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on High Resolution Molecular Spectroscopy

HighRus-2015

June 30–July 4, 2015

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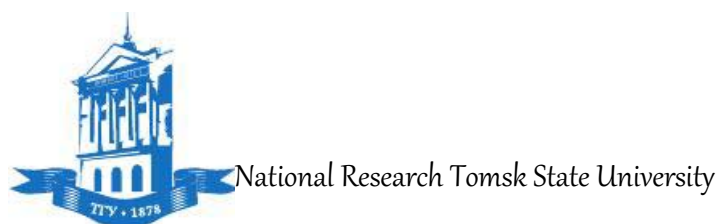
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V.I. Perevalov – *chair*

B.A. Voronin

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Symposium Schedule

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

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Session Program

June 30, 2015, Tuesday

Invited Lectures A, 11⁰⁰–12³⁰

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, 14³⁰–16⁰⁰

Chair: Vladimir G. Tyuterev

- B1 A new triplet transition of the V₂ 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 NO₂ 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, 16¹⁵–18⁰⁰

- C1 Millimeter-wave measurements and ab initio calculations of the NH₃–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 S¹⁸O₂ spectrum: The ν_1 and ν_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 ν_6 band of the CH₂=CD₂ molecule
K.B. Berezkin, N.V. Kashirina
- C6 The absorption spectrum of ¹⁷O enriched water vapor by CRDS between 5850 and 6670 cm⁻¹
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 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 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 GeH_4 molecule
A.A. Rodina, A.V. Nikitin, M. Rey, V.I.G. Tyuterev
- C10 First principles calculation of rovibrational spectra for 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 SO_2
B.A. Voronin
- C16 Retrievals of the CH_4 and 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 CO_2 clusters relevant to CO_2 -rich atmospheres
T.N. Sinyakova, R.E. Asfin, D.V. Oparin, N.N. Filippov, J.V. Buldyreva
- C18 Temperature dependence of self-, N_2 -broadened line widths of methyl cyanide vibrational lines
A.S. Dudaryonok, N.N. Lavrentieva, J.V. Buldyreva
- C19 Study of the H_2O – H_2O line broadening in 15 500–16 000 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 H_2 , He and CO_2 broadening and shifting parameters and their temperature dependences. Part 1: SO_2 , NH_3 , HF, HCl, OCS, and C_2H_2
J.S. Wilzewski, I.E. Gordon, L.S. Rothman, R.V. Kochanov, C. Hill
- C22 Broadening parameters for H_2O 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. Patrakeev, 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 μm 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 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, 17⁰⁰–18³⁰

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, 9⁰⁰–10³⁰

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, 11⁰⁰–12³⁰

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, 14³⁰–16⁰⁰

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 cm^{-1} and 5900 cm^{-1}
A. Rausch, O. Werhahn, V. Ebert
- G3 D_2O 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 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 NH₃
M.R. Cherkasov

Poster Session H, 16¹⁵–18⁰⁰

- H1 Analysis of six new bands of ¹⁸O₃ recorded by CRDS technique in the 7400–7920 cm⁻¹ 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 N₂O 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 C₂H₂D₂-*trans*: the ν₈+ν₁₀ (Au) band
A.G. Litvinovskaya, N.I. Raspopova, F. Zhgan
- H4 Nitrogen dioxide high temperature line list in the 466–3374 cm⁻¹ region
A.A. Lukashevskaya, V.I. Perevalov, A. Perrin
- H5 Fourier transform absorption spectrum of D₂¹⁶O in 14 800–15 200 cm⁻¹ 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 CO₂ near 1.7 μm
S. Kassi, D. Mondelain, H. Tran, A. Campargue
- H8 Calculation of rotation-vaibaron 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 ¹⁶O¹⁸O¹⁶O and ¹⁸O¹⁶O¹⁸O 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 PH₃ absorption spectrum in the Octad range between 2800 and 3600 cm⁻¹
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 AB₄, ABC₃ type molecules
A.V. Nikitin, B.M. Krishna, M. Rey, Vl.G. Tyuterev
- H13 Radiative properties of the low-lying states of Rb₂ and Cs₂ 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 (C₂H₂)
O.M. Lyulin, V.I. Perevalov
- H17 ¹²C¹⁶O 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 μm 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 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. Kolobyanin
- 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. Pereslavytseva, 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 μm 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, 17⁰⁰–18⁴⁵

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, 9⁰⁰–10³⁰

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, 11⁰⁰–12³⁰

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, 9⁰⁰–10³⁰

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, 11⁰⁰–12³⁰

Chair: Jonathan Tennyson

- M1 Rotational spectrum of the NH₃–H₂ 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 H₂O molecule: New experimental data and their comparative analysis
M.Yu. Tretyakov, T.A. Odintsova, P. Roy, O. Pirali
- M4 H₂CO 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, 14³⁰–16⁰⁰

Chair: Andrei V. Stolyarov

- N1 Analyses of ¹⁶O¹⁶O¹⁸O asymmetric ozone isotopic species in the whole 800–6500 cm⁻¹ 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–O₂ as a new channel of singlet oxygen O₂(¹Δ_g)
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, 16¹⁵–18⁰⁰

- O1 Rotational study of the CH₄–CO van der Waals complex in the millimeter-wave range
I.V. Tarabukin, V.A. Panfilov, L.A. Surin
- O2 CRDS spectrum of the 3ν₁ + 3ν₂ + ν₃ band of NO₂ near 7587 cm⁻¹
A.A. Lukashevskaya, O.V. Naumenko, V.I. Perevalov, D. Mondelain, S. Kassi, A. Campargue
- O3 High-resolution study of the ν₁₀ + ν₁₂ – ν₁₀ "hot" band of the ¹³C₂H₄
G.A. Onopenko, N.V. Kashirina, A.G. Litvinovskaya
- O4 High resolution analysis of the ν₁₂ band and re-analysis of the ground vibrational state of *cis*-d₂-ethylene
Yu.V. Chertavskikh, A.S. Belova, I.A. Konov
- O5 Assignment and modeling of ¹³CH₄ from 5853 to 6200 cm⁻¹: Preliminary results
E.N. Starikova, A.V. Nikitin, S.A. Tashkun, M. Rey, V.I.G. Tyuterev
- O6 Line parameters of HD¹⁶O from LED-based Fourier transform spectroscopy between 11 200 cm⁻¹ and 12 400 cm⁻¹
L.N. Sinitsa, 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 H₃⁺: 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 ¹⁷O enriched water vapor between 12277 and 12894 cm⁻¹
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⁻¹ 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 cm^{-1} region
A.V. Nikitin, M. Rey, S.A. Tashkun, Vi.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 H_2O line profiles near 0.8 μm
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 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, 17³⁰–19⁰⁰

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, 9⁰⁰–10³⁰

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, 11⁰⁰–12³⁰

Chair: Mikhail Yu. Tretyakov

- R1 Application of methane saturated dispersion resonances near 2.36 μm 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 CO₂ 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 μm 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 μm 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 μm bands
I.V. Ptashnik, T.E. Klimeshina

School Lectures S, 14³⁰–16¹⁵

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, 16³⁰–18⁰⁰

Chair: Igor V. Ptashnik

Molecular complexes $(\text{H}_2\text{S})_n$, $n = (1-6)$

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Studies of the molecular structure for the complexes $(\text{H}_2\text{S})_n$, $n = 1-6$ were carried out at the MP2 level of theory and at the DFT level using the density functionals B3LYP, CAM-B3LYP, B97D3, and PBE0 with the aug-cc-pvtz basis. As a result, the stable configurations of considered complexes were found. As an example, Fig. 1 shows the two stable configurations of H_2S trimer. The harmonic frequencies of all studied complexes and anharmonic frequencies for the dimer and trimer are reported. The harmonic frequencies for

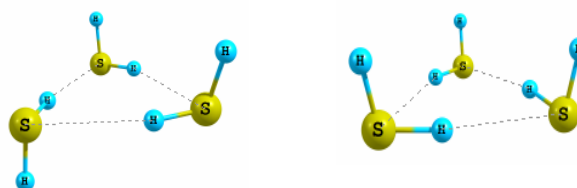


Fig.1. Stable configurations of $(\text{H}_2\text{S})_3$. (on the left – like in [1], on the right – new found).

the most stable configurations calculated with the B3LYP functional are given in Fig. 2. Analysis of the figure shows that the largest frequency shifts ($\sim 2550-2690 \text{ cm}^{-1}$) for considered complexes are related to the symmetric vibration ν_1 of H_2S . It is also noticeable that with the increasing of the size of a complex the frequencies related to the ν_1 and ν_3 bands of H_2S are shifted to the lower ones. At the same time, the bands related to the bending vibration ν_2 of H_2S are shifted in both directions.

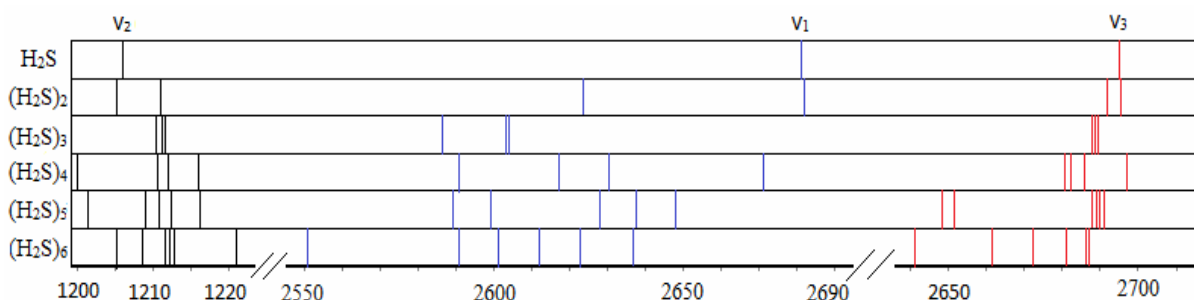


Fig. 2. Harmonic frequencies of the molecular complexes $(\text{H}_2\text{S})_n$, $n = (1-6)$.

We also report the multipole electric moments and polarizabilities of studied complexes. The simulated Raman and IR spectra of considered complexes are presented. The analysis of the polarization properties of Raman scattering was carried out.

References

1. M. Joze, M. Enrique, *J. Chem. Phys.* **122**, 204315 (2005).