medical diagnostics, well production optimization, asset allocation and decision making for M\&A, strategies for product innovation, and consumer behavior prediction.

The latest advances in computational linguistics will continue to improve the usability of "smart" systems that allow us to communicate with computers using natural language. These are just a few of the ways that systems that are supported by computational linguistics are already changing how we communicate with people, companies and technology:

- Rather than going through an exhaustive telephone menu system, many companies, especially banks, are offering natural language based customer service to handle simple queries (connecting with Q\&A knowledge bases or how-to type information) that the customer can speak or write in his or her own language.
- Digital personal assistants or other intelligent agents use a combination of approaches, including computational linguistics, to perform a variety of functions, from limited conversational dialogue, to responding to requests, typing out dictated text (such as for text messages or emails), or retrieving information, like Apple's Siri [5].
- Combined with artificial intelligence mechanisms, such systems can go one step further to actually take action upon our requests, to make restaurant reservations, set up meetings or arrange other services. Among other abilities such as recognizing moving objects, faces and gestures, Honda's robot assistant, ASIMO, verbally responds to questions in different languages as part of its human-like interaction.

Conclusion. Internet of Things systems combined with voice-recognition technologies are being developed to complement home-based electronics systems for temperature control, internet, electricity, sound and more, creating a new market of high-end, smart-home devices. Amazon's Echo is a version of one aspect of this, serving as a voice command device that can play audio (music, podcasts, audio books), provide real-time information on the weather, traffic, etc. or set alarms, or communicate with other smart devices.
The future of computational linguistics is full of interesting applications that will continue to transform the way we live and work.

## References

1. Alan Bailin: Artificial Intelligence and Computer-Assisted Language Instruction: A Perspective. University of Western Ontario - New York. - 2015. 567 p.
2. Igor Bolshakov and Alexander Gelbukh: Computational linguistics: Models, Resources, Applications. - Berlin. - 2004. - 129 p.
3. Linguistic Society of America. Association for Computational Linguistics: "Computers and Language", 2009. - Vol. 5. - p.13-14.
4. https://linguistics.stanford.edu
5. https://www.aclweb.org/website/cljournal

## CHEMICAL SCIENCES

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## CRYSTAL STRUCTURE OF DOUBLE SODIUM-COPPER (II) PARATUNGSTATE B: $\mathrm{Na}_{2} \mathrm{Cu}_{3}(\mathrm{CuOH})_{2}\left[\mathrm{~W}_{12} \mathrm{O}_{40}(\mathrm{OH})_{2}\right] \cdot \mathbf{3 2} \mathrm{H}_{2} \mathrm{O}$

The objective of the paper considered is to find the synthesis of double sodiumcopper(II) paratungstate $\mathrm{B} \mathrm{Na}_{2} \mathrm{Cu}_{3}(\mathrm{CuOH})_{2}\left[\mathrm{~W}_{12} \mathrm{O}_{40}(\mathrm{OH})_{2}\right] \cdot 32 \mathrm{H}_{2} \mathrm{O}$ conditions and to characterize them by chemical analysis, FTIR spectroscopy and single crystal X-ray diffraction study.

From the solution of the $\mathrm{Na}_{2} \mathrm{WO}_{4}-\mathrm{HNO}_{3}-\mathrm{Cu}\left(\mathrm{NO}_{3}\right)_{2}-\mathrm{H}_{2} \mathrm{O}$ system acidified to $\mathrm{Z}=v\left(\mathrm{H}^{+}\right) / v\left(\mathrm{WO}_{2}{ }^{4-}\right)=1.17$, the light blue crystals of sodium-copper(II) paratungstate B $\mathrm{Na}_{2} \mathrm{Cu}_{3}(\mathrm{CuOH})_{2}\left[\mathrm{~W}_{12} \mathrm{O}_{40}(\mathrm{OH})_{2}\right] \cdot 32 \mathrm{H}_{2} \mathrm{O}$ are isolated.

The example presented below corresponds to the formation of the paratungstate $B$ anion:
$12 \mathrm{WO}_{2}{ }^{4-}+14 \mathrm{H}^{+}=\left[\mathrm{W}_{12} \mathrm{O}_{40}(\mathrm{OH})_{2}\right]^{10-}+6 \mathrm{H}_{2} \mathrm{O}$
The results of synthesis and subsequent chemical and FTIR spectroscopic analysis show that in the aqueous solution of $\mathrm{Na}_{2} \mathrm{WO}_{4}$ acidified to $\mathrm{Z}=1.17$ and lasted for one month after addition of $\mathrm{Cu}\left(\mathrm{NO}_{3}\right)_{2}$ (ratio $\left.v(\mathrm{Cu}): v(\mathrm{~W})=0.00625: 0.01\right)$. As a result, the formation of crystalline precipitate of copper(II) paratungstate B $\mathrm{Cu}_{5}\left[\mathrm{~W}_{12} \mathrm{O}_{40}(\mathrm{OH})_{2}\right] \cdot 35 \mathrm{H}_{2} \mathrm{O}$ occurs. Wt \% was calculated: CuO 10.0 (10.39), $\mathrm{WO}_{3}$ 72.5 (72.67), $\mathrm{H}_{2} \mathrm{O} 16.5$ (16.94). FTIR, $\mathrm{cm}^{-1}: 426 \mathrm{w}\left(\delta(\mathrm{W}-\mathrm{O}-\mathrm{W})\right.$ ), 507w $531\left(\mathrm{lib}\left(\mathrm{H}_{2} \mathrm{O}\right.\right.$, $\mathrm{OH})$ ), 690s 742sh 790s $840 \mathrm{~s} 874 \mathrm{~s}(\mathrm{v}(\mathrm{W}-\mathrm{O}-\mathrm{W})$ ), $943 \mathrm{~s}(\mathrm{v}(\mathrm{W}=\mathrm{O}))$, 1092 w 1167 w $(\delta(\mathrm{W}-\mathrm{O}-\mathrm{H}))$, $1627 \mathrm{~s}\left(\delta\left(\mathrm{H}_{2} \mathrm{O}\right)\right)$, $3427 \mathrm{~s} \mathrm{~b}\left(v\left(\mathrm{H}_{2} \mathrm{O}\right)\right)$. It should be noted that the addition of $\mathrm{Cu}\left(\mathrm{NO}_{3}\right)_{2}$ to the freshly acidified to $\mathrm{Z}=1.17$ aqueous solution of $\mathrm{Na}_{2} \mathrm{WO}_{4}$ results in the formation of not an individual compound but a mixture of crystallohydrates of copper(II) orthotungstate and paratungstate B.

In three months, from the tightly closed mother liquor, light blue crystals were withdrawn, which according to the data of chemical and FTIR spectroscopic analysis, the formula of double sodium-copper(II) paratungstate B $\mathrm{Na}_{2} \mathrm{Cu}_{3}(\mathrm{CuOH})_{2} \cdot\left[\mathrm{~W}_{12} \mathrm{O}_{40}(\mathrm{OH})_{2}\right] \cdot 32 \mathrm{H}_{2} \mathrm{O}$ corresponds to. Wt \% was calculated: $\mathrm{Na}_{2} \mathrm{O}$ 1.6 (1.61), CuO 10.2 (10.32), $\mathrm{WO}_{3} 72.0$ (72.18), $\mathrm{H}_{2} \mathrm{O} 15.8$ (15.89). FTIR, cm-1: 438w ( $\delta(\mathrm{W}-\mathrm{O}-\mathrm{W})$ ), 502 w 533 w (lib ( $\left.\mathrm{H}_{2} \mathrm{O}, \mathrm{OH}\right)$ ), 621sh 702s 801s 886s b ( $v(\mathrm{~W}-\mathrm{O}-$ W) ), 947s ( $v(\mathrm{~W}=\mathrm{O})$ ), 1113w $1165 \mathrm{w}\left(\delta(\mathrm{W}-\mathrm{O}-\mathrm{H})\right.$ ), 1624s $\left(\delta\left(\mathrm{H}_{2} \mathrm{O}\right)\right)$, 3453s b 3520 w ( $\mathrm{v}(\mathrm{H} 2 \mathrm{O})$ ).

By the positions of the absorption peaks of stretching vibrations in the $\mathrm{W}-\mathrm{O}-\mathrm{W}$ framework, the FTIR spectra of the separated salts reliably fit with those previously determined for the salts with the anion of paratungstate B and different cations.

It should be noted that we have failed to solve the structure of copper (II) paratungstate $\mathrm{B} \mathrm{Cu}_{5}\left[\mathrm{~W}_{12} \mathrm{O}_{40}(\mathrm{OH})_{2}\right] \cdot 35 \mathrm{H}_{2} \mathrm{O}$ separated in the process. We have failed to select a single crystal suitable for direct X-ray diffraction analysis from the fine crystalline precipitate.

At the same time, the crystals of sodium-copper(II) paratungstate B $\mathrm{Na}_{2} \mathrm{Cu}_{3}(\mathrm{CuOH})_{2}\left[\mathrm{~W}_{12} \mathrm{O}_{40}(\mathrm{OH})_{2}\right] \cdot 32 \mathrm{H}_{2} \mathrm{O}$ been formed in the mother liquor after the separation of $\mathrm{Cu}_{5}\left[\mathrm{~W}_{12} \mathrm{O}_{40}(\mathrm{OH})_{2}\right] \cdot 35 \mathrm{H}_{2} \mathrm{O}$, appeared to be bigger in size and stable when storing in the air.

By single crystal X-ray diffraction analysis, the structure of $\mathrm{Na}_{2} \mathrm{Cu}_{3}(\mathrm{CuOH})_{2}\left[\mathrm{~W}_{12} \mathrm{O}_{40}(\mathrm{OH})_{2}\right] \cdot 32 \mathrm{H}_{2} \mathrm{O}$ is solved: triclinic, space group P 1 , $\mathrm{a}=10.6836(4) \AA, \mathrm{b}=12.9066(6) \AA, \mathrm{c}=13.6475(5) \AA, \alpha=73.561(4)^{\circ}, \beta=75.685(3)^{\circ}$, $\gamma=67.666(4)^{\circ}, \mathrm{V}=1648.68(12) \AA 3$ at $\mathrm{T}=293 \mathrm{~K}, \mathrm{Z}=1, \mathrm{~d}_{\text {calc }}=3.882 \mathrm{~g} / \mathrm{cm}^{3}$. The paratungstate B anion in the structure is surrounded by two centrosymmetric pairs of octahedra $\left\{\mathrm{Na}\left(\mu-\mathrm{H}_{2} \mathrm{O}\right)_{2}\left(\mathrm{H}_{2} \mathrm{O}\right)_{3} \mathrm{O}\right\}$ and $\left\{\mathrm{Cu}(4)(\mu-\mathrm{OH})_{2}\left(\mathrm{H}_{2} \mathrm{O}\right)_{3} \mathrm{O}\right\}$ and six $\mathrm{CuO}_{6}$ octahedra forming a three-dimensional structure, in the voids of which uncoordinated $\mathrm{H}_{2} \mathrm{O}$ molecules are located.

Conclusions. The possibility of formation of individual copper (II) paratungstate $\mathrm{B} \mathrm{Cu}_{5}\left[\mathrm{~W}_{12} \mathrm{O}_{40}(\mathrm{OH})_{2}\right] \cdot 35 \mathrm{H}_{2} \mathrm{O}$ and double sodium-copper(II) paratungstate B $\mathrm{Na}_{2} \mathrm{Cu}_{3}(\mathrm{CuOH})_{2}\left[\mathrm{~W}_{12} \mathrm{O}_{40}(\mathrm{OH})_{2}\right] \cdot 32 \mathrm{H}_{2} \mathrm{O}$ as the result of self-assembly in the $\mathrm{Cu}\left(\mathrm{NO}_{3}\right)_{2}-\mathrm{Na}_{2} \mathrm{WO}_{4}-\mathrm{HNO}_{3}-\mathrm{H}_{2} \mathrm{O}$ solution at $\mathrm{Z}=1.17$ 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

