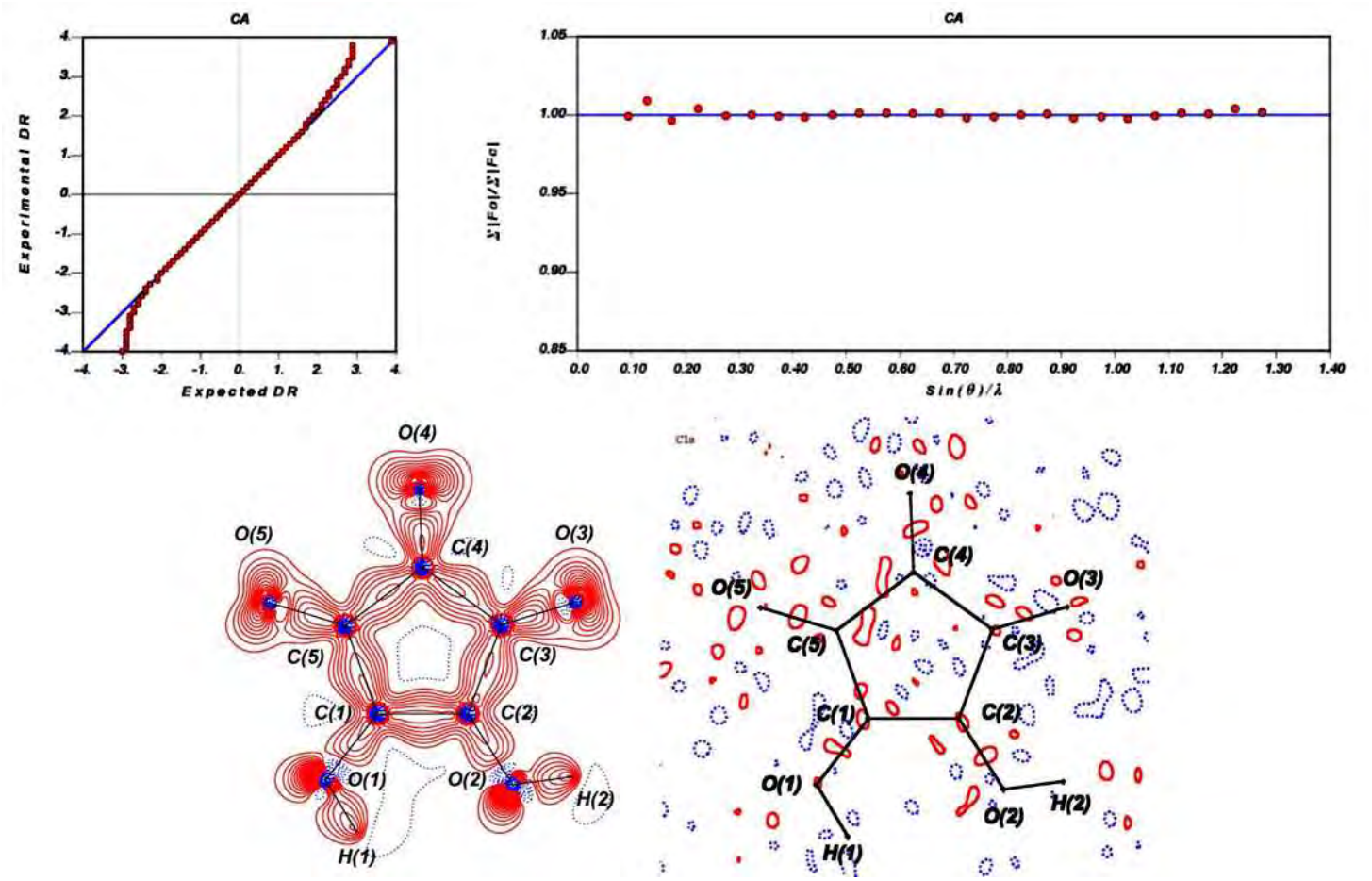
The constant progress in both X-ray source and detector technology has clearly led not only to faster data collection, but also to improvements in data quality. As we move towards the unattainable “holy grail” of error free diffraction data, it is possible to address ever more subtle questions concerning the electron density distribution and associated properties. Current applications to the study of weak interactions, core polarization, heavy element compounds, anharmonic atomic displacements, and anisotropic motion of hydrogen atoms will be presented. The reliability of these studies will be discussed based on evaluations of data quality and refinement statistics.



Keywords: experimental charge density