International Journal of Advanced Chemistry, 7 (2) (2019) 77-81

International Journal of Advanced Chemistry

Website: www.sciencepubco.com/index.php/IJAC

Research paper

Calculation by UFF method of frequencies and vibrational temperatures of the unit cell of the rhodochrosite crystal

Ricardo Gobato [1], Marcia Regina Risso Gobato [2], Alireza Heidari [3*]

[1] Laboratory of Biophysics and Molecular Modeling Genesis, State Secretariat of Education of Parana, 86130-000, Parana, Brazil
[2] Green Land Landscaping and Gardening, Seedling Growth Laboratory, 86130-000, Parana, Brazil
[3] Faculty of Chemistry, California South University, 14731 Comet St. Irvine, CA 92604, USA
**Corresponding author E-mail: Scholar.Researcher.Scientist@gmail.com*

Abstract

The electronic oscillator circuit that uses the mechanical resonance of a vibrating crystal of piezoelectric material to create an electrical signal with a precise frequency is a crystal oscillator. Particularly one using a quartz crystal works by distorting the crystal with an electric field, when voltage is applied to an electrode near or on the crystal. Other crystals such as rhodochrosite also have piezoelectric properties. The rhodochrosite as crystal oscillator for being an alternative to those of quartz. The rhodochrosite (MnC03) shows complete solid solution with siderite (FeC03), and it may contain substantial amounts of Zn, Mg, Co, and Ca. A molecular dynamic via molecular mechanics using the UFF (Universal Forces Field) provided the vibrational frequencies of the fundamental structure of the crystal molecule. The frequencies and vibrational temperatures of the unit cell of rhodochrosite obtained by UFF were calculated in the range from 0.6059 to 1,731.38 cm-1 and 0.87 to 2,491.06 K, respectively.

Keywords: *Rhodochrosite; UFF; Synchrotron Radiation; Quartz Crystal; RLC Circuit; Cancer Cells.*

1. Introduction

The electric charge that accumulates in certain solid materials, such as crystals, certain ceramics, and biological matter such as bone, DNA and various proteins) in response to applied mechanical stress, phenomenon called piezoelectricity. [1]
The electronic oscillator circuit that uses the mechanical resonance of a vibrating crystal of piezoelectric material to create an electrical signal with a precise frequency is a crystal oscillator. The most common type of piezoelectric resonator used is the quartz crystal, so oscillator circuits incorporating them became known as crystal oscillators. Particularly one using a quartz crystal works by distorting the crystal with an electric field, when voltage is applied to an electrode near or on the crystal. This property is known as electrostriction or inverse piezoelectricity. [2] When the field is removed, the quartz - which oscillates in a precise frequency - generates an electric field as it returns to its previous shape, and this can generate a voltage. The result is that a quartz crystal behaves like an RLC circuit (resistor (R), inductor (L), and capacitor (C)), but with a much higher Q factor. Quartz crystals are manufactured for frequencies from a few tens of kilohertz to hundreds of megahertz. More than two billion crystals are manufactured annually. Most are used for consumer devices such as wristwatches, clocks, radios, computers, cellphones, signal generators and oscilloscopes. [3 - 5]
But other crystals such as rhodochrosite also have piezoelectric properties. The rhodochrosite as crystal oscillator for being an alternative to those of quartz. The rhodochrosite ($MnC0_3$) shows complete solid solution with siderite ($FeC0_3$), and it may contain substantial amounts of Zn, Mg, Co, and Ca. The Kutnohorite [$CaMn\ (C0_3)_2$] is a dolomite group mineral intermediary between rhodochrosite and calcite. [3 - 5]

Fig. 1: Rolled Rhodochrosite from Argentina. Ruler in Centimeters [6].

2. Methods

A molecular dynamic via molecular mechanics using the UFF (Universal Forces Field) may provide the vibrational frequencies of the fundamental structure of the crystal molecule in an Bases set Zero Differential Overlap (ZDO) [7-10].
In short the goal of molecular mechanics is to predict the detailed structure and physical properties of molecules. Examples of physical properties that can be calculated include enthalpies of formation, entropies, dipole moments, and strain energies. Molecular mechanics calculates the energy of a molecule and then adjusts the energy through changes in bond lengths and angles to obtain the minimum energy structure. [7-10].

$$E_{se} = E_{str} + E_{bend} + E_{str-bend} + E_{oop} + E_{tor} + E_{vdW} + E_{qq} \quad (1)$$

The steric energy, bond stretching, bending, stretch-bend, out of plane, and torsion interactions are called bonded interactions because the atoms involved must be directly bonded or bonded to a common atom. The van der Waals and electrostatic (qq) interactions are between non-bonded atoms. [7-10]

2.1. Hardware and software

For calculations a computer models was used: Intel® Core™ i3-3220 CPU @ 3.3 GHz x 4 processors [12], Memory DDR3 4 GB, HD SATA WDC WD7500 AZEK-00RKKA0 750.1 GB and DVD-RAM SATA GH24NS9 ATAPI, Graphics Intel® Ivy Bridge [13].
For calculations of computational dynamics, the Ubuntu Linux version 16.10 system was used [14] and the software used for the molecular dynamics was GAMESS [15-16],

3. Results

Calculations using Molecular Mechanics and methods ab initio in this direction, based on the unit molecular structure of the rhodochrosite crystal, Figure (2), and experimental measurements could provide data from the pros and against the use of a crystal rhodochrosite oscillator, in an RLC circuit, replacing a crystal quartz oscillator.

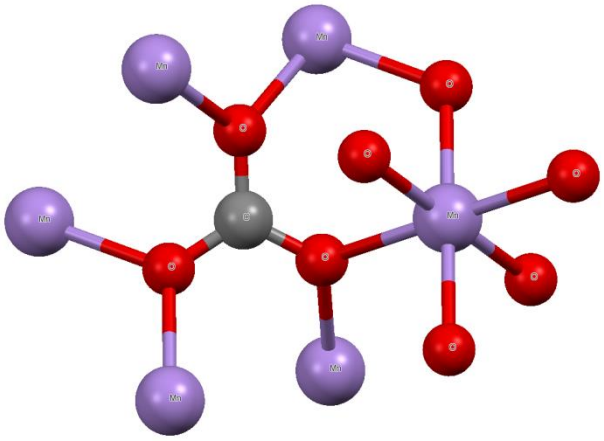

Fig. 2: Cell Structure of A Rhodochrosite Crystal. Represented in Red Color, Oxygen; in the Dark Gray Color, the Carbon and in the Purple Color, The Manganese. [74-78].

Table 1: Rhodocrosite Crystal Vibrational Energy

E (Thermal)	E (Thermal) (KCal/Mol)	CV (Cal/Mol-Kelvin)	S (Cal/Mol-Kelvin)
Electronic	0	0	0
Translational	0.889	2.981	44.328
Rotational	0.889	2.981	35.975
Vibrational	28.592	69.641	254.549
Total	30.369	75.602	334.852

Table (1) shows the vibrational, rotational and translational energies for rhodocrosite crystal, obtained by UFF.

Table 2: Vibrational Temperatures (Kelvin) of Rhodochrosite Crystal

0.87	3.71	5.08	5.64	6.82
7.87	8.73	9.77	9.91	11.31
12.73	12.92	14.57	16.34	17.54
17.89	19.18	20.57	20.88	25.23
28.44	29.85	32.62	34.25	35.06
38.6	40.11	41.18	45.99	47.52
51.25	58.92	62.25	271.71	996.22
996.4	1287.09	2491.01	2491.06	

Table (2) shows the temperatures in Kelvin the crystal of rhodochrosite, obtained by UFF.

Table 3: Vibrational Frequencies (Cm^{-1}) of Rhodochrosite Crystal

0.6059	2.5772	3.5287	3.9185	4.7399	5.4673	6.069

6.7922	6.8885	7.8622	8.8445	8.9819	10.1271	11.3539
12.193	12.4363	13.3317	14.2963	14.51	17.5325	19.7635
20.7445	22.6701	23.8052	24.3696	26.83	27.8756	28.6216
31.9667	33.0292	35.622	40.949	43.268	188.85	692.41
692.534	894.574	1731.34	1731.38	-	-	-

Table (3) shows the vibrational frequencies in Kelvin the crystal of rhodochrosite, obtained by UFF.

4. Conclusion

The total thermal energy of the rhodochrosite crystal is 30.369 (KCal/Mol), its specific heat is 75.602 (Cal /Mol-Kelvin) and its entropy is 334.852 (Cal/Mol-Kelvin).
The frequencies and vibrational temperatures of the unit cell of rhodochrosite obtained by UFF were calculated in the range from 0.6059 to 1,731.38 cm^{-1} and 0.87 to 2,491.06 K, respectively.
Later studies could check the advantages and disadvantages of rhodochrosite versus quartz crystal, such as crystal oscillator.

References

[1] *F. James Holler, Douglas A. Skoog and Stanley R. Crouch. Principles of Instrumental Analysis (6th ed.). Cengage Learning. 200, p. 9. ISBN 978-0-495-01201-6.*
[2] Fox Electronics. Quartz Crystal Theory of Operation and Design Notes. Oscillator Theory of Operation and Design Notes. 2008. Available in: April 16, 2019. URL: https://web.archive.org/web/20110725032851/http://www.foxonline.com/techdata.htm
[3] R. E. Newnham. Properties of materials. Anisotropy, Simmetry, Structure. Oxford University Press, New York, 2005.
[4] C. D. Gribble and A. J. Hall. A Practical Introduction to Optical Mineralogy. 1985. https://doi.org/10.1007/978-94-011-7804-4.
[5] Creative Commons. (CC-BY 4.0). *Wikipedia, The Free Encyclopedia*, May 2019. URL: https://creativecommons.org/licenses/by/4.0/,
[6] Talismã de Cristal, Porto Alegre, Rio Grande do Sul, 2019. Available in April 09, 2019. URL: http://www.talismadecristal.com.br/Produto/Relacionamentos/213.
[7] A. K. Rappe, C. J. Casewit, K. S. Colwell, W. A. Goddard III, W. M. Skiff. "UFF, a Full Periodic Table Force Field for Molecular Mechanics and Molecular Dynamics Simulations". *J.Am. Chem. Soc.* 114 (1992) 10024–10035. https://doi.org/10.1021/ja00051a040.
[8] E. Eliav. Elementary introduction to Molecular Mechanics and Dynamics, Jun 2013.
[9] W. J. Hehre. A Guide to Molecular Mechanics and Quantum Chemical Calculations, Wavefunction. Inc., Irvine, CA, 2003.
[10] I. N. Levine. Quantum Chemistry. Pearson Education (Singapore) Pte. Ltd., Indian Branch, 482 F. I. E. Patparganj, Delhi 110 092, India, 5th ed edition, 2003.
[11] W. D. Cornell; P. Cieplak; C. I.Bayly; I. R. Gould; K. M. Merz Jr.; D. M. Ferguson; D. C. Spellmeyer; T. Fox; J. W. Caldwell and P. A. Kollman. A Second-Generation Force Field for the Simulation of Proteins, Nucleic Acids, and Organic Molecules. J. Am. Chem. Soc., 117:5179–5197, 1995. https://doi.org/10.1021/ja00124a002.
[12] Creative Commons, (CC BY 4.0), https://creativecommons.org/licenses/by/4.0/. "List of Intel Core i3 microprocessors", https://en.wikipedia.org/wiki/List_of_Intel_Core_i3_microprocessors, Access in: August 30, 2018.
[13] "Ivy Bridge", https://pt.wikipedia.org/wiki/Ivy_Bridge, Access in: August 31, 2018.
[14] "Ubuntu (operating system)", https://en.wikipedia.org/wiki/Ubuntu_(operating_system), Access in: August 31, 2018.
[15] M. S. Gordon and M. W. Schmidt. Advances in electronic structure theory: GAMESS a decade later. Theory and Applications of Computational Chemistry: the first forty years. Elsevier. C. E. Dykstra, G. Frenking, K. S. Kim and G.E. Scuseria (editors), pages 1167–1189, 2005. Amsterdam. https://doi.org/10.1016/B978-044451719-7/50084-6.
[16] M. S. Gordon et al. General Atomic and Molecular Electronic Structure System (GAMESS). J. Comput. Chem., 14:1347–1363, 1993. https://doi.org/10.1002/jcc.540141112.
[17] R. Gobato, A. Gobato, D. F. G. Fedrigo, "Inorganic arrangement crystal beryllium, lithium, selenium and silicon". In XIX Semana da Física. Simpósio Comemorativo dos 40 anos do Curso de Física da Universidade Estadual de Londrina, Brazil, 2014. *Universidade Estadual de Londrina* (UEL).
[18] R. Gobato, "Benzocaína, um estudo computacional", Master's thesis, *Universidade Estadual de Londrina* (UEL), 2008.
[19] R. Gobato, "Study of the molecular geometry of Caramboxin toxin found in star flower (*Averrhoa* carambola L.)". *Parana J. Sci. Edu,* 3(1):1–9, January 2017.
[20] R. Gobato, A. Gobato, D. F. G. Fedrigo, "Molecular electrostatic potential of the main monoterpenoids compounds found in oil Lemon Tahiti - (*Citrus Latifolia* Var Tahiti)". *Parana J. Sci. Edu.*, 1(1):1–10, November 2015.
[21] R. Gobato, D. F. G. Fedrigo, A. Gobato, "Allocryptopine, Berberine, Chelerythrine, Copsitine, Dihydrosanguinarine, Protopine and Sanguinarine. Molecular geometry of the main alkaloids found in the seeds of *Argemone Mexicana Linn". Parana J. Sci. Edu.*, 1(2):7–16, December 2015.
[22] R. Gobato, A. Heidari, "Infrared Spectrum and Sites of Action of Sanguinarine by Molecular Mechanics and *ab initio* Methods", *International Journal of Atmospheric and Oceanic Sciences*. Vol. 2, No. 1, 2018, pp. 1-9. https://doi.org/10.11648/j.ijaos.20180201.11.
[23] R. Gobato, D. F. G. Fedrigo, A. Gobato, "Molecular geometry of alkaloids present in seeds of mexican prickly poppy". *Cornell University Library.* Quantitative Biology, Jul 15, 2015. arXiv:1507. 05042.
[24] R. Gobato, A. Gobato, D. F. G. Fedrigo, "Study of the molecular electrostatic potential of D-Pinitol an active hypoglycemic principle found in Spring flower Three Marys (*Bougainvillea species*) in the Mm+ method". *Parana J. Sci. Educ.*, 2(4):1–9, May 2016.
[25] R. Gobato, D. F. G. Fedrigo, A. Gobato, "Avro: key component of Lockheed X-35", *Parana J. Sci. Educ*., 1(2):1–6, December 2015.
[26] R. Gobato, D. F. G. Fedrigo, A. Gobato, "LOT-G3: Plasma Lamp, Ozonator and CW Transmitter", *Ciencia e Natura*, 38(1), 2016. https://doi.org/10.5902/2179460X19387.
[27] R. Gobato, "Matter and energy in a non-relativistic approach amongst the mustard seed and the faith. A metaphysical conclusion". *Parana J. Sci. Educ.*, 2(3):1–14, March 2016.
[28] R. Gobato, A. Gobato, D. F. G. Fedrigo, "Harnessing the energy of ocean surface waves by Pelamis System", *Parana J. Sci. Educ.*, 2(2):1–15, February 2016.
[29] R. Gobato, A. Gobato, D. F. G. Fedrigo, "Mathematics for input space probes in the atmosphere of Gliese 581d", *Parana J. Sci. Educ.*, 2(5):6–13, July 2016.
[30] R. Gobato, A. Gobato, D. F. G. Fedrigo, "Study of tornadoes that have reached the state of Parana". *Parana J. Sci. Educ.*, 2(1):1–27, 2016.
[31] R. Gobato, M. Simões F. "Alternative Method of RGB Channel Spectroscopy Using a CCD Reader", *Ciencia e Natura*, 39(2), 2017. https://doi.org/10.5902/2179460X25617.
[32] R. Gobato, A. Heidari, "Calculations Using Quantum Chemistry for Inorganic Molecule Simulation $BeLi_2SeSi$", *Science Journal of Analytical Chemistry*, 5(5):76–85, September 2017. https://doi.org/10.11648/j.sjac.20170505.13.

[33] M. R. R. Gobato, R. Gobato, A. Heidari, "Planting of Jaboticaba Trees for Landscape Repair of Degraded Area", *Landscape Architecture and Regional Planning*, 3(1):1–9, March 18, 2018. https://doi.org/10.11648/j.larp.20180301.11.

[34] R. Gobato, "The Liotropic Indicatrix", 2012, 114 p. Thesis (Doctorate in Pysics). *Universidade Estadual de Londrina*, Londrina, 2012.

[35] R. Gobato, A. Heidari, "Calculations Using Quantum Chemistry for Inorganic Molecule Simulation $BeLi_2SeSi$", *Science Journal of Analytical Chemistry*, Vol. 5, No. 6, Pages 76–85, 2017. https://doi.org/10.11648/j.sjac.20170505.13.

[36] M. R. R Gobato, R. Gobato, A. Heidari, "Planting of Jaboticaba Trees for Landscape Repair of Degraded Area", *Landscape Architecture and Regional Planning*, Vol. 3, No. 1, 2018, Pages 1–9, 2018. https://doi.org/10.11648/j.larp.20180301.11.

[37] R. Gobato, A. Heidari, "Molecular Mechanics and Quantum Chemical Study on Sites of Action of Sanguinarine Using Vibrational Spectroscopy Based on Molecular Mechanics and Quantum Chemical Calculations", *Malaysian Journal of Chemistry*, Vol. 20(1), 1–23, 2018. https://doi.org/10.11648/j.ijaos.20180201.11.

[38] A. Heidari, R. Gobato. "A Novel Approach to Reduce Toxicities and to Improve Bioavailabilities of DNA/RNA of Human Cancer Cells–Containing Cocaine (Coke), Lysergide (Lysergic Acid Diethyl Amide or LSD), Δ⁹–Tetrahydrocannabinol (THC) [(–)–trans–Δ⁹–Tetrahydrocannabinol], Theobromine (Xantheose), Caffeine, Aspartame (APM) (NutraSweet) and Zidovudine (ZDV) [Azidothymidine (AZT)] as Anti–Cancer Nano Drugs by Coassembly of Dual Anti–Cancer Nano Drugs to Inhibit DNA/RNA of Human Cancer Cells Drug Resistance", *Parana Journal of Science and Education*, v. 4, n. 6, pp. 1–17, 2018.

[39] A. Heidari, R. Gobato, "Ultraviolet Photoelectron Spectroscopy (UPS) and Ultraviolet–Visible (UV–Vis) Spectroscopy Comparative Study on Malignant and Benign Human Cancer Cells and Tissues with the Passage of Time under Synchrotron Radiation", *Parana Journal of Science and Education*, v. 4, n. 6, pp. 18–33, 2018.

[40] R. Gobato, A. Heidari, "Using the Quantum Chemistry for Genesis of a Nano Biomembrane with a Combination of the Elements Be, Li, Se, Si, C and H", *J Nanomed Res.*, 7 (4): 241-252, 2018.

[41] S. K. Agarwal, S. Roy, P. Pramanick, P. Mitra, R. Gobato, A. Mitra, "*Marsilea quadrifolia*: A floral species with unique medicinal properties", *Parana J. Sci. Educ*., v.4, n.5, (15–20), July 1, 2018.

[42] A. Mitra, S. Zaman, R. Gobato. "Indian Sundarban Mangroves: A potential Carbon Scrubbing System". *Parana J. Sci. Educ.*, v.4, n.4, (7–29), June 17, 2018.

[43] O. Yarman, R. Gobato, T. Yarman, M. Arik. "A new Physical constant from the ratio of the reciprocal of the "Rydberg constant" to the Planck length". *Parana J. Sci. Educ*., v.4, n.3, (42–51), April 27, 2018.

[44] R. Gobato, M. Simões F., "Alternative Method of Spectroscopy of Alkali Metal RGB", *Modern Chemistry*. Vol. 5, No. 4, 2017, pp. 70–74. https://doi.org/10.11648/j.mc.20170504.13.

[45] D. F. G. Fedrigo, R. Gobato, A. Gobato, "Avrocar: a real flying saucer", *Cornell University Library*. 24 Jul 2015. arXiv:1507.06916v1 [physics.pop–ph].

[46] M, Simões F., A. J. Palangana, R. Gobato, O. R. Santos, "Micellar shape anisotropy and optical indicatrix in reentrant isotropic—nematic phase transitions", *The Journal of Chemical Physics*, 137, 204905 (2012); https://doi.org/10.1063/1.4767530.

[47] A. Heidari, R. Gobato, "Putrescine, Cadaverine, Spermine and Spermidine–Enhanced Precatalyst Preparation Stabilization and Initiation (EPPSI) Nano Molecules", Parana Journal of Science and Education (PJSE)–v.4, n.5, (1–14) July 1, 2018. https://doi.org/10.15761/GII.1000162.

[48] R. Gobato, A. Heidari, "Molecular Mechanics and Quantum Chemical Study on Sites of Action of Sanguinarine Using Vibrational Spectroscopy Based on Molecular Mechanics and Quantum Chemical Calculations", Malaysian Journal of Chemistry, Vol. 20 (1), 1–23, 2018. https://doi.org/10.11648/j.ijaos.20180201.11.

[49] R. Gobato, A. Heidari, A. Mitra, "The Creation of C13H20BeLi2SeSi. The Proposal of a Bio–Inorganic Molecule, Using Ab Initio Methods for the Genesis of a Nano Membrane", Arc Org Inorg Chem Sci 3 (4). AOICS.MS.ID.000167, 2018. https://doi.org/10.32474/AOICS.2018.03.000167.

[50] R. Gobato, A. Heidari, A. Mitra, "Using the Quantum Chemistry for Genesis of a Nano Biomembrane with a Combination of the Elements Be, Li, Se, Si, C and H", ResearchGate, See discussions, stats, and author profiles for this publication at: https://www.researchgate.net/publication/326201181, 2018.

[51] A. Heidari, R. Gobato, "First–Time Simulation of Deoxyuridine Monophosphate (dUMP) (Deoxyuridylic Acid or Deoxyuridylate) and Vomitoxin (Deoxynivalenol (DON)) ((3α,7α)–3,7,15–Trihydroxy–12,13–Epoxytrichothec–9–En–8–One)–Enhanced Precatalyst Preparation Stabilization and Initiation (EPPSI) Nano Molecules Incorporation into the Nano Polymeric Matrix (NPM) by Immersion of the Nano Polymeric Modified Electrode (NPME) as Molecular Enzymes and Drug Targets for Human Cancer Cells, Tissues and Tumors Treatment under Synchrotron and Synchrocyclotron Radiations", Parana Journal of Science and Education, Vol. 4, No. 6, pp. 46–67, 2018.

[52] R. Gobato, M. R. R. Gobato, A. Heidari, A. Mitra, "Spectroscopy and Dipole Moment of the Molecule C13H20BeLi2SeSi via Quantum Chemistry Using Ab Initio, Hartree–Fock Method in the Base Set CC–pVTZ and 6–311G**(3df, 3pd)", Arc Org Inorg Chem Sci 3 (5), Pages 402–409, 2018. https://doi.org/10.32474/AOICS.2018.03.000171.

[53] R. Gobato, M. R. R. Gobato, A. Heidari, A. Mitra, "Spectroscopy and Dipole Moment of the Molecule C13H20BeLi2SeSi via Quantum Chemistry Using Ab Initio, Hartree–Fock Method in the Base Set CC–pVTZ and 6–311G**(3df, 3pd)", American Journal of Quantum Chemistry and Molecular Spectroscopy, Vol. 2, No. 1, pp. 9–17, 2018. https://doi.org/10.32474/AOICS.2018.03.000171.

[54] R. Gobato, M. R. R. Gobato, A. Heidari, "Raman Spectroscopy Study of the Nano Molecule C13H20BeLi2SeSi Using ab initio and Hartree–Fock Methods in the Basis Set CC–pVTZ and 6–311G** (3df, 3pd)", International Journal of Advanced Engineering and Science, Volume 7, Number 1, Pages 14–35, 2019. https://doi.org/10.32474/AOICS.2018.03.000171.

[55] A. Heidari, R. Gobato, "Evaluating the Effect of Anti–Cancer Nano Drugs Dosage and Reduced Leukemia and Polycythemia Vera Levels on Trend of the Human Blood and Bone Marrow Cancers under Synchrotron Radiation", Trends in Res, Volume 2 (1): 1–8, 2019.

[56] A. Heidari, R. Gobato, "Assessing the Variety of Synchrotron, Synchrocyclotron and LASER Radiations and Their Roles and Applications in Human Cancer Cells, Tissues and Tumors Diagnosis and Treatment", Trends in Res, Volume 2 (1): 1–8, 2019. https://doi.org/10.23880/MACIJ-16000111.

[57] A. Heidari, R. Gobato, "Pros and Cons Controversy on Malignant Human Cancer Cells, Tissues and Tumors Transformation Process to Benign Human Cancer Cells, Tissues and Tumors", Trends in Res, Volume 2 (1): 1–8, 2019.

[58] A. Heidari, R. Gobato, "Three–Dimensional (3D) Simulations of Human Cancer Cells, Tissues and Tumors for Using in Human Cancer Cells, Tissues and Tumors Diagnosis and Treatment as a Powerful Tool in Human Cancer Cells, Tissues and Tumors Research and Anti–Cancer Nano Drugs Sensitivity and Delivery Area Discovery and Evaluation", Trends in Res, Volume 2 (1): 1–8, 2019.

[59] A. Heidari, R. Gobato, "Investigation of Energy Production by Synchrotron, Synchrocyclotron and LASER Radiations in Human Cancer Cells, Tissues and Tumors and Evaluation of Their Effective on Human Cancer Cells, Tissues and Tumors Treatment Trend", Trends in Res, Volume 2 (1): 1–8, 2019. https://doi.org/10.23880/MACIJ-16000111.

[60] A. Heidari, R. Gobato, "High–Resolution Mapping of DNA/RNA Hypermethylation and Hypomethylation Process in Human Cancer Cells, Tissues and Tumors under Synchrotron Radiation", Trends in Res, Volume 2 (2): 1–9, 2019.

[61] R. Gobato, M. R. R. Gobato, A. Heidari, "Storm Vortex in the Center of Paraná State on June 6, 2017: A Case Study", Sumerianz Journal of Scientific Research, Vol. 2, No. 2, Pages 24–31, 2019.

[62] R. Gobato, M. R. R. Gobato, A. Heidari, "Attenuated Total Reflection–Fourier Transform Infrared (ATR–FTIR) Spectroscopy Study of the Nano Molecule C13H20BeLi2SeSi Using ab initio and Hartree–Fock Methods in the Basis Set RHF/CC– pVTZ and RHF/6–311G** (3df, 3pd): An Experimental Challenge to Chemists", Chemistry Reports, Vol. 2, No. 1, Pages 1–26, 2019. https://doi.org/10.32474/AOICS.2018.03.000171.

[63] R. Gobato, M. R. R. Gobato, A. Heidari, A. Mitra, "New Nano–Molecule Kurumi–C13H 20BeLi2SeSi/C13H19BeLi2SeSi, and Raman Spectroscopy Using ab initio, Hartree–Fock Method in the Base Set CC–pVTZ and 6–311G** (3df, 3pd)", J Anal Pharm Res. 8 (1): 1-6, 2019. https://doi.org/10.32474/AOICS.2018.03.000171.

[64] R. Gobato, M. R. R. Gobato, A. Heidari, "Evidence of Tornado Storm Hit the Counties of Rio Branco do Ivaí and Rosario de Ivaí, Southern Brazil", Sci Lett 7 (1), 9 Pages, 2019.
[65] Moharana Choudhury, Pardis Fazli, Prosenjit Pramanick, Ricardo Gobato, Sufia Zaman, Abhijit Mitra, "Sensitivity of the Indian Sundarban mangrove ecosystem to local level climate change", Parana Journal of Science and Education. Vol. 5, No. 3, 2019, pp. 24-28.
[66] Arpita Saha, Ricardo Gobato, Sufia Zaman, Abhijit Mitra, "Biomass Study of Mangroves in Indian Sundarbans: A Case Study from Satjelia Island", Parana Journal of Science and Education. Vol. 5, No. 2, 2019, pp. 1-5.
[67] Nabonita Pal, Arpan Mitra, Ricardo Gobato, Sufia Zaman, Abhijit Mitra, "Natural Oxygen Counters in Indian Sundarbans, the Mangrove Dominated World Heritage Site", Parana Journal of Science and Education. Vol. 5, No. 2, 2019, pp. 6-13.
[68] Ricardo Gobato, Victoria Alexandrovna Kuzmicheva, Valery Borisovich Morozov, ―Einstein's hypothesis is confirmed by the example of the Schwarzschild problem", Parana Journal of Science and Education, Vol. 5, No. 1, 2019, pp. 1-6.
[69] Sufia Zaman, Ricardo Gobato, Prosenjit Pramanick, Pavel Biswas, Uddalok Chatterjee, Shampa Mitra, Abhijit Mitra, "Water quality of the River Ganga in and around the city of Kolkata during and after Goddess Durga immersion", Parana Journal of Science and Education, Vol. 4, No. 9, 2018, pp. 1-7.
[70] Ozan Yarman, Metin Arik, Ricardo Gobato, Tolga Yarman, Clarification of "Overall Relativistic Energy" According to Yarman's Approach.", Parana Journal of Science and Education., v.4, n.8, 2018, pp. 1-10. https://doi.org/10.1016/j.rinp.2018.06.058.
[71] Sufia Zaman, Utpal Pal, Ricardo Gobato, Alekssander Gobato, Abhijit Mitra, "The Changing Trends of Climate in Context to Indian Sundarbans", Parana Journal of Science and Education, Vol. 4, No. 7, 2018, pp. 24-28.
[72] Suresh Kumar Agarwal, Sitangshu Roy, Prosenjit Pramanick, Prosenjit Mitra, Ricardo Gobato and Abhijit Mitra. Parana Journal of Science and Education. Vol. 4, No. 5, 2018, pp. 15-20.
[73] Ricardo Gobato and Marcia Regina Risso Gobato, "Evidence of Tornadoes Reaching the Countries of Rio Branco do Ivai and Rosario de Ivai, Southern Brazil on June 6, 2017", Climatol Weather Forecasting 2018, 6:4. DOI: 10.4172/2332-2594.1000242.
[74] Ricardo Gobato. "New Nano-Molecule Kurumi and Raman Spectroscopy using ab initio, Hartree-Fock Method" Am J Biomed Sci & Res. 2019 - 2(4). AJBSR.MS.ID.000594. https://doi.org/10.34297/AJBSR.2019.02.000594.
[75] D. L. Graf, Rhodochrosite, Crystallographic tables for the rhombohedral carbonates, American Mineralogist 46 (1961) 1283-1316.
[76] E. N. Maslen, V. A. Streltsov, N. R. Streltsova, N. Ishizawa, Electron density and optical anisotropy in rhombohedral carbonates. III. Synchrotron X-ray studies of CaCO3, MgCO3 and MnCO3, Acta Crystallographica B51 (1995) 929-939. https://doi.org/10.1107/S0108768195006434.
[77] R. Wyckoff, The crystal structures of some carbonates of the calcite group, American Journal of Science 50 (1920) 317-360. https://doi.org/10.2475/ajs.s4-50.299.317.
[78] Avogadro: an open-source molecular builder and visualization tool. Version 1.1.1. http://avogadro.cc/
[79] D. Marcus, D. E. Hanwell, D. C. Curtis, T. V Lonie, E. Zurek, G. R. Hutchison, "Avogadro: An advanced semantic chemical editor, visualization, and analysis platform" *Journal of Cheminformatics* 2012, 4:17. https://doi.org/10.1186/1758-2946-4-17.