Minutes of the Salamanca Meeting of the Task Group

Salamanca, Spain, September 16-17, 2005

In attendance: The following 10 members, out of 14, of the Task Group were present at the meeting. Alain Campargue (Grenoble, France), Attila Császár (ELTE, Hungary), Robert Gamache (Lowell, USA), Joseph Hodges (NIST, USA), Alain Jenouvrier (Reims, France), Oleg Polyansky (Ulm, Germany), Laurence Rothman (Harvard, USA), Jonathan Tennyson (UCL, UK), Ann Carine Vandaele (Brussels, Belgium), and Nikolai Zobov (Nizhny Novgorod, Russia).

Guest participants: Sergei Shirin (Nizhny Novgorod, Russia), Vladimir Tyuterev (Reims, France), Roman Tolchenov (UCL, UK), Boris Voronin (UCL, UK), Svetlana Voronina (UCL, UK)

Absentees: Peter Bernath (Waterloo, Canada), Michel Carleer (Brussels, Belgium), Olga Naumenko (Tomsk, Russia), and Robert Toth (JPL, USA).

Location: The workshop was held at the campus of the university in Salamanca. Help provided by Rafael Escribano is gratefully acknowledged. Accommodation was provided at different hotels and in Collegio del Oviedo in Salamanca.

AGENDA OF THE SALAMANCA MEETING

September 16, 2005

Presentations and discussions

14:00 Introduction (J. Tennyson)
14:10 A database for water transitions from experiment and theory (J. Tennyson)
15:05 CW-CRDS of water (A. Campargue, D. Romanini, S. Kassi, O. Naumenko, S.N. Mikhailenko, P. Macko)
15:25 Near infrared water vapor line intensities measured using frequency-stabilized cavity ring-down spectroscopy (J. Hodges)
15:45 Break
16:15 New Edition of the HITRAN Spectroscopic Database Compilation (L. Rothman)
18:20 Introduction and some recent results from the Budapest group (A. Császár)
18:35 Adjournment
20:15 Dinner

September 17, 2005

Presentations and discussions

9:00 Line shape of H_2O via complex Robert-Bonamy theory (R. Gamache)
9:30 Experimental measurements of water vapor and its isotopologues (A. C. Vandaele, C. Hermans, M. Carleer, P.-F. Coheur, S. Fally, and A. Jenouvrier)
10:15 Water: potentials and analysis (O. Polyansky)
11:00 Break
11.15 Improved theoretical treatment of hot and cold water spectra (V. Tyuterev)
11:45 Using more theory in fitting spectral line parameters (R. Tolchenov)
12:00 General discussion
13:10 Adjournment

Resolutions

- All tasks should be carried out by individuals or by small groups of individuals. Each person from a particular group represents the whole group.
- The deliverable of the TG will be a well designed critically evaluated relational database. Design principles should be discussed with Marie-Lise Dubernet-Tuckey (LERMA, Paris, France) who is coordinating efforts to make database standards for spectral linelists (see http://www.ivoa.net/twiki/bin/view/IVOA/SpectralLineLists). Discussions should also be carried out with Dr. Alex Fazliev (Tomsk).
- The following subgroups have been established:

  Cold water (**C**, leader: Larry Rothman, members: Peter Bernath, Alain Campargue, Michel Carleer, Alain Jenouvrier, Olga Naumenko, Oleg Polyansky, Jonathan Tennyson, Robert Toth, Ann Carine Vandaele, Nikolai Zobov).

  Hot water (**H**, leader: Peter Bernath, members: Alain Campargue, Michel Carleer, Oleg Polyansky, Larry Rothman, Jonathan Tennyson, Nikolai Zobov).

  Line profiles (**L**, leader: Bob Gamache, members: Joseph Hodges, Larry Rothman).

  Database (**D**, leader: Attila Császár, members: Olga Naumenko, Oleg Polyansky, Larry Rothman, Jonathan Tennyson).

  Theoretical computations (**T**, leader: Oleg Polyansky, members: Attila Császár, Bob Gamache, Jonathan Tennyson, Nikolai Zobov).

  Validation and standardization (**V**, leader: Joe Hodges). It is understood that all members of the TG will take part in the validation process.

- Subgroup leaders are responsible for reporting to the TG leader all works and results performed within their area of expertise related to the TG.
- The subgroups overlap too much to make official separate (parallel) group meetings practical.
- The TG limits itself to transitions between 0 and 30.000 cm^{-1} even for $H_2{}^{16}O$.
- The water linelist will be made available both for room temperature (**C**, 296 K) and for hot (**H**) water. The temperature for **H** has not been decided.
- The TG aims at a complete inclusion of intensities in the database though completeness should be maintained only above 10^{-29} cm molecule^{-1} in natural abundance. It is possible that different cutoffs will be selected for the different isotopologues.
- A comprehensive database is to be built for $H_2{}^{16}O$. The order of importance of the singly and doubly substituted isotopologues also to be included in the final database: $HD^{16}O$, $H_2{}^{18}O$, $H_2{}^{17}O$, $D_2{}^{16}O$, $HD^{17}O$, and $HD^{18}O$. No triply substituted isotopologue will be considered.
- A master database is prepared for all isotopologues. Critical evaluation and annotation means that the database will capture the origin, possible time-dependence, and other salient properties of the measurements and the computed values, as well. Both 'old' and 'new' data are to be archived and made readily accessible. To help modelers, special care must be taken to distinguish lines which do have assigned quantum numbers from those which do not.
- A web site is to be set up and maintained in Budapest, Hungary. This should be linked to the official web site of the TG maintained by IUPAC and Mrs. Fabienne (http://www.iupac.org/projects/2004/2004-035-1-100.html).
- Line profiles: Broadening parameters γ and δ for self-broadening, as well as.
- Dependence of the line shapes with pressure (0 – 3 atm) and temperature (200 – 300 K) must be investigated both experimentally and computationally. The use of both Lorentz and Voigt profiles will be investigated. Broadening parameters for self- and foreign-broadening, including N_2, O_2, air, and H_2, will be included in the database.

PUBLICATIONS STRATEGY

It has been concluded that the primary product of the efforts of the TG is a large size relational database containing all critically evaluated data, both experimental and theoretical, available at the end of the mandate of the TG. Relevant issues related to the relational database should be written up and published in the scientific literature. The authorship of any publications resulting from efforts of the TG will be discussed at the next meeting in 2006.

All TG members are asked to include the following sentence in their publications related to the work of the IUPAC TG: "This research forms part of an effort by a Task Group of the International Union of Pure and Applied Chemistry (IUPAC, Project no. 2004-035-1-100) on 'A database of water transitions from experiment and theory'."

BUDGET AND NEXT MEETING

The precise budget is not known because (*i*) the accounts of expenses of the Salamanca Meeting will be made in the next days, and (*ii*) the exhange rate used by IUPAC Secretariat is not known. An estimate of the expenses shows that we have used up so far about 30% of the total funding available. This means that without extra funding we could organize two more meetings. Special thanks go to all those who used other types of funding to attend this meeting and thus saved money for the next meetings.

The next meeting will be held around 26-29 June, 2006 in conjunction with the next HITRAN conference, organized by Larry Rothman, in the USA. No decision is made about the third meeting, to be held sometimes in the fall of 2007.

30th September, 2005

Attila Császár and Jonathan Tennyson