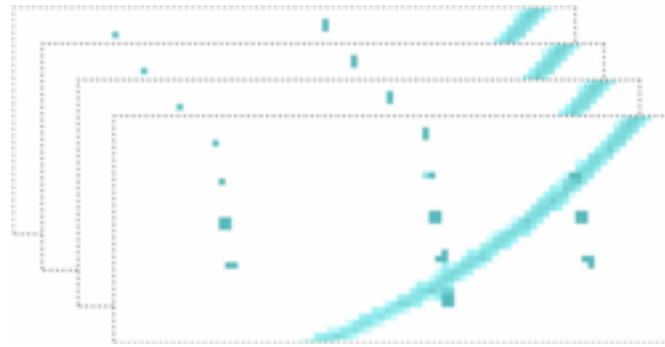




Review of the Status of imgCIF

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ImgCIF Workshops

Tuesday, 14 Aug 2007, 12:45 – 13:45 Barbirolli Room

- 12:45 – 13:00 Introduction and review of status of imgCIF – Herbert J. Bernstein
- 13:00 – 13:15 Experience with imgCIF for the Pilatus 6M detector at SLS – Clemens Schulze-Briese
- 13:15 – 13:30 “imgCIF: a developers perspective” -- Graeme Winter

Friday, 17 Aug 2007, 12:30 – 17:00, room 1.17 Diamond House, Diamond Light Source, Didcot, Chilton

- 12:30 – 12:45 imgCIF and the interaction with NeXus – Herbert J. Bernstein
- 12:45 – 13:00 Experience with imgCIF at Diamond – Alun Ashton
- 13:00 – 13:15 HDF – Mike Folk
- 13:15 – 13:30 Status of Data Formats in Cryo-electron Microscopy – Matt Dougherty
- 13:30 – 13:45 (Topic to be announced) – Chris Nielsen
- 13:45 – 14:00 Break
- 14:00 – 15:00 Discussion – interaction among imgCIF, NeXus, HDF and XML
- 15:00 – 15:30 Discussion – open issues in imgCIF
- 15:30 – 16:30 Formulation of recommendations
- 16:30 – 16:45 Future plans

Introduction

What is imgCIF/CBF?

1. A clearly defined set of terms to use in describing raw diffraction images (data) and the way in which they were collected (metadata); and
2. A workable and efficient format in which to record, archive and transmit data and metadata; and
3. Support software (e.g. CBFlib)

Status?

Little use, some support (fit2d, mosflm, adxv)

Community uses dozens of distinct formats

Use starting now at SLS and Diamond

Introduction (cont.)

Pending Issues?

Integration with other data frameworks

NeXus, XML, HDF

Integration with SAS

Axis definitions without a goniometer

MiniCBFs

Just the data with
the metadata gathered under just one tag

Jiffies

Cylindrical Detectors

New category for axis origins

Versioning

Why Does imgCIF/CBF exist?

Issue:

Managing massive amounts of data
in structural biology; e.g. in proteomics

Problem:

Many different data formats.

Practical Solution:

Provide a common approach to interchange
Crystallographic Information Framework (CIF)

Crystallographic Information Framework (CIF)

Started in 1990 by the International Union of Crystallography to reduce friction in managing structural data

[Hall, Allen, Brown 1991] [Hall, McMahon 2005]

Great success in handling of structural data for small molecules

Clarified the terms for macromolecules

mmCIF, PDBML

Effort to bring similar organization to synchrotron image data

imgCIF/CBF

Other Important Frameworks

CCP4 [CCP4 1994]

Collaborative Computational Project, No. 4, (CCP4) is a suite for protein crystallography. It “is a set of separate programs which communicate via standard data files”. Many programs have been adapted to CCP4 file formats

XML [Bray, Paoli, Sperberg-McQueen 98]

The eXtensible Markup Language is a text-based approach to marking up documents that has become a standard tool for managing data about data (metadata), e.g. in PDBML and CML.

Other Important Frameworks

NeXus [Klosowski et al. 1998].

“NeXus is a data format for the exchange of neutron and synchrotron scattering data between facilities and user institutions. It has been developed by an international team of scientists and computer programmers from neutron and X-ray facilities around the world. The NeXus format uses the hierarchical data format (HDF) that is portable, binary, extensible and self-describing. The NeXus format defines the structure and contents of these HDF files in order to facilitate the visualization and analysis of neutron and X-ray data. In addition, an application program interface (API) [was] produced in order to simplify the reading and writing of NeXus files. The details of the format are available at <http://www.neutron.anl.gov/NeXus/>”.

What Makes CIF Different

CIF clearly defines its terms in dictionaries

core CIF, powder CIF, modulated structures CIF,
electron density CIF, macromolecular CIF, image
CIF, symmetry CIF

**The same terms can then be used in multiple
formats with no loss of information**

e.g. mmCIF vs PDBML

CIF is very database-friendly

CIF is documented (International Tables Volume G)

CIF supports arrays, binary and compression well

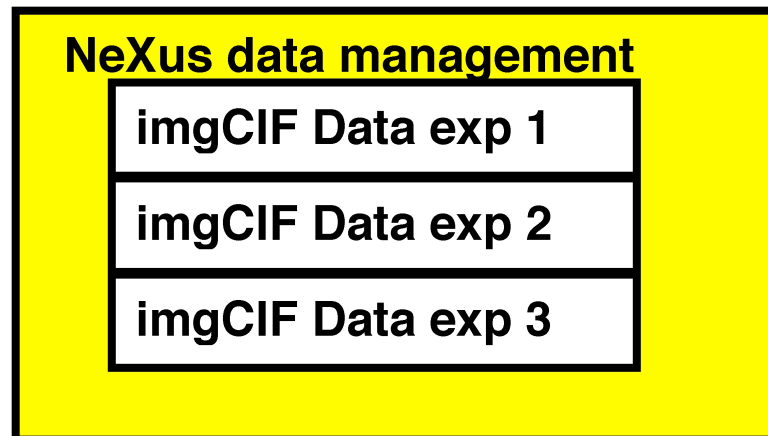
What Makes CIF Relevant?

“Diamond intends to provide their PX beam lines with imgCIF data, but to work to having a true [NeXus] infrastructure. Soleil intends to produce imgCIF for their PX beam lines and simply to encapsulate the imgCIF data sets as data (headers and all) within a [NeXus] infrastructure. ISIS is working purely in [NeXus]. At the moment, the critical need seems to be for both [NeXus] and imgCIF instrument definitions. [NeXus] seems to be well equipped with neutron instrument tokens and the X-ray tokens are a work soon to be in progress. ...”

-- from email summary for the group by HJB subsequent to a meeting at Diamond, 10 January 2006

Where Should imgCIF, NeXus and mmCIF fit?

imgCIF dictionary extends mmCIF to manage data images
NeXus to provide a data framework within which to manage
multiple sets of experimental data for multiple experiments
mmCIF provides the base within which to manage the entire
crystallographic experiment



Integration of imgCIF with NeXus

ImgCIF is tightly structured

makes it easy to map from imgCIF to other frameworks with less structure

makes it hard to map from less structured frameworks to imgCIF

Matches need to be found between

NeXus groups and data items versus

imgCIF categories and tags

not just for the items, but for their relationships

Details to be discussed Friday

Integration with SAS

1998 -- 2007 -- cif_sas.dic Marc Malfois, Dmitri Svergun, revisions by I. D. Brown

Needs work to align with imgCIF, mmCIF

Major issue: axis definitions

If there is no goniometer the standard imgCIF definition of X does not work. We keep the origin in the sample, but use an X derived from the fast axis of the detector if there is no principal goniometer axis.

miniCBFs

Issues

Not all information is available at time of data collection

Time constraints may limit complexity of what can be written

Processing programs may need a minimal header

Issues came to a head in setting up for SLS detector

Proposed solution

Write miniCBF at collection

Convert to full imgCIF with convert_minicbf program

Jiffies

Small programs to convert to/from imgCIF

Recommended by Hawaii imgCIF workshop in 2006

Conversion to imgCIF from MAR, ADSC and SLS
miniCBFs working

Work on Bruker-AXS starting

2 year project funded by DOE starting now

Cylindrical Detectors

Issue raised by James Hester

Can be done using the current dictionary
but requires implicit definition of the origin direction
for rotation axes.

Better approach

new category, `AXIS_ROTATION_ORIGIN`

give a unit vector at right angles to the rotation axis
representing the direction of the rotation axis at its
zero setting.

Versioning

After (or even during) initial data collection we may have multiple versions of the same items, e.g. beam center

```
loop_
  _variant.variant
  _variant.role
  _variant.timestamp
  _variant.variant_of
  _variant.details
.      "raw data" 2007-08-03T23:20:00 . .
indexed "preferred" 2007-08-04T01:17:28 .
      "indexed cell and refined beam center"
```

Software status

CBFlib (<http://www.bernstein-plus-sons.com/CBF>) provides

- API (C function library, under GPL or LGPL, your choice)
- more compressions, major speedup, support for maps

- Manual

- Sample files

- Utilities (under GPL only)

 - convert_image (works for Mar or ADSC)

 - convert_miniCBF (e.g. for SLS images)

 - cif2cbf

 - vcif2

mosflm (<http://www.mrc-lmb.cam.ac.uk/harry/mosflm/>) supports imgCIF

adxv (<http://www.scripps.edu/~arvai/adxv.html>) supports imgCIF

People Involved

Frances C. Bernstein

imgCIF Workshops:

Dowling: HJB

BNL: Robert M. Sweet

ARCiB Lab:

Dowling College: HJB, Isaac Awuah Asiamah, Darina Boycheva, Georgi Darakev, Nikolay Darakev, John Jemilawon, Nan Jia, Greg McQuillan, Dan O'Brien, Georgi Todorov

SVEVSL Project:

Dowling College: ARCiB Lab group

RIT: Paul A. Craig, Jared Carter, Brett Hanson, Scott Mottarella, Charlie Westin

And many more over the years.

Additional Material

**Additional material to help in understanding imgCIF
is provided on the slides that follow**

Status of CIF in PX

Core CIF (used for ligands):

An effective, working standard, heavily used

mmCIF (macromolecular structures):

Some use, community prefers old PDB format.

imgCIF (synchrotron data images, other images):

Little use, some support (fit2d, mosflm, adxv)

Community uses dozens of distinct formats

Use starting now at SLS and Diamond

Problem

Use of many different data formats causes delay and confusion; may lead to errors

Synchrotron image data formats:

Wladek Minor is “dealing with 197 (!!!!) frame formats” [email Wladek Minor to H. J. Bernstein, 15 May 2006].

2003 Denzo manual lists 107 available detector formats [Gewirth 2003] [Otwinowski, Minor 1997]

An Impractical Solution (The Esperanto Solution)

**Mandate one perfect format for everyone to
use for everything (internals and externals)**

Not workable:

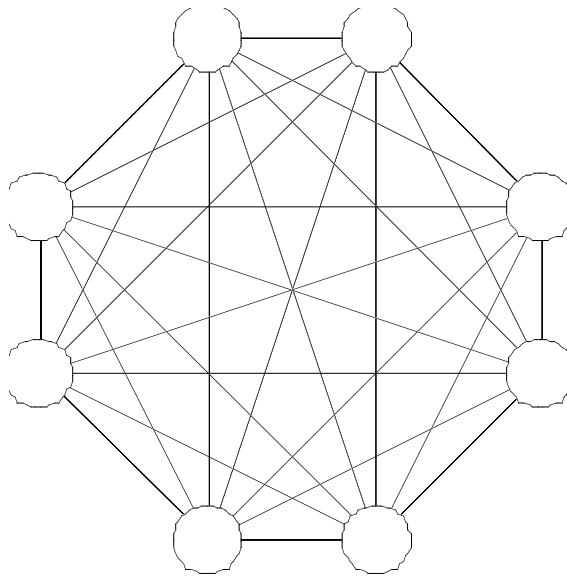
Might suppress new ideas and good science

**There is no agreement on the “perfect” format
What is perfect for the internals of one
project might be imperfect for the internals
of another project**

A Solution: Focus on Interchange

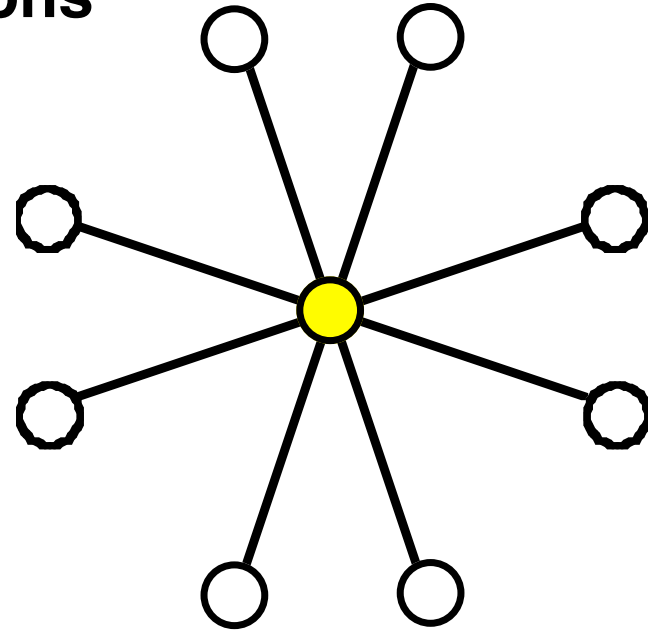
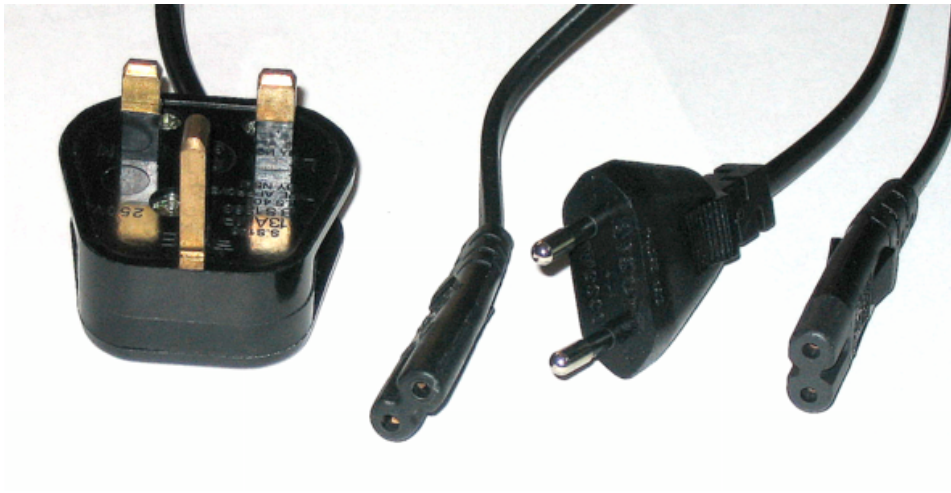
Include adapters with/in each system to handle many formats

For N systems with N-1 foreign formats, need
 $N*(N-1)$ adapters



A Better Solution

Provide a common format for interchange (e.g. CIF)
Instead of $N*(N-1)$ conversions
We only need $2N$ conversions



The Basics of imgCIF

There are multiple types of CIF

DDL1 CIFs (e.g. coreCIF, pdCIF)

DDL2 CIFs (e.g. mmCIF, imgCIF)

DDL3 is coming

CIF Dictionaries define the terms that can be used and their relationships.

Users can add terms of their own, but you should not use an existing term with a meaning that conflicts with the meaning in a dictionary or in a way that could be confused with terms that have been officially adopted.

For all CIFs:

Information is organized into blocks of data

Each block of data is managed essentially in terms of tables

Tables are called “categories” or “loops”

The column headings are called tags” or “data names”

Some tables have only one row of data

then each tag can be put with its value

Some tables have multiple rows of data

A given tag can appear only once in a block

DDL1 CIFs treat all categories similarly

DDL2 CIFs explicitly state relationships

e.g. parent-child relationships

imgCIF is a DDL2 dictionary that extends the macromolecular CIF (mmCIF) dictionary.

imgCIF Categories

ARRAY_DATA

presents the actual numeric data
(e.g. the numeric values of the pixels in an image)

ARRAY_INTENSITIES

tells you what you need to do to recover
intensities from ARRAY_DATA values

ARRAY_STRUCTURE

how the bits and bytes are organized

ARRAY_STRUCTURE_LIST

how the array dimensions are organized

ARRAY_STRUCTURE_LIST_AXIS

how axis settings relate to array indices

AXIS

the physical parameters of each axis

imgCIF Categories (cont.)

DIFFRN

mmCIF category describing diffraction data

DIFFRN_DATA_FRAME

details about each frame of data

DIFFRN_DETECTOR

information about each detector

DIFFRN_DETECTOR_AXIS

information about each detector axis

DIFFRN_DETECTOR_ELEMENT

layout of detector elements

DIFFRN_MEASUREMENT

goniometer information

DIFFRN_MEASUREMENT_AXIS

information about each goniometer axis

imgCIF Categories (cont.)

DIFFRN_RADIATION

incident radiation (crossfire, polarization, etc.)

DIFFRN_REFLN

reflection-by-reflection parameters for each frame

DIFFRN_SCAN

relationship of axis settings to scans

DIFFRN_SCAN_FRAME

relationship of particular frames to scans

DIFFRN_SCAN_FRAME_AXIS

relationship of axis settings to particular frames

imgCIF Categories (cont.)

Categories under development

MAP

density maps and masks

MAP_SEGMENT

bricks, slices and other segments of maps

Similar categories for compressed binary arrays are being considered.

CIF Syntax

A collection of data blocks

Each data block contains data names (tags) and their values

White space delimits tokens

Tags start with a leading underscore ("_") to distinguish them from values

Values that might be confused with data names or keywords or that contain whitespace are quoted

Quoting

single quote (single line only)

double quote (single line only)

semicolon in column 1 (multiple lines OK)

terminal quote mark must be followed by whitespace

Characters with special meaning

Underscore

Quote marks

Period (".") or question mark ("?") (null value)

Hash mark ("#") (comment)

Reserved words

"global_", "data_", "loop_", "stop_", and "save_"

In addition to the underscore, and the three quote marks, three other characters have special meaning: the period ("."), the question mark ("?") and the hash mark ("#"). The period is used when no value is specified. The question mark is used when a value is desired but not available. The hash mark indicates that the remaining characters on that line are part of a comment.

There are a small number of reserved words:

"global_", "data_", "loop_", "stop_", and "save_".

The last two reserved words are not used by CIF but are reserved to prevent conflict with the language from which CIF is derived (STAR). "global_" and "data_" mark the start of a data block.

"data_" should be followed immediately with the name of the block, without intervening whitespace.

If "loop_" appears, it is followed by a sequence of tags without intervening data values. Those tags are considered as the column headings of a table. These are followed by rows of data values corresponding to those column headings.

Outside of a table, tags and data values appear in simple alternation. Within a data block a given tag may appear only once.

The meaning of a CIF document is not altered by changing the order of presentation of data blocks nor is it altered by changing the order of presentation of tags within a block.

There are two styles of CIF in use for crystallography: DDL1 and DDL2.

DDL1 CIF (e.g. coreCIF, pdCIF)

Partial example of a small molecule coordinate list [Longridge 98]

```
loop_  
_atom_site_label  
_atom_site_fract_x  
_atom_site_fract_y  
_atom_site_fract_z  
_atom_site_U_iso_or_equiv  
_atom_site_adp_type  
_atom_site_calc_flag  
_atom_site_refinement_flags  
_atom_site_occupancy  
_atom_site_disorder_assembly  
_atom_site_disorder_group  
_atom_site_type_symbol  
Fe1 1 0 1 .0084(2) Uani d S 1 . . Fe  
Na1 .50907(11) .13980(8) 1.09450(9) .0185(3) Uani d . 1 . . Na  
Na2 .89904(10) .37128(8) 1.21657(9) .0171(3) Uani d . 1 . . Na  
C1 .7997(2) -.01740(18) 1.0419(2) .0110(4) Uani d . 1 . . C  
N1 .6788(2) -.02885(18) 1.0696(2) .0166(4) Uani d . 1 . . N  
C2 .9306(3) -.01004(16) .8075(3) .0130(4) Uani d . 1 . . C
```

DDL2 CIF (e.g. mmCIF, imgCIF)

Partial example of a macromolecular CIF (1CRN) as converted to mmCIF by the program pdb2cif [Bernstein et al. 98]

```
loop_
_atom_site.label_seq_id
_atom_site.group_PDB
_atom_site.type_symbol
_atom_site.label_atom_id
_atom_site.label_comp_id
_atom_site.label_asym_id
_atom_site.auth_seq_id
_atom_site.label_alt_id
_atom_site.cartn_x
_atom_site.cartn_y
_atom_site.cartn_z
_atom_site.occupancy
_atom_site.B_iso_or_equiv
_atom_site.footnote_id
_atom_site.label_entity_id
_atom_site.id
1
ATOM N N THR * 1 . 17.047 14.099 3.625 1.00 13.79 . 1 1
1
ATOM C CA THR * 1 . 16.967 12.784 4.338 1.00 10.80 . 1 2
```

ImgCIF Binary Data

```
_array_structure.id ARRAY1  
_array_structure.encoding_type "signed 32-bit integer"  
_array_structure.compression_type packed  
_array_structure.byte_order little_endian  
_array_data.array_id ARRAY1  
_array_data.binary_id 1  
_array_data.data  
;  
--CIF-BINARY-FORMAT-SECTION--  
Content-Type: application/octet-stream;  
conversions="x-CBF_PACKED"  
Content-Transfer-Encoding: BINARY  
X-Binary-Size: 3745758  
X-Binary-ID: 1  
X-Binary-Element-Type: "signed 32-bit integer"  
Content-MD5: 1zsJjWPfol2GYl2V+QsXrw==  
' []P«q «q FA• f¡Æ• àR~u<~>k2`b |5ß ...
```

Background

Imagine trying to do electronics without any agreement as to how to draw schematics.

That is how we have managed massive amounts of data in structural biology.

Some points of coherence in the chaos:

BNL Protein Data Bank format

[Bernstein et al. 1977]

de facto standard for macromolecular coordinates

CCDC's Cambridge Structural Database

[Allen et al. 1973]

de facto standard for small molecules

Background (cont.)

In general

- Each vendor of data collection equipment

- Each group maintaining a software package has their own approach to representing and storing raw data

This causes delays and confusion -- friction -- in working with data in so many different formats

Is the Problem Real?

Date: Sat, 06 Jan 2007 16:32:12 -0500

From: Arun Malhotra <malhotra@miami.edu>

To: CCP4 Bulletin Board <ccp4bb@dl.ac.uk>

“One common source of errors is changes made in reflection or coordinate files... For example, only recently, someone in my lab just manually edited out a hkl format file to change a few reflections from the exponential format into the standard F format, so that it could be converted into the mtz format. ... Format conversions (hkl to mtz or vice-versa) or simple manual edits to coordinate files are very common, and are fertile places for mistakes to creep in. Once such mistakes are made, they are not often easy to catch since there is no easy way to compare files....”

Is the Problem Real?

Date: Sun, 07 Jan 2007 11:25:26 +0900

From: Charlie Bond <Charles.Bond@uwa.edu.au>

To: ccp4bb@dl.ac.uk

“... Often at the synchrotron one is in a tired hurry to get an image indexed and processed. If the wrong parameters are used (eg the ones from the home lab with a bit of editing), a dataset in the wrong hand can be quickly produced

“Increasingly beamlines automatically prepare the correct parameter files for you, but it is cases where images are difficult to process (low resolution, disorder) that processing may occur later at home and the details of the beamline may be disregarded.

“Correct me if I'm wrong, but even the deposition of images would not help this as the critical information is the geometry of the beamline set up which is probably not recor[d]ed with the images.

...”

14 August 2007

Bernstein: Current Status imgCIF

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Frequently Asked Questions

Can I change it?

Yes, please do. We would appreciate:

New ideas

New items for the dictionary

New support software

Bug fixes and improvements

Translations to and from other presentations

Please don't use existing terms in ways that conflict with their meanings; define a new term with a new name instead

Frequently Asked Questions (Cont.)

The BIG Frequently Asked Question Can I make proprietary software using imgCIF and CBFlib?

**Yes, the API in CBFlib is available under the
LGPL.**

**If you change CBFlib itself, you must publish the
changed source code under the LGPL, but even
if you change CBFlib, you do not have to make
your program into an open source program.**

How to Make Changes to the imgCIF Dictionary

- 1. Get the best current version of the dictionary from the IUCr**
- 2. Check that what you propose is not already there, or if there is at least an appropriate category**
- 3. To avoid conflicts with others doing the same thing, get a prefix from Brian McMahon (bm@iucr.org)**
- 4. If you are going to be sending files to other people, discuss your new definition with them and, please, on the imgcif-I list**
- 5. If this will remain just a local change, use it in good health**
- 6. If you think this should be added to the main dictionary for community use, please say so on the imgcif-I list, and, if appropriate, on other lists**
- 7. If there is sentiment to add it to the main imgCIF dictionary, we will post a revised dictionary for comments, and then, if the dictionary working group agrees, forward the dictionary to COMCIFS for adoption**

How to Use and Make or Propose Changes to CBFLib

Use:

1. Download the package (source or binary)
2. If source, build for your machine
3. If you need help building, contact yaya@dowling.edu
4. If you are using the utilities, install them in your favorite location for binaries and use them
5. If you are building an application against the API, install the library in your favorite location and use it

Changes:

1. Changes in your own programs that just use the API:
Just do it (LGPL)
2. Changes to the API or Program
Do it, but follow the GPL/LGPL rules on changes
(making source available, carrying the license forward)

Credit

**We would appreciate a credit and knowing about changes.
Please cite [Bernstein, Ellis 2005] (see below)**

Where to Find imgCIF Information

IUCr Crystallographic Information Framework:

International Tables, Volume G

<http://www.iucr.org/iucr-top/cif/index.html>

official copies of dictionaries and stable releases of software

Image CIF/Crystallographic Binary File (imgCIF/CBF)

<http://arcib.dowling.edu/CBF>

<http://www.bernstein-plus-sons.com/software/CBF>

development versions of dictionary and software

<http://www.iucr.org/iucr-top/cif/cbf/imgcif-I>

<http://scripts.iucr.org/mailman/listinfo/imgcif-I>

imgCIF discussion list (please join)

Management of Experimental Data in Structural Biology (MEDSBIO)

<http://www.medsbio.org>

A broader perspective (imgCIF, NeXus, ...) concentrating on interfaces

<http://www.medsbio.org/meetings>

information on this workshop and future ones of interest

<http://scripts.iucr.org/pipermail/medsbio-I/>

<http://scripts.iucr.org/mailman/listinfo/medsbio-I>

MEDSBIO discussion list (please join)

Protein Data Bank

<http://www.pdb.org>

Information on dictionaries and file format, BioSync, etc.

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