



The First Working Group 4 Meeting of
the COST Action MOLIM: Molecules in Motion

“Active Databases”



MINUTES

July 25, 2015

Windsor – United Kingdom

Minutes of the First WG4 Meeting

Talks (see Book of Abstracts)

Round table discussion

WG4 attendees:

S. Yurchenko
H. Müller
J. Tennyson
C. Hill
A. Ross
A. Fateev
T. Furtenbacher
A. G. Császár
V. Boudon

Introduction of the WG4 members (including new ones) and their roles:

Sergey Yurchenko (ExoMol)
Attila Császár (MARVEL)
Isabelle Kleiner (astro-applications)
Miguel Carvajal (astro-applications)
Viktor Szalay (theory)
Per Jensen (spectroscopic data)
Roman Ciurylo (line profiles)
Alberto Garcia-Vela (molecular dynamics, quantum control)
Jonathan Tennyson (ExoMol, electron scattering)
Christian Hill (VAMDC)
Tibor Furtenbacher (MARVEL)
Vincent Boudon (MeCaSDa and ECaSDa databases)
Holger Müller (CDMS database)
Volker Ebert (PTB, metrology)
Alexander Fateev (industrial applications)
Amanda Ross (spectroscopic data for diatomics, MH)

The results of the intensive round-table discussion can be summarized as follows:

Possible roles and goals and deliverables of WG4:

- Virtual Atomic and Molecular Data Centre (VAMDC) as a goal for WG4: the data producers from MOLIM may want to join VAMDC or VAMDC nodes
- development of a cloud model (metadata) for storing the data: advantage is easy to maintain and access (google-like search), disadvantage is the trust of the data; the metadata format should be developed
- Development of benchmarks for variational codes, PESs, DMSs, etc.

- Acknowledging MOLIM@COST in publications related to the action
- Money/reimbursement: 120+120+20+20 EUR

Possible topics for Task Groups

- the iCloud model is too risky and non-efficient, VAMDC is a better alternative although requires much more efforts to maintain and to follow the VAMDC standards
- a suggestion for a Task Group: “Big data” (development of methods efficiently treating huge amount of data) and “Benchmarks” (variational codes, PESs, DMSs, diverse applications)
- a library of PESs or even bibliography as part of the agenda for this Task Group
- other possible topics for a Task Group: line profiles, spectroscopy for metrology, Raman database (no decision made)

To do list:

- prepare the minutes (S. Yurchenko)
- prepare suggestions for Task Groups and discuss them with WG4 members via emails (A. Császár, S. Yurchenko, J. Tennyson)
- publish the WG4 book of abstract on the MOLIM website (T. Furtenbacher)
- distribute minutes among WG4 and MC members (S. Yurchenko/A. Császár)
- recruit new members augmenting the expertise of the WG4 (S. Yurchenko/A. Császár)
- look for possible contacts with industry (A. Fateev)