

# **XXII International Conference on Chemical Thermodynamics in Russia**

**June 19-23, 2019  
Saint Petersburg, Russia**



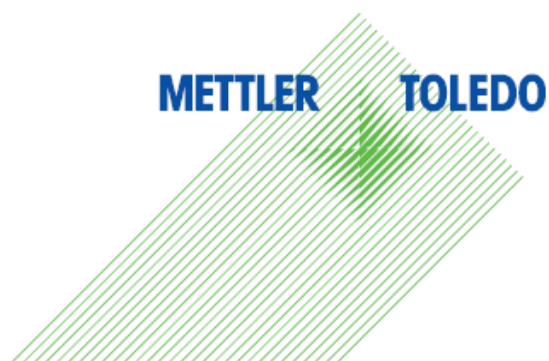
**RCCT-2019**

## **BOOK OF ABSTRACTS**

**Saint Petersburg State University  
Ministry of Science and Higher Education  
Kurnakov Institute of General and Inorganic Chemistry of the Russian Academy  
of Sciences  
Russian Academy of Sciences  
The Mendeleev Russian Chemical Society  
Interregional Innovative Development Center (INNO-MIR) LLC**



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## PREFACE

### **XXII International Conference on Chemical Thermodynamics in Russia, RCCT-2019 June 19-23, 2019, St.Petersburg, Russia: Abstracts.**

This book contains the scientific program and the abstracts of presentations at the XXII International Conference on Chemical Thermodynamics in Russia (RCCT-2019). The conferences on chemical thermodynamics are among the largest conferences held in Russia since 1961. Until 1977 a conference of this series was called "All-Union Conference on Calorimetry" and later, until 1992, "All-Union Conference on Calorimetry and Chemical Thermodynamics". After a long break the tradition of holding these conferences was revived in St.Petersburg (2002). Today the RCCT International Conferences are organized every two years by large Russian scientific centers that have included Moscow (2005, 2013), Ivanovo (2007), Kazan (2009), Samara (2011), Nizhny Novgorod (2015) and Novosibirsk (2017). Every RCCT is a unique and important scientific event both for Russian and international thermodynamic communities. The conference traditionally covers all aspects of chemical thermodynamics from fundamentals to applications, including multidisciplinary approaches and related fields of science.

RCCT2019 takes place in the year declared "The International Year of Periodic Table of Chemical Elements" that marks the 150th anniversary of the publication of Mendeleev's Periodic Table of Chemical Elements in 1869; you can see the original Mendeleev's lifetime Periodic Table right at its birthplace in one of the meeting rooms of RCCT2019. Our conference brings together around 300 scientists from 22 different countries; many of them are young researches, including undergraduate and graduate students. Two junior poster awards have been established by the organizers for the best poster presentations: the RCCT-2019 junior poster award "Excellence in Chemical Thermodynamics" and "Mikhail M. Schultz award", a special award dedicated to 100 years from the birthday of Acad. Mikhail M. Schultz.

The scientific program of RCCT2019 includes plenary and invited lectures, 3 parallel sessions of oral presentations and 3 poster sessions. These contributions reflect the latest trends in Chemical Thermodynamics, including the development and application of theory, new experimental techniques and computer simulation for a variety of different systems.

It is our pleasure to thank all the participants of RCCT2019 and to welcome you in St.Petersburg. We only hope that the treacherous St.Petersburg's weather will not prevent us from enjoying the beauty of our city and its magnificent "white" nights.

On behalf of the organizers,

Alexey Victorov, RCCT2019 Vice-chair





# **CONFERENCE TIMETABLE**



**WEDNESDAY, 19.06.2019**

17.00 – 19.30	Arrivals <b>Registration</b> (Ceremony Hall, main building)
19.30	Welcome reception

**THURSDAY, 20.06.2019**

09.00 – 09.15	<b>Opening</b> (Ceremony Hall, main building)		
<b>Plenary session</b> (Ceremony Hall, main building) Chair: Sadowski G., Coutinho J.			
09.15 – 9.50	Sadowski G. (p. 4)		
9.50 – 10.25	Coutinho J. (p. 5)		
10.25 – 11.00	Anisimov M. (p. 6)		
11.00 – 11.30	Coffee break		
	<b>Section 2: Thermodynamics of Liquids, Fluid Mixtures, and Phase Equilibria</b> (Ceremony Hall, main building) Chair: Anisimov M., Kleiber M.,	<b>Section 1: Development of General Methods and Tools of Chemical Thermodynamics: New Experimental Techniques, Theory and Computer Simulation</b> (Room 133, main building) Chair: Yagofarov M., Kiselev M.	<b>Section 5: Thermodynamics of Functional Materials and Engineered Self- Assembly</b> (Mendeleev Center building) Chair: Markarian Sh., Bykov A.
11.30 – 11.50	Nikitin E. (p. 8)	Schawe J. (p. 16)	Bykov A. (p. 24)
11.50 – 12.10	Khodov I. (p. 9)	Nagrimanov R. (p. 17)	Schick C. (p. 25)
12.10 – 12.30	Chuev G.N. (p. 10)	Yagofarov M. (p. 18)	Antina L (p. 26)
12.30 – 12.50	Shilov I. (p. 11)	Chua Y. (p. 19)	Emelianova K. (p. 27)
12.50 – 13.10	Kleiber M. (p. 12)	Schick C. (p. 20)	Markarian Sh. (p. 28)
13.10 – 13.30	Polishuk I. (p. 13)	Toikka A (p. 21)	Kuznetsov V (p. 29)
13.30 – 13.50	Davydov A. (p. 14)	Asadov M. (p. 22)	Milyaeva O. (p. 30)
13.50 – 15.30	Lunch		
<b>Plenary session</b> (Ceremony Hall, main building) Chair: Ciach A., Brilliantov N.			
15.30 – 16.05	Kiselev M. (p. 32)		
16.05 – 16.40	Idrissi A. (p. 33)		
16.40 – 17.00	Schawe J.E.K. (p. 34)		
17.00 – 18.30	<b>Poster Session 1</b> (p. 125)		
20.00 – 23.00	Gala Dinner (Grand Duke's Palace, next to the Hermitage)		

**FRIDAY, 21.06.2019**

<b>Plenary session (Ceremony Hall, main building)</b> Chair: Victorov A., Shchekin A.			
09.00 – 09.35	Budkov Yu. (p. 36)		
09.35 – 10.10	Ciach A. (p. 37)		
10.10 – 10.45	Brilliantov N. (p. 38)		
10.45 – 11.15	Coffee break		
	<b>Section 2: Thermodynamics of Liquids, Fluid Mixtures, and Phase Equilibria</b> (Ceremony Hall, main building) Chair: Banerjee T., Sineva S.	<b>Section 4: Thermodynamics of Interfacial and Confined Phenomena</b> (Room 90, main building) Chair: Barannikov V., Idrissi A.	<b>Section 5: Thermodynamics of Functional Materials and Engineered Self- Assembly</b> (Mendeleev Center building) Chair: Marczak W, Sizova A.
11.15 – 11.35	Vorozhtcov V. (p. 40)	Shchekin A. (p. 48)	Amashaev R. (p. 56)
11.35 – 11.55	Sineva S. (p. 41)	Barannikov V. (p. 49)	Sizova A. (p. 57)
11.55 – 12.15	Shner N. (p. 42)	Kopanichuk I. (p. 50)	Asabina E. (p. 58)
12.15 – 12.35	Banerjee T. (p. 43)	Akimenko S. (p. 51)	Marczak W. (p. 59)
12.35 – 12.55	Nikfarjam S. (p. 44)	Sizov V. (p. 52)	Mosyagina S. (p. 60)
12.55 – 13.15	Rychkov D. (p. 45)	Baidakov V. (p. 53)	Vasileva A. (p. 61)
13.15 – 13.35	Alekseeva O. (p. 46)	Samsonov V. (p. 54)	Voznesenskiy M. (p. 62)
13.35 – 15.00	Lunch		
	<b>Section 2: Thermodynamics of Liquids, Fluid Mixtures, and Phase Equilibria</b> (Ceremony Hall, main building) Chair: Pimerzin A., Gabrielyan L.	<b>Section 1: Development of General Methods and Tools of Chemical Thermodynamics: New Experimental Techniques, Theory and Computer Simulation</b> (Room 90, main building) Chair: Cicciooli A., Ustinov E.	<b>Section 5: Thermodynamics of Functional Materials and Engineered Self- Assembly</b> (Mendeleev Center building) Chair: Kurapova O., Zherikova K.
15.00 – 15.20	Pimerzin A. (p. 64)	Medvedev N. (p. 72)	Gavrichev K. (p. 80)
15.20 – 15.40	Gabrielyan L. (p. 65)	Ustinov E. (p. 73)	Zherikova K. (p. 81)
15.40 – 16.00	Miroshnichenko E. (p. 66)	Ukhov S. (p. 74)	Lozanov V. (p. 82)
16.00 – 16.20	Cherkasov D. (p. 67)	Varfolomeev M. (p. 75)	Zavrzhnov A. (p. 83)
16.20 – 16.40	Oparin R. (p. 68)	Khvan A. (p. 76)	Kurapova O. (p. 84)
16.40 – 17.00	Sineva M. (p. 69)	Cicciooli A. (p. 77)	Mikhailov O. (p. 85)
17.00 – 19.00	<b>Poster Session 2 (p. 191)</b>		

**SATURDAY, 22.06.2019**

<b>Plenary session (Ceremony Hall, main building)</b> Chair: Neau E., Smirnova I.			
09.00 – 09.35	Monte M. (p. 88)		
09.35 – 10.10	Smirnova I. (p. 89)		
10.10 – 10.45	Skorb E. (p. 90)		
10.45 – 11.15	Coffee break		
	<b>Section 2: Thermodynamics of Liquids, Fluid Mixtures, and Phase Equilibria</b> (Ceremony Hall, main building) Chair: Smirnova I., Skorb E.	<b>Section 4: Thermodynamics of Interfacial and Confined Phenomena</b> (Room 90, main building) Chair: Gor G., Noskov B.	<b>Section 3: Thermochemistry and Databases</b> (Mendeleev Center building) Chair: Verevkin S., Vecchio Cipriotti S.
11.15 – 11.35	Orekhov M. (p. 92)	Noskov B. (p. 100)	Zelenina L. (p. 108)
11.35 – 11.55	Fomin Yu. (p. 93)	Kolesnikov A. (p. 101)	Dávalos J. (p. 109)
11.55 – 12.15	Brazhkin V. (p. 94)	Tavares F.W. (p. 102)	Samosudova Ya. (p. 110)
12.15 – 12.35	Toikka M. (p. 95)	Lasich M. (p. 103)	Verevkin S. (p. 111)
12.35 – 12.55	Smotrov M. (p. 96)	Tsiok E. (p. 104)	Vecchio Cipriotti S. (p. 112)
12.55 – 13.15	Adamova T. (p. 97)	Talyzin I. (p. 105)	Morozov I. (p. 113)
13.15 – 13.35	Abdulagatov I. (p. 98)	Baidakov V. (p. 106)	Miroshnichenko E. (p. 114)
13.35 – 15.00	Lunch		
	<b>Special session “100 Years from Birthday of Acad. Mikhail M. Schultz”</b> (Ceremony Hall, main building) Chair: Toikka A, Stolyarova V.		
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15.35 – 16.10	Toikka A. (p. 117)		
16.10 – 16.45	Stolyarova V. (p. 118)		
16.45 – 18.45	<b>Poster Session 3 (p. 265)</b>		

**SUNDAY, 23.06.2019**

<b>Plenary session (Ceremony Hall, main building)</b> Chair: Gor G., Gavrichev K.	
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09.35 – 10.10	Kramarenko E. (p. 121)
10.10 – 10.45	Gor G. (p. 122)
10.45 – 11.15	Coffee break
11.15 – 11.50	Vishnyakov A (p. 123)
11.50 – 12.25	Samsonov V. (p. 124)

12.25 – 12.40	Solomonov B.N. <b>Presentation of the 23th RCCT</b>
12.40 – 13.00	<b>Conference Closure</b>
13.10 – 14.40	Lunch
	Departure

Sectional talks: 20 min (15 min for talk + 5 min for questions)

Plenary talks: 35 min (30 min for talk + 5 min for questions)

# **SCIENTIFIC PROGRAM**





**THURSDAY, 20.06.2019**

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Chair persons: Anisimov M., Kleiber M.

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Chair persons: Banerjee T., Sineva S.

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