Infrared Spectroscopy of the two esters from 2,3,4,5-Tetrahydro-oxepine derivatives, new nano molecules

Ricardo Gobato[1,*], Alireza Heidari[2], Lauro Figueroa Valverde[3] Abhijit Mitra[4], Marcela Rosas Nexticapa[5], Maria López Ramos[3], Maria Virginia del Socorro Mateu Armad[5], Magdalena Alvarez Ramirez[5], Francisco Díaz Cedillo[6], Ibtihal Kadhim Kareem Dosh[7]

[1]Green Land Landscaping and Gardening, Seedling Growth Laboratory, 86130-000, Parana, Brazil.

[2]Faculty of Chemistry, California South University, 14731 Comet St. Irvine, CA 92604, USA, United States of America.

[3]University Autonomous of Campeche (Faculty of Chemical-Biological Sciences), Calle Av. Agustín Melgar s/n, Buenavista, 24039 Campeche, Mexico.

[4]Department of Marine Science, University of Calcutta, 35 B. C Road, Kolkata, 700019, West Bengal, India.

[5]Facultad de Nutrición, Universidad Veracruzana, Médicos y Odontologos s/n C.P. 91010, Unidad del Bosque, Xalapa, Veracruz, Mexico.

[6]Escuela Nacional de Ciencias Biológicas del Instituto Politécnico Nacional. Prol. Carpio y Plan. de Ayala s/n Col. Santo Tomas, D.F. C.P. 11340, Mexico.

[7]Kufa University, Faculty of Education, Department of Chemistry, An Najaf, Iraq.

[*]Corresponding author: ricardogobato@hotmail.com; ricardogobato@gardener.com

Abstract—The work focused on determining the Infrared spectroscopy (IRS) of the two compounds calculated are from two esters (compounds C1 and C2) from 2,3,4,5-Tetrahydro-oxepine derivatives, here called C1 and C2. The IRS was obtained via computational methods *ab initio* Restricted Hartree-Fock. Optimization of molecular structure via UFF, followed by PM3, RHF/EPR-II and RHF/STO-6G, thus obtaining a stable structure, in STP. The molecule was obtained, whose composition is C: 81.7%; H: 7.1%; N: 3.4%; O: 7.8%, 411.53536 g, and molecular formula: $C_{28}H_{29}NO_2$, for C1 and C: 70.6%; H: 7.4%; N: 10.3%; O: 11.7%, 544.68439 g, and molecular formula: $C_{32}H_{40}N_4O_4$. The highest vibrational absorbance frequency peaks for the C1 and C2 molecule are found at the frequency of 1793.58 cm^{-1}, 1867.14 cm^{-1} and 1956.39 cm^{-1}, for C1 and 1368.99 cm^{-1}, 1409.43 cm^{-1} and 1790.47 cm^{-1}, for C2, respectively. Limitations our study has so far been limited to computational simulation via quantum mechanics (QM) an applied theory. Our results and calculations are compatible with the theory of QM.

Index Terms—Restricted Hartree-Fock method, Infrared spectroscopy, IR spectroscopy, UFF, PM3, EPR-II.

I. INTRODUCTION

The Infrared spectroscopy (IRS) is the measurement of the interaction of infrared radiation with matter by absorption, emission, or reflection. It is used to study and identify chemical substances or functional groups in solid, liquid, or gaseous forms. The method or technique of IRS is conducted with an instrument called spectrophotometer which produces an IRS. An IRS can be visualized in a graph of infrared light absorbance (or transmittance) on the vertical axis vs. frequency or wavelength on the horizontal axis. [1], [2], [3]

The work focused on determining the IRS [1], [2], [3] of the three compounds here named C1 and C2, where the IRS was obtained via computational methods *ab initio* Restricted Hartree-Fock. [4], [5], [6], [7], [8], [9], [10], [11], [12], [13] [14], [15], [16].

The molecules was obtained experimentally in the laboratory of the University Autonomous of Campeche (Faculty of Chemical-Biological Sciences) Valverde et al. [17], [18], [19], [20], [21] and are characterized by two-ester structures: 2,3,4,5-Tetrahydro-oxepine derivatives, compounds C1 and C2.

II. METHODS

A. *Methodology*

Its structure and chemical conformation and its IRS were obtained from computational chemistry calculations, using the GAMESS software. [15], [22]

The methods used initially were UFF (Universal Force Field) [23], [24], [22], [25], obtaining the lowest energy molecular structure. Optimization of molecular structure via UFF, followed by PM3 (Parametric Method 3) [26], [27], [28], [29], followed by Restricted Hartree-Fock [4], [5], [6], [7], [8], [9], [10], [11], [12], [13] [14], [15], [16] RHF/EPR-II

GOBATO, R. *et al.*: INFRARED SPSCTROSCOPY OF THE TWO ESTERS FROM 2,3,4,5-TETRAHYDRO-OXEPINE DERIVATIVES, NEW NANO MOLECULES

2

and RHF/STO-6G[1], thus obtaining a stable structure, in STP (Standard Temperature and Pressure) [23], [24], [22], [25].

The molecular Hartree-Fock [4], [5], [6], [7], [8], [9], [10], [11], [12], [13] [14], [15], [16] wave function is written as an antisymmetrized product (Slater determinant) of spin-orbitals, each spin-orbital being a product of a spatial orbital φ_i and a spin function (either α or β) was used. The basis sets of Barone [30] which are optimized for the computation of hyperfine coupling constants. EPR-II (Electron Paramagnetic Resonance II) is a double zeta basis set with a single set of polarization functions.

B. *Hardware and Software*

For calculations the computer used a Desktop with SUSE Linux Enterprise Desktop[2], AMD Ryzen 7 1800X processor [31], ASUS Prime A320M-K motherboard [32], 16GB of RAM, with 500GB SSD [33].

The *ab initio* calculations have been performed to study the equilibrium configuration of C1 and C2 molecules. The set of programs GaussView 5.0.8 [34], HyperChem 8.0.6 Evaluation [35], are the advanced semantic chemical editor, visualization, and analysis platform and GAMESS [15], [22], [34] is a computational chemistry software program and stands for General Atomic and Molecular Electronic Structure System [15], [34], BIOVIA Draw 2017 [36], CHARMM22 [37], [38], and OriginLab ®2018 Evaluation Licence [39], set of programs were used.

III. RESULTS

The molecular structure of C1 and C2 molecules, were obtained through computationally calculated obtained after molecular optimization, using the *ab initio* Hartree-Fock (HF) method, Figure (1) left side.

The names of the two compounds calculated are from two esters (compounds C1 and C2) from 2,3,4,5-Tetrahydro-oxepine, Figure (1), right side shows, obtained experimentally in the laboratory of the University Autonomous of Campeche (Faculty of Chemical-Biological Sciences) Valverde et al. [17], [18], [19], [20], [21].

The Table (1) on the shows the properties of compounds C1 and C2, obtained BIOVIA Draw 2017 software [36].

The Compound C1 presents normalized absorption peaks of 20-25% between frequencies 410-530 cm^{-1}, 25-70% between 1230-1550 cm-1, 40-100% between 1740-1960 cm^{-1} and 15-35% between 3170-3250 cm^{-1}, Figure (2).

The Compound C2 exhibits normalized sinusoidal absorption peaks of 5-15% between frequencies 360-1360 cm^{-1}. Normalized absorption peaks of 35-100% between frequencies
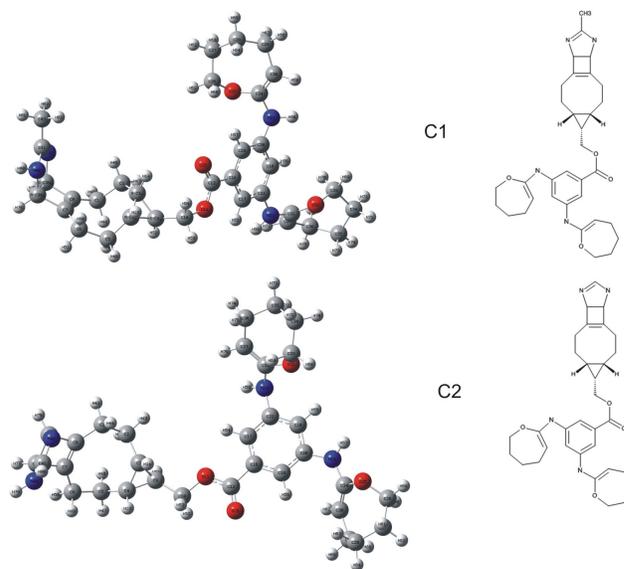
Fig. 1: Representation of the structure of the C1 and C2 molecules, obtained experimentally at the University Autonomous of Campeche (Faculty of Chemical-Biological Sciences) Valverde et al. [17], [18], [19], [20], [21], side right. On the left, the figures of the molecular structures of compounds C1 and C2, obtained after molecular optimization, using computational quantum chemistry methods, using the computer programs GAMESS [15], [22]. Subsequently, the UFF, PM3, *ab initio* RHF/EPR-II and RHF/STO-6G methods were used. Atoms are numbered and represented in colors: in blue the Nitrogen atom; in red the Oxygen atoms; in gray the Carbon atoms; blank Hydrogen atoms, side left.
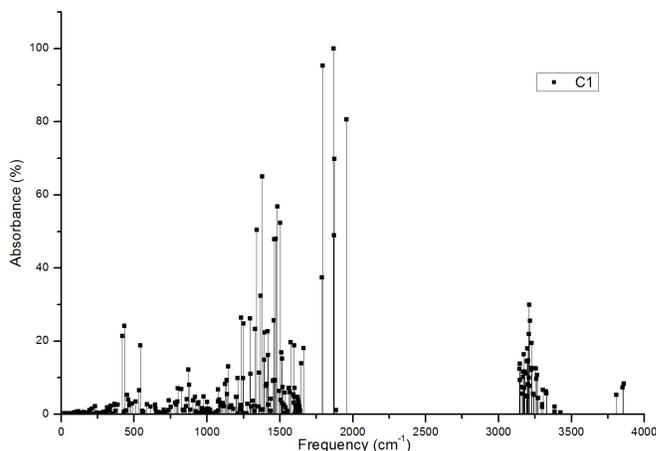
Fig. 2: The graph represents the infrared spectrum of the C1 molecule. Have the absorbance (%) normalized x frequency (cm^{-1}), obtained after molecular optimization, using computational quantum chemistry methods, using the computer programs GAMESS [15], [22]. Subsequently, the UFF, PM3, ab initio RHF/EPR-II and RHF/STO-6G methods were used. Graphic edited in OriginLab®2018 Evaluation software [39].

---

[1]STO-nG basis sets are minimal basis sets, where n primitive Gaussian orbitals are fitted to a single Slater-type orbital (STO). The *n* originally took the values 2–6.

[2]Suse. SUSE Linux Enterprise Desktop. Available in August 28, 2021. URL: https://www.suse.com/download/sled/
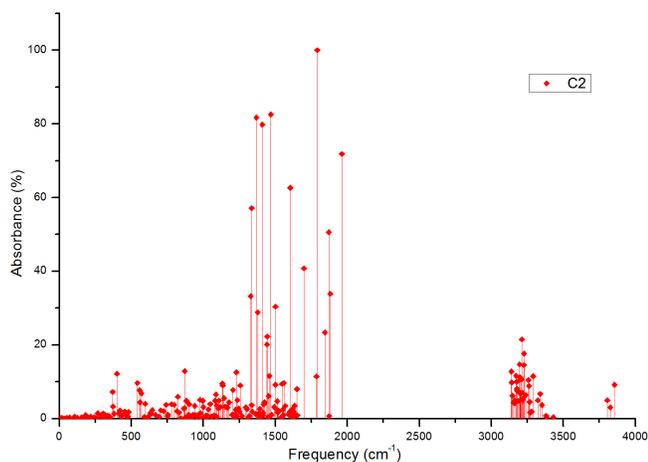
Fig. 3: The graph represents the infrared spectrum of the C2 molecule. Have the absorbance (%) normalized x frequency (cm^{-1}), obtained after molecular optimization, using computational quantum chemistry methods, using the computer programs GAMESS [15], [22]. Subsequently, the UFF, PM3, ab initio RHF/EPR-II and RHF/STO-6G methods were used. Graphic edited in OriginLab®2018 Evaluation software [39].
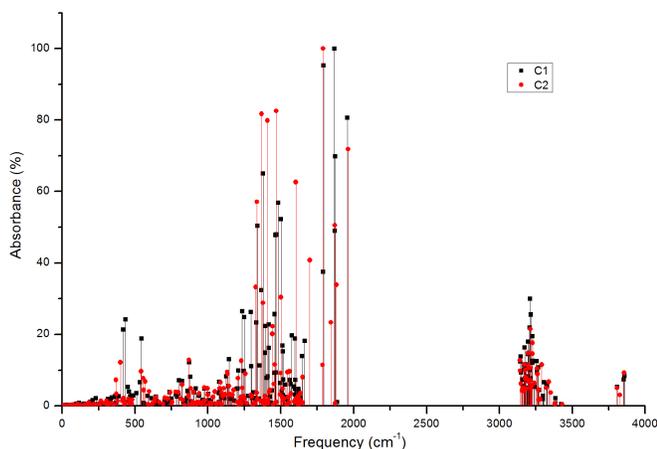
Fig. 4: The graph represents the infrared spectrum of the C1 and C2 molecules. Have the absorbance (%) normalized x frequency (cm^{-1}), obtained after molecular optimization, using computational quantum chemistry methods, using the computer programs GAMESS [15], [22]. Subsequently, the UFF, PM3, ab initio RHF/EPR-II and RHF/STO-6G methods were used. Graphic edited in OriginLab®2018 Evaluation software [39].

1300-1965 cm^{-1}, and parabolic absorption peaks of 10-25% between frequencies 3140-3250 cm^{-1}, Figure (3).

As expected, the infrared spectrum frequencies of compounds C1 and C2 are considerably similar, as they are derived from the same compound and have similar structures, Figure (4).

For C2 molecule, they present normalized sinusoidal absorption peaks that are amortized and energized between

TABLE I: The peaks with the highest absorbance intensity. Absorbance (km/mol) in function of vibrational frequencies (cm^{-1}) of C1 and C2 molecules for RHF/EPRII basis set

C1 (cm^{-1})	C1 I (km/mol)	C2 (cm^{-1})	C2 I (km/mol)
1340.31	199.9386	1328.81	172.3762
1378.75	258.0679	1335.90	296.3096
1789.38	148.5676	1368.99	423.6898
1793.58	377.9173	1409.43	414.0385
1867.14	396.7230	1698.92	211.5513
1871.04	194.1433	1790.47	518.6190
1873.74	277.0964	1844.08	121.3860
1956.39	319.7612	1870.87	262.2486
		1881.07	175.8778

5-25%, between frequencies 300-1200 cm^{-1}. Two expressive normalized absorption peaks between 18-83% and 40-100%, between frequencies 1200-1700 cm^{-1} and 1700-1960 cm^{-1}, respectively. Normalized absorption peaks of 5-30%, between frequencies 3150-3450 cm^{-1}. There are also small normalized absorption peaks between 5-10%, between 3800-3900 cm^{-1}, Figure (3).

The Representation of the molecular structure of the compounds C1 and C2, Figure (1), side left, obtained after molecular optimization, using computational quantum chemistry methods, using the computer programs GAMESS [15], [22]. Subsequently, the UFF, PM3, *ab initio* RHF/EPR-II and RHF/STO-6G methods were used. The Graphics edited in OriginLab®2018 Evaluation software [39].

The highest vibrational absorbance frequency peaks for the C1 molecule are found at the frequency of 1793.58 cm^{-1}, 1867.14 cm^{-1} and 1956.39 cm^{-1}, of intensity I 377.9173 km/mol, 396.7230 km/mol and 319.7612 km/mol, respectively, Table (1).

The highest peak vibrational absorbance frequency peaks for the C2 molecule are found at the frequency of 1368.99 cm^{-1}, 1409.43 cm^{-1} and 1790.47cm^{-1}, of intensity I 423.6898 km/mol, 414.0385 km/mol and 518.6190 km/mol , respectively, Table (1).

All Using computer programs GAMESS [15], [22], the calculations obtained in the *ab initio* RHF method.

IV. CONCLUSIONS AND CHALLENGES

The Infrared spectrum of the two 2,3,4,5-Tetrahydro-oxepine derivatives (Compounds C1 and C2) was calculated, indicating the characteristic of the nano-molecule genesis. Characterized was infrared spectrum quantum calculated, accepted by quantum chemistry parameters, with *ab initio* methods, in the RHF methods.

The molecule is named 2,3,4,5-Tetrahydro-oxepine derivatives (Compounds C1 and C2); of composition: C: 70.9%; H: 7.6%; N: 10%; O: 11.5%, formula weight: 558.71097g, and molecular formula: $C_{33}H_{42}N_4O_4$; of composition: C: 70.9%; H: 7.6%; N: 10%; O: 11.5%, formula

weight: 544.68439 g, and molecular formula: $C_{32}H_{40}N_4O_4$.

The highest vibrational absorbance frequency peaks for the C1 molecule are found at the frequency of 1793.58 cm^{-1}, 1867.14 cm^{-1} and 1956.39 cm^{-1}, of intensity I 377.9173 km/mol, 396.7230 km/mol and 319.7612 km/mol, respectively.

The highest peak vibrational absorbance frequency peaks for the C2 molecule are found at the frequency of 1368.99 cm^{-1}, 1409.43 cm^{-1} and 1790.47cm^{-1}, of intensity I 423.6898 km/mol, 414.0385 km/mol and 518.6190 km/mol , respectively.

Limitations our study has so far been limited to computational simulation via quantum mechanics (QM) an applied theory. Our results and calculations are compatible with the theory of QM, but their physical experimental verification depends on experimental data that should be laboratory for experimental biochemical.

REFERENCES

[1] D. A. Burns and E. W. Ciurczak, *Handbook of Near-infrared Analysis. Series: Practical spectroscopy 27*. M. Dekker ISBN: 0824705343,9780824705343,9780585417875., 2001.

[2] R. C. N. R., *Chemical Applications of Infrared Spectroscopy*. Academic Press, ISBN: 9780125802505,0125802501., 1963.

[3] H.-U. Gremlich and B. Yan, *Infrared and Raman Spectroscopy of Biological Materials. Series: Practical spectroscopy 24*. M. Dekker, ISBN: 0824704096,9780824704094, 2001.

[4] 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.

[5] A. Szabo and N. S. Ostlund, *Modern Quantum Chemistry*. Dover Publications, New York, 1989.

[6] W. Kohn and L. J. Sham, "Self-consistent equations including exchange and correlation effects," *Phys. Rev.*, vol. 140, p. A1133, 1965.

[7] J. M. Thijssen, *Computational Physics*. Cambridge University Press, Cambridge, 2001.

[8] T. H. D. Jr., "Gaussian basis sets for use in correlated molecular calculations, the atoms boron through neon and hydrogen," *J. Chem. Phys.*, vol. 90, pp. 1007–23, 1989.

[9] D. E. Woon and T. H. D. Jr., "Gaussian-basis sets for use in correlated molecular calculations. the atoms aluminum through argon," *J. Chem. Phys.*, pp. 1358–73, 1993.

[10] A. K. Wilson, T. van Mourik, and T. H. D. Jr., "Gaussian basis sets for use in correlated molecular calculations. sextuple zeta correlation consistent basis sets for boron through neon," *J. Mol. Struct. (Theochem)*, vol. 388, p. 339–49, 1996.

[11] E. Polak, *Computational Methods in Optimization*. v. 77. Elsevier, 111 Fifth Avenue, New York, New York 1000, 1971.

[12] T. H. D. Jr. and P. J. Hay, *Modern Theoretical Chemistry*. v. 3. Plenum, New York, 1977.

[13] E. Eliav, *Elementary introduction to Molecular Mechanics and Dynamics*. Jun. 2013.

[14] W. J. Hehre, *A Guide to Molecular Mechanics and Quantum Chemical Calculations, Wavefunction*. Inc., Irvine, 2003.

[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," p. 1167–1189, 2005.

[16] F. Weigend and R. Ahlrichs, "Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for h to rn: Design and assessment of accuracy," *Phys. Chem. Chem. Phys.*, vol. 7, p. 3297–305, 2005.

[17] L.-R. Maria, F.-V. Lauro, D.-C. Francisco, G. Ricardo, H. Alireza, R.-N. Marcela, M.-A. M. Virginia, and A. R. Magdalena, "Synthesis of two 2,3,4,5-tetrahydrooxepin-7-ylamino)benzoate derivatives as antibacterial agents against escherichia coli and staphylococcus aure.," *Vietnam Journal of Chemistry*, 2021(Accept).

[18] M. Lopez-Ramos, L. Figueroa-Valverde, F. Diaz-Cedillo, M. Rosas-Nexticapa, M. V. Mateu-Armand, E. Montano-Tapia, and E. García-Cervera., "Facile synthesis of some oxazepine- steroid using three component system," *Parana J. Sci. Educ.*, vol. 6, no. 1, pp. 34–45, 2018.

[19] L. Figueroa-Valverde, F. Díaz-Cedillo, M. López-Ramos, M. Rosas-Nexticapa, V. Mateu-Armad, A. Garcimarrero, and R. Cauich-Carrillo, "Experimental and theoretical evaluation of two indol-steroid-cyclobuta-imidazole derivatives as antibacterial drugs," *Bioniterface Res. Appl. Chem.*, vol. 9, no. 5, pp. 4405–4415, 2019.

[20] L. Figueroa-Valverde, F. Díaz-Cedillo, and A. A. Camacho-Luis, "Synthesis of a succinate–dihydrotestosterone–dihydropyrimidine conjugate," *Monats. Für Chem.*, vol. 141, no. 1, pp. 75–78, 2010.

[21] L. Figueroa-Valverde, M. Rosas-Nexticapa, M. Lopez-Ramos, and Diaz-Cedillo, "Synthesis of a new dioxaspiro [bicyclo [3.3. 1] nonane-oxabicyclo [6.2. 0] deca-1 (10), 8-dien-4-one derivative using some chemical strategies," *Lett. Org. Chem.*, vol. 17, no. 5, pp. 393–402, 2020.

[22] M. S. G. et al., "General atomic and molecular electronic structure system (gamess)," *J. Comput. Chem.*, vol. 14, p. 1347–1363, 1993.

[23] R. Gobato, A. Heidari, L. F. Valverde, A. Mitra, M. R. Nexticapa, M. L. Ramos, M. V. del Socorro Mateu Armad, M. A. Ramirez, and F. D. Cedillo, "1h nmr spectroscopy of the new xalapa molecule," *ResearchGate.net*, 2021.

[24] R. Gobato, M. R. R. Gobato, and 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," *International Journal of Advanced Engineering and Science*, vol. 7, no. 1, pp. 14–35, 2019.

[25] R. Gobato and 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, pp. 1–9, 2018.

[26] J. J. P. Stewart, "Optimization of parameters for semiempirical methods i. method," *J. Comput. Chem.*, vol. 10, no. 2, p. 209–220, 1989.

[27] J. J. P. Stewart, "Optimization of parameters for semiempirical methods ii. applications," *J. Comput. Chem.*, vol. 10, no. 2, p. 221–264, 1989.

[28] J. J. P. Stewart, "Optimization of parameters for semiempirical methods. iii extension of pm3 to be, mg, zn, ga, ge, as, se, cd, in, sn, sb, te, hg, tl, pb, and bi," *Journal of Computational Chemistry*, vol. 12, no. 3, p. 320–341, 1991.

[29] J. J. P. Stewart, "Optimization of parameters for semiempirical methods iv: Extension of mndo, am1, and pm3 to more main group elements," *Journal of Molecular Modeling*, vol. 10, no. 2, p. 155–64, 2004.

[30] V. Barone, *in Recent Advances in Density Functional Methods, Part I*. Ed. D. P. Chong (World Scientific Publ. Co., Singapore,, 1996.

[31] A. A. M. Devices, "Amd advanced micro devices (2021), inc processador amd ryzentm 7 1800x," p. Available in: Aug. 28, 2021.

[32] "Asus. amd am4 uatx motherboard with led lighting, ddr4 3200mhz, 32gb/s m.2, hdmi, sata 6gb/s, usb 3.0," Available in: Aug. 28, 2021.

[33] T. F. E. Wikipedia, "Solid-state drive," Wikipedia, The Free Encyclopedia, Available in: Aug. 28, 2021.

[34] R. Dennington, T. Keith, and J. Millam., "Gaussview, version 5," 2009.

[35] "Molecular modeling system. hyperchemtm 7.5 evaluation (2003) hypercube.," 2003.

[36] C. results obtained using software programs from Dassault Systèmes BIOVIA. The ab initio calculations were performed with the DMol3 program and graphical displays generated with Draw, "Biovia draw 2017 enterprise. mdl draw editor 17.1.0.900. ",," 2017.

[37] R. Brooks, R. E. Bruccoleri, B. D. Olafson, D. J. States, and S. Swaminathan, "Charmm: A program for macromolecular energy, minimization, and dynamics calculations," *J. Comp. Chem.*, vol. 4, pp. 187–217, 1983.

[38] M. Karplus, B. R. Brooks, C. L. B. III, A. D. M. Jr., L. Nilsson, R. J. Petrella, B. Roux, Y. Won, and e. a. M. Karplus, "Charmm: The biomolecular simulation program," *J. Comput. Chem*, vol. 30, pp. 1545–1614, 2009.

[39] "Originlab2018 evaluation licence, graphing & analysis, originlab corporation,"