

**Saturday
March 6, 2010**

3:00 – 10:00 PM Registration/Reception, Radisson Austin North Hotel, Room 920

**Sunday Morning Session
March 7, 2010**

Chair: **Peter Weber**, Brown University, Providence, Rhode Island, U.S.A.

8:30 **James E. Boggs**: Introductory remarks

8:45 SM1 **R. J. Dwayne Miller**
University of Toronto, Toronto, Ontario, Canada
“Making the molecular movie”: quest for the structure-function correlation in biology”

9:45 SM2 **David Gruzman, Amir Karton and Jan M. L. Martin**
Weizmann Institute of Science, Rehovot, Israel
“Conformational equilibria in linear and branched alkanes: surprisingly difficult targets for density functional methods”

10:05 SM3 **Peter Zajac^a, Dong Xu^b, and Andrew L. Cooksy^a**
^aSan Diego State University, San Diego, California, U. S. A.
^bNational Biomedical Computational Resource, San Diego, California, U.S.A.
“Vibrational states on relocalization surfaces of hydrocarbon free radicals”

10:25 Break

10:55 SM4 **Anthony M. Reilly, Carole A. Morrison, Derek A. Wann and David W. H. Rankin**
University of Edinburgh, Edinburgh, United Kingdom
“Equilibrium structures of gases and solids”

11:15 SM5 **Luis Rivera-Rivera, Blake A. McElmurry, K. Wayne Smith, Z. Wang, F. F. Willaert, I. I. Leonov, Robert R. Lucchese and John W. Bevan**
Texas A & M University, College Station, Texas, U.S.A.
“New perspectives from morphing potentials for hydrogen bonded interactions”

11:35 SM6 **Norman Craig**
Oberlin College, Oberlin, Ohio, U.S.A.
“A proposal for a general method for determining semi-experimental equilibrium structures of carbon atom backbones”

11:55 Lunch

**Sunday Afternoon Session
March 7, 2010**

Chair: **Carole Morrison**, Edinburgh University, Edinburgh, United Kingdom

- 1:30 SA1 **Paul R. Raithby**
University of Bath, Bath, United Kingdom
“Photocrystallography: from static to dynamic”
- 2:30 SA2 **Elfi Kraka**
Southern Methodist University, Dallas, Texas, U.S.A.
“Unified reaction valley approach: new insights into chemical reaction mechanism”
- 2:50 SA3 **Dines Christen^a, Alexander Konrad^a, Frank Blockhuys^b, Karla Tersago^b, Sergey A. Shlykov^c, and Peter Groner^d**
^aInstitut für Physikalische und Theoretische Chemie der Universität Tübingen, Germany
^bUniversity of Antwerp, Antwerp, Belgium
^cIvanovo State University of Chemistry and Technology, Ivanovo, Russia
^dUniversity of Missouri at Kansas City, Missouri, U. S. A.
“Microwave spectroscopy at the University of Tübingen”
- 3:10 SA4 **Alan R. Ford and Peter Pulay^b**
^aAlakai Defense Systems, Fort Leonard Wood, Missouri, U. S. A.
^bUniversity of Arkansas, Fayetteville, Arkansas, U. S. A.
“Infrared spectra of polycondensed aromatic hydrocarbons”
- 3:30 SA5 **Frank J. Lovas^{a,b}, David F. Plusquellic^a, and Susanna L. Widicus Weaver^{b,c}**
^aNational Institute of Standards and Technology, Gaithersburg, Maryland, U.S.A..
^bUniversity of Virginia, Charlottesville, Virginia, U.S.A.
^cEmory University, Atlanta, Georgia, U.S.A.
“Spectral study of dimethyl carbonate, a low energy isomer in the family with empirical formula C₃H₆O₃”
- 3:50 - 5:30 **Poster session I**
Posters 1 - 12

POSTER SESSION I
SUNDAY, MARCH 7, 2010
3:50-5:30 PM

- P1 **Sean C. Smith, S. A. Alexander and Walter M. Potter**
Southwestern University, Georgetown, Texas, U.S.A.
“Finding molecules with large molecular hyperpolarizabilities”
- P2 **Karissa A. Utzat^a, R. K. Bohn^a, J. A. Montgomery, Jr.^a, H. H. Michels^a, and Walther Caminati^b**
^aUniversity of Connecticut, Storrs, Connecticut, U.S.A.
^bUnivesità di Bologna, Bologna, Italy
“Rotational spectrum and tunneling motions of benzyl alcohol”
- P3 **S. A. Cooke**
University of North Texas, Denton, Texas. U.S. A.
“Facilities for microwave spectroscopy at the University of North Texas”
- P4 **Norman C. Craig^a, Deacon J. Nemchick^a, Ethan C. Glor^a, Drew F. K. Williamson^a, Thomas A. Blake^b, and Robert L. Sams^b**
^aOberlin College, Oberlin, Ohio, U.S.A.
^bPacific Northwest National Laboratory, Richland, Washington, U.S.A.
“Rotational analysis of bands in the high-resolution infrared spectra of *trans,trans*- and *cis,cis*-1,4-difluorobutadiene-2-*d*₁”
- P5 **Masaru Fukushima^{a,b} and Michael C. L. Gerry^a**
^aThe University of British Columbia, Vancouver, British Columbia, Canada.
^bHiroshima City University, Hiroshima, Japan
“Fourier transform microwave spectroscopy of AISH”
- P6 **L. L. Griffin^a, S. Vijayakumar^b, N. H. March^{c,d}, D. J. Klein^a**
^aTexas A&M University at Galveston, Galveston, Texas, U.S.A.
^bBar-Ilan Univesity, Ramat Gan, Israel
^cUniversity of Antwerp, Antwerp, Belgium
^dOxford University, Oxford, England
“Defected graphene-like molecules: relative energies and structures”
- P7 **Natalja Vogt and Jürgen Vogt**
Universität Ulm, Ulm, Germany
“New features of the MOGADOC database”

- P8 **Drahomir Hnyk, Jan Machacek and Michael G. S. Londesborough**
Institute of Inorganic Chemistry of the ASCR, Rez, Czech Republic
“Two decaboranes together: *syn*- and *anti*-B₁₈H₂₂ revisited. Structural and ¹¹B NMR consequences of their deprotonation”
- P9 **Russell D. Johnson III**
National Institute of Standards and Technology, Gaithersburg, Maryland, U.S.A.
“NIST computational chemistry comparison and benchmark database”
- P10 **Yang Liu, Isaac B. Bersuker, Wenli Zou, and James E. Boggs**
The University of Texas at Austin, Austin, Texas, U.S.A.
“Pseudo Jahn-Teller versus Renner-Teller effects in instability of linear triatomic molecules”
- P11 **Davood Nori-Shargh^{a,b}, Abolfazl Shiroudi^b, and James E. Boggs^a**
^aThe University of Texas at Austin, Austin, Texas, U.S.A.
^bIslamic Azad University, Tehran, Iran
“Theoretical study of the pressure dependent rate constants of the isomerization reactions of vinylcyclopropane and perfluorovinylcyclopropane to their corresponding cyclopentenes”
- P12 **Juana Vázquez and John F. Stanton**
The University of Texas at Austin, Austin, Texas, U.S.A.
“Exploiting symmetry for the computation of infrared spectroscopic features”

**Monday Morning Session
March 8, 2010**

Chair: **David W. H. Rankin**, University of Edinburgh, Edinburgh, United Kingdom

8:30 MM1 **Joshua Sebree, Chirantha P. Rodrigo, William H. James III, and Timothy S. Zwier**

Purdue University, Lafayette, Indiana, U.S.A.

“Laser probes of structure and dynamics in the complexity gap”

9:30 MM2 **Attila G. Császár^a, Edit Mátyus^{a,b}, Gábor Czako^{a,c}, Csaba Fábri^a, Tibor Furtenbacher^a, and Tamás Szidarovszky^a**

^aEötvös University, Budapest, Hungary

^bEidgenössische Technische Hochschule, Zürich, Switzerland

^cEmory University, Atlanta, Georgia, U.S.A.

“Quantum spectroscopy”

9:50 MM3 **Peter M. Weber, Michael P. Minitti, Sanghamitra Deb, Christine Bühler**
Brown University, Providence, Rhode Island, U.S.A.

“Ultra structural dynamics in tertiary amines and cyclic dienes”

10:10 Break

10:40 MM4 **Sarah L. Masters**

University of Edinburgh, Edinburgh, United Kingdom

“Hot Stuff: FVP-GED”

11:00 MM5 **Ray Hefferlin**

Southern Adventist University, Collegedale, Tennessee, U.S.A.

“Spectroscopic constants systematics and predictions using least squares and neural networks”

11:20 MM6 **Michael E. Harding^{a,b}, Juana Vázquez^{a,b}, Gregor Diezemann^b, John F. Stanton^a, and Jürgen Gauss^b**

^aThe University of Texas at Austin, Austin, Texas, U.S.A.

^bUniversität Mainz, Mainz, Germany

“Vibrational energy levels and vibrationally averaged properties using a mixed approach of numerical and analytical integration”

11:40 MM7 **Xinzheng Yang and Michael B. Hall**

Texas A&M University, College Station, Texas, U.S.A.

“Unusual involvement of a ruthenium complex’s pincer ligand in promoting the splitting of water”

12:00 Lunch

**Monday Afternoon Session
March 8, 2010**

Chair: **Elfi Kraka**, Southern Methodist University, Dallas, Texas. U.S.A.

- 1:30 MA1 **Jens-Uwe Grabow**
Gottfried-Wilhelm-Leibniz-Universität, Hannover, Germany
“Delivering local structure information via long distance communication to a large amplitude motion site: molecular rotation spectra”
- 2:30 MA2 **Cristina Puzzarini**
Università di Bologna, Bologna, Italy
“Molecular structure determination from quantum-chemical calculations: extrapolation to the complete basis set limit and additivity approximation”
- 2:50 MA3 **R. Bakova^b, S. Zális^b, E. Gindensperger^a and Chantal Daniel^a**
^aUniversité de Strasbourg, Strasbourg, France
^bAcademy of Sciences of Czech Republic, Prague, Czech Republic
“Ultra-fast intersystem crossings in transition metal complexes: a theoretical analysis based on *ab initio* calculations”
- 3:10 MA4 **John F. Stanton**
The University of Texas at Austin, Austin, Texas, U.S.A.
“The B-X Band System of NO₃”
- 3:30 Break
- 4:00 MA5 **Kenneth Hedberg**
Oregon State University, Corvallis, Oregon, U.S.A.
“How accurate are parameter values determined by gas-phase electron diffraction?”
- 4:20 MA6 **Jean Demaison**
Université de Lille, Villeneuve d’Ascq, France
“Do we need accurate rotational constants?”
- 6:30 **Social Hour**
- 7:15 **Symposium banquet**
- Presentation of Dr. Barbara Mez-Starck Prize**
Jürgen Vogt, Universität Ulm, Ulm, Germany
- Banquet Speaker: Carl Lineberger**
University of Colorado at Boulder, U. S. A.
“Forty years of molecular structure”

**Tuesday Morning Session
March 9, 2010**

Chair: **Christina Puzzarini**, Univesità di Bologna, Bologna, Italy

- 8:30 TM1 **Robert J. McMahon**
University of Wisconsin, Madison, Wisconsin, U. S. A.
“Photochemistry and spectroscopy of organic reactive intermediates”
- 9:30 TM2 **Harald Møllendal and Alexey Konovalov**
University of Oslo, Oslo, Norway
“Microwave spectrum of 2-aminooxazole, a compound of potential prebiotic and astrochemical interest”
- 9:50 TM3 **Esther J. Ocola^a, Abdulaziz A. Al-Saadi^b, and Jaan Laane^a**
^aTexas A & M University, College Station, Texas, U.S.A.
^bKing Fahd University of Petroleum & Minerals, Dhahran, Saudi Arabia
“Spectroscopic and *ab initio* investigation of intramolecular π -type hydrogen bonding ”
- 10:10 TM4 **Cyril Párkányi^a, Zuzana Zajícková^b, Omar R. Martínez^{a,c}, and Marwan Dakkouri^d**
^aFlorida Atlantic University, Boca Raton, Florida, U.S.A.
^bBarry University, Miami Shores, Florida, U.S.A.
^cResidencias Palma Real, Puerto La Cruz, Venezuela
^dUniversität Ulm, Ulm, Germany
“Nitropyridine N-oxides – a theoretical and experimental study”
- 10:30 Break
- 11:00 TM5 **Dieter Cremer**
Southern Methodist University, Dallas, Texas, U.S.A.
“Collaboration between experiment and theory: the Cal-X methods”
- 11:20 TM6 **Manfred Fink^a, Philip Varghese^b, Tamara Pease^c**
^aPhysics Department, The University of Texas at Austin, Austin, Texas, U.S.A.
^bAeromechanics Research Center, The University of Texas at Austin, Austin, Texas, U.S.A.
^cMarine Science Institute, The University of Texas at Austin, Port Aransas, Texas, U.S.A.
“Superior analyzer for Raman spectra with high acceptance cone, high resolution, high transmission, high quantum efficiency and strong background reduction, simultaneously”

11:40 TM7 **Stephen A. Alexander^a, Sumita Datta^b, R. L. Coldwell^c**

^aSouthwestern University, Georgetown, Texas, U.S.A.

^bS. N. Bose National Centre for Basic Sciences, Salt Lake, Calcutta, India

^cUniversity of Florida, Gainesville, Florida, U.S.A.

“Visualizing the hydrogen molecule using Monte Carlo methods”

12:00 Lunch

**Tuesday Afternoon Session
March 9, 2010**

Chair: **Juana Vázquez**, The University of Texas at Austin, Austin, Texas, U.S.A.

1:30 TA1 **Eleanor E. B. Campbell**^{a,c}, **Niklas Olofsson**^b, **Johan Ek Weis**^a, **Oleg A. Nerushev**^a, **Anders Eriksson**^b, **Sang Wook Lee**^c

^aEdinburgh University, Edinburgh, United Kingdom

^bGothenburg University, Gothenburg, Sweden

^cKonkuk University, Seoul, Korea

"Structure and dynamical properties of carbon nanotubes"

2:30 TA2 **William Klemperer**

Harvard University, Cambridge, Massachusetts, U.S.A.

"Comparison of complexes of hydrogen with those of hydrogen fluoride"

2:50 TA3 **Carole A. Morrison**, **Anthony M. Reilly** and **David W. H. Rankin**

University of Edinburgh, Edinburgh, United Kingdom

"Atomic probability distribution functions from molecular dynamics simulations"

3:10 TA4 **Marion L. Ellzey, Jr.**

The University of Texas at El Paso, El Paso, Texas, U.S.A.

"Symmetry averaging a molecular Hamiltonian by tensorial matrix expansion"

3:30 TA5 **Suresh C. Mehrotra**

Dr. Babasaheb Ambedkar Marathwada University, Aurangabad, India

"Structural study of polar liquids through dielectric study using time domain reflectometry"

3:50 - 5:30 **Poster session II**

Posters 14 – 26

**POSTER SESSION II
TUESDAY, MARCH 9, 2010
3:50-5:30 PM**

- P14 **G. Smitty Grubbs II^a, Stephen A. Cooke^a, and Wei Lin^b**
^aUniversity of North Texas, Denton, Texas, U.S.A.
^bUniversity of Texas at Brownsville and Texas Southmost College, Fort Brown, Brownsville, Texas, U.S.A.
“Chirped-pulse Fourier transform microwave spectroscopy of perfluorobutyryl fluoride, C₃F₇COF”
- P15 **Laurent Margulès^a, Jean Demaison^a, Heinz Dieter Rudolph^b**
^aUniversité de Lille, Villeneuve d’Ascq, France
^bUniversität Ulm, Ulm, Germany
“Accurate determination of an equilibrium structure in the presence of a small coordinate: the case of dimethylsulfide”
- P16 **Joseph A. Fournier^a, Robert K. Bohn^a, John A. Montgomery, Jr.^a, and Masao Onda^b**
^aUniversity of Connecticut, Storrs, Connecticut, U.S.A.
^bSophia University, Tokyo, Japan
“Perfluoropentane is helical but C₃F₈ and HC₃F₇ are not”
- P17 **C. T. Dewberry, G. S. Grubbs II, and S. A. Cooke**
University of North Texas, Denton, Texas, U.S.A.
“The pure rotational spectrum of lead monochloride, X²[] PbCl, recorded using a chirped pulse, Fourier transform microwave spectrometer equipped with a laser ablation source”
- P18 **G. S. Grubbs II^a, A. Agnew^b, W. C. Bailey^c and S. A. Cooke^a**
^aUniversity of North Texas, Denton, Texas, U.S.A.
^bGannon University, Erie, Pennsylvania, U.S.A.
^cKean University, Union, New Jersey, U.S.A.
“Observed doubling in the pure rotational spectra of hexafluoroisobutene, (CF₃)₂C=CH₂, hexafluoroacetone imine, (CF₃)C=NH, and also 1-iodoperfluorobutane, C₄F₁₁I”
- P19 **R. J. Mawhorter^a, Arolyn Conwill^a, Zack Lasner^a, Lukas Alpei^b and Jens-Uwe Grabow^b**
^aPomona College, Claremont, California, U.S.A.
^bLeibniz University, Hannover, Germany
“Fluoride diatomics & the shape of the electron”

- P20 **Luis A. Rivera-Rivera, Robert R. Lucchese, and John W. Bevan**
Texas A & M University, College Station, Texas, U.S.A.
“A four-dimensional compound-model morphed potential for the OC:HBr complex”
- P21 **Davood Nori-Shargh, and James E. Boggs**
^aThe University of Texas at Austin, Austin, Texas, U.S.A.
“Hybrid-DFT study and NBO interpretation of the enantiomerization energy profile of chloromethyl methyl ether and its analogues containing Cl, Br and I atoms”
- P22 **Maxim Abaev^{a,b}, Natalja Vogt^a, Igor F. Shishkov^b, Jürgen Vogt^a, Anatolii N. Rykov^b, Lev V. Vilkov^b, Heinz Oberhammer^c**
^aUniversität Ulm, Ulm, Germany
^bMoscow State University, Moscow, Russia
^cUniversität Tübingen, Tübingen, Germany
“Equilibrium structure and conformational composition of succinic acid from gas phase electron diffraction (GED) and quantum chemical studies”
- P23 **Nobuhiko Kuze, Yoji Yanagawa, Noriaki Uchida, Takeshi Sakaizumi, Osamu Ohashi**
Sophia University, Tokyo, Japan
“Molecular conformation, dipole moment, quadrupole coupling constants and barriers to C-C rotation of 2-methyl-2-propenal oxime by rotational spectroscopy and quantum chemical calculation”
- P24 **Derek A. Wann^a, Anthony M. Reilly^a, Paul D. Lickiss^b and David W. H. Rankin^a**
^aUniversity of Edinburgh, Edinburgh, United Kingdom
^bImperial College, London, United Kingdom
“Gas-phase equilibrium structures of silsesquioxanes”
- P25 **Wenli Zou, Yang Liu and James E. Boggs**
The University of Texas at Austin, Austin, Texas, U.S.A.
“Relativistic ab initio study of HePtF: bonded structures of helium”
- P26 **Jon Baker**
Parallel Quantum Solutions, Fayetteville, Arkansas, U.S.A.
“Geometry Optimization of Molecular Clusters”

SUPPLEMENTARY ABSTRACTS

- S1 **Caiping Liu and Michael B. Hall**
Texas A & M University, College Station, Texas, U.S.A.
“Solvent effects on infrared spectra of N-heterocyclic carbene substituted diiron complexes”
- S2 **Praveenkumar Boopalachandran^a, Jaan Laane^a, and Norman C. Craig^b**
^aTexas A&M University, College Station, Texas, U.S.A.
^bOberlin College, Oberlin, Ohio, U.S.A.
“Raman spectra and internal rotation potential energy function of butadiene and its deuterated isotopomers”
- S3 **Vladimir S. Mastryukov**
The University of Texas at Austin, Austin, Texas, U.S.A.
“Gas-phase electron diffraction turns 80”
- S4 **D. G. G. Merchante, A. Tamara, M. Alcolea Palafox, and N. Iza**
Universidad Complutense, Madrid, Spain
“Conformational study of thymidine in the isolated state and under hydration”
- S5 **C. González-Martínez and M. Alcolea Palafox**
Universidad Complutense, Madrid, Spain
“Conformational study of the iododeoxyuridine (IUdR) anticancer drug”
- S6 **M. C. Álvarez-Ros^a, M. Alcolea Palafox^b, M De La Fuente^a and N. Iza^b**
^aUniversidad Nacional de Educación a Distancia, Senda del Rey, Spain
^bUniversidad Complutense, Madrid, Spain
“Conformational stability of the six main tautomers of hypoxanthine under hydration”
- S7 **A. Tamara, D. G. G. Merchante, and M. Alcolea Palafox**
Universidad Complutense, Madrid, Spain
“Conformational study of the anti-HIV drug Nikavir”
- S8 **M. Alcolea Palafox^a, J. Talaya^a, V. K. Rastogi^b, A. Guerrero-Martínez^a and G. Tardajos^a**
^aUniversidad Complutense, Madrid, Spain
^bChoudhury Charan Singh University, Meerut, India
“Quantum chemical study of the vibrational spectra, geometries and tautomerism of hydrated 2-thiouracil”
- S9 **Zulfiya G. Bazhanova, Yury I. Tarasov, Dmitry M. Kovtun, Igor V. Kochikov, Alexander I. Boltalin, Boris K. Novosadov**
Moscow State University, Moscow, Russia
“B3LYP structure of Ag(I) fluoroacetate oligomers compared with X-ray data”

- S10 **Yury I. Tarasov, Igor V. Kochikov, Dmitry M. Kovtun**
 Moscow State University, Moscow, Russia
“Internal rotation in nitroethane molecule: the unusual relation between LAM dependent amplitudes”
- S11 **Yury I. Tarasov, Igor V. Kochikov, Dmitry M. Kovtun, Arkady A. Ivanov**
 Moscow State University, Moscow, Russia
“Quantum chemical and electron diffraction study of the structure and internal rotation in 2-methyl-2-nitropropane”
- S12 **Yury I. Tarasov, Igor V. Kochikov, Dmitry M. Kovtun, Arkady A. Ivanov**
 Moscow State University, Moscow, Russia
“Comparison of the structure and internal rotation in methyl substituted nitromethanes”
- S13 **Dmitry M. Kovtun, Igor V. Kochikov, Arkady A. Ivanov, Yury I. Tarasov**
 Moscow State University, Moscow, Russia
“Internal rotation and equilibrium structure of 2-chloro-3-nitrothiophene from gas electron diffraction and quantum chemistry”
- S14 **Igor V. Kochikov,^a A. V. Stepanova^b, G. M. Kuramshina^b**
^aScientific Research Computer Centre, Moscow State University, Moscow, Russia
^bDepartment of Physical Chemistry, Moscow State University, Moscow, Russia
“Scaling procedure for correction of *ab initio* molecular force fields in Cartesian coordinates”
- S15 **Denis N. Ksenafontov, Natalia F. Moiseeva, Igor F. Shishkov, Nikolay M. Karasyov, Lyudmila V. Khristenko, Lev V. Vilkov**
 Moscow State University, Moscow, Russia
“Structure and conformations of piracetam (2-oxo-1-pyrrolidineacetamide): gas-phase electron diffraction and quantum chemical calculations”
- S16 **A. S. Alikhanyan^a, K. V. Didenko^a, G. V. Girichev^b, N. I. Giricheva^c, O. A. Pimenov^b, S. A. Shlykov^b, G. A. Zhurko^b**
^aKurnakov Institute of General and Inorganic Chemistry, Moscow, Russia
^bIvanovo State University of Chemistry and Technology, Ivanovo, Russia
^cIvanovo State University, Ivanovo, Russia
“Molecular structure of copper(I) pivalate dimer $Cu_2O_4C_{10}H_{18}$ ”
- S17 **G. V. Girichev^a, N. I. Giricheva^b, N. V. Tverdova^a, E. D. Pelevina^b, N. P. Kuzmina^c, O. V. Kotava^c**
^aIvanovo State University of Chemistry and Technology, Ivanovo, Russia
^bIvanovo State University, Ivanovo, Russia
^cLomonosov Moscow State University, Moscow, Russia
“Molecular structure of N, N’ -o-phenylene-bis(salicylideneaminato)zinc (II), Zn(saloph), in gas-phase and in crystal”

- S18 **N. I. Giricheva^a, Ju. S. Medvedeva^a, G. V. Girichev^b, V. M. Petrov^a, A. V. Bardina^a, S. N. Ivanov^a**
^aIvanovo State University, Ivanovo, Russia
^bIvanovo State University of Chemistry and Technology, Ivanovo, Russia
“Molecular structure of 2-nitrobenzenesulphonamide by gas electron diffraction and quantum chemical calculations”
- S19 **V. M. Petrov^a, N. I. Giricheva^a, G. V. Girichev^b, V. N. Petrova^b, A. V. Bardina^a, S. N. Ivanov^a**
^aIvanovo State University of Chemistry and Technology, Ivanovo, Russia
^bIvanovo State University, Ivanovo, Russia
“Molecular structure of 2-ortho-nitrobenzenesulphonic acid by gas-phase electron diffraction and quantum chemical calculations”
- S20 **Alexander E. Pogonin, Yury V. Minenkov, Sergei A. Shlykov, Alexander S. Semeikin and Georgiy V. Girichev**
Ivanovo State University of Chemistry and Technology, Ivanovo, Russia
“The structure of tin(II) octamethylporphyrin: a gas-phase electron diffraction and quantum chemical study”
- S21 **S. A. Shlykov^a, N. I. Giricheva^b, E. A. Lapykina^b, H. Oberhammer^c and G. V. Girichev^a**
^aIvanovo State University of Chemical Technology, Ivanovo, Russia
^bIvanovo State University, Ivanovo, Russia
^cUniversität Tübingen, Tübingen, Germany
“The molecular structure of some lanthanide triiodides by gas-phase electron diffraction and quantum chemical calculations”
- S22 **Yuriy A. Zhabanov^a, Sergey A. Shlykov^a, Georgiy V. Girichev^a and Nina I. Giricheva^b**
^aIvanovo State University of Chemistry and Technology, Ivanovo, Russia
^bIvanovo State University, Ivanovo, Russia
“Structure and thermodynamics of beryllium dihalides”
- S23 **Yuriy A. Zhabanov^a, Alexander V. Zakharov^a and Mikhail K. Islyaikin^b** ^a
^aDepartment of Physics, Ivanovo State University of Chemistry and Technology, Ivanovo, Russia
^bDepartment of Fine Organic Synthesis, Ivanovo State University of Chemistry and Technology, Ivanovo, Russia
“Tautomerism in thiadiazole-containing expanded heteroazaporphyrinoids”

- S24 **Alexander V. Belyakov^a, Alexander N. Khramov^a and Victor A. Naumov^b**
^aTechnological Institute, Saint-Petersburg, Russia
^bArbuzov Institute of Organic and Physical Chemistry, Kazan, Tatarstan, Russia
**“Molecular structure and conformational preferences of dibromo-
(methylthio)phosphite, Br₂PSCH₃, as studied by gas electron diffraction and
quantum-chemical calculations”**
- S25 **Victor G. Solomonik and Andrew A. Mukhanov**
Ivanovo State University of Chemistry and Technology, Ivanovo, Russia
“Complete basis set coupled cluster study of CoF₃”
- S26 **Victor G. Solomonik and Alexander N. Smirnov**
Ivanovo State University of Chemistry and Technology, Ivanovo, Russia
**“The LaF₃ non-rigid molecular structure, inversion spectrum, and
thermodynamic functions”**