Metadata standards in x-ray crystallography

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Experimental methods in crystallography are only becoming more diverse, and the metadata that must describe them is growing in complexity at the same time. Crystals are analyzed using rotational methods at synchrotrons on advanced goniometers, or with random orientations in serial crystallography at synchrotrons and XFELs. Beams are monochromatic, Laue, SASE, multi-color, or stochastic, are continuous or pulsed, and have profiles large and small, focused using a terrific variety of lenses and mirrors. Detectors are using counting and integrating methods, have single panels or hundreds of panels in complex configurations, differing efficiencies, materials, sensor thicknesses, pixel sizes, binning methods, gain/pedestal calibrations, and framing speeds. Users can even bring in multiple detectors at arbitrary positions for advanced methods. Finally, users adapt their experiments according to the constraints of the facility, but also spread their work across many facilities, taking advantage of available beamtime and endstation configurations. Therefore they need their data to be as cross compatible with their software as possible. How can facilities ensure the data they create is usable outside of their own custom environments? For this talk/panel discussion we will focus on standardization issues for metadata at crystallographic beamlines and how facilities can move together to common methods for metadata organization and storage, using technologies such as ISPyB and NeXus.