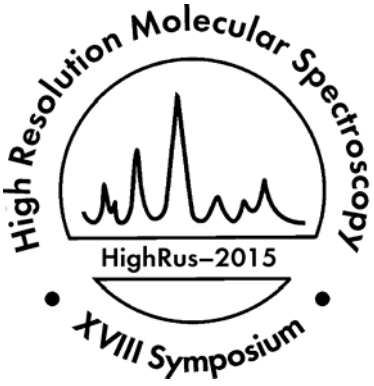

XVIII Symposium and School

on High Resolution Molecular Spectroscopy

HighRus-2015

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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		

Contents

Session Program

June 30, 2015, Tuesday

Invited Lectures A, 11^{00}–12^{30}

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^{30}–16^{00}

Chair: Vladimir G. Tyuterev

B1 A new triplet transition of the V_2 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_2 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^{15}–18^{00}

C1 Millimeter-wave measurements and ab initio calculations of the NH_3–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 $S^{18}O_2$ 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 v6 band of the CH_2=CD_2 molecule
K.B. Berezkin, N.V. Kashirina

C6 The absorption spectrum of ^{17}O 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 $^{12}C^{18}O_2$ and $^{16}O^{12}C^{18}O$ 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, Vl.G. Tyuterev

C10 First principles calculation of rovibrational spectra for SiH_4 molecule
Y.S. Chizhmakova, A.V. Nikitin, M. Rey, Vl.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 $^{16}O^{12}C^{32}S$ 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, Vl.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, 17^{00}–18^{30}

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^{00}–10^{30}

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^{00}–12^{30}

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^{30}–16^{00}

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 ← 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_3
M.R. Cherkasov

Poster Session H, 16^{15}–18^{00}

H1 Analysis of six new bands of $^{18}O_3$ 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 N_2O 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 $C_2H_2D_2$-*trans*: the $\nu_8+\nu_{10}$ (Au) band
A.G. Litvinovskaya, N.I. Raspopova, F. Zhgan

H4 Nitrogen dioxide high temperature line list in the 466–3374 $см^{-1}$ region
A.A. Lukashevskaya, V.I. Perevalov, A. Perrin

H5 Fourier transform absorption spectrum of $D_2{}^{16}O$ 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 CO_2 near 1.7 μm
S. Kassi, D. Mondelain, H. Tran, A. Campargue

H8 Calculation of rotation-vaibarion 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 $^{16}O^{18}O^{16}O$ and $^{18}O^{16}O^{18}O$ 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_3 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 AB_4, ABC_3 type molecules
A.V. Nikitin, B.M. Krishna, M. Rey, Vl.G. Tyuterev

H13 Radiative properties of the low-lying states of Rb_2 and Cs_2 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_2H_2)
O.M. Lyulin, V.I. Perevalov

H17 $^{12}C^{16}O$ 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. Tretyakov

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. Pereslavtseva, 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, 17^{00}–18^{45}

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^{00}–10^{30}

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^{00}–12^{30}

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^{00}–10^{30}

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^{00}–12^{30}

Chair: Jonathan Tennyson

M1 Rotational spectrum of the NH_3–H_2 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_2O molecule: New experimental data and their comparative analysis
M.Yu. Tretyakov, T.A. Odintsova, P. Roy, O. Pirali

M4 H_2CO 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
Vl.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^{30}–16^{00}

Chair: Andrei V. Stolyarov

N1 Analyses of $^{16}O^{16}O^{18}O$ asymmetric ozone isotopic species in the whole 800–6500 cm^{-1} infrared spectral region
A. Barbe, M.-R. De Backer, X. Thomas, Vl.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_2 as a new channel of singlet oxygen $O_2(^1\Delta_g)$
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. Wcisło, J.S. Wilzewski, I.E. Gordon, L.S. Rothman

Poster Session O, 16^{15}–18^{00}

O1 Rotational study of the CH_4–CO van der Waals complex in the millimeter-wave range
I.V. Tarabukin, V.A. Panfilov, L.A. Surin

O2 CRDS spectrum of the $3\nu_1 + 3\nu_2 + \nu_3$ band of NO_2 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 $\nu_{10} + \nu_{12} - \nu_{10}$ "hot" band of the $^{13}C_2H_4$
G.A. Onopenko, N.V. Kashirina, A.G. Litvinovskaya

O4 High resolution analysis of the ν_{12} band and re-analysis of the ground vibrational state of *cis*-d_2-ethylene
Yu.V. Chertavskikh, A.S. Belova, I.A. Konov

O5 Assignment and modeling of $^{13}CH_4$ from 5853 to 6200 cm^{-1}: Preliminary results
E.N. Starikova, A.V. Nikitin, S.A. Tashkun, M. Rey, Vl.G. Tyuterev

O6 Line parameters of $HD^{16}O$ 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 H_3^+: 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, Vl.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 ^{17}O 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 $^{12}CH_4$ spectra at 80 K in the 6539–6800 cm^{-1} region
A.V. Nikitin, M. Rey, S.A. Tashkun, Vl.G. Tyuterev, S. Kassi, A. Campargue

O16 Molecular complexes $(H_2S)_n$, 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. Pereslavtseva, A.Yu. Klimchuk

O22 Dependence of H_2O–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^{30}–19^{00}

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^{00}–10^{30}

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^{00}–12^{30}

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 CO_2 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, 14^{30}–16^{15}

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^{30}–18^{00}

Chair: Igor V. Ptashnik

O27

Electronic spectra of molecular quasicrystals with Frank-Kasper structure

Anna K. Drozdova, Alexander V. Nyavro, Victor N. Cherepanov

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The considered quasicrystal structures are an alloy of iron-manganese-carbon (86% Fe; 13% Mn; 1% C). Under the influence of dynamic loading or as a result of cryomechanical processing the crystal lattice of Hadfield's steel is destroyed and some fragments are appeared which have the icosahedral structure (the symmetry axis of order 5 is appeared which is forbidden for ideal crystals). So, these fragments have the molecular quasicrystal structure. They are also called as the Frank-Kasper (FK) structures [1].

In this work the electron states both for clusters of the ideal twelve vertex polyhedron structure (FK12) and the clusters with the atoms Fe, Mn and C have been considered. The calculations carried out by the method of scattered waves [2, 3] show that in contrast to an ideal crystal the molecular clusters have magnetic properties.

The spectra of single-electron states for each of the spin subsystems were calculated. The curves of the state density have been found.

The measurements of the absorption spectra of thin films of the alloy $Fe_{86}Mn_{13}C$ after cryomechanical processing were carried out the use ShimadzuUV-3600 spectrometer.

The good agreement between the calculated and experimental spectra confirms the appearance of the molecular quasicrystals with the Frank-Kasper structures.

References

1. L.I. Kveglis, R.B. Abylkalykova, F.M. Noskov, V.G. Arhipkin, V.A. Musikhin, V.N. Cherepanov, A.V. Niavro. Local electron structure and magnetiztion in beta-$Fe_{86}Mn_{13}C$, *Superlattices Microstruct.* **46**, 116–120 (2009).
2. V.V. Hemoshkalenko, Yu.N. Kucherenko, Methods of computational physics in the theory of solids. Electronic states in nonideal crystals, Kiev: Naukova Dumka, 1986.
3. A.V. Nyavro, The evolution of the electronic states: atom—molecule—cluster—crystal, Tomsk: TSU Publishing House, 2013.