

The ACA imgCIF/CBF Workshop

22 July 2006

The Charge to the Workshop:

Organize the adoption of a standard, self-documenting format for diffraction image files.

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ACA Data, Standards, and Computing Committee



A little history: There has been over a decade of discussion and activity on this question.

- March '95 – The subject of internally documented images was raised in a workshop on GUT's at BNL.
- July '95 – The SR-SIG endorsed a standard format with header at the ACA meeting.
- Early '96 – Intense E-mail discussions made progress.
- August '96 – Report from this group at Seattle IUCr mtg CIF wkshp.
- October '97 – Major workshop at BNL. Led to two years of off-line work to establish the imgCIF/CBF standard.
- August '99 – Reported to IUCr COMCIFS.
- July '00 – Submitted to COMCIFS
- December '00 – Approved by COMCIFS
- May '05 – ACA data committee says, "Let's get on with it!"



The point of this workshop:

- The diffraction experiment for small molecules is like spectroscopy – give the specimen to the machine; hit <Enter>; look at the answer; submit the CIF file to the Cambridge Crystallographic Data Centre.
- High-Throughput macromolecular crystallography is approaching this situation.
- May '05 – ACA data committee says, "Let's get on with it!"

