

XVIII Symposium and School

on High Resolution Molecular Spectroscopy

HighRus-2015

June 30–July 4, 2015

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### Symposium

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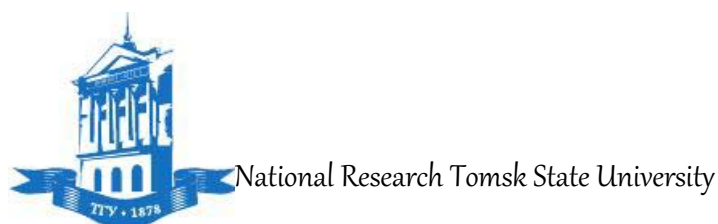
O.Yu. Ponomareva

### School

V.I. Perevalov – *chair*

B.A. Voronin

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## Symposium Schedule

<b>Time</b>	<b>Tuesday, June 30</b>	<b>Wednesday, July 1</b>	<b>Thursday, July 2</b>	<b>Friday, July 3</b>	<b>Saturday, July 4</b>
<b>9:00 – 10:30</b>	Registration	<b>Invited Lectures E</b>	<b>Invited Lectures J</b>	<b>Invited Lectures L</b>	<b>Invited Lectures Q</b>
<b>10:30 – 11:00</b>	Opening	Coffee Break	Coffee Break	Coffee Break	Coffee Break
<b>11:00 – 12:30</b>	<b>Invited Lectures A</b>	<b>Invited Lectures F</b>	<b>School Lectures K</b>	<b>Oral Session M</b>	<b>Oral Session R</b>
<b>12:30 – 14:30</b>	Lunch Break	Lunch Break	Lunch Break	Lunch Break	Lunch Break
<b>14:30 – 16:00</b>	<b>Oral Session B</b>	<b>Oral Session G</b>	Excursion	<b>Oral Session N</b>	<b>School Lectures S</b>
<b>16:00 – 16:15</b>	Coffee Break	Coffee Break		Coffee Break	Coffee Break
<b>16:15 – 18:00</b>	<b>Poster Session C</b>	<b>Poster Session H</b>		<b>Poster Session O</b>	<b>Round Table T</b>
<b>17:30 – 19:00</b>	<b>School Lectures D</b>	<b>School Tutorials I</b>		<b>Round Table P</b>	Closing
<b>19:00 – 22:00</b>	Cocktail party		Banquet		

## Contents

Session Program .....	7
Invited Lectures A, Tuesday, June 30, 11:00 .....	16
Oral Session B, Tuesday, June 30, 14:30 .....	18
Poster Session C, Tuesday, June 30, 16:15 .....	24
School Lectures D, Tuesday, June 30, 17:00 .....	51
Invited Lectures E, Wednesday, July 1, 09:00 .....	53
Invited Lectures F, Wednesday, July 1, 11:00 .....	55
Oral Session G, Wednesday, July 1, 14:30 .....	57
Poster Session H, Wednesday, July 1, 16:15 .....	63
School Tutorials I, Wednesday, July 1, 17:00 .....	92
Invited Lectures J, Thursday, July 2, 09:00 .....	95
School Lectures K, Thursday, July 2, 11:00 .....	97
Invited Lectures L, Friday, July 3, 09:00 .....	99
Oral Session M, Friday, July 3, 11:00 .....	101
Oral Session N, Friday, July 3, 14:30 .....	107
Poster Session O, Friday, July 3, 16:15 .....	113
Round Table P, Friday, July 3, 17:30 .....	142
Invited Lectures Q, Saturday, July 4, 09:00 .....	145
Oral Session R, Saturday, July 4, 11:00 .....	147
School Lectures S, Saturday, July 4, 14:30 .....	154
Round Table T, Saturday, July 4, 16:00 .....	156
Author Index .....	157
E-mail Address Book .....	160

## Session Program

**June 30, 2015, Tuesday**

**Invited Lectures A, 11<sup>00</sup>–12<sup>30</sup>**

*Chair: Yurii N. Ponomarev*

- A1 Microwave Coherence Spectroscopy: How to use real high resolution – and why  
**Jens-Uwe Grabow**
- A2 Laser spectroscopy of some MH molecules with astrophysical "overtones"  
**Amanda Ross**

**Oral Session B, 14<sup>30</sup>–16<sup>00</sup>**

*Chair: Vladimir G. Tyuterev*

- B1 A new triplet transition of the V<sub>2</sub> molecule  
**A.S.C. Cheung, Yue Qian, Y.W. Ng**
- B2 Accurate non-adiabatic corrections to ro-vibrational levels of small molecules through effective nuclear masses  
**J.R. Mohallem, L. Diniz, L. Adamowicz, A. Alijah**
- B3 A database of NO<sub>2</sub> spectral line parameters at  $T = 1000$  K  
**O.K. Voitsekhovskaya, O.V. Egorov, D.E. Kashirskii**
- B4 Numerical construction of symmetry-adapted ro-vibrational basis sets for variational nuclear motion calculations  
**S.N. Yurchenko**
- B5 Nitrous Oxide Spectroscopic Databank (NOSD)  
**S.A. Tashkun, V.I. Perevalov, N.N. Lavrentieva**
- B6 High-resolution spectra of polarized thermal radiation in atmosphere: simulation for satellite remote sensing  
**B.A. Fomin, V.A. Falaleeva**

**Poster Session C, 16<sup>15</sup>–18<sup>00</sup>**

- C1 Millimeter-wave measurements and ab initio calculations of the NH<sub>3</sub>–CO complex  
**L.A. Surin, A.V. Potapov, S. Schlemmer, A.A. Dolgov, I.V. Tarabukin, V.A. Panfilov, Yu.N. Kalugina, A. Faure, A. van der Avoird**
- C2 High resolution analysis of S<sup>18</sup>O<sub>2</sub> spectrum: The  $\nu_1$  and  $\nu_3$  interacting bands  
**Yu.V. Krivchikova, V.A. Zamotaeva, S.A. Zhdanovich**
- C3 The disagreements between calculation results of water vapor spectral characteristics at high temperatures  
**O.K. Voitsekhovskaya, O.V. Egorov, D.E. Kashirskii**
- C4 On the "expanded local mode" approach applied to ethylene  
**A.S. Belova, A.L. Fomchenko, Yu.S. Aslapovskaya**
- C5 High resolution analysis of the  $\nu_6$  band of the CH<sub>2</sub>=CD<sub>2</sub> molecule  
**K.B. Berezkin, N.V. Kashirina**
- C6 The absorption spectrum of <sup>17</sup>O enriched water vapor by CRDS between 5850 and 6670 cm<sup>-1</sup>  
**S.N. Mikhailenko, A. Campargue, D. Mondelain, S. Kassi, E.V. Karlovets**

- C7 High resolution absorption spectra of  $^{12}\text{C}^{18}\text{O}_2$  and  $^{16}\text{O}^{12}\text{C}^{18}\text{O}$  in the 11 260–11 430  $\text{cm}^{-1}$  wavenumber range  
**L.N. Sinitsa, A.A. Lugovskoi, V.I. Serdyukov, S.A. Tashkun, V.I. Perevalov**
- C8 High sensitivity cavity ring down spectroscopy of  $\text{CO}_2$  overtone bands near 830 nm  
**Y. Tan, X.-Q. Zhao, J. Wang, A.-W. Liu, S.-M. Hu, O.M. Lyulin, S.A. Tashkun, V.I. Perevalov**
- C9 *Ab initio* calculation of ro-vibrational spectra for  $\text{GeH}_4$  molecule  
**A.A. Rodina, A.V. Nikitin, M. Rey, V.I.G. Tyuterev**
- C10 First principles calculation of rovibrational spectra for  $\text{SiH}_4$  molecule  
**Y.S. Chizhmakova, A.V. Nikitin, M. Rey, V.I.G. Tyuterev**
- C11 Combined effect of small- and large-angle scattering collisions on a spectral line shape  
**V.P. Kochanov**
- C12 Accuracy and precision of line center frequency measurements of  $^{16}\text{O}^{12}\text{C}^{32}\text{S}$  rotational lines of in MM and Sub-MM wave range  
**G.Yu. Golubiatnikov, S.P. Belov, A.V. Lapinov**
- C13 Numerical model of Zeeman splitting of ro-vibrational lines in the NO fundamental band  
**Yu.G. Borkov, O.N. Sulakshina, Yu.M. Klimachev**
- C14 Wave functions and lifetimes of ozone metastable states above the dissociation threshold: Impact on the dynamics  
**V. Kokoouline, D. Lapierre, A. Alijah, V.I.G. Tyuterev, R.V. Kochanov, J. Blandon**
- C15 Estimations for line parameters of  $\text{SO}_2$   
**B.A. Voronin**
- C16 Retrievals of the  $\text{CH}_4$  and  $\text{CO}_2$  atmospheric amount from the high resolution absorption spectra of solar radiation with the use of different spectroscopic databanks  
**T.Yu. Chesnokova, A.V. Chentsov, N.V. Rokotyan, V.I. Zakharov**
- C17 Evidence of stable Van Der Waals  $\text{CO}_2$  clusters relevant to  $\text{CO}_2$ -rich atmospheres  
**T.N. Sinyakova, R.E. Asfin, D.V. Oparin, N.N. Filippov, J.V. Buldyreva**
- C18 Temperature dependence of self-,  $\text{N}_2$ -broadened line widths of methyl cyanide vibrational lines  
**A.S. Dudaryonok, N.N. Lavrentieva, J.V. Buldyreva**
- C19 Study of the  $\text{H}_2\text{O}$ – $\text{H}_2\text{O}$  line broadening in 15 500–16 000  $\text{cm}^{-1}$  region  
**L.N. Sinitsa, V.I. Serdyukov, A.P. Shcherbakov, N.N. Lavrentieva, A.S. Dudaryonok**
- C20 Contribution of different components of bimolecular absorption to the water vapour continuum in rotational and fundamental rovibrational spectral bands  
**T.A. Odintsova, E.A. Serov, M.A. Koshelev, M.Yu. Tretyakov**
- C21 Addition of the  $\text{H}_2$ , He and  $\text{CO}_2$  broadening and shifting parameters and their temperature dependences. Part 1:  $\text{SO}_2$ ,  $\text{NH}_3$ , HF, HCl, OCS, and  $\text{C}_2\text{H}_2$   
**J.S. Wilzewski, I.E. Gordon, L.S. Rothman, R.V. Kochanov, C. Hill**
- C22 Broadening parameters for  $\text{H}_2\text{O}$  lines perturbed by argon in infrared region  
**T.M. Petrova, A.M. Solodov, A.A. Solodov, V.M. Deichuli, V.I. Starikov**
- C23 DRIADA—compact high-resolution spectrometer for atmospheric monitoring of greenhouse gases in near IR  
**A.Yu. Trokhimovskiy, O.I. Korablev, I.A. Dzyuban, A. Patrakeeve, A.A. Fedorova, S. Mantsevich, A. Shapkin, Yu.V. Smirnov, M.A. Poluarshinov**
- C24 Integrated cavity output spectroscopy using reflected radiation  
**P.V. Korolenko, I.V. Nikolaev, V.N. Ochkin, S.N. Tskhai, A.A. Zaytsev**
- C25 A cavity ring down spectrometer for high sensitivity absorption in the 2.35  $\mu\text{m}$  atmospheric window  
**S.S. Vasilchenko, D. Mondelain, S. Kassi, P. Cermak, A. Campargue**



- C26 New features of FT spectrometer using LED sources  
**L.N. Sinitsa, V.I. Serdyukov**
- C27 Fine structure of  $Q$ -branch  $\nu_1+\nu_3$  band of  $\text{UF}_6$  absorption spectra: Tunable QCL and FTIR spectroscopy studies  
**Sh.Sh. Nabiev, V.M. Semenov, P.L. Men'shikov, L.I. Men'shikov, G.Yu. Grigor'iev, D.B. Stavrovskii, Ya.Ya. Ponurovskii**

**School Lectures D, 17<sup>00</sup>–18<sup>30</sup>**

*Chair: Valery I. Perevalov*

- D1 The diatomic spectroscopy of excited states beyond adiabatic approximation  
**Elena A. Pazyuk**
- D2 High resolution spectra of molecules with variational methods  
**Sergei N. Yurchenko**

**July 1, 2015, Wednesday**

**Invited Lectures E, 9<sup>00</sup>–10<sup>30</sup>**

*Chair: Alain Barbe*

- E1 Rotational action spectroscopy in cryogenic ion traps  
**Sandra Brünken, L. Kluge, A. Stoffels, P. Jusko, O. Asvany, S. Schlemmer**
- E2 Molecular line lists for exoplanets and other atmospheres  
**Jonathan Tennyson**

**Invited Lectures F, 11<sup>00</sup>–12<sup>30</sup>**

*Chair: Alain Campargue*

- F1 Coherent effects in the terahertz region and their spectroscopic applications  
**Evgeni N. Chesnokov, P.V. Koshlyakov, V.V. Kubarev**
- F2 Using synchrotron radiation for high resolution molecular spectroscopy in the terahertz  
**Olivier Pirali**

**Oral Session G, 14<sup>30</sup>–16<sup>00</sup>**

*Chair: Leonid A. Surin*

- G1 A hot spot in the high resolution spectroscopy of methanol  
**S.P.Belov, G.Yu.Golubiatnikov, A.V. Lapinov, V.V. Ilyushin, E.A. Alekseev, A.A. Mescheryakov, J.T. Hougen, Li-Hong Xu**
- G2 Self broadening and foreign broadening of methane lines in the tetradecade between  $5880\text{ cm}^{-1}$  and  $5900\text{ cm}^{-1}$   
**A. Rausch, O. Werhahn, V. Ebert**
- G3  $\text{D}_2\text{O}$  dimers in silicon airgel nanopores  
**A.A. Lugovskoi, V.I. Serdyukov, L.N. Sinitsa**
- G4 Predissociation of high-lying Rydberg states of molecular iodine via ion-pair states  
**A.S. Bogomolov, A.V. Baklanov, B. Grüner, M. Mudrich, S.A. Kochubei**
- G5 Speed dependence, velocity change and line mixing in self-colliding  $\text{CO}_2$  under high pressures in the  $30013 \leftarrow 00001$  band: Measurements and test of models  
**V.A. Kapitanov, K.Yu. Osipov, A.E. Protasevich, Ya.Ya. Ponurovskii**

G6 Self-broadening and collision mixing of the spectral lines in the fundamental bands of NH<sub>3</sub>  
**M.R. Cherkasov**

**Poster Session H, 16<sup>15</sup>–18<sup>00</sup>**

- H1 Analysis of six new bands of <sup>18</sup>O<sub>3</sub> recorded by CRDS technique in the 7400–7920 cm<sup>-1</sup> spectral range  
**E.N. Starikova, A. Barbe, Vl.G. Tyuterev, D. Mondelain, S. Kassi, A. Campargue**
- H2 High sensitivity cw-cavity ring down spectroscopy of N<sub>2</sub>O near 1.22 μm  
**E.V. Karlovets, A. Campargue, S. Kassi, S.A. Tashkun, V.I. Perevalov**
- H3 A high resolution analysis of weak absorption bands of C<sub>2</sub>H<sub>2</sub>D<sub>2</sub>-*trans*: the ν<sub>8</sub>+ν<sub>10</sub> (Au) band  
**A.G. Litvinovskaya, N.I. Raspopova, F. Zhgan**
- H4 Nitrogen dioxide high temperature line list in the 466–3374 cm<sup>-1</sup> region  
**A.A. Lukashevskaya, V.I. Perevalov, A. Perrin**
- H5 Fourier transform absorption spectrum of D<sub>2</sub><sup>16</sup>O in 14 800–15 200 cm<sup>-1</sup> spectral region  
**I.A. Vasilenko, O.V. Naumenko, V.I. Serdyukov, L.N. Sinitsa**
- H6 Intensities and self-broadening coefficients of the strongest water vapour lines in 2.7 and 6.25 μm absorption bands  
**I.V. Ptashnik, R.A. McPheat, K.M. Smith, K.P. Shine**
- H7 High pressure Cavity Ring Down spectroscopy: Application to the absorption continuum of CO<sub>2</sub> near 1.7 μm  
**S. Kassi, D. Mondelain, H. Tran, A. Campargue**
- H8 Calculation of rotation-vibration energy levels of the ammonia molecule based on an *ab initio* potential energy surface  
**O.L. Polyansky, R.I. Ovsyannikov, A.A. Kyuberis, N.F. Zobov, L. Lodi, J. Tennyson, A.A. Yachmenev, S.N. Yurchenko**
- H9 The line lists of the <sup>16</sup>O<sup>18</sup>O<sup>16</sup>O and <sup>18</sup>O<sup>16</sup>O<sup>18</sup>O ozone isotopologues of the S&MPO database  
**A. Barbe, S.N. Mikhailenko**
- H10 Small molecules in external magnetic fields  
**H.M. Cobaxin, A. Alijah, J.C. López Vieyra, A.V. Turbiner**
- H11 Present status and perspectives of line-by-line analyses of the PH<sub>3</sub> absorption spectrum in the Octad range between 2800 and 3600 cm<sup>-1</sup>  
**Y.A. Ivanova, A.V. Nikitin, S.A. Tashkun, M. Rey, Vl.G. Tyuterev, L.R. Brown**
- H12 First principles calculation of energy levels and spectra for AB<sub>4</sub>, ABC<sub>3</sub> type molecules  
**A.V. Nikitin, B.M. Krishna, M. Rey, Vl.G. Tyuterev**
- H13 Radiative properties of the low-lying states of Rb<sub>2</sub> and Cs<sub>2</sub> based on *ab initio* calculations  
**E.A. Pazyuk, E. Revina, A.V. Stolyarov**
- H14 Speed-dependent spectral line profile including line narrowing and mixing  
**V.P. Kochanov**
- H15 Calculating the "hot" line intensities ( $Ka \leq 25, J \leq 30$ ) of water vapor (000)–(000) band  
**O.V. Egorov, O.K. Voitsekhovskaya, D.E. Kashirskii**
- H16 Global modeling of high-resolution spectra of acetylene (C<sub>2</sub>H<sub>2</sub>)  
**O.M. Lyulin, V.I. Perevalov**
- H17 <sup>12</sup>C<sup>16</sup>O line profile parameters for Mars and Venus atmospheres  
**N.N. Lavrentieva, B.A. Voronin, A.A. Fedorova**
- H18 Broadening, shifting and speed dependence coefficients of diagnostic water lines  
**I.N. Vilkov, M.A. Koshelev, G.V. Fedoseev, M.Yu. Tretvakov**

- H19 Hitran.org : new website, new structure, new interface for the HIRAN spectroscopic database  
**C. Hill, I.E. Gordon, R.V. Kochanov, J.S. Wilzewski, P. Wcisło, L.S. Rothman**
- H20 Water vapour self-continuum absorption within 0.94 and 1.13  $\mu\text{m}$  bands at high temperatures  
**I.V. Ptashnik, A.A. Simonova, R.A. McPheat, K.M. Smith, K.P. Shine**
- H21 The line shape problem of high-precision spectra of self-colliding  $\text{CO}_2$  molecules in the pressure range between 0.002 and 1 atm: Measurements and test of models  
**V.A. Kapitanov, K.Yu. Osipov, A.E. Protasevich, Yu.N. Ponomarev, Ya.Ya. Ponurovskii**
- H22 Measurements of absorber density based on examination of spectral line shape  
**Yu.A. Adamenkov, Yu.V. Kolobyaniin**
- H23 He-broadening and -shift parameters of the water vapor spectral lines in the wide spectral range  
**T.M. Petrova, A.M. Solodov, A.A. Solodov, V.I. Starikov**
- H24 Diode-laser spectrometer concept for Martian atmosphere studies  
**I.I. Vinogradov, Yu.V. Lebedev, A.V. Rodin, A.Yu. Klimchuk, V.M. Semenov, O.V. Benderov, A.A. Pereslavl'tseva, M.V. Spiridonov, V.V. Barke**
- H25 Reference wavenumbers and assessment of trust in spectral database  
**O.V. Naumenko, A.I. Privezentsev, N.A. Lavrentiev, A.Z. Fazliev**
- H26 A W@DIS-based data quality analysis of the energy levels and wavenumbers of isotopologues of the water molecule  
**A.Z. Fazliev, O.V. Naumenko, A.I. Privezentsev, A.Yu. Akhlyostin, N.A. Lavrentiev, A.V. Kozodoev, S.S. Voronina, A.V. Apanovich, A.G. Császár, J. Tennyson**
- H27 Measurements of carbon dioxide isotopic ratio in ambient air using an optical cavity and tunable diode laser in 1.605  $\mu\text{m}$  area  
**I.V. Nikolaev, V.N. Ochkin, S.N. Tskhai, A.A. Zaytsev**
- H28 Feature of IR spectra of ICAO taggants in the vapor state  
**Sh.Sh. Nabiev, L.A. Palkina, D.B. Stavrovskii, E.N. Golubeva, V.L. Zbarskii, N.V. Yudin, V.M. Semenov**

### School Tutorials I, 17<sup>00</sup>–18<sup>45</sup>

*Chair: Igor V. Ptashnik*

- I1 Retrieving spectroscopic data from Virtual Atomic and Molecular Data Center (VAMDC)  
**Mikhail V. Doronin**
- I2 W@DIS information system. Spectral data analysis  
**Alexander Z. Fazliev**
- I3 SPECTRA—An interactive tool for molecular spectroscopy  
**Semen N. Mikhailenko**

### July 2, 2015, Thursday

### Invited Lectures J, 9<sup>00</sup>–10<sup>30</sup>

*Chair: Iouli E. Gordon*

- J1 Infrared quantitative spectroscopy and atmospheric satellite measurements  
**Jean-Marie Flaud**
- J2 Cold molecules and high-resolution spectroscopy: Experiments on two-, three- and four-electron molecules  
**P. Jansen, S. Scheidegger, L. Semeria, Frédéric Merkt**

## School Lectures K, 11<sup>00</sup>–12<sup>30</sup>

*Chair: Yury I. Baranov*

- K1 Remote sensing of the atmosphere using satellite and ground-based high resolution spectrometers in IR  
**Vyacheslav I. Zakharov**
- K2 Importance of the proper data presentation in submitted manuscripts and a look beyond the impact factor of the journal: Primer of JQSRT  
**Iouli E. Gordon, L.S. Rothman**

## July 3, 2015, Friday

### Invited Lectures L, 9<sup>00</sup>–10<sup>30</sup>

*Chair: Nikolai N. Filippov*

- L1 Challenges and applications of synchrotron based and laser based - line shape studies  
**Adriana Predoi-Cross**
- L2 Calculation of rovibrational line broadening and shifting of symmetric and asymmetric top molecules  
**Nina N. Lavrentieva**

### Oral Session M, 11<sup>00</sup>–12<sup>30</sup>

*Chair: Jonathan Tennyson*

- M1 Rotational spectrum of the NH<sub>3</sub>–H<sub>2</sub> van der Waals complex  
**L.A. Surin, I.V. Tarabukin, V.A. Panfilov, S. Schlemmer, A. Breier, T. Giesen, M.C. McCarthy**
- M2 Influence of nanoconfinement on the line parameters for 2–0 absorption band of CO  
**A.A. Solodov, Yu.N. Ponomarev, T.M. Petrova, A.M. Solodov**
- M3 Water vapor continuum in the range of rotational spectrum of H<sub>2</sub>O molecule: New experimental data and their comparative analysis  
**M.Yu. Tretyakov, T.A. Odintsova, P. Roy, O. Pirali**
- M4 H<sub>2</sub>CO molecule vibrational energy spectrum. Re-summation of divergent perturbation series for highly excited states  
**A.N. Duchko, A.D. Bykov**
- M5 Combining *ab initio*, variational and contact transformation methods for accurate spectra predictions: from three- to six-atomic molecules  
**Vi.G. Tyuterev, M. Rey, T. Delahaye, A.V. Nikitin, S.A. Tashkun, R.V. Kochanov, E.N. Starikova**
- M6 Spectral sensitivity of Fourier transform spectrometer based on relative intensity measurements and *ab initio* calculations  
**A. Kruzins, I. Klincare, O. Nikolayeva, M. Tamanis, R. Ferber, E.A. Pazyuk, A.V. Stolyarov**

### Oral Session N, 14<sup>30</sup>–16<sup>00</sup>

*Chair: Andrei V. Stolyarov*

- N1 Analyses of <sup>16</sup>O<sup>16</sup>O<sup>18</sup>O asymmetric ozone isotopic species in the whole 800–6500 cm<sup>-1</sup> infrared spectral region  
**A. Barbe, M.-R. De Backer, X. Thomas, Vi.G. Tyuterev, E.N. Starikova, A. Campargue, D. Mondelain, S. Kassi**

- N2 Sub-THz molecular spectroscopy with radioacoustic detection and high-power radiation source  
**M.A. Koshelev, A.I. Tsvetkov, M.V. Morozkin, M.Yu. Glyavin, M.Yu. Tretyakov**
- N3 Tunable diode laser absorption spectroscopy for the measurement of accurate and traceable line strengths of different analytes  
**A. Pogány, A. Klein, O. Werhahn, V. Ebert**
- N4 FTIR spectrometer with 30-m base length absorption cell for spectra investigation in wide spectral region: improvement of optical setup  
**A.M. Solodov, T.M. Petrova, Yu.N. Ponomarev, A.A. Solodov**
- N5 UV-Photoexcitation of oxygen encounter complexes X–O<sub>2</sub> as a new channel of singlet oxygen O<sub>2</sub>(<sup>1</sup>Δ<sub>g</sub>)  
**A.P. Pyryaeva, A.V. Baklanov, S.A. Kochubei, V.G. Goldort**
- N6 Introduction to HITRAN Application Programming Interface (HAPI)  
**R.V. Kochanov, C. Hill, P. Wcislo, J.S. Wilzewski, I.E. Gordon, L.S. Rothman**

**Poster Session O, 16<sup>15</sup>–18<sup>00</sup>**

- O1 Rotational study of the CH<sub>4</sub>–CO van der Waals complex in the millimeter-wave range  
**I.V. Tarabukin, V.A. Panfilov, L.A. Surin**
- O2 CRDS spectrum of the 3ν<sub>1</sub> + 3ν<sub>2</sub> + ν<sub>3</sub> band of NO<sub>2</sub> near 7587 cm<sup>-1</sup>  
**A.A. Lukashevskaya, O.V. Naumenko, V.I. Perevalov, D. Mondelain, S. Kassi, A. Campargue**
- O3 High-resolution study of the ν<sub>10</sub> + ν<sub>12</sub> – ν<sub>10</sub> "hot" band of the <sup>13</sup>C<sub>2</sub>H<sub>4</sub>  
**G.A. Onopenko, N.V. Kashirina, A.G. Litvinovskaya**
- O4 High resolution analysis of the ν<sub>12</sub> band and re-analysis of the ground vibrational state of *cis*-d<sub>2</sub>-ethylene  
**Yu.V. Chertavskikh, A.S. Belova, I.A. Konov**
- O5 Assignment and modeling of <sup>13</sup>CH<sub>4</sub> from 5853 to 6200 cm<sup>-1</sup>: Preliminary results  
**E.N. Starikova, A.V. Nikitin, S.A. Tashkun, M. Rey, V.I.G. Tyuterev**
- O6 Line parameters of HD<sup>16</sup>O from LED-based Fourier transform spectroscopy between 11 200 cm<sup>-1</sup> and 12 400 cm<sup>-1</sup>  
**L.N. Sinita, V.I. Serdyukov, E.R. Polovtseva, B.A. Voronin, A.P. Shcherbakov, A.D. Bykov**
- O7 Approximation of Voigt contour for atmosphere transmission spectra calculation  
**A.Ya. Sukhanov**
- O8 Vibrational states of the triplet electronic state of H<sub>3</sub><sup>+</sup>: the role of non-adiabatic Jahn-Teller coupling  
**A. Alijah, V. Kokoouline**
- O9 Methane high-*T* partition function from contact transformations and variational calculations  
**B.M. Krishna, A.V. Nikitin, M. Rey, S.A. Tashkun, V.I.G. Tyuterev**
- O10 Absorption spectra of combustion products of aircraft and rocket engines  
**O.K. Voitsekhovskaya, D.E. Kashirskii, O.V. Egorov, O.V. Shefer**
- O11 CRDS absorption spectrum of <sup>17</sup>O enriched water vapor between 12277 and 12894 cm<sup>-1</sup>  
**A.-W. Liu, S.-M. Hu, X.-Q. Zhao, J. Wang, S.N. Mikhailenko**
- O12 Reanalysis of line centers of HCl isotopologues in the ground electronic state  
**T.I. Velichko, S.N. Mikhailenko**
- O13 FTIR spectra of Ne I in 1300–7000 cm<sup>-1</sup> range: Rydberg *h*-states  
**S. Civiš, P. Kubelik, A. Pastorek, E.M. Zanozina, L. Juha, V.T. Chernov, A.A. Voronina**
- O14 Fourier transform spectrum of water vapor in the 3–5 μm transparency window  
**T.M. Petrova, A.M. Solodov, A.A. Solodov, O.V. Naumenko**

- O15 Modeling of CRDS  $^{12}\text{CH}_4$  spectra at 80 K in the 6539–6800  $\text{cm}^{-1}$  region  
**A.V. Nikitin, M. Rey, S.A. Tashkun, Vl.G. Tyuterev, S. Kassi, A. Campargue**
- O16 Molecular complexes  $(\text{H}_2\text{S})_n$ ,  $n = (1-6)$   
**D.A. Sunchugashev, Yu.N. Kalugina, V.N. Cherepanov**
- O17 Conformational analysis of the *N*-methylformamide molecule in the ground  $S_0$  and lowest excited  $S_1$  and  $T_1$  electronic states  
**N.V. Tukachev, V.A. Bataev, I.A. Godunov**
- O18 Retrieving the ratios of soft to hard velocity-changing collision's frequencies from  $\text{H}_2\text{O}$  line profiles near 0.8  $\mu\text{m}$   
**V.P. Kochanov, L.N. Sinitsa**
- O19 NO absorption dynamics in gas mixtures excited by pulsed electric discharge  
**S.P. Derevyashkin, A.A. Ionin, Yu.M. Klimachev, I.O. Kinyaevskiy, A.A. Kotkov, A.Yu. Kozlov, A.K. Kurnosov**
- O20 Simulation of the atmospheric radiative transfer in the water vapor near-infrared absorption bands  
**T.Yu. Chesnokova, A.V. Chentsov, B.A. Voronin**
- O21  $\text{CO}_2$  absorption lines measuring in the Earth's atmosphere using NIR heterodyne spectrometer  
**A.A. Pereslavl'tseva, A.Yu. Klimchuk**
- O22 Dependence of  $\text{H}_2\text{O}-\text{N}_2$  broadening coefficients on the vibrational quantum indices  
**L.N. Sinitsa, V.I. Serdyukov, N.N. Lavrentieva, A.S. Dudaryonok**
- O23 Broadening parameters of water vapor lines induced by hydrogen and helium pressure  
**A.S. Dudaryonok, N.N. Lavrentieva, J. Tennyson, E. Barton, S.N. Yurchenko**
- O24 The dependence of the optical parameters XeCl-excilamp of the dynamic pressure jump  
**M.V. Didenko**
- O25 *Ab initio* calculation of the photodissociation processes in the NaO molecule  
**A. Berezhnoy, A.A. Buchachenko, V.V. Meshkov, A.V. Stolyarov**
- O26 Application of a near-IR tunable diode laser absorption spectroscopy (TDLAS) for temperature and concentration measurements of methane at various pressures  
**Sh.Sh. Nabiev, V.M. Semenov, G.Yu. Grigor'iev, D.B. Stavrovskii, Ya.Ya. Ponurovskii**
- O27 Electronic spectra of molecular quasicrystals with Frank-Kasper structure  
**A.K. Drozdova, A.V. Nyavro, V.N. Cherepanov, L.I. Kveglis**
- O28 Electronic structure and spectra of 3-nitroformazan  
**P.V. Petunin, P.S. Postnikov, M.E. Trusova, A.K. Drozdova, R.R. Valiev, V.N. Cherepanov**

### Round Table P. Quality of spectral data, 17<sup>30</sup>–19<sup>00</sup>

*Chair: Leonid N. Sinitsa*

- P1 On the accuracy of atomic and molecular data needed for stellar spectroscopy  
**Tatiana A. Ryabchikova**
- P2 How to compile line lists from diverse experimental and theoretical sources while letting through a minimum of errors  
**Iouli E. Gordon, L.S. Rothman**
- P3 Expert spectral data quality  
**Alexander Z. Fazliev**

## July 4, 2015, Saturday

### Invited Lectures Q, 9<sup>00</sup>–10<sup>30</sup>

*Chair: Frédéric Merkt*

- Q1 High-resolution spectroscopy to study the atmospheres of terrestrial planets  
**Anna A. Fedorova**
- Q2 Molecular spectroscopy as a probe for quantum water potentials  
**Claude Leforestier**

### Oral Session R, 11<sup>00</sup>–12<sup>30</sup>

*Chair: Mikhail Yu. Tretyakov*

- R1 Application of methane saturated dispersion resonances near 2.36  $\mu\text{m}$  over the temperature range 77–300 K for optical frequency standards  
**V.A. Lazarev, M.K. Tarabrin, V.E. Karasik, A.N. Kireev, Yu.V. Korostelin, Yu.P. Podmarkov, M.P. Frolov, A.S. Shelkovnikov, V.I. Kozlovsky, M.A. Gubin**
- R2 Spectral line-shape model tests with precision spectroscopy of hydrogen molecule  
**Y. Tan, A.-W. Liu, J. Wang, C.-F. Cheng, S.-M. Hu**
- R3 Band wing shape calculation using spectral characteristics of collision-induced rotational perturbations: application to CO and CO<sub>2</sub> infrared spectra  
**D.V. Oparin, I.M. Grigoriev, N.N. Filippov**
- R4 The water self- and foreign- continua in the 2.3 and 1.6  $\mu\text{m}$  atmospheric windows  
**D. Mondelain, S.S. Vasilchenko, S. Kassi, D. Romanini, I. Ventrillard, A. Campargue**
- R5 Retrieval of the water vapour continuum absorption from the high-resolution Fourier spectra in 2.7 and 6.25  $\mu\text{m}$  bands  
**I.V. Ptashnik, T.E. Klimeshina, T.M. Petrova, A.A. Solodov, A.M. Solodov**
- R6 Spectral composition of the water vapour self-continuum absorption in 2.7 and 6.25  $\mu\text{m}$  bands  
**I.V. Ptashnik, T.E. Klimeshina**

### School Lectures S, 14<sup>30</sup>–16<sup>15</sup>

*Chair: Sergei N. Yurchenko*

- S1 Collision-induced absorption of IR-radiation by the major atmospheric species  
**Yury I. Baranov**
- S2 Water vapour continuum absorption: History, hypotheses, experiment  
**Igor V. Ptashnik**

### Round Table T. Water vapour continuum absorption, 16<sup>30</sup>–18<sup>00</sup>

*Chair: Igor V. Ptashnik*

## Electronic structure and spectra of 3-nitroformazan

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Formazan dyes are considerable interest as organic reactants and widely known for several decades. In addition to its value as synthetic intermediates in the preparation tiocarbazon, tetrazolium salts and verdazyl radicals [1], they are also promising dyes to form the brightly colored compounds due to their ability to form stable complexes with various metals [2].

Some characteristics of the electronic absorption spectra of formazan molecules with nine different substituents have been calculated using the RI-CC2 and TDDFT quantum chemical methods (see table and figure). Also, the electronic absorption spectra have been measured. The experimental electronic energies and oscillator strengths are agreed well with the theoretical results obtained by the both methods. The discrepancies are not exceeded of  $800\text{ cm}^{-1}$ . Therefore, the use of these methods for the modeling of the electronic properties and spectra of considered molecules is adequate.



Fig. 3-nitroformazan structure.

Table. Wave numbers of the  $S_0 \rightarrow S_1$  transitions and Hammett and Brown constants for 3-nitroformazan

Substituent	Hammett constant $\sigma_{\text{para}}$	Wavenumber, $\text{cm}^{-1}$ TDDFT/B3LYP/6-31G(d,p)	Brown constant $\sigma_{\text{para}}^+$	Wavenumber, $\text{cm}^{-1}$ TDDFT/B3LYP/6-31G(d,p)
-O-C <sub>2</sub> H <sub>5</sub>	-0.28	19406.00	-0.78	19406.00
-C <sub>4</sub> H <sub>9</sub>	-0.16	18818.00	-0.33	18818.00
-C <sub>2</sub> H <sub>5</sub>	-0.14	18817.00	-0.31	18817.00
-H	0.00	18650.00	0	18650.00
-Ph	0.05	18564.00	-0.179	18564.00
-Br	0.26	18583.00	0.15	18583.00
-COO-C <sub>2</sub> H <sub>5</sub>	0.44	17988.00	0.48	17988.00
-CN	0.70	17900.00	0.66	17900.00
-NO <sub>2</sub>	0.81	17600.00	0.79	17600.00

The calculations show that the electronic donor groups -C<sub>2</sub>H<sub>5</sub>, -C<sub>4</sub>H<sub>9</sub>, -O-C<sub>2</sub>H<sub>5</sub>, and -H increase the electronic density at LUMO orbitals increasing the wavenumbers of the transition  $S_0 \rightarrow S_1$ . In turn, the electron-accepter substituents -CN, -COO-C<sub>2</sub>H<sub>5</sub>, C<sub>2</sub>H<sub>5</sub>, -NO<sub>2</sub> attract the electronic density of LUMO orbitals to itself decreasing the calculated wavenumbers for the transition  $S_0 \rightarrow S_1$ .

The found high correlation between Hammett and Brown constants and the wavenumber changes shows that the proposed model may be used to calculate the spectra of 3-nitroformazan.

### References

1. J.B. Gilroy, M.J. Ferguson, R. McDonald, R.G. Hicks, Synthesis and characterization of palladium complexes of 3-nitroformazans, *Inorg. Chim. Acta* **361**, 3388–3393 (2008).
2. J. Sokolowska-Gajda, H.S. Freeman, A. Reife, Synthetic Dyes Based on Environmental Considerations. Part 2: Iron Complexed Formazan Dyes, *Dyes Pigm.* **30**, 1–20 (1996).