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BOOK OF ABSTRACTS

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SEMI-EXACT, QUASI-EXACT AND CONDITIONALLY-EXACT SOLUTIONS OF THE SCHRÖEDINGER EQUION

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Usually one-particle eigenvalue problems have to be solved numerically. Several exactly solvable models (harmonic oscillator, hydrogen atom) play a fundamental role in quantum chemistry. Quasi-exactly solvable equations, where a finite number of solutions (usually just one) may be expressed analytically, have been intensively studied over last two decades. For equations referred to as conditionally-exactly-solvable the complete set of analytic solutions may be obtained for some specific values of the potential parameters. In the case of semi-exactly-solvable equations, an analytical expression is obtained for the general solution. This expression depends on the unconstrained energy parameter and, in general, does not fulfill the boundary conditions in the infinity. The discrete values of the energy parameter for which the solution is square integrable, equal to the eigenvalues of the Hamiltonian, have to be found numerically. The last two kinds of problems attracted some attention only recently [1,2]

One-particle potentials expressed as polynomials of the radial variable are known as the power potentials. It is demonstrated that the Schrödinger equations with power potentials are semi-exactly-solvable and their solutions may be expressed in terms of the Hessenberg determinants [2]. Conditions under which the equations with power potentials are either exactly or quasi-exactly solvable are also derived and examples of solutions are presented.

References:

- [1] A. M. Ishkhanyan, *Phys. Lett.* **A380** (2016) 3786-3790.
- [2] J. Karwowski and H. A. Witek, *Mol. Phys.* **114** (2016) 932-940.

SOLITONIC NATURAL ORBITALS

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Natural orbitals (NOs) and their occupancies constitute a convenient and conceptually appealing representation of the one-electron reduced density matrix from which all one-electron properties (including the majority of indices of interest to chemists) follow. However, their importance notwithstanding, some of the properties of the NOs are not fully understood. In particular, the existence of unoccupied NOs (UNOs) has been the subject of several studies with contradictory conclusions.

This talk focuses on our recent investigation of the elusive UNOs that employs a combination of rigorous analysis and extensive highly accurate numerical calculations aiming at elucidation of the sign patterns exhibited by the natural amplitudes pertaining to the NOs of two-electron systems in singlet ground states. First, the universal presence of exactly one positive-valued natural amplitude (“the normal sign pattern”) in systems with electron-electron interactions sufficiently weak in comparison to those with the external potential is rigorously proven. This result assures the vanishing of the occupation numbers of the NOs at certain values of the nuclear charge in the helium iso-electronic series or/and at certain internuclear distances in the H₂ molecule. Second, the evolution of the natural amplitudes of the harmonium atom in its ground state with the confinement strength ω is thoroughly studied. The presence of the normal sign pattern for all $\omega \geq \frac{1}{2}$ is demonstrated. Even more importantly, the existence of unusual weakly occupied NOs corresponding to positive-valued natural amplitudes at weak confinements is revealed. These solitonic NOs, whose shapes remain almost invariant as their radial positions drift toward infinity upon the critical values of ω being approached from below, exhibit strong radial localization. Their asymptotic properties are extracted from the numerical data and their relevance to electronic structure calculations on fully Coulombic systems is discussed.

Analytical form of helium wave function

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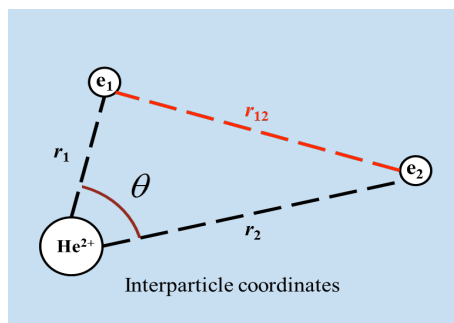
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Implicit analytical form of the ground state wave function for helium

$$\Psi(r_1, r_2, \theta) = 0 \infty r_1 r_2 + 0 r_1 r_2 \ln r_1 r_2 + 0 r_1 r_2 \cdot \cos \theta r_1 r_2 - 0 r_1 r_2 + 0 r_1 r_2 \cos \theta + 0 r_1 r_2 - 0 r_1 r_2 \cos \theta$$

was proposed by Fock in 1954 [1]. Explicit determination of the angular Fock coefficients Ψ_{lm} turned out to be a complex task; only few of them are found up to date [1–6]. The Fock series can be considered as an extended Taylor series of the exact wave function in the coordinates $r = r_1 r_2$, $\ln r$, $\cos \theta$, $\cos \theta$ around the triple coalescence point $r = 0$. The current talk will show how the Fock series emerges. In particular, it will show how the logarithmic terms appear in low-order Fock coefficients in order to guarantee physical behavior (continuity and finiteness) of the resulting wave function. We will address also the question of Fock expansion for helium in states with non-zero angular momentum and for helium without the Born-Oppenheimer approximation.



References:

- [1] V. A. Fock, *Norske Vidensk. Selsk. Forh.*, **31**, 138–152 (1958). (English translation of earlier Russian paper: V. A. Fock, *Izv. Akad. Nauk*, **18**, 161–172 (1954).)
- [2] A. M. Ermolaev, *Vest. Len. Univ.* **16**, 19–33 (1961).
- [3] P. C. Abbott, *PhD Thesis*, Univ. Western Australia, Perth 1986.
- [4] P. C. Abbott and E. N. Maslen, *J. Phys. A*, **20**, 2043–2075, (1987); J. E. Gottschalk, P. C. Abbott, and E. N. Maslen, *J. Phys. A*, **20**, 2077–2104, (1987); J. E. Gottschalk and E. N. Maslen, *J. Phys. A*, **20**, 2781–2803, (1987).
- [5] P. Pluvinaige, *J. Physique*, **43**, 439–458, (1982); R. C. Forrey, *Phys. Rev. A* **69**, 022504 (2004); E. Z. Liverts, *Phys. Rev. A* **89**, 032506 (2014).
- [6] E. Z. Liverts and N. Barnea, *Phys. Rev. A* **92**, 042512 (2015); E. Z. Liverts, *Phys. Rev. A* **94**, 022504 (2016).
- [7] B.-H. He and H. A. Witek, *J. Chin. Chem. Soc.* **63**, 69–82 (2016)

Structural origin of thermodynamic anomalies in liquids

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Thermodynamic and kinetic anomalies are often encountered in tetrahedral liquids, most famously in water (for example, the density anomaly), but also in SiO₂, BeF₂, Si and many other liquids that have different interaction types between constituent atoms. Several thermodynamic theories and scenarios have been proposed that link behaviour of anomalous properties to the existence of a liquid-liquid critical point [1] but none of them provide any links or insights into the structure itself. Stillinger-Weber (SW) potentials are often employed to model covalent tetrahedral liquids (Si, Ge, carbon). These potentials are composed of a standard pairwise term and a many-body term which penalizes deviations from ideal tetrahedral angle[2]. In recent years the critical point for SW silicon has been uncovered [3] and loci of anomalous properties calculated for constant pressure for different strengths of many-body term in SW potential[4]. In this study we take a systematic approach to explore the parameter space of the many-body term in the SW potential at various temperatures, pressures and densities. This enables us to more thoroughly understand the appearance of thermodynamic anomalies in tetrahedral liquids and make a connection between the anomalies and the network structure of the liquid. We also model MX₂ molten salt system made of 2+ charged cation and 1- charged anion using polarisable ion model. We vary polarisability of the potential to track the changes in anomalous behavior and structure of the liquid. An attempt is made to connect results from two different potentials through structural similarity between two radically different systems.

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References:

- [1] S. Sastry, P.G. Debenedetti, F. Sciortino and H.E. Stanley, *Phys. Rev. E* **1996**, 53(6), 6144–6154.
- [2] F.H. Stillinger and T. Weber, *Phys. Rev. B*, **1985**, 31(8), 5262–5271.
- [3] V.V. Vasisht, S. Saw and S. Sastry, *Nature Physics*, **2011**, 7(7), 549–553.
- [4] W. Hujo, B.S. Jabes, V.K. Rana, C. Chakravarty and V. Molinero, *Journal of Statistical Physics*, **2011**, 145, 293–312.

MODELING THE BONDING OF QUANTUM DOTS (BONDOTS) ON FULLERENIC GRAPHENE BY RAMAN SPECTROSCOPY

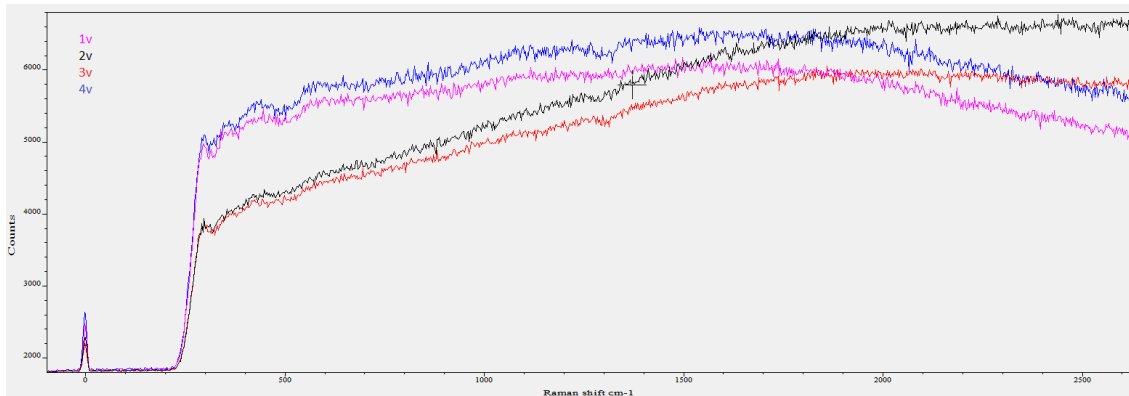
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The quantum electronic current intensity $i(\varepsilon) = -\frac{2e}{\hbar} \int_{\varepsilon}^{\infty} f(E_D) dE_D$ is for the first time computed for the bonding of quantum dots, emerging into the so called bondots (\mathcal{D}) [1], with the aid of the comb function $f(E_D) \cong \sum_{q=-\infty}^{q=+\infty} \delta(q - E_D)$ modeling the Coulomb blockade of bondots on the fullerenic graphenes, as recorded by the allied Raman shifts on various graphenic oxides samples [2] (1v-to-4v variants, see figure).



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References:

- [1] M.V. Putz, M.C. Mirica, Eds. (2016). *Sustainable Nanosystems Development, Properties, and Applications*, IGI Global, Hershey Pasadena, USA.
- [2] M.V. Putz, P. Svera, A.M. Putz, F. Cataldo, *Fullerenes, Nanotubes and Carbon Nanostructures* **26** (2018) 330–341.

MODELING THE QUANTUM-RELATIVISTIC PHASE TRANSITIONS ON FULLERENIC GRAPHENE BY ATOMIC FORCE MICROSCOPY

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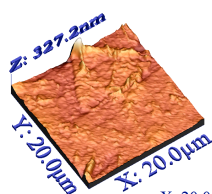
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The so called chemical field, in terms of applied potential $V(x, y, z)$ producing the density of states $\rho_n(x, y, z)$ at the Boltzmann thermal energy $\beta = 1/Tk_B$, i.e.

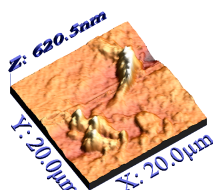
$$j_n[V(x, y, z)] = (\hbar\beta V(x, y, z))^{-1} \iint \hat{f}_n(x, y, z) V(x, y, z) dx dy dz,$$

it is for the first time computed in close relation with the quantum probability super-current $j_e = (-e)j_n$ towards identifying the critical temperature triggering the relativistic fullerenic graphenic phase transition from the fermionic quantum statistics $\rho_{Fermi-Dirac}(x, y, z)$ to the pairing of electrons into the so called bosonic bondon (B) statistics $\rho_{Bosonic-Bondon}(x, y, z)$ [1], in various graphenic oxide-reduction environments, as recorded by the Atomic Force Microscopy [2] experiments (see figures).



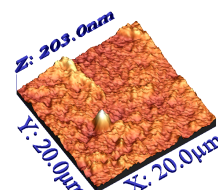
X: 20.0µm
Y: 20.0µm
Z: 327.2nm

Graphene oxide dissolved in water - "Graphenea" in isopropyl alcohol solution



X: 20.0µm
Y: 20.0µm
Z: 620.5nm

Graphene oxide dissolved in water- "Graphenea" in ethylene glycol solution



X: 20.0µm
Y: 20.0µm
Z: 203.0nm

Graphene oxide dissolved in water - "Graphenea" in water

Acknowledgement: Work supported by research project PED123/2017 of UEFISCDI-Romania.

References:

[1] M.V. Putz, D.L. Buzatu, M.C. Mirica, O. Ori, *Fullerenes, Nanotubes And Carbon Nanostructures* **26** (2018) 303–314.

[2] M.V. Putz, M.C. Mirica, Eds. (2016). *Sustainable Nanosystems Development, Properties, and Applications*, IGI Global, Hershey Pasadena, USA.

Exploring and Evaluating Reaction Mechanisms Using Graph Transformation

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The study of the reaction mechanisms in detail is a core part of understanding chemical systems. This has been supported computationally for decades using models based on quantum chemistry. While those methods give accurate results they are computationally intensive, and it is therefore of interest to investigate methods on a higher level of abstraction that trades away accuracy for the potential of faster algorithms.

We model molecules as labelled graphs and classes of reactions can be modelled as formal graph transformation rules.¹ This allows for a concise description of chemical systems as graph grammars, from which explicit reaction networks can be generated. While this ignores the spacial embedding of molecules it is still possible to include stereochemical features.² Using this framework we here present a method for exploring and evaluating decompositions of overall reactions into simpler patterns of electron movement, described by given transformation rules. Importantly the transformation system makes the exact atom maps of each step of the decomposition explicitly available. It is thus readily possible to define arbitrary evaluation functions that takes the context of rule application into account. Using a pathway model based on integer hyperflows³ we can search for not only decompositions that are optimal with respect to the chosen evaluation function, but also near-optimal solutions, that can be use for subsequent study.

To illustrate the potential of the framework we use transformation rules that encode charge separation and charge combination. Individual steps resulting from composition are evaluated using the partial charges of each atom.

References:

- [1] J.L. Andersen, C. Flamm, D. Merkle, P.F. Stadler. *Int. Conf. Graph Transformation* (2016)
- [2] J.L. Andersen, C. Flamm, D. Merkle, P.F. Stadler. *Int. Conf. Graph Transformation* (2017)
- [3] J.L. Andersen, C. Flamm, D. Merkle, P.F. Stadler. *Trans. Comp. Biol. and Bioinf.* (2017)

THE USE OF SQUARE OF CORRELATION COEFFICIENT (q^2) FOR ESTIMATING THE QUALITY OF MODELS IN CHEMISTRY: A 30 YEARS OLD QUESTION

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Correlation coefficient (or its square) has been used as the most common statistical parameter for estimating the quality of models in chemistry. It is usually calculated in each of three main validation procedure: fitting (r^2), cross-validation (q^2), and prediction on an external test set (222222). Wide use of q^2 in cross-validation technique was initiated by a very often cited paper by Cramer et al. [1], in which comparative molecular field analysis based on partial least squares method was introduced in chemical modeling. The use of q^2 was additionally accelerated by its involvement in the regulatory perspectives of the U.S.A. Environmental Protection Agency (EPA) [2] and in the Guidance document of OECD principles on the validation of (quantitative) structure-activity relationship ((Q)SAR) models [3]. In latter applications of q^2 several researchers noticed its strange properties like overestimation or underestimation when applied on external (test) data set. Therefore, two additional alternative variants of q^2 [4,5] were proposed, but the problem remains unsolved.

All these results are reviewed and their statistical foundations are re-analysed, considering all three validation procedures, i.e. fitting, cross-validation and prediction. Obtained results will be illustrated on literature data sets. It comes out that the best estimate of the model quality can be obtained by simultaneous calculation and comparison of root-mean-square errors of fit, cross-validation and prediction

- [1] R. D. Cramer et al., Comparative molecular field analysis (CoMFA). 1. Effect of shape on binding of steroids to carrier proteins. *J. Am. Chem. Soc.* 110 (1988) 5959–5967.
- [2] M. Zeeman, et al., U.S. EPA regulatory perspectives on the use of QSAR for new and existing chemical evaluations, *SAR QSAR Environ. Res.* 3 (1995) 179–201.
- [3] OECD guidelines concerning QSARs, 2007, pp. 55–65.
[http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?doclanguage=en&cote=env/jm/mo\(2007\)2](http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?doclanguage=en&cote=env/jm/mo(2007)2), accessed: May 25, 2018.
- [4] G. Schüürmann et al., External validation and prediction employing the predictive squared correlation coefficient - test set activity mean vs training set activity mean. *J. Chem. Inf. Model.* 48 (2008) 2140–2145.
- [5] V. Consonni et al., Comments on the definition of the q^2 parameter for QSAR validation. *J. Chem. Inf. Model.* 49 (2009) 1669–1678.

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IMPROVED INTERPRETATION OF THERMAL STABILITY MODELS OF NITROAROMATICS BY AN EFFICIENT SELECTION OF DESCRIPTORS AND BY THE USE OF CHEMICAL SHIFTS AS DESCRIPTORS

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Nitroaromatic compounds, like nitrobenzene derivatives can be considered as the typical energetic molecules [1]. Some of them are commonly used as explosives like TNB (1,3,5-Trinitrobenzene) or TNT (2,4,6-trinitrotoluene) [2]. For the suitability of an explosive substance in a specific use, better understanding of physico-chemical attributes of its structure which are related to compound's stability is a very important task. Many structure-thermal stability models have been developed in the last ten years for this class of compounds. The largest data sets used are those published by Fayet et al. [3] based (primarily) on the set of semi-empirical molecular descriptors calculated by the MOPAC program [4], and by Li et al. [2] selected from the large pool of molecular descriptors calculated by the Dragon 5.5 program [5].

To achieve better physico-chemical interpretation of models, in addition to descriptors calculated and used in previous models we calculated and used additional descriptors like (1) those given in the PubChem database [5], (2) experimental or calculated ¹H and ¹³C chemical shifts of nitroaromatics and (3) the number of specific connectivity terms in molecular skeleton. Also, an improved selection of molecular descriptors was performed in attempt to develop simpler structure-property models (having a smaller number of descriptors). Performing descriptor selection, whenever it was possible and statistically reasonable, we considered the possibility of inclusion of simpler molecular descriptors into the final models instead of more complex ones or those computed from 3D structure. As an interesting results we found that the maximal ¹H chemical shift of hydrogens attached to aromatic ring is a significant descriptor, as well as the number of multiple bonds in a compound. Obtained results were compared with other models from literature showing that presented approach is a promising way of selecting statistically good structure-thermal stability models of nitroaromatics, which are more informative and easy to interpret.

- [1] G. Fayet, et al., A theoretical study of the decomposition mechanisms on substituted orthonitrotoluenes. *J. Phys. Chem. A* 113 (2009) 13621–13627.
- [2] J. Li et al., Structure-Activity Relationship Analysis of the Thermal Stabilities of Nitroaromatic Compounds Following Different Decomposition Mechanisms. *Mol. Inf.* 32 (2013) 193 – 202.
- [3] G. Fayet, P. et al., Development of a QSPR model for predicting thermal stabilities of nitroaromatic compounds taking into account their decomposition mechanisms. *J. Mol. Model.* 17 (2011) 2443–2453.
- [4] MOPAC2016, J. J. P. Stewart, Stewart Computational Chemistry, web: <http://OpenMOPAC.net>
- [5] R. Todeschini, V. Consonni (2006) DRAGON Professional 5.4 program, TALETE srl, Milano, Italy, 2006, (<http://www.talete.mi.it/dragon.htm>).
- [6] S. Kim et al., PubChem substance and compound databases. *Nucl. Acid Res.* 44 (2016) D01202-D01213.

MODELING TOXICITY OF NITROAROMATICS: COMPARATIVE ANALYSIS OF DIFFERENT VARIABLE AND MODEL SELECTION METHODS

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The study of nitrobenzene derivatives like nitroaromatic compounds is a very important task, due to their increased influence on living organisms and environment, in general [1]. These compounds and their derivatives and metabolic products show mutagenic and carcinogenic effects, as well as allergic reactions, endocrine system impairment and skin irritation [2]. In recent study the authors performed a comprehensive quantitative structure-toxicity relationship study on rats using a set of 90 nitroaromatics whose structures were described by three sets having ~ 800, 20000 and 1500 different descriptors (based on 1D, 2D and 3D structures) calculated by the PaDEL, HiTQSAR and Dragon program, respectively [2]. Among them Dragon set contains the largest portion of 3D descriptors. Additionally, two smaller sets of 3D descriptors based on semiempirical and DFT structure were also calculated and all descriptors were selected into Multivariate Linear Regression (MLR) models by the method based on genetic algorithm, as implemented in QSARIns [3]. In modeling, experimental values of concentrations which had lethal toxic outcome for 50% tested organisms were used as endpoints (LD50). In summary, better models were obtained from sets of descriptors composed mostly of 1D or 2D descriptors (HiTQSAR, PaDEL), and if data sets contain only smaller sub-sets of 3D descriptors (Dragon). The worst models were those based on semi-empirical and DFT 3D descriptors. To test the possibility of improvement of models obtained in [2] we performed an analysis using only Dragon 5.5 set of descriptors and extended previous study by: (1) enlarging data set by 100 novel nitroaromatics obtained from the LD50 database involved into the program TEST 4.2.1 [4] (given on U.S. Env. Protection Agency web site), (2) the use of an additional algorithm which performs detailed descriptor selection by considering all combinations of fixed size subsets of descriptors [5], and (3) by the use of more robust Partial Least Square (PLS) method for selection of models [6]. The novel set of 100 nitroaromatics contains compounds having high similarity with 90 compounds from ref. [2]. This set was used as an additional set for testing external predictivity of developed models. As the main result we have found that the Root Mean Squared Error (RMSE) of prediction by U.S. EPA method TEST 4.2.1 for 10 compounds (out of 90 nitroaromatics from [2]) which are not involved in the TEST 4.2.1 database is ~1.17 log units, what is significantly higher error than it was obtained for the training set used for development of corresponding toxicity models in TEST 4.2.1. This fact justifies the existence of need for improvement of existing models of nitroaromatics. RMSEs of fit or cross-validation of LD50 values for 90 nitroaromatics were between 0.28 - 0.7 on log scale in all considered PLS and MLR models. But, for the novel test set of 100 nitroaromatics RMSEs are ~0.75 - 1.0 (for all models). However, the lowest RMSE of prediction on 100 compounds of complex PLS models having 13 components (that are formed by ~40 initial descriptors) is 0.75, and the best one-descriptor (the number of phosphorous atoms) MLR model gives fairly low RMSE of 0.89. Almost all obtained MLR and PLS models have RMSEs in prediction on large external set comparable or even lower than the TEST 4.2.1 program, thus confirming that there is a space for improvement of structure-toxicity models of nitroaromatics.

[1] P.-Z. Lang, G.-H Lu, *Chem. J. Chin. Univ.* 16 (1995) 1083–1087.

[2] A. Gooch *et al.*, *Environ. Toxicol. Chem.* 36 (2017) 2227–2233.

[3] P. Gramatica *et al.*, *J. Comput. Chem.* 34 (2013) 2121–2132.

[4] TEST 4.2.1 program, 2016, <https://www.epa.gov/chemical-research/toxicity-estimation-software-tool-test>.

[5] B. Lučić, N. Trinajstić, *J. Chem. Inf. Comput. Sci.* 39 (1999) 121–132.

[6] K. Roy, P. Ambure, *Chemom. Intell. Lab. Syst.* 159 (2016) 108–126.

QSAR OF RADICAL INACTIVATION BY SELECTED ANTHRAQUINONES

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Anthraquinones are natural antioxidants capable to combat the progression of various diseases [1]. Among underlying health promoting mechanisms, radical scavenging could be operative *via* several possible processes [2]. In building QSAR models, among thousands molecular descriptors we preferred those with clear physicochemical meaning related to antiradical mechanisms, e.g., bond dissociation enthalpy (BDE) as a general parameter for (poly)phenolics radical scavenging activity, ¹³C NMR chemical shift of C atom adjacent to phenolic OH group [3], aromaticity indices (e.g. ring current index, RCI [4]), hydrogen bonding indices, etc.

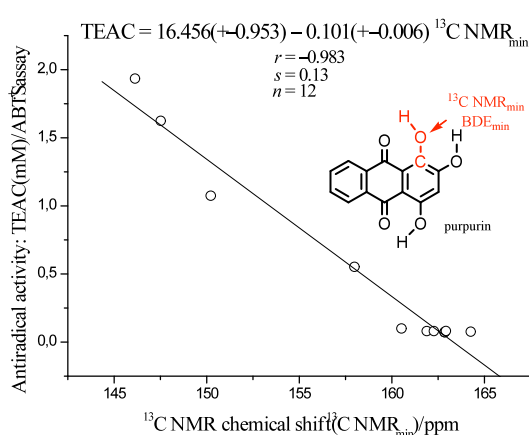


Figure 1.

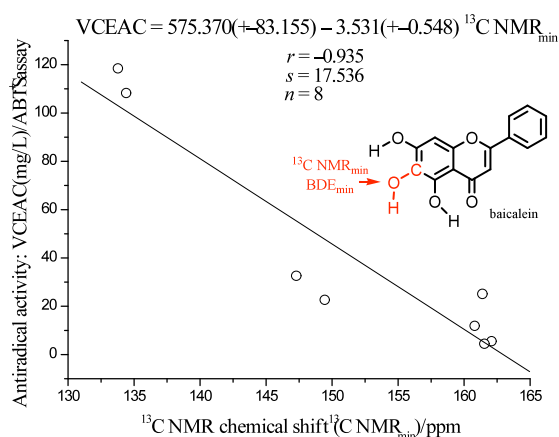


Figure 2.

Due to limited number of compounds (12 anthraquinones [5]), only models with one or two descriptors are acceptable. The best one descriptor model, using ¹³C NMR_{min} chemical shift ($r = -0.983$, $r_{cv} = -0.969$), is presented in Fig. 1. The phenolic OH group with more abstractable H atom shielded the ¹³C nucleus from the external magnetic field more effectively than the OH group with less abstractable H atom. One descriptor models using BDE and RCI, are slightly inferior: $r = -0.934$ ($r_{cv} = -0.904$) and $r = 0.914$ ($r_{cv} = -0.848$), respectively. The best two descriptor model embraces ¹³C NMR_{min} chemical shift and RDF055m descriptor (related to the 3D positions of the atoms) and possesses only slightly better statistics: $r = -0.990$, $r_{cv} = -0.979$. It should be emphasized that obtained model(s) are transferable to flavones [6], another class of (poly)phenols, Fig 2.

References:

- [1] S. Jeremić, A. Amić, M. Stanojević-Pirković, Z. Marković, *Org. Biomol. Chem.* **16** (2018) 0000–0000.
- [2] S. Jeremić, S. Radenković, M. Filipović, M. Antić, A. Amić, Z. Marković, *J. Mol. Graph. Model.* **72** (2017) 240–245.
- [3] B. Lučić, V. Stepanić, D. Plavšić, A. Amić, D. Amić, *Monatsh. Chem.* **145** (2014) 457–463.
- [4] K. Jug, *J. Org. Chem.* **48** (1983) 1344–1348.
- [5] Y.-Z. Cai, M. Sun, J. Xing, Q. Luo, H. Corke, *Life Sci.* **78** (2006) 2872–2888.
- [6] D.-O. Kim, C.Y. Lee, *Crit. Rev. Food Sci. Nutr.* **44** (2004) 253–273.

DFT AND PM7 STUDY OF RADICAL INACTIVATION BY SELECTED HETEROCYCLIC COMPOUNDS WITH COUMARIN CORE

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Coumarin (2H-1-benzopyran-2-one, 2H-chromen-2-one, 1,2-benzopyrone) and coumarine derivatives are polyphenolic compounds widely distributed in plant kingdom and have a great significance as natural fragrances, having a characteristic odour like vanilla beans [1]. These compounds also possess a number of various biological activities, such as anticoagulant, anti-inflammatory, anti-HIV, anticancer, antiviral etc. [2]. Additionally, hydroxycoumarins have been identified as powerful antioxidants that can prevent radical induced damage by scavenging reactive oxygen species [3].

The antioxidative potential of 15 compounds containing coumarin core was investigated theoretically. Reaction enthalpies related to hydrogen atom transfer (HAT) and electron transfer followed by proton transfer (ET-PT) mechanisms were calculated using MOPAC2012 COSMO PM7 and Gaussian 09 DFT/M05-2X/6-311++G(d,p), in conjunction with the SMD continuum solvation model in polar and nonpolar medium [4]. For building QSAR models Dragon and ADMEWorks Programs were used. The effect of the position of the hydroxyl group, as well as other present groups, on the antioxidative activity was examined. Based on the computational results, compounds containing catechol and guaiacol group exhibit the highest radical scavenging properties.

References:

- [1] M.M. Darla, B.S. Krishna, K.U. Rao, N.B. Reddy, M.K. Srivash, K. Adeppa, C.S. Sundar, C.S. Reddy, K. Misra, *Res. Chem. Intermed.* **41** (2015) 1115–1133.
- [2] S.S. Sahoo, S. Shukla, S. Nandy, H.B. Sahoo, *Eur. J. Exp. Biol.* **2** (2012) 899–908.
- [4] M.J. Frisch, G.W. Trucks, H.B. Schlegel et al., Gaussian 09, Wallingford, CT, 2009.
- [3] M. Paya, B. Halliwell, J.R. Hoult. *Biochem. Pharmacol.* **44** (1992) 205–214.

Computer Aided Design of Bio-macromolecular Systems

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Everyday increasing of the computer performances combined with development of efficient and reliable algorithms for modelling of biological macromolecules enables us to widen our understanding of various processes at cellular level, like protein aggregation, different cellular pathways, enzyme function, protein-ligand interactions ...

Molecular dynamics (MD) simulations is becoming an ubiquitely used methods in research of all kind of biomolecular systems. The workshop is designed for 'no-experts in MD simulations', aiming to explain basic philosophy of MD simulations to the audience, and to explain what are the main things that should be taken in consideration during MD simulations of macromolecules. Besides classical MD simulations the methods designed to improve efficiency of the conformational space sampling will be presented as well (like coarse grained, accelerated, RAMD, steered and replica exchange MD simulations). Also, importance of using the experimental results as constraints and/or reference points during MD simulations will be discussed.^{1,2}

Beside MD simulations, some other molecular modelling methods, like homology modelling, docking, and the free energy calculations will be also mentioned during the workshop.

Finally, several examples³⁻⁹ of using MD simulations in study of protein structure, dynamics and function will be presented.

REFERENCES

1. Tus, A.; Rakipović, A.; Peretin, G.; Tomić, S.; Šikić, M., *Nucleic acids research*. **v40** (Web Server Issue) (2012).
2. Kazazić S., Karacčić Z., Sabljčić I., Agić D., Tomin M., Abramić M., Dadlez M, Tomić A., Tomić S., *RSC Adv*. **8** (2018), 13310-13322.
3. Tomić, A; Gonzalez, M.; Tomić, S., *Journal of chemical information and modeling*. **52** (2012); 1583-1594.
4. Brkić, H., Kovačević, B., Tomić, S., *Molecular biosystems*. **11** (2015), 898-907.
5. Gershberg J., Radić Stojković M., Škugor M., Tomić S., Rehm T.H., Rehm S., Saha-Möller C. R., Piantanida I, Würthner F., *Chemistry - A European Journal*. **21** (2015); 7886-7895.
6. Tomić, A; Berynskyy, M.; Wade, C. R.; Tomić, S., *Mol. BioSyst*. **11** (2015); 3068-3080.
7. Smolko, A.; Šupljika, F.; Martinčić, J.; Jajčanin-Jozić, N.; Grabar- Branilović, M.; Tomić, S.; Ludwig-Müller, J.; Piantanida, I.; Salopek- Sondi, B., *Physical Chemistry Chemical Physics*. **18** (2016); 8890-8900.
8. Hromić-Jahjefendić A., Jajčanin Jozić N., Karačić Z., Schrittwieser J., Mohan Padmanabha Das K., Kazazić S., Grabar Branilović M., Tomin M., Oberer M., Gruber K., Abramić M., and Tomić S., *PLoS ONE* **12** (2017), e0188915.
9. Sabljčić I, Tomin M, Matovina M, Sućec I, Tomašić Paić A, Tomić A, et al., *PLoS ONE* **13**(2) (2018), e0192488.

COMPUTATIONAL CHEMISTRY METHODS AS A TOOL FOR ANALYSIS AND PREDICTON OF SUPRAMOLECULAR INTERACTIONS IN COORDINATION COMPOUNDS

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Today computational chemistry methods are used to interpret experimental observations and illustrate chemical concepts. However, applications of these principles are also chosen to predict structures, calculate molecular properties and to help us in design of new materials. Ferrocene peptide conjugates are unique by their properties to form intra- and intermolecular hydrogen bonds and mimicking secondary structures of proteins, especially turn-like motifs. In order to predict their secondary structures, we need to fully understand their conformational properties, employing experimental but also computational chemistry methods.[1] Introduction of two ferrocene units can alter their conformational and optical properties in comparison with their mononuclear analogs.

Delivery of materials with a targeted physical property or response is one of the primary challenges of practical crystal engineering. A deeper insight into supramolecular interactions, hydrogen and halogen bonds, can help us in targeting of specific molecular arrangements in three-dimensional architectures, thus resulting with desired properties of materials. Molecular electrostatic potential values are quite useful method for ranking affinities of hydrogen and halogen bond donors toward acceptors. This approach is very often used for purely organic systems, however it also becomes useful for the explanation of supramolecular interactions between metal complexes. In order to extend this approach from discrete single molecules to one-dimensional coordination polymers, for example Cd(II) halides equipped with functionalized pyridyl-based ligands, we proposed a new approach for relatively fast calculation of electrostatic potential values of such infinite chains.[2]

References:

- [1] M. Čakić Semenčić, I. Kodrin, L. Barišić, M. Nuskol, A. Meden, *Eur. J. Inorg. Chem.* **2** (2017) 306–317.
- [2] M. Đaković, Ž. Soldin, B.-M. Kukovec, I. Kodrin, C. B. Aakeröy, N. Baus, T. Rinkovec, *IUCrJ* **5** (2018) 13–21.

Acknowledgements

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LINKING HYDROCARBON AND BORON HYDRIDE CHEMISTRIES AND BIDIMENSIONAL AND THREE-DIMENSIONAL AROMATICITIES

Miquel Solà,^a Jordi Poater,^{b,c} Clara Viñas^d and Francesc Teixidor^d

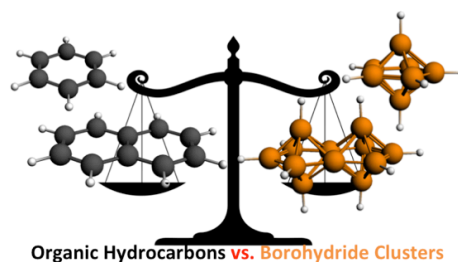
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In the first part of the lecture, a link between the hydrocarbon and boron hydride chemistries will be established by showing that hydrocarbons and boron hydrides have a common root regulated by the number of valence electrons in a confined space [1]. Application of the proposed electronic confined space analogy (ECSA) method to archetypal hydrocarbons leads to well-known boron hydrides but, more importantly, it allows the design of new interesting boron-containing molecules that can be a source of inspiration for synthetic chemists. In the second part, we apply the ECSA method to archetypal polycyclic aromatic hydrocarbons (PAH) to conclude that the $4n+2$ Wade-Mingos rule for three-dimensional closo boranes is equivalent to the $(4n+2)\pi$ Hückel rule for bidimensional PAHs [2,3].



References:

- [1] J. Poater, M. Solà, M.; C. Viñas and F. Teixidor, *Chem. Eur. J.* **19** (2013) 4169–4175.
- [2] J. Poater, M. Solà, C. Viñas and F. Teixidor, *Angew. Chem. Int. Ed.* **53** (2014) 12191–12195.
- [3] J. Poater, M. Solà, M.; C. Viñas and F. Teixidor, *Chem. Eur. J.* **22** (2016) 7437–7443.

30th Math/Chem/Comp Conference
June 18–23, 2018, Dubrovnik, Croatia

The Conundrum of the C₄H₇⁺ Cation

Dedicated to George A. Olah

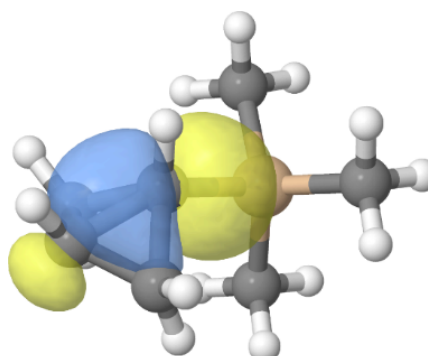
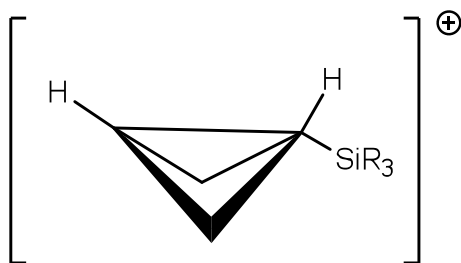
Hans-Ullrich Siehl

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Nobel Laureate George A. Olah passed away March 8, 2017 at the age of 89. George Olah was a true legend in the field of chemistry. His pioneering research created an entire new field of chemistry of considerable theoretical and practical importance. The work on carbocations fundamentally redefined the field of physical organic chemistry and revolutionized the understanding of organic chemistry, leading to new discoveries, new fields of research and countless applications.

This contribution will mainly review some retrospective and recent results from our group focused on experimental and computational NMR Spectroscopy of highly reactive carbocations such as the Bicyclobutonium C₄H₇⁺ and related cations.



References H.-U. Siehl, The Interplay between experiment and theory: Computational NMR Spectroscopy of Carbocations, in *Adv. Phys. Org. Chem.*, Vol. 42, Ed. J.P. Richard, Academic Press, 2008.

Holzschuh, C. Freudenberger, H.-U. Siehl, submitted.

BEHAVIOR OF CHLOROGENIC ACID DIANION TOWARDS FREE RADICALS IN WATER SOLUTION

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At physiological pH chlorogenic acid (5-*O*-caffeoylquinic acid, **5CQA**) exists in monoanionic (87%) and dianionic (13%) forms. Although the monoanions of **5CQA** are present in larger concentration at pH = 7.4, the effect of dianions on overall antioxidative activity is significant [1]. The thermodynamic and kinetic investigations of hydrogen atom transfer (HAT), radical adduct formation (RAF), sequential proton loss-electron transfer (SPLET) and single electron transfer-proton transfer (SET-PT) mechanisms for the reaction of **5CQA** dianion with HO[•] and CH₃OO[•] radicals in water solution were examined. It was found that in presence of HO[•] dianion spontaneously transfers to radical anion which can further react through PT, HAT and RAF mechanisms. It was showed that in all three cases reactions are diffusion-controlled. Dianion of **5CQA** can react with CH₃OO[•] only via HAT mechanism. The results obtained for the reactions with HO[•] are in very good agreement with experimental findings [2]. All calculations were carried out at the M06-2X/6-311++G(d,p) level of theory in conjunction with CPCM polarizable continuum solvation model.

References:

- [1] J. Tošović, S. Marković, J. M. Dimitrić Marković, M. Mojović, D. Milenković, *Food. Chem.* **237** (2017) 390–398.
- [2] Y. Kono, K. Kobayashi, S. Tagawa, K. Adachi, A. Ueda, Y. Sawa, H. Shibata, *Biochim. Biophys. Acta* **1335** (1997) 335–342.

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MICROWAVE IRRADIATION ENHANCES MISFOLDING OF PEPTIDES

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Microwaves have been experimentally shown to affect the folding dynamics of peptides and proteins. Using molecular dynamics we performed all-atom simulations of a model β -peptide in aqueous solution where the individual degrees of freedom of solvent molecules were decoupled to allow for investigation at non-equilibrium microwave-irradiated conditions.[1] Elevated rotational temperature of the water medium was found to significantly affect the conformation of the peptide due to the weakened interactions with the surrounding solvent molecules. Cluster analysis revealed that microwave irradiation can indeed act as a catalyst in the formation of new misfolded peptide chains, which are generally associated with the onset of several neurodegenerative disorders (Alzheimer's, Parkinson's, Huntington's, Creutzfeldt–Jakob diseases as well as several cancer types like amyloidosis).

References:

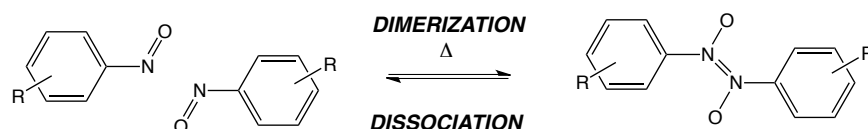
[1] T. Mohorič and U. Bren, *J. Chem. Phys.* **146** (2017) 044504.

Reactions in crystalline molecular solids: activation parameters and the nature of transition state

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Using the dimerization-dissociation of aromatic C-nitroso compounds as a molecular model (Scheme) we have developed the method for studying the reaction mechanisms in the molecular crystals. By detailed studies of the thermodynamics and kinetics of these thermally induced reactions we have found that the most important parameter, which modify the chemical reactivity is activation entropy. Variation in activation entropy could be explained by softening of the reactive zone around the transition state within the crystal. Since the analogous entropic effect of the variable rigidity has been found also for the transition state encapsulated in the enzyme cavity, our investigations of the solid-state reaction mechanisms by using convenient models could be of more general importance in physical organic chemistry.



References

- Vančik, H., *Aromatic C-Nitroso Compounds*; Springer Verlag: Dordrecht, Berlin, New York, 2013.
Biljan, I.; Vančik, H. *Crystals* **2017**, *7*, 376.
Halasz, I.; Meštrović, E.; Čičak, H.; Mihalić, Z.; Vančik, H. *J. Org. Chem.* **2005**, *70*, 8461-8467.
Varga, K.; Volarić, J.; Vančik, H. *CrystEngComm* **2015**, *17*, 1434-1438.

Acknowledgements

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AROMATIC DINITROSO DERIVATIVES: INTERACTIONS THROUGH AZODIOXIDE BONDS IN SOLUTION, SOLID STATE AND ON GOLD SURFACE

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Aromatic C-nitroso compounds and their *Z*- and/or *E*-azodioxy dimers exist in equilibrium in solution, which is usually shifted towards the monomers at ambient conditions.^[1] Dimers can be formed by lowering the solution temperature or by crystallization. Compounds with two or more nitroso groups are able to form oligomers and polymers by interactions through multiple azodioxide bonds.

Recently, we prepared several new aromatic dinitroso derivatives differing in spacer between two phenyl rings. Inspection of IR spectra revealed that in solid state these compounds are mostly present as *E*- or *Z*-oligomers. In order to investigate their possible dimerization or oligomerization in solution, we recorded one- and two-dimensional ¹H NMR spectra at ambient and low temperatures. Analysis of NMR spectra indicated that aromatic dinitroso derivatives dimerize at low temperatures affording a mixture of nitroso monomers and *Z*- and/or *E*-azodioxides. The proton chemical shifts of nitroso monomer-azodioxide mixtures were assigned and validated by DFT calculations. In almost all cases, a preference towards the formation of *Z*-azodioxy isomer was found.

In addition, we recently investigated self-assembly and possible dimerization of sulfur-containing aromatic dinitroso derivatives on gold surface by using polarization modulation infrared reflection-absorption spectroscopy (PM-IRRAS), atomic force microscopy (AFM), scanning tunneling microscopy (STM), ellipsometry and water contact angle goniometry.^[2] The results obtained suggested that aromatic dinitroso compounds are able to dimerize on gold surface through *E*-azodioxide bonds. In comparison to their mononitroso counterparts, adsorption of aromatic dinitroso derivatives on gold surface results in the formation of less ordered layers.

References:

- [1] H. Vančik, *Aromatic C-Nitroso Compounds*, Springer Verlag, New York, 2013.
- [2] T. Klačić, K. Varga, M. Kralj, I. Delač Marion, H. Vančik, I. Biljan, *Colloids Surf. A* (2018) 10.1016/j.colsurfa.2018.05.024.

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MULTI-WAY ANALYSIS OF POTENTIAL ENERGY SURFACES

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Multi-way analysis (MWA) is the numerical analysis of large data sets represented as multidimensional array (or a higher order tensor). This tensor is composed from sequences of calculated potential energy surfaces (PES) spanned in relevant torsional angles for investigated compounds. Each PES is finally represented as only one point in the reduced space.

MWA was carried out using the 3-way TUCKER decomposition model

$$\underline{\mathbf{X}} = \underline{\mathbf{A}} \underline{\mathbf{G}} \underline{\mathbf{B}} \otimes \underline{\mathbf{C}} + \underline{\mathbf{E}}$$

where \mathbf{A} , \mathbf{B} , and \mathbf{C} are 1st-way, 2nd-way, and the 3rd-way loadings matrices, respectively (\otimes represents Kronecker matrix product). The \mathbf{G} matrix (*core-array*) is associated with the amount of variation explained by loadings in the different modes (Fig. 1).

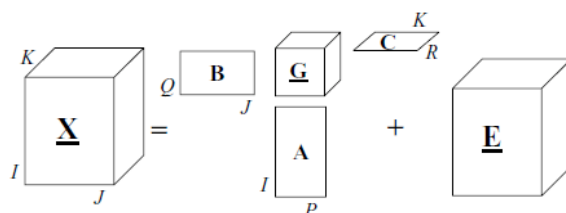


Figure 1. Graphical representation of the TUCKER3 model.

Results obtained for different classes of molecules and different types of PES will be presented and discussed. All *multi-way* analyses were performed by using our own code.

Acknowledgement: This work was supported by the Croatian Science Foundation (Project No: IP-2016-06-3775, Activity and *in silico* guided design of bioactive small molecules, ADESIRE).

Geometric Order of the Atom Based on 3,4 & 6 axes of Symmetry

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Marla Jeanne Wagner e-mail groundgardendesign@gmail.com

The use of the cube as a philosophy to describe space is incomplete in its representation of nature. We present a paradigm shift for the geometry of the atomic particles, via a new philosophy of space based on a combination of tetrahedrons and octahedrons, see Figure 1.

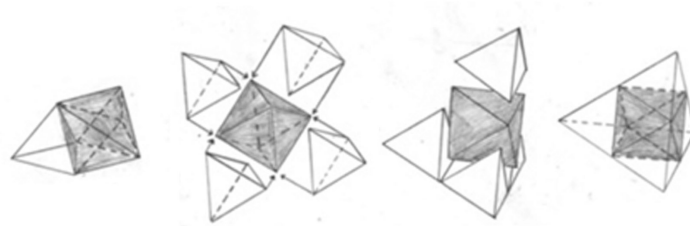


Figure 1

We are familiar with the (x,y,z) coordinate system with three axes symmetry based on 90 degrees angles. Crystallography visualizes the 3 axes of symmetry of the cube. See Figure 2.

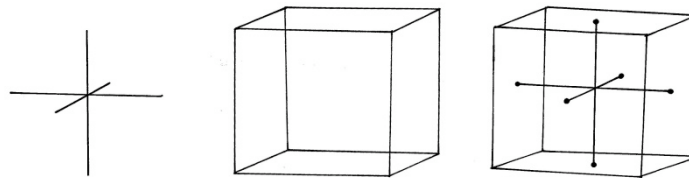


Figure 2

When the opposite corners of the cube are connected, 4 additional axis are formed. These four axes of symmetry are equidistant at 108° angles. See Figure 3.

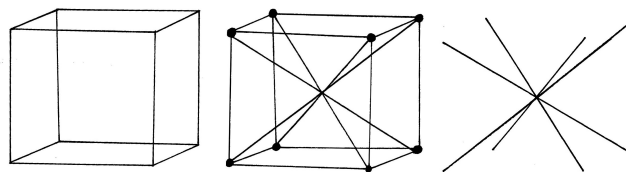


Figure 3

When the corners of the cube are truncated, a triangular face is revealed. The four axes of symmetry also connect the opposite centers of these triangular faces. See Figure 4.

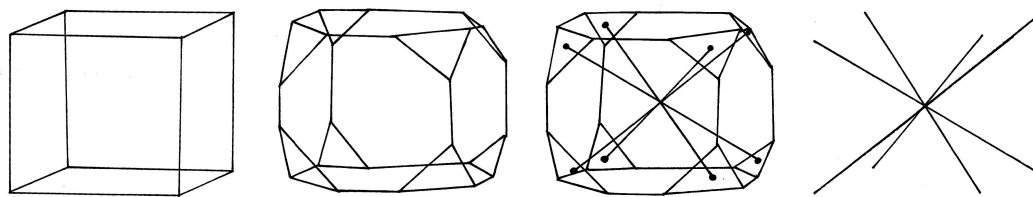


Figure 4

When the cube is truncated 12 points are visualized where the vertices of the triangular faces meet on 6 axes of symmetry. When the twelve opposite vertices of the cuboctahedron are connected, the six dimensions are revealed. These six dimensions are at equidistant 60° angles. See Figure 5.

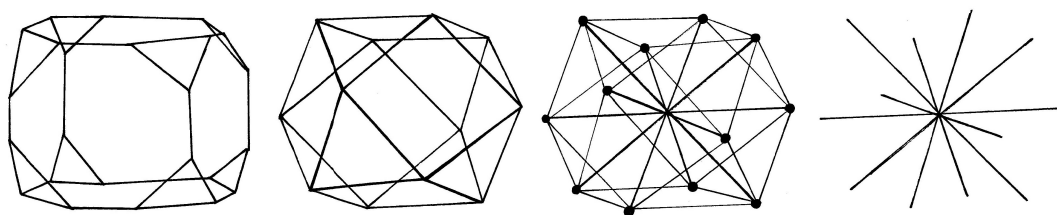


Figure 5

We present a six-dimensional coordinate system, based on tetrahedral geometry. Nature utilizes triangular polyhedrons : tetrahedron, octahedron, cuboctahedron, icosahedron, dodecahedron, truncated octahedron, see Figure 6. Nature's true patterns consists of equilateral triangles.

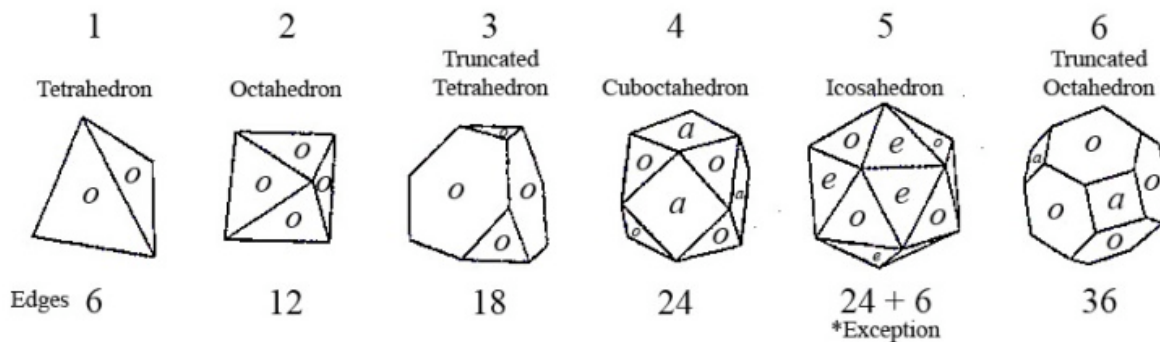


Figure 6

References:

- 1) ISIS International Society for the Interdisciplinary Study of Symmetry 1998 Haifa Israel, pp 97-100.
- 2) International Journal of Chemical Modeling vol 4 number 2-3 2012 pp 369 -
- 3) Registered: Mihai V. PUTZ (AAP Editor): Kindly confirm Invitation Contributing/EXPLICATIVE DICTIONARY of NANOCHEMISTRY

Counting Nucleons as Atomic Mass Numbers for the Atomic Elements and Isotopes

James Sawyer Marla Wagner

The spherical nucleon theory of Linus Pauling presented a paradigm shift for the structure of the nucleus of the atom and it is our foundation for a triangular polyhedral nuclear geometry within the Periodic Table of the Elements. We established a direct connection between atomic mass numbers and the number of spherical nucleons for many key Elements. The tetrahedral/ octahedral coordinate system accurately numbers nuclear Quantum Space for many isotopes. Example: diamond as Carbon 12 by definition is presented as a 12 atomic mass spherical units, packed into 4 triangular number planes in a tetrahedral octahedral matrix pattern representing 6 triangular dimensions algebraically as (r,s,t,u,v,w) edges. This stacking of spheroids as theoretical nucleons in triangular numbers produces symmetrical polyhedrons with three fold, four fold and six fold symmetry as a cuboctahedron. We see a theoretical carbon 12 nucleus composed of 12 quarks in four triangular sets of three spinning quarks. The spherical packing theory of Linus Pauling numerically agrees with atomic mass numbers for a Carbon atomic mass of 12 nucleons as being 12 spinning quarks. There would be 4 axes of symmetry through the centroids of the triple set of spinning quarks. This agrees with the primary characteristic property of carbon atoms bonding in four directions in tetrahedral space found in organic chemistry. This triangular/ tetrahedral packing fits nicely for

Number	Element	Atomic Mass
1) 10	Neon	20
2) 18	Argon	40
3) 20	Calcium	44
4) 30	Zink	68
5) 36	Krypton	92
6) 54	Xenon	128
7) 56	Barium	140
8) 58	Cerium	140
9) 60	Neodemium	146
10) 98	Californium	250
11) 122	Marlanium	298

Please note: We are predicting a new Stable Element that we shall call Marlanium. After Lisa Mitner a derivation of Mitner, Lisa and Marla (discovered by Marla Wagner). It would be the nuclear fusion of 98 Californium 248 and 24 Chromium 50 = 122 Marlanium atomic mass 298. A stable polyhedral Element 122 Marlanium atomic mass 298.

