

In the Rapidly Advancing Field of MicroED, What Should be Done About Past Data?

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The topic of data archiving should be at the forefront of the minds of people working in the MicroED / 3D ED field. This field has seen a recent explosion of interest with new structure depositions climbing each year, especially for small molecules. Many groups, including my own, are using crystallography tools built for X-ray diffraction to process MicroED data, a process that regularly produces structures but has substantial room for improvement. The opportunity to re-process old raw data with improved data processing tools is extremely enticing and hopefully holds the key to improving MicroED structures and bringing our R-factors better in line with those from single crystal X-ray diffraction (scXRD). Recent advances in electron diffraction data processing tools have allowed for absolute configuration determination via dynamical refinement, demonstrated the differences in hydrogen inter-atomic distances for MicroED data relative to scXRD and have opened the door to charge state refinement. I expect the coming years to build on these advances and I look forward to continuing to improve on structures derived from previously collected data. This of course begs the question of what data should be archived and where it should be stored (the 3DED/MicroED Datasets community on Zenodo.org is one such option). Publicly available raw data is extremely important for software developers, especially in a field moving as quickly as ours. I look forward to exploring these topics with those within and outside the MicroED field.