

EMOL Group Evaluation Activities

B. J. Braams with thanks to N. J. Mason (OU)

22nd Data Centre Network meeting

IAEA, Vienna, 4-6 Sep 2013



IAEA

International Atomic Energy Agency

eMOL Project

- Project to **develop methodology** for analysing, validating and recommending **electron molecule collision** data sets.
- Will review 12-15 data sets in three years (2013-2015).
- Form part of a **Roadmap** for A+M data evaluation, recommendation and dissemination.
- Proposed and organized as a **community activity**; the community is assembled like a journal board. Current “Board” is 43 people.
- Each evaluation is a **small group project** by 4-7 people.
- Aim to provide recommended datasets that are **self-consistent** and **complete** (entire energy range, all processes).
- Will publish recommendations in EPJD and on website.
- Approach follows Christoforou and Olthoff at NIST (e.g. C_3F_8 published in J Phys Chem Ref Data, 1998).

eMOL Project, ...

eMOL evaluations schedule, subject to change.

H₂O: May 2013, Vienna.

Biomolecules I, THF and nucleobases: May 2013, Gdansk.

Fluorocarbons (*) I: July 2013, Japan.

Fluorocarbons II: Sept 2013, Trieste.

Fluorocarbons III: January 2014, Slovenia.

N₂ (and N₂⁺?): December 2013, Vienna.

SO₂ and Ozone: May 2014.

N₂O: June 2014, Bratislava.

NH₃: September 2014, location tbd.

Biomolecules II Pyrimidine, THFA: December 2014, tbd.

Maybe still O₂, others.

(*) Includes CF₄, CHF₃, C₂F₄, C₂F₆, C₃F₈, C₄F₈ and SF₆

First evaluation, H₂O

8-10 May 2013, one joint day with our Code Centre Network meeting.



First evaluation, H₂O, ...

Based on previous review by Itikawa and Mason, 2005. Assignments:

- **Dissociation:** S Matejcik, P Limao Vieira and B Marinkovic
- **DEA:** S Denifl, N J Mason and P Limao Vieira
- **Elastic:** B Marinkovic, G Karwasz and Y Itikawa
- **Electronic excitation:** G Karwasz, B Marinkovic and S Matejcik
- **Emission:** S Matejcik S Denifl and P Limao Vieira
- **Inelastic:** J Tennyson, G Karwasz and Y Itikawa
- **Ionisation:** S Denifl, S Matejcik and P Limao Vieira
- **Momentum Transfer:** G Karwasz, Y Itikawa and B Marinkovic
- **Rotational excitation:** Y Itikawa, J Tennyson and N J Mason
- **Total:** N J Mason, J Tennyson, G Karwasz
- **Vibrational Excitation:** J Tennyson, B Marinkovic and N J Mason

Evaluation process

Procedure for one review.

- Assemble the papers. Ideally there is an earlier review.
- Divide review by processes: total, elastic, ionisation, DEA, etc..
- Assemble review team and divide into sub-teams.
- Meet face to face – discuss and agree ‘best values’.
- Post meeting: check datasets for consistency, consider scaling or corrections.
- Agree on uncertainty assignments for recommended data sets.
- Produce paper to be submitted to EPJD.
- Online archive and updates. Website is scheduled for 2014.
- Subsequent updates: expected about every 5 years.

H₂O example: One more discussion at GEC (Oct 2013); then wrap-up.

The End..