

# Theoretical Studies on the Isomers of Quinazolinone by first Principles

Srivastava Rajesh Kumar, Narayan Vijay, Kumar Amarendra, Prasad Onkar and Sinha Leena\*  
Physics Department, University of Lucknow, Lucknow, INDIA

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## Abstract

The present communication is aimed at comparing the molecular structural properties, vibrational and energetic data of 2- and 4- quinazolinone, the two isomers of Quinazolinone, a biologically active heterocyclic compound, in gas phase, due to their pharmacological activities and applications. The ground state properties of the two isomers have been calculated employing DFT/ B3LYP level of theory using the basis sets 6-311G(d), 6-311+G(d,p), 6-311++G(d,p). The dipole moment and mean polarizability are calculated to be 6.4687 Debye and 110.202/a.u. in case of 2- quinazolinone and for 4-quinazolinone these values are 1.4611 Debye and 107.663/a.u. at B3LYP/ 6-311++G(d,p) level of theory. MESP surfaces have also been drawn and compared. In order to obtain a complete description of molecular dynamics, vibrational wavenumber calculation along with the normal mode analysis, have been carried out at the DFT level.

**Keywords:** Quinazolinone, frontier orbitals, MESP surface, normal mode analysis

## Introduction

Quinazolinone and its derivatives constitute an important class of heterocyclic compounds. These compounds are reported to have physiological and pharmacological activities and applications in the treatment of several diseases such as cancer and mental disorders and also exhibit a wide range of activities, such as antibacterial, analgesic, anti-inflammatory, antifungal, antimalarial, antihypertensive, CNS depressant, anticonvulsant, antihistaminic and local anaesthetic, antiparkinsonism, antiviral<sup>1-9</sup>. There are two structural isomers, 2-quinazolinone and 4-quinazolinone, with the 4-isomer being the more common. Very recently Fang-Tsao Hong et.al. have filed a patent "2-Quinazolinone compounds and methods of use" vide no. US7935709; Issue date May 3, 2011, in which the invention comprises a new class of compounds with 2-Quinazolinone core, useful for the prophylaxis and treatment of protein kinase mediated diseases, including inflammation and related conditions. Looking at the biological significance of quinazolinones, the present communication deals with the investigation of the structural, electronic and vibrational properties of 2-quinazolinone and 4-quinazolinone. The electronic structures and harmonic frequencies have been determined and analyzed at DFT level employing the basis set 6-311+G(d,p). The optimized geometry of 2-quinazolinone and 4-quinazolinone and their molecular properties such as equilibrium energy, frontier orbital energy gap, molecular electrostatic potential energy map, dipole moment, polarizability, first static hyperpolarizability have also been used to understand the properties and their activity. The normal mode analysis has also been carried out for better understanding of the vibrational dynamics of the molecules under investigation.

## Material and Methods

Geometry optimization is one of the most important steps in the theoretical calculations. The model molecular structure of 4-quinazolinone and 2-quinazolinone were built in gauss-view using the X-ray data of 4-quinazolinone derivative (CCDC-680038)<sup>10</sup> and were used to optimize the structures. The molecules under investigation have been analyzed with density functional theory (DFT)<sup>11</sup>, employing Becke's three parameter hybrid exchange functionals with Lee-Yang-Parr correlation functionals (B3LYP)<sup>12-14</sup>. All the calculations were performed using the Gaussian 09 program<sup>15</sup>. The model molecular structures of 2-quinazolinone and 4-quinazolinone are given in figure-1. Positive values of all the calculated vibrational wave numbers confirmed the geometry to be located on true local minima on the potential energy surface. As the DFT hybrid B3LYP functional tends to overestimate the fundamental normal modes of vibration, a scaling factor of 0.9679<sup>16</sup> has been applied. By combining the results of the Gaussview's program package<sup>17</sup> with symmetry consideration, vibrational frequency assignments were made with a high degree of accuracy. For the precise vibrational assignments, the normal modes have also been analyzed using the VEDA 4 program<sup>18</sup>.

## Results and Discussion

**Geometric Structure:** The electronic structures of 2-quinazolinone and 4-quinazolinone have been investigated, in order to assess the effect of changing the position of electron withdrawing carbonyl group (C=O) with respect to nitrogen atom. The optimized molecular structures with numbering scheme of the atoms are shown in figure-1. The ground state optimized parameters at different basis sets are reported in table-1. As the calculated vibrational spectra has no imaginary frequency, the optimized geometry is confirmed to be located at

the local minima on potential energy surface. The benzene ring C-C bond distances in two molecules are between 1.38 Å to 1.42 Å which are close to standard value 1.40 Å for benzene ring<sup>19</sup>. The C(2)-C(3) in 2-quinazolinone and C(2)-C(4) in 4-quinazolinone are equal to 1.43 Å and 1.47 Å respectively. These are carbon-carbon single bonds between two sp<sup>2</sup> hybridized carbon atoms (standard value 1.47 Å). The C=N bond lengths in two molecules are found to be at 1.24 Å and C-N single bond lengths vary between 1.35 Å to 1.42 Å. The C(9)-N(1) bond in 4-quinazolinone shows some double bond character. The C=O bond lengths for two molecules are at 1.21 Å (standard value 1.22 Å). The optimized benzene ring C-H bond lengths are 1.08 Å in two molecules. In two molecules, all the C-C-C angles of benzene rings lie between 119.02° to 120.82°. The C-N-C angle at N(1) in two molecules are approximately same at 121° but at N(4) in 2-quinazolinone and at N(5) in 4-quinazolinone are at 125.94° and 118.40° respectively. All the dihedral angles in two molecules are close to either at 0° or 179° showing the planar structure of the two molecules.

**Electronic Properties:** The basic electronic parameters related to the orbitals in a molecule are the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) and their resulting energy gap. These orbitals not only determine the way the molecule interacts with other species, but their energy gap (frontier orbital gap) helps characterize the chemical reactivity and kinetic stability of the molecule. A molecule with a small frontier orbital gap is more polarizable and is generally associated with a high chemical reactivity, low kinetic stability and is also termed as soft molecule<sup>20</sup>. Table-1 shows that the frontier orbital gap in case of 2-quinazolinone is lower than 4-quinazolinone molecule calculated at three basis sets 6-311G(d), 6-311+G(d,p) and 6-311++G(d,p). This makes 2-quinazolinone a soft and more polarizable molecule as compared to 4-quinazolinone molecule. The HOMO is the orbital that primarily acts as electron donor and the LUMO is the orbital that largely acts as the electron acceptor. The 3D plots of the frontier orbitals HOMO and LUMO, electron density (ED) and the molecular electrostatic potential map (MESP) for both molecules are shown in figure-2 and figure-3.

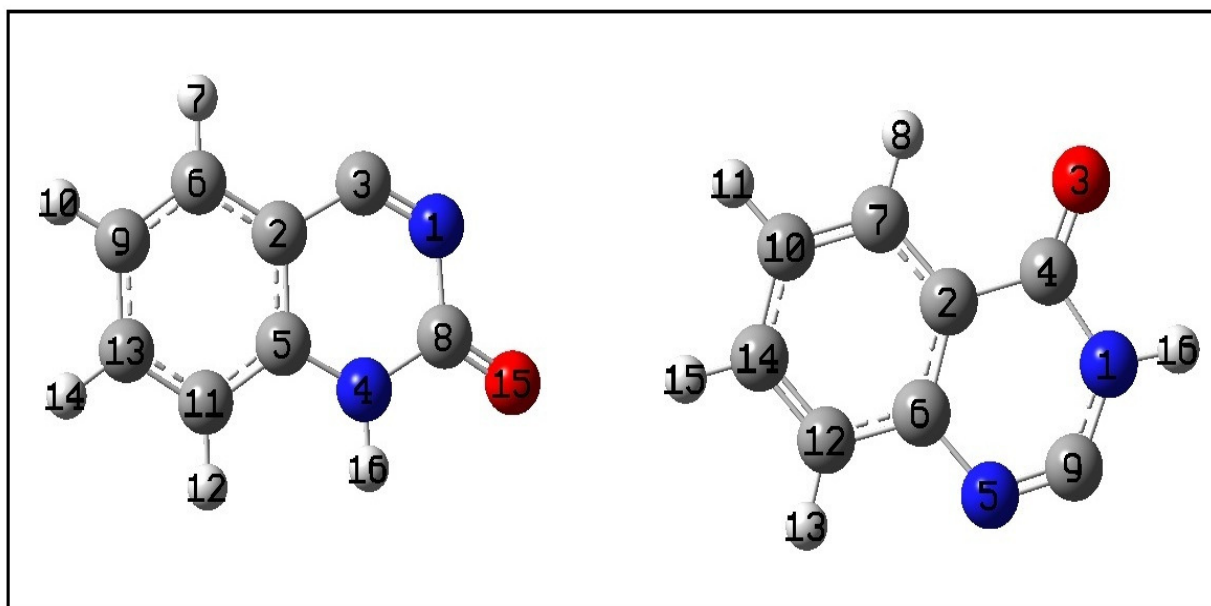


Figure-1  
 Optimized structures of 2-quinazolinone and 4-quinazolinone at B3LYP/6-311++G (d,p)

Table 1  
 Parameters corresponding to optimized geometry of 2-Quinazolinone and 4-Quinazolinone at DFT/B3LYP level of theory

| Basis set      | Ground State Energy<br>(Hartree) |                 | Frontier Orbital Energy Gap<br>(Hartree) |                 | Dipole Moment<br>(Debye) |                 |
|----------------|----------------------------------|-----------------|--|-----------------|--------------------------|-----------------|
|                | 2-Quinazolinone                  | 4-Quinazolinone | 2-Quinazolinone                          | 4-Quinazolinone | 2-Quinazolinone          | 4-Quinazolinone |
| 6-311G (d)     | -492.6516                        | -492.6551       | 0.14328                                  | 0.18536         | 6.0889                   | 1.2051          |
| 6-311+G (d,p)  | -492.6706                        | -492.6732       | 0.14282                                  | 0.18269         | 6.4686                   | 1.4607          |
| 6-311++G (d,p) | -492.6707                        | -492.6734       | 0.14281                                  | 0.18268         | 6.4687                   | 1.4611          |

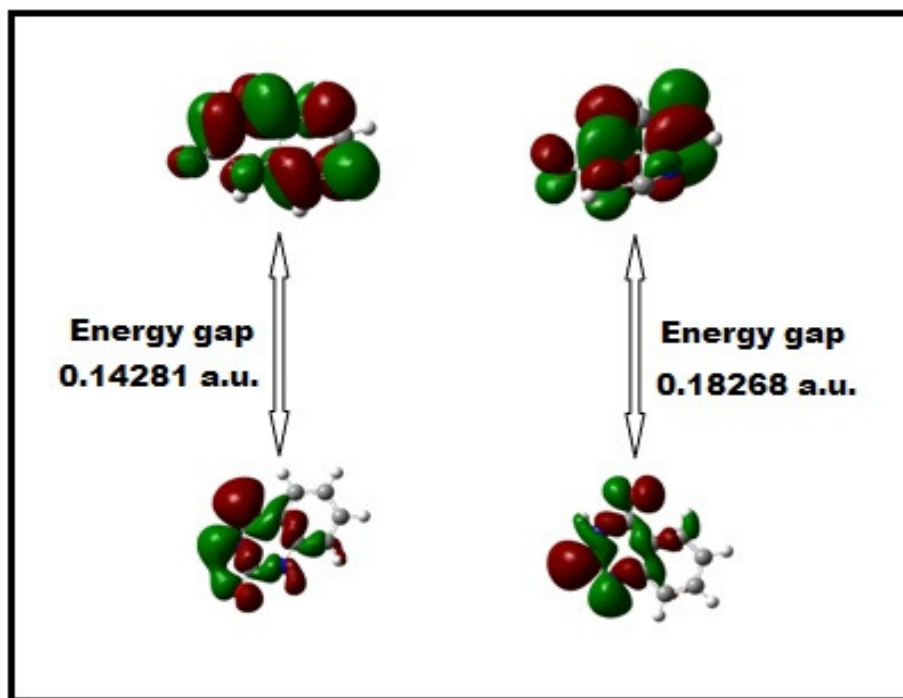


Figure-2  
Plots of Homo, Lumo and the energy gap in 2-quinazolinone & 4-quinazolinone

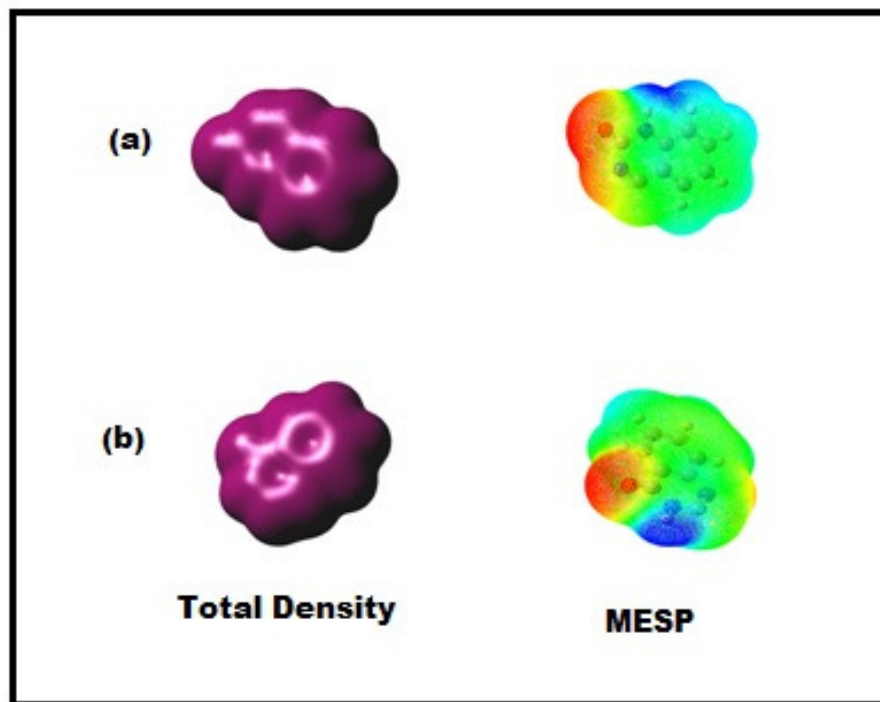


Figure-3  
Total Density and MESP of 2-Quinazolinone and 4-Quinazolinone

It can be seen from the figures that LUMO's of both the molecules are distributed uniformly over the entire molecules and show antibonding characters. The HOMO's of both the molecules are shifted mainly towards heterocyclic ring (containing the carbonyl group) and some part of benzene ring. The HOMO's of both the molecules show considerable sigma bond characters. The nodes in HOMO's and LUMO's are placed almost symmetrically. The molecular electrostatic potential surface MESP which is a plot of electrostatic potential mapped onto the iso-electron density, simultaneously displays molecular shape, size and electrostatic potential values and has been plotted for both the molecules. The molecular electrostatic potential (MESP) mapping is very useful in the investigation of the molecular structure with its physiochemical property relationships<sup>21-26</sup>. A portion of the molecule that has a negative electrostatic potential is susceptible to electrophilic attack. The red and blue regions in the MESP map refer to the regions of negative and positive potentials and correspond to the electron-rich and electron-deficient regions respectively whereas the green colour signifies the neutral electrostatic potential. The MESP map in case of 4-quinazolinone suggests that there are two regions of negative potential characterized by red and yellow colour, viz. one around carbonyl oxygen atom and one at nitrogen N(5) atom, whereas in case of 2-quinazolinone a relatively larger region around carbonyl oxygen atom represents the most negative potential region (dark red) and is responsible for electrophilic interaction. The hydrogen atom attached to nitrogen bear the maximum brunt of positive charge (dark blue). The most of the region of the two molecules seem to present almost neutral potential as represented by green colour.

**Electric Moments:** The dipole moment in a molecule is an important property that is mainly used to study the intermolecular interactions involving the bonded type dipole-dipole interactions, because higher the dipole moment, stronger will be the intermolecular interactions. The calculated dipole moment for both the molecules are given in Table-1. Table-1 shows that the calculated value of dipole moment in case of 2-quinazolinone is found to be quite higher than 4-quinazolinone. The lower frontier orbital energy gap and very high dipole moment for the 2-quinazolinone are manifested in its high reactivity and consequently higher selectivity for the derivatives of 2-quinazolinone in cancer treatment. According to present calculations, the mean polarizability of 2-quinazolinone (110.202 a.u., refer to Table -2) is found slightly higher than 4-quinazolinone (107.66 a.u.) calculated at the same level of theory as well as same basis set 6-311++G(d,p). This is related very well to the smaller frontier orbital energy gap of 2-quinazolinone as compared to 4-quinazolinone.

**Vibrational Spectral Analysis:** As the molecules under study exhibits no special symmetries, all the normal modes are both infrared and Raman active. A total of 42 (3N-6) normal modes of vibration of both the isomers of quinazolinone are distributed among the functional and the fingerprint region. The computed vibrational wave numbers, their IR intensity and Raman activity

and the detailed description of each normal mode of vibration of 2- and 4-quinazolinone and their contribution to the total potential energy are given in Table-3(a) and Table-3(b). It is well known that ab-initio and DFT systematically overestimate the vibrational wavenumbers. These discrepancies can be corrected either by computing anharmonic correlations explicitly, by introducing a scaled field or even by directly scaling the calculated wavenumbers with proper factor<sup>16</sup>. The vibrational wavenumbers are calibrated accordingly with scaling factor of 0.9679 for DFT at B3LYP.

**Table-2**  
**Polarizability data for 2-Quinazolinone and 4-Quinazolinone at DFT/B3LYP**

| Polarizability           | 2-Quinazolinone | 4-Quinazolinone |
|--------------------------|-----------------|-----------------|
| $\alpha_{xx}$            | 165.103         | 147.337         |
| $\alpha_{yy}$            | -1.984          | -0.435          |
| $\alpha_{zz}$            | 109.973         | 120.065         |
| $\alpha_{xy}$            | 0.600           | 0.001           |
| $\alpha_{yz}$            | -0.001          | -0.001          |
| $\alpha_{zx}$            | 55.550          | 55.588          |
| $\langle \alpha \rangle$ | 110.202         | 107.663         |

In atomic units. Conversion factor to the SI units,  $1e^2 a_0^2 E_h^{-1} = 1.648778 \times 10^{41} C^2 m^2 J^{-1}$

**N-H vibrations:** The N-H stretching of nitrogen containing ring of 2-quinazolinone/ 4-quinazolinone is calculated at 3483/3482  $cm^{-1}$ . The N-H stretching of heterocyclic six-membered ring of tegafur, having two nitrogen atoms has also been calculated at 3477  $cm^{-1}$ <sup>27</sup>. As expected, this is a pure stretching mode and is evident from P.E.D. table contributing 100% to the total P.E.D.. The N-H wagging mode in 2-quinazolinone is calculated at 586  $cm^{-1}$  contributing 72% to the total P.E.D whereas in the case of 4-quinazolinone this mode is at higher wavenumber at 637  $cm^{-1}$ .

**C-C and C-H vibrations:** The four C-H stretching vibrations of benzene ring for both the isomers are found in the region 3099-3066  $cm^{-1}$  having 100% contribution to the total P.E.D. in calculation. First vibration at 3099  $cm^{-1}$  is the symmetric vibration and remaining three vibrations are asymmetric vibrations. The C-C stretching vibrational modes are observed in the frequency range 1585  $cm^{-1}$  to 1000  $cm^{-1}$ .

**C=O and C-N vibrations:** The appearance of a strong band in IR spectra around 1700  $cm^{-1}$  show the presence of carbonyl group in the molecule and is due to the C=O stretch. The frequency of the stretch due to carbonyl group mainly depends on the bond strength which in turn depends upon inductive, conjugative, field and steric effects. The effect of electron withdrawing oxygen and nitrogen atoms attached to the carbonyl group is to increase the strength of the C=O bond hence in case of 2-quinazolinone the vibration occurs at relatively higher value 1737  $cm^{-1}$  due to presence of two nitrogen atoms adjacent to C=O bond. In case of 4-quinazolinone the corresponding vibration occurs at lower value 1706  $cm^{-1}$  due to presence of one nitrogen atom adjacent to C=O bond. The C-N stretching in case of 2-quinazolinone are calculated as mixed modes at 1442, 1231, 1090 and 852  $cm^{-1}$ .

**Table 3(a)**  
**Theoretical unscaled and scaled wavenumbers (in  $\text{cm}^{-1}$ ) for 2-Quinazolinone**

| S.No. | Cal. Unsc. wave no. in $\text{cm}^{-1}$ | Infrared Intensity | Raman Activity | Sc. wave no. in $\text{cm}^{-1}$ | Assignment of dominant modes in order of decreasing potential energy distribution (PED)   |
|-------|---|--------------------|----------------|----------------------------------|---|
| 1     | 3598                                    | 44.87              | 119.89         | 3483                             | v (N(4)-H(16))Hr(100)   |
| 2     | 3202                                    | 7.79               | 258.68         | 3099                             | $\nu_s(\text{C-H})\text{R}(100)$  |
| 3     | 3198                                    | 5.37               | 81.57          | 3095                             | $\nu_{as}(\text{C-H})\text{R}(100)$   |
| 4     | 3182                                    | 4.17               | 118.76         | 3080                             | $\nu_{as}(\text{C-H})\text{R}(100)$   |
| 5     | 3168                                    | 2.80               | 50.80          | 3066                             | $\nu_{as}(\text{C-H})\text{R}(100)$   |
| 6     | 1795                                    | 387.86             | 21.49          | 1737                             | v(C8=O15)Hr(76)   |
| 7     | 1769                                    | 985.16             | 100.23         | 1712                             | v (N(1)-C(3))Hr(65)   |
| 8     | 1646                                    | 48.44              | 25.73          | 1593                             | v (C-C)R(68)  |
| 9     | 1604                                    | 39.31              | 30.98          | 1553                             | v(C(5)-C(2))R(22) + v(C(13)-C(9))R(27) + $\Phi(\text{H}(16)-\text{N}(4)-\text{C}(5))\text{Hr}(19)$  |
| 10    | 1517                                    | 0.70               | 8.16           | 1468                             | v(C(11)-C(13))R(11) + v(C(2)-C(6))R(14) + $\Phi(\text{H}(16)-\text{N}(4)-\text{C}(8))\text{Hr}(13)$ + $\Phi(\text{H}(10)-\text{C}(9)-\text{C}(13))\text{R}(21)$   |
| 11    | 1490                                    | 32.24              | 27.50          | 1442                             | v(N(4)-C(5))Hr(14)+ $\Phi(\text{H}(12)-\text{C}(11)-\text{C}(13))\text{R}(17)$ + $\Phi(\text{H}(14)-\text{C}(13)-\text{C}(11))\text{R}(15)$ + $\Phi(\text{H}(7)-\text{C}(6)-\text{C}(2))\text{R}(13)$                                     |
| 12    | 1437                                    | 4.49               | 22.05          | 1391                             | $\Phi(\text{H}(16)-\text{N}(4)-\text{C}(8))\text{Hr}(37)$ + $\Phi(\text{H}(14)-\text{C}(13)-\text{C}(11))\text{R}(16)$  |
| 13    | 1357                                    | 8.53               | 73.83          | 1313                             | v (C-C)R(65)  |
| 14    | 1300                                    | 14.90              | 14.39          | 1258                             | v(C(2)-C(6))R(19) + $\Phi(\text{H}(7)-\text{C}(6)-\text{C}(9))\text{R}(29)$   |
| 15    | 1272                                    | 13.87              | 1.23           | 1231                             | v(C(5)-C(11))R(14)+v(N(4)-C(5))Hr(16)+ $\Phi(\text{H}(14)-\text{C}(13)-\text{C}(11))\text{R}(12)$ + $\Phi(\text{H}(16)-\text{N}(4)-\text{C}(8))\text{Hr}(23)$   |
| 16    | 1238                                    | 28.55              | 15.70          | 1198                             | v(C(2)-C(3))Hr(12)+ $\Phi(\text{H}(5)-\text{C}(11)-\text{C}(12))\text{R}(24)$ + $\Phi(\text{H}(7)-\text{C}(6)-\text{C}(2))\text{R}(14)$ + $\Phi(\text{H}(10)-\text{C}(9)-\text{C}(6))\text{R}(18)$  |
| 17    | 1192                                    | 25.40              | 6.01           | 1154                             | $\Phi(\text{H}(10)-\text{C}(9)-\text{C}(13))\text{R}(18)$ + $\Phi(\text{H}(12)-\text{C}(11)-\text{C}(13))\text{R}(22)$ + $\Phi(\text{H}(14)-\text{C}(13)-\text{C}(11))\text{R}(33)$   |
| 18    | 1140                                    | 19.82              | 0.63           | 1103                             | v(C(11)-C(13))R(13)+ $\Phi(\text{H}(7)-\text{C}(6)-\text{C}(9))\text{R}(16)$ + $\Phi(\text{H}(10)-\text{C}(9)-\text{C}(6))\text{R}(19)$ + $\Phi(\text{C}(2)-\text{C}(6)-\text{C}(9))\text{R}(11)$   |
| 19    | 1126                                    | 40.92              | 38.43          | 1090                             | v(N(4)-C(8))Hr(30) + v(C(2)-C(3))Hr(12)   |
| 20    | 1046                                    | 3.32               | 21.70          | 1012                             | v (C-C)R(60)  |
| 21    | 995                                     | 0                  | 0.04           | 963                              | $\omega(\text{C-H})\text{R}(88)$  |
| 22    | 966                                     | 1.56               | 0.06           | 935                              | $\omega(\text{C-H})\text{R}(89)$  |
| 23    | 923                                     | 15.39              | 2.51           | 893                              | Triangular bending(R)(65)   |
| 24    | 880                                     | 12.67              | 5.97           | 852                              | v(N(1)-C(8))Hr(30)+ $\Phi(\text{C}(3)-\text{N}(1)-\text{C}(8))\text{Hr}(21)$ + $\Phi(\text{C}(11)-\text{C}(13)-\text{C}(9))\text{R}(12)$  |
| 25    | 862                                     | 0.16               | 0.03           | 834                              | $\omega(\text{C-H})\text{R}(91)$  |
| 26    | 780                                     | 5.96               | 22.87          | 755                              | Ring-breathing(Hr)(52)+ $\Phi(\text{C}(5)-\text{C}(11)-\text{C}(13))\text{R}(11)$ + $\Phi(\text{C}(11)-\text{C}(13)-\text{C}(9))\text{R}(19)$   |
| 27    | 768                                     | 69.09              | 0.46           | 743                              | $\omega(\text{C-H})\text{R}(90)$  |
| 28    | 743                                     | 52.66              | 0.28           | 719                              | $\Psi(\text{N4}-\text{C8}-\text{N1})(49)$ + $\omega(\text{C-H})\text{R}(17)$  |
| 29    | 725                                     | 8.71               | 6.08           | 702                              | v(C(5)-C(11))R(10)+ $\Phi(\text{C}(3)-\text{N}(1)-\text{C}(8))\text{Hr}(33)$ + $\Phi(\text{O}(15)-\text{C}(8)-\text{N}(1))\text{Hr}(11)$ + $\Phi(\text{C}(13)-\text{C}(9)-\text{C}(6))\text{R}(13)$                                       |
| 30    | 722                                     | 7.36               | 0.03           | 699                              | Phenyl Ring torsion (67) + $\Psi(\text{H}(16)-\text{N}(4)-\text{C}(5))\text{Hr}(13)$  |
| 31    | 634                                     | 15.40              | 1.13           | 614                              | $\Phi(\text{N}(1)-\text{C}(3)-\text{C}(2))\text{Hr}(18)$ + $\Phi(\text{C}(6)-\text{C}(9)-\text{C}(13))\text{R}(28)$ + $\Phi(\text{C}(2)-\text{C}(6)-\text{C}(9))\text{R}(23)$ + $\Phi(\text{C}(5)-\text{C}(11)-\text{C}(13))\text{R}(20)$ |
| 32    | 605                                     | 47.92              | 1.39           | 586                              | $\omega(\text{N-H})(72)$  |
| 33    | 570                                     | 2.29               | 4.22           | 552                              | $\Phi(\text{C}(11)-\text{C}(13)-\text{C}(9))\text{R}(12)$ + $\Phi(\text{C}(5)-\text{C}(2)-\text{C}(6))\text{R}(16)$ + $\Phi(\text{O}(15)-\text{C}(8)-\text{N}(1))\text{Hr}(43)$   |
| 34    | 540                                     | 1.75               | 0.20           | 523                              | $\tau(\text{H}(16)-\text{N}(4)-\text{C}(5)-\text{C}(2))\text{Hr}(23)$ + $\tau(\text{C}(11)-\text{C}(13)-\text{C}(9)-\text{C}(6))\text{R}(12)$   |
| 35    | 493                                     | 2.21               | 13.51          | 477                              | $\Phi(\text{N}(4)-\text{C}(5)-\text{C}(11))\text{Hr}(12)$ + $\Phi(\text{C}(8)-\text{N}(4)-\text{C}(5))\text{Hr}(27)$  |
| 36    | 468                                     | 7.20               | 0.49           | 453                              | Hr ring torsion(36)+Phenyl ring torsion(31)   |
| 37    | 448                                     | 4.17               | 6.39           | 434                              | $\Phi(\text{N}(1)-\text{C}(8)-\text{N}(4))\text{Hr}(23)$ + $\Phi(\text{C}(5)-\text{C}(2)-\text{C}(3))\text{Hr}(20)$ + $\Phi(\text{C}(5)-\text{C}(11)-\text{C}(13))\text{R}(14)$   |
| 38    | 406                                     | 0.003              | 0.68           | 393                              | $\tau(\text{C}(3)-\text{N}(1)-\text{C}(8)-\text{N}(4))\text{Hr}(28)$ + $\tau(\text{C}(11)-\text{C}(13)-\text{C}(9)-\text{C}(6))\text{R}(18)$ + $\tau(\text{C}(2)-\text{C}(6)-\text{C}(9)-\text{C}(13))\text{R}(18)$                       |

**Table 3(b)**  
**Theoretical unscaled and scaled wavenumbers (in  $\text{cm}^{-1}$ ) for 4-Quinazolinone**

| S.No. | Cal. Unsc. wave no. in $\text{cm}^{-1}$ | Infrared Intensity | Raman Activity | Scaled Wave. No in $\text{cm}^{-1}$ | Assignment of dominant modes in order of decreasing potential energy distribution (PED)  |
|-------|---|--------------------|----------------|-------------------------------------|--|
| 1     | 3597                                    | 92.06              | 157.20         | 3482                                | v (N(1)-H(16))Hr(100)  |
| 2     | 3202                                    | 6.80               | 275.10         | 3099                                | vs(C-H)R (100)   |
| 3     | 3198                                    | 3.58               | 32.58          | 3095                                | vas (C-H)R(100)  |
| 4     | 3186                                    | 5.32               | 100.34         | 3084                                | vas (C-H)R(100)  |
| 5     | 3172                                    | 3.68               | 68.46          | 3070                                | vas (C-H)R(100)  |
| 6     | 1787                                    | 248.22             | 95.63          | 1729                                | v (N(5)-C(9))Hr(81)  |
| 7     | 1762                                    | 508.30             | 59.27          | 1706                                | v (C4=O3)Hr(83)  |
| 8     | 1642                                    | 100.83             | 20.85          | 1589                                | v(C-C)R(79)  |
| 9     | 1596                                    | 4.59               | 31.73          | 1545                                | v(C-C)R(48) + $\Phi$ (C(6)-C(12)-C(14))R(10)+ $\Phi$ (C(2)-C(7)-C(10))R(12)  |
| 10    | 1492                                    | 59.57              | 4.00           | 1444                                | $\Phi$ (H(8)-C(7)-C(10))R(20)+ $\Phi$ (H(13)-C(12)-C(14))R(25)+ $\Phi$ (H(15)-C(14)-C(12))R(20)                                  |
| 11    | 1490                                    | 30.89              | 1.06           | 1442                                | v(C-C)R(36) + $\Phi$ (H(11)-C(10)-C(14))R(24)+ $\Phi$ (H(15)-C(14)-C(12))R(14)   |
| 12    | 1423                                    | 23.05              | 15.27          | 1377                                | v(N(1)-C(9))Hr(16) + $\Phi$ (H(16)-N(1)-C(9))Hr(63)  |
| 13    | 1344                                    | 19.14              | 30.07          | 1301                                | v(C-C)R(85)  |
| 14    | 1310                                    | 45.62              | 0.64           | 1268                                | $\Phi$ (H(8)-C(7)-C(10))R(22)+ $\Phi$ (H(13)-C(12)-C(14))R(25)+ $\Phi$ (H(15)-C(14)-C(12))R(28) + $\Phi$ (H(11)-C(10)-C(7))R(19) |
| 15    | 1246                                    | 18.80              | 43.18          | 1206                                | v(C(2)-C(7))R(11) + v(N(5)-C(6))Hr(34) + $\Phi$ (H(8)-C(7)-C(10))R(13)   |
| 16    | 1234                                    | 11.58              | 35.10          | 1194                                | v(N(1)-C(4))Hr(11) + $\Phi$ (C(2)-C(7)-C(10))R(13)   |
| 17    | 1180                                    | 6.0 $\tau$ 4       | 6.09           | 1142                                | v(C(14)-C(10))R(10)+ $\Phi$ (H(11)-C(10)-C(14))R(22)+ $\Phi$ (H(13)-C(12)-C(14))R(12) + $\Phi$ (H(15)-C(14)-C(12))R(29)          |
| 18    | 1127                                    | 25.33              | 1.14           | 1091                                | $\Phi$ (H(8)-C(7)-C(10))R(26)+ $\Phi$ (H(13)-C(12)-C(14))R(18)+ $\Phi$ (H(11)-C(10)-C(14))R(15) + $\Phi$ (C(2)-C(7)-C(10))R(15)  |
| 19    | 1121                                    | 25.76              | 5.42           | 1085                                | v(N(1)-C(9))Hr(38)+ $\Phi$ (H(16)-N(1)-C(9))Hr(10)+ $\Phi$ (H(13)-C(12)-C(14))R(18)  |
| 20    | 1075                                    | 32.64              | 11.13          | 1041                                | v(N(1)-C(4))Hr(36) + $\Phi$ (C(12)-C(14)-C(10))R(10) + $\Phi$ (C(2)-C(7)-C(10))R(15)   |
| 21    | 1040                                    | 17.68              | 17.73          | 1007                                | v(C(14)-C(10))R(34)  |
| 22    | 1006                                    | 0.02               | 0.08           | 974                                 | $\omega$ (C-H)(R)(86)  |
| 23    | 986                                     | 1.80               | 0.02           | 955                                 | $\omega$ (C-H)(R)(91)  |
| 24    | 892                                     | 0.46               | 0.01           | 863                                 | $\omega$ (C-H)(R)(92)  |
| 25    | 852                                     | 11.57              | 6.09           | 824                                 | v(N(5)-C(6))Hr(15)+ $\Phi$ (C(7)-C(10)-C(14))R(26)+ $\Phi$ (C(12)-C(14)-C(10))R(12)  |
| 26    | 805                                     | 48.36              | 9.94           | 779                                 | $\Phi$ (N(1)-C(9)-N(5))Hr(33)+ $\Phi$ (C(9)-N(5)-C(6))Hr(15)+ $\Phi$ (C(4)-N(1)-C(9))Hr(13)                                      |
| 27    | 798                                     | 8.35               | 0.18           | 772                                 | $\Psi$ (N1-C4-C2)(18)+ $\Psi$ (O3-C4-C2)(17)+ $\omega$ (C-H)(R)(16)  |
| 28    | 775                                     | 50.65              | 0.42           | 750                                 | $\omega$ (C-H)(R)(34)+ $\Psi$ (N1-C4-C2)(11)+ $\Psi$ (C2-C6-N5)(10)  |
| 29    | 729                                     | 2.38               | 25.15          | 705                                 | $\Phi$ (C(6)-C(12)-C(14))R(22) + $\Phi$ (C(12)-C(14)-C(10))R(25)   |
| 30    | 711                                     | 75.07              | 0.003          | 689                                 | (C-C-C)R torsion(24)+ $\Psi$ (C2-C4-O3)(16)+ $\tau$ (H16-N1-C9-N5)(13)   |
| 31    | 658                                     | 25.76              | 0.36           | 637                                 | $\omega$ (N-H)(59)   |
| 32    | 584                                     | 9.36               | 4.15           | 566                                 | v(N(1)-C(4))Hr(11)+ $\Phi$ (C(6)-C(12)-C(14))R(20)+ $\Phi$ (C(2)-C(7)-C(10))R(12)+ $\Phi$ (O(3)-C(4)-N(1))Hr(25)                 |
| 33    | 536                                     | 9.85               | 1.62           | 519                                 | $\Phi$ (C(7)-C(10)-C(14))R(12)+ $\Phi$ (C2-C(6)-C(12))R(15)+ $\Phi$ (O(3)-C(4)-N(2))Hr(26)                                       |
| 34    | 526                                     | 2.88               | 1.49           | 509                                 | Ring torsion (70) + $\tau$ (H(16)-N(1)-C(9)-N(5))Hr(18)  |
| 35    | 504                                     | 2.16               | 6.02           | 488                                 | $\Phi$ (C12-C14-C10))R(16)+ $\Phi$ (C(4)-C(2)-C(6))Hr(32)+ $\Phi$ (N(1)-C(9)-N(5))Hr(26)   |
| 36    | 472                                     | 3.23               | 12.46          | 457                                 | v(C(6)-C(12))R(12) + $\Phi$ (C(9)-N(5)-C(6))Hr(42)+ $\Phi$ (N(5)-C(6)-C(12))Hr(13)   |
| 37    | 468                                     | 4.92               | 2.29           | 453                                 | Ring torsion (R)(62)+ $\tau$ (H(16)-N(1)-C(9)-N(5))Hr(32)  |
| 38    | 420                                     | 10.16              | 1.73           | 407                                 | $\tau$ (H(16)-N(1)-C(9)-N(5))Hr(12)+ $\tau$ (C(2)-C(7)-C(10)-C(14))R(33)+ $\tau$ (C(6)-C(12)-C(14)-C(10))R(11)                   |

Note - Abbreviations used here have following meaning. v: stretching; vs: symmetric stretching; vas: asymmetric stretching;  $\Phi$ : in plane bending;  $\Psi$ : out of plane bending;  $\tau$ : torsion;  $\omega$ : wagging;  $\gamma$ : twisting; R; Benzene ring.; Hr; Ring involving nitrogen atom.

## Conclusion

In the present work we have calculated the equilibrium geometries, vibrational wavenumbers, frontier orbitals, MESP of 2-quinazolinone and 4-quinazolinone at DFT level employing the 6-311++G(d,p) basis set. The lower frontier orbital energy gap, the higher dipole moment and polarizability values make 2-quinazolinone the more reactive and more polar as compared to the 4-quinazolinone. The present quantum chemical study may further play an important role in understanding of dynamics of these molecules.

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