Infrared Spectrum of New Nano-molecule Silicon-based

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November 21, 2026

Abstract

Through of restricted Hartree-Fock (RHF) computational simulation, the work was to determine the infrared spectrum and the stability of a silicon-based analog of the uracil molecule, in which all carbon atoms were replaced by silicon. A preliminary structural analysis was performed using molecular mechanics (MM) with UFF (Universal Force Field) to identify the most stable conformation. Subsequently, quantum chemical calculations were carried out using the RHF method, alongside molecular dynamics simulations, employing various basis sets: STO-3G (Slater-Type Orbital - 3 Gaussians) and cc-pVnZ (n = double, triple, quadruple and quintuple-zeta, respectively, *i.e.*, correlation-consistent polarized valence n-zeta). The infrared spectrum was obtained for each of these basis sets, and the molecule was found to possess a stable structure.cc-pVnZ. The maximum absorbance peaks for infrared spectrum in the STO-3G, cc-pVDZ, cc-pVTZ, cc-pVQZ and cc-pV5Z set basis are present at the frequencies 1121.08 cm^{-1}, 1399.34 cm^{-1}, 1430.56 cm^{-1}, 1430.38 cm^{-1}, 1428.02 cm^{-1}, with a normalized intensity of 100%, respectively.

Keywords: Hartree-Fock Methods, Uracil, Silicon, STO-3G, cc-pVnZ, Infrared spectrum, RNA.

1 Introduction

The objective of this work was to determine the infrared spectrum and the stability of a silicon-based analog of the uracil molecule, in which all carbon atoms were replaced by silicon. A preliminary structural analysis was performed using molecular mechanics (MM) with UFF (Universal Force Field) [1, 2] to identify the most stable conformation. Subsequently, quantum chemical calculations were carried out using the restricted Hartree-Fock (RHF) method [3-7], alongside molecular dynamics simulations, employing various basis sets: STO-3G (Slater-Type Orbital - 3 Gaussians) [8, 9], cc-pVDZ (correlation-consistent polarized valence double-zeta), cc-pVTZ (correlation-consistent polarized valence triple-zeta), cc-pVQZ correlation-consistent polarized valence quadruple-zeta and cc-pV5Z (correlation-consistent polarized valence 5-zeta) [10-13]. The infrared spectrum was obtained for each of these basis sets, and the molecule was found to possess a stable structure.

Ribonucleic acid (RNA) is a polymeric molecule that is essential for most biological functions, either by performing the function itself (non-coding RNA) or by forming a template for the production of proteins (messenger RNA). RNA and deoxyribonucleic acid (DNA) are nucleic acids. The nucleic acids constitute one of the four major macromolecules essential for all known forms of life. RNA is assembled as a chain of nucleotides. Cellular organisms use messenger RNA (mRNA) [14] to convey genetic information (using the nitrogenous bases of guanine, uracil, adenine, and cytosine, denoted by the letters G, U, A, and C) that directs synthesis of specific proteins. Many viruses encode their genetic information using an RNA genome. [15]

Uracil (symbol U or Ura) is one of the four nucleobases in the nucleic acid RNA. The others are adenine (A), cytosine (C), and guanine (G). In RNA, uracil binds to adenine via two hydrogen bonds. In DNA, the uracil nucleobase is replaced by thymine (T). [16] Uracil is a demethylated form of thymine. Common and naturally occurring pyrimidine derivative. [17] The name "uracil" was coined in 1885 by the German chemist Robert Behrend, who was attempting to synthesize derivatives of uric acid. [18] Originally discovered in 1900 by Alberto Ascoli, it was isolated by hydrolysis of yeast nuclein; [19] it was also found in bovine thymus and spleen, herring sperm, and wheat germ. [20] It is a planar, unsaturated compound that has the ability to absorb light. [21]

1.1 Properties chemical of Uracil

Formula $C_4H_4N_2O_2$,, molar massa 112.08676 g/mol, solid, density 1.32 g/cm^3, melting point 335 °C (635 °F; 608 K) and water soluble. Other Names for this Substance: 2,4(1H,3H)-Pyrimidinedione; Uracil; 2,4-Dioxopyrimidine; 2,4-Pyrimidinediol; 2,4-Dihydroxypyrimidine; Pyrod; Pirod; 2,4-Pyrimidinedione; Hybar X; NSC 3970; 4-Hydroxyuracil; 1,2,3,4-Tetrahydropyrimidine-2,4-dione. [22]

2 Methods

2.1 Hartree-Fock Methods

The Hartree-Fock self–consistent method [23-27] is based on the one-electron approximation in which the motion of each electron in the effective field of all the other electrons is governed by a one-particle Schrodinger¨ equation. The Hartree-Fock approximation takes into account of the correlation arising due to the electrons of the same spin, however, the motion of the electrons of the opposite spin remains uncorrelated in this approximation. The methods beyond self-consistent field methods, which treat the phenomenon associated with the many-electron system properly, are known as the electron correlation methods.

The vast literature associated with these methods suggests that the following is a plausible hierarchy:

$HF << MP2 < CISD < CCSD < CCSD\,(T) < FCI$

The extremes of 'best', FCI, and 'worst', HF, are irrefutable, but the intermediate methods are less clear and depend on the type of chemical problem being addressed. [18] The use of HF in the case of FCI was due to the computational cost.

The molecular Hartree-Fock 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).

The expression for the Hartree-Fock molecular electronic energy E_{HF} is given by the variation theorem as $E_{HF} = \left\langle D|_{el}^{H} + \ V_{NN}|\, D \right\rangle$

where D is the Slater-determinant Hartree-Fock wave function and $\widehat{\mathbf{H}}_{el}$ and V_{NN} are given by

$$\widehat{\mathbf{H}}_{el} = -\frac{\hbar^2}{2m_e}\sum_i \nabla_i^2 - \sum_\alpha \sum_i \frac{Z_\alpha e'^2}{r_{i\alpha}} + \sum_j \sum_{i>j} \frac{e'^2}{r_{ij}}$$

$$V_{NN} = \sum_\alpha \sum_{\beta>\alpha} \frac{Z_\alpha Z_\beta e'^2}{r_{\alpha\beta}}$$

Since V_{NN} does not involve electronic coordinates and ***D*** is normalized, then

$$\langle D|V_{NN}|D\rangle = V_{NN}\,\langle D|D\rangle = V_{NN}\ .$$

The operator $\widehat{\mathbf{H}}_{el}$ is the sum of one-electron operators $\widehat{f}_i$ and two-electron operators $\widehat{g}_{ij}$; we have

$\widehat{\mathbf{H}}_{el} = \sum_i \widehat{f}_i + \sum_j \sum_{i>j} \widehat{g}_{ij}$, where

$\widehat{f}_i = -\frac{1}{2}\nabla_i^2 \sum_\alpha \sum_\alpha / r_{i\alpha}$ and $\widehat{g}_{ij} = \frac{1}{r_{ij}}$.

The Hamiltonian $\widehat{\mathbf{H}}_{el}$ is the same as the Hamiltonian $\widehat{\mathbf{H}}$ for an atom except that $\sum_\alpha \sum_\alpha / r_{i\alpha}$ replaces Z/r_i in $\widehat{f}_i$. Hence

$$E = \left\langle D\middle|\widehat{\mathbf{H}}\middle|D\right\rangle = 2\sum_i^{n/2} \left\langle \phi_i(1)\middle|\widehat{f}_i\middle|\phi_i(2)\right\rangle +$$

$$+ \sum_{j=1}^{n/2}\sum_{i=1}^{n/2} (2\mathbf{J}_{ij} - \mathbf{K}_{ij})$$

where

$$\mathbf{J}_{ij} = \left\langle \phi_i(1)\phi_j(2)\middle|\frac{e'^2}{r_{12}}\middle|\phi_i(1)\phi_j(2)\right\rangle$$

and

$$\mathbf{K}_{ij} = \left\langle \phi_i(1)\phi_j(2)\middle|\frac{e'^2}{r_{12}}\middle|\phi_j(1)\phi_i(2)\right\rangle$$

$$\widehat{f}_i = -\left(\frac{\hbar^2}{2m_e}\right)\nabla_i^2 - Z\frac{e'^2}{r_1}$$

can be used to give $\left\langle D\middle|\widehat{\mathbf{H}}_{el}\middle|D\right\rangle$.

Therefore, the Hartree-Fock energy of a diatomic or polyatomic molecule with only closed shells is

$$\mathbf{E}_{HF} = 2\sum_{i=1}^{n/2}\mathbf{H}_i^{core} + \sum_{j=1}^{n/2}\sum_{i=1}^{n/2}(2\mathbf{J}_{ij} - \mathbf{K}_{ij}) + \mathbf{V}_{NN}$$

$$\mathbf{H}_i^{core} \equiv \left\langle \phi_i(1)\middle|\widehat{\mathbf{H}}^{core}(1)\middle|\phi_i(1)\right\rangle \equiv$$

$$\equiv \left\langle \phi_i(1)\middle| -\frac{1}{2}\nabla_i^2 \sum_{\alpha} Z_\alpha / r_{1\alpha}\middle|\phi_i(1)\right\rangle$$

$$\mathbf{J}_{ij} \equiv \left\langle \phi_i(1)\phi_j(2)\middle|\frac{1}{r_{12}}\middle|\phi_i(1)\phi_j(2)\right\rangle$$

and

$$\mathbf{K}_{ij} \equiv \left\langle \phi_i(1)\phi_j(2)\middle|\frac{1}{r_{12}}\middle|\phi_j(1)\phi_i(2)\right\rangle$$

where the one-electron-operator symbol was changed from $\widehat{f}_i$ to $\widehat{\mathbf{H}}^{core}(1)$. [23-27]

3 Hardware and Software

For calculations a computer models was used: Intel® Core™ i5-1135G7 Processor, Memory 8 GB, Intel(R) Iris(R) Xe Graphics (128 MB). [28]

For calculations of computational dynamics, the Ubuntu Linux version 16.10 system was used [29] and the software used for the molecular dynamics was GAMESS [30-31]. For analisys Avogadro [32] and GaussView version 3.0 [33].

4 Results

The Uracil-Si molecule has:

PSA: 58,2;
ALogP: 4,7246;
Stereo Center Count: 0;
Axial Stereo Count: 0;
Hydrogen Acceptor Count: 2;
Hydrogen Donor Count: 2;
Composition: H: 23.00% N: 15.900% O: 18.100% Si: 63.700%;
Molecular Weight: 176.38596;
Exact Mass: 175.934983508;
Molecular Formula: $H_4N_2O_2Si_4$;
IUPAC Name: 1,3-dihydro-1,3,2,4,5,6-diazatetrasiline 2,4-dioxide.

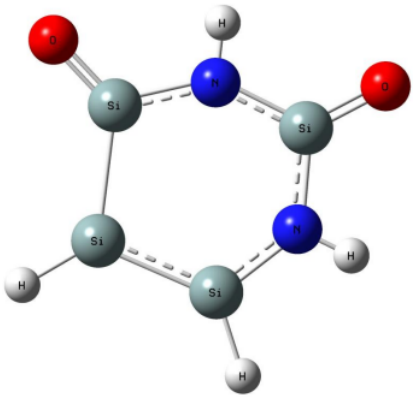

Figure 1: *Representation of Uracil-Si molecule, obtained after molecular dynamics via Restricted Hartree-Fock method, in basis set cc-pVTZ.* ***Source****: Authors.*

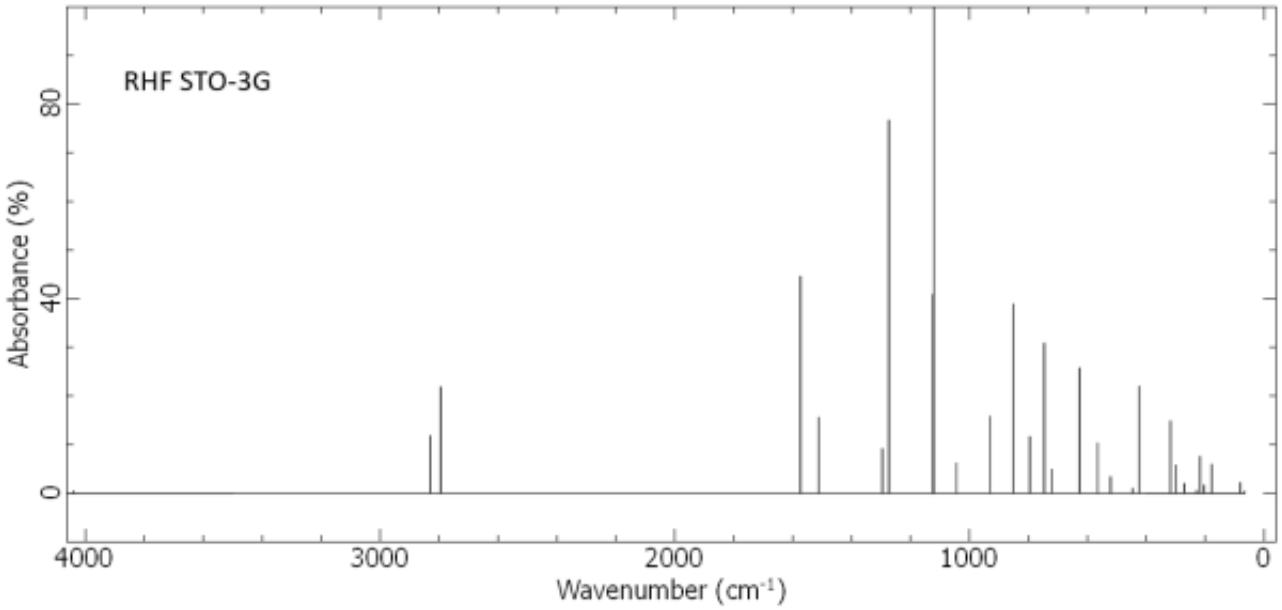

Figure 2: *Infrared spectrum of the Uracil-Si molecule, following molecular dynamics using the RHF (Restricted Hartree-Fock) method with the STO-3G basis set.* ***Source****: Authors.*

Table 1: *Peaks maximum absorption intensity by the frequency given for infrared spectrum. Absorbance frequency as a function of vibrational frequencies of Uracil-Si molecule for RHF for basis set: STO-3G, cc-pVDZ, cc-pVTZ, cc-pVQZ and cc-pV5Z.*

	ν (cm^{-1})	I (%)	ν (cm^{-1})	I (%)	ν (cm^{-1})	I (%)	ν (cm^{-1})	I (%)	ν (cm^{-1})	I (%)
STO-3G	1121.08	100	1273.53	76.6510	1573.55	44.5802	1123.75	40.8105	850.145	38.8692
cc-pVDZ	1399.34	100	1321.06	39.0939	989.247	37.5607	1015.44	37.1828	788.419	27.8868
cc-pVTZ	1430.56	100	1369.05	42.5267	1043.98	28.2888	795.899	25.2680	699.496	22.5232
cc-pVQZ	1430.38	100	1371.77	43.5624	1043.17	26.8241	1024.40	24.7101	799.199	24.3736
cc-pV5Z	1428.02	100	1364.82	42.1744	1020.66	29.8791	1040.35	29.4462	701.495	28.8338

ν = Frequency (cm^{-1}); I = Normalized Intensity (%). **Source** = Authors.

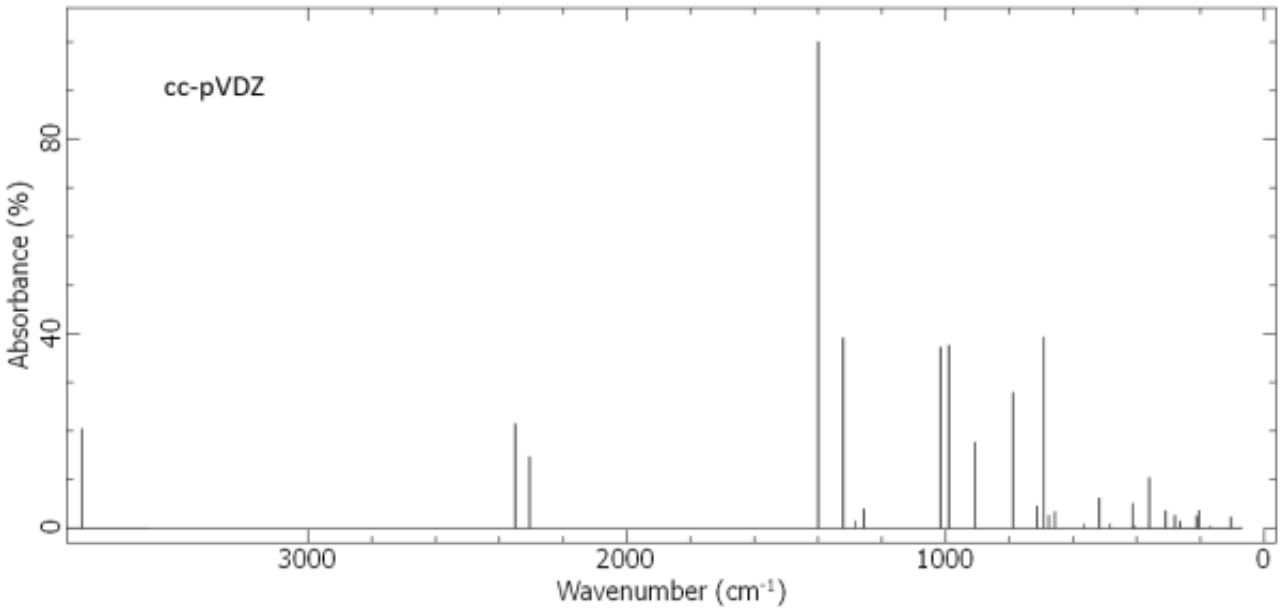

Figure 3: *Infrared spectrum of the Uracil-Si molecule, following molecular dynamics using the RHF method with the cc-pVDZ basis set.* ***Source****: Authors.*

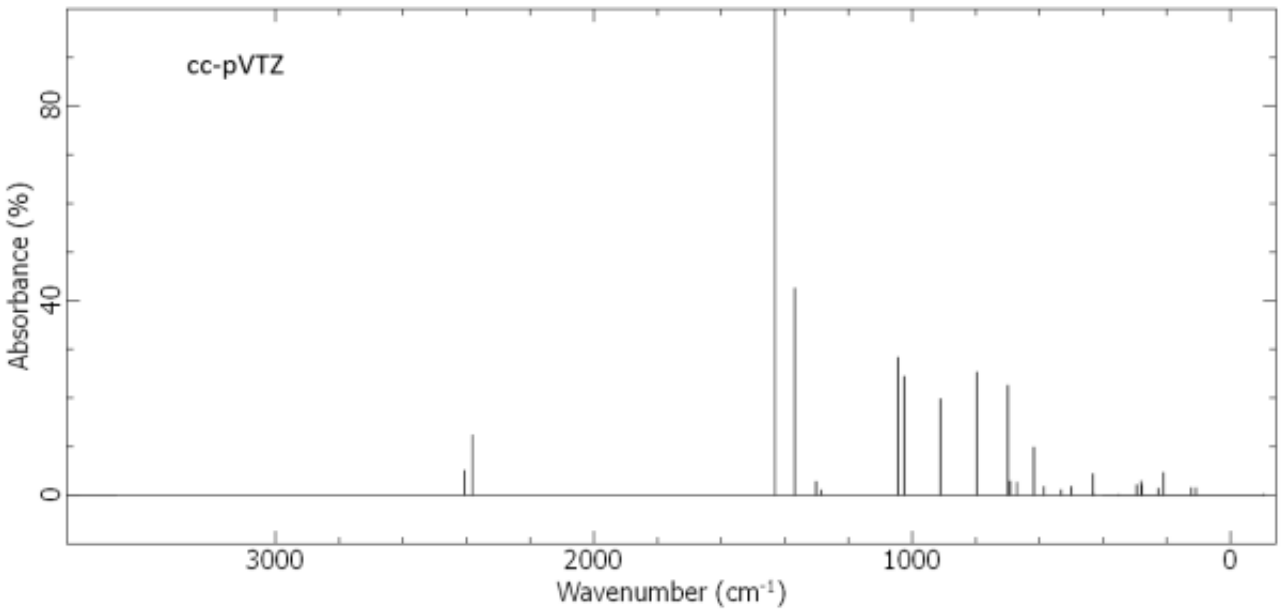

Figure 4: *Infrared spectrum of the Uracil-Si molecule, following molecular dynamics using the RHF method with the cc-pVTZ basis set.* ***Source****: Authors.*

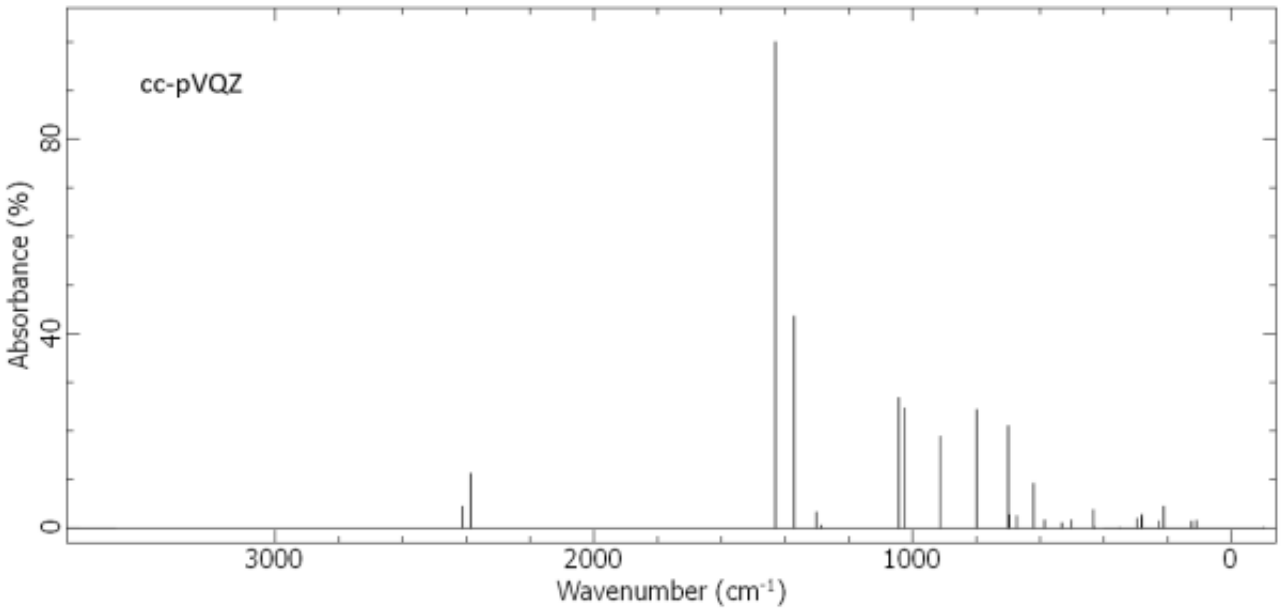

Figure 5: *Infrared spectrum of the Uracil-Si molecule, following molecular dynamics using the RHF method with the cc-pVQZ basis set.* ***Source****: Authors.*

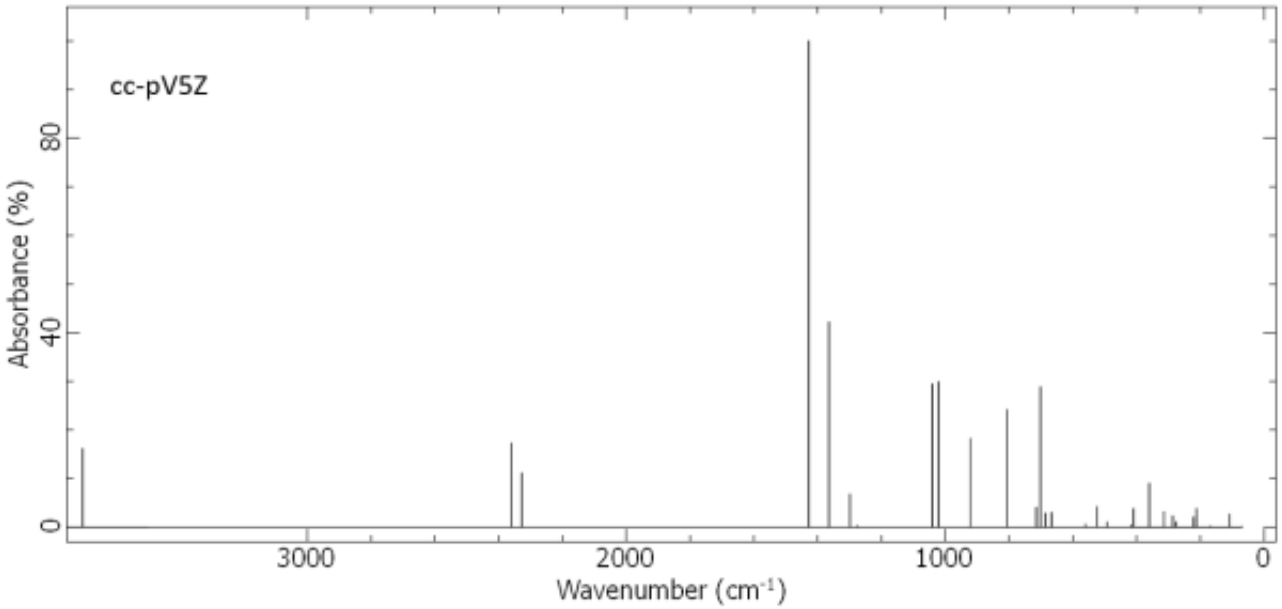

Figure 6: *Infrared spectrum of the Uracil-Si molecule, following molecular dynamics using the RHF method with the cc-pV5Z basis set.* ***Source****: Authors.*

The Table (1) show the maximum absorbance peaks for infrared spectrum in the STO-3G, cc-pVDZ, cc-pVTZ, cc-pVQZ and cc-pV5Z set basis are present at the frequencies 1121.08 cm^{-1}, 1399.34 cm^{-1}, 1430.56 cm^{-1}, 1430.38 cm^{-1}, 1428.02 cm^{-1}, with a normalized intensity of 100%, respectively.

5 Analisys and Conclusions

The Figure (1) representsof Uracil-Si molecule, obtained after molecular dynamics via Restricted Hartree-Fock method, in basis set cc-pVTZ.

The Figures (2) to (6) represents of Uracil-Si molecule, obtained after molecular dynamics via Restricted Hartree-Fock method, in basis set STO-3G, cc-pVDZ, cc-pVTZ, cc-pVQZ, cc-pV5Z, respectively.

The Table (1) represents to peaks maximum absorption intensity by the frequency given. Absorbance frequency as a function of vibrational frequencies of Uracil-Si molecule for RHF for basis set: STO-3G, cc-pVDZ, cc-pVTZ, cc-pVQZ and cc-pV5Z. respectively.

The maximum absorbance peaks for infrared spectrum in the STO-3G, cc-pVDZ, cc-pVTZ, cc-pVQZ and cc-pV5Z set basis are present at the frequencies 1121.08 cm^{-1}, 1399.34 cm^{-1}, 1430.56 cm^{-1}, 1430.38 cm^{-1}, 1428.02 cm^{-1}, with a normalized intensity of 100%, respectively.

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