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A Multi-Data-Set Data Collection Strategy Using Dose Derived Exposures for Optimum Data Acquisition.
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In estimating the $\sigma(I)$ for a measured intensity (I), two factors are generally taken into consideration: a counting statistics term, proportional to the square root of the measured photon counts, and an “experimental factor”, proportional to the measured photon counts. The $I/\sigma(I)$ for a reflection, in theory, increases with increased photon counts and thus the longer the exposure time the better the signal in the data. However, in practice, the radiation damage cannot be avoided. Thus, a crystal has a fixed dose related lifetime after which data quality deteriorates rapidly. In addition, we also need to consider the detector’s DQE effects.

We are exploring a dose derived exposure strategy where we collect N data sets using an X/N exposure time instead of one data set with a total exposure time of X. This strategy in theory should reduce the “experimental error” described above, thus, increasing the $\langle I/\sigma(I) \rangle$ and anomalous $\langle S/N \rangle$ in the data. This expectation is now confirmed using Zn-free insulin’s anomalous scattering data collected at SER-CAT. Both the theoretical and experimental aspects of this approach will be discussed.