



ITMO UNIVERSITY



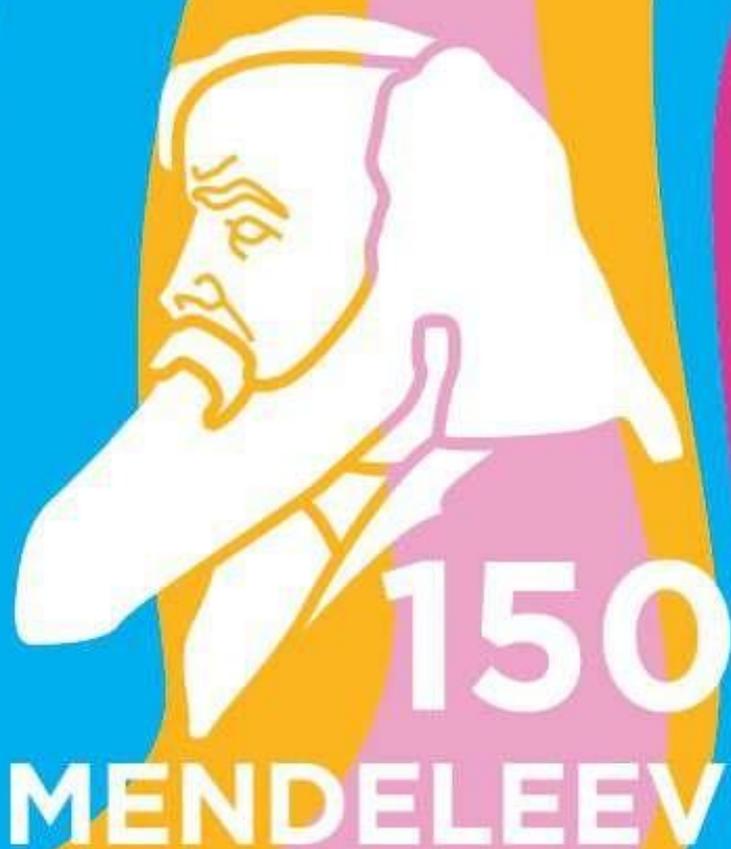
SCAMT

49 Kronverksky Pr.,
Saint Petersburg, 197101

4th International Conference on the Periodic Table endorsed by IUPAC

July 26–28/2019
Saint Petersburg

Book of Abstracts

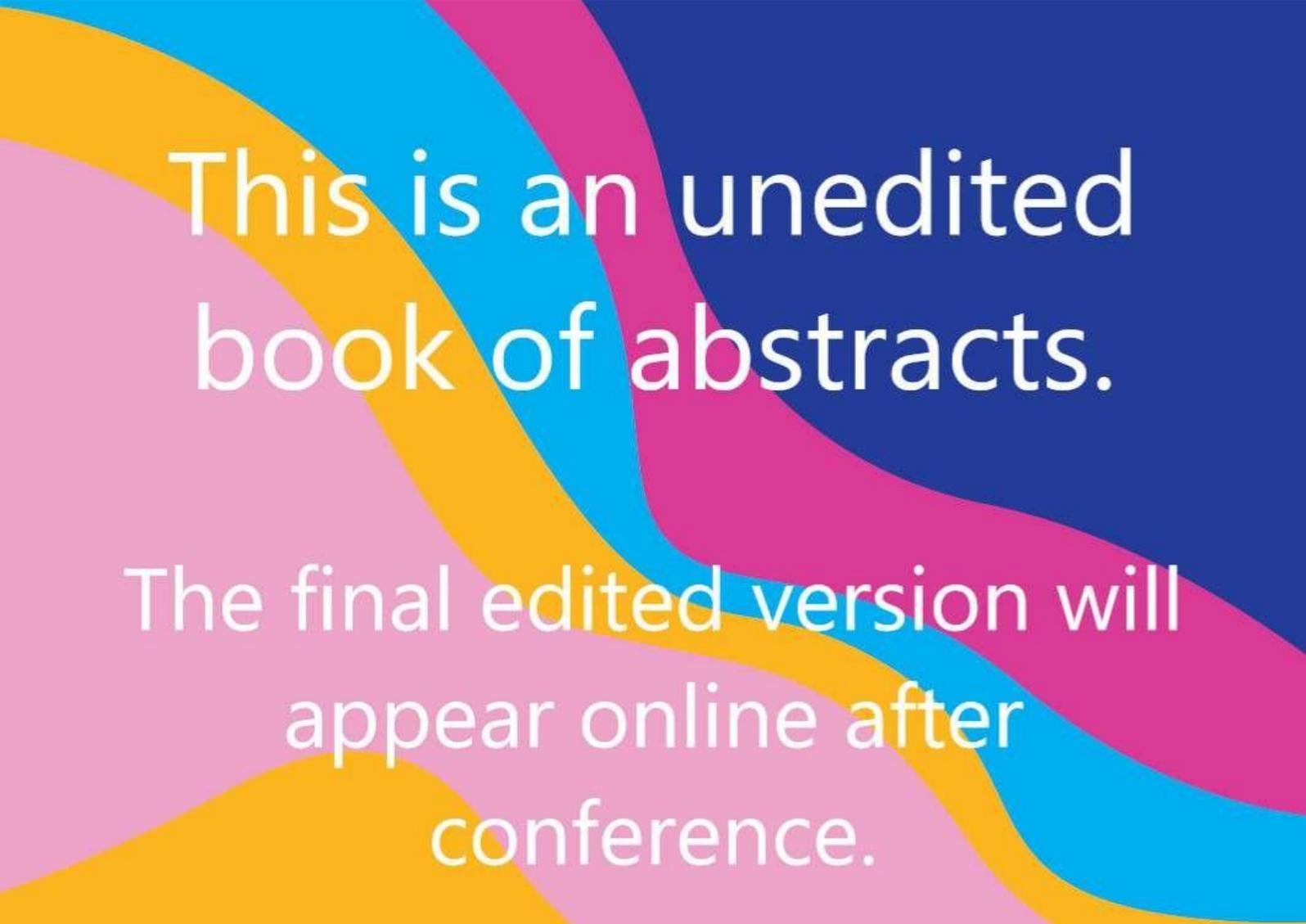


abocr



**MEL
Science**





This is an unedited
book of abstracts.

The final edited version will
appear online after
conference.

**Fourth International Conference on the Periodic Table
July 26-29, 2019, St Petersburg, Russia**

THE PERIODIC TABLE: SEEKING ORDER IN CHAOS

Abhinav Godavarthi¹ and Swaminathan Sivaram²

¹ 5853 Pebblestone Ln, Plano, TX 75093, USA ² Indian Institute of Science Education and Research Dr Homi Bhabha Road, Pune, 411 008, India.

ABSTRACT

In a short communication published in Zeitschrift fur Chemie, volume 12, pp 405-406, 1869, titled, “On the relationship of the properties to the atomic weights of the elements” Mendeleev announced a startling discovery that would revolutionize chemistry forever. The Periodic Table revealed a pervasive order in nature, one that always existed, but was hidden till Mendeleev expounded it

In this presentation, we shall briefly trace the origins of the discovery with a retrospective view of what led Mendeleev to this epochal discovery . We illustrate the conception of the Periodic Table as a classical Kuhnian scientific revolution; that is, a discovery made according to the paradigm of the scientific time period as a whole. To this end, we observe and analyze the greater trends in science during the era of Mendeleev and his immediate influences. Moreover, we address how the lexicon in the field of chemistry and chemical analysis today allows for a broad interpretation of the current paradigm, and that this qualitative aspect of “the central science” enables for unique creative contributions. Finally, we investigate alternative historical models for the discovery of the Periodic Table, compare such models, and present an approach to scientific inquiry going forward in an era dominated by computational power and artificial intelligence.

Applications of spectroscopy in the study of elements of the Periodic Table

In This study the applications of spectroscopy in the identification of chemical elements of the Periodic Table, present in different light sources used in everyday life, are proposed.

Since Isaac Newton (1666) adopted the name "Spectrum", noting that the white light of the sun could disperse into a continuous series of colours, using a prism, to Gustav Robert Kirchoff and Robert Wilhelm Eberhard von Bunsen (1859) who found that spectral lines were unique to each chemical element, other researchers such as William Hyde Wollaston (1802) and Joseph von Fraunhofer (1814) observed dark lines present in the solar spectrum, with the invention of the first grid spectroscope of diffraction.

The objectives of the study are summarized in the design and construction of a desktop spectroscope, in the transformation of the mobile phone into a spectrophotometer diffraction grid and in the investigation of applications of spectroscopy in the Identification of chemical elements of the Periodic Table present in different light sources.

In order to develop the objectives of the study, once the search for materials required in the design and construction of spectroscopes has been completed, the process of assembling them has been carried out. Upon completion of this last step, observations of light spectra emitted by different light sources (incandescent light, halogen light, cold and warm light consumption, and fluorescent light) have been carried out.

Once the observations have been completed, the results obtained (calibration of spectroscopes) were analysed by comparing the emission spectra obtained through desktop spectroscopy and the mobile transformed into a spectrophotometer, with the real emission spectra of the chemical components existing inside the light sources analysed.

Checked the usefulness of spectroscopy in the identification of chemical elements, it can be concluded that spectroscopy can help us to observe different chemical components present in the light sources used in the daily life. On the other hand, it can propose other fields in which it may be useful: to study the chemical components that provoke atmospheric pollution in a given area or even in the analysis of the chemical composition of stars.

СОЗДАНИЕ ТЕОРИИ СПЕЦИФИЧЕСКИХ ВЗАИМОДЕЙСТВИЙ ОРГАНИЧЕСКИХ СОЕДИНЕНИЙ НА ОСНОВЕ НОВЫХ ИДЕЙ ОБОБЩЕНИЯ

А.К. Баев

Институт Химии Растворов им. Г. А. Крестова РАН

E-mail: alexeibaev@mail.ru

Мой учитель проф. С.А. Щукарев последователь Д.И. Менделеева писал в 1965 г. (Петербург Г.У). “В настоящее время наука о веществе переживает особый момент, принципиально сходный с тем, который история человеческой культуры прошла 100 лет тому назад, в эпоху открытия Д.И. Менделеевым Периодической системы химических элементов. Тогда невидимые гипотетические атомы...поднялись в глазах мыслящего человечества как глубокая в своем содержании реальность, на высоту нового обобщения, и появилась возможность предсказывать свойства еще не открытых элементов“. В данной лекции мы обосновываем необходимость выдвижения новых, нестереотипных идей, обеспечивающих вскрытие природы специфических межмолекулярных взаимодействий и проникновение в более глубокое их понимание и восприятие для создания и развития самой теории типов таких взаимодействий, установление их энергетических параметров, в которых так нуждались ученые. Под специфическими взаимодействиями следует понимать взаимодействие между связевыми вакансиями атомов контактирующих молекул. Основой для обоснования таких взаимодействий явились термодинамические исследования фазовых преобразований процессов испарения и сублимации алкильных соединений элементов III-VI и ZnR_2 групп Периодической таблицы и изучение состояния соединений в газовой фазе, обосновавшие получение энергетических параметров специфических взаимодействий мономерных форм, закономерности их изменения и вытекающие из них выводы. Экспериментальное обоснование присутствия в парах димерных форм у алкилов алюминия с высокими энергиями диссоциации димеров $Al_2(CH_3)_6$ и $Al_2(C_2H_5)_6$ соответственно является неоспоримым доказательством участия пентакоординированного атома углерода в качестве связевой вакансии в формировании взаимодействия [1]. В то же время снижение стабильности энергии специфического взаимодействия с увеличением числа атомов углерода в алкильной цепи является следствием формирования обратной дативной связи центральным атомом комплекса.

1. Пентакоординированный атом углерода формирует специфические межмолекулярные взаимодействия в широком диапазоне величин энергией, с более трехкратным превышением энергии водородной связи $10.99 \text{ кДж моль}^{-1}$ жидкой воды [1];
2. Новый тип внутримолекулярного взаимодействия – обратная дативная связь между атомом углерода С лиганда и центральным атомом А в комплексе $AR_k C(2e) \rightarrow A(0e)$ [1, 2];
3. Несостоятельность модели $sp^3(C)$ – гибридизации электронной конфигурации атома углерода;
4. Наличие существенно неподеленной $2s^2(C)$ – электронной пары атома углерода, способной смещать электронную плотность на атом акцептора и с атома донора [1];
5. Все связевые вакансии молекулы принимают участие в формировании специфических взаимодействий [3];
6. Энтальпия (энтропия) испарения (сублимации) взаимосвязана с числом и энергией формируемых молекулой специфических взаимодействий [3, 4].

Разработанные основополагающие представления позволили создать систему согласующихся энергетических параметров различных типов специфических взаимодействий и классов органических соединений, обсуждаемых в докладе.

1. Baev, A. K. Pentacoordinated Carbon Atom at Intermolecular Interactions. Russian Journal of Coordination Chemistry. 1996, V. 22. № P.399. 2. Baev A.K., Korolkov D.V., Book of Abstract the XVth FECHEM Conference on Organometallic Chemistry. University of Zurich. Svizeland.(2003) 350. 3. Baev A. K. Specific Intermolecular Interactions of Organic Compounds. Springer. Hiedelberg, Dordrecht, London, New York. 2012. 434 p. 4. Baev A.K. Specific Intermolecular Interactions of Element-Organic Compounds. Springer. Hiedelberg, Dordrecht, London, New York. 2014. 278 p.

CREATION OF THEORY SPECIFIC INTERACTIONS OF ORGANIC COMPOUNDS ON THE BASE OF GENERALIZATION OF NEW IDIES

Alexei K. Baev

G.A.Krestov Institute of Solution Chemistry of the RAS
Ivanovo. E-mail: alexeibaev@mail.ru

My scientist S.A. Schukarev, of the follower of D.I. Mendeleev, wrote at 1965 year (Sc. Petersburg, Univ.): “In the present time the science about substance survive special moment, in principle similar with that, which the history of human culture passed 100 years ago, at epoch of discovery by D.I. Mendeleev of the Periodical system chemical elements. Then invisible hypothetical atoms ... roused at the eyes of the thinking humanity as deep at own maintenance reality on the height of new generalization, and appeared possibility to foretell the properties of still not open elements.” In this lecture we substantiate the necessity to proposal a new, non-stereotypic ideas, secured expose of the nature of specific intermolecular interactions and penetration in more deep of their understanding and apprehension for substantiation and development of theory types of this interactions, establish of values energetic parameters at which scientists required so march. Ander specific interactions follow to understand the interaction by bonding vacancies’ of atoms contacted molecules. Basis of substantiation of this interactions are thermodynamic investigations of phase reorganization of the processes vaporization and sublimation of alkyl compounds of the elements III – VI and ZnR_2 groups, another organic compounds and investigations [1, 2] of condition compounds in gas phase, determination the energetic parameters of specific interactions monomer forms, law- governed nature of their changing and with all that this implies. Substantiated dimirisation at gas phase of alkyls aluminum with high dissociations energy dimer $Al_2(CH_3)_6$ и $Al_2(C_2H_5)_6$ correspondingly, are incontestable evidence participation pentacoordinated carbon atom at quality bonding vacancies at formation specific interactions [1]. At the same time the reduction of stability energy of specific interaction with grooving of number carbon atom at alkyl chain is consequence of the formation of reverse dative bond by central atom complex. Using new ideas, we created system specific interactions, enrich chemical sciences, its theoretical and experimental directions:

1. Pentacoordinated carbon atom forms specific intermolecular interactions at wide range values energies, more tree-time overstepping of energy hydrogen bond $10.99 \text{ kJ} \cdot \text{mol}^{-1}$ of H_2O ;
2. Novel kind of intramolecular interaction - rivers dative bond between carbon atom C alkyl ligand R and central atom A in complex $AR_k C(2e) \rightarrow A(0e)$, in its electron structure is consist;
3. Substantiated refusal from $sp^3(c)$ -hybridization model of electron configuration of carbon atom;
4. Existence of essential no divided $2s^2(c)$ -electron pair,
5. All bonding vacancies of a molecule must take part at a formation of specific intermolecular interactions;
6. Enthalpy (entropy) vaporization (sublimation) is interconnected with a number and energy of formed molecule of specific interactions [3, 4].

It is discussed of the develop problems of theories of different types of specific intermolecular interactions of organic compounds.

1. Baev, A. K. Pentacoordinated carbon atom at Intermolecular Interactions. Russian Journal of Coordination Chemistry. 1996, V. 22. № P.399.
2. Baev A.K., Korolkov D.V., Book of Abstract the XVth FEICHEM Conference on Organometallic Chemistry. University of Zurich. Svizeland.(2003) 350.
3. Baev A. K. Specific Intermolecular Interactions of Organic Compounds. Springer. Hiedelberg, Dordrecht, London, New York. 2012. 434 p.
4. Baev A.K. Specific Intermolecular Interactions of Element-Organic Compounds.Springer. Hiedelberg, Dordrecht, London, New York. 2014. 278 p.

MENDELEEV'S WORK – A SOURCE OF INSPIRATION FOR BULGARIAN STUDENTS

We humbly admire and look up to Mendeleev – a genius, one of his kind. Without even having a slight idea about the existence of protons, he managed to accurately identify the atomic number of all known elements at the time and it was not until the discoveries of Rutherford and Moseley half a century later, that all of his ideas turned out to match reality. Mendeleev is a master of intuitive thinking. What is extremely fascinating in its educative manner is that he kept in mind the fact that chemical knowledge was limited, and therefore left empty spaces for new, undiscovered elements. It is important for our students to know that even if something is unfamiliar or unknown, it still might exist and could most probably be explained.

With that said, we would like to take the opportunity to introduce you to the work of the students of three Bulgarian high schools, who drew their inspiration from the Periodic table, as well as the discovery of new elements, and implemented numerous out of class activities.

To begin with, we celebrated the International Year of Chemistry, 2011. The students created a periodic table with simple substance samples and a poster, regarding the importance of some elements for life as we know it. A competition also took place, where some students came up with logical and experimental problems for the two competing teams.

During “The Teenager – a young scientist” project, the students conveyed a water research, for water is a substance we use on a daily basis, and even though we think we know nearly everything about it, it never fails to impress with its unique properties; as ubiquitous as it is, water is also used for grouping substances and understanding some basic concepts in chemistry. The participants regarded to one another with the nickname Hydromaniacs.

Moreover, for the anniversary of Marie Curie's birthday, as well as for the completion of the 7th period of the Periodic Table and naming the remaining elements, a group of enthusiastic students produced a large, hand-made Periodic Table wall chart for the Chemistry classroom. It was probably the first actualised Periodic Table of its size in our country.

Our future plans include the following events:

1. Honouring Mendeleev's birthday with a presentation for his life and times
2. A contest for Mendeleev's doppelganger
3. Creating a logo for the jubilee
4. Creating a video series about the Periodic Table on YouTube.
5. Creating a catalogue of different Periodic Tables
6. Creating a Periodic Table board game
7. Creating a “Living Periodic Table”
8. Establishing an annual celebration, called “The Periodic table – an ingenious product of a magical science”

Key words: Periodic Table, students, out of class activities, create, inspiration, work.

PARTICIPANTS

1. Kalinka Benova

"Geo Milev" High School of Mathematics, Pleven, Bulgaria

kalina.benova@gmail.com

2. Antoaneta Hineva

“Dr. Petar Beron” High School of Mathematics, Varna, Bulgaria

anthineva@gmail.com

3. Violeta Konstantinova

“Vasil Drumev” High School of Mathematics and Natural Science, Veliko Tarnovo, Bulgaria

vili7070@abv.bg

4. Momchil Benov - presenter

Sofia University “St. Kliment Ohridski”, Sofia, Bulgaria

momchil.benov@gmail.com

CORRECTION OF THE CONCEPT OF PERIODICITY AND THE SIMPLEST EQUATIONS FOR THE NATURAL PERIODIC TABLE

Yury Bukayev

We'll consider how our development¹ of the concept of periodicity first creates the natural PT, the simplest equations for it: E, PE.

There are two types of breaks in the half-long PT before non-periodic zones: empty cells, breaks between periods. Equations can't suit if PT-cells are empty: we fill them by Nu ($Z=0$)¹. $Z \neq 0$ puts an element into the certain period, $Z=0$ can't do it.

PT doesn't reflect radical differences among noble gases (NG). We prove¹: there are twenty groups. We call H-position in gr-17 as 'primary relative', other elements' positions (excluding NG- in gr-18, gr-20, Nu-) as 'absolute'. Kr, Xe etc. have their primary relative position in gr-18, Ar - in gr-19, He, Ne - in gr-20¹. NG' absolute positions are in gr-19¹. Both positions of each NG are in the same period. The rest of gr-18, gr-20 consists of dualistic positions (Nu-, secondary relative NG-). Going to E, we exclude non-periodic zones (La etc.), fix the numbers: G – of passed groups in the period, D_s – of earlier passed relative positions of elements (H in gr-17, NG in gr-18, gr-20 and Nu) in PT, N_r – of repeated passages through the group. E is

$$G=Z+D_s-20N_r$$

for absolute positions.

We up-date this structure by separation of non-periodic zones. Further, going to structures without breaks, we transform it into plane cyclic 20-sectored structures (e.g. into the Archimedean spiral, where its turn coincides with a period, or into the circle, where its circuit coincides with one), where all positions are equidistant from 'horizontal' neighbours.

The difference of groups with s-, p-elements from d-groups isn't reflected so we transform 20-sectored structures into following 10-sectored 'multilayered' complex continuous structures (MLPT): concentric circles, the Archimedean spiral, the circle, where superposed cells of different 'layers' (A (s-, p-elements), B (d-elements) are one-'layered' individual structures) form one cell with a vector/matrix of elements. We have continuous 20-celled periods, two types of continuous 10-celled periods in MLPT (including the basic type formed by a turn of A or B separately). E works in MLPT too.

We prove that MLPT is a natural PT by two ways¹. Going to one of them, we fix and call two following different quantities as 'real pseudovalentoid number (PVN) of s-, p- and d-elements' (they are fully related, have equal values).

1) PVN is a sum of electrons on a filling d-sublevel (if it exists) of a free atom, and on its top level, and on a filled d-sublevel (if it exists) if the level having it is a top. We call such electrons as 'pseudovalentoid' (PV-).

2) PVN is a degree of plurality of PV-electrons' interactions.

Other (internal) electrons form the whole participant of interactions. PVN is reflected by positions including ones of Nu. Moreover, there are groups (17-20), where one element (H, He) has a value of PVN (1, 2), that differs from the value for other elements of such group (7, 8). We fix¹ the quantity 'seeming pseudovalentoid number (PVN_{seem}) of s-, p- and d-elements'. $PVN_{seem}(H)=7$, $PVN_{seem}(He)=8$. Positions of H, He in these groups reflect PVN_{seem} , instead of PVN. We fix¹ the quantity 'generalized pseudovalentoid number (PVN_{gen}) of the position of s-, p- and d-elements' (or 'large chemical number (LN)'). Its values for positions of 20-celled period are 1,2,3,4,5,6,7,8,9,10,1,2,3,4,5,6,7,8,8,8, for ones of 10-celled period of A are 1,2,3,4,5,6,7,8,8,8, for ones of B are 1,2,3,4,5,6,7,8,9,10. There are periodic function and periods of a mathematical concept of periodicity. Going to PE for LN, we fix the numbers: S_r – of repeated passages through the sector of A+B in the 20-celled

period, C_r – of earlier passed elements with the same electron structure and chemistry in the 20-celled period. This PE is

$$LN = G - 10S_r - C_r = Z + D_s - 20N_r - 10S_r - C_r \quad .$$

After fixing¹ of ‘small chemical number (SN)’ and ‘resultant chemical number (RN)’ (SN, $RN = LN + SN$ are also such periodic functions, where SN=2 for gr-20, SN=1 for gr-19, SN=0 for other groups) we have the other PE:

$$RN = LN + C_r = Z + D_s - 20N_r - 10S_r \quad .$$

References

1. Bukayev Yu.V. Chemical Elements: the New Laws. Correction, Mathematization of the Periodic Law, Tables, Tests. The New Form of the Fajans-Soddy Law. Moscow: IMGRE, 2019 – ISBN 978-5-4472-7764-2.

THE PERIODIC TABLE OF THE POLYHEDRA AND NETWORK UNIVERSE

M.BURT, PROF. EMERITUS, FACULTY OF ARCHITECTURE & T.P, TECHNION,
ISRAEL INSTITUTE OF TECHNOLOGY, HAIFA-32.000, ISRAEL

ABSTRACT:

The diversity of structural forms that meets the eye is overwhelming. They shape our environment: physical, mental, intellectual. Theirs is a dynamic milieu; time induced transformation and the evolutionary development of the perceiving mind. Our study of natural forms, the essence of structural morphology, is part a wider science, dealing with forms which are **theoretically imaginable**, to imply: **causal-rational forms**. A particular interest should be focused on two principal categories of structure-forms.

1. Structures that are shaped like polyhedral solids (continuous enveloping tessellated surfaces). Conspicuous are those relating to sponge-like labyrinthine polyhedral surfaces, which until quite recently were not even considered as a worthy research topic.
2. Structures describing polyhedral interrelating and interconnected arrays of (sometimes energized) point-wise entities, with a network characteristics, that may represent the structure of almost any abstract or physical plurality that may exist in the world of phenomena of the biological-physical and chemical-crystallographic domains.

It is these polyhedral and network lattice structures, with their periodic order and symmetry constraints, and their extended derivatives, the number of which extends to infinity, that are at the core of this investigation.

The Periodic Table of the Polyhedral and Network Universe was inspired by Mendeleev and conceived to provide an overview of its evolving complexity, and gain insights into it's defining topological-Symmetrical-structural properties, their hierarchical characteristics and order.

Arranged on the basis of **primary parameters** of polyhedra and the networks phenomenon (when expressed as unihedra), considered to be: Valency (val.); $\Sigma\alpha$ (in a vertex) and genus (g), a Cartesian environment is constructed, in which every polyhedral and network configuration has a **unique point-representation**, and all **shared properties** (order, stability, e.c.t) of various groupings of geometrical structures **are posing as mathematically embraced location patterns**, mostly of a topological nature.

The fantastic story of Rare-earths

Alice Carlotto and Marco Dalla Tiezza

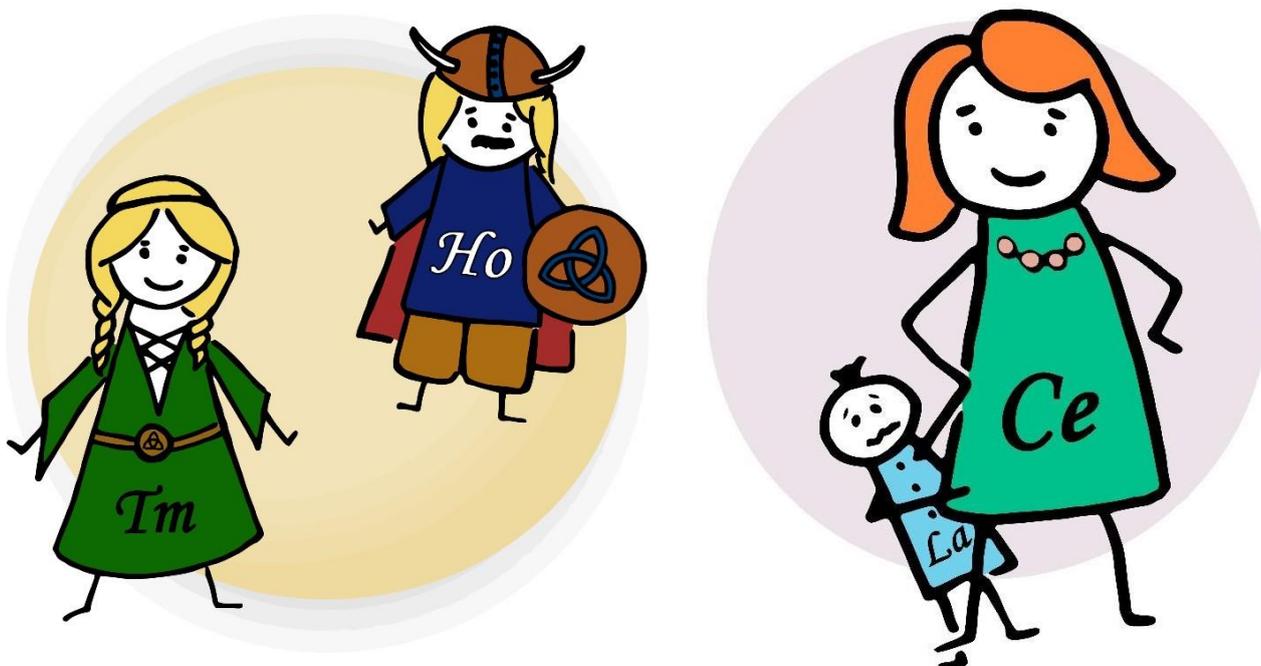
Dep. of Chemical Sciences, University of Padova, Via F. Marzolo 1, 35131 Padova, Italy

E-mail: alice.carlotto@phd.unipd.it

“Lanthanons – these elements perplex us in our researches, baffle us in our speculations, and haunt us in our very dreams. They like an unknown sea before us; mocking, mystifying and murmuring strange revelation and possibilities.”^{1,2}

This is not a tale as old as time, but surely an extraordinary adventure in a little-known world, not so big, but full of wonders.

The Rare-earths were bashful creatures, they often hid themselves with each other as Cerium with Lanthanum (*lanthanein*, to lie hidden) or the little twins Neodimium and Praseodimium (*didimos*, twin). Others lived together in the little village of Ytterby (Terbium, Erbium, Ytterbium) or were difficult to reach as Dysprosium (*dysprositos*, hard to get). Then, there were four that shone of the rainbow colors. During this almost 200 years old story, we will reveal the secrets of the lanthanides and, although these mysterious elements have remained hidden for a long time, we will discover that nowadays you can find the Rare-earths where you least expect them. They are in the microphones, computers, and guitars, but also in colored glasses, aircrafts, lamps and even in the euro banknotes. They can be employed to obtain very special magnets, lasers or thermometers. Nevertheless, all of these are only few application examples, the Rare-earths story is only at the beginning and who can say what the next chapter will be.



1. J. Emsley, Nature's Building Blocks An A-Z Guides to the Elements, Oxford University Press, 2003.

2. C. Baskerville, Science 19 (1904) 88.

Innovative 3D model of periodic table consisting of each individual element in the form of atom having electronic configuration with rotating orbits

Deepti Dhaygude, Vaishali Dhaygude, Dr.Sanjeev Joshi, Yudhavir Mahindrakar and Krantivir Mahindrakar.

Dhygude Science Activity Centre(D-SAC),Kunthanaka, Solapur, 413003,India

deeptisjoshi@yahoo.com, vaishalidhaygude@yahoo.com

Abstract

In the history of periodic table from Mendeleev to modern Periodic table two dimensional text format is used for presentation. Such a format is difficult for teachers to teach and the perception of atomic structures goes beyond the imagination at student level. The understanding would be more clear and easy to remember if a three dimensional model of each element can be put in front of the students.

This article emphasizes on the description and use of our 3D innovative periodic table model. This model contains each element in its atomic form with central nucleus: having protons and neutrons and, rotating orbits with respective electrons.

In preparing the model, care was taken to see that different orbits can be freely rotated to show that they can have different orientations in space. Metal wires are used for orbits of different radii while different colored beads are used to represent natures of the elements.

A foldable frame of 17 x 6 feet was constructed on which all the individual element models can be mounted easily and gives exact idea of the 18 groups and 7 periods. Using these models, formation of ionic and covalent bonds can be shown using the individual atom models. This gives an interactive and joyful experience to the students.

It took around 8 months to construct the model. An overwhelming response from students and teachers of schools, colleges, and scientists from science institutes motivated us to present it at international level. It is an effective teaching aid as well as an asset to science labs and museums.

In further development of the 3D model, we will be attempting to incorporate s,p,d,f orbital which will facilitate learning of hybridization, polar molecules etc. We acclaim it to be the biggest interactive 3D Periodic Table model which will build interest even in the lay man's mind to learn the alphabets of Chemistry.

Gennady G. Dlyasin (Dlyasin, Gennady Gennad'evich), Master's degree in Chemistry; PhD (Moscow, 1996); Associate Professor of Social Technologies (Moscow, 2001).

445008 Russia, Samara region, Togliatti city, Matrosova str. 14 – 33. E-mail: gensin777@yandex.ru

The symmetry concept of the periodic system of elements, according to the complementarity principle.

The principle of periodicity remains the main law of the periodic system of elements, which longs for the new approach and perusal. The system is essentially spiral and symmetrical. 15 elements are divided into 4 groups of 4, which is tetrad-effect. 4 multiplied by 4 equals 16, elements are 14, but the effect is working on 15. Number 14 here is odd-even. Such analysis does not exist, on the opposite – the “intuitive obviousness” is a common approach. The symmetry of the U-turn around the carbon on the series Lithium – Fluorine usually referred to as a sequence of “bounces and steadiness” [Khimiya i periodicheskaya... , 1982, s.67, 68] or “horizontal” periodicity. [Stepin B. D. and Tsvetkov A. A. 1994, s. 54] The conceptual and terminological confusion is obvious.

The goal of the study – to construct the concept of symmetry, correlating to the periodicity based on the principle of complementarity. The method of research is a comparison of the curves of the properties of elements.

+Objectives: To conceptually analyze curves relations of changes in properties in periodicity and other transformations (1); To develop glossary of the symmetry concept of the system (2); Examine all the many theories of symmetry, including tetrad-effect.

The researchers of tetrad-effect have mentioned that it works everywhere in the system. We have shown exactly that. We have picked and followed 5 transformations of symmetry – external vector translation (periodicity), internal translation, and also mirror symmetry. We have introduced formulas of symmetry. We have established that the changes of the properties in series, which are packets (with maximal layout and unification) is full of all kinds of symmetry. The possibility of it links with the properties of co-symmetry (author's concept: not complete in-phase, mutual bending) – conditional “force” of interaction.

As a result we have discovered and shown hidden symmetries of the system, and also the effectiveness of the idea of co-symmetry as a method; we have formulated the concept, established the terms and formulas of symmetry. Tetrads and triads on a “staves” of tetrad effects are like cryptograms of some “chemical semiotics”. The symmetries shown (and concepts, including 2 new laws, which we only mentioned) are to be seen as a new object of future research. They also demand justification in the terms of quantum mechanics.

Khimiya i periodicheskaya tablitsa / K. Sayto, S. Khayakava, F. Takei i dr. Pod. Red. K. Sayto [Chemistry and Periodic Table]. M. Mir, 1982. 320 s.

Stepin B. D. Tsvetkov A. A. Neorganicheskaya khimiya. [Inorganic chemistry] M. Vysshaya shkola, 1994. 608 s.



(Recent Photograph)

Title: The Story of Hypervalent Iodine Catalysis

Toshifumi Dohi

College of Pharmaceutical Sciences, Ritsumeikan University, Japan

td1203@ph.ritsumei.ac.jp, +81-77-561-4908

Type of Presentation: Oral

Abstract:

Halogens are sometimes incorporated into many useful organic molecules and fine chemicals utilized in a wide range of scientific fields, such as natural products, biologically-active compounds, and organic materials. With long history since their findings and isolations, halogens as well as halogenated organic compounds continue to play important roles as the resources that make the lives of humans more prosperous.

Among them, **iodine**, first discovered in 1811, is a chemical element with symbol **I** and atomic number 53. Due to the large atomic size, it can take a variety of the oxidation states ranging from -1 to +7. Recently, hypervalent iodine(III) and (V) reagents are popularly used for many oxidation reactions and cross-couplings as a greener alternative to heavy metal oxidants as well as transition metal catalysts in virtue of their low toxicities and ready availabilities. They generally show high reactivities over molecular iodine and can oxidize substrates with more stable monovalent iodine formation as the driving force.

After discovery of the first hypervalent iodine compound (Willgerodt's reagent) more than 100 years ago, they have become useful in many synthetic applications, but stoichiometric amounts were usually employed in their use. The catalytic utilization of hypervalent iodine reagent, largely in consideration of economic and environmental viewpoints, is thus a desired goal in 21th century. Gratefully, new reliable catalytic methods have emerged since 2005 that can broaden the scope of the catalytic concept. For these contributions, catalytic strategy is now available for performing many representative types of oxidative bond-forming reactions and alcohol oxidations mediated by hypervalent iodines, some of which even include key transformations for the synthesis of natural products. This lecture highlights the historical background and the efforts made to realize the catalytic utilization of these reagents, especially with focus on iodine(III).

Biography: Toshifumi Dohi received his MS in 2002 (Prof. S. Murai) and PhD in 2005 (Prof. Y. Kita), subsequently became Assistant Professor at Osaka University, and was promoted to Professor (PI) in 2019 at Ritsumeikan University. He received the IUPAC-ICOS 15 Poster Award for most excellent presentation, the PSJ Award for Young Scientists (2009), Banyu Chemist Award (2013), Thieme Chemistry Journal Award (2014), and GSC Encouragement Award (2015). His current research interest is focused on the hypervalent iodine chemistry in organic synthesis. For more details, see homepage: <http://www.ritsumei.ac.jp/pharmacy/dohi/>.

The properties periodicity of transition metals π -allyl complexes in the norbornadiene allylation reaction

Durakov S.A., Flid V.R.

MIREA - Russian technological university, Institute of Fine Chemical Technologies named after M.V. Lomonosov, Moscow, Russia
s.a.durakov@mail.ru

Allyl complexes of transition metals are of great interest in organic synthesis and catalysis. They are intermediate compounds in many reactions involving unsaturated compounds of unsaturated compounds that occur in the presence of transition metal complexes, such as carbonylation, isomerization, hydrogenation, oxidation, oligo- and polymerization. The important role of allyl complexes in these processes is due to their ability to easily enter the district with CO, olefins, acetylenes and other unsaturated compounds. Such metal-ligand bonding reactions through allyl intermediate derivatives are often key in catalytic processes.

The norbornadiene (NBD) allylation reacton with allyl complexes of transition metals is not similar to the well-known allylic substitution reactions [1]. The peculiarity of this reaction is the controlled variation in the nature of the addition of an allyl fragment to the NDB, which can undergo significant changes, up to the breaking of the C-C bond. This reaction opens up exceptional opportunities for single-stage synthesis of a wide range of strained polycyclic hydrocarbons containing methylene, vinyl, methylenecyclobutane and allyl fragments.

Using the example of the behavior of Fe, Co, Ni, Rh, Pd, Pt allyl complexes in the NBD allylation reaction, a change in the periodicity of their properties is demonstrated. It is shown that the stoichiometric reaction with the participation of allyl complexes of these metals makes it possible to obtain a huge amount of substituted derivatives of NBD [2]. It was investigated that with an increase in the atomic number, the stability of the intermediates formed in the reaction increases, which makes it possible to carry out not only a stoichiometric but also a catalytic process. Using Ni, Pd, Pt as an example, it is shown that, when moving in a group from top to bottom, the reducing properties of the complexes increase.

A detailed study and comparison of the catalytic properties of systems based on Ni and Pd in this reaction was carried out. On the basis of a complex of physicochemical, kinetic, electrochemical, and isotopic methods, the schemes of the mechanisms of allylation reactions NBD in the presence of nickel and palladium complexes are substantially supplemented and specified. The directions and the variability of the stages of β -hydride transfer in the interaction of NBD and allyl formate are experimentally established [3,4]. The effect of the nature of the metal on the direction of the β -hydride transfer stage in the reaction is shown.

Acknowledgement. This work was supported by the Russian Science Foundation (RSF), grant № 18-13-00415.

References:

- [1] N.A. Butt, W.Zhang, Chem. Soc., Rev. 44, (2015), 7929
- [2] V.R. Flid, O.S. Belov, A.A. Grigoriev, J. Organomet. Chem., 4, (1991), 864
- [3] S. A. Durakov, R. S. Shamsiev, V. R. Flid, A. E. Gekhman, Russ. Chem. Bull., 67, (2018), 2234.
- [4] S. A. Durakov, R. S. Shamsiev, V. R. Flid, A. E. Gekhman, Kinet. Katal., 60, (2019), 1.

A MOBILE APPLICATION TO LEARN ATOMIC MODELS

Mustafa ERGUN

Science Education, University of Ondokuz Mayıs, Samsun, Turkey

mergun@omu.edu.tr

Human have always sought to understand the smallest constituent part of the matter that surrounds us either by the reflection of philosophers or by experimentation. The concept and the model of the atom were always questioned by scientists.

The history of the evolution of the models of the atom shows us the existence of different representations of the atom in the history of science, especially in chemistry. An atomic model is a theoretical representation of the properties of the atom and each model has characteristics that are valid in its time. As the history of modeling the atomic structure shows us the difficulties of understanding this concept, the learning of atomic concept modeling is not easy for students. Many studies of students' conceptions on atomic structure have shown the persistence of obstacles in learning. For the last ten years, the integration of technology (software and mobile applications) into learning has allowed teachers to better understand the obstacles that prevent them from understanding the concept involved.

The purpose of this study is to know the usefulness of a mobile application created for the learning of models of the atom in the teaching of chemistry in middle and high school. Our mobile application was prepared based on Mobil-D, a mobile application development model, which was developed by Abrahamsson et al. (2004), and Spataru (2010).

We have created a mobile application called "atomic model" that allows to see the first thirty-six chemical elements with five different models (Dalton, Thomson, Rutherford, Bohr and Quantum). Our mobile application allows the user to see the particles of the same chemical element in each model successively. Once the application is downloaded on mobile or tablet, it's not necessary to have the internet connection.

In this mobile application, user can see the structure of the carbon element according to five different atomic models from the following figures. Each shape contains images of the same element with respect to different models. For example, if the carbon atom is explained by the Dalton's atomic model, solid sphere model, it is understood that subatomic particles such as electrons and protons in their structure are not visible and atoms aren't indivisible (Figure 1).

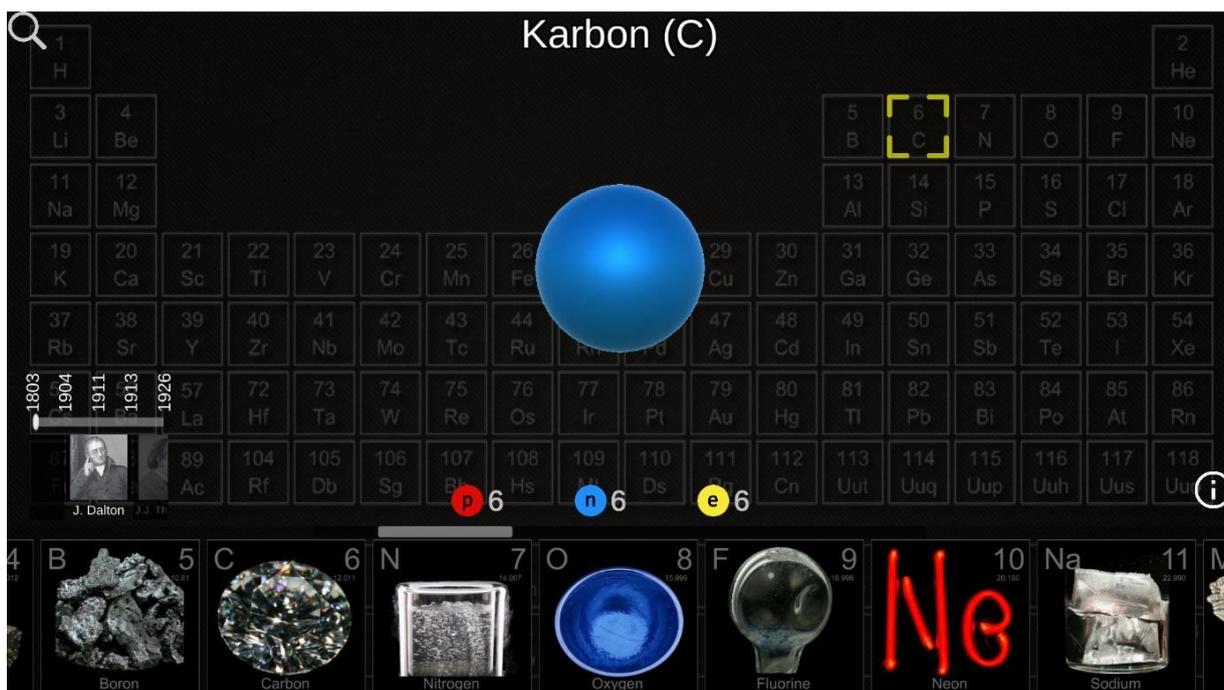


Figure 1. Mobile Application Screen Shot of Carbon Element According to Dalton's atomic model.

If the structure of the carbon element is explained by the Thomson's model, plum pudding model, it is understood that as the subatomic particles only charged particles are visible and have a total neutral structure and there is no nucleus (Figure 2).

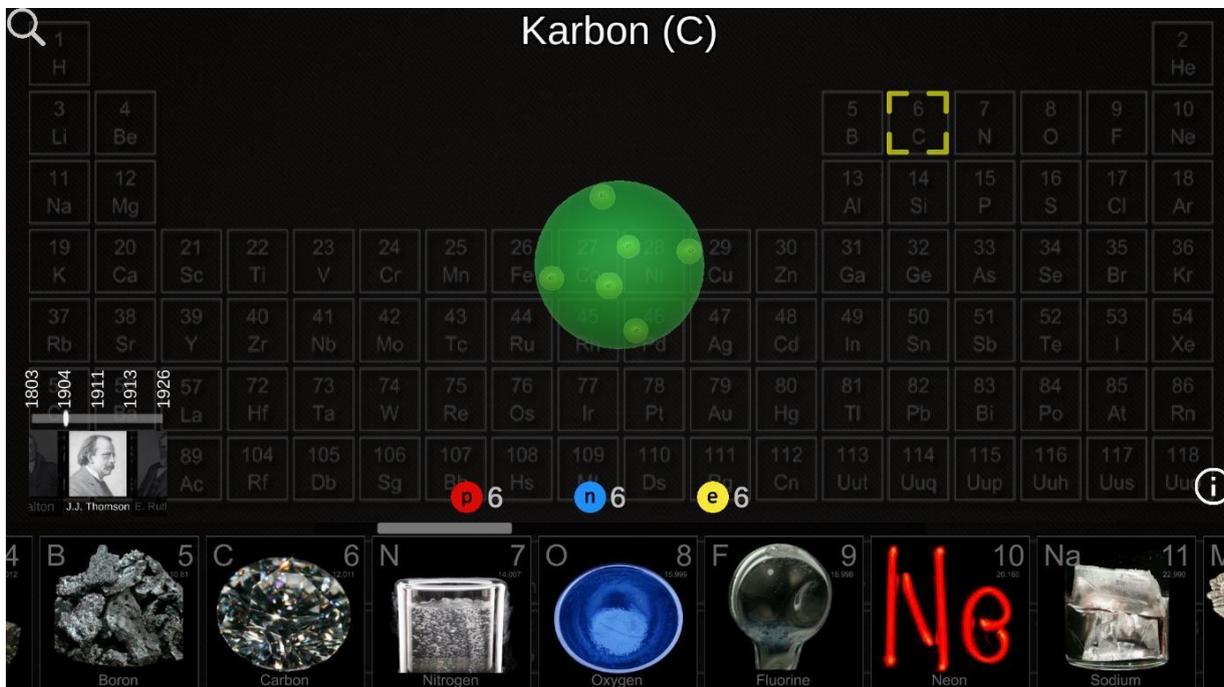


Figure 2. Mobile Application Screen Shot of Carbon Element According to Thomson's model.

According to the Rutherford's model, nuclear model, it is understood that protons in the structure of carbon element are inactive localized in the nucleus and electrons are surrounded by protons. It is also understood that there is not a nucleus concept in the model (Figure 3).

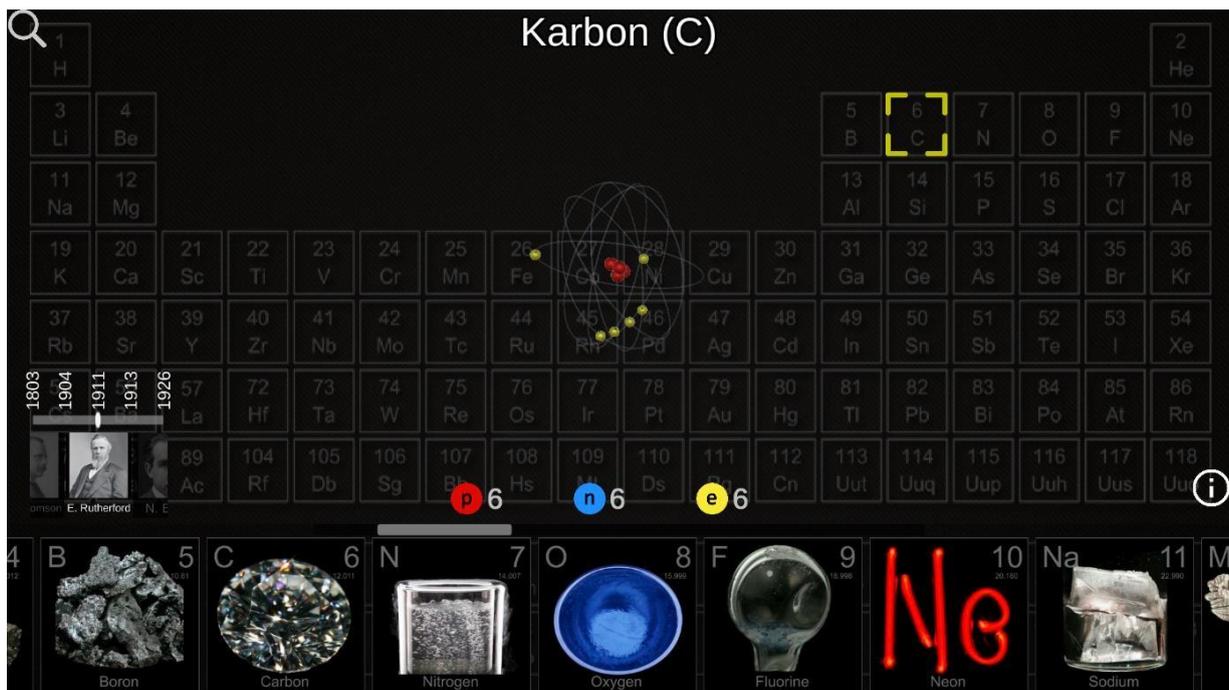


Figure 3. Mobile Application Screen Shot of Carbon Element According to Rutherford's model.

In the Bohr's model, planetary model, it is understood that the protons in the structure of the carbon element are in nucleus, electrons move around the nucleus in orbits and this model not work for heavier atoms (Figure 4).

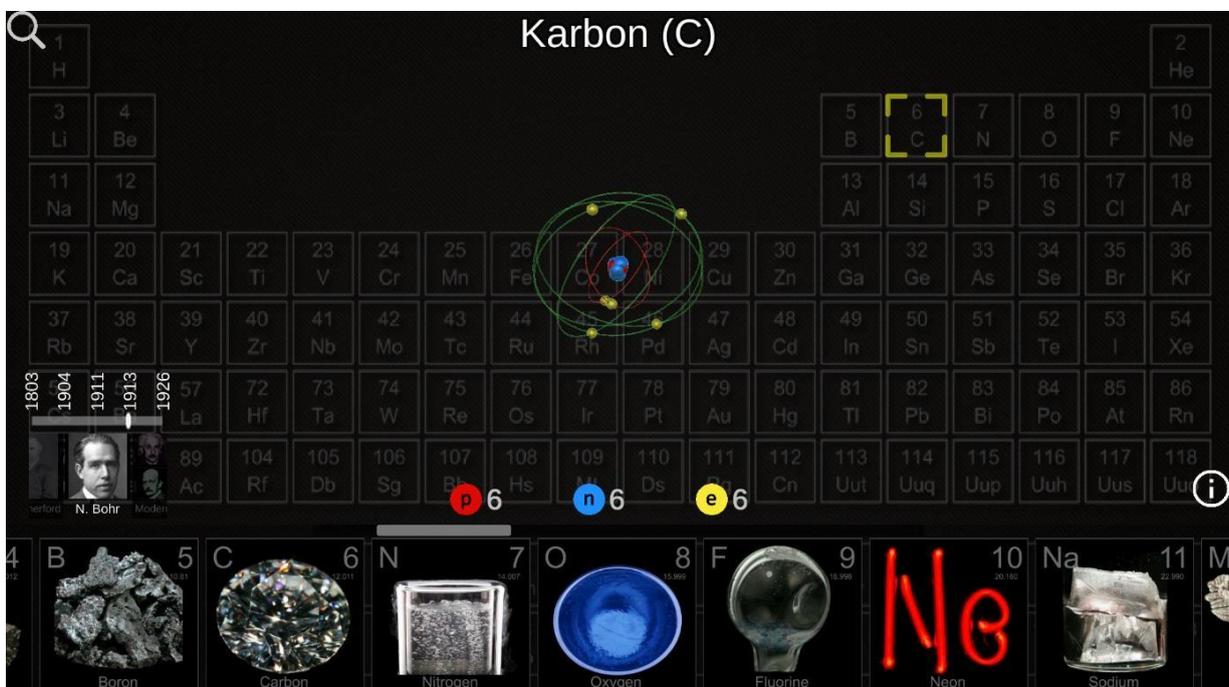


Figure 4. Mobile Application Screen Shot of Carbon Element According to Bohr's model.

In the quantum model, Schrödinger's model, it is shown that the protons and neutrons in the structure of carbon are present in the nucleus and the electrons don't move around the nucleus

in the orbits but in clouds where their position is uncertain. It is impossible and know the exact location of the electrons instead clouds of probability orbitals (Figure 5).

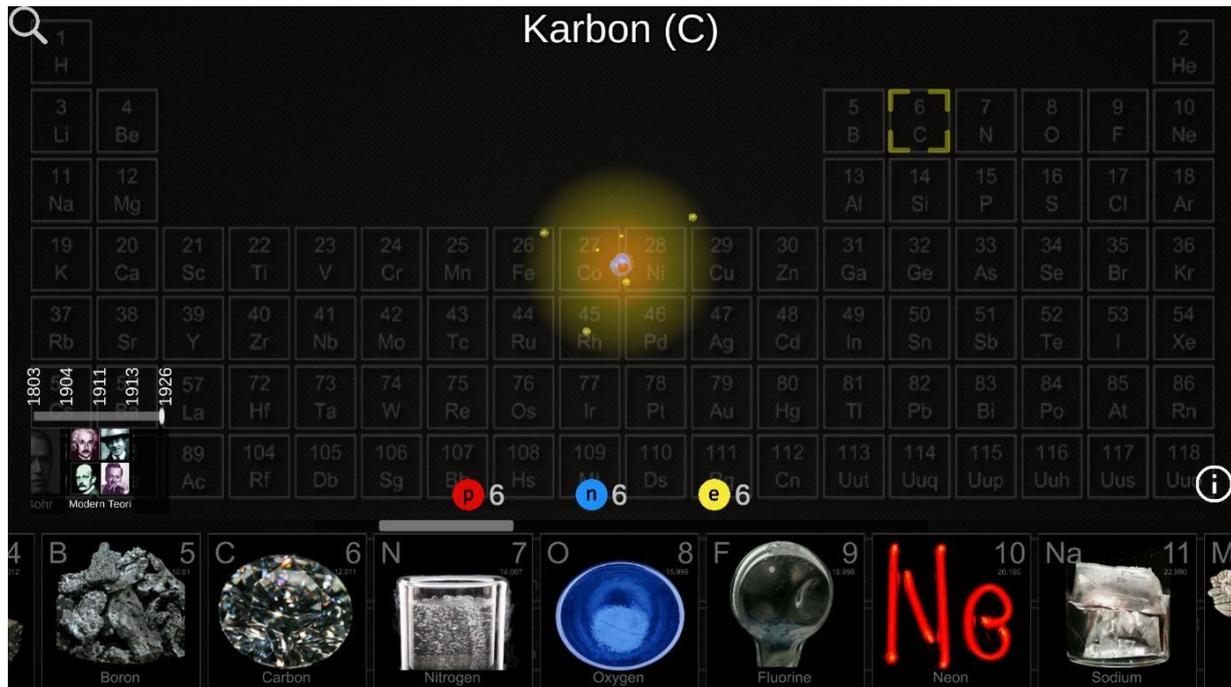


Figure 5. Mobile Application Screen Shot of Carbon Element According to Quantum Model

We conducted a descriptive survey of eighty-two prospective science teachers to evaluate the usefulness of our mobile application. In this questionnaire, we asked 13 questions (5 open-ended question, 8 multiple choice questions).

The results we have obtained allow us to conclude that this mobile application helps to learn atomic models. Using this mobile application in the course increases the motivation of the learner. There are difficulties identified by the user regarding the size of the screen.

Abrahamsson, P., Hanhineva, A., Hulkko, H., Ihme, T., Jäälinoja, J., Korkala, M., Koskela, J., Kyllönen, P & Salo, O. 2004, Mobile-D: an agile approach for mobile application development. Conference on Object Oriented Programming Systems Languages and Application; Companion to the 19th annual ACM SIGPLAN conference on Object-oriented programming systems, languages, and applications (pp. 174-175). Vancouver: ACM.

Spataru, A.C.: 2010, "Agile development methods for mobile applications", School of Informatics, University of Edinburgh, Yüksek Lisans tezi.

Using the Periodic Table of Elements and quantum chemical calculations 2-substituted-1,3,2-dioxarsenites and 1,3,2-dioxarsolanes for to search new chemical reactions

Francisco Fernandez, Tudor Spataru, Aibassov Yerkin, Yemelyanova Valentina

Natural Sciences Department, Hostos College, 500 Grand Concourse, New York, 10451, USA,

The basis of the periodic system of chemical elements is the fundamental law of nature. The value of any scientific theory is not only that it explains already known facts, but also that it opens up the possibility of predicting new facts, laws and reactions.

We used the periodic system of elements to search for new chemical reactions of arsenic, antimony and bismuth.

As a result, we discovered new reactions of arsenic, antimony and bismuth.

Thus, we have shown the possibility of using the Periodic Table of the elements of the I-VIII groups to search for new reactions (1) - (6):

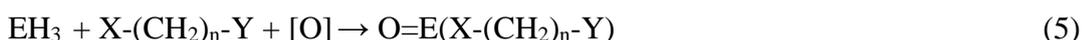
In the first reaction, an element E with a valency of 0 is oxidized to a valence (+3).



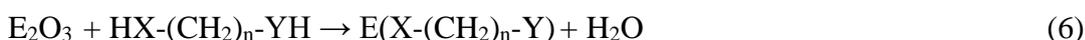
In the second reaction, the compound M_3E_2 with a valence (+3) is converted into a derivative with a valence (+3) or (+5).



In the third reaction, the hydride of the element EH_3 valency (-3) is oxidized to valence (+3) or (+5).



In the fourth reaction, the trioxide of the element E_2O_3 of valency (-3) is converted into a compound of valence (+3) or (+5).



We performed DFT geometry optimization in the frame of B3LYP approximation.

Basis set of 6-31++G** for light atoms and 6-311G** for As and halogens have been used within all geometry optimization processes.

The results of the quantum chemical calculation of 2-substituted-1,2,3-dioxarsolane, 2-substituted-1,2,3-oxaarsolane, 2-substituted-1,2,3-oxathiaarsolanes showed that these reactions proceed without changing the valence of arsenic.

Thus, the Periodic Law allows to systematize the reactions, to give an explanation to them and to anticipate new, still unknown reactions.

Fe vs. Ru Tetrahydrides with PNP-, CNC-, NNN-Pincer Ligands as Acids, Bases, and H[•] Donors

Gazimagomedov M.A.¹, Polynski M.V.¹, Pidko E.A.^{1,2}

¹TheoMAT group, ITMO University, Saint Petersburg, Russia

²ISE group, Delft University of Technology, Delft, Netherlands

The chemistry of transition metal hydrides offers new ways for renewable energy conversion and storage. They are efficient catalysts for the sustainable reduction of multiple C-heteroatom bonds in esters, nitriles, ketones, and (no less importantly) carbon dioxide [1]. Their reactivity in reduction reactions can be estimated both experimentally and computationally by means of hydricity and acidity values [2]. From the perspective of computational chemistry, hydricity calculation is a straightforward way to make a universal and experimentally verifiable prediction of a transition metal reactivity in reduction reactions.

In the present work, we calculated hydricity and acidity of Fe- and Ru- tetrahydrides with PNP-, CNC-, and NNN- pincer ligands, as well as the Gibbs free energies of the H[•] transfer to TEMPO molecules. (Figure 1a-c) with DFT methods. Main binding motifs of H₂ to the transition metal centers were determined (Figure 1d, e).

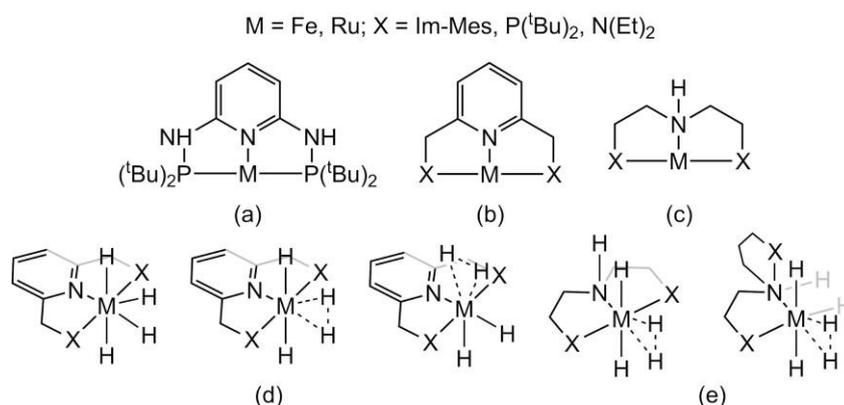


Figure 1.

(a)-(c) – structures of the modelled tetrahydride complexes;

(d) – from left to right: classic tetrahydride complex, equatorial and axial H₂ molecules coordination;

(e) – mer- and fac- coordination of the ligands depicted in Figure 1c.

The obtained values (Figure 3) correspond to Gibbs free energies of hydride/proton transfer from the metal complex to the implicit solvent specie (Figure 2):



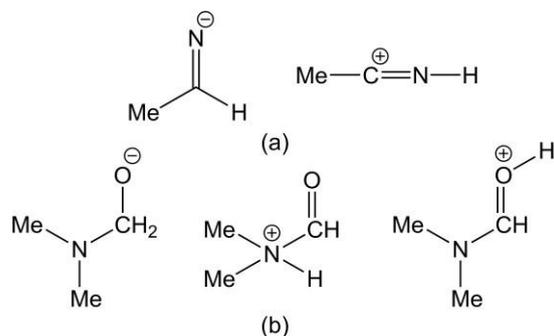


Figure 2.

(a) – left to right: structure of acetonitrile- H^- anion and protonated acetonitrile cation;
 (b) – left to right: structure of DMF- H^- anion and protonated DMF cations.

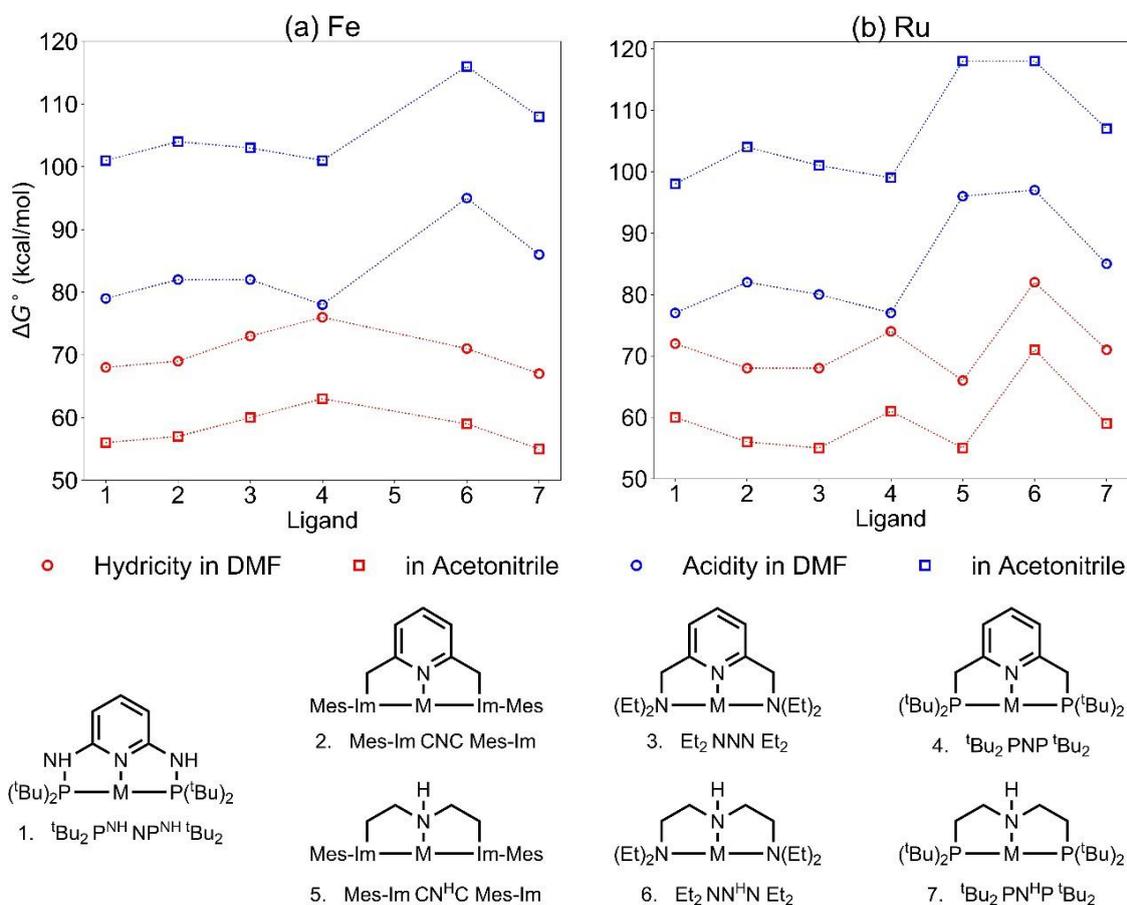


Figure 3.

Hydricity (red) and acidity (blue) of pincer complexes in DMF (circle) and acetonitrile (square).
 The values were computed with TPSS functional and COSMO-RS

We used the ORCA 4.0 program package[3] to perform unrestricted Kohn-Sham calculations at the B97-3c [4] and TPSS-D3/ma-def2-TZVP//TPSS-D3/ma-def2-SVP [5, 6] levels of theory. Vibrational frequencies were computed with the finite difference algorithm validate the optimized geometries as true minima, as well as to calculate the Gibbs free energies. Bulk solvent effects effects were calculated with conductor-like screening model for realistic solvation (COSMO-RS) [7], [8] as implemented in the COSMOTerm [9], [10] and TURBOMOLE V7.2 [11] programs.

References:

- [1] M. A. Esteruelas, A. M. López, and M. Oliván, "Polyhydrides of Platinum Group Metals: Nonclassical Interactions and σ -Bond Activation Reactions," *Chem. Rev.*, vol. 116, no. 15, pp. 8770–8847, 2016.
- [2] E. S. Wiedner, M. B. Chambers, C. L. Pitman, R. M. Bullock, A. J. M. Miller, and A. M. Appel, "Thermodynamic Hydricity of Transition Metal Hydrides," *Chem. Rev.*, vol. 116, no. 15, pp. 8655–8692, 2016.
- [3] F. Neese, "The ORCA program system," *Wiley Interdiscip. Rev. Comput. Mol. Sci.*, vol. 2, no. 1, pp. 73–78, Jan. 2012.
- [4] J. G. Brandenburg, C. Bannwarth, A. Hansen, and S. Grimme, "B97-3c: A revised low-cost variant of the B97-D density functional method," *J. Chem. Phys.*, vol. 148, no. 6, p. 064104, Feb. 2018.
- [5] J. Tao, J. P. Perdew, V. N. Staroverov, and G. E. Scuseria, "Climbing the density functional ladder: Nonempirical meta-generalized gradient approximation designed for molecules and solids," *Phys. Rev. Lett.*, vol. 91, no. 14, p. 146401, Sep. 2003.
- [6] J. Zheng, X. Xu, and D. G. Truhlar, "Minimally augmented Karlsruhe basis sets," *Theor. Chem. Acc.*, vol. 128, no. 3, pp. 295–305, Feb. 2011.
- [7] A. Klamt, "Conductor-like Screening Model for Real Solvents: A New Approach to the Quantitative Calculation of Solvation Phenomena," *J. Phys. Chem.*, vol. 99, no. 7, pp. 2224–2235, Feb. 1995.
- [8] Andreas Klamt, † Volker Jonas, and Thorsten Bürger, and J. C. W. Lohrenz, "Refinement and Parametrization of COSMO-RS," 1998.
- [9] F. Eckert and A. Klamt, "Fast Solvent Screening via Quantum Chemistry: COSMO-RS Approach," *AIChE J.*, vol. 48, no. 2, pp. 369–385, Feb. 2002.
- [10] COSMOtherm, C3.0, release 16.02, COSMOlogic GmbH & Co KG, <http://www.cosmologic.de>
- [11] TURBOMOLE V7.2 2017, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989–2007, TURBOMOLE GmbH, since 2007, available from <http://www.turbomole.com>

Novel bimetallic iridium dyad as a single molecule white light emitter

Anastasia Yu. Gitlina, Elena V. Grachova

Iridium is a transition metal of platinum group with atomic number 77. Since the opening of the metal its chemistry has been developing rapidly. Thus, compounds in oxidation states between -3 and +9 involving complexes with coordination numbers between 4 and 6 were synthesized. Nevertheless, the most attractive compounds are organometallic iridium(III) complexes.

Cyclometalated iridium(III) complexes demonstrate remarkable properties which determine a wide range of applications. In particular, these are unique luminescent properties. The best illustration is that iridium(III) complexes are the components of the electroluminescent devices such as organic light-emitting diodes [1].

Nowadays, the most popular trend is obtaining of white light emitters. Even in that iridium(III) complexes were successful. For instance, white emitting device was constructed by mixing in active layer of two cyclometalated iridium(III) complexes with green and red emission bands, combination of which led to the effect [2].

However, in our research group a single molecule white light emitter was obtained. It is a dyad which contains two cyclometalated iridium(III) centers with ligands having different electronic properties. The metals are connected by ancillary organic linker that complements the coordination sphere. The dyad demonstrates a number of emission bands in visible spectrum, combination of which leads to white emission under UV conditions. Obtained compounds were characterized by NMR and HR mass spectra and elemental analysis.

Great acknowledgements express to the Russian Science Foundation grant 16-13-10064. The work was carried out using equipment of Saint Petersburg State University Research Park: Centers of Magnetic Resonance, Chemical Analysis and Materials Research.

References:

1. E. Zysman-Colman, *Iridium(III) in Optoelectronic and Photonics Applications*, 2017, 2, 736 p.;
2. S.Tang, J. Pan, H. Buchholz, *White Light-Emitting Electrochemical Cell*, ACS Appl. Mater. Interfaces, 2011, 3(9), 3384–3388.

Beryllium as p block element in superconductors ZrBe_2 and HfBe_2

Dr. Maarten G. Goesten, Division of Physical Science and Engineering, KAUST, Saudi Arabia

The first report on π -bonding between two s block elements came in 2018, in a theoretical description of $\text{Be}_2(\mu_2\text{-X})_4$ complexes.¹ These complexes have not been synthesized as yet. In this work, it is shown that π -bonding between beryllium atoms had been experimentally realized already in the 1960s and 1970s, in ZrBe_2 and HfBe_2 .^{2,3} Stoichiometrically, these look like ordinary alloys, but a closer look at the P_6/mmm structures reveals a hexagonal honeycomb Be sublattice, held together by fully delocalized π -bonds. The electronic band structure of this Be sublattice is topologically similar to that found in graphite, or the boron sublattice in MgB_2 .

MgB_2 and graphite intercalation compounds (GICs) form a well-known family of conventional superconductors. It is herein predicted that ZrBe_2 and HfBe_2 are superconductors as well, with computed critical temperatures of 11 K (ZrBe_2) and 9 K (HfBe_2). These are unusually high values for metal alloys at ambient pressure, and a detailed inspection of the phonon-mediated superconductivity discloses a mechanistic similarity to that found in MgB_2 and GICs.

This work shows that the elements which construct exotic, aromatic 2D materials (graphene, borophene, silicene), stretch beyond the p block. Peculiar beryllium startles again.⁴

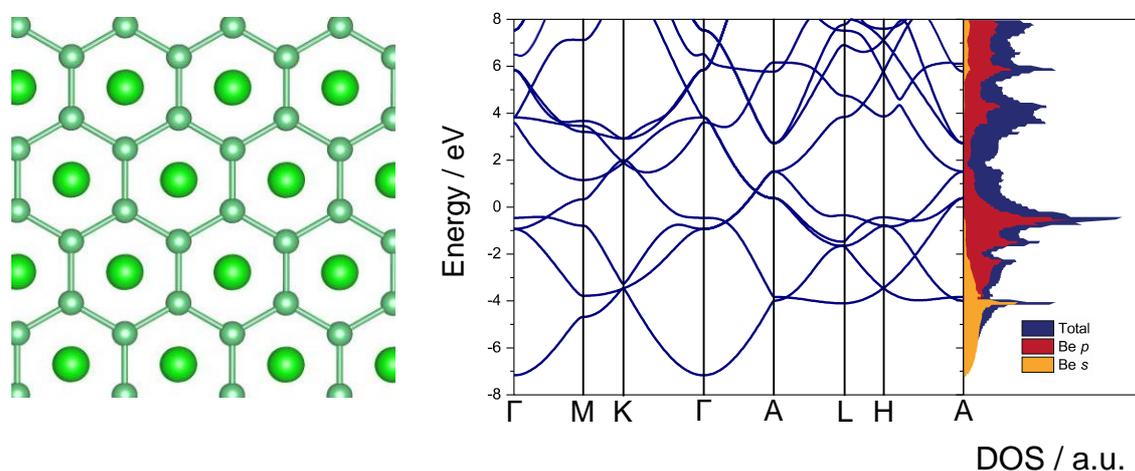


Figure 1. (Left) Zr ions (large green spheres) and the honeycomb Be lattice in ZrBe_2 . (Right) the band structure of ZrBe_2 , and the Be s and p orbital contribution to the density-of-states. The Fermi level is set at 0 eV.

References

- (1) Liu, X.; Zhang, M.; Yu, S.; Geng, Y.; Zhang, X.; Ding, Y.; Su, Z. *Physical Chemistry Chemical Physics* **2018**, 20 (37), 23898.
- (2) Zalkin, A.; Sands, D. E.; Bedford, R. G.; Krikorian, O. H.; IUCr. *Acta Crystallogr* **1961**, 14 (1), 63.
- (3) Stuemke, M.; Petzow, G. *Zeitschrift fuer Metallkunde* **1975**, 66 (5), 292.
- (4) Frenking, G. *Nature* **2015**, 522 (7556), 297.



Title: The importance of semiotic representations in the teaching of chemistry

Name: Marcos Aurélio Gomes da Silva
federal University Juiz de fora, BRA

Abstract

The motivation to do this work was to reflect on the use of chemical language in the classroom, since my focus is to work with scientific literacy and language contributes significantly in this subject.

This work intends to bring reflections and applications on the importance of the use of chemical symbology in the classroom, since students have a great difficulty in the use and interpretation of symbols used in chemical language. For this we will use as theoretical support the bases of the semiotic theory of Charles Peirce that deals precisely on the relations between the representations and their axes of signification.

Semiotics is the science of meaningful processes (semiosis), linguistic signs and languages. We approach the representations of chemical formulas first in a historical way starting with the symbology used by the alchemists and passing through chemical languages used by chemists like Dalton and Berzelius arriving until the current symbology.

We analyzed contents such as organic and inorganic compound nomenclatures, periodic table and chemical reactions from the observation of the symbology used allowing students to reflect on the importance of symbols and representations in the construction of chemistry.

we understand and discuss the concept of common sense in the construction of chemical language. we use computational molecular models to help us to have a greater and interactive dimension to the processes of representations of chemical language.

he chosen theme allowed a significant approach to the teaching of chemistry and first a diagnostic evaluation was made in order to trace the profile of previous knowledge regarding the subject from basic concepts on the subject containing 9 questions related to the content of organic chemistry and general chemistry .

Presenting author details

Full name: Marcos Aurelio Gomes da Silva

Category: Poster

Email id: marcosaurelijf@hotmail.com

Design of polychromatic molecular emitters based on lanthanide complexes

Elena V. Grachova

Lanthanides are series of unique chemical elements with similar chemical properties and amazing photonic. Luminescence of molecular emitters based on lanthanide(III) has a few practically important advantages in compare with traditional organic phosphors and luminescent complexes of d-elements, such as a narrow emission bands, high photostability, and long lifetimes of the excited state.

From the other hand, construction of luminescent compounds which can demonstrate multiply emission and partial intramolecular energy transfer is one of the most interesting and demanded trend in coordination chemistry, and some features of lanthanide(III) sensitization make possible to use these metalcenters to create discrete molecular polychromatic emitters.

Based on a heterofunctional polydentate ligands decorated by bipyridine moiety we prepared a set of d-f heterometallic emissive complexes that demonstrate unusual combination of different nature emission from one molecule.

Using of luminescent complexes of d-metals as building blocks for design of luminescent d-f heterometallic molecular assemblies will be discussed, and some general principles of d-f molecular polychromatic emitters design will be presented in the framework of the lecture.

This work was supported by the Russian Science Foundation (grant 16-13-10064) and was carried out using equipment of St. Petersburg State University Research Park: Centers of Magnetic Resonance, Optical and Laser Materials Research, Chemical Analysis and Materials Research; Physical Methods of Surface Investigation, and the X-ray Diffraction Centre.

Diverse structures of Al and Ga halide complexes with *bpe* and *bpa*: a search for synthetic efficiency

Gugin Nikita

Student, 1 master degree course

Saint-Petersburg State University

Institute of Chemistry, Saint-Petersburg, Russia

E-mail: nikita.gugin@yandex.ru

Scientific supervisor: Dr. Davydova E.I.

Group 13 element trihalides are strong Lewis acids which form stable donor-acceptor (DA) complexes with bifunctional N-donors. Resultant 13-15 DA complexes can have molecular structures or produce group 13 metal-organic frameworks (MOF-13) of different kinds. The former complexes are prospective single-source precursors for the CVD of nitrides [1], whereas the latter can be used as materials for sorption, separation, heterogeneous catalysis, sensing etc. [2]. Most of 13-MOFs described are built using poly-carboxylate linkers, but there are only a few examples of using N-donors. Thereby synthesis and characterization of new 13-15 complexes built up with bifunctional N-donors are important tasks.

In order to comply with the 'green fabrication' principles all complexes were synthesized by direct interaction of MX_3 ($\text{M}=\text{Al, Ga}$; $\text{X}=\text{Cl, Br}$) with 1,2-bis(4-pyridyl)ethylene (*bpe*) or 1,2-bis(4-pyridyl)ethane (*bpa*) without the use of organic solvents (or with the addition of minor quantities of fluid molecules). Because of the moisture and air sensitivity of group 13 element halides and of the reaction products, all synthetic operations were carried out in whole glass apparatuses under vacuum. Solid state structures of molecular adducts ($\text{MX}_3 \cdot \text{LL} \cdot \text{MX}_3$, $\text{LL}=\textit{bpe}$: $\text{M}=\text{Al, Ga}$, $\text{X}=\text{Cl, Br}$; $\text{LL}=\textit{bpa}$: $\text{M}=\text{Al, Ga}$; $\text{X}=\text{Cl}$) as well as coordination polymers (e.g. ${}^1_{\infty}[\text{MCl}_2(\textit{bpa})_2]^+[\text{MCl}_4]^-$ ($\text{M}=\text{Al, Ga}$), ${}^2_{\infty}[\text{Al}_2\text{Br}_4(\textit{bpe})_5]^{2+}[\text{AlBr}_4]^- \cdot \textit{bpe}$) were established by single crystal X-ray analysis. Due to remarkable diversity of the possible reaction products, the development of the efficient selective method for the DA complex synthesis is an exceptional task. Therefore, different conditions of the complexation process were varied: the components ratios; the temperature regime and the synthetic method (dry melt synthesis or fluid-assisted synthesis). The bulk products obtained were characterized by X-ray Powder Diffraction.

We are grateful to M. Bodensteiner, A.V. Virovets and E.V. Peresyphkina (University of Regensburg) for the X-ray structure determination. X-ray powder diffraction measurements were performed at the Research park of St Petersburg State University.

References

1. A.Y. Timoshkin, H.F. Schaefer // Chem. Record, 2, 319 (2002).
2. Y. Liu et al. // J. Solid State Chem., 223, 84 (2015).

TOPIC: BINODIC PERIODIC SYSTEM, NEW APPROACH

AUTHOR: Julio Antonio Gutiérrez Samanez, Chemical Engineer.

COUNTRY: Peru.

ABSTRACT

This paper aims to understand the periodic chemical system as a matrix of diachronic and synchronic functions, which lead to a general mathematical function, which we call: "Binodic function", formed by pairs of periods, dyads or binodes, that describe Mendeleev's Periodic Law as a growing or progressive function of the main quantum number (n), with order and ordered rank, and that by unity and opposition of negative principles, generate in their dynamics: first, gradual or evolutionary quantitative changes (without variation of the format) and, second, radical quantitative changes, with the appearance of new quantum transitions, with growth of the format and qualitative or of binodo change. For whose understanding the analytical method and the geometric or graphic method were used. This rationalization restates Mendeleev's Law, which is only a literal statement, by placing the size of the pairs of symmetric or binary periods (Y) and the continuous elementary series (Z), as a function of their correlative number (B) or (n).

Likewise, they support this thesis: a 2D graphic representation of a self-similar spiral function of the distribution of the elements, under a geometric growth pattern, and, to 3D animation that shows a conical helical function that describes the position of each of the chemical elements, according to two growth laws: $(2n^2)$ and $(4n^2)$. This new approach to articulation and systematization constitutes a new conception of the Periodic System and the Periodic Table of Chemistry, synthesized in a concrete mathematical form: The Binodic law.

Julio Antonio Gutiérrez Samanez

N-Substituted Phosphine-Imine Ligands for The Palladium(II) Catalyzed Mizoroki-Heck C-C Coupling Reactions

Sevilay Yılmaz, Bilgehan Güzel

e-mail: bilgehan@cu.edu.tr

Çukurova University, The Faculty of Arts and Sciences, Chemistry Department, 01330, Adana, TURKEY

Mizoroki-Heck C-C coupling reactions have been used for the instruction of new carbon-carbon bonds for the synthesis of important intermediates such as fine chemicals, pharmaceuticals, polymers and agrochemicals. These reactions are generally catalyzed with Pd(0) or Pd(II) complexes which have phosphine or carben ligands [1,2]. Otherwise, palladium-(phosphine-imine) complexes have been rarely used as catalyst for the Mizoroki-Heck C-C coupling reactions, although such complexes are known to be versatile catalysts for many different catalytic reactions. In this study, we have prepared a series of Pd(II) complexes from phosphine-imine ligands containing both phosphorus and nitrogen donors (Scheme 1) and we applied these complexes for the Mizoroki-Heck C-C coupling reactions as catalyst (Table 1).

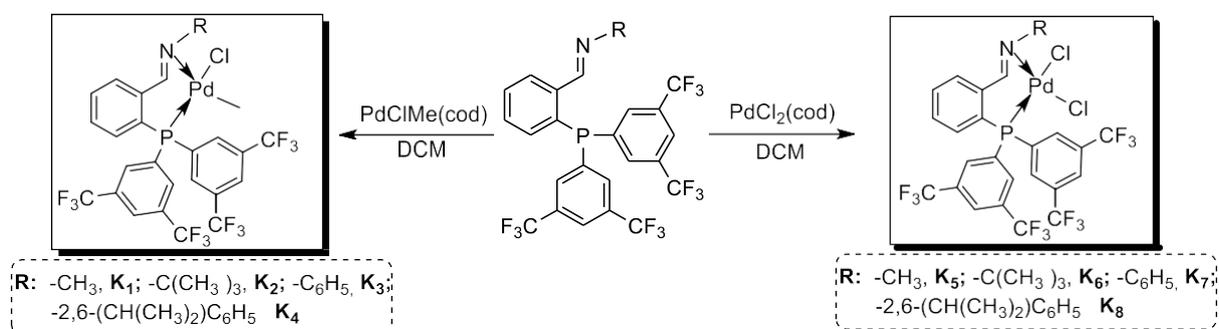


Table 1. The effect of Pd(II) catalysts (**K**₁₋₈) on the Mizoroki-Heck C-C coupling reactions of deactivated aryl bromides and styrene*

Entry	ArBr	Product	Yield (%) ^a							
			K ₁	K ₂	K ₃	K ₄	K ₅	K ₆	K ₇	K ₈
1			94	69	75	40	80	76	70	28
2			88	77	68	54	74	66	70	36
3			92	84	76	51	81	48	72	45
4			91	91	67	61	82	70	68	38

^aReaction conditions: Aryl bromide (0.1 mmol), Styrene (1.2 mmol), Cs₂CO₃ (1.2 mmol), Catalyst, (0.002 mol%), T: 80 °C, Time: 6 h. Yields were given for isolated products after column chromatography on silica gel.

Scheme 1. Synthesis of Pd(II)-phosphine-imine complexes

Acknowledgement: This study was supported by the Research Fund of Çukurova University in Turkey with Project Number: FDK-2016-7521.

- [1] L. Kurti, B. Czako, *Strategic Applications of Name Reactions in Organic Synthesis*; Elsevier Academic Press, Boston, (2005).
- [2] N. Miyaura, *Cross-coupling reactions: a practical guide*, *Top. Curr. Chem.* 219 (2002) 11.

Phosphorus — The Devil's Element?

Evamarie Hey-Hawkins, John Popp, Axel Straube, Toni Grell, and Volker Eilrich

Faculty of Chemistry and Mineralogy, Institute of Inorganic Chemistry, Leipzig
University, Leipzig, Germany

The chemical element phosphorus was discovered by the German alchemist Hennig Brand in 1669 on attempting to create the fabled Philosopher's stone through distillation of urine. He produced the white form of phosphorus, which glows upon exposure to oxygen. This characteristic led to its name, which means "light bearer" in Greek. Until the process for manufacturing red phosphorus, which is far less flammable and much less toxic, was discovered, the use of white phosphorus resulted in many murders, suicides and accidental poisonings [1].

The chemistry of phosphorus is, without a doubt, one of the most intriguing fields of inorganic and organic chemistry. It comprises a vast number of classes of compounds with many elements in the periodic table and combinations thereof. Phosphorus compounds are widely used in fertilisers, food additives, detergents, flame retardants, pharmaceuticals, pesticides and insecticides, to name but a few. Furthermore, phosphane ligands play an important role in homogeneous catalysis, especially chiral ones, which can improve significantly the efficiency, specificity and selectivity of catalysts. Metal phosphides, on the other hand, find applications in materials science. Besides an overview on the element phosphorus and its remarkable chemistry, examples of switchable catalysts [2] and suitable precursors for phosphorus-rich metal phosphides [3] will be presented.

[1] J. Emsley, *The 13th Element*, John Wiley & Sons, Inc. 2000.

[2] P. Neumann, H. Dib, A.-M. Caminade, E. Hey-Hawkins, *Angew. Chem. Int. Ed.* **2015**, *54*, 311-314

[3] T. Grell, D. M. Yufanyi, A. K. Adhikari, M. B. Sárosi, P. Lönnecke, E. Hey-Hawkins, *Pure Appl. Chem.* **2019**, DOI: <https://doi.org/10.1515/pac-2018-1013>

Scandium(III) trifluoromethanesulfonate – an efficient Lewis acid catalyst for organic and organometalloidal synthesis

Grzegorz Hreczycho, Krzysztof Kuciński, Joanna Kaźmierczak, Hanna Stachowiak, Dariusz Lewandowski

Adam Mickiewicz University in Poznań, Umultowska 89b, 61-614 Poznań, Poland
E-Mail: g.h@amu.edu.pl

Scandium (Sc) is placed in group 3 of the periodic table (along with yttrium, lanthanum and actinium), and has the smallest radius across all rare-earth elements. Its chemical properties are known to be intermediate between that of aluminum and lanthanides. Scandium is not rare element in the Earth's crust and its concentration is comparable to that of cobalt. However, Sc is relatively uncommon due to the lack of rich sources and difficulties in its separation. Despite this fact, the application of scandium and its compounds is quite significant. In particular, the scandium(III) trifluoromethanesulfonate [Sc(OTf)₃, scandium(III) triflate] is well-known as highly efficient Lewis acid catalyst for organic and organometalloidal synthesis.

It is noteworthy that Sc(OTf)₃ differs significantly from typical Lewis acid representatives (e.g., AlCl₃, BF₃, etc.). Specifically, scandium(III) triflate is stable in the presence of water unlike classic Lewis acids. As the result, none of reactions must be carried out under strictly anhydrous conditions. In comparison to other lanthanide triflates, scandium salt also shows the highest catalytic activity and selectivity in the vast majority of cases.

The aim of this communication is to demonstrate high activity and selectivity of scandium(III) trifluoromethanesulfonate in the synthesis of various organometalloidal compounds [1-3].

Acknowledgements:

This work was supported by The National Science Centre (Poland) under Grant no 2015/19/B/ST5/00240

[1]. G. Hreczycho, P. Pawluć, B. Marciniak, *New J. Chem.*, 2011, **35**, 2743-2746.

[2]. G. Hreczycho, K. Kuciński, P. Pawluć, B. Marciniak, *Organometallics*, 2013, **32**, 5001-5004.

[3]. J. Kaźmierczak, K. Kuciński, G. Hreczycho, *Inorg. Chem.*, 2017, **56**, 9337-9342.

Periodic law: new formulation and equation description

Imyanitov N.S., Sankt Petersburg, Russia

The atomic weight, nuclear charge, electron configuration of an atom and the total number of *i*-electrons in an atom belonging to *i*-block (*i* = *s*, or *p*, or *d*, or *f*) are considered as the fundamental characteristics of an element (atom). Only in the latter case, the true periodicity is achieved: the repetitions occurs at regular intervals. The total number of *i*-electrons in an atom belonging to *i*-block is used as the new basis for the description of the periodicity. This made possible to propose a new formulation of the Periodic law and to describe the Periodic law by an equation. One equation quantitatively describes the selected property of all atoms of a given block of the Periodic table. For another property or another block, the same equation is applied, but with different parameters.

The suitability of the equation is exemplified by the description of the properties of atoms, such as ionization energy, electron affinity, proton affinity, electronegativity, covalent atomic radii and the enthalpy of formation of elements in the gas phase. The equation makes it possible to describe also the properties of compounds and their fragments: the acidic properties of compounds with hydrogen of elements of groups 14, 15, 16 and 17; the acidic properties of protonated atoms of group 18 as well as molecules derived from elements of groups 15, 16 and 17; gas-phase basicity and proton affinity for compounds of elements of groups 2, 13, 14, 15, 16 and 17; inductive effects of ligands in coordination chemistry and substitutes in organic chemistry (derivatives of elements of groups 1-17); electronic parameters of 222 neutral ligands (compounds of elements of groups 14, 15, 16 and 17); the electron effect constants of coordinating metals of groups 3-17.

The new formulation and the equation retain their correctness upon fundamental changes in the composition and mutual arrangement of the blocks and periods. New broad areas for the application of the equation are discussed.

Title of Talk: Green Organosulfur Chemistry

Due to the profound significance of sulfur-containing molecules in organic chemistry and chemical biology, development of novel sulfurating reagents to access sulfur-containing compounds via mild, concise, and efficient approaches is necessary. The introduction of sulfur atoms into target molecules is an important area in organic synthesis, particularly in the synthesis of pharmaceutical and material compounds. Our group has explored the smellless, stable and sustainable (3S) green sulfuration reactions, and developed a set of new sulfurating reagents and corresponding methodologies. Through their strategies, the construction of C-S, C=S, S-S, S-N, S=O, and O=S=O bonds in natural products and pharmaceuticals was achieved comprehensively.^[1] In 2018, he was selected as Ambassador of "Sulfur" in "Periodic Table of Younger Chemists" by IUPAC. In 2019, he was selected as "Asian Representative Speaker of Young Outstanding Scientists of the World" by UNESCO in Opening Ceremony of International Year of Periodic Table of Chemical Elements.

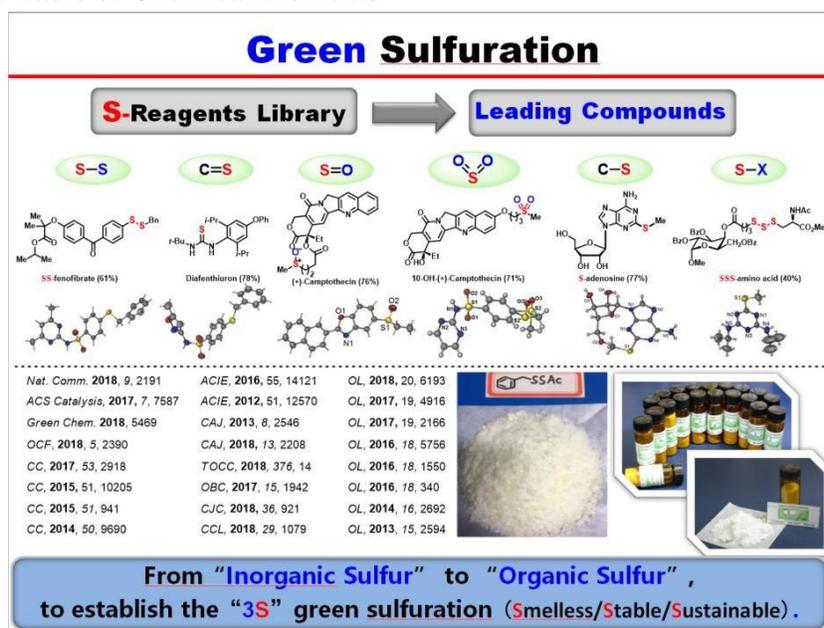


Figure: Our sulfur atom transfer strategy

References

[1] (a) Xiao, X.; Xue, J.; Jiang X. *Nat. Commun.* **2018**, 9, 2191. (b) Xiao, X.; Feng, M.; Jiang, X. *Angew. Chem. Int. Ed.* **2016**, 55, 14121. (c) Qiao Z.; Jiang X. *Org. Biomol. Chem.* **2017**, 15, 1942. (d) Liu, H.; Jiang X. *Chem. Asian. J.* **2013**, 8, 2546.

Applications of spectroscopy in the study of elements of the Periodic Table

This study proposes some of the applications of spectroscopy, in the identification of chemical elements of the Periodic Table, present in different light sources used in everyday life.

Since Isaac Newton (1666) adopted the name "Spectrum", noting that the white light of the sun could disperse into a continuous series of colours, using a prism, to Gustav Robert Kirchoff and Robert Wilhelm Eberhard von Bunsen (1859) who found that spectral lines were unique to each chemical element, other researchers such as William Hyde Wollaston (1802) and Joseph von Fraunhofer (1814) observed dark lines present in the solar spectrum, with the invention of the first grid spectroscope of diffraction.

The objectives of the study are summarized in the following steps: design and construction of a desktop spectroscope, transformation of the mobile phone into a spectrophotometer diffraction grid and investigation of applications of spectroscopy, in the identification of chemical elements of the Periodic Table present in different light sources.

In order to develop the objectives of the study, once the search for materials required in the design and construction of spectroscopes has been completed, the process of assembling them has been carried out. Upon completion of this last step, observations of spectra emitted by different light sources (incandescent light, halogen light, cold and warm light consumption, and fluorescent light) have been achieved.

Once the observations have been completed, the results obtained were analysed by comparing the emission spectra obtained through desktop spectroscope and the mobile transformed into a spectrophotometer, with the real emission spectra of the chemical components existing inside the light sources analysed (calibration of spectroscopes)

Checked the usefulness of spectroscopy in the identification of chemical elements, it can be concluded that spectroscopy can help us to observe different chemical components present in the light sources used in the daily life. Moreover, other fields where it can be useful, can be proposed, such as to study the chemical components that provoke atmospheric pollution in a given area or even in the analysis of the chemical composition of stars.

Europium. Luminescence and chemical properties.

Keskinova M.V., Sychov M.M.

Europium, Eu, chemical element of the third group of the Periodic Table, is related to the lanthanides. Europium was isolated in 1901 and is named after the continent of Europe.

There are 2 oxidation states of Eu (+2 and +3) in compounds. The materials with trivalent europium usually are synthesized in air. While compounds with divalent europium require reducing atmosphere. Luminescent materials with divalent europium usually are synthesized in hydrogen atmosphere or under layer of coal.

The main properties of phosphors contained Eu ions associated with the processes of light absorption or light emission processes or luminescence, are determined by intraconfigurational transitions between 4f states of Eu^{3+} ion, as well as interconfigurational transitions between 4f and 5d states of Eu^{2+} ion.

Due to fully filled $5s^2$ and $5p^6$ shells in Eu ions, electrons located at the 4f levels of the shell are almost completely screened from the influence of an external crystalline field. The weak interaction of the 4f shell electrons with the crystal field and, accordingly, the weak electron-phonon interaction leads to the fact that the optical and luminescent spectra characterizing the transitions between different states of the 4f configuration have a linear structure, very small displacements when going from one crystal to the other, a small broadening of the lines (about $10\text{--}100\text{ cm}^{-1}$).

The 4f-4f electron transitions of Eu^{3+} in $\text{Zr}_{0,95}\text{Y}_{0,05}\text{O}_2:\text{Eu}^{3+}$ phosphor and the emission spectrum of $\text{Zr}_{0,95}\text{Y}_{0,05}\text{O}_2:\text{Eu}^{3+}$ phosphor are shown in Fig. 1.

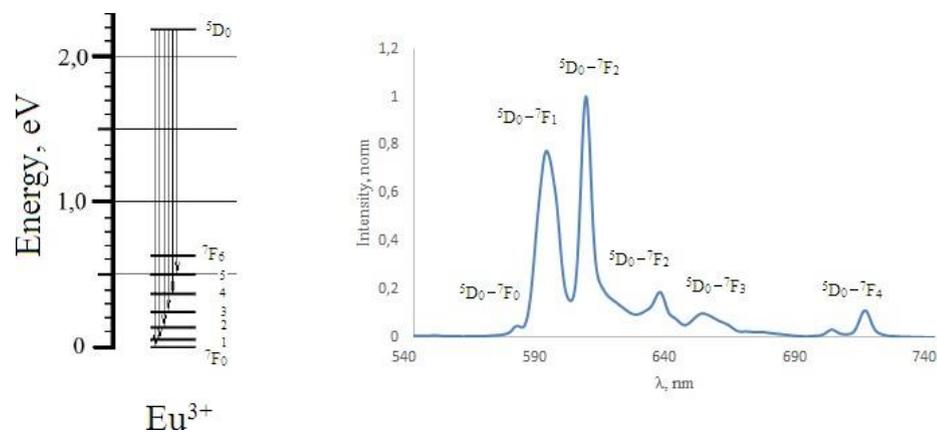


Fig. 1 The electron transitions of Eu^{3+} in $\text{Zr}_{0,95}\text{Y}_{0,05}\text{O}_2:\text{Eu}^{3+}$ phosphor and the emission spectrum of $\text{Zr}_{0,95}\text{Y}_{0,05}\text{O}_2:\text{Eu}^{3+}$ phosphor

The interconfigurational $4f^7 - 4f^65d^1$ transitions of Eu^{3+} lead to the appearance of wide bands in the absorption and luminescence spectra [1].

The $4f^7 - 4f^65d^1$ electron transitions of Eu^{2+} in $\text{NaBaPO}_4:\text{Eu}^{2+}$ phosphor and the emission spectrum of phosphor $\text{NaBaPO}_4:\text{Eu}^{2+}$ [2] are shown in Fig. 2.

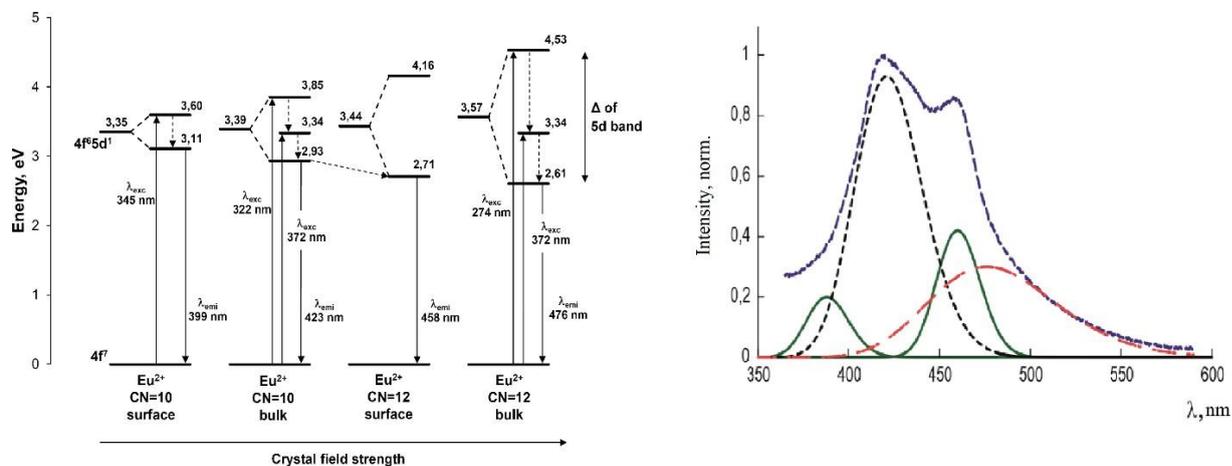


Fig.2 The electron transitions of Eu^{2+} in $\text{NaBaPO}_4:\text{Eu}^{2+}$ phosphor and the emission spectrum of phosphor $\text{NaBaPO}_4:\text{Eu}^{2+}$

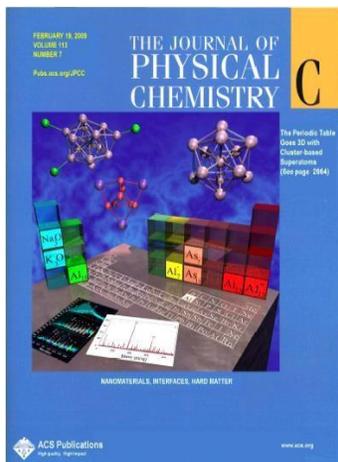
Literature:

1. Pustovarov, V.A. Spectroskopiya redkozemel'nih ionov/ V.A. Pustovarov. – URFU, 2016. – 69 P. (rus)
2. Bakhmet'ev, V.V. Synthesis of finely dispersed $\text{NaBaPO}_4:\text{Eu}^{2+}$ phosphors and structural investigation of their centers of luminescence/ V.V. Bakhmet'ev, V.V. Malygin, L.A. Lebedev, M.V. Keskinova, M.M. Sychev// Journal of Optical Technology. – 2017. – V. 84. – № 9. – P. 642-646.

Superatoms: A New Kind of Alchemy with Potential for Novel Materials

S. N. Khanna

Department of Physics, Virginia Commonwealth University, Richmond, VA 23284-2000



Size selected stable clusters have the potential to mimic the chemistry of elements in the periodic table and can be regarded as “superatoms” forming a third dimension to the periodic table. The physical, chemical, electronic and magnetic properties of superatoms can vary, sometimes severely, by the size, symmetry, composition, and the charged state with a further control provided by the addition of ligands. The talk will focus on this intriguing discovery and its implication for unifying nanoscience and potential for creating nanoscale materials with tunable characteristics. Specific examples illustrating how the clusters of the most easily oxidized solids can display extreme resistance to oxidation, clusters with specific symmetry that can split alcohols, and clusters that display novel magnetic properties will be presented. I will talk about our recent efforts where the superatoms ligated with charge transfer ligands can

lead to motifs that can donate or accept multiple electrons with low energies and with first ionization energies lower than any element in the periodic table. Recent protocols that enable us to synthesize materials from the new building blocks and the potential offered by the new materials will be highlighted. The talk will cover our recent work on metal-chalcogenide superatomic clusters that can lead to novel semiconductors with tunable band gaps.

References:

- [1] "Al cluster superatoms as halogens in polyhalides and as alkaline earth in iodide salts", D. E. Bergeron, P. J. Roach, A. W. Castleman, Jr., N. O. Jones, and S. N. Khanna, *SCIENCE* **307**, 231 (2005).
- [2] "Complementary Active Sites are Responsible for the Size-Selective Reactivity of Aluminum Cluster Anions with Water", P. J. Roach, W. H. Woodward, A. W. Castleman, Jr, A. C. Reber, and S. N. Khanna, *SCIENCE* **323**, 492-495 (2009).
- [3] "Designer magnetic superatoms", J. Ulises Reveles, P. A. Clayborne, A. C. Reber, S. N. Khanna, K. Pradhan, P. Sen, and M. R. Pederson, *Nature Chemistry* **1**, 310-315 (2009).
- [4] "Controlling the Band Gap Energy of Cluster-Assembled Materials". S. Mandal, A.C. Reber, M. Qian, P.S. Weiss, S.N. Khanna, A. Sen. *Accounts of Chemical Research* **46**, 2385-2395 (2013).
- [5] "A Systematic Framework and Nanoperiodic Concept for Unifying Nanoscience: Hard/Soft Nano-Elements, Super Atoms, Meta-Atoms, New Emerging Properties, Periodic Property Patterns, Predictive Mendeleev-Like Nanoperiodic Tables", D. A. Tomalia and S. N. Khanna, *Chem. Rev.* **116**, 2705-2774 (2016).
- [5] "Strong lowering of ionization energy of metallic clusters by organic ligands without changing shell filling.", V. Chauhan, A.C. Reber, and S.N. Khanna. *Nature Communications* **9**, 2357 (2018).

References

1. *Kononov L.O.* RSC Adv. **5**(58), 46718-46734 (2015).
2. *Ghibaudi E., Cerruti L.* Found. Chem. **19**(2), 97-123 (2017).
3. *Xu R.R.* National Sci. Rev. **5**(1), 1 (2018).
4. *Burdge J.* Chemistry. / 2nd Ed. / N.Y.: The McGraw-Hill Companies, Inc.; 2011, p. 86.
5. UDC: Universal decimal classification. Standard edition. / 2 volumes / London: BSI; 2005.
6. *van der Asdonk P., Kouwer P.H.J.* Chem. Soc. Rev. **46**(19), 5935-5949 (2017).
7. *Mendeleev D.* Zh. Rus. Khim. Obshchestva. **1**(2), 60-77 (1869).
8. *Mendelejeff D.* Z. Chem. **12**, 405-406 (1869).
9. *Mallard E., Le Châtelier A.L.* Ann. Mines. **4**(5), 276-295 (1883).
10. *Mendelejeff D.* Ann. Physik. **214**(10), 230-279 (1869).
11. *Mendeleev D.I.* Investigation of aqueous solutions by specific weight. Saint-Petersburg: Tipografiya V. Demakova; 1887 (in Russian).
12. *Klyucharev V.V., Klyuchareva S.V.* J. Therm. Anal and Calorim. **119**(3), 1633-1651 (2015).
13. *Tretyakov Y.D.* Vysshee Obrazovanie v Rossii. (2), 47 (2002).
14. *Döbereiner J.W.* The elements of chemistry and stoichiometry. Jena: Cröker; 1819 (in German).
15. *Döbereiner J.W.* Pogg. Ann. **15**(2), 301-307 (1829).
16. *Mendeleeff J.* Chem. Soc. Trans. **55**, 634-656 (1889).
17. *Mendeleev D.I.* The principles of chemistry. / 8th Ed. / Saint-Petersburg: Tipo-litographiya M.P. Frolovoi; 1906 (in Russian).
18. *Imyanitov N.S.* Found. Chem. **18**(2), 153-173 (2016).
19. *Andriiko A.A., Lunk H.J.* ChemTexts. **4**, 4 (2018).
20. *Putz M.V.* Quantum nanochemistry. Volume II: Quantum atoms and periodicity. Oakville: Apple Academic Press, Inc; 2016.
21. Mendeleev to Oganesson. A multidisciplinary perspective on the periodic table. / *Scerri E., Restrepo G. (Eds.)* / N.Y.: Oxford University Press; 2018.
22. *Oganov A.R.* Faraday Disc. **211**, 643-660 (2018).
23. *Semenok D.V., Kvashnin A.G., Kruglov I.A., Oganov A.R.* J. Phys. Chem. Lett. **9**(8). 1920-1926 (2018).
24. *Fias S., Chang S., Anatole von Lilienfeld O.* J. Phys. Chem. Lett. **10**(1), 30-39 (2019).
25. *Brosi F., Vent-Schmidt T, Kieninger S., Schlöder T., Beckers H., Riedel S.* Chem. Eur. J. **21**(46), 16455-16462 (2015).
26. *Zhang Q.N., Hu S.X., Qu H., Su J., Wang G.J., Lu J.B., Chen M.H., Zhou M.F., Li J.* Angew. Chem. **55**(24), 6896-6900 (2016).
27. *Su J., Hu S.X., Huang W., Zhou M.F.* Sci. China Chem. **59**(4), 442-451 (2016).
28. *Hu S.X., Jian J.W., Su J., Wu X., Li J., Zhou M.F.* Chem. Sci. **8**(5), 4035-4043 (2017).
29. *Dingle A.* Nature Chem. **10**(5), 576 (2018).
30. *Johnson D.A., Nelson P.G.* Found. Chem. **20**(1), 15-27 (2018).
31. *Savin, V.D., Elyutin A.V., Mikhailova N.P.* Abstr. of 6th All-Russ. meeting "High temperature chemistry of silicates and oxides". Leningrad: Nauka; 1988, p. 174-176 (in Russian).
32. *Savin, V.D., Elyutin A.V., Mikhailova N.P., Eremenko Z.V.* Zh. Neorg. Khim. **33**(9), 2190-2195 (1988).
33. *Savin, V.D., Elyutin A.V., Mikhailova N.P., Eremenko Z.V., Opolchenova N.L., Stepareva N.N.* Tsvetnye Metally. (3), 76-82 (1989).
34. *Savin V.D., Elyutin A.V., Mikhailova N.P.* Tsvetnye Metally. (11), 74-79 (1989).
35. *Gorokh A.V.* Dokl. Akad. Nauk SSSR. **292**(3), 597-601 (1987).
36. *Gorokh A.V.* Dokl. Akad. Nauk SSSR. **318**(3), 581-585 (1991).
37. *Gorokh A.V.* Periodical system of chemical elements. Genetic aspect. Donetsk: DonFTI NANU. 2002 (in Russian).
38. *Wiese G., Böse D.* Z. Naturforsch. B. **27**(8), 897-902 (1972).
39. *Didyk Y.K.* Trudy NVII. (15), 37-62 (1973).

(YOUR LETTERHEAD)

Dec 23 2018

Prof. Haresh Lalvani
Director, Center for Experimental Structures
School of Architecture
Pratt Institute, Brooklyn,
New York, NY 11205

Dear Prof. Lalvani,

We are pleased to invite you to present your periodic table of chemical elements at **Mendeleev 150: 4th International Conference on the Periodic Table** endorsed by IUPAC (International Union of Pure and Applied Chemistry), to be held at ITMO University, Saint Petersburg, Russia, July 26-28, 2019.

This will be a very exciting event during the International Year of the Periodic Table (IYPT) to celebrate the 150th anniversary of the publication of Mendeleev's periodic table. We have organized leading experts and pioneers in the field and this will be a good opportunity for you to share your work with this community.

We hope you will be able to join us and look forward to seeing you in St Petersburg next July.

Sincerely,

Prof. Eric Scerri
Dept. of Chemistry and Biochemistry, UCLA
Organizer, Mendeleev 150

Sol-gel synthesis super active catalysts on core-shell organomodified silica

A.R. Latypova¹, M.D. Lebedev¹, E.A. Kopoleva¹,

Yu. S. Marfin¹, E.V. Romyantsev¹, A.V. Bykov², V.Yu. Doluda^{1,2}

¹*Ivanovo State University of Chemistry and Technology, Sheremetevsky ave.7, Ivanovo, Russian Federation*

²*Tver State Technical University, Nab. A. Nikitina 22, Tver, Russian Federation*

LatAdel@yandex.ru

Abstract: Obtain submicron and nanoscale particles it is one of the most important directions in materials. Based of them scientists create a new functional materials with adjusted structure and morphology parameters. In particular the nanoparticles of Pt and Cu groups the most widespread in applied catalysis. It is associated with catalytic properties of these chemical elements in different chemical process. However, the use of these nanoparticles in the native form does not seem appropriate because of the significant metal losses in the separation of the reaction products from the catalyst.

In this research is developing a method for synthesis composite materials of the core-shell type and organic modified silica particles. In case of core-shell particles the nickel was used as a magnetic core and silica as a shell. Silica particles were modified by aminopropyl- groups and the aminopropylthreemethoxysilane was used as precursor in sol-gel synthesis. The materials were obtained by sol-gel synthesis using the modified Schober method. For materials with a core-shell structure, the first stage was to obtain a suspension of nickel metal particles stabilized by cetyl trimethylammonium bromide. Synthesis of Pd based catalysts was made by precipitation of palladium hydroxide due to hydrolysis reaction by addition of 3 mM H_2PdCl_4 solution to a 1 gramm of support suspended in 40 ml aqueous solution of 0.1 M Na_2CO_3 . Obtained materials were studied by Fourier transform infrared spectroscopy, hydrogen pulse chemisorption, X-ray photoelectron spectroscopy and scanning electron microscopy.

Acknowledgements

This work is supported by the Russian Science Foundation grant №18-79-10157.

**The problem of "zero elements" in the works of D.I. Mendeleev.
Neutron matter and its place in the Periodic Table of Chemical Elements**

Ryazantsev G.B., Dr. Khaskov M.A., Prof. Dr. Lavrenchenko G.K., Prof. Dr. Beckman I.N.

Lomonosov Moscow State University, Moscow, Russia

All-Russian Institute of Aviation Materials, Moscow, Russia

Institute of Low-Temperature Energy Technologies, Odessa, Ukraine

anis-mgu@rambler.ru

D.I. Mendeleev wrote about the elements in front of hydrogen: *"The chosen subject long occupied my thoughts, but for various reasons I didn't want to talk about it, especially because those few clarifications that I thought could withstand criticism did not satisfy me, and I expected everything from the experiments with which I intended to continue my first attempts, answers that were more encouraging in the correctness of the born conclusions. However, the years went away, the more persistent ones were torn me off, and no one touched on a question that seemed burning to me, so I decided to say in relation to it what and how I can do, without pretending at all about his decision"*. Elements before hydrogen inevitably fall into the zero group. *"This position of argon analogs in the zero group is a strictly logical consequence of understanding the periodic law,"* stated D.I. Mendeleev. He allowed the existence of elements - X ("**newtonium**") and Y ("**coronium**") before hydrogen in the zero group. It should be recalled that Mendeleev had not been mistaken in his predictions of new elements! *"When I applied a periodic law to analogues of boron, aluminum and silicon, I was 33 years younger, I had complete confidence that sooner or later the foreseeable elements must certainly be justified, because everything was clearly visible to me there. Justification came sooner than I could have hoped. Then I did not risk, now I risk. This needs resoluteness. It came when I saw radioactive phenomena ... and when I realized that it was already impossible for me to postpone and that, perhaps, my imperfect thoughts would lead someone on a path more faithful than the possible one that seems to my weakening sight. "*

DI. Mendeleev did not have time to solve this problem, and his students and followers tried to forget this topic as "erroneous". It should be noted that after D.I. Mendeleev's question about "zero" elements was repeatedly raised by many authors both in the past and in the present centuries, however, for brevity, we only mention the very first and most famous ones: for example, Ernest Rutherford in 1920 and Andreas von Antropoff in 1926 as the designation for a hypothetical element with atomic number zero, which it placed at the beginning of the periodic table. A. Antropoff was the first to suggest the term "**neutronium**". Currently, neutron matter, like neutron stars, is a recognized reality in astro- and nuclear physics. Neutron matter from the standpoint of General chemistry can be classified as chemically simple (that is, it cannot be decomposed into simpler chemical means), then inevitably the question arises about the Element corresponding to it, and its place in the Periodic System. Based on the logic of the Periodic Law - (ordinal number - electric charge) - the ordinal number of neutron matter will correspond to zero, which makes us remember

a
n
d

d
e
v
e
l
o
p

t
h
e

***“Elementouch”* and three-dimensional periodic tables**

Yoshiteru Maeno

Department of Physics, Kyoto University, Kyoto 606-8502, Japan

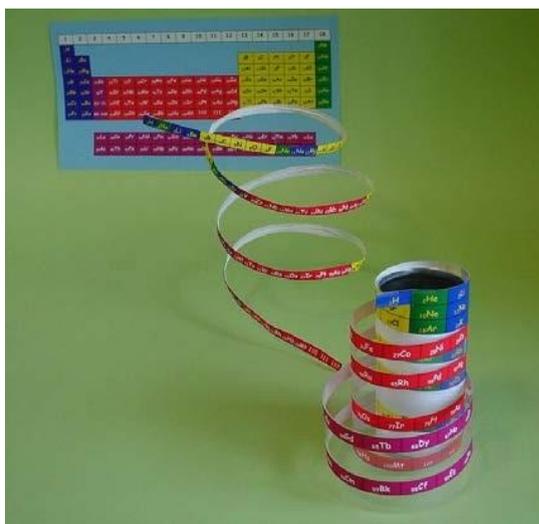
e-mail: maeno@scphys.kyoto-u.ac.jp

The arrangement in Mendeleev’s short-period periodic table of the elements reflects how each element forms oxides. In contrast, the long-period table widely used now expresses configuration of electron orbitals. It is introduced as early as in 1905 by a Swiss chemist, Alfred Werner [1]. In addition to many other variations of the periodic tables proposed, there have also been efforts to better represent the periodicity in three-dimensional forms. In this talk, I will briefly review these efforts to improve the periodic table since Mendeleev’s version, in special focus on the three-dimensional versions. I will then describe how the three-dimensional periodic table *“Elementouch”* can resolve some of the shortcomings of the widely-used Werner’s table [2]. Namely, (1) all the elements are arranged continuously, (2) electron orbitals can be visualized better, and (3) grouping of elements based on their chemical valences as in Mendeleev’s table is recovered.

[1] J. W. van Spronsen, “The periodic system of chemical elements”, Elsevier (1969).

[2] <http://www.ss.scphys.kyoto-u.ac.jp/elementouch/index.html>

Presented at Japanese Physical Society Meeting, March 24, 2002; and at American Physical Society Meeting, March 15, 2010.



日本物理学会誌

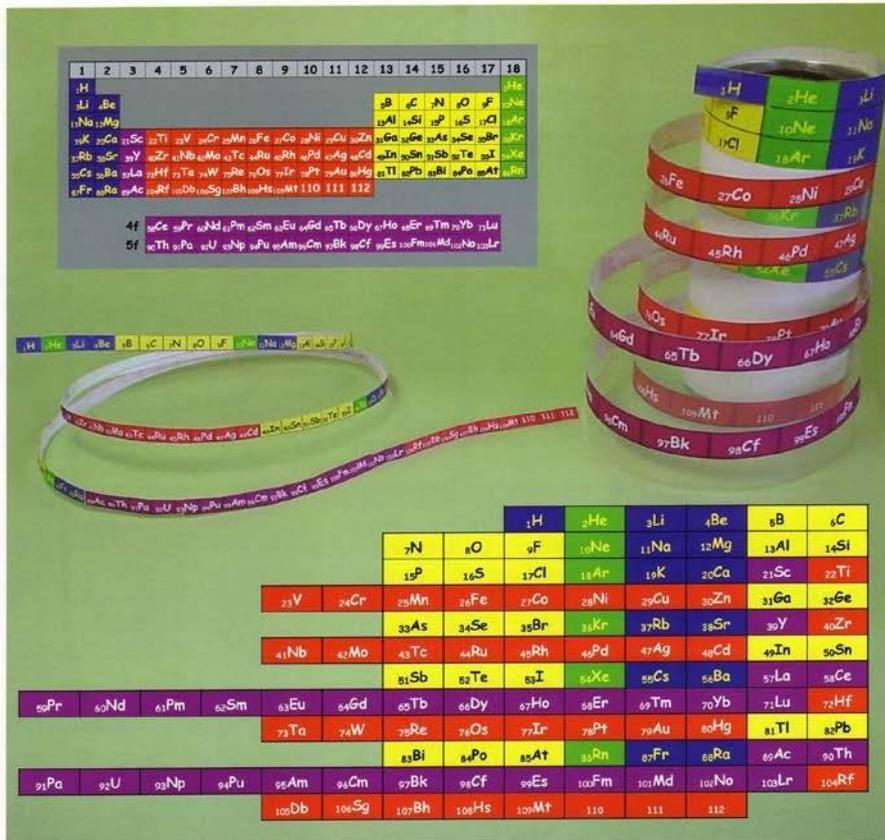
- X線による原始星の研究
- 複合ペロブスカイト酸化物の巨大圧電効果
- 高次元時空の世界から4次元時空の世界を眺める

BUTSURI

昭和30年6月13日 第3種郵便物認可
平成14年9月5日発行 毎月5日発行
第57巻 第9号 ISSN 0029-0181

2002 VOL. 57 NO.

9



<http://wwwsoc.nii.ac.jp/jps/>

Cover of "Butsuri", the JPS counterpart of "Physics Today" of APS.

Diamond — a modification of carbon with unique properties
Makogon A.I*^{1,2}, ***Balabanov S.V.¹, ***Perevislov S.N.***^{1,2}**

¹*Institute of Silicate Chemistry of the Russian Academy of Sciences*

²*Saint-Petersburg State Institute of Technology*

e-mail:makogon422833@gmail.com

Diamond is an allotropic modification of carbon, the mineral known first of all for its extremely high hardness ($H\mu = 80-100$ GPa). High hardness and fragility considerably limit possible scopes of materials based on diamonds.

According to periodic law properties and forms of compounds are in periodic dependence on the charge of nucleus. Both C and Si are elements of 14th group. They have some familiar properties. Their familiarities, predicted by periodic law, made it possible to create the unique material representing composition of diamond powder with various fractional structures and silicon carbide.

The silicon carbide also has unique properties, among them are low density and TEC ($\rho = 3,21$ g/sm³, $a = 3,4 \cdot 10^{-6}$ K⁻¹), high hardness ($H\mu = 31$ GPA), thermal stability and corrosion resistance and also it perfectly combines in contact with diamond. The most common form is α -SiC, with a Wurzite lattice, however in the context of this work a β -SiC interests us, which is a low-temperature form with a cubic lattice.

In this work used synthetic diamonds with sizes from 30 to 200 microns. Usage of powders of various fractional structure allows to consolidate preparations of materials to more dense state. At high-temperature impregnation of porous diamond preparation by fusion of liquid silicon the space between particles of diamond was filled β -SiC, formed in interaction of liquid silicon with carbon (a product of pyrolysis of organic binding).

In our work the original method of creating products on the basis of diamond powders is realized. It is shown that this material surpasses, on the level of mechanical properties, the majority of the known ceramics. It is offered to use the developed material as frictional units for pumps, sanding snuffles, shovels of gas-turbine engines, etc.

The research was made at the expense of a grant of the Russian scientific fund (project No. 17-13-01382).

Promoting Public Understanding of Periodic Table and Chemical Elements in IYPT
2019

Mei-Hung Chiu
National Taiwan Normal University
Graduate Institute of Science Education
mhchiu@gapps.ntnu.edu.tw

United Nations proclaimed the "International Year of the Periodic Table of Chemical Elements (IYPT2019)" to celebrate the 150th anniversary of discovery of the Periodic Table of Chemical Elements by Dmitri Mendeleev in 1869. It intends to recognize how the nature and properties of chemical elements contribute to change and enhance the life quality of humankind. The Periodic Table of Chemical Elements is considered as the totem of chemistry that many scientists contributed their wisdom and effort to this significant product for humankind. However, negative image the general public hold about chemistry, with connotations of toxicity, danger, or explosions, has prevented people from developing a better understanding and positive attitude towards a scientific/chemical view of their environment. To join the global event of IYPT, Taiwan has various celebratory activities on Periodic Table and Chemical Elements for school children, students, teachers, and the public. They are aimed to increase participants' cognition of chemistry, foster a positive attitude towards chemistry, and promote motivation and awareness of sustainability about chemistry. To provide different channels for conveying values and contributions of chemistry to citizen is the main design principle for IYPT 2019 activities and interventions.

Modification of natural polymer cellulose with metals of IB group

A. Mikhailidi¹, B.M. Tofanica², N. Kotelnikova³

¹St. Petersburg State University of Industrial Technologies and Design, St. Petersburg, Russia

²Gheorghe Asachi Technical University of Iasi, Iasi, Romania

³Institute of Macromolecular Compounds, Russian Academy of Sciences, St. Petersburg, Russia

Polymer nanocomposites which consist of metal (Me) nanophase dispersed in a polymer scaffold are one of the major application areas for nanoscale technology. The presence of the metal nanoparticles imparts electrical and magnetic properties to polymer nanocomposites. Last decades, the use of natural polymer cellulose to prepare biobased composites with transition metals was developed to prepare environmentally-friendly materials for various applications.

Transition metals attracted exceptional attention due to their high reactivity and specific properties. In our study we used the metals of IB group, i.e. semi-noble copper and noble silver and gold that exhibit oxidation states of +1, +2, and +3. According to the secondary periodicity, their properties within a subgroup vary, as follows: properties of gold are closer to these of copper than of silver.

Intercalation of copper, silver and gold into the cellulose matrix was carried out via two-stage process: diffusion of metal ions from aqueous solutions and their subsequent reduction. The process has resulted in intercalation of Me(0) nanoparticles to the cellulose. The type of cellulose matrices and the reducers strongly affected content of Me(0) in the composites (not exceeded 3 wt%).

The mechanism of redox reactions was proposed and the physico-chemical properties of the obtained nanocomposites were studied with a microscopy, WAXS, FTIR and XPS spectroscopy. The cellulose matrix served as a neutral nanoreactor and a stabilizer of non-aggregated Me(0) nanoparticles.

The modification of the cellulose support with the incorporated metal nanoparticles led to obtaining bionanocomposites with antibacterial and catalytic properties that offer novel advantageous opportunities for various applications.

THE PERIODICITY OF CHEMICAL ELEMENTS AND THE MATERIALS PERFORMANCE: A COMPLEMENT FOR THE COMPREHENSION OF THE PERIODIC TABLE.

Virginia E. Noval, José G. Carriazo y Manuel F. Molina C.

Departamento de Química, Facultad de Ciencias, Universidad Nacional de Colombia, Ciudad Universitaria, Carrera 30 No. 45-03, Bogotá, Colombia

e-mail: : venovall@unal.edu.co, jcarriazog@unal.edu.co, mfmolinac@unal.edu.co

The United Nations (UN) proclaimed 2019 as the International Year of the Periodic Table of Chemical Elements (IYPT 2019). For this reason, it is considered pertinent to highlight the importance of the periodic system in the scientific and technological development of chemistry; therefore, we carry out a discussion of some applications of the periodicity of the elements to design new materials. We discuss some periodic trends of molecules and complex structures of materials, by selecting different cases of chemical periodicity applied to improve and design steels with greater resistance to wear, prepare refractory materials and synthesize chalcogenide glasses, among others. We show that the periodic regularities observed in materials of interest are a consequence of the individual periodicity of the chemical elements. The periodicity in materials is highlighted as a complement to the understanding of the periodic table and it is considered appropriate to address the thematic nuclei related to molecular periodicity and its influence on the formation of clusters and nanoparticles, the influence of the variation of the atomic number of elements added in the grain boundaries of steels, the effect of periodicity in refractory materials, in the formation of chalcogenide glasses and in some materials based on coordination compounds. Finally, the proposed topics and the regularities discussed are considered complementary contexts of exceptional interest to motivate the significant learning of the periodic table taking into account current scientific and technological research.

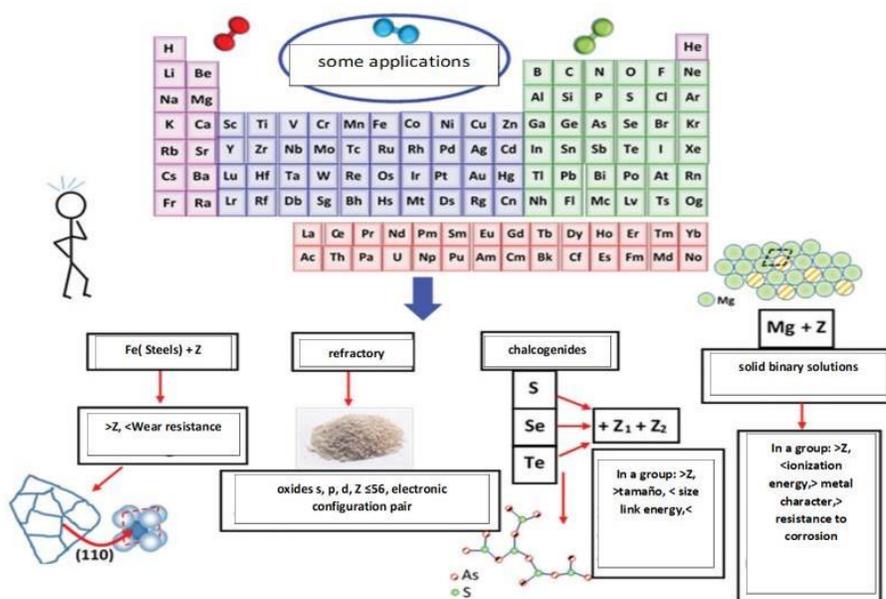


Figure 1. Some cases of chemical periodicity in materials

The chemical elements take a selfie!

Maristella Cestaro,^a Alessandra De Togni,^b Lucia Giuffreda,^c Rossella Romualdi,^d Marco Bortoli,^e
Marco Dalla Tiezza,^e Cecilia Muraro,^e Giovanni Parolin,^e Cristina Tubaro,^e Laura Orian^e

^a IIS 'Veronese- Marconi' – Sede associata di Cavarzere, via Tullio Serafin 15, 30014 Cavarzere (Ve), Italy.

^b IIS Ferraris-Fermi di Verona, Via del Pontiere 40, 37122 Verona, Italy.

^c IIS Duca degli Abruzzi, Via Merlin 1, 35143 Padova, Italy.

^d IIS 'Pacinotti' Chimica dei materiali articolazione Biotecnologie ambientali, via Caneve 93, 30173 Mestre (Ve), Italy.

^eDip. Scienze Chimiche Università degli Studi di Padova Via Marzolo 1 35131 Padova, Italy.

E-mail: cristina.tubaro@unipd.it, laura.orian@unipd.it

Almost 400 students of 25 secondary schools of our region have prepared an original periodic table, dressing like chemical elements, creating themed scenarios and finally taking pictures. Conceived for the web (<https://pls.scienze.unipd.it/tavolaperiodica/>), this creation, developed in the framework of a national educational project (Piano nazionale Lauree Scientifiche), aims at attracting young students and at divulging basic notions of the chemistry of the elements, which are present in our daily life or exist only for very short times in a lab.

Acknowledgements

Piano nazionale Lauree Scientifiche – Chimica (MIUR) is gratefully acknowledged for financial support to this project, which was developed by: Rosella Cavalcanti, Daniela Napoli, Annalisa Scalvi, Anita Paghera, Barbara Ballarini, Federica Stazi, Rita Mellere, Sandra Taschetti, Federica Dal Molin, Paola Baron Toaldo, Monica Vianello, Annalisa Piazzesi, Manuela Fistarol, Rossella Romualdi, Michela Cadorin, Laura Gianni, Roberta Predonzan, Mariapaola Colleselli, Lucia Pucci, Paola Meneghetti, Ornella Priolisi, Maristella Cestaro, Maria Rosa D'Acunto, Lucia Giuffreda, Riccardo Lambini, Carlo Santi, Marco Bortoli, Marco Dalla Tiezza, Cecilia Muraro, Giovanni Parolin, Cristina Tubaro, Laura Orian and ... the students of 25 schools of the Italian Veneto region.

Oxygen-containing derivatives of coumarins as biologically active compounds

Kinga Ostrowska

Medical University of Warsaw, Faculty of Pharmacy, Department of Organic Chemistry, Banacha 1, Warsaw 02-097, Poland

Oxygen is the most widespread element on Earth - the oxygen content in its shell is 46.4%. It is also a major component of the Earth's atmosphere and in the form of compounds with other elements it is part of the hydrosphere and lithosphere. Oxygen is the building block of many inorganic compounds, and organic compounds very often contain additional atoms of this element. Oxygen-containing heterocyclic compounds, including coumarins are an important class of natural compounds. Coumarin (*2H*-1-benzopyran-2-one) is a plant-derived natural product known for its pharmacological properties such as cytotoxic, antibacterial, antifungal, antimalarial, anti-tuberculosis, anti HIV and antitumor activities. Coumarin derivatives have drawn considerable attention from researchers due to their role in natural and synthetic organic chemistry, and their interesting biological activities. In the scientific literature there are many examples of coumarin-piperazine derivatives, especially with arylpiperazines linked to a coumarin system via an alkyl linker, that can modulate 5-HT, D and α_{1A} receptors. Numerous studies have revealed that the inclusion of a piperazine moiety could occasionally provide unexpected improvements in the bioactivity of various biologically active compounds. The piperazine analogs have been shown to have a potent antimicrobial activity and they can also act as BACE-1 inhibitors. On the other hand, arylpiperazines linked to a coumarin system have been shown to have antiproliferative activity against leukemia, lung, colon, breast, and prostate tumors. Recently, it has been reported that coumarin-piperazine derivatives exhibit a neuroprotective effect by their antioxidant and anti-inflammatory activities and they also show activity as acetylcholinesterase inhibitors and antifilarial activity. In view of the widespread interest in the activity spectrum and profile of coumarins and in continuation of our work on the synthesis of new compounds of pharmacological and biological interest we present the preparation and spectroscopic characterization of some new coumarin-piperazine derivatives as biologically active compounds.

Adventures Attempting to Synthesize Group 14, a Catorcane

Keith Pannell and Hemant Sharma

Department of Chemistry, The University of Texas at El Paso, El Paso, TX. 79968-0513, USA

Within the history of the Periodic Table of the Elements, Germanium, Ge, plays a pivotal rôle. In 1869, Mendeleev simply predicted a missing element, noted as eka-silicon (экасилиций), one place below Silicon, Si, in his Table of the elements. The discovery of Ge in 1886 cemented the scientific community's belief and pleasure in the Table. In our laboratory we have a focused interest on the chemistry of Ge along with that of its Group 14 partners, Si, Sn, and Pb. Since a characteristic of these elements is the concept of catenation, chain formation, we suggest that, alone in the Periodic Table of the elements, we should be able to synthesize Group 14 in the appropriate sequence, C-Si-Ge-Sn-Pb. We have synthesized, structurally characterized, and revealed the chemistry of many of the intra-group 14 element bonds. For example a range of Si-Si, Si-Ge, Si-Sn, Ge-Sn bonded materials, synthesized a molecule with a central C atom bonded to each of the other group 14 elements, and reported an 80% catorcane, C-Si-Ge-Sn. The final step of including a Sn-Pb bond is problematic; a possible solution will be discussed and presented.

Oligopyridine ligands with transition metal ions

Violetta Patroniak, Aleksandra Bocian, Adam Gorczyński, Marta Fik

Adam Mickiewicz University in Poznań, Umultowska 89b, 61-614 Poznań, Poland

E-Mail: violapat@amu.edu.pl

During the years, oligopyridine ligands like pyridines, bipyridines, terpyridines and quaterpyridines [1] were the subject of broad interest due to their coordination behavior, analytical chemistry and commercial purposes .

It has always been a challenge to create metal coordination complexes with unusual frameworks and controlled characteristics. The decisive role is played by the choice of the organic ligand with suitable distribution of the donor atoms that leads to the formation of the architectures with required structures and properties . The tpy ligands usually exhibit the meridional binding mode, thus surrounding the metal ion with three, near-coplanar nitrogen donor atoms in the all-*cisoidal* conformation.

Due to the applicative relevance of the tpy type ligands and the structural diversity of coordination compounds including 6,6''-dimethyl-2,2':6',2''-terpyridine **L**, there were chosen transition metal salts (Co(II), Au(III), Ag(I), Zn(II) and Cd(II)) and synthesised with characterization new coordination compounds, mostly with unexpected structure or characteristics. [2, 3, 4] Unusual assemblies were observed in the presence of Au(III) or Cd(II) salts, thus leading to compounds with full/partial protonation of ligand **L** or rare mixed solid state solutions, respectively. Luminescent properties of them were investigated. What is more, due to complexation with silver(I) ions there were obtained new fluorescent dinuclear double helicates with *in vitro* antiproliferative activity.

Acknowledgements:

This research was carried out as a part of the project No. 2016/21/B/ST5/00175 supported by Polish National Science Centre.

References:

1. A. Gorczyński, J. Harrowfield, V. Patroniak, A. R. Stefankiewicz, Chem. Rev., 116, 14620 (2016)
2. A. Bocian, D. Brykczyńska, M. Kubicki, Z. Hnatejko, M. Wałęsa-Chorab, A. Gorczyński, V. Patroniak, Polyhedron, 157,1,249 (2019)
3. M. A. Fik, A. Gorczyński, M. Kubicki, Z. Hnatejko, A. Fedoruk-Wyszomirska, E. Wyszko, M. Giel-Pietraszuk, V. Patroniak, Eur. J. Med. Chem., 86, 456 (2014)
4. A. Gorczyński, M. Zaranek, S. Witomska, A. Bocian, A.R. Stefankiewicz, M. Kubicki, V. Patroniak, P. Pawluć, Catal. Commun. 78, 71 (2016).

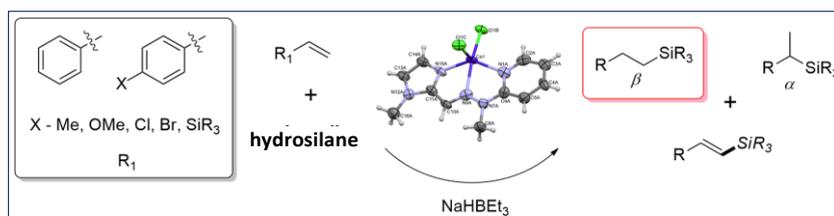
First-row transition metal complexes as an alternative for platinum group metal catalysts in hydrosilylation of olefins

*Piotr Pawluć, Maciej Skrodzki, Aleksandra Bocian, Aleksandra Skoczeń,
Maciej Zaranek*

*Adam Mickiewicz University in Poznań, Umultowska 89b, 61-614 Poznań, Poland
E-Mail: piotrpaw@amu.edu.pl*

Silicon compounds are used in many areas of economy and technology, from the most popular in cleaners, detergents, cosmetics, to more spectacular in medicine, electronics, car industry and airplane industry. Hydrosilylation is one of the most important catalytic reactions used in a large industrial scale for the synthesis and modification of silicon compounds.¹ The commonly used catalysts in this process are platinum compounds, however, high price of platinum and impossibility of its reuse in technological processes, have prompted us to search for alternative cheaper solutions, based on other elements, but of similar effectiveness.

An inspiration to solve this problem comes from the use of catalytic systems based on first-row transition elements (*3d* metals) such as iron,² cobalt³ and nickel⁴ that are more abundant in the nature. In the communication we present our results in the synthesis and application of new effective and selective catalytic systems for hydrosilylation of alkenes based on the *3d*-electron metals (Fe, Co, Ni) with the tridentate ligands of Schiff bases type and trialkylhydroborates of metals from group I of the periodic table ($M^I HBR_3$)⁵.



Acknowledgements:

This work was supported by The National Science Centre (Poland) under Grant no 2016/23/B/ST5/00177

1. B. Marciniak, H. Maciejewski, C. Pietraszuk, P. Pawluć, *Hydrosilylation: a Comprehensive Review on Recent Advances*, Springer, (2009)
2. M.D. Greenhalgh, A.S. Jones, S.P. Thomas, *ChemCatChem*, 7 (2015) 190.
3. J. Sun, L. Deng, *ACS Catal*, 6 (2016) 290.
4. Y. Nakajima, K. Sato, S. Shimada, *Chem. Record*, 16 (2016) 2379.
5. A. Gorczyński, M. Zaranek, S. Witomska, A. Bocian, A.R. Stefankiewicz, M. Kubicki, V. Patroniak, P. Pawluć, *Catal. Commun.* 78 (2016) 71.

Different Versions of the Periodic Table

K. PCHOLKINA, E. ALEKSANDROVA

Saint Petersburg State Institute of Technology (Technical University)

Abstract to the poster session

The first version of the Periodic table was proposed by D. I. Mendeleev in his "Fundamental Chemistry" in 1869. Now over 400 versions of the table are known. In this work the most interesting and improbable ideas of the scientists, who proposed their own design of the table, were examined.

The Periodic tables often differ in accommodation of separate groups of analogous elements and the way to display the Periodic law. In some of them the group of noble gases is placed in the right part, in others - in the left, in the third - in the middle of the table. There are tables, where the elements are located not according to the filling of electronic levels in atoms, but as consecutive arrangement in its left part the groups of s- and p-elements, in the right part - all groups of d- and f-elements. Sometime the first period is located at the bottom of the table, and over it the elements of subsequent periods; that symbolizes gradual complication of an electron shell of atoms are known. Authors of a number of tables divide the groups of elements into 3 or 4 subgroups, including f-elements in these additional subgroups.

However, the majority of these tables, highlighting the frequency of changes in these or other properties of elements and their connections, do not bring something essentially new in the design of the Periodic system. Changes of properties of the elements are connected with the structure of electron shell in atom, more precisely, with a capacity of electronic levels to be equal 8, 18 and 32. As a result, three main versions of the cellular image of a system dominate, when the elements are located according to the increase of atomic nucleus charge or number of electrons. Tables with 8-, 18- or 32-elements periods are the basis for their construction.

Role of Iron in Biological Systems

Elizaveta S. Perepelitca, Tatiana B. Lisitskaia

Saint Petersburg State Institute of Technology (Technical University)

Abstract to the poster session

Transition metals occupy a large section of the Periodic table. Several elements of this block are known to have biological functions. Iron is the most familiar example, as it is also known as one of the most common elements on Earth. Biological properties of iron are attributable to its redox abilities, wide range of oxidation states, and variety of coordination compounds. Those, conversely, can be explained by the electronic configuration of iron.

It is notorious that there are proteins and enzymes that contain iron, such as hemoglobin, cytochrome and catalase. They are used for vital processes, including oxygen transport and protection of the cell from oxidative damage.

Deficiency of this element or iron overdose have observable effect on human and animal health and can lead to various diseases. However, not only the higher organisms rely on iron. This metal is a critical nutrient for microorganisms or, more precisely, bacteria as well.

Bacteria utilize iron in two main metabolic processes: energy generation and anaerobic respiration.

Representatives of such genera of bacteria as *Thiobacillus* and *Leptospirillum* oxidize ferrous iron to produce energy. Iron-oxidizing bacteria typically proliferate in water bodies with massive concentrations of iron. These reservoirs can be highly polluted as a result of such bacteria's activities. Iron-oxidizing bacteria *Leptothrix*, *Sphaerotilus*, *Crenothrix*, *Gallionella*, *Siderocapsa* have a low catalase activity to enzymes and use iron to destroy excess of hydrogen peroxide.

Some of the other bacteria (for instance, *Geobacter metallireducens*) use iron for respiration instead of oxygen. These microorganisms metabolize organic matter and move electrons on ferric iron, carrying out a reducing reaction.

Moreover, magnetic properties of iron find a use in magnetotactic bacteria. Crystals of magnetite, that are present in such organisms are called magnetosomes. They act like compasses and allow bacteria to move along the lines of Earth's magnetic field.

Chemical Quest: general knowledge and popular culture quizzes about the elements in a board game for the class

Maristella Cestaro,^a Alessandra De Togni,^b Lucia Giuffreda,^c Rossella Romualdi,^d Marco Bortoli,^e
Marco Dalla Tiezza,^e Laura Orian^e

^a IIS 'Veronese- Marconi' – Sede associata di Cavarzere, via Tullio Serafin 15, 30014 Cavarzere (Ve), Italy.

^b IIS Ferraris-Fermi, Via del Pontiere 40, 37122 Verona, Italy.

^c IIS Duca degli Abruzzi, Via Merlin 1, 35143 Padova, Italy

^d IIS 'Pacinotti' Chimica dei materiali articolazione Biotecnologie ambientali, via Caneve 93, 30173 Mestre (Ve), Italy.

^eDip. Scienze Chimiche Università degli Studi di Padova Via Marzolo 1 35131 Padova, Italy

E-mail: laura.orian@unipd.it

Chemical Quest is an innovative trivia game based on the 102 elements of the periodic table from H to No, developed collaboratively by secondary school and university teachers with the aim of increasing the interest of young students in chemistry. As part of the project, a software version of the game was successfully played in 24 classes. 'Challenging, sometimes difficult, highly instructive, relaxing, captivating,' are some of the positive comments by students and teachers. In addition, Chemical Quest was conceived to be adaptable since the rules can be modified and the cards can be selected to match the educational objectives.

Acknowledgements

Piano nazionale Lauree Scientifiche – Chimica (MIUR) is gratefully acknowledged for financial support to this project, which was developed by: Antonella Balasso, Giovanni Carta, Maristella Cestaro, Viviana Colla, Alessandra De Togni, Giulio Gallani, Cristina Giacometti, Laura Gianni, Lucia Giuffreda, Manuela Granella, Marina Iarabek, Enrico Lion, Giuseppe Mazzi, Caterina Migale, Stefano Milan, Paola Molesini, Mara Moretto, Roberta Predonzan, Ornella Priolisi, Rossella Romualdi, Cristina Rubini, Sandra Scarfi, Elena Tobaldini, Marco Bortoli, Marco Dalla Tiezza, Enrico Nale, Massimo Bellanda, Gordon Kennedy, Gianpietro Sella, Laura Orian.

Process Orientated Guided Inquiry Learning (POGIL) in Qatar: A practitioner's perspective on students' engagement and learning of content relating to the Periodic Table

*Sheila Qureshi, Pre-medical Education,
Weill Cornell Medicine in Qatar (WCM-Q)*

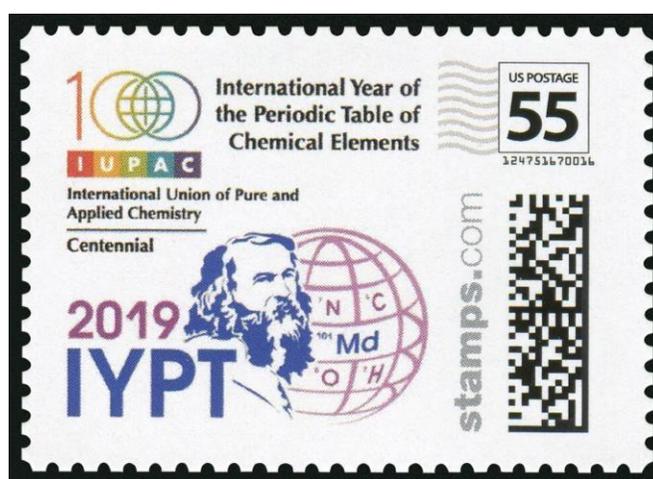
The aim of the poster is threefold: 1) it provides an introduction to Process Orientated Guided Inquiry Learning (POGIL) and opportunities for chemistry educators to explore the benefits of this approach to active learning in the general chemistry classroom; 2) it informs outcomes from a recently concluded chemistry education research project implemented in the foundation chemistry course at Weill Cornell Medicine in Qatar and selected high schools for students to develop key process skills such as teamwork, collaboration, and critical thinking, which foster lifelong learning skills; and 3) to show case POGIL activities related to the theme of the conference such as 'atomic structure', 'the periodic table', 'allotropy', 'the industrial importance of halogens and their compounds'. Most of these activities were written specifically for year 10 high school students and translated into Arabic in accordance with the Qatari curriculum. Students found some of these topics challenging and it helped engage their interest in chemistry. This poster further incorporates a POGIL practitioner's reflections on the development and utilization of highly structured learning materials (focusing concepts relevant to item #3).

Hydrogen to Oganesson: A Philatelic Tour of the Periodic Table

Daniel Rabinovich

ABSTRACT

The International Year of the Periodic Table of the Chemical Elements (IYPT), which marks the sesquicentennial of its introduction by Dmitri Mendeleev in 1869, can be celebrated in many ways. A key goal of these endeavors is to highlight the contributions of chemistry to society while introducing the general public to the history and value of the periodic table, perhaps the most recognizable symbol of the central science. This presentation will rely on the use of postage stamps to illustrate some of the most interesting aspects of the development of the periodic table and the discovery of several chemical elements. For example, stamps have been issued in France, Portugal, Germany, and other countries to recognize earth, water, air and fire, *i.e.*, the four classical elements in Greece. The work of several alchemists has also been depicted on stamps, including the successful isolation of elemental phosphorus by Hennig Brand 350 years ago (1669). This presentation will showcase several scientists who contributed to the development of the modern periodic table (Döbereiner, Gmelin, Mendeleev) and the discovery of various chemical elements (Berzelius, Davy, Gadolin, Marie Curie, Scheele, Vauquelin). Even some of the most recent additions to the periodic club, such as flerovium, nihonium, and oganesson, have been honored with postage stamps, which will also be briefly described in this presentation.



The Accumulation of Heavy Metals in Microorganisms

A. A. Romanova, M. M. Shamtsyan

Saint Petersburg State Institute of Technology (Technical University)

Abstract to the poster session

The ability of microorganisms to accumulate heavy metals and the use of this quality in the industry was reviewed in this work. The biotechnological industry is quickly developing.

There are 90 chemical elements in the nature, 53 of which are heavy metals. With the exception of noble metals, these include metals with a density of $8 \cdot 10^3 \text{ kg / m}^3$ and more. In very low concentrations, heavy metals have a beneficial effect.

Heavy metals Cd, Hg, Zn, Ni, Cu, Pb belong to the group of toxic, but to feel their toxic effects on the organism, it is necessary that the concentration of their ions reaches at least 1 nMol/l .

It is interesting to notice that all these toxic elements occupy the positions of transition metals in the Periodic table. Their toxicity is related to their variable degrees of oxidation.

For almost all d-elements, which have 2 valence electrons on the external ns-sublevel, the oxidation state is +2. Starting with the d-elements of Group III of the Periodic System, the elements in the lowest oxidation state form demonstrate the basic properties in their compounds, in the highest - acidic, in the intermediate - amphoteric.

Microorganisms are able to accumulate heavy metals and can passivate their ions. Bio-accumulators of heavy metals, in addition to some active strains of bacteria, are also mushrooms and algae. The issues of bioremediation of polluted soils and biological wastewater treatment are the subject of environmental biotechnology. The concentration of heavy metals in nature is quite low, so the use of bacteria that accumulate them is much more beneficial. Polymetallic ores that are in no use in metal mining may be employed.

It is cheaper to leach metals from ores than to obtain them by traditional methods, as it is quite enough natural conditions for the work of bacteria. The speed of microbial enzymes is much higher. This is an environmentally safe production, which also eliminates the adverse effects of metallurgical production: dumps of substandard and poor breeds.

Microorganisms have great potential both in metallurgy and environmental remediation.

Three-dimensional (3-D) version of the Periodic system of chemical elements: Mendeleev's Flower

Ryazantsev G.B., Dr. Khaskov M.A., Prof. Dr. Lavrenchenko G.K., Prof. Dr. Beckman I.N.
Lomonosov Moscow State University, Moscow, Russia
All-Russian Institute of Aviation Materials, Moscow, Russia
Institute of Low-Temperature Energy Technologies, Odessa, Ukraine
anis-mgu@rambler.ru

A three-dimensional version of the Periodic System (PS) of chemical elements is proposed. It is based on the early works of Russian and French scientists: Mendeleev and de Chancourtois, while preserving the idea of consistency and continuity of a number of chemical elements. The resulting system resembles a "flower" with petals, which are elements with a certain orbital quantum number. The historical sequence of development of the idea of the spatial representation of PS chemical elements and the contribution of various authors are considered. D.I. Mendeleev was the true discoverer of the Periodic Law (PL) precisely because he first saw in it the Fundamental law of nature, and not just the formal system of classification of chemical elements that existed already long before him. Moreover, the idea of the periodicity of elements itself was known before. He felt the unity of the elements and forces of the Nature in the PL, and therefore the PS displaying the PL should have been a single whole, organically linking empirically isolated elements. According to the logic of the development of science at that time, it was quite natural that the PS could graphically be represented as the Periodic Table (PT). D.I. Mendeleev, strictly following to the principle of consistency and continuity, did so, and the first PTs were built. One can confidently say, that the principle of consistency and continuity at that moment was the main Heuristic principle in the work of a scientist, which can be also named as the principle of integrity.

And this principle brought overwhelming success and worldwide recognition to D.I. Mendeleev and to the PL. Since, according to the Mendeleev's belief, the PS is a single organically connected whole, any omissions and voids between the elements are absolutely unacceptable. It can be argued that Dmitry Ivanovich felt that the "infinity" of the PL cannot be adequately (strictly following the principles of consistency and continuity) expressed in a flat rectangular PT. The scientist foresaw that "... the system requires a bodily form that allows for approaching from all directions." The spatial spiral shape was first proposed by the French scientist Alexander Emile de Chancourtois, one of the predecessors of D.I. Mendeleev in the discovering of the PL. It should be noted that after de Chancourtois many prominent scientists spoke and wrote about the volumetric form of PS. For example, academician A. Fersman proposed to erect a monumental monument (in the form of a spatial spiral) to both the PS and D.I. Mendeleev. The legendary physicist George Gamow used the spatial form of PS in his popular books on science. This spatial form was patented by Roy Alexander. The model proposed in this work, in principle, is similar to the models of Gamow and Alexander, but there are certain differences: the s- and p- elements form separate independent petals (the previous authors combined them into one cylinder) and all the petals extend from the same axis (the lines "growth"). The volumetric model of PS can be performed in various versions and can be

r
e
c
o
m
m
e
n
d
e
d

a

Abstract for an invited talk at
Mendeleev 150: 4th International Conference on the Periodic Table
Sankt-Peterburg, Russia, 2019 July 26-28 (Fr-Su)

"Physical explanation of horizontal and vertical periodicities in the system of elements"

W. H. Eugen Schwarz* and Jun Li

Theoretical Chemistry Center, Tsinghua University, Beijing, China

Chemistry Department, Southern University of Science and Technology, Shenzhen, China

Chemistry Department, University of Siegen, Germany

eugen.schwarz@uni-siegen.de, junli@tsinghua.edu.cn

Half a century after experimental realization (Lavoisier) of the modern concept of chemical elements (Boyle), the then verified half a hundred of elements were ordered empirically (Gmelin): the unique elements H, N, O; the different groups of electronegative halogens, chalcogens, pnictogens and the electronpositive alkali, alkaline earth and earth metals; and the large group of rather similar transition metals. The first complete Periodic Table, designed by MENDELEYEV one and a half centuries ago followed this pattern by cutting the continuous array of elements (Cannizzaro) between the most different groups of halogens and alkali metals and placing them at the edges with the more similar elements in the broad center, as supported by numerical plots of properties (Lothar Meyer).

The strong variations of properties from the halogens to the noble gases to the alkali metals fixing the *Horizontal Principal Periodicity*, and the non-smooth variation of properties down from period to period defining the *Vertical Secondary Periodicity*, have both their physical origin in the peculiar pattern of atomic orbital *energies and radii* that are determined by idiosyncratic quantum mechanics and Pauli exclusion principle through atomic number governing nucleus-electron and electron-electron interactions. Formal Janet-Madelung-Klechkowski rule does not provide physical rationalization. The qualitative trends can be explained however on general physical grounds, while the quantitative details that produce the qualitative pattern are due to the numerical orbital values that can be deduced from experimental measurement or quantum theoretical calculation. It is typical for any complex field of reality that the full details cannot be completely reproduced or even understood from paper and pencil models only.

Synthesis of E, E-4- [4- (4-aminophenyl) buta-1,3-dienyl] aniline and its ability to modify silver nanoparticles, studied using SERS

Aleksei A.N., Odintsova O.V., Solovyeva E.V.

Saint Petersburg State University, Saint Petersburg, Russia
Student
alexnicksmirnow@gmail.com

The properties of noble metals, which distinguish this group from others, are very remarkable, and one of the most unusual is their ability to exist in a colloidal form in the form of pure metal nanoparticles. Despite the fact that Faraday first described this phenomenon about 150 years ago, there is now a new surge of scientific interest in these systems (Faraday, 1857.). For example, silver nanoparticles can serve as a substrate that demonstrates the characteristics of plasmon resonance, which opens up the possibility of assembling sensitive optically active materials after modification with the corresponding compounds.

This report is dedicated to the developed synthetic route of obtaining 4-[4-(4-aminophenyl)buta-1,3-dienyl]aniline (DABUDEN) from simple compounds and its ability to serve as the plasmon substrates modifier. This work is part of the bigger project, dedicated to the obtaining and investigation of nanostructures, obtained by interaction of aminostilbene derivatives with silver nanoparticles in hydrosol. We already demonstrated the ability of 4,4'-diaminostilbene to chemically adsorb on the silver surface in such systems, which leads to the great enhancement of Raman signal (Solovyeva et. al, 2018.). Moreover it is able to serve as the «molecular linker» between two different nanoparticles. We were interested in studying the dependence of the morphology of the obtained adsorption layers on the length of the conjugation between the phenyl rings. The compound of interest, DABUDEN, according to literature data was obtained only once from non-common components, so we decided to find simple way of synthesis. Despite the fact that our method consists of eight stages it has relatively high yield in virtue of applying of convergent pathway and don't require any special conditions except photoisomerisation of the final product. This compound was investigated by SERS in silver hydrosol and the results are comparable with our previous study.

Faraday, M. 1857. *Philos. Trans. R. Soc. London*, 147, 145–181.

Solovyeva, E. V., Ubyivovk, E. V. and Denisova, A. S. 2018. *Colloids Surfaces A Physicochem. Eng. Asp.* Elsevier, 538, 542–548.

HIGH TEMPERATURE BEHAVIOR OF HAFNATE SYSTEMS ACCORDING TO D.I. MENDELEEV PREDICTION

V.L. Stolyarova

*Saint Petersburg State University, Universitetskaya nab. 7/9, Saint Petersburg, 199034, Russia
v.stolyarova@spbu.ru*

Oxide ceramics based on hafnium and rare-earth oxides are extremely promising for development of high temperature materials of new generation for aircraft and aerospace engineering, for nuclear applications, for thermal barrier coatings and casting molds for gas turbine engine blades, since substitution of zirconia by hafnia in traditionally applied ZrO_2 -based materials allows their working temperature ranges to be increased significantly. Review on the available experimental data on vaporization processes and thermodynamic properties of binary and ternary hafnia and rare-earth oxide containing systems obtained at the temperatures up to 3000 K by Knudsen effusion mass spectrometric method is presented.

Vaporization regularities of hafnia and rare-earth oxide containing systems are considered according to the features of electronic structure and position of rare-earth element in the D.I. Mendeleev Periodic Table. This analysis allows predicting the features of vaporization of unstudied systems as well as thermodynamic behavior.

Thermodynamic data found in these systems were discussed using acid-base concept of vaporization of oxide systems considered in details earlier [1]. This approach allows to predict and to identify the ternary hafnia-containing system as the most suitable for development of refractory materials [2]. The results obtained in the present study enable one to choose the optimal compositions of ceramics for production of thermal barrier coatings with enhanced performance capacities, to find the least volatile concentration ranges in the systems studied for development of synthetic and application routes of the refractory materials and to derive the comprehensive thermodynamic description of the systems using various model approaches.

Acknowledgements The financial support of the present study was carried out by the Russian Foundation for Basic Research according to Project No. 19-03-00721.

- [1] V.L. Stolyarova and G.A. Semenov, *Mass spectrometric study of the vaporization of oxide systems*, 1994, 494, Wiley&Sons, Chichester, Great Britain.
- [2] V.L. Stolyarova, V.A. Vorozhtcov and S.I. Lopatin, *Trudy Kolyskogo Nauchnogo Tcentra RAN*, 2018, 9, 104.

HIGH TEMPERATURE BEHAVIOR OF HAFNATE SYSTEMS ACCORDING TO D.I. MENDELEEV PREDICTION

V.L. Stolyarova

*Saint Petersburg State University, Universitetskaya nab. 7/9, Saint Petersburg, 199034, Russia
v.stolyarova@spbu.ru*

Oxide ceramics based on hafnium and rare-earth oxides are extremely promising for development of high temperature materials of new generation for aircraft and aerospace engineering, for nuclear applications, for thermal barrier coatings and casting molds for gas turbine engine blades, since substitution of zirconia by hafnia in traditionally applied ZrO_2 -based materials allows their working temperature ranges to be increased significantly. Review on the available experimental data on vaporization processes and thermodynamic properties of binary and ternary hafnia and rare-earth oxide containing systems obtained at the temperatures up to 3000 K by Knudsen effusion mass spectrometric method is presented.

Vaporization regularities of hafnia and rare-earth oxide containing systems are considered according to the features of electronic structure and position of rare-earth element in the D.I. Mendeleev Periodic Table. This analysis allows predicting the features of vaporization of unstudied systems as well as thermodynamic behavior.

Thermodynamic data found in these systems were discussed using acid-base concept of vaporization of oxide systems considered in details earlier [1]. This approach allows to predict and to identify the ternary hafnia-containing system as the most suitable for development of refractory materials [2]. The results obtained in the present study enable one to choose the optimal compositions of ceramics for production of thermal barrier coatings with enhanced performance capacities, to find the least volatile concentration ranges in the systems studied for development of synthetic and application routes of the refractory materials and to derive the comprehensive thermodynamic description of the systems using various model approaches.

Acknowledgements The financial support of the present study was carried out by the Russian Foundation for Basic Research according to Project No. 19-03-00721.

- [1] V.L. Stolyarova and G.A. Semenov, *Mass spectrometric study of the vaporization of oxide systems*, 1994, 494, Wiley&Sons, Chichester, Great Britain.
- [2] V.L. Stolyarova, V.A. Vorozhtcov and S.I. Lopatin, *Trudy Kolyskogo Nauchnogo Tcentra RAN*, 2018, 9, 104.

A.S. Terteryan, D.I. Mustafin
Mendeleev University of Chemical Technology of Russia
UNESCO department "Green chemistry for sustainable development", Moscow
dmustafin@hotmail.com

NEW VERSION OF THE PERIODIC TABLE OF D.I. MENDELEYEV

The Periodic Table by D.I. Mendeleev gives us chance to understand the idea of regularity and also understanding of what has to be the idea of display of this regularity. D.I. Mendeleev, of course, understood that time will enter amendments into its system. We made such attempt of its development and constructed the table based on the new data obtained by chemists and physicists. At the same time were used the following parameters:

1) number of electronic level (the period, - the amount of the periods is equal to eight);
2) number or a symbol of a sublevel (is a group -the number of groups is equal to four - s, p, d, f); 3) the power sequence of atomic orbitals which, as we know, has the following appearance: 1s,2s,2p,3s,3p,4s,3d,4p,5s,4d,5p,6s,4f,5d,6p,7s,5f,6d,7p,8s. As a result we received essentially new configuration of the table, surprisingly harmonious, complete, symmetric, and, after all, mathematically reasonable. Besides, the discrepancy of borders of the periods with borders of consecutive electron shells (which were revealed by N. Bohr) as it appeared, has the strict sequence and frequency. As for lanthanides and actinoids, they were logically built in the table. And almost complete symmetry allows to draw a conclusion about it almost completeness.

А.С.Тертерян, Д.И.Мустафин
Российский химико-технологический университет имени Д.И.Менделеева
Кафедра Юнеско «Зеленая химия для устойчивого развития», Москва
dmustafin@hotmail.com

НОВАЯ ВЕРСИЯ ПЕРИОДИЧЕСКОЙ СИСТЕМЫ ХИМИЧЕСКИХ ЭЛЕМЕНТОВ Д.И. МЕНДЕЛЕЕВА

Открытие Д. И. Менделеевым Периодической системы химических элементов даёт нам шанс понять саму идею закономерности, а также понимание того, какова должна быть идея отображения этой закономерности. Д. И. Менделеев, конечно, понимал, что время будет вносить коррективы в его систему. Мы предприняли такую попытку её развития и построили таблицу, основанную на новых данных, полученных химиками и физиками. При этом нами были использованы следующие параметры: 1) номер электронного уровня - это период (количество периодов равно восьми); 2) номер или символ подуровня - это группа (количество групп равно четырём - s,p,d,f); 3) энергетическая последовательность атомных орбиталей, которая, как известно, имеет следующий вид: 1s,2s,2p,3s,3p,4s,3d,4p,5s,4d,5p,6s,4f,5d,6p,7s,5f,6d,7p,8s. В результате нами получена принципиально новая конфигурация таблицы, удивительно стройная, целостная, симметричная, и, к тому же, математически обоснованная. Кроме того, несовпадение границ периодов с границами последовательных электронных оболочек, которые выявил Н. Бор, как оказалось, имеет строгую последовательность и периодичность. Что касается лантаноидов и актиноидов, то они оказались логически встроенными в саму таблицу. А практически завершённая симметричность позволяет сделать вывод о её почти завершённости.

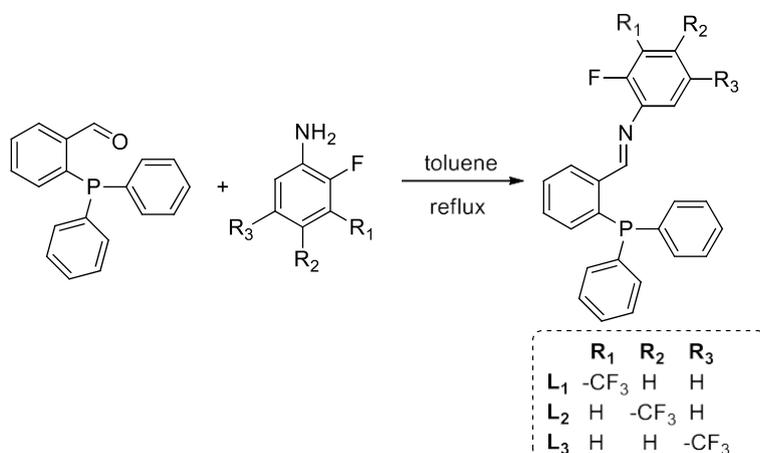
TWO DONOR ATOMS: “P” AND “N”

Burcu Tezcan, Saliha Baran, Bilgehan Güzel

*Chemistry Department, Çukurova University, 01330, Adana, Turkey
burcudarendeli@gmail.com*

The bidentate and polydentate phosphines are important ligands in coordination chemistry and homogeneous catalysis. The most important and widely used of heterodentate ligands are those which bear phosphorus and nitrogen as their donor atoms. The π -acceptor character of the phosphorus can stabilize a metal center in a low oxidation state, while the nitrogen σ -donor ability makes the metal more susceptible to oxidative addition reactions¹. This combination can help to stabilize intermediate oxidation states or geometries which form during a catalytic cycle.

Also, bonding the phosphorus directly to a more electronegative atom such as oxygen or nitrogen will lessen its electron-donating ability while also enhancing its π -acceptor capacity. Alternatively, the presence of an imino group rather than an amino group will result in a nitrogen donor atom of greater σ -donating capabilities and this will result in a greater electronic disparity between the donor atoms. According to this information, in this study, three different PN-type (imine N donor and phosphine P donor) ligands were synthesized for utilizing them as a catalyst in C-C coupling reactions (Scheme 1).



Scheme 1: Structures of PN-type ligands

References:

1. Guiry, P. J.; Saunders, C. P., *Advanced Synthesis & Catalysis* **2004**, 346 5, 497-537.

Acknowledgment

This work was supported by the Scientific Research Projects Program (BAP No: FBA-2018-10690), Çukurova University, Turkey.

Third-generation periodic table of elements

<u>G</u> 1	<u>G</u> '	<u>G</u> '1	<u>G</u> '2	<u>G</u> '3	<u>G</u> '4	<u>G</u> '5	<u>G</u> "	1 <u>G</u> '	2 <u>G</u> '	3 <u>G</u> '	4 <u>G</u> '	5 <u>G</u> '	6 <u>G</u> '	7 <u>G</u> '	8 <u>G</u> '	9 <u>G</u> '	<u>G</u> '	1,1 <u>G</u> '	2,1 <u>G</u> '	3,1 <u>G</u> '	4,1 <u>G</u> '	5,1 <u>G</u> '	6,1 <u>G</u> '	7,1 <u>G</u> '	8,1 <u>G</u> '	9,1 <u>G</u> '	10,1 <u>G</u> '	11,1 <u>G</u> '	12,1 <u>G</u> '	13,1 <u>G</u> '	1 <u>G</u> '	
<u>U</u> 1	<u>U</u> '																															
<u>B</u> 1 francium	<u>B</u> ' radium	<u>B</u> '1 nihonium	<u>B</u> '2 flerovium	<u>B</u> '3 tennessine	<u>B</u> '4 oganeson	<u>B</u> '5 tennessine	<u>B</u> " oganeson																									
<u>T</u> 1 caesium	<u>T</u> ' barium	<u>T</u> '1 thallium	<u>T</u> '2 lead	<u>T</u> '3 bismuth	<u>T</u> '4 polonium	<u>T</u> '5 astatine	<u>T</u> " radon	1 <u>B</u> ' actinium	2 <u>B</u> ' thorium	3 <u>B</u> ' protactinium	4 <u>B</u> ' thorium	5 <u>B</u> ' protactinium	6 <u>B</u> ' thorium	7 <u>B</u> ' protactinium	9 <u>B</u> 1 actinium	<u>B</u> 1 actinium	<u>B</u> ' actinium															
- <u>Q</u> 1 rutherfordium	- <u>Q</u> ' rutherfordium	<u>Q</u> '1 indium	<u>Q</u> '2 tin	<u>Q</u> '3 antimony	<u>Q</u> '4 tellurium	<u>Q</u> '5 iodine	<u>Q</u> " xenon	1 <u>T</u> ' lanthanum	2 <u>T</u> ' cerium	3 <u>T</u> ' praseodymium	4 <u>T</u> ' neodymium	5 <u>T</u> ' promethium	6 <u>T</u> ' europium	7 <u>T</u> ' gadolinium	9 <u>T</u> 1 platinum	<u>T</u> 1 gold	<u>T</u> ' mercury	2 <u>B</u> ' thorium	2,1 <u>B</u> ' thorium	3,1 <u>B</u> ' protactinium	4,1 <u>B</u> ' thorium	6, <u>B</u> ' plutonium	7, <u>B</u> ' americium	7,1 <u>B</u> ' curium	9, <u>B</u> ' berkelium	10, <u>B</u> ' californium	11, <u>B</u> ' einsteinium	12, <u>B</u> ' fermium	13, <u>B</u> ' mendelevium	<u>B</u> ' nobelium	1 <u>B</u> ' actinium	
- <u>q</u> 1 actinium	- <u>q</u> ' calcium	<u>q</u> '1 gallium	<u>q</u> '2 zinc	<u>q</u> '3 arsenic	<u>q</u> '4 selenium	<u>q</u> '5 bromine	<u>q</u> " krypton	1 <u>Q</u> ' yttrium	2 <u>Q</u> ' zirconium	4 <u>Q</u> 1 niobium	5 <u>Q</u> 1 molybdenum	5 <u>Q</u> ' niobium	7 <u>Q</u> 1 rhenium	8 <u>Q</u> 1 rhenium	<u>Q</u> actinium	<u>Q</u> 1 silver	<u>Q</u> ' cadmium	1,1 <u>T</u> ' cerium	3,1 <u>T</u> ' praseodymium	4,1 <u>T</u> ' neodymium	5,1 <u>T</u> ' promethium	6, <u>T</u> ' europium	7,1 <u>T</u> ' gadolinium	9,1 <u>T</u> ' terbium	10,1 <u>T</u> ' dysprosium	11,1 <u>T</u> ' holmium	12,1 <u>T</u> ' erbium	13,1 <u>T</u> ' thulium	<u>T</u> ' ytterbium	1 <u>T</u> ' lutetium		
<u>t</u> 1 sodium	<u>t</u> ' magnesium	<u>t</u> '1 aluminium	<u>t</u> '2 silicon	<u>t</u> '3 phosphorus	<u>t</u> '4 sulfur	<u>t</u> '5 chlorine	<u>t</u> " argon	1 <u>q</u> ' lanthanum	2 <u>q</u> ' cerium	3 <u>q</u> ' praseodymium	5 <u>q</u> 1 molybdenum	5 <u>q</u> ' niobium	6 <u>q</u> ' iron	7 <u>q</u> ' cobalt	8 <u>q</u> ' nickel	9 <u>q</u> ' copper	<u>q</u> ' zinc															
<u>b</u> 1 lithium	<u>b</u> ' beryllium	<u>b</u> '1 boron	<u>b</u> '2 carbon	<u>b</u> '3 nitrogen	<u>b</u> '4 oxygen	<u>b</u> '5 fluorine	<u>b</u> " neon																									
<u>u</u> 1 hydrogen	<u>u</u> ' helium																															

Key –

1. Core of code = u and U represent uni i.e. s subshell, b and B represent bi i.e. s and p subshells, t and T represent tri i.e. s, p and d subshells and q and Q represent quad i.e. s, p, d and f subshells.
2. Any number at Immediate left, left, right and immediate right position with receptive to core represent that number of electrons in (P-2)f, (P-1)d, (P)s and (P)p subshell respectively.
3. Comma in a code is for presence of (P-2)f and (P-1)d subshells while hyphen is for presence of (P-1)d subshell.
4. Inverted comma in a code at immediate left, left, right and immediate right position with respect to core represents filled (P-2)f, (P-1)d, (P)s and (P)p subshell respectively.

Influence of Element Position in Periodic Table on Its Properties.

S. TIKHANOVA, E. ALEKSANDROVA

Saint Petersburg State Institute of Technology (Technical University)

Abstract to the poster session

According to the Periodic law, proposed by D. I. Mendeleev in 1869, the position of each element in the Periodic table is determined by its electronic structure and influences the chemical properties.

In the secondary subgroup of the VIII group of the Periodic system, there are nine elements: iron, cobalt, nickel, ruthenium, rhodium, palladium, osmium, iridium, platinum. Elements of this group are similar to each other in the same period and form so-called triads. The elements iron, cobalt and nickel form an iron group, and the remaining elements of group VIII form the groups of palladium and platinum.

The iron group is unique, since none of its elements forms compounds of oxidation state + 8, appropriating the group number, that feature can be considered exceptional. This oxidation state is achieved only for two elements of the group, ruthenium and osmium located under the iron in the Periodic table (in RuO_4 [1], OsO_4 for example). For the others, the oxidation states + 2 and +3 are the most stable, and for nickel and cobalt, the oxidation state + 2 is the most typical.

Inability to form compounds in oxidation state + 8 is explained by the kaysymmetry[2] of the 3d shell for the elements in the iron group and the consequent increased strength of the interaction between electrons and the nucleus. In addition, due to the increase of electrons number at d-sublevels, the increase in the level stability occurs, which explains inability to form compounds in the highest oxidation state.

Finally, we can say that despite the existence of exceptions, the regularities laid down by the Periodic law are also observed in the eighth group, since ruthenium and osmium exhibit the highest degree of oxidation.

1. Vorobiev, A. F., General and Inorganic Chemistry. Vol. 1. Theoretical Foundations of Chemistry / A.A. F. Vorobiev, N. T. Kuznetsov, A. Yu. Tsivadze and others. - ICC Academicbook Moscow, 2004. - 373 p.

2. Shukarev, S. A. Inorganic chemistry: a textbook for universities in 2 tons. T. 2. / S. A. Shukarev. - M.: High School, 1974. - 382

The rise (and no sign of fall) of Ruthenium

Ruthenium, which original name comes from Ruthenia, the Latin word for Rus/Russia, was an element with obscure use for the large parts of the 19th century. That has rapidly changed with the rise of electronics and, more recently, when its amazing catalytic properties have been discovered. Today it's hard to imagine the 21st century catalysis without Ruthenium, which plays a vital role in such different processes as asymmetric hydrogenation (Nobel Prize in chemistry in 2001), olefin metathesis (Nobel Prize in chemistry in 2005) and C-H activation. The best part – it's just getting started, as the number of ruthenium complexes, particularly with the emerging carbenes, the ideal counterpart for catalysis, is growing exponentially. In this presentation I'll give a short overview of this fascinating element and the latest trends in ruthenium chemistry.

Maria Vinogradova (scicom.ru)

Cosmogonic way of Periodic Mendeleev's system forming

Abstracts

Conception of delivery of substance atoms and heavenly bodies in single process of starry cyclic synthesis was promoted by Russian scientist A.E. Khod'kov (1909-2003). On base of cosmogonic essence of Periodic Mendeleev's system it was observed the peculiarity of atom's structures, formed in the definite star (the Jupiter or the Sun), which explained with help of notion about dipole's atom structure and her interaction with celestial ether. Just the interaction with celestial ether across alteration of frequency of dipole's pulsation explains the processes do not attended by quantum chemistry. It was arise necessity to investigate deeper our notion about nature of caught by the Earth (possessing jupiterian origin) strange abiogenetic carbon matter provoking antagonism of earthy entrails to biosphere.

Vinogradova M.G. About cosmogonic essence of Periodic Mendeleev's system of chemical elements /on Russian. Novosibirsk. Academpublish. 2019. 236 p.

A brief history of time in chemistry

Gregory S. Yablonsky^{1*}, Guy B. Marin²

¹*Department of Energy, Environmental and Chemical Engineering,*

Washington University in St. Louis, 1 Brookings Drive, St. Louis, MO 63130

USA

gy@wustl.edu; gregoryyanlonsky@yahoo.com

²*Laboratory for Chemical Technology, Gent University, Technologiepark 914, B-9052, Gent, Belgium*

guy.marin@ugent.be

**corresponding author*

An evolution of the concept of “chemical time” will be presented. Different milestones in introducing this concept into chemistry will be described – from combustion and alchemy to complex chemistry of our days, giving a emphasis on the discovery of catalysis and development of chemical kinetics [13]. Three typical meanings of “chemical time” will be explained: (1) “external time” of the chemical system, i.e. temporal scale of our observations; (2) “internal”, or “intrinsic” time; (3) transport time (“residence” time).

A big influence of mechanical concepts on chemical kinetics will be stressed, i.e. ideas of “mass-action-law”, “equilibrium”, “mechanism”, “transition-state-theory” et al. The theoretical basis of contemporary chemical kinetics is presented as an interplay between different paradigms, ‘pro-mechanical’ (Guldberg-Waage), ‘pro-chemical’ (van’t Hoff) and thermodynamic (Boltzmann and Onsager). It will be done an attempt to distinguish time as a framework for demonstrating the chemical transformations and time as a manifestation of the chemical complexity.

Essential characteristics are given for different periods of chemical kinetics:

XIX century was a period of formulating the basic subjects and laws of chemical kinetics

XX century can be defined as a period with a focus on the “chemical complexity” (gaseous chain reactions, Semenov and Hinshelwood; heterogeneous catalytic reactions, Langmuir and Temkin; oscillating reactions and chemical bifurcations (Zhabotinskii, Prigogine), theory of chemical networks (Aris, Horn)

In contemporary temporal chemistry, state-of-the-art can be characterized by the “*stop-time-trend*” with two approaches, (I) ‘Chemical Calculus’-approach in which the advanced millisecond pulse-response technique (Temporal Analysis of Products, TAP- technique) is used for active material *non-destructive* characterization and studying the mechanism of complex catalytic reactions [4-5] (II) ‘Joint Kinetics’ – approach which focuses on the analysis of combination of special dual experiments aiming the search of *kinetic temporal invariants* [6-7].

References

1. .G.S. Yablonskii, V.I. Bykov, A.N. Gorban' and V.I. Elokhin, "Kinetic Models of Catalytic Reactions, in series"Comprehensive Chemical Kinetics," vol. 32, Amsterdam-Oxford- New York - Tokyo: Elsevier, 1991, 396 pp
2. G. B. Marin, G. Yablonsky “Kinetics of Chemical Reactions. Decoding Complexity”, Wiley-VCH (2011) 428 pp; G. B. Marin, G. Yablonsky, D. Constales, “Kinetics of Chemical Reactions. Decoding Complexity”, 2nd edition, Wiley-VCH (2019, in press)

3. A.N. Gorban, G.S. Yablonsky, "Three Waves of Chemical Dynamics", *Math. Model. Nat. Phenom.*, 2015, 10, 5, 1-5
4. J.T. Gleaves, G.S. Yablonskii, P. Phanawadee and Y. Schuurman, "TAP-2. Interrogative Kinetics Approach", *Applied Catalysis A: General*, 160, 55-88 (1997)
5. G. S. Yablonsky, M. Olea, G. Marin, "Temporal Analysis of Products: Basic Principles, Applications, and Theory", *J. of Catalysis*, 216, 120-134 (2003)
6. G. Yablonsky, A.N. Gorban, D. Constaes, V. Galvita and G.B. Marin, "Reciprocal Relations Between Kinetic Curves", *Euro Physics Letters (EPL)* 93(2011) 20004-20007
7. G. Yablonsky, D. Constaes and G. B. Marin, "New Types of Complexity in Chemical Kinetics: Intersections, Coincidences and Special Symmetric Relationships", "*Advances in Chemical Physics*", v. 157 (2014)69-73

About the secondary criterion of periodic classification: the proposal of periodicity trees

Alfio Zambon

Universidad Nacional de la Patagonia San Juan Bosco (Argentina)

azambon@infovia.com.ar

Abstract

Periodic tables are constructed based on two criteria: a) a primary criterion, generally horizontal, that orders chemical elements in a sequentially increasing way; and b) a secondary criterion, generally vertical, that allows grouping the elements into chemically similar families. The first gives rise to the periods and the second to the groups in the Standard Periodic Table. The first periodic tables developed in the late nineteenth or early twentieth century (such as Mendeleev, Meyer or Werner) had as a primary criterion the atomic weight, and secondary criteria were used as the maximum valence in the formation of oxides, or similarities in the chemical reactivity (Van Spronsen, 1969). From the discovery of the atomic number by Henry Moseley, and the development of electronic configurations, in the first decades of the twentieth century, the developed Tables took as their primary criterion the atomic number, and as secondary the electronic configuration of the neutral atom.

Scerri (2007, 2008) reformulated the concept of triads, moving from atomic weight to atomic number for its definition, resulting in accurate triads. He also suggested the use of atomic number triads as a possible secondary categorical criterion, based on the fact that the atomic number is the only essential property of the chemical elements if they are considered as basic substances and not as simple substances. Zambon (2018) proposed a representation of the periodic system where the primary criterion is the increasing order of atomic numbers, and the secondary criterion is established by the formation of atomic number triads, although the proposed table is based on triads of atomic numbers, the fundamental relationship in the architecture of the table is given by the "trees of periodicity": symmetric systems of interrelated elements by means of the triads, which contain 20 elements each and they take the place of traditional groups.

In this work, we will develop the proposal of "trees of periodicity"; we will analyze each structure independently and discuss the implications in the context of the teaching and communication of chemistry. Also, given that the proposed structures are based on a dual conception of the chemical element concept, we will study the challenges of transmitting the concept in this system. Finally, we will reflect on the answer to the traditional problems of periodic classification within the framework of this proposal and we will discuss the advantages and limitations of it.

References

Scerri, E. (2007). *The Periodic Table – Its Story and Its Significance*, New York: Oxford University Press.

Scerri, E. (2008). “The role of triads in the evolution of the periodic table: past and present”. *Journal of Chemical Education*, **85**: 585-589.

Van Spronsen, J. W. (1969). *The Periodic System of Chemical Elements - A History of the First Hundred Years*, Amsterdam: Elsevier Publishing Company.

Zambon, A. (2018). “A Representation of the Periodic System based on atomic-number triads” *Foundation of Chemistry*, **20**: 51-74.