At the same time, the crystals of sodium-copper(II) paratungstate B $Na_2Cu_3(CuOH)_2[W_{12}O_{40}(OH)_2]\cdot 32H_2O$ been formed in the mother liquor after the separation of $Cu_5[W_{12}O_{40}(OH)_2]\cdot 35H_2O$, appeared to be bigger in size and stable when storing in the air.

By single crystal X-ray diffraction analysis, the structure of $Na_2Cu_3(CuOH)_2[W_{12}O_{40}(OH)_2]\cdot 32H_2O$ is solved: triclinic, space group P1, a=10.6836(4) Å, b=12.9066(6) Å, c=13.6475(5) Å, α=73.561(4)°, β=75.685(3)°, γ=67.666(4)°, V=1648.68(12) Å3 at T=293 K, Z=1, $d_{calc}$=3.882 g/cm$^3$. The paratungstate B anion in the structure is surrounded by two centrosymmetric pairs of octahedra $\{Na(\mu\text{-}H_2O)_2(H_2O)_3O\}$ and $\{Cu(4)(\mu\text{-}OH)_2(H_2O)_3O\}$ and six $CuO_6$ octahedra forming a three-dimensional structure, in the voids of which uncoordinated $H_2O$ molecules are located.

*Conclusions.* The possibility of formation of individual copper (II) paratungstate B $Cu_5\ [W_{12}O_{40}(OH)_2]\cdot 35H_2O$ and double sodium-copper(II) paratungstate B $Na_2Cu_3(CuOH)_2[W_{12}O_{40}(OH)_2]\cdot 32H_2O$ as the result of self-assembly in the $Cu(NO_3)_2$–$Na_2WO_4$–$HNO_3$–$H_2O$ solution at Z = 1.17 was found. The separated double salt was characterized by chemical analysis, FTIR spectroscopy and single crystal X-ray diffraction study.

## References


1. G. M. Rozantsev, S. V. Radio, and N. I. Gumerova, Pol. J. Chem., 82, No. 11, 2067 (2008).
2. B.-Z. Lin, Y.-M. Chen, and P.-D. Liu, Dalton Trans., No. 12, 2474 (2003).
3. Y.-W. Li, Y.-H. Wang, Y.-G. Li, E.-B. Wang, W.-L. Chen, Q. Wu, and Q. Shi, Inorg. Chim. Acta., 362, No. 4, 1078 (2009).
4. S. V. Radio, M. A. Kryuchkov, E. G. Zavialova, V. N. Baumer, O.V. Shishkin, and G. M. Rozantsev, J. Coord. Chem., 63, No. 10, 1678 (2010).


## BIOLOGICAL SCIENCES


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## RESEARCH IN SILICO REDOX METABOLISM OF HUMAN ERYTHROCYTES

*Introduction.* Metabolic modeling is a promising *in silico* approach to predict cell functioning based on the relationships and interactions of cellular components. Many attempts of computer modeling of metabolic networks have been made for better understanding of the cell molecular networks at the system level (system biology). Because of the simplicity of the structure, components and availability of

kinetic information, the erythrocyte metabolism has been in the center of mathematical modeling for more than three decades and it is a key example of mathematical modeling not only for understanding the biochemical regulation, but also as a basis for creating other metabolic networks.

*The objective of the paper* is to discuss the peculiarities of researching redox metabolism of human erythrocytes. Models of metabolism of red blood cells could foresee an importance of glutathione de novo synthesis and its role in cells with of glucose-6-phosphate dehydrogenase (G6PDH) deficiency, the effects of G6PDH and piruvatkinase enzymopathies.

They could show the differences between patients with chronic and motor and psychic activity anemia and deficiency of these two enzymes. Models of red blood cells metabolism were used to analyze the physiological role of the two enzyme methemoglobin – renewable systems and processes clustering protein band 3 with oxidative stress. The most famous kinetic models of metabolic models of human erythrocytes are Holzhütter (Holzhütter, 2004) and Mulquiney & Kuchel (Mulquiney P.J., Kuchel P.W., 1999) and are freely available (http://www.jjj.bio.vu.nl/database). The purpose of scientific work was to elaborate a kinetic mathematical model for studies of redox metabolism in red blood cells, developed by H. Holzhütter (Holzhütter, 2004).

The mathematical model of erythrocyte metabolism, including glycolysis (Embden- Meyerhoff pathway), pentose phosphate pathway, ways of restoring metHb and reactions of $H_2O_2$ metabolism consists of 50 reactions and 60 metabolites. Within the model the change in the activity of certain enzymes and metabolites concentrations in the steady state was investigated. They participated in the process of disposal of reactive oxygen species and restoration of methemoglobin, depending on the number of exogenous and endogenous $H_2O_2$. The threshold nature of studied parameters changes indicates that the cells may be long enough at almost physiological condition while external conditions are changing.

*Conclusion.* The estimation of redox state in the red blood cells at oxidative stress was made. The changes of $E_{GSSG/2GSH}$, $E_{NADP^+/NADPH}$ and $E_{NAD^+/NADH}$ depending on the concentration of endogenous $H_2O_2$ were shown. It was established that there are high slope changes $E_{GSSG/2GSH}$ in the investigated range of endogenous $H_2O_2$ concentrations that cannot be detected for $E_{NADP^+/NADPH}$ and other redox couples.

The simulation results coincide with existing views on the functioning of antioxidant enzymes in human erythrocytes and indicate the possibility of practical application of the model.

## References

1. Kuchel P.W. Current status and challenges in connecting models of erythrocyte metabolism to experimental reality/ P.W. Kuchel // Prog. Biophys. Mol. Biol.– 2004.–v.85.–P. 325–342.

2. Kauffman K.J. Description and analysis of metabolic connectivity and dynamics in the human red blood cell / K.J. Kauffman, J.D. Pajerowski, N. Jamshidi, B.O. Palsson, J.S. Edwards // Biophys. J.– 2002.–v.83.–P. 646–662.

3. Wiback S.J. Extreme pathway analysis of human red blood cell metabolism / S.J. Wiback, B.O. Palsson // Biophys. J.– 2002.–v.83.–P. 808–818.

4. Price N.D. Network-based analysis of metabolic regulation in the human red blood cell / N.D. Price, J.L. Reed, J.A. Papin, S.J. Wiback, B.O. Palsson // J. Theor. Biol.– 2003.–v. 225.–P. 185– 194.

5. Price N.D. Uniform sampling of steady-state flux spaces: means to design experiments and to interpret enzymopathies / N.D. Price, J. Schellenberger, B.O. Palsson // Biophys. J.– 2004.–v.87.–P. 2172–2186.

6. Nakayama Y. Dynamic simulation of red blood cell metabolism and its application to the analysis of a pathological condition / Y. Nakayama, A. Kinoshita, M. Tomita // Theor. Biol. Med. Model.– 2005.–v.2.–P. 18.

## MATHEMATICAL SCIENCES

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## GAUSSIAN STATIONARY QUASI ORNSTEIN–UHLENBECK PROCESS AND ITS SIMULATION

*Introduction*. In the paper we apply representations of random processes in the form of random series with uncorrelated members, obtained in the work [2], for the construction of models of stochastic processes, which approximates the processes with given reliability and accuracy in spaces $C\left(\left[0,T\right]\right)$ and $L_p\left(\left[0,T\right]\right), p \geq 1$. Thus, *the objective of the paper* is to briefly discuss Gaussian stationary quasi Ornstein-Uhlenbeck process and its simulation.

We construct models that approximate the quasi Ornstein-Uhlenbeck process, which is a centered stationary Gaussian process with the correlation function $R(\tau) = \sigma^2 \cdot \exp\left\{-a|\tau|^2\right\}$, with given reliability $1-\alpha$, $0 < \alpha < 1$, and accuracy $\beta > 0$ in spaces $C\left(\left[0,T\right]\right)$ and $L_p([0,T]), p \geq 1$.