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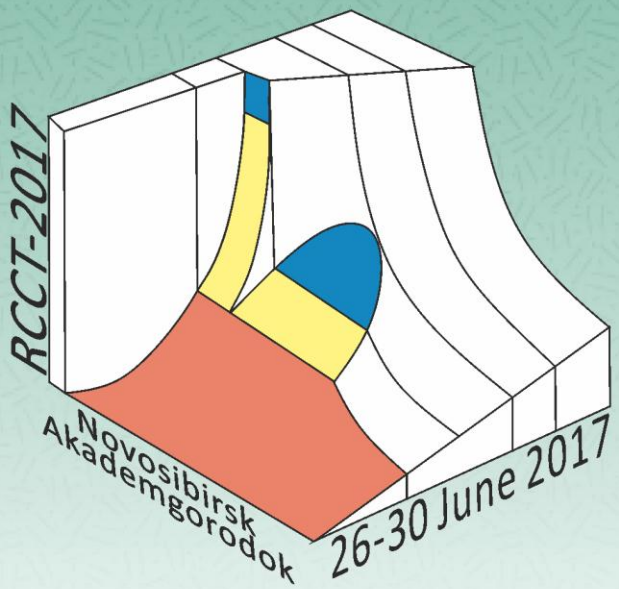
ABSTRACTS

XXI International Conference on Chemical Thermodynamics in Russia

School-Conference on Chemical Thermodynamics for Young Scientists



June 26-30, 2017,
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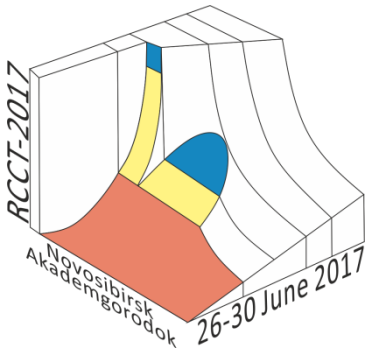

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School-Conference on Chemical Thermodynamics for Young Scientists

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This book presents abstracts of the participants of the XXI International Conference on Chemical Thermodynamics in Russia (RCCT-2017). The conferences on chemical thermodynamics are among the largest conferences held in Russia since 1961. Till 1977 the conference was called "All-Union conference on calorimetry", further, till 1992 - "All-Union conference on calorimetry and chemical thermodynamics", then after a long break the tradition of holding the conference was revived in 2001.

At present the RCCT International Conferences take place every two years in various large Russian scientific centers such as Moscow, St. Petersburg, Nizhny Novgorod, Novosibirsk, Kazan, Samara and others. At present the RCCT International Conferences take place every two years in various large Russian scientific centers such as Moscow, St. Petersburg, Nizhny Novgorod, Novosibirsk, Kazan, Samara and others. Every RCCT is unique and significant event both for Russian and for world thermodynamic community as a whole. The conference traditionally covers all the aspects of chemical thermodynamics: from fundamental to applied areas, including multidisciplinary approaches and related areas of science.

RCCT-2017 scientific program includes plenary and invited lectures, oral presentations, poster sessions and virtual contributions

Electronic version of the book can be found at:
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THE EXPERIMENTAL AND COMPUTATIONAL DETERMINATION OF THE HENRY'S LAW CONSTANT FOR THE SOLUTIONS OF NOBLE GASES IN METHANOL, ETHANOL AND PROPAN-2-OL AT HIGH TEMPERATURES

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Noble gases are found in a wide range of applications in medicine, environmental chemistry or lighting. The solubility and the phase behaviour of noble gases in water and organic solvents was studied rather widely, however, for many systems the available information is not complete. Particularly, data on the solubility of noble gases in primary and secondary alcohols are present only for a very limited temperature range. In the present work the experimentally determined Henry's law constant for the solutions of argon and helium in propan-2-ol at 360, 420 and 480 K, as well as the Henry's law constant for the solutions of neon, krypton, argon and xenon in methanol, ethanol and propan-2-ol at temperatures ranging from 50% to 95% of the solvent's critical temperatures are reported.

The experimental setup for the high temperature gas solubility measurements and the experimental procedure were described previously [1]. The density of argon and propan-2-ol as well as the saturated vapour pressure of pure propan-2-ol at these temperatures were calculated according to the corresponding equations of state [2, 3].The measured Henry's law constant data are listed in Table 1.

The Henry's law constant is related to the residual chemical potential at infinite dilution that can be calculated by molecular simulation. The molecular models for noble gases [4], methanol [5] and ethanol [6] were developed previously. In this study the modified Lorentz-Berthelot rule was applied; the simulation procedure and details were described previously [7]. A state-independent binary parameter ξ was adjusted such that the differences between the simulation results, the present experimental values and the literature data were minimal; its values for the binary systems are listed in Table 2. The simulations were carried out with the *ms2* software [8]. The calculated Henry's law constant dtat are presented in Figure 1.

Table 1. *Henry's law constants of argon and helium in propan-2-ol*

T, K	$H_{Ar/2\text{-}PrOH}$, MPa	$H_{He/2\text{-}PrOH}$, MPa
360	114.0 ± 1.5	600.9 ± 43.5
420	98.5 ± 2.5	334.1 ± 13.6
480	57.6 ± 2.1	142.1 ± 6.3

Table 2. *Estimated values of the binary parameter ξ in the modified Lorentz–Berthelot rule for binary systems*

Component	Ne	Ar	Kr	Xe
Methanol	0.53	1	1	0.978
Ethanol	0.60	1.02	1.027	1
Propan-2-ol	1	0.964	1	0.97

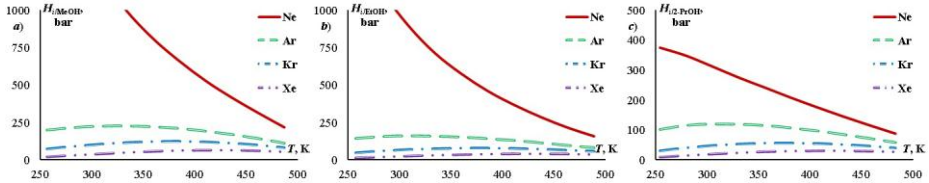

Figure 1. *Henry's law constant of noble gases in a) methanol, b) ethanol, and c) propan-2-ol at temperatures between 250 and 480 K from molecular simulation*

[1] Windmann T., Linnemann M., Vrabec J., J. Chem. Eng. Data, 2014, 59(1), 28–38.
[2] Tegeler C., Span R., Wagner W., J. Phys. Chem. Ref. Data, 1999, 28(3), 779–850.
[3] Gross J., Sadowski G., Ind. Eng. Chem. Res., 2002, 41(22), 5510–5515.
[4] Vrabec J., Stoll J., Hasse H.,. J. Phys. Chem. B., 2001, 105(48), 12126–12133.
[5] Schnabel T., Srivastava A., Vrabec J., Hasse H., J. Phys. Chem. B, 2007, 111(33), 9871–9878.
[6] Schnabel T., Vrabec J., Hasse H., Fluid Phase Equilib., 2005, 233(2), 134–143.
[7] Schnabel T., Vrabec J., Hasse H., J. Mol. Liquids, 2007, 135(1–3), 170–178.
[8] Glass C. W. et al. Comput. Phys. Commun., 2014, 185(12), 3302 – 3306.