

Draft minutes of the COMCIFS closed meetings at the IUCr Congress in Florence, August 23-31, 2005.

David Brown (Chair)

#### Meeting of the Chair with the Executive Committee

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I met briefly with the Executive Committee and pointed out that we needed to extend our Terms of Reference beyond the current and limited purpose of 'maintaining the integrity of CIF' on behalf of the Union. The terms should also include the ability to establish standards that would allow crystallographic information in electronic form to be accessed by other related disciplines. The Executive Committee was receptive to this idea, and I will shortly circulate a proposed rewording for discussion and approval.

I also pointed out that after 15 years the CIF project was at a crossroads and needed to move into new directions; I expected the meetings of COMCIFS at the present Congress would set the agenda for the next five or more years. The Executive Committee was appreciative of the work we had done and expressed its confidence in what we might propose for the future.

The Executive Committee did, however, express some reservations about the lack of new and younger voting members on COMCIFS. While they appreciated that this critical juncture was not the time for a large turn-over of members, we were urged to consider bringing in new blood at the next Congress.

#### COMCIFS Closed Meetings

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In addition to the COMCIFS open meeting and the microsposium hosted by the Computing Commission and COMCIFS, which will be reported in the IUCr Newsletter, COMCIFS held two closed meetings. The following were present at one or both meetings: David Brown (as chair), Brian McMahon, Herbert Bernstein, Simon Coles, Howard Flack, Ralf Grosse-Kunstleve, Syd Hall, James Hester, Owen Johnson, Peter Murray-Rust, Nick Spadaccini, Brian Toby and John Westbrook,

Following a report on my discussions with the Executive Committee, the meeting agreed with the proposal that COMCIFS should take responsibility for the maintenance of the orphaned DDL1 (Dictionary Definition Language 1). Discussion on the interoperability between CIF and XML led naturally to Syd Hall's presentation on starDDL, and in turn to a general discussion of the requirements for the next version of CIF. In brief, these include a more structured hierarchy of concepts, better linking between concepts, the introduction of vector and matrix items, the introduction of methods which would allow an item to be calculated from other items present in the CIF, and interoperability with XML while maintaining full compatibility with the existing CIF archives written using DDL1 or DDL2 dictionaries. It was however recognized that some significant investment would be needed in open source tools if the project is to be accepted by the community. While early versions of CIF could be prepared on a word processor, a factor crucial to CIF's original acceptance by the crystallographic community, the new generation of CIFs would need creation and editing tools to ensure that their more complex structure fully

conformed to the new dictionaries.

The second meeting opened with a review by John Westbrook of the current status of CIF in the Protein Data Bank, highlighting their requirements in any new version of CIF (e.g., XML and backward CIF compatibility). In the discussion following there was a consensus on the requirements of the next generation of CIF and that starDDL provided a suitable basis for the development of a new generation of dictionaries. These would be compatible with the current CIF archive and would add the functionality required in the future. There was also agreement that the dictionaries needed to be divided on an hierarchical principle rather than following the ad hoc arrangement that had grown up during the early development stages.

In order to move rapidly forward, Syd Hall, Nick Spadaccini and John Westbrook agreed to post a version of starDDL to serve as the basis for future development. Syd also agreed to provide software to transform the current dictionaries into starDDL compliant dictionaries (though warning that manual editing of these would also be necessary). David Brown and Brian McMahon agreed to work on the rearrangement of items into dictionaries that followed the hierarchy of crystallographic concepts. Protocols for the merging of dictionaries would be needed. David Brown and Brian McMahon also agreed to prepare a timeline for the development of the new standard, indicating what features (dictionaries, software, etc.) would be needed at each point, and what resources would need to be found.

As we finished, John Westbrook suggested that the acronym CIF should be reinterpreted as Crystallographic Information Framework. This was given a favourable reception (as it had been in Geneva). A formal motion to effect this change will be presented to COMCIFS.

I. David Brown  
Chair