Minutes of the closed COMCIFS meetings held on 25 and 28 August 2008 at the Grand Cube Convention Center in Osaka.

Present: David Brown (chair), Herbert Bernstein, Ralf Grosse-Kunstleve, Ilia Guzei, Syd Hall, James Hester, Brian McMahon, Nick Spadaccini and John Westbrook.

1. David Brown reported on his meeting with the Executive Committee of the IUCr at which he recommended the following be appointed as voting members of COMCIFS for the coming triennium: James Hester (chair), Herbert Bernstein, Ralf Grosse-Kunstleve, Brian McMahon, Nick Spadaccini and John Westbrook. The Executive Committee had no specific recommendations for COMCIFS and subsequent to this meeting the Executive Committee approved our list of nominees.

2. Brian McMahon reported on recent work in the Chester office, specifically adding to publCIF facilities for displaying and manipulating interactive figures, as well as the development of standards for CIF submissions to Acta Cryst. D and F.

3. John Westbrook described the work of the Biomedical Ontology Working Group which is developing a formal ontology for biological databases at a more abstract level than that provided by mmCIF. He emphasized the importance of developing a link between mmCIF and the biomedical ontology. A working group consisting of Westbrook (chair), Bernstein, McMahon and Spadaccini will examine the problems and report back to COMCIFS.

4. Herbert Bernstein reported that agreement had been reached at a meeting of the relevant manufacturers earlier in the week on a CIF based standard for reporting diffraction (and other) images.

5. The main part of the meeting was taken up with discussion of matters raised during the evaluation of DDLm. Reports were received from Spadaccini and Hester, who were the most actively involved in the review process. Hester gave an overview of the issues raised during the review, and stated that in his opinion and subject to some minor technical corrections, both DDLm and dREL were fit for purpose. He recommended that they be accepted by COMCIFS.

5.1 Westbrook expressed concern that the conventions, such as quoted containers, adopted for text items should not compromise the parsing of text used in mmCIF. It was agreed that Unicode could be used within **(text?)** strings.

5.2 Bernstein pointed out the importance of archival CIFs adopting a tight

structure, one that could be relaxed during CIF manipulation.

5.3 Westbrook emphasized the importance of maintaining proper parent-child relationships.

5.4 It was agreed that dREL and datanames should in future be case sensitive, but to avoid confusion, legacy datanames would continue to be treated as case insensitive and no duplication of letter sequences in datanames would be permitted.

5.5 There was discussion on the unambiguous identification of characters in the specifications, specifically the ASCII slash and backslash characters. In line with the proposal 5.1 to adopt Unicode within text strings, these might best be identified by the Unicode character codes and descriptions 002F (solidus) and 005C (reverse solidus). The correct form of a file URI is file://host/path; where host is not given (implying an address on the local filesystem) the URI appears with three leading slash characters file:///path."

5.6 As ordering of loop packets may sometimes be important, especially where those loop packets describe some sort of imperative behaviour (e.g. importing dictionaries) it was proposed that a DDLm key may have type 'ordinal' and, when that key is missing, the ordering will be implicit. Spadaccini will develop a formal description of this addition.

5.7 McMahon described the inclusion of Jmol script within a CIF, Bernstein described a graphics script which includes an imgCIF.

5.8 It was agreed that the methods included in the CIF dictionaries represent the formal definition of the item and therefore a strict hierarchy of items derived from the set of primitive items should be observed.

6. It was agreed to continue with the development of DDLm and its dictionaries as follows:

6.1 A description of the new version of the STAR file structure describing the DDLm text delimiters and containers is needed and this should be published. Hall and Spadaccini agreed to arrange this.

6.2 The current DDLm dictionary and dREL specifications were approved for alpha release.

6.3 Work to continue on the DDLm core dictionary. Brown to reactivate the coreCIF maintenance group and the working group on description of chemical entities in CIF. Hall and Westbrook to be added to this list.

6.4 The above decisions to be announced in the IUCr Newsletter, the

various COMCIFS Discussion lists and the IUCr web page **(Brown to initiate?)**

The first meeting continued informally for another hour in the hallways, the second meeting was more formally adjourned.