Report on IUCr CSMD Commission meeting 14 July 2010

During the last GRC on Electron Distribution and Chemical Bonding, Mount Holyoke College (MA), USA, 11-16 July 2010, a meeting of the IUCr CSMD Commission took place.

Members which were present :

C. Gatti
L. J. Farrugia
B. Gillon
D. Jayatilaka
U. Pietsch

Consultant :

A. Pinkerton

We have reported or discussed the following:

a) **IUCr Madrid 2011 Meeting** : the information provided through e-mail by K. Hamäläinen has been reported. The Commission thanks Keijo for his precious work and success.

b) **IXS-2010 Meeting** : the information provided through e-mail by K. Hamäläinen has been reported. The Commission expresses its wishes for a successful conference. If possible, it would be advisable to receive a short report after the meeting, as just received from the GRC chair (see below) for GRC meeting.

c) **CD school as a IuCr Madrid 2011 satellite:** the material provided by Claude Lecomte and Fernando Lahoz (school chairs) has been discussed. The Commission expresses its thanks for the very important initiative and suggests contacting soon (Fall 2010?) the teachers and to possibly focus and restrict a little bit the topics to be treated.

d) **ECDM-VI** : it will take place in Slovakia (close to Bratislava or close to the border with Poland in the Tatra mountains) in 2012. It should be planned so as not to interfere with the Sagamore meeting (Japan, date and location not yet available) and the next international conference of magnetism (ICM2012, 8-13 July, Korean, http://www.icm2012.org/).

e) **GRC :** we have discussed about the imperative request from the GRC staff to switch the Electron Distribution and Chemical Bonding GRC from a triennial to a biennial cycle. There are no possible alternatives, unless giving up with such a conference and with such an opportunity for our Commission. Clearly the biennial cycle impacts negatively with the present organization, with all main conferences for this Commission (IUCr General Assembly, GRC, Sagamore, IXS) being based on a triennial cycle. Since we had the possibility to have the next GRC in 2012 or 2013 it was stated to select the second option. This enables us to not impact with the present organization of meeting (Madrid, Sagamore, etc.) for the next three years and gives us some more time to take a decision whether to continue or give up with GRC after 2013.
We discussed also at length the best candidates as co-chair for next GRC. Wolfang Scherer (Germany) was selected as the best candidate for this role. Indeed Wolfgang Scherer has then been

elected during the GRC business meeting. The Commission expresses its thanks to Wolfgang Scherer for accepting such an important duty.
A report on the GRC 2010, presented by the chairs (Piero Macchi and Dylan Jayatilaka) is appended to this meeting report.

f) **Commission projects :**

Old projects : the chair (CG) has kindly solicited Dylan Jayatilaka to prepare an intermediate report on his project, which should be presented not later than at IUCr 2011. CG believes that Dylan could simply collect materials from the various groups participating to the project and prepare from such a material a distilled short report illustrating the main results thus far obtained. This report could represent the first draft for a final report to be published on Acta Cryst at due time.

New projects : CG has solicited the Commission members to propose new projects for the future and has indicated a number of projects that, to his advise, could start soon: a) a project on some target material (corundum again?) where the synergic help from different exp and theor techniques is mandatory. Recent developments in efficiently filtering the inelastic component of CBED data (see PRB 81 115135 (2010)) and progresses made in ab-initio computations of solids could call for a renewal in some form of the old project. Philip NH Nakashima has expressed his willingness and enthousiasm to be responsible of such project; b) a project on a organometallic compound of medium size, focussed on verifying the quality of data coming from various laboratories, the differences in refinements on such data, the differences in chemical interpretations of the resulting static (and dynamic) densities, using the many topological approaches. In addition, comparative work within the various labs on the same set of data could also be accomplished. Louis Farrugia has accepted to be responsible of such project. Two other projects have been discussed, one on CD databanks (Dylan Jayatilaka should contact the various groups involved in this topic to explore whether they would be interested in) and another one on joint charge/spin/momentum density refinements (proposed by B. Gillon). Concerning this latter, it has been suggested to postpone it for the moment, since at present there are three groups in competition on this topic and the time for a joint Commission project appears premature.
The discussion has been concluded by asking to the thus far designed responsible (Nakashima and Farrugia) to send a written informal proposal (one page) to the Commission chair. After acceptance from the Commission members the proposal will become an official project of the Commission.

Other suggestions for future projects are clearly welcome.

14 July 2010,
For the commission : C Gatti (chair)